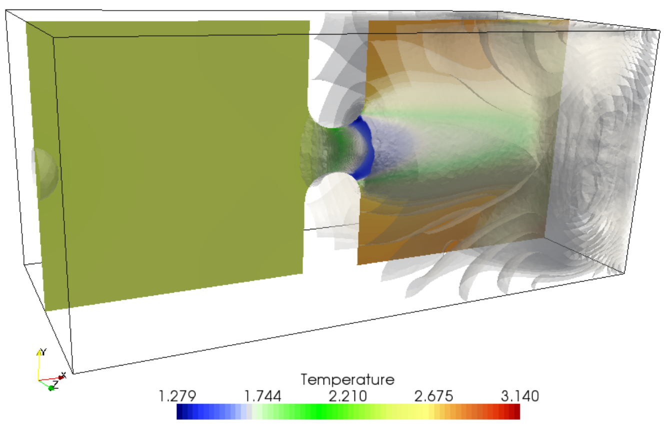
Computational Thermodynamics



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January 10, 2012

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Part I

Short Story

Chapter 1

Prelude: Entropy Turbulence

> I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is turbulent motion of fluids. And about the former I am rather optimistic. (Horace Lamb, 1932)

> The steam engine having furnished us with a means for converting heat into motive power, and our thoughts being thereby led to regard a certain quantity of work as an equivalent for the amount of heat expended in its production, the idea of establishing theoretically soem fixed relation bewteen a quantity of heat and the quantity of work whcih it can possibly produce, from which relation conclusions regarding the nature of heat itself may be deduced, naturally presents itself. (Clausius 1851)

1.1 Entropy

Modern physics was born from the work by the German physicist Ludwig Boltzmann (1844-1906) on *thermodynamics* in the late 19th century. Boltzmann had taken on the mission to solve the main open problem of physics of his time of deriving the *2nd Law of Thermodynamics* from Newtonian mechanics of a gas viewed as a large collection of atoms or molecules interacting by collisions.

The 2nd Law had been formulated by Rudolf Clausius in 1865 in terms of the new concept of *entropy*, motivated from urgent practical needs of improving the efficiency of steam engines as *heat engines* transforming heat energy into mechanical energy, see Fig. 1.1. Clausius postulated that only transformations with non-decreasing (increasing or constant) entropy were possible, with entropy something which could only accumulate but never be destroyed.

A transformation with strictly increasing entropy would then be *irreversible*, which in particular would explain why mechanical energy once transformed into heat energy by friction cannot be retrieved and thus put a limit on the efficiency of heat engines working in a cycle.

Clausius could not explain the physical meaning of entropy and his 2nd Law, and this was required to keep physics and mathematics as the King and Queen of Rational Science. The challenge was taken on by the young ambitious Boltzmann in what was to become the project of his life, starting from the at his time still unproven atomistic hypothesis of a gas as a large collection of atoms.

However, the task showed to be overwhelming and Boltzmann felt forced to give up classical deterministic Newtonian mechanics and replace it with a new form of *statistical mechanics*, and in the end to give up his own life as he lost faith in his creation. Classical deterministic Newtonian is formally reversible and thus must be modified to show irreversibility. Boltzmann's resorted to statistics and paid the price. In this book we shall consider a much less brutal modification in the form of *finite precision computation* at an affordable necessary cost.

But statistical mechanics survived and is today viewed to offer a scientific definition of entropy as a "measure of disorder" in some statistical sense. Statistical mechanics was boosted by the discovery of atoms and prepared the statistical interpretation of the wave function of quantum mechanics as a probability of particle configuration, commonly believed to be an inevitable aspect of modern physics. But statistics represents a form capitulation away from prediction by cause-effect, which is the heart of rational science.

1.2 Turbulence

There is another fundamental problem of classical mechanics, namely the problem of *turbulence* in a gas or fluid seen as a large collection of gas/fluid particles or atoms/molecules interacting by pressure and friction forces. Turbulent flow is not determinstic as concerns pointwise values in space and time, and thus has been approached by statistical methods, however with meager

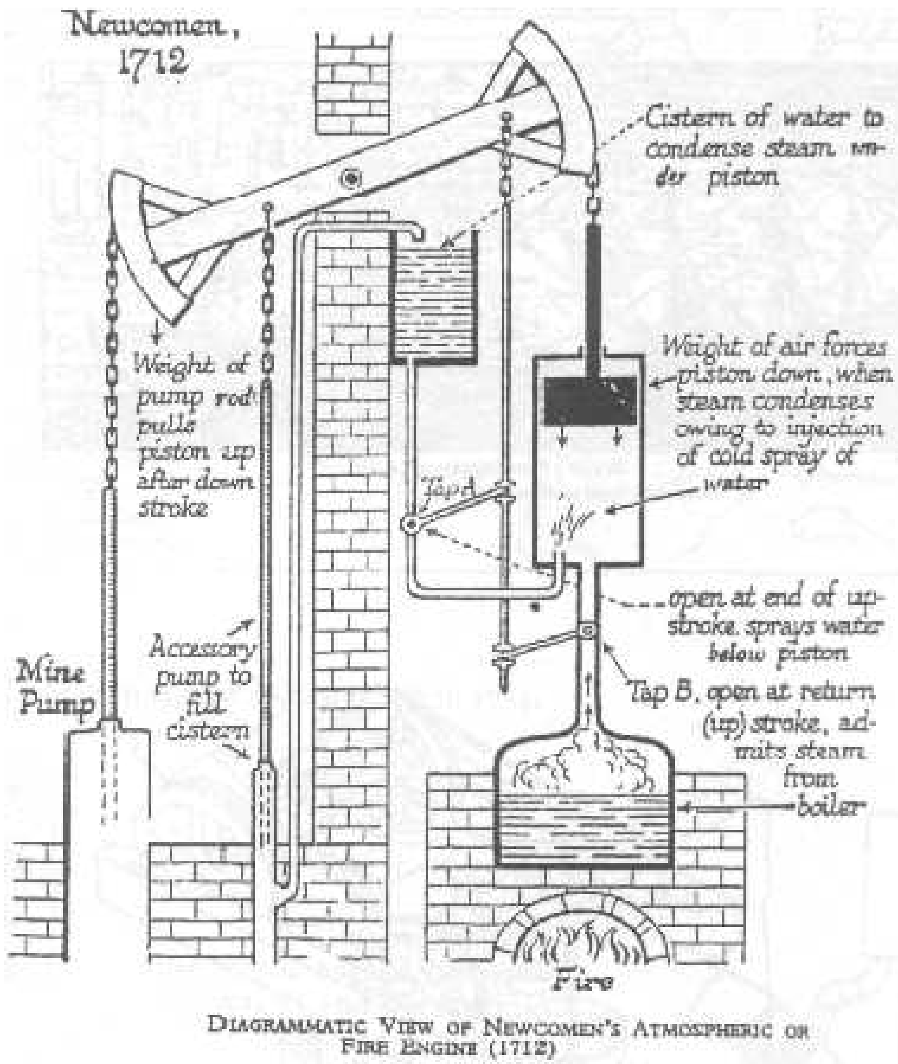

Figure 1.1: Converting heat to kinetic (mechanical) energy in 1712.

concrete results.

There are thus two main open problems of classical mechanics

- entropy,
- turbulence,

which have not been found a resolution within a deterministic framework, and to be honest not really within a statistical framework either as evidenced in quotations below.

But there is midway between full determinism and full indeterminism or statistics, which we explored in our previous book *Computational Turbulent Incompressible Flow* [20]. We showed that mean-value quantities such as drag and lift in turbulent bluff body flow, can be computed deterministically without resort to statistics, by solving the Euler/Navier-Stokes equations by a certain computational method named *EG2* as an acronym for *Euler General Galerkin* finite element method.

EG2 opens to an exploration of turbulent flow viewing EG2 as direct model of physics with an automatic turbulence model introducing a certain *turbulent dissipation*. EG2 thus resolves the problem of turbulence in the sense of offering a computable understandable mathematical model of turbulence.

EG2 shows to satisfy a certain 2nd Law formulated without the concept of entropy, using only the known concepts of heat energy, kinetic energy, work toghether with *turbulent dissipation*, and thus offers a resolution of the problem of formulating a 2nd Law in physical terms.

EG2 essentially replaces entropy by turbulent dissipation and the 2nd Law comes out simply as a consequence of the inevitable presence of turbulent dissipation in certain processes.

EG2 thus opens to a resolution of the two main problems of macroscopic mechanics of turbulence and 2nd Law, by showing that the problems are essentially the same and can approached by deterministic computation.

1.3 EG2 as Model of Thermodynanics

In this book we extend the scope of [20] to compressible flow described by the Euler/Navier-Stokes equations solved by EG2 into *Computational Thermodynamics*. We thus use EG2 in an exploration of basic processes of thermodynamics in heat engines, heat pumps and refrigerators with turbulent dissipation setting limits of efficiency.

1.4 Icarus Education

This book is part of *Icarus Education* originating in the *Body&Soul* educational project [2] and including:

- Computational Calculus.
- Computational Turbulent Incompressible Flow [20].
- Mathematical Theory of Flight.
- Mathematical Theory of Sailing.
- Mathematical Physics of Blackbody Radiation.
- Many-Minds Relativity
- Many-Minds Quantum Mechanics
- Dr Faustus of Modern Physics.
- The Clock and the Arrow: A Brief Theory of Time.

1.5 EG2 Software: FEniCS: Unicorn

Open source software implementing EG2s available as the *FEniCS* application *Unicorn* [14].

1.6 Outline

Part I Short Story recapitulates the questions and answers of classical thermodynamics and briefly presents the new answers offered by computational thermodynamics. Joule's experiment from 1845 with a gas expanding to double volume is used to illustrate a basic problem of thermodynamics and its resolution by EG2.

Part II World of Thermodynamics briefly covers some of the very many applications of thermodynamics from small to large scales.

Part III Mathematics presents a basic mathematical analysis of solutions the Euler/Navier-Stokes equations, which we follow up in Part IV Computation with an analysis of EG2. The 2nd Law is proved and the limits of mean-value determinism are by a posteriori error estimation based on solving a dual lineraized problem.

Part V Model Analysis is a study of some model problems by analytical mathematics.

Part VI Applications reaches the main goal of computing the efficiency of heat engines, heat pumps and refrigerators in prototype form.

Chapter 2

Objective

> You can fool all the people some time, and some of the people all the time, but you cannot fool all people all the time. (Abraham Lincoln)

The physicist Arnold Sommerfeld (1868-1951) gave the following account of his experience of thermodynamics as a scientific discipline:

- *Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you any more.*

The greatest mystery is the *2nd Law of Thermodynamics*, which has haunted many great scientists into obsession including Maxwell, Boltzmann, Planck, Mach, Ostwald and Prigogine, ever since it was formulated in 1865 by Clausius.

The 2nd Law states that a certain quantity named *entropy* cannot decrease with increasing time, and when strictly increasing characterizes an *irreversible* thermodynamic process, which cannot be reversed in time, since the reversed process would have a strictly decreasing entropy violating the 2nd Law. A direction of time or *Arrow of time* would thus be defined by irreversible thermodynamics. Max Planck (1858-1947) expressed the role of the 2nd Law as follows:

- *Were it not for the existence of irreversible processes, the entire edifice of the 2nd Law would crumble.*

Newtonian deterministic mechanics *without* viscosity/friction, as well as quantum mechanics, is formally time reversible, since the basic equations are invariant under time reversal, and Planck pointed to the need of explaining how irreversibility can arise in a formally reversible deterministic system, more precisely how it can be that a *macroscopic* process based on reversible *microscopic* mechanics, can be irreversible.

Newtonian mechanics *with* slight viscosity from microscopic viscosity, is easily seen to be irreversible as a consequence of the smoothing effect of viscosity; it is of course not surprising that a processes *with* viscosity shows effects *of* viscosity. What physicists of the late 19th century were asking was *how* effects of friction/viscosity can arise in a macroscopic system based on reversible microscopic particle/quantum mechanics *without* viscosity.

Ludwig Boltzmann (1844-1906) took on the challenge and came up with a resolution in the form of *statistical mechanics* based on an assumption of *molecular chaos*, or molecular games of roulette, supposedly reflecting a tendency of thermodynamical processes to evolve from *ordered* towards *disordered* states, or from *less probable* towards *more probable* states, identified by increasing entropy. But a molecular game of roulette introduces a microscopic viscous effect *by assumption*, and thus is similar to deterministic mechanics *with* microscopic viscosity with the same lack of explicative power of irreversibility, as noted in early criticism by Loschmidt [33] and expressed by Eisenschitz in the introduction of his *Statistical Theory of Irreversible Processes* from 1958:

- *The irreversible nature of the approach to equilibrium is apparently incompatible with the reversibility of molecular dynamics. In resolving this paradox the theory faces difficulties that have not yet been fully overcome.*

Further, observations of *self-organization* and *emergence* of order out of chaos contradict steady increase of disorder/entropy. Nevertheless, in the absence of a better explanation, statistical mechanics is today viewed by the physics community as the foundation of thermodynamics offering a justification of both the 2nd Law, irreversibility and the Arrow of time. But statistical mechanics is difficult to understand and to use: The modern text-book [31] prepares the student for (very) tough studies:

- *Statistical thermodynamics is a challenging discipline... It demands an incredible diversity of skills, from probability theory to quantum me-*

> *chanics to molecular modeling...transport phenomena and physical optics. With continuing study and reflection you can rest assured that a practical symbiosis will eventually bloom that simultaneously reinforces and expands your appreciation of both microscopic and macroscopic thermodynamics.*

The objective of this book is to develop a deterministic foundation of thermodynamics in the form of *computational thermodynamics*, which does not rely on any form of statistical mechanics. We show that computational thermodynamics offers accurate simulation and scientific understanding of complex real thermodynamical processes, without requiring any "incredible diversity of skills". In short, we show that thermodynamics can be made both understandable and applicable. The basic idea is to view physical processes as some form of *finite precision analog computation*, which can be simulated by *finite precision digital computation*.

We shall see that computational thermodynamics opens new possibilities to progess with new questions and answers, in particular concerning the phenomena of *turbulence* and *shocks* typically occuring in the thermodynamics of slightly viscous flow dominating applications. The basic novelty is that turbulent/shock solutions are computed and thus are available to inspection, which means that the focus of the science of thermodynamics can be shifted from *a priori* predictions based on analytical mathematics to *a posteriori* analysis of computed turbulent solutions, which can be viewed as a veritable shift of paradigm.

The new computational foundation is based on a *1st Law of Thermodynamics* in the form of the *Euler equations of an ideal gas* expressing *conservation of mass, momentum and energy*, combined with *finite precision computation* in the form of a *least squares stabilized finite element method* referred to as *Euler General Galerkin* or *EG2*. We prove a *2nd Law of Thermodynamics* without the concept entropy to be a consequence of the 1st Law combined with finite precision computation.

With a 2nd Law in this form we avoid the (difficult) main task of statistical mechanics of specifying the physical significance of entropy and motivating its tendency to increase by probabilistic considerations based on (tricky) combinatorics. Yet, we achieve the main goal of the 2nd Law of giving a rational expression and explanation of irreversibility in macroscopic systems based on formally reversibe microscopic mechanics. Thus using *Ockham's razor* [34], we rationalize a scientific theory of major importance making it both more understandable and more useful. The new 2nd Law is closer to classical Newtonian mechanics than the 2nd Law of statistical mechanics, and thus can be viewed to be more fundamental.

We shall see that EG2 is not just any ad hoc computational method for the Euler equations, but is designed to capture the fundamentals of thermodynamics including turbulence and shocks. We will thus view EG2 as a constructive physical model of thermodynamics, in distinction from a classical non-constructive mathematical model without computational solution procedure.

A fundamental question concerns *wellposedness* in the sense of Hadamard, that is what aspects or *outputs* of turbulent/shock solutions are *stable* under perturbations, that is what outputs change little under small perturbations including perturbations from the computational discretization and mesh. We show that wellposedness of EG2 solutions can be tested a posteriori by computationally solving a *dual linearized problem*, through which the output sensitivity of non-zero Euler residuals can be estimated. We find that mean-value outputs such as drag and lift and total turbulent dissipation are wellposed, while point-values of turbulent flow are not. We can thus a posteriori case by case assess the quality of EG2 solutions as solutions of the Euler equations.

Chapter 3

Classical Thermodynamics

> Heat, a quantity which functions to animate, derives from an internal fire located in the left ventricle. (Hippocrates, 460 B.C.)

3.1 Classical 1st and 2nd Laws

Thermodynamics is fundamental in a wide range of phenomena from macroscopic to microscopic scales. Thermodynamics essentially concerns the interplay between *heat energy* and *kinetic energy* in a *gas* or *fluid*. Kinetic energy, or *mechanical energy*, may generate heat energy by *compression* or *turbulent dissipation*. Heat energy may generate kinetic energy by *expansion*, but not through a *reverse* process of turbulent dissipation. The industrial society of the 19th century was built on the use of *steam engines*, and the initial motivation to understand thermodynamics came from a need to increase the efficiency of steam engines for conversion of heat energy to useful mechanical energy. Thermodynamics is closely connected to the dynamics of *slightly viscous* and *compressible* gases, since substantial compression and expansion can occur in a gas, but less in fluids (and solids).

The development of classical thermodynamics as a rational science based on logical deduction from a set of axioms, was initiated in the 19th century by Carnot [7], Clausius [**?**] and Lord Kelvin [25], who formulated the basic axioms in the form of the *1st Law* and the *2nd Law* of thermodynamics. The 1st Law states (for an isolated system) that the *total energy*, the sum of kinetic and heat energy, is conserved. The 1st Law is naturally generalized to include also conservation of mass and Newton's law of conservation of momentum and then can be expressed as the *Euler equations* for a gas/fluid with *vanishing viscosity*.

The 2nd Law has the form of an inequality $dS \geq 0$ for a quantity named *entropy* denoted by S, with dS denoting change thereof, supposedly expressing a basic feature of real thermodynamic processes. The classical 2nd Law states that the entropy cannot decrease; it may stay constant or it may increase, but it can never decrease (for an isolated system).

The role of the 2nd Law is to give a scientific basis to the many observations of *irreversible* processes, that is, processes which cannot be reversed in time, like running a movie backwards. Time reversal of a process with strictly increasing entropy, would correspond to a process with strictly decreasing entropy, which would violate the 2nd Law and therefore could not occur. A perpetum mobile would represent a reversible process and so the role of the 2nd Law is in particular to explain *why* it is imposssible to construct a perpetum mobile, and *why* time is moving forward in the direction an *arrow of time*, as expressed by Max Planck [35, 36, 37]: *Were it not for the existence of irreversible processes, the entire edifice of the 2nd Law would crumble.*

While the 1st Law in the form of the Euler equations expressing conservation of mass, momentum and total energy can be understood and motivated on rational grounds, the nature of the 2nd Law is mysterious. It does not seem to be a consequence of the 1st Law, since the Euler equations seem to be time reversible, and the role of the 2nd Law is to explain irreversibility. We repeat the questions from above since they are so central:

- If the 2nd Law is a new independent law of Nature, how can it be justified?
- What is the physical significance of that quantity named entropy, which Nature can only get more of and never can get rid of, like a steadily accumulating heap of waste?
- What mechanism prevents Nature from recycling entropy?
- How can irreversiblity arise in a reversible system?
- How can viscous dissipation arise in a system with vanishing viscosity?
- Why can a gas by itself expand into a larger volume, but not by itself contract back again, if the motion of the gas molecules is governed by

the reversible Newton's laws of motion?

- Why is there an arrow of time?

3.2 The Mystery of Entropy

These were the questions which confronted scientists in the late 19th century, after the introduction of the concept of entropy by Clausius in 1865, and these showed to be tough questions to answer. After much struggle, agony and debate, the agreement of the physics community has become to view *statistical mechanics* based on an assumption of *molecular chaos* as developed by Boltzmann [4], to offer a rationalization of the classical 2nd Law in the form of a tendency of (isolated) physical processes to move from improbable towards more probable states, or from ordered to less ordered states.

Boltzmann's assumption of molecular chaos in a dilute gas of colliding molecules, is that two molecules about to collide have independent velocities, which led to the *H-theorem* for *Boltzmann's equations* stating that a certain quantity denoted by H could not decrease and thus could serve as an entropy defining an arrow of time.

Increasing disorder would thus represent increasing entropy, and the classical 2nd Law would reflect the eternal pessimistists idea that things always get more messy, and that there is really no limit to this, except when everything is as messy as it can ever get. Of course, experience could give (some) support this idea, but the trouble is that it prevents things from ever becoming less messy or more structured, and thus may seem a bit too pessimistic.

No doubt, it would seem to contradict the many observations of *emergence* of ordered non-organic structures (like crystals or waves and cyclons) and organic structures (like DNA and human beings), seemingly out of disordered chaos, as evidenced by the physics Nobel Laureate Robert Laughlin [26].

Most trained thermodynamicists would here say that emergence of order out of chaos, in fact does not contradict the classical 2nd Law, because it concerns "non-isolated systems". But they would probably insist that the Universe as a whole (isolated system) would steadily evolve towards a "heat-death" with maximal entropy/disorder (and no life), thus fulfilling the pessimists expectation. The question from where the initial order came from, would however be left open.

The standard presentation of thermodynamics based on the 1st and 2nd Laws, thus involves a mixture of deterministic models (Boltzmann's equations with the H-theorem) based on statistical assumptions (molecular chaos) making the subject admittedly difficult to both learn, teach and apply, despite its strong importance.

This is primarily because the question *why* necessarily $dS \geq 0$ and never $dS < 0$, is not given a convincing understandable answer. In fact, statistical mechanics allows $dS < 0$, although it is claimed to be very unlikely. The basic objective of statistical mechanics as the basis of classical thermodynamics, thus is to (i) give the entropy a physical meaning, and (ii) to motivate its tendency to (usually) increase.

Before statistical mechanics, the 2nd Law was viewed as an experimental fact, which could not be rationalized theoretically. The classical view on the 2nd Law is thus either as a statistical law of large numbers or as a an experimental fact, both without a rational deterministic mechanistic theoretical foundation. The problem with thermodynamics in this form is that it is understood by very few, if any, as indicated by the above quotes.

Chapter 4

Telling the Truth

To motivate the that thermodynamics needs a new foundation, we here collect some of the many expresssions in the literature giving evidence that classical thermodynamics is a mess:

- *Every mathematician knows it is impossible to understand an elementary course in thermodynamics.* (V. Arnold)

- *...no one knows what entropy is, so if you in a debate use this concept, you will always have an advantage.* (von Neumann to Shannon)

- *As anyone who has taken a course in thermodynamics is well aware, the mathematics used in proving Clausius' theorem (the 2nd Law) is of a very special kind, having only the most tenous relation to that known to mathematicians.* (S. Brush [**?**])

- *Where does irreversibility come from? It does not come form Newton's laws. Obviously there must be some law, some obscure but fundamental equation. perhaps in electricty, maybe in neutrino physics, in which it does matter which way time goes.* (Feynman [13])

- *For three hundred years science has been dominated by a Newtonian paradigm presenting the World either as a sterile mechanical clock or in a state of degeneration and increasing disorder...It has always seemed paradoxical that a theory based on Newtonian mechanics can lead to chaos just because the number of particles is large, and it is subjectivly decided that their precise motion cannot be observed by humans... In* *the Newtonian world of necessity, there is no arrow of time. Boltzmann found an arrow hidden in Nature's molecular game of roulette.* (Paul Davies [10])

- *The goal of deriving the law of entropy increase from statistical mechanics has so far eluded the deepest thinkers.* (Lieb [32])

- *There are great physicists who have not understood it.* (Einstein about Boltzmann's statistical mechanics)

- *...thermodynamics is a dismal swamp of obscurity... a prime example to show that physicists are not exempt from the madness of crowds... Clausius' verbal statement of the second law makes no sense...All that remains is a Mosaic prohibition; a century of philosophers and journalists have acclaimed this commandment; a century of mathematicians have shuddered and averted their eyes from the unclean...Seven times in the past thirty years have I tried to follow the argument Clausius offers and seven times has it blanked and gravelled me. I cannot explain what I cannot understand.* (Truesdell [41])

- *The second law of thermodynamics is, without a doubt, one of the most perfect laws in physics. Any reproducible violation of it, however small, would bring the discoverer great riches as well as a trip to Stockholm. The world's energy problems would be solved at one stroke. It is not possible to find any other law (except, perhaps, for super selection rules such as charge conservation) for which a proposed violation would bring more skepticism than this one. Not even Maxwell's laws of electricity or Newton's law of gravitation are so sacrosanct, for each has measurable corrections coming from quantum effects or general relativity. The law has caught the attention of poets and philosophers and has been called t he greatest scientific achievement of the nineteenth century. Engels disliked it, for it supported opposition to Dialectical Materialism, while Pope Pius XII regarded it as proving the existence of a higher being.* (Bazarov in *Thermodynamics*, 1964)

- *If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equations, then so much the worse for Maxwell's equations. If it is found to be contradicted by observation, well, these experimentalists do bungle things sometimes. But if your* *theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation* (Sir Arthur Stanley Eddington in *The Nature of the Physical World*, 1915)

- *A good many times I have been present at gatherings of people who, by the standards of the traditional culture, are thought highly educated and who have with considerable gusto been expressing their incredulity at the illiteracy of scientists. Once or twice I have been provoked and have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative.* (C. P. Snow in 1959 Rede Lecture entitled *The Two Cultures and the Scientific Revolution*).

From *Challenges to the 2nd Law of Thermodynamics* by V. Capek and D. P. Sheenan:

- *This monograph is the first to examine modern challenges to the 2nd Law. For more than a century this field has lain fallow and beyond the pale of legitimate scientific inquiry due to both a dearth of scientific results and to a surfeit of peer pressure against such inquiry.*

- *It is remarkable that 20th century physics, which embraced several radical paradigm shifts, was unwilling to wrestle with this remnant of 19th century physics, whose foundations were admittedly suspect and largely unmodified by the discoveries of the succeeding century.*

- *This failure is due in part to the many strong imprimaturs placed on it by prominent scientists like Planck, Eddington and Einstein. There grew around the second law a nearly inpentrable mystique which only now is being pierced.*

- *The 2nd Law has no general theoretical proof and, like all physical laws, its status is tied ultimately to experiments.*

- *Inquiry into its status should not be stifled by certain unscientific attitudes and practices that have operated thus far.*

From *A History of Thermodynamics: The Doctrine of Energy and Entropy* by Ingo Müller:

- *A physicist likes to be able to grasp his concepts plausibly and on an intutive level. In that respect, however, the entropy - for all its proven an recognized importance - is a disappointment. The formula* $dS = \frac{dQ}{T}$ *does not lend itself to a suggestive interpretation.*

From *Classical Thermodynamics as Theory of Heat Engines* by C. Truesdell and S. Bharatha:

- *I do not think it s possible ton write a history of a science until that science itself shall have been understood, thanks to a clear, explicit, and decent logical structure. The exuberance of dim, involute, and undisciplined historical essays upon classical thermodynamics reflects the confusion of the theory itself.*

- *Thermodynamics was born in obscurity and disorder, not to say confusion, and there the common presentations of it has remained.*

From *Tragicomical History of Thermodynamics* by C. Truesdell:

- *Thermodynamics is the kingdom also of running current history as well as polemics, not to mention verbosity. In no other discipline have the same equations been published over and over again so many times by different authors in different ill-defined notations and therefore claimed as his own by each; in no other has a single author seen fit to publish essentially the same ideas over and over again within a perieod of twenty years; and nowhere is else is the ratio of talk and excuse to reason and result so high...*

Chapter 5

Old Questions

> Those who have talked of "chance" are the inheritors of antique superstition and ignorance...whose minds have never been illuminated by a ray of scientific thought. (T. H. Huxley)

5.1 The Enigma

While the 1st Law in the form of conservation of energy can be viewed as a definition of internal energy, and as such cannot be disputed, the nature of the 2nd Law posed a main challenge to the scientists of the late 19th century with the following basic questions:

- Is the 2nd Law a law of Nature which can be justified, or is it an experimental fact beyond rationalization?
- What is the physical significance of that quantity named entropy, which Nature can only get more of and never can get rid of, like a steadily accumulating heap of waste? What mechanism prevents Nature from recycling entropy?
- How can irreversibility arise in reversible mechanics?

The enigma Boltzmann set out to solve was to explain *how* in reversible mechanics there can be irreversible processes with an Arrow of time, and his solution was "Natures molecular game of roulette" or molecular chaos in a *particle model* of a dilute gas of elastically colliding molecules, *assuming* pairs of molecules about to collide to have statistically independent velocities *before* collision, but not after. From the statistical particle model Boltzmann derived a deterministic *kinetic model* in the form of *Boltzmann's equation* for the particle density as a function of position, velocity and time as independent variables. Boltzmann proved that solutions satisfy a 2nd Law referred to as the *H-theorem*, as a consequence of the assumption of molecular chaos. Boltzmann's solution was immediately heavily criticized, in particular by Loschmidt [33], who pointed to the (obvious) fact that assuming statistical independence *before* collision, effectively defines an Arrow of time and thus assumes what is to be demonstrated.

5.2 From Boltzmann to Planck

In "an act of despair" Max Planck stimulated by statistical mechanics proposed to explain the irreversible nature of *black-body radiation* in terms of statistics of light quanta, which initiated quantum mechanics. Boltzmann was annihilated by the criticism, but not his atomic games of roulette, which became the signum of the physics of the 20th century.

5.3 Emergence

However, the criticism remains into our days: Molecular games of roulette with steadily increasing disorder is incompatible with *emergence* of ordered structures (like crystals, waves and cyclons or DNA and human beings), as pointed out by many including the physics Nobel Laureate Robert Laughlin [26].

5.4 Microscopics of Microscopics

Microscopics of macroscopics in the form of games of roulette requires its own microscopics, which leads to a neverending chain of microscopics upon microscopics. Einstein and Schrödinger never accepted the statistical *Copenhagen interpretation* of quantum mechanics forefully advocatd by in particular Nils Bohr, who dismissed their criticism as an early onset of senility. However, an (informal) poll taken at the 1997 UMBC quantum mechanics workshop gave the Copenhagen interpretation less than half of the votes (http://space.mit.edu/home/tegmark/).

5.5 2nd Law by Statistics

The objective of statistical mechanics as the basis of classical thermodynamics, is to give entropy a physical meaning, and to motivate its tendency to increase. Before statistical mechanics, the 2nd Law was viewed as an experimental fact, which could not be rationalized theoretically.

To sum up, the accepted view on the 2nd Law is either as a statistical law of large numbers or simply as an experimental fact, both without a rational deterministic mechanistic theoretical foundation.

Chapter 6

New Answers

> What we observe as material bodies and forces are nothing but shapes and variations in the structure of space. Particles are just schaumkommen (appearances). ... Let me say at the outset, that in this discourse, I am opposing not a few special statements of quantum physics held today (1950s), I am opposing as it were the whole of it, I am opposing its basic views that have been shaped 25 years ago, when Max Born put forward his probability interpretation, which was accepted by almost everybody... I don't like it, and I'm sorry I ever had anything to do with it. (Schrödinger [39])

6.1 Computational Turbulence

In this book we present a foundation of thermodynmaics where the basic assumption of statistical mechanics of molecular chaos, is replaced by *deterministic finite precision computation*, more precisely by a *least squares stabilized finite element method* for the Euler/Navier-Stokes equations, referred to as *Euler General Galerkin* or *EG2*. In the spirit of Dijkstra [?], we thus view EG2 as the physical model of thermodynamics, that is the Euler equations together with a computational solution procedure, and not just the Euler equations without constructive solution procedure as in a classical non-computational approach.

Using EG2 as a model of thermodynamics changes the questions and answers and opens new possibilities of progress together with new challenges to mathematical analysis and computation. The basic new feature is that EG2 solutions are computed and thus are available to inspection. This means that the analysis of solutions shifts from *a priori* to *a posteriori*; after the solution has been computed it can be inspected.

Inspecting computed EG2 solutions we find that they are *turbulent* and have *shocks*, which is identified by pointwise large Euler residuals, reflecting that pointwise solutions to the Euler equations are lacking. The enigma of thermodynamics is thus the enigma of turbulence (since the basic nature of shocks is understood). Computational thermodynamics thus essentially concerns computational turbulence.

The fundamental question concerns *wellposedness* in the sense of Hadamard, that is what aspects or *outputs* of turbulent/shock solutions are stable under perturbations in the sense that small perturbations have small effects. We show that wellposedness of EG2 solutions can be tested a posteriori by computationally solving a *dual linearized problem*, through which the output sensitivity of non-zero Euler residuals can be estimated. We find that mean-value outputs such as drag and lift and total turbulent dissipation are wellposed, while point-values of turbulent flow are not. We can thus a posteriori in a case by case manner, assess the quality of EG2 solutions as solutions of the Euler equations.

6.2 Basic 2nd Law Without Entropy

We formulate a 2nd Law for EG2 without the concept of entropy, in terms of the basic physical quantities of kinetic energy K, heat energy E, rate of *work* W and shock/turbulent dissipation $D > 0$. The new 2nd Law reads in the case of no exterior forcing:

$$\dot{K} = W - D, \quad \dot{E} = -W + D, \tag{6.1}$$

where the dot indicates time differentiation. Slightly viscous flow always develops turbulence/shocks with $D > 0$, and the 2nd Law thus expresses an irreversible transfer of kinetic energy into heat energy, while the total energy $\epsilon = E + K$ remains constant as seen by summing the two equations:

$$\dot{\epsilon} = \dot{K} + \dot{E} = 0. \tag{6.2}$$

We see that the work W transforms heat energy into kinetic energy or kinetic energy into heat energy depending on the sign of W:

- In expansion with $W > 0$, heat energy transforms into kinetic energy,

- In compression with $W < 0$, kinetic energy transforms into heat energy.

On the other hand, since $D > 0$, turbulent dissipation only transforms kinetic energy into heat energy, and not heat energy to kinetic energy. When you rub your hands they get warm, but you cannot get your hand rubbing by only heating them. Motion can generate heat by friction, but heat cannot generate motion by an inverse process of friction. In this book you will discover a mathematical explanation of this familiar experience based on finite precision digital computation, which represents a new way of viewing physics as a form of analog computation of finite precision.

You will find that the 2nd Law in the form (6.1) is easy to grasp intuitively as expressing a basic balance between heat energy and kinetic energy, with unidirectional flow of turbulent dissipation energy from kinetic to heat energy, but also reflects a rather deep mathematical principle.

With the 2nd Law in the form (6.1), we avoid the (difficult) main task of statistical mechanics of specifying the physical significance of entropy and motivating its tendency to increase by probabilistic considerations based on (tricky) combinatorics. Thus using *Ockham's razor* [34], we rationalize a scientific theory of major importance making it both more understandable and more useful. The new 2nd Law is closer to classical Newtonian mechanics than the 2nd Law of statistical mechanics, and thus can be viewed to be more fundamental.

The new 2nd Law is a consequence of the 1st Law in the form of the Euler equations combined with EG2 finite precision computation effectively introducing viscosity and viscous dissipation. These effects appear as a consequence of the non-existence of pointwise solutions to the Euler equations reflecting instablities leading to the development shocks and turbulence in which large scale kinetic energy is transferred to small scale kinetic energy in the form of heat energy. The viscous dissipation can be interpreted as a penalty on pointwise large Euler residuals arising in shocks/turbulence, with the penalty being directly coupled to the violation following a principle of criminal law exposed in [15]. EG2 thus explains the 2nd Law as a consequence of the non-existence of pointwise solutions with small Euler residuals.

This offers an understanding to the emergence of irreversible solutions of the formally reversible Euler equations. If pointwise solutions had existed, they would have been reversible without dissipation, but they don't exist, and the existing computational solutions have dissipation and thus are irreversible.

Chapter 7

Joule's 1845 Experiment

> The most convincing proof of the conversion of heat into living force [vis viva] has been derived from my experiments with the electro-magnetic engine, a machine composed of magnets and bars of iron set in motion by an electrical battery. I have proved by actual experiment that, in exact proportion to the force with which this machine works, heat is abstracted from the electrical battery. You see, therefore, that living force may be converted into heat, and that heat may be converted into living force, or its equivalent attraction through space.

7.1 The Essence of Thermodynamics

We shall now discover the essence of thermodynamics as transformation between heat energy and kinetic energy in a basic experiment performed by the James Prescott Joule (17874-1858), a manager of a brewery and hobby scientist with special interest in electricity. Joule reflected about replacing the brewery's steam engine by the newly invented electrical motor and thus became interested in the efficiency of different forms of energy conversion. *Joule's Law* gives the heat Q generated by an electrical current I through a resistor R as $Q = I^2R$.

In his basic thermodynamics experiment, Joule considered a gas initially at rest, or in equilibrium, at a certain temperature and density in a certain volume immersed into a container of water, see Fig. 7.1. At initial time a valve was opened and the gas was allowed to expand into the double volume while the temperature change in the water was carefully measured by Joule.

To the great surprise of both Joule and the scientific community, no change of the temperature of the water could be detected, in contradiction with the expectation that the gas would cool off under expansion. Moreover, the expansion was impossible to reverse; the gas had no inclination to contract back to the original volume.

We assume that the gas is a *ideal gas* satisfying the gas law

$$p = \gamma\rho T \tag{7.1}$$

where p is pressure, ρ is density and T is absolute temperature and where $0 < \gamma < 1$ is a gas constant. This law come out as a combination of Boyle's law stating that pressure and density under constant temperature are proportional and Charles law stating that absolute temperature and density under constant pressure are inversely proportional.

We simulate Joule's experiment computationally using EG2: At initial time a valve is opened in a channel connecting two cubical chambers, a left and a right chamber, filled with gas of the same temperature but different density/pressure with high density/pressure in the left and low in the right chamber. Fig. 7.2-7.3 display the time-evolution of mean temperature, density, kinetic energy, pressure and turbulent dissipation in the left and right chambers, while Fig. 7.5-**??** give snapshots of the distribution of temperature, speed, turbulent dissipation at an intermediate time.

We see that temperature drops in the left chamber as the gas expands with heat energy transforming to kinetic energy with a maximal temperature drop in the channel. When the cool expanding gas hits the wall opposite to the channel inlet in the right chamber, it is heated in recompression and turbulent/shock dissipation. The mean temperature thus drops in the left chamber and increases in the right and after a slight rebounce settles to a remaining density/temperature gap as the gas comes to rest with the same pressure in the left and right chambers and the same total heat energy as before expansion. Joule measured the total heat energy of the initial and final equilibrium states and found them to be equal. Joule did not seek to measure the dynamics of the process, nor the remaining temperature/density gap.

From the 1st Law alone there are many different possible end states with varying gaps in density/temperature. It is the 2nd Law which determines the size of the gap, which relates to the amount of turbulent/shock dissipation in the left and right chambers, which is determined by the dynamics of the process including the distribution of turbulence/shock dissipation.

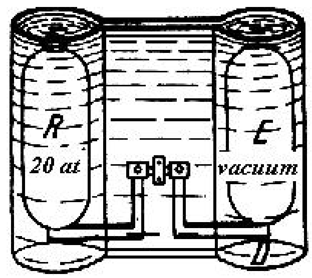

Fig. 358 Concerning overflowing experiment of Joule (Scientific Papers). *R* contains at first air compressed to 20 atm, *E* is initially a vacuum, *D* the tube

Figure 7.1: Joule's 1845 experiment

Classical thermodynamics focussing on equiblium states does not tell which from a range of possible equlibrium end states with varying gaps, will actually be realized, because the true end state depends on the dynamics of the process. If anything, classical thermodynmics would predict an end state with zero gap, which we have seen is incorrect. In short, classical equilibrium thermodynamics excluding the dynamics cannot correctly predict transition from one equlibrium state to another, and thus has little practical value.

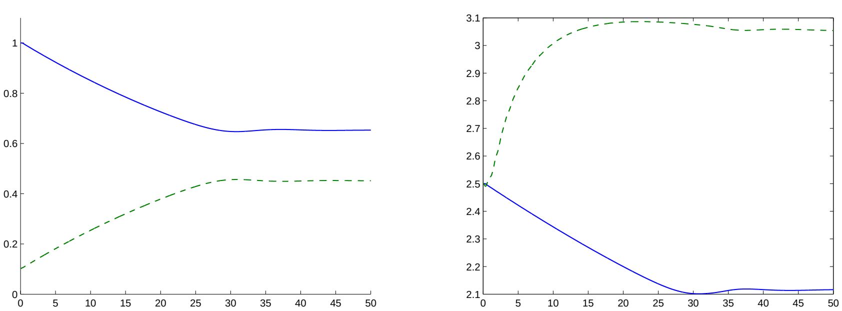

Figure 7.2: Mean density and temperature in left and right chambers as functions of time.

The 2nd Law states that reversal of the process with the gas contracting back to the original small volume, is impossible because the only way the

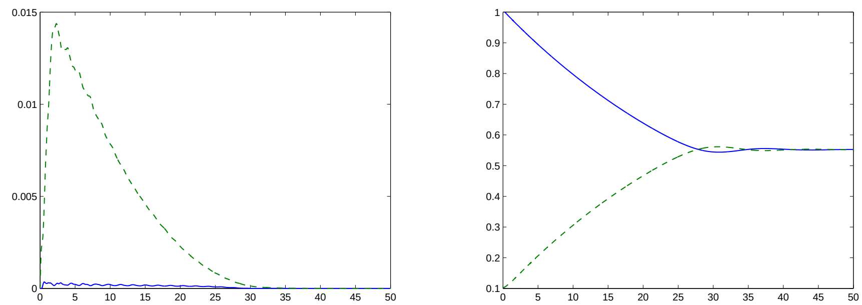

Figure 7.3: Mean kinetic energy and pressure in left and right chambers as functions of time.

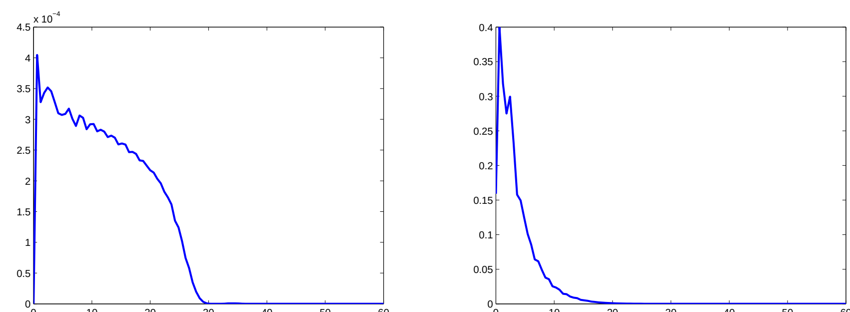

Figure 7.4: Mean turbulent dissipation in left and right chambers as functions of time.

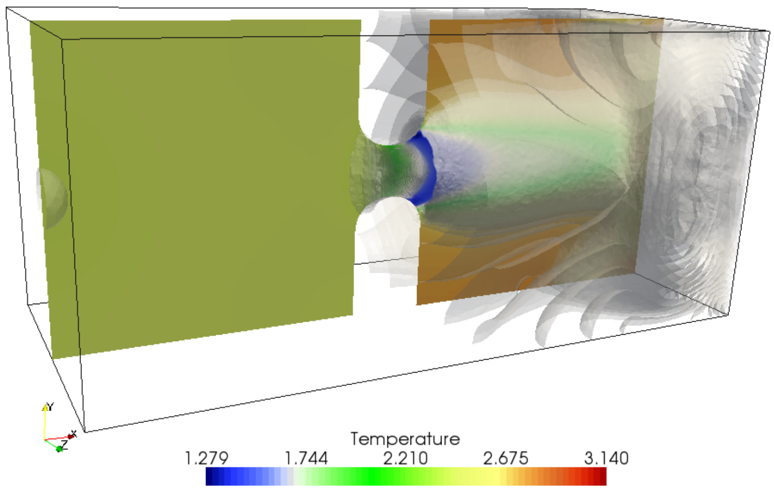

Figure 7.5: Distribution of gas temperature at $T = 3$

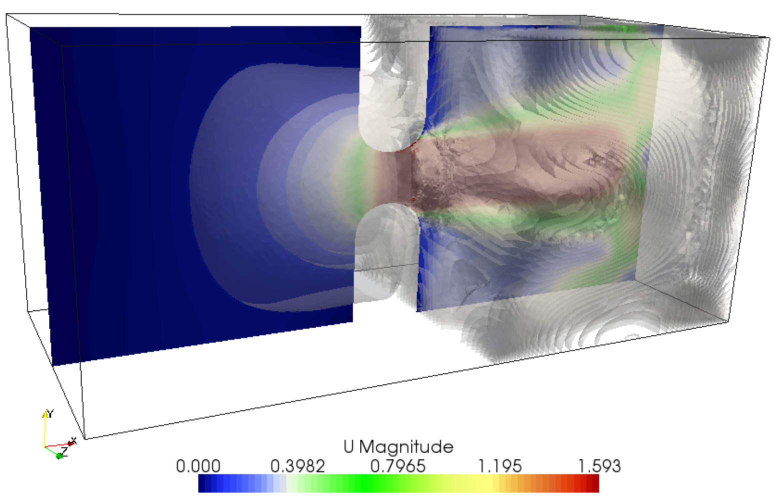

Figure 7.6: Distribution of gas speed at $T = 3$

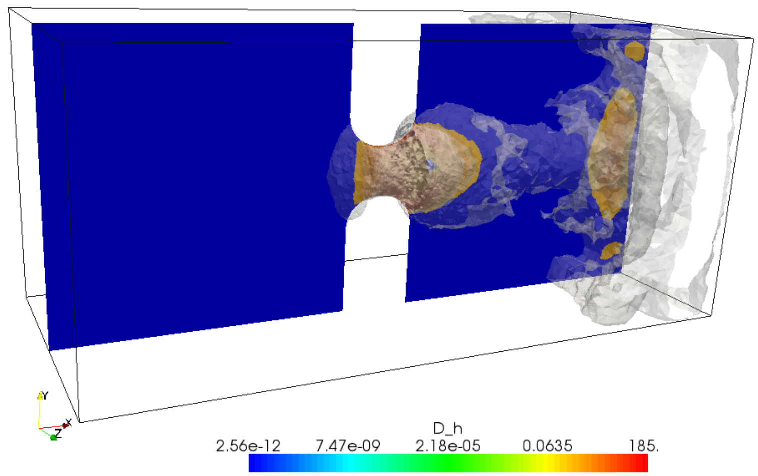

Figure 7.7: Distribution of turbulent dissipation at $T = 3$

gas can be put into motion without external forcing is by expansion: Self-expansion is possible, but not self-constraction.

We are thus able to analyze and understand the dynamics of the Joule experiment using the 1st and the new form of the 2nd law. The experiment displays the expansion phase of a compression refrigerator with heat being moved by expansion from the left chamber in contact with the inside of the refrigerator, into the right chamber in contact with the outside. The cycle is closed by recompression under outside cooling. The efficiency connects to the temperature drop in the left chamber and the gap, with efficiency suffering from rebounce to small gap.

7.2 Computation of Efficiency as Refrigerator

Thermodynamics was developed to understand the functioning of heat engines transforming heat energy to mechanical energy, and heat pumps and refrigerators moving heat energy from a reservoir of low temperature to reservoir of higher temperature at the expenense of mechanical work. We can view these devices as different forms of a heat engine as a transformer between mechanical energy and heat energy.

We can use the Joule experiment as a idealized model of a heat pump refrigerator working in a cycle absorbing heat from the exterior in the left chamber and delivering heat to the exterior from the right chamber, corresponding to moving heat from the inside of a refigerator to the outside. We consider a model consisting of the following steps starting with a gas at rest with $\rho = T = 1$ in a left box of unit volume connected to a right empty box of the same volume through a channel with a valve closed at the start of the cycle.

1. Open the valve and let gas expand to the double volume as in the Joule experiment to rest state with mean temperature $T_l < 1$ in the left chamber and $T_r > 1$ in the right.

2. Close the valve and let the gas absorb heat in the left chamber from exterior and deliver heat in the right chamber to the exterior to restore mean temperature $T = 1$.

3. Compress the gas in left and right chamber under heat exchange with the exterior at $T = 1$ until $\rho = 1$ and open the valve. Return to 1.

For simplicity we assume that the rest states are constant in space, so that in particular T_l and T_r are the constant tempeartures, and ρ_l and ρ_r the constant densities, in the left and right chambers after the expansion in step 1. We have the following balance equations assuming the gas law $p = \bar{\gamma}\rho T$:

$$\rho_l T_l = \rho_r T_r = \frac{1}{2} \quad \rho_l + \rho_r = 1 \tag{7.2}$$

since also $\rho_l T_l + \rho_r T_r = 1$ by conservation of heat energy. We conclude that

$$T_l = \frac{1}{2\rho_l} \quad T_r = \frac{1}{2(1-\rho_l)}. \tag{7.3}$$

The heat Q_l absorbed in the left chamber in step 2 equals

$$Q_l = \rho_l(1 - \frac{1}{2\rho_l}) = \rho_l - \frac{1}{2} \tag{7.4}$$

and the work W_l and W_r performed in the left and right chambers step 3 is given by

$$W_l = -\int p dV = \bar{\gamma}\int_{\rho_l}^{1} \frac{d\rho}{\rho} \qquad W_r = -\int p dV = \bar{\gamma}\int_{1-\rho_l}^{1} \frac{d\rho}{\rho}. \tag{7.5}$$

The efficency η of the device viewed as a refrigerator is the given by

$$\eta = \frac{Q_l}{W_l + W_r} = \frac{\rho_l - \frac{1}{2}}{-\log(\rho_l(1-\rho_l))} \tag{7.6}$$

We see that η depends on the temperature drop T_l with $\eta = 0$ in the extreme cases of $\rho_l = \frac{1}{2}$ and $T_l = 1$ and $\rho_l = 1$ and $T_r = \infty$. Maximal efficiency ≈ 0.387 is obtained for $\rho \approx 0.85$ with a gap $T_r - T_l \approx 0.3$.

The efficiency as a heat pump becomes the same if we view the useful heat that which is delivered to the exterior from the right chamber in step 2. Including some of heat from compression in step 3 as useful heat increases the efficiency as a heat pump. We get the indication that it is easier to construct an efficient heat pump than an efficient refrigerator.

Classical thermodynamics would, if anything, predict $\rho_l = \rho_r = \frac{1}{2}$ and $T_l = T_r = 1$ and thus $\eta = 0$. In order to find the correct rest state after adiabatic expansion, it is necesary to follow the dynamics of the expansion with the amount of turbulenct/shock dissipation in the two chambers determining the resulting gaps in temperature and density. Classical thermodynamics only considers equilibrium states leaving out the turbulence/shock dynamics and thus is basically useless for prediction of efficiency of heat engines, which was the original goal of thermodynamics.

In the above model we set for simplicity the interior rest temperature equal to the exterior temperature = 1, viewing the heat Q absorbed in the left chamber as excess heat introduced into the refrigerator to be moved to the outside. We can obviously extend the above computation to the more realistic case of a lower interior rest temperature. In this case less heat Q would be absorbed in step 2 decreasing the efficiency.

In a real refrigerator the expansion comes along with vaporization which increases the temperature drop and thus the efficiency. In the applications part we will consider more realistic heat engines including heat pumps and refrigerators.

Note that the rapidity of the process of moving heat from the left to the right chamber is crucial. By heat conduction alone it would be possible to move exces heat from left to right, but that would be a slow process. With the compression and expansion of the gas heat can quickly be transported and that is a crucial aspect as concerns the capacity of the device.

Classical thermodynamics focussing on equilibrium states considers transitions between equalibrium states to be very slow and thus does not cover useful applications.

7.3 Conclusions from Joule's Experiment

We have used Joule's experiment to illustrate basic features of thermodynamics including the essence of both aspects *thermo* and *dynamics*. We have seen that computational thermodynamics is capable of simulating the dynamics including turbulence and shocks, in particular during expansion where the amount and distribution of turbulent/shock dissipation determines the gap in density-temperature after expansion, which determines the efficiency as a refrigerator or heat pump. We have seen the 2nd Law explain why expansion from rest is possible without interaction with the exterior, while compression requires exterior work.

We have found no need of any concept of entropy: The concepts of kinetic energy, heat energy, work and turbulent dissipation which are physical quantities which can be measured, are sufficient to describe thermodynamics, and entropy serves no purpose and has no physical meaning.

Chapter 8

New Foundation

Heat, a quantity which functions to animate, derives from an internal fire located in the left ventricle. (Hippocrates, 460 B.C.)

8.1 The Euler and Navier-Stokes Equations

The *Navier-Stokes equations* for a compressible gas express *conservation of mass, momentum and total energy* as a system of partial differential equations with position and time as independent variables, together with *constitutive laws* defining *pressure*, *viscous forces* and *diffusive heat fluxes* in terms of *mass density*, *velocity* and *heat/internal energy*, combined with *initial conditions* and *boundary conditions*. In a *perfect gas* the pressure is proportional to the internal energy. With vanishing viscosity and heat conductivity the Navier-Stokes equations reduce to the *Euler equations*. The Euler/Navier-Stokes equations represent a *fluid mechanics model* of thermodynamics, as compared to a kinetic model with also particle velocity as an independent variable.

Conservation of mass, momentum and total energy in the Euler equations formally arise by averaging over velocities in Boltzmanns kinetic model. However, the constitutive laws of the Navier-Stokes equations including coefficients of *viscosity* and *heat conductivity* show to be solution dependent and thus difficult to determine *ab initio* from a kinetic model, or in experiments. In a *Newtonian fluid* the viscosity is *assumed* to be constant, but this assumption is questionable for slightly viscous fluids with vastly different effects of viscosity in turbulent and laminar flow. The *existence* and *uniqueness* (or the converse of *non-existence*) of solutions to the incompressible Navier-Stokes equations for a Newtonian fluid represent one of the open Clay Mathematics Institute Millenium Problems [**?**].

Solutions of the Navier-Stokes equations for a perfect gas *formally* satisfy a 2nd Law expressing that a specific scalar entropy defined in terms of mass density and internal energy is strictly increasing with increasing time, as an expression of a loss of kinetic energy by *positive viscous dissipation* formally obtained by forming the scalar of the momentum equation including viscous stresses with the velocity. The 2nd Law with strictly increasing entropy for solutions of Navier-Stokes equations enforcing irreversibility, is thus formally equivalent to the presence of non-vanishing viscosity. For the Euler equations, the entropy (formally) stays constant as an expression of vanishing viscosity and reversibility.

For the Navier-Stokes equations *with* viscous dissipation, we might thus simply forget the entropy inequality, because it is an automatically satisfied *derived relation*.

This reduces the enigma of the 2nd Law to explaining how effects of viscous dissipation and irreversibility can arise in a formally reversible system such as a system of elasticly colliding particles without viscosity. Simply claiming that viscous effects must come from somewhere is not informative. Neither is to claim that they come from quantum mechanics (or neutrino physics like Feynman), since quantum mechanics is formally reversible. Nor is simply assuming constitutive laws for viscous stresses of some form, e.g. simply assuming the fluid to be Newtonian.

Boltzmann's answer was molecular games of roulette, but it is an answer which poses more questions than it resolves.

8.2 Computational Thermodynamics

In this book we present a *constructive deterministic* fluid mechanics model of the thermodynamics of a slightly viscous gas/fluid based on *finite precision computation* by a *weighted least squares stabilized finite element method* for the *Euler/Navier-Stokes equations* with *slip boundary conditions* at solid boundaries, referred to as *Euler General Galerkin* or *EG2*. For definiteness we consider a perfect gas/fluid, but extension to more general state equations for the pressure is possible.

Note that we start from the Euler equations with vanishing viscosity and heat conductivity and we thus do not need input of constitutive laws for viscous stresses and heat diffision, only a law of state for the pressure.

The least squares stabilization in EG2 penalizes large Euler residuals by viscosity acting in the streamline direction as a form of *bulk viscosity* of order h, and is complemented by a higher-order residual dependent isotropic *shear viscosity* of order $h^{3/2}$ in turbulent regions, where h is the mesh size, together referred to as *EG2 viscosity*.

EG2 is a *constructive model* in the form of the Euler equations *together* with a computational solution procedure including EG2 viscosity, guaranteeing existence by computational construction, to be distinguished from a *formal model* e.g. in the form of the Navier-Stokes equations without constructive solution procedure and requiring input of viscosity.

EG2 automatically introduces solution dependent viscosity and thus circumvents the difficult problem of specifying viscosity (and heat conductivity) in a Navier-Stokes model. The only input in this regard is that the flow is *slightly viscous* with *Reynolds number* larger than say 10^6, which covers many important applications in aero- and hydrodynamics.

We discover by computation that EG2 solutions are *turbulent* and have *shocks*, both phenomena being identified by substantial (positive) *EG2 turbulent/shock dissipation* from EG2 viscosity with pointwise large (but weakly small) Euler residuals. Turbulence/shocks are thus identified by substantial EG2 turbulent/shock dissipation, which reflects pointwise large Euler residuals, which reflects non-existence of pointwise solutions with pointwise vanishing Euler residuals. We observe turbulence in EG2 solutions with slip boundary conditions, and conclude that turbulence does not (primarily) originate from microscopic boundary layers with no-slip boundary conditions, contrary to state-of-the art boundary layer theory by Prandtl and Schlichting [**?**, **?**], but from macroscopic instability.

We motivate using slip boundary conditions (or more generally a friction boundary condition with small friction) by the computationally and experimentally verified fact that the *skin friction* of a turbulent boundary layer tends to zero with viscosity and thus is (comparatively) small for slightly viscous flow.

We prove that EG2 solutions satisfy a 2nd Law expressed in terms of kinetic energy, internal energy, work and (positive) turbulent/shock dissipation. We realize that irreversibility is a consequence of substantial turbulent/shock dissipation, which is consequence of pointwise instability of slightly viscous flow, which is reflected by non-existence of pointwise solutions to the Euler equations. We thus justify a 2nd Law without resort to any ad hoc assumption of positive viscous dissipation or molecular chaos.

Existence of EG2 solutions is guaranteed by construction. Uniqueness relates to *wellposedness* in the sense of Hadamard, which concerns what aspects or *outputs* of EG2 turbulent/shock solutions are stable under perturbations in the sense that small perturbations have small output effects. We define a EG2 output to be wellposed if it is insensitive to mesh refinement and thus can be computed with finite mesh size. We show that wellposedness of EG2 solutions can be tested a posteriori by computationally solving a *dual linearized problem*, through which the output sensitivity of non-zero Euler residuals can be estimated. We find that mean-value outputs such as drag and lift and total turbulent dissipation are wellposed, while point-values of turbulent flow are not. We can thus a posteriori assess the quality of EG2 solutions as solutions of the Euler equations and identify what outputs are wellposed and converge with decreasing mesh size.

EG2 solutions can be viewed either as exact Euler solutions subject to perturbations from non-vanishing Euler residuals, or alternatively as approximate Navier-Stokes solutions with specific viscosity given by the mesh-dependent EG2 viscosity, combined with slip/friction boundary conditions.

We emphasize that EG2 contributes its own mesh/solution-dependent EG2 viscosity and thus does not require any input of viscosity (or heat conductivity) coefficients, or turbulence model.

8.3 EG2 as Automatic Turbulence Model

EG2 can be viewed as a form of *Large Eddy Simulation LES* for slightly viscous/high Reynolds number flow with an *turbulence model* given by the least squares stabilization for interior turbulence and the slip boundary condition for turbulent boundary layers.

We recall that *Direct Numerical Simulation DNS* by computational solution of Navier-Stokes equations with resolution of all turbulent scales including thin boundary layers, is today possible for Reynolds numbers up to 10^4, while reaching 10^6 is estimated to take another 50 years [**?**, **?**].

Some form of LES with turbulence modeling is therefore needed for high Reynolds number flow, but the design of turbulence models is an open problem since more than hundred years. EG2 offers an automatic turbulence model based on computational principles, with automatic assessment of wellposedness by duality.

EG2 thus gives an answer to the enigma of the origin of viscosity in terms of of finite precision computational simulation of turbulent flow. EG2 finite precision computation is not statistics, because statistical ensembles of outputs do not appear, only mean-values in space-time of individual trajectories/solutions.

8.4 From Probable to Necessary

The stabilization/viscous dissipation in EG2 is necessary because without stabilization EG2 solutions cease to exist in blowup as they inevitably go turbulent, while physical flows continue to exist without blowup even after transition to turbulence. Viscous dissipation thus comes out from an *inevitable* development of turbulence/shocks as a result of an inherent instability of slightly viscous flow, and a *necessity* to avoid blowup into non-existence, because non-existence is not an option: The show must go on, which is not a question of probability. EG2 viscous dissipation is thus a necessity, and not the result of a game of roulette.

EG2 viscosity transfers kinetic energy into internal energy by pointwise large but weakly small violation of conservation as the characterstic of turbulence. By necessity, as a characteristic of turbulence, the pointwise violation is large, yet in a sense smallest possible to prevent blowup and thus generic and not ad hoc.

8.5 The Spirit of Dijkstra

We follow the device of the famous computer scientist Dijkstra:

- *Originallly I viewed it as the function of the abstract machine to provide a truthful picture of the physical reality. Later, however, I learned to consider the abstract machine as the* true *one, because that is the only one we can think; it is the physical machine's purpose to supply a working model, a (hopefully) sufficiently accurate physical simulation of the true, abstract machine.*

We thus view EG2 as a constructive mathematical model (abstract machine) of a physical reality (physical machine). We are then led to interprete the digital finite precision computation as some form of analog physical computation, and digital EG2 viscosity as some form of analog physical viscosity.

We compare with a classical formal mathematical model in the form of the Navier-Stokes equations including an ad hoc model of viscosity, e.g. a Newtonian model with constant shear viscosity. We are thus led to turn around the common view of computational viscosity as “artificial” viscosity and Newtonian viscosity as “physical” viscosity, and instead interprete EG2 viscosity as physical (and then Newtonian viscosity as artificial), following von Neumann who opened compressible flow to computational simulation by introducing artificial viscosity on physical grounds.

EG2 thus offers a model of fluid flow, which can be inspected, analyzed, understood, utilized and evaluated, while the true physics of turbulent flow may remain inaccessible to inspection and analyzis. Even if the mechanics of turbulent flow in principle can be reduced to quantum mechanics on atomic scales, such a model seems useless for predictions on macroscopic scales. For example, determining the viscosity of water from quantum mechanics is still an open problem.

We remark that the role of viscosity coefficients in classical modeling is to define viscous force in terms of fluid velocity (strain). If now EG2 automatically supplies viscous forces, without input of viscosity, there is no longer any need to define viscosity coefficients, or the Reynolds stresses of turbulence modeling, and EG2 thus offers a simplification of fluid mechanics and a way out of a stalemate.

Using EG2 as a model of thermodynamics changes the questions and answers and opens new possibilities of progress together with new challenges to mathematical analysis and computation. EG2 solutions are contructed/computed and thus are available to inspection, which means that the analysis of solutions shifts from *a priori* to *a posteriori*; after solutions have been computed they can be inspected, their qualities can be evaluated and interpreted in physical terms.

8.6 The Power of EG2

In related work [**?**, **?**, 20] we have demonstrated the new capabilities offered by EG2 in resolutions of both dAlemberts paradox from 1752 and the Clay Millenium Problem on existence and uniquenes of the incompressible Euler/Navier-Stokes equations: In short, existence follow by construction and uniqueness from wellposedness, both being consequences of the basic structure of EG2 as a midway between the Scylla/Galerkin of weak solution, which is too weak, and the Carybdis/least squares of strong solution, which is too strong. With the proper weighting of the least squares stabilization, EG2 manages to combine accuracy with wellposedness and thus produce meaningful outputs.

More precisely, we will see below that output variation is bounded by $S\|hR\|_0$, where S is a stability factor, h is the mesh size, R is the Euler residual and $\|\cdot\|_0$ is a space-time L_2-norm. This results from the Galerkin orthogonality of EG2, which together with least squares stabilization introducing a bound on $\|\sqrt{h}R\|_0$, enforces control of output variation up to a tolerance $S\sqrt{h}$. We shall find that for mean-value outputs such as drag/lift and total turbulent dissipation, $S << h^{-1/2}$ which implies wellposedness. The unique design of EG2 with a combination of Galerkin orthogonality and weighted least squares stabilization, thus can be motivated on rational grounds towards the goal of producing wellposed outputs, and can then as such be interpreted in physical terms.

EG2 shows to be a computationally affordable useful model for slightly viscous (compressible and incompressible) flow, because mean-value outputs can be computed without resolving boundary layers and interior turbulence to physical scales. This reflects that mean-value outputs in slightly viscous turbulent flow, can vary little with the viscosity (beyond the drag crisis), as long as the viscosity is sufficiently small or the Reynolds is number sufficiently large, as observed in both physical experiment and computation.

EG2 allows accurate prediction of the turbulent losses in a heat engine and the drag/lift of a car and airplane with millions of mesh points [**?**, **?**], instead of the trillions required with DNS according to state-of-the art [**?**]. EG2 offers automatic turbulence modeling and assessment of wellposedness. Adopting EG2 as a model of thermodynamics can be seen as a return to Eulers original idea of using inviscid flow as a model of slightly visocus flow, but with new insight and capabilities.

8.7 2nd Law for EG2

As already indicated, we formulate a 2nd Law for EG2 without the concept of entropy, in terms of the basic physical quantities of kinetic energy K, heat energy E, rate of work W and shock/turbulent dissipation $D > 0$, of the form

$$\dot{K} = W - D, \quad \dot{E} = -W + D, \tag{8.1}$$

where the dot indicates time differentiation. Slightly viscous flow always develops turbulence/shocks with $D > 0$, and the 2nd Law thus expresses an irreversible transfer of kinetic energy into heat energy, while the total energy $E + K$ remains constant because $\dot{E} + \dot{K} = 0$.

8.8 Irreversibility and Finite Precision

The 2nd Law (8.1) with $D > 0$ describes a process which is irreversible with a forward Arrow in time, since the reversed process would correspond to $D < 0$. We can understand the irreversibility as a consequence of finite precision computation combined with a certain form of wellposedness as follows: We have noted that in viscous dissipation with $D > 0$ kinetic energy is transformed into smaller scale kinetic energy in the form of internal/heat energy. This process is wellposed e.g. in the sense that the total viscous dissipation is insensitive to mesh refinement/vanishing viscosity. This can be seen as feature of a process of smashing larger units into smaller pieces with certain mean-value outputs being insensitive to the precision of the smashing procedure.

On the other hand, in the reversed process small pieces would have to be put together into larger units in a precise way, and such a process is very sensitive to the precision of the assembly.

The 2nd Law (6.1) based on finite precision computation thus can be viewed to reflect that smashing into pieces is insensitive to the precision of the smashing, while the reversed process of reassembly is sensitive to the precision of the assembly. The 2nd Law thus expresses a familar phenomenon without any mystery of molecular games of roulette, just finite precision construction/computation.

8.9 Viscosity Solutions

An EG2 solution can be viewed as particular *viscosity solution* of the Euler equations, which is a solution of *regularized Euler equations* augmented by additive terms modeling viscosity effects with small viscosity coefficients.

The effective viscosity in an EG2 solution typically may be comparable to the mesh size.

For incompressible flow the existence of viscosity solutions, with suitable solution dependent viscosity coefficients, can be proved a priori using standard techniques of analytical mathematics. Viscosity solutions are pointwise solutions of the regularized equations. But already the most basic problem with constant viscosity, the incompressible Navier-Stokes equations for a Newtonian fluid, presents technical difficulties, and is one of the open Clay Millennium Problems.

For compressible flow the technical complications are even more severe, and it is not clear which viscosities would be required for an analytical proof of the existence of viscosity solutions [**?**] to the Euler equations. Furthermore, the question of wellposedness is typically left out, as in the formulation of the Navier-Stokes Millennium Problem, with the motivation that first the existence problem has to be settled. Altogether, analytical mathematics seems to have little to offer a priori concerning the existence and wellposedness of solutions of the compressible Euler equations. In contrast, EG2 computational solutions of the Euler equations seem to offer a wealth of information a posteriori, in particular concerning wellposedness by duality of turbulent/shock solutions.

An EG2 solution thus can be viewed as a specific viscosity solution with a specific regularization from the least squares stabilization, in particular of the momentum equation, which is necessary because pointwise momentum balance is impossible to achieve in the presence of shocks/turbulence. The EG2 viscosity can be viewed to be the minimal viscosity required to handle the contradiction behind the non-existence of pointwise solutions. For a shock EG2 could then be directly interpreted as a certain physical mechanism preventing a shock wave from turning over, and for turbulence as a form of automatic computational turbulence model.

Part II

World of Thermodynamics

Chapter 9

Transformations of Energy

> God has chosen that which is the most simple in hypotheses and the most rich in phenomena. (Leibniz, Discours de métaphysique, VI, 1686)

> The sight of day and night, and the months and the revolutions of the years, have created number and have given us conception of time, and the power of inquiring about the nature of the Universe. (Plato in *Timaeus*)

> ... in a purely mechanical world, the tree could become a shoot and a seed again, the butterfly turn back into a caterpillar, and the old man into a child. No explanation is given by the mechanistic doctrine for the fact that it does not happen. (Ostwald)

> ... a complete explanation of the arrow requires explaining why the universe started out as it did. It is a problem in cosmology. (Hawking)

9.1 Kinetic Energy and Heat Energy

Thermodynamics is fundamental in a wide range of phenomena from macroscopic to microscopic scales. Thermodynamics essentially concerns the interplay between *kinetic energy* and *heat energy* in a *gas* or *fluid*, where heat energy is a form of small scale kinetic energy. Thermodynamics thus concerns transformations between large scale kinetic energy and small scale kinetic energy in the form of heat. Large scale kinetic energy, or *mechanical energy*, may generate heat energy by *compression* or *turbulent dissipation*.

Heat energy may generate (large scale) kinetic energy by *expansion*, but not through a *reverse* process of turbulent dissipation. Thermodynamics is closely connected to the dynamics of *slightly viscous* and *compressible* gases, since substantial compression and expansion can occur in a gas, but less in fluids (and solids).

9.2 Cosmology and Big Bang

Cosmology is the scientific study of the large scale properties of the *Universe* as a whole, including its origin, evolution and ultimate fate. The *Big Bang* model postulates that 12 to 14 billion years ago, the universe was in a very hot very dense state, which expanded along with galaxies and stars being formed by gravitation from variations in density, see Fig. 9.1. It is believed that we can see remnants of the hot dense matter as the now very cold cosmic microwave background radiation, which still pervades the universe as a slightly varying glow across the entire sky, see Fig. 9.2, a discovery made by the Cosmic Background Explorer COBE-telescope, which gave the Nobel Prize in 2006 to John Mather and George Smoot. Cosmology is basically a very (very) large scale application of thermodynamics as an interplay of mass, momentum and energy governed by gravitational and inertial forces and driven by nuclear reactions.

9.3 Astronomy and Nuclear Energy

The *stars* were formed in the early Universe by accretion of mass by gravitational collaps increasing the temperature of a central core and thus igniting the star in a nuclear fusion process with first deuterium and then hydrogen being transformed to helium under intense release of energy (according to Einsteins famous formula $E = mc^2$) increasing the pressure and counterbalancing the gravitational collaps. *Planets* may be formed from heavier atoms and molecules created in nuclear processes in stars, and under favorable conditions give rise to (intelligent) *life* and theories of thermodynamics. Stars of 0.4-10 times the mass of our own Sun expand into red giant very bright stars, when the supply of hydrogen in the core is empty and fusion starts in an outer core. Our own Sun thus eventually will swallow the Earth into a fusion process, but this is estimated to be a couple of billion years away.

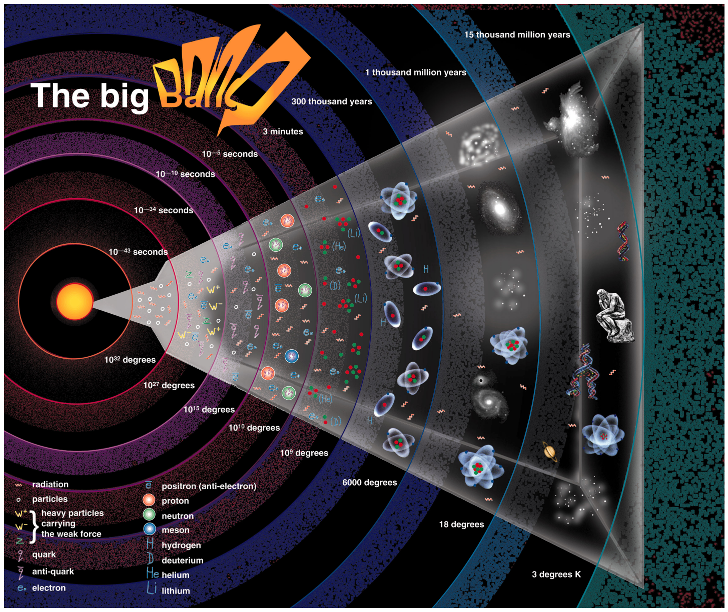

Figure 9.1: Thermodynamics of Big Bang from 10^{-41} seconds to 15 billion years.

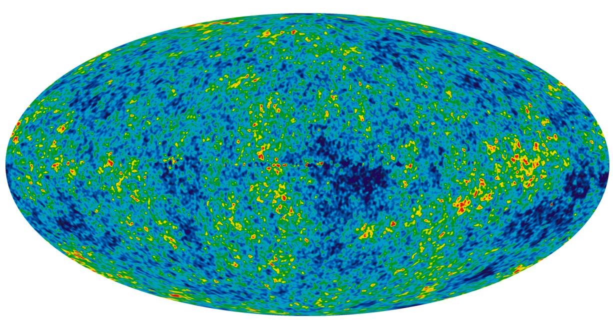

Figure 9.2: Cosmic back-ground radiation according to COBE.

The thermodynamics of the Sun thus is the basis of both life and death of the Earth.

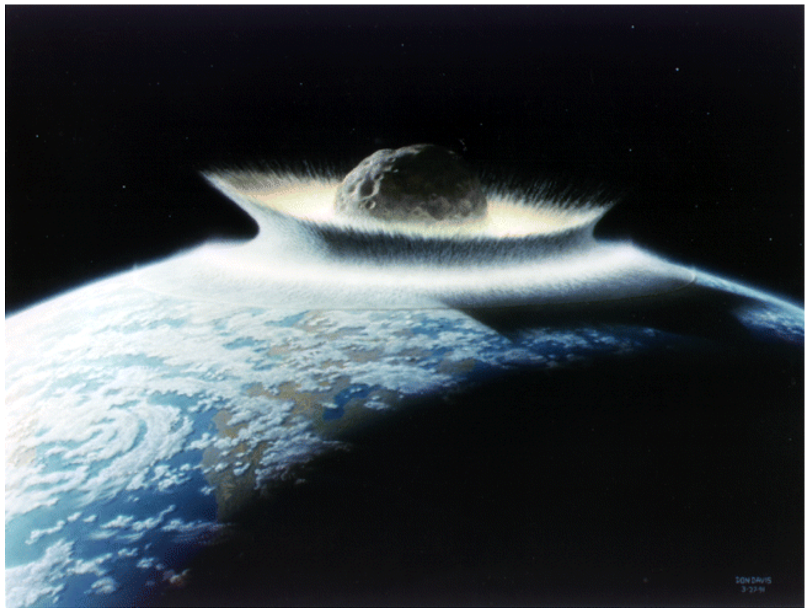

Figure 9.3: Asteroid impact on the surface of the Earth with irreversible transfer of large scale kinetic energy into small scale kinetic energy in the form of heat energy.

9.4 Geology and Global Warming

Geology or earth science contains the subfields of geophysics, glaciology, volcanology, climatology and meteorology connecting to the the central issue of the thermodynamics of *global warming*. Computational simulation of global climate change has a very important role to play to find out what actions are beneficial for sustainable development and long-time survival.

9.5 Black Body Radiation and the Sun

A *black body* absorbs incoming white light of all frequencies, from high frequency ultraviolet to low frequency infrared, but only radiates low frequency

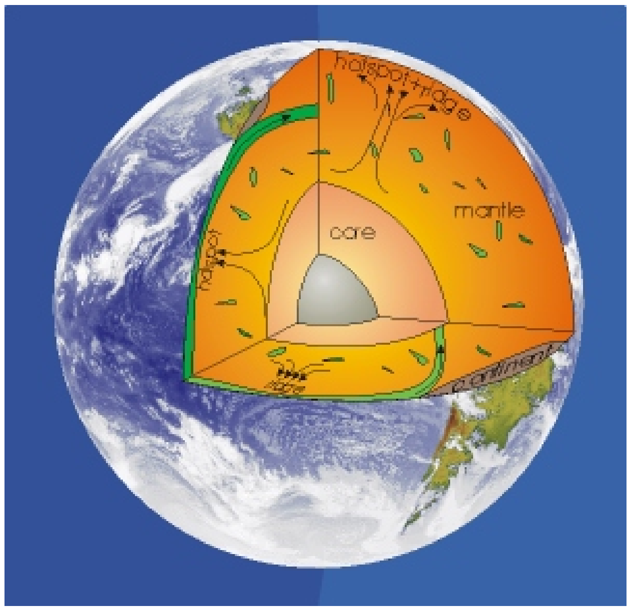

Figure 9.4: The Earth

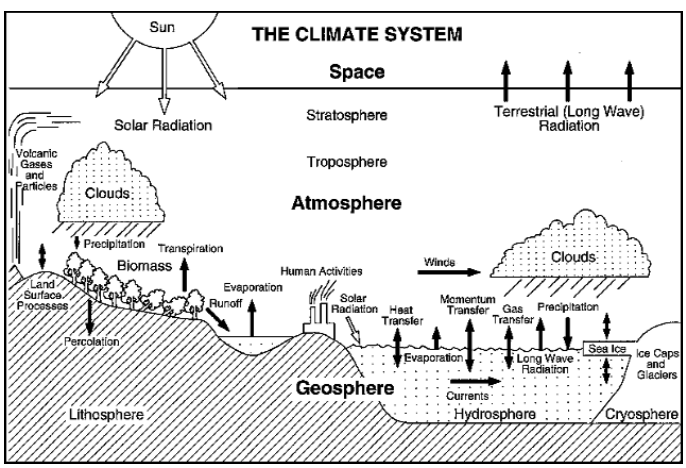

Figure 9.5: Global heat balance.

light (with color depending on the temperature of the body). This is the basis of the gross energy balance of the Earth absorbing white light from the hot Sun and radiating low frequency light into empty space. One can view black body absorption/emission as an (irreversible) thermodynamic process transforming high frequency light energy to low frequency (long wave) light energy [24].

Figure 9.6: Life in action.

9.6 Biology and Life

Most forms of biological processes build on conversion of chemical energy into heat and kinetic energy, and thus ultimately on Solar energy converted to chemical energy in the *photo-synthesis*.

Muscle contraction occurs when a muscle fiber generates tension through *actin and myosin cross-bridge cycling* shortening the fiber fueled by *Adanenosine TriPhosphate ATP*. Locomotion in most higher animals is possible only through the repeated contraction of many muscles at the correct times controlled by the central nervous system, the brain and spinal cord. Voluntary muscle contractions are initiated in the brain, while the spinal cord initiates involuntary reflexes.

The emergence of biological life may naively appear to contradict the 2nd Law in its classical form, by creating ordered structures out of disordered,

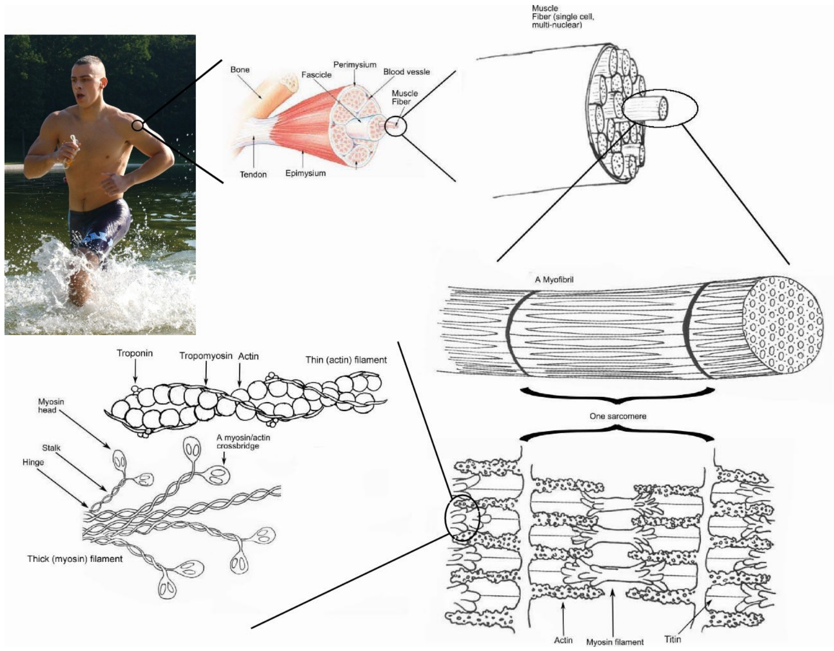

Figure 9.7: Muscle contraction by actin-myosin twitch fueled by ATP.

while the death of a living organism when order dissolves into disorder, reflects the classical 2nd Law very well. We shall see that in the new formulation of the 2nd Law not relying on notions of ordered/unordered, there is nothing (in principle) that prevents ordered structures to develop from unordered (for example in Irak), assuming there is some input of energy (oil).

9.7 Molecular Biology and Protein Folding

Biology builds on cell microbiology based on the thermodynamics of chemical reactions of *protein synthesis* from amino acid molecules according to the instructions of *DNA*. Computational thermodynamics of the cell is becoming an increasingly important tool in medicine and drug design.

9.8 Quantum Physics and Chemistry

The thermodynamics of chemical reactions and radiation build on the *quantum mechanics* of electrons, and the thermodynamics of nuclear reactions

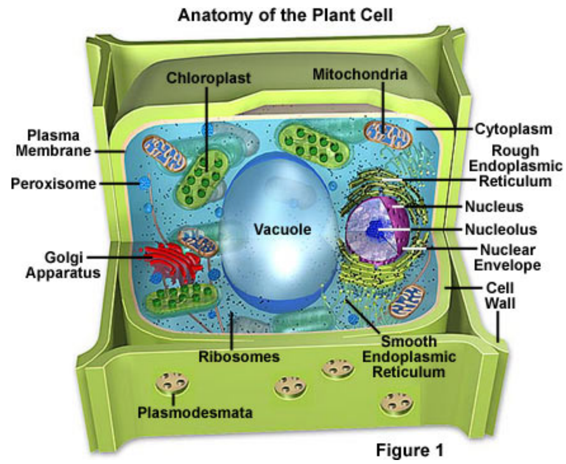

Figure 9.8: Inside a plant cell.

build on quantum electrodynamics of elementary particles. Computational solution of the equations of quantum mechanics presents a tough challenge, because of the richness of the the wave function solution with in principle three independent space coordinates for each particle (electron) involved. Methods reducing the dimensionality are today routinely used in massive computations in *quantum chemistry*, and could open to new insights of the nature of the quarks of elementary particle physics.

9.9 Energy Generation and Consumption

Our *industrial society* is based on production and consumption of energy in thermodynamic energy conversion processes of the form:

- nuclear/fossile/biological/chemical → heat/kinetic/electric,
- wind/wave kinetic → electric,
- solar radiation → heat/electric.
- electric → heat/kinetic.

In all conversion of energy, minimization of *losses* into useless heat is of prime concern, for which computational thermodynamics opens new possibilities.

9.10 Heat Engines and Industrialization

The industrial society of the 19th century was built on the use of *steam engines*, and the initial motivation to understand thermodynamics came from a need to increase the efficiency of steam engines for conversion of heat energy to useful mechanical energy. A steam engine is a particular form of a *heat engine* converting heat to mechanical work in a thermodynamical process. The modern *combustion engine* in a car is a form of heat engine generating kinetic energy from explosive burning of fuel. The efficiency of a heat engine is of prime importance, and can be studied by computational thermodynamics. The necessary *cooling* of a car engine represents a loss of energy which is not transformed into useful mechanical work.

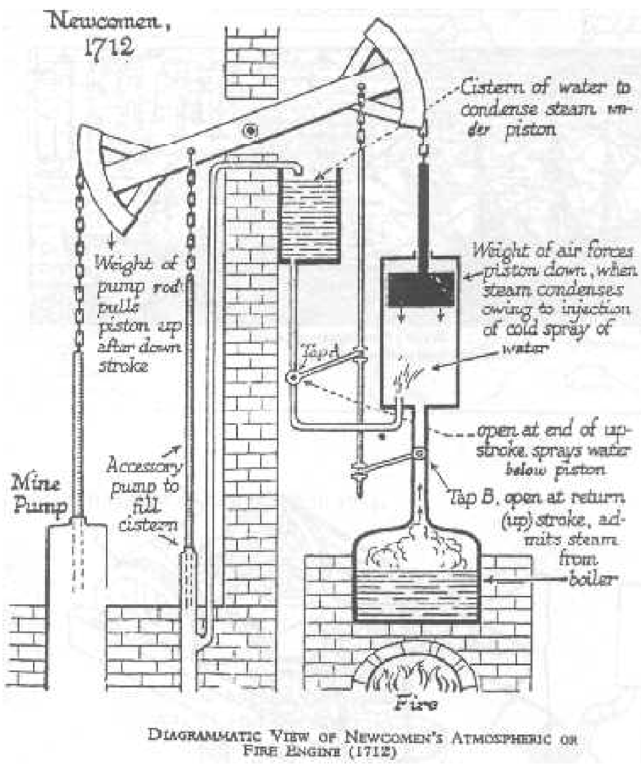

Figure 9.9: Converting heat to kinetic (mechanical) energy in 1712.

9.11 Heat Pumps and Oil Crisis

The *heat pump* is replacing the increasingly expensive oil for heating of houses. A heat pump converts low temperature heat energy from the earth or the air to higher temperature useful heat energy, by supplying the necessary conversion energy from electricity. The efficiency is today typically around 2/3, that is, for 1/3 unit of electric energy, you get out 1 unit of useful heat energy. You can thus reduce your electrical bill by a factor of 3 by changing from full electrical heating of your house to heating by an efficient heat pump. Of course, it is of interest to seek to increase the efficieny even more. Can we reach 99% efficiency, and if not why? We will address this question below.

9.12 Refrigerators and Urban Civilization

A *refrigerator* is a form of heat pump taking heat from the inside of the refrigerator and delivering it to the exterior at higher temperature. The refrigerator is an absolute necessity of modern urban civilization.

The standard design builds on cycling a fluid alternating between *expansion/evaporation* to gas phase with temperature drop, and *compression/condensation* to liquid phase with temperature increase, with the cold gas in contact with the interior of the refrigerator and the warm liquid phase in contact with the exterior. The cooling process with heat flowing from cold to hot (contrary to its natural tendency to flow from hot to cold) is thus maintained by an (electric) *compressor* consuming energy.

The first design of an *absorption refrigerator*, without compressor and moving parts and thus silent, was invented by the two young Swedish engineering students Carl Munters and Baltzar von Platen during their class in thermodynamics at the Royal Institute of Technology in 1922 (although they slept through the lectures working all night on their invention). This invention together with a vacuum cleaner gave the impetus of the quick expansion of the Electrolux company. The production of the Munters-Platen refrigerator has continued at Motala in Sweden uninterrupted since 1925 with today a total of 10 million units being produced. We hope this book may be useful for young minds of today for new inventions.

Figure 9.10: Inside a refrigerator: The principle of preservation of food.

9.13 Information and Communication

Information theory was created by Shannon [40] in the 1940s borrowing the concept of *entropy* from *thermodynamics*, with the idea of measuring communication channel capacity requirements for different types of information. Random information would then represent information with maximal entropy, in principle requiring maximal capacity (although random information would seem like useless information).

Alternatively, one can view communication of information as a thermodynamic flow with the heat energy representing loss or destruction of information during the communication. More generally, not only creation but also destruction of information represent fundamental aspects of physical and biological processes.

9.14 Economy and Welfare

One can also view an evolving economy as a thermodynamic flow process transforming resources into utilities. In (a free) economy turbulent dissipation could be viewed as a measure of necessary losses during the process, in the form of interest rates, taxes, bribes, thefts, which cannot (fully) be avoided. The flow of the World economy represents a complex process of prime importance to all of us. An economist with (some) understanding of

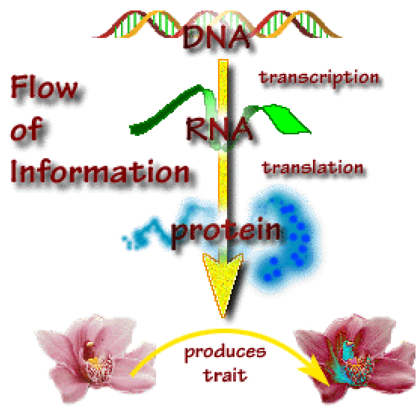

Figure 9.11: Flow of information in a flower.

the process can be raised to fame and fortune.

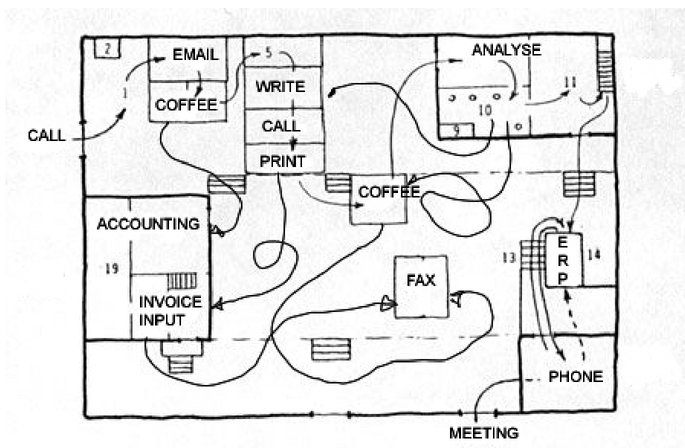

Figure 9.12: Flow of information in an office of the last century.

9.15 Emergence: A New Approach to Physics

Ilya Prigogine received the Nobel Prize in Chemistry in 1977 for his work on *non-equlibrium thermodynamics* proposing a new (statistical) approach to the 2nd Law allowing ordered structures to develop from non-ordered, see

Fig. 9.13 and 9.14. Even if Prigogine did not convince the physics community at large, he at least showed the severe short-coming of the classical 2nd Law seemingly preventing order from develping from chaos.

Emergence is the process of complex pattern formation from more basic constituent parts or "particles", that is the formation of order out of chaos. Turbulence shows phenomena of both emergence and featureless chaos, none of which can be understood by considering only a single fluid particle, only by considering the interaction of many. The (new) 2nd Law expresses a collective behavior of many fluid particles to form turbulent flow with an irreversible transfer of large scale kinetic energy to heat energy. Thus thermodynamics naturally connects to the new approach to physics based on emergence, which is now developing (emerging) with input from e.g. 1988 Nobel Laurate Robert Laughlin [26], and which is radically different from the *reductionist* approach of elementary particle physics completely dominating the scene since the birth of quantum mechanics in the beginning of the last century.

Since emergence concerns the interaction of many particles, analytical methods fall short (which lies behind the reductionist obsession with a single particle hopefully allowing analytical mathematical description), while computational methods open new possiblities of simulating emergent and turbulent phenomena, as is shown in this book.

9.16 The Battle between Growth and Decay

We shall see that turbulent flow and thus thermodynamics (the World) can be viewed as a battle between a growth process of *differentiation by advection* and a decay process of *mixing by diffusion* according to:

- *growth: increase difference-differentiate-separate: advection*
- *decay: decreasse difference–uniformize-mix: diffusion.*

The classical 2nd Law captures the diffusion process with mixing and decreasing difference. But it does not capture the advection process allowing increasing difference and separation, which is a severe short-coming. The new 2nd Law captures both processes. In the thermodynamics of Prigogine the two processes are represented by "Unstable Dynamical Systems" and "Dissipative Structures", but Prigogine sticks to "Randomness", see Fig. 9.13.

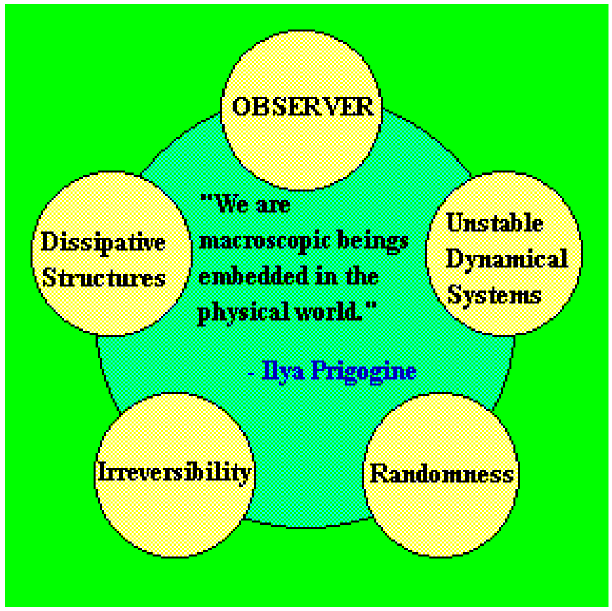

Figure 9.13: The World according to Ilya Prigogine.

Figure 9.14: Ilya Prigogine receiving the Nobel Prize in Chemistry in 1977 from the hands of King Karl XVI Gustav.

9.17 Physics: Flow of Information: Computation

The basic idea of this book is to view thermodynamics as a form of analog computation, which can be simulated by digital computation. Both analog physics and digital computation can be seen as flows of information reflecting the flow of mass, momentum and energy in a physical system and the flow of digits from input to output in the execution of a subroutine of the computational code.

For a computer programmer the information flow is represented in the flow chart of a computer code, which is essential for the understanding of the code. Likewise, a flow chart of the analog computation of a physical process can help the physicist to understanding.

9.18 Thermodynamics as a "Best of Worlds"

The above survey indicates that thermodynamics is a fundamental part of science and technology and thus serves a very important role in our society. Thermodynamics is maybe the scientific field closest to Leibniz' definition of a *Best of Worlds* as a world, which is richest in variation of ordered complex structures or emergence, such as different forms of life and conscience, while being governed by simplest possible principles or laws.

> I say that I am strongly inclined to believe that heat is of the same kind, and that material things which make us hot and feel hot (such as we call by the general name *fire* are a multitude of tiny corpuscles of such and such a shape, and moving at such and such a speed. When they meet our bodies, they penetrate them with their extreme subtlety, and the way they touch our substance as they pass through it is sensed by us as the affection we call "heat". It is pleasant or unpleasant in proportion to the number and speed of the particles as they prick and penetrate it. This penetration is pleasant if it is beneficial to our insensible vital functions, and unpleasant when it causes too much of a separation and dissolution of our substance. (Galieo in *The Assayer*, 1623)

Chapter 10

Classical Thermodynamics

> Neither Herr Boltzmann nor Herr Planck has given a defnition of W... Usually W is put equal to the number of complexions. In order to calculate W, one needs a *complete* (molecular-mechanical) theory of the system under consideration. Therefore it is dubious whether the Boltzmann principle has any meaning without a *complete* molecular-mechanical theory or some other theory which describes the elementary processes (and such a theory is missing). (Einstein)

> The reversibility of the mechanical theory suggested for many years that any observable motion should have a twin reverdes motion which can also be observed. The consequences of reversibility, however, seem contrary to our intuition: Although salt spontaneously dissolves in water, no one has ever seen salt precipitate from an unsaturated solution. (Joel Keizer in *Statistical Thermodynamics of Nonequilibrium processes*)

> Mechanically, the task seems impossible, and we will just have to get used to it (statistics of quanta) (Planck 1909).

10.1 The 1st and 2nd Laws of Thermodynamics

The development of classical thermodynamics was initiated in the 19th century by Carnot [7], Clausius [8, 9] and Lord Kelvin [25], who formulated basic axioms in the form of the *1st Law* and the *2nd Law* of thermodynamics. The

1st Law states conservation of total energy as the sum of kinetic, potential and heat energy. The 1st Law can be viewed as a definition of heat energy as any loss of kinetic/potential energy in conserved total energy. The classical 2nd Law has several forms from the formulation by Carnot in terms of *heat engines* to that by Clausius in terms of entropy:

- Carnot 1824: *No heat engine can be more efficient than a Carnot engine with efficiency* $1 - t_c/t_h$ *operating between two temperatures* t_h *and* $t_c < t_h$.

- Clausius 1850: *It is impossible for heat to flow from a colder body to a warmer body without any work having been done to accomplish the flow. Energy will not flow spontaneoulsy from a low temperature object to a higher temperature object.*

- Kelvin-Planck 1851 [25]: *It is impossible to obtain a process that, operating in cycle, produces no other effect than the subtraction of a positive amount of heat from a reservoir and the production of an equal amount of work.*

- Clausius 1865: *In any cyclic process the entropy cannot decrease.*

Clausius', Kelvin-Planck's and Carnot's formulations are negative and express impossibilitities, which are tricky to dechiffer: If somebody claims having constructed an engine more efficient than a Carnot engine, then Carnot would say that it is not a heat engine. Or if we observe heat flow from a cold to a warm body (which we will do below), then Clausius would say that it is not spontaneous and Kelvin-Planck that some other effect must have been produced.

The only statement of the above versions of the 2nd Law which is positive in form, is the last one about entropy. But this formulation requires a specification of the physical significance of entropy, and this has shown to be very difficult, if not impossible to achieve. In particular, nobody has found any sensor of entropy in Nature, and the physical mechanism preventing entropy from decreasing has remained mysterious.

To give perspective we recall the presentations of thermodynamics and statistical mechanics from the standard source Wikipedia representing a form of common understanding as of today.

Figure 10.1: Sadi Carnot: *No heat engine can be more efficient than a Carnot engine.*

Figure 10.2: Rudolf Clausius: *The energy of the world is constant. Its entropy tends to a maximum.*

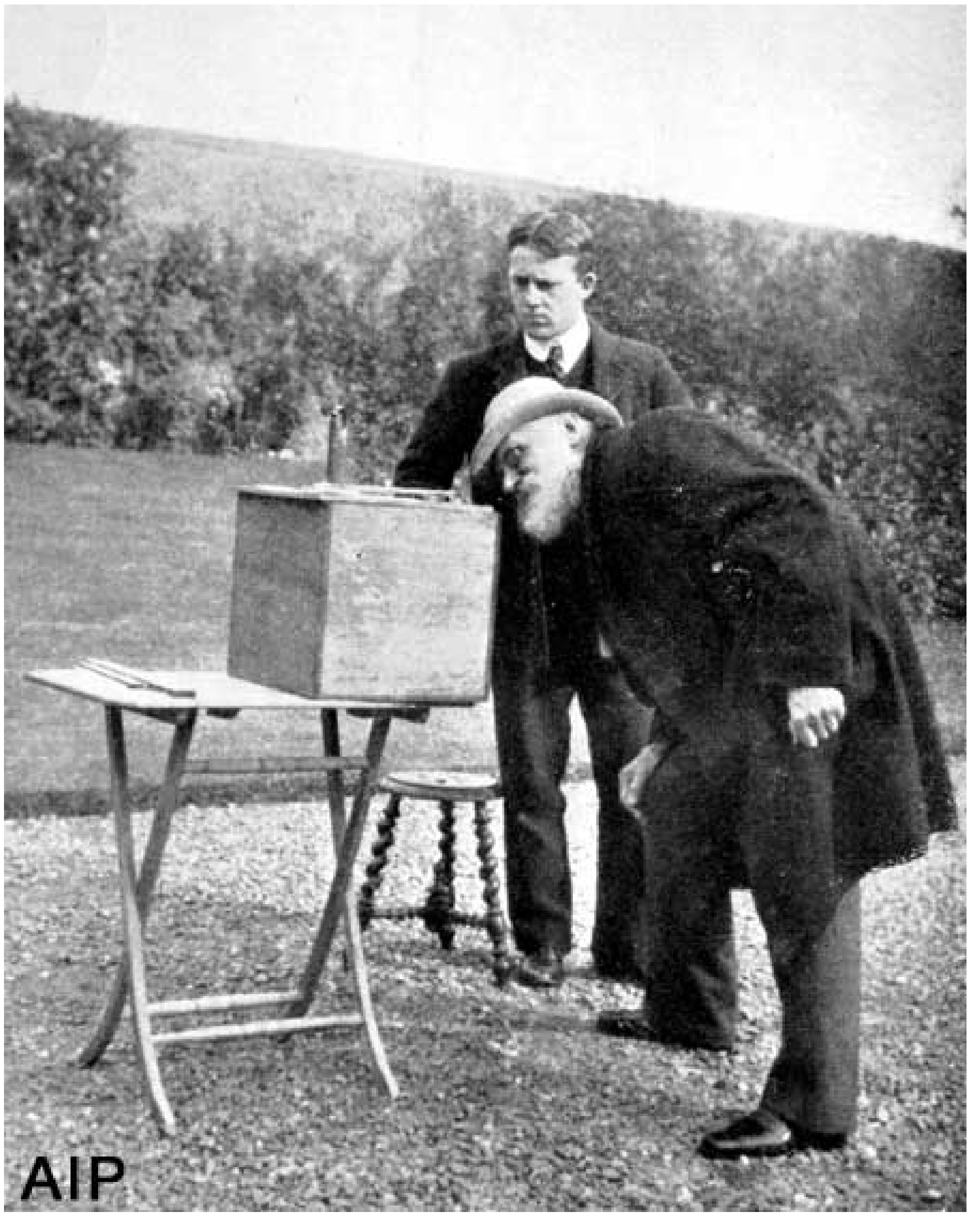

Figure 10.3: Lord Kelvin to assistent while making observations: *I am never content until I have constructed a mechanical model of what I am studying. If I succeed in making one, I understand; otherwise I do not.*

10.2 Thermodynamics in Wikipedia

Thermodynamics (from the Greek thermos meaning heat and dynamis meaning power) is a branch of physics that studies the effects of changes in temperature, pressure, and volume on physical systems at the macroscopic scale by analyzing the collective motion of their particles using statistics. Roughly, heat means "energy in transit" and dynamics relates to "movement"; thus, in essence thermodynamics studies the movement of energy and how energy instills movement. Historically, thermodynamics developed out of the need to increase the efficiency of early steam engines.

The starting point for most thermodynamic considerations are the laws of thermodynamics, which postulate that energy can be exchanged between physical systems as heat or work. They also postulate the existence of a quantity named entropy, which can be defined for any system. In thermodynamics, interactions between large ensembles of objects are studied and categorized. Central to this are the concepts of system and surroundings. A system is composed of particles, whose average motions define its properties, which in turn are related to one another through equations of state. Properties can be combined to express internal energy and thermodynamic potentials are useful for determining conditions for equilibrium and spontaneous processes.

With these tools, thermodynamics describes how systems respond to changes in their surroundings. This can be applied to a wide variety of topics in science and engineering, such as engines, phase transitions, chemical reactions, transport phenomena, and even black holes. The results of thermodynamics are essential for other fields of physics and for chemistry, chemical engineering, cell biology, biomedical engineering, and materials science to name a few.

10.3 Statistical Mechanics in Wikipedia

Statistical mechanics is the application of statistics, which includes mathematical tools for dealing with large populations, to the field of mechanics, which is concerned with the motion of particles or objects when subjected to a force.

It provides a framework for relating the microscopic properties of individual atoms and molecules to the macroscopic or bulk properties of materials that can be observed in everyday life, therefore explaining thermodynamics

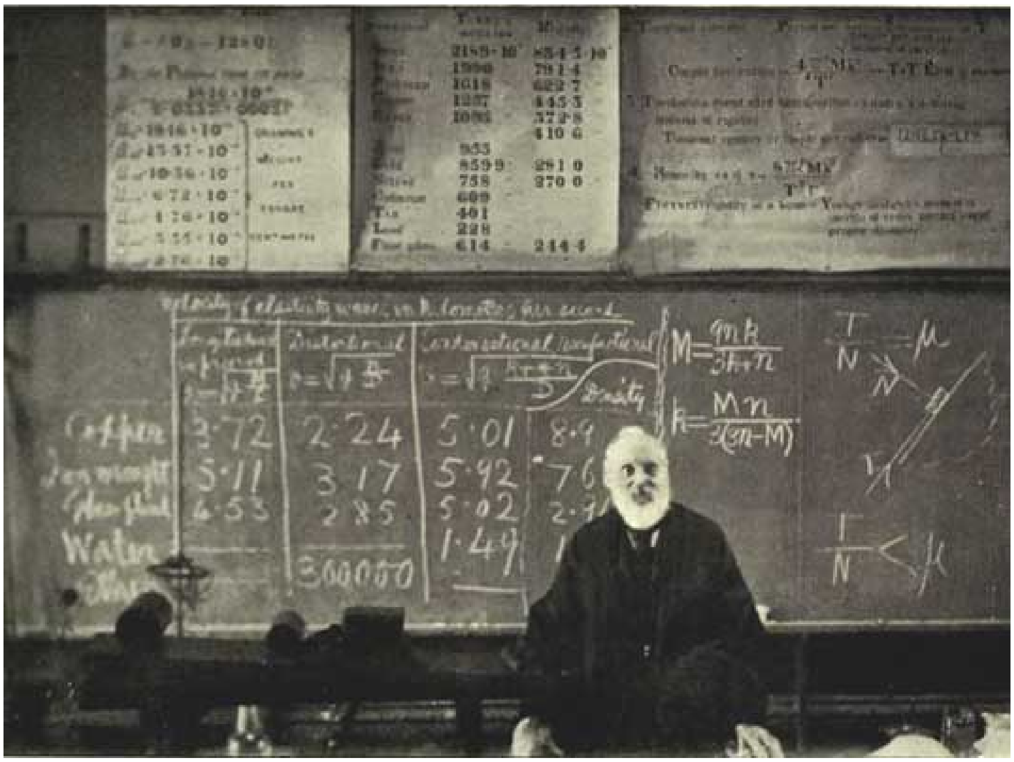

Figure 10.4: Lord Kelvin in his last lecture: *Do not imagine that mathematics is hard and crabbed, and repulsive to common sense. It is merely the etherialization of common sense.*

as a natural result of statistics and mechanics (classical and quantum) at the microscopic level. In particular, it can be used to calculate the thermodynamic properties of bulk materials from the spectroscopic data of individual molecules.

This ability to make macroscopic predictions based on microscopic properties is the main asset of statistical mechanics over thermodynamics. Both theories are governed by the second law of thermodynamics through the medium of entropy. However, Entropy in thermodynamics can only be known empirically, whereas in Statistical mechanics, it is a function of the distribution of the system on its micro-states.

Figure 10.5: Ludwig Boltzmann: *Available energy is the main object at stake in the struggle for existence and the evolution of the world.*

10.4 The 2nd Law in Popular Science

In *The Cosmic Blueprint* by the physicist Paul Davies, we read on statistical mechanics and the 2nd Law:

- *One of the states will represent "maximal disorder", which is the state*

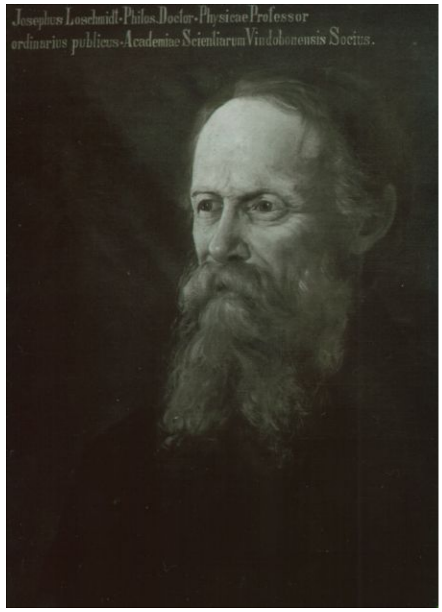

Figure 10.6: Loschmidt: *I consider irreversibility in reversible systems to be paradoxical. Indeed very paradoxical, yes.*

attainable in a maximal number of ways, or the macro-state with a maximal number of corresponding micro-states.

- *The maximally disordered state thus corresponds to thermodynamic equilibrium.*
- *One can define a statistical quantity representing the "degree of disorder" of a (macro)state, in terms of the number of corresponding microstates.*
- *Boltzmann showed that if the molecular collisions are chaotic (in a rather precise sense), this quantity will with an overwhelming probability increase.*
- *Boltzmann had thus found a quantity in statistical mechanics corresponding to thermodynamic entropy.*
- *Boltzmann thus gave a demonstration, at least in a simple gas model, of "why" entropy tends to increase.*

Davies description illustrates that there are two different notions of entropy and two corresponding versions of the 2nd Law, one in classical thermodynamics and one in statistical mechanics. The 2nd Law in classical thermodynamics is usually considered to represent an experimental (deterministic) fact without rational theoretical basis, while the 2nd Law in statistical mechanics is motivated by combinatorics. Boltzmann's goal thus was to rationalize the 2nd Law of thermodynamics by replacing it with the 2nd Law of statistical mechanics.

10.5 The 2nd Law for Young Scientists

There are several educational sites directed to young scientists seeking to explain the 2nd Law, where you can read:

- *The 2nd Law is the most misunderstood, abused, and needlessly confused principle of physics.* (www.ftexploring.com)
- *There are as many forms of the 2nd Law as there have been discussions of it* (P.W. Bridgman, 1941)
- *Nothing in life is certain, except death, taxes and the 2nd Law* (Seth Lloyd)
- *We have people making decisions at a government level who don't know the 2nd Law. Who does?* (Sting)

10.6 Reflections on the 2nd Law

A popular idea when presenting the 2nd Law to non-specialists of thermodynamics is to say that it represents a "general tendency (of energy) to spread out or disperse", or a "general tendency to decrease difference by mixing". The ambition to justify the 2nd Law this way without reference to entropy or combinatorics is admirable, but it only captures one side of the truth, and is similar in spirit to ad hoc viscous regularization also decreasing difference.

Thus, to say to a young eager student searching for knowledge, that the 2nd Law expresses that "differences tend to decrease", will not be convincing, in particular not in academics or sports. If you believe it should be, try it out and notice the dissapointment of the student, when you cannot answer the natural question: *Why* do differences have to decrease and if they have to, *how* can differences emerge and increase? We believe that students thirst for knowledge should be acknowledged and satisfied, and this book seeks to fill this need.

If now the 2nd Law is so difficult to formulate and justify, why has it been formulated at all? We have already said that it is a common belief that without a 2nd Law of some form or the other, there would be no Arrow of time pointing forward in time. Processes would seem to be reversible and there would seem to be no limitation on the possibilitities of transforming one form of energy to another, as long as the total energy is constant. But this is not what we observe: time is always moving forward and transforming heat energy generated by friction from kinetic or potential energy, back to kinetic or potential energy, seems impossible: We may observe that a stone dropped to the ground heats up, but nobody has ever observed a stone on the ground lifting itself by cooling off. Or a smashed Chinese vase reassembling by itself (although some biological organisms seem to have this capacity). Certain processes thus seem to be *irreversible* with *time reversal* being impossible, which gives time a direction forward and thus defines an Arrow.

On the other hand, classical Newtonian or Hamiltonian mechanics (without friction and viscosity) appears to be reversible with no preferred direction of time and no Arrow, and the question then comes up what the mechanics behind irreversibility might be, if it is not Newtonian or Hamiltonian? This is the puzzle of *Loschmidt's paradox*, to which we will return below. Simply adding viscosity in an ad hoc fashion does not give a good answer.

Scientists in the late 19th century thus were searching for foundation of thermodynamics in the form of a 2nd Law expressing that a certain quantity named entropy could never decrease and when increasing strictly would signfy irreversibility. The scientific challenge became to give the entropy a physical molecular-mechanistic meaning, which could justify the 2nd Law. This turned out to be very difficult to achieve, and as a last resort statistical methods were introduced by Boltzmann. Many prominent scientists including Maxwell had a hard time following Boltzmann's arguments, and statistical mechanics was initially viewed with considerable suspicion. During the 20th century the critics and their criticism gradually faded, and statistical mechanics is today often presented as an accepted truth, seemingly questioned by few even if not understood by many.

More precisely, there was (and still is) a desperate need to find a 2nd Law defining an Arrow; without any scientific explanation of such a seemingly simple thing as why time is always moving forward and not backward, physics and mathematics risk to loose credibility at a very high cost. The accepted way out of the dilemma is statistical mechanics. In this book we present a new resolution with based on deterministic finite precision computation instead of statistics. In statistical mechanics microscopical particles play roulette, while our particles follow deterministic laws albeit with finite precision. One can view finite precision computation as a very primitive form of statistics, so primitive that it is not statistics any more, and thus it is free of the complications of statistics.

Chapter 11

Classical vs Basic 2nd Law

> Emergence means complex organizational structure growing out of simple rules. Emergence means stable inevitability in the way certain things are. Emergence means unpredictability, in the sense of small events (possibly) causing great and qualitative changes in larger ones. (Robert Laughlin in *A Different Universe*, 2005)

Classical thermodynamics is based on a 1st Law stating conservation of total energy combined with a 2nd Law involving entropy in the form

$$\tau dS = dE + pdV, \quad dS \geq 0, \tag{11.1}$$

where τ is (absolute) temperature, S entropy, E internal energy, p pressure and V volume, and d represents change. The enigma of classical thermodynamics is to give the entropy S a physical meaning and to motivate why $dS \geq 0$.

Computational thermodynamics is based on a 1st Law stating conservation of mass, momentum and total energy combined with a 2nd Law without entropy in the form

$$dE + pdV = D \geq 0 \tag{11.2}$$

which is a different way of expressing $\dot{E} + W = D \geq 0$, the second equation of (6.1), including equality. Since the temperature $\tau > 0$, we see that the two forms of the 2nd Law effectively express the same relation

$$\tau dS = D \geq 0.$$

We refer to the 2nd Law in the form (15.1) as the *Classical 2nd Law* and in the form (15.1) as the *Basic 2nd Law*. The basic features of the Basic 2nd Law are

(B1) it is a consequence of the 1st Law and finite precision computation,

(B2) it is formulated in terms of the physical concepts of internal energy, work and turbulent dissipation, and does not involve entropy.

The basic difficulties of the Classical 2nd Law are:

(C1) the entropy S has unclear physical significance,

(C2) the inequality $dS \geq 0$ requires a motivation.

We see that the role of entropy change dS in the Classical 2nd Law is in the Basic 2nd Law taken over by turbulent diffusion D. While D has a direct physical meaning as a mechanism of generating heat, which can be observed and computed, change of entropy dS has not. Altogether (B1-2) offer great advantages over (C1-2).

11.1 The Seduction of the Classical 2nd Law

If now entropy is such a difficult concept, why was it introduced at all through the relation $\tau dS = dE + pdV$? To find out, let us see what the mathematics of Calculus says: For a *perfect gas* with $pV = \gamma\tau$, with $0 < \gamma < 1$ a *gas constant*, and $E = \tau$ assuming normalization to unit *specific heat*, the Classical 2nd law

$$dS = \frac{dE}{\tau} + \frac{pdV}{\tau} = \frac{d\tau}{\tau} + \gamma\frac{dV}{V}$$

is an *exact differential* and thus defines (up to a constant)

$$S = \log(\tau V^{\gamma})$$

as a *state variable* in terms of τ and V. For a Calculus enthousiast, and the thermodynamicists of the 19th century were, this is irresistible: It invites to use a 2nd Law in the form $dS \geq 0$ to identify irreversible processes between different *equilibrium states* defined by certain combination of the state variables of temperature τ and volume V. Only processes with non-decreasing entropy S could be physically possible and a strictly increasing entropy would identify and irreversible process. Wonderful! It suggested that the complex dynamics from one equilibrium state to another could be left out, and the thermodynamisist would (miracously) be able to say if a process would be possibel or not. Not bad!

Processes could thus be predicted to move from equilibrium states with low entropy (small S) to equilibrium states with higher entropy (larger S), but not the other way. In short, it captured a form of thermodynamics without dynamics, which however showed to be too simplistic.

We shall see, as can be expected, that the true dynamics must be taken into account and then the new 2nd Law without entropy serves the same role as the classical 2nd Law with entropy. Whereas temperature and volume have a clear physical significane, entropy has not, and why $dS \geq 0$ has remained mysterious. Moreover for a general gas, $dS = \frac{dE}{\tau} + \frac{pdV}{\tau}$ may not be exact, and then S is not a state variable and then the main reason to introduce S disappears.

> The second law of thermodynamics is, without a doubt, one of the most perfect laws in physics. Any reproducible violation of it, however small, would bring the discoverer great riches as well as a trip to Stockholm. The world's energy problems would be solved at one stroke. It is not possible to find any other law (except, perhaps, for super selection rules such as charge conservation) for which a proposed violation would bring more skepticism than this one. Not even Maxwell's laws of electricity or Newton's law of gravitation are so sacrosanct, for each has measurable corrections coming from quantum effects or general relativity. The law has caught the attention of poets and philosophers and has been called t he greatest scientific achievement of the nineteenth century. Engels disliked it, for it supported opposition to Dialectical Materialism, while Pope Pius XII regarded it as proving the existence of a higher being. (Bazarov in *Thermodynamics*, 1964)

> There is at present in the material world a universal tendency to the dissipation of mechanical energy. — We have the sober scientific certainty that the heavens and earth shall "wax old as doth a garment." — Although mechanical energy is indestructible, there is a universal tendency to its dissipation, which produces throughout the system a gradual augmentation and diffusion of heat, cessation of motion and exhaustion of the potential energy of the material Universe. — Any restoration of mechanical energy, without more than an equivalent of dissipation, is impossible in inanimate material processes, and is probably never effected by means of organized matter, either endowed with vegetable life, or subjected to the will of an animated creature. — Nothing can be more fatal to progress than a too confident reliance

on mathematical symbols; for the student is only too apt to take the easier course, and consider the formula not the fact as the physical reality. — I have no satisfaction in formulas unless I feel their numerical magnitude. (Lord Kelvin)

11.2 Lord Kelvin

We recall Lord Kelvin:

- *There is at present in the material world a universal tendency to the dissipation of mechanical energy*
- *We have the sober scientific certainty that the heavens and earth shall "wax old as doth a garment." — Although mechanical energy is indestructible, there is a universal tendency to its dissipation, which produces throughout the system a gradual augmentation and diffusion of heat, cessation of motion and exhaustion of the potential energy of the material Universe*
- *Any restoration of mechanical energy, without more than an equivalent of dissipation, is impossible in inanimate material processes, and is probably never effected by means of organized matter, either endowed with vegetable life, or subjected to the will of an animated creature.*
- *Nothing can be more fatal to progress than a too confident reliance on mathematical symbols; for the student is only too apt to take the easier course, and consider the formula not the fact as the physical reality.*
- *I have no satisfaction in formulas unless I feel their numerical magnitude.*

11.3 Classical Analysis of Joule's Experiment

Let us now see what classical thermodynamics can offer to help us understand Joule's experiment.

We recall that classical thermodynamics concerns transformations between *equilibrium states*. The initial state, denoted by subindex i, with the gas at rest in the left chamber is an equilibrium state with $u_i = 0$ and say

$\rho_i = 1$, $V_i = 1$, $\tau_i = 1$ and thus $p_i = \gamma$ and $S_i = \log(\tau V^\gamma) = 0$. Clearly, in the final state, denoted by a subindex f, $\rho_f = 1/2$ and $V_f = 2$, but classical thermodynamics does not specify the temperature τ_f, nor the velocity u_f. If we *assume* that $\tau_f = 1$, which by energy conservation is the same as assuming that $u_f = 0$, then we find $S_f = \gamma \log(2) > S_i = 0$ and thus the transformation from the initial equilibrium state $(\rho_i, V_i, \tau_i, u_i) = (1, 1, 1, 0)$ to the equilibrium state $(\rho_f, V_f, \tau_f, u_f) = (0.5, 2, 1, 0)$ in the double volume, satisfies the classical 2nd Law.

We compare assuming instead $\tau_f = 1/2$ (and $p_f = 1/4$), which gives $S_f = \log(2^{\gamma-1}) < 0 = S_i$, which violates the 2nd Law. But as soon as $\tau_f \geq 2^{-\gamma}$ the 2nd Law $dS \geq 0$ will be satisfied. Thus any $\tau_f \geq 2^{-\gamma}$ seems to be possible, while we know that only $\tau_f = 1$ actually occurs. The classical 2nd Law does not supply the information that $u_f = 0$, because it does not involve the dynamics taking one equilibrium state into another. On the other hand, taking as above the dynamics including turbulent dissipation into account, shows that $u_f = 0$ and $\tau_f = 1$.

The objective of statistical mechanics is to motivate that $dS \geq 0$ viewing the final state as being "less ordered" or "more probable", because the gas "is more spread out", and the reverse process with the gas contracting back to the initial small volume, if not completely impossible, would be "improbable". But to say that a probable state is is more probable than an improbable state, or that things "in general tend to spread out", is not science.

We conclude that taking the true dynamics of the process and the new 2nd Law into account including in particular the second phase with heat generation from shocks or turbulence, we can understand the observation of constant temperature and irreversibility in a deterministic fashion without using any mystics of entropy ultimately based on mystics of statistics.

Part III

Mathematics

Chapter 12

The Euler Equations

> However sublime are the researches on fluids which we owe to Messrs Bernoulli, Clairaut and d'Alembert, they flow so naturally from my two general formulae that one cannot sufficiently admire this accord of their profound meditations with the simplicity of the principles from which I have drawn my equations ...(Euler 1752)

> I know that most men, including those at ease with problems of the highest complexity, can seldom accept even the simplest and most obvious truth if it be such as would oblige them to admit the falsity of conclusions which they have delighted in explaining to colleagues, which they have proudly taught to others, and which they have woven, thread by thread, into the fabric of their lives. (Tolstoy)

12.1 Conservation of Mass, Momentum and Energy

Computational thermodynamics is based on a 1st Law in the form of the Euler equations for an ideal perfect gas/fluid expressing conservation of mass, momentum and total energy as a system of partial differential equations. We formulate these equations for a gas/fluid enclosed in a fixed (open) domain Ω in three-dimensional space $\mathbb{R}^3$ with boundary Γ over a time interval $[0, T]$ with intial time zero and final time T (from now on T denotes final time and not temperature as above). The Euler equations model a gas/fluid with vanishing (very small) viscosity and heat conductivity. The Euler equations then represent a Hamiltonian system.

We seek the *density* ρ, *momentum* $m = \rho u$ with $u = (u_1, u_2, u_3)$ the *velocity*, and the *total energy* ϵ as functions of $(x,t) \in \Omega \cup \Gamma \times [0,T]$, where $x = (x_1, x_2, x_3)$ denotes the coordinates in $\mathbb{R}^3$ and u_i is the velocity in the x_i-direction. The Euler equations for $\hat{u} \equiv (\rho, u, \epsilon)$ read with $Q = \Omega \times I$ and $I = (0,T]$:

$$\begin{aligned}
\dot{\rho} + \nabla \cdot (\rho u) &= 0 && \text{in } Q,\\
\dot{m}_i + \nabla \cdot (m_i u) + p_{,i} &= f_i && \text{in } Q, \quad i = 1,2,3,\\
\dot{\epsilon} + \nabla \cdot (\epsilon u + p u) &= g && \text{in } Q,\\
u \cdot n &= 0 && \text{on } \Gamma \times I,\\
\hat{u}(\cdot, 0) &= \hat{u}^0 && \text{in } \Omega,
\end{aligned} \tag{12.1}$$

where $p = p(x,t)$ is the *pressure* of the fluid, $v_{,i} = \frac{\partial v}{\partial x_i}$ is the partial derivative with respect to x_i, $\dot{v} = \frac{\partial v}{\partial t}$ is the partial derivative with respect to time t, n denotes the outward unit normal to Γ and $f = (f_1, f_2, f_3)$ is a given *volume force* (like gravity) acting on the fluid, g is a given heat source, and $\hat{u}^0 = \hat{u}^0(x)$ represent initial conditions. Further, the total energy $\epsilon = k + e$, where

$$k = \frac{\rho |u|^2}{2}$$

is the *kinetic energy* with $|u|^2 = \sum_{i=1}^3 u_i^2$, and

$$e = \rho \tau$$

is the *internal energy* or *heat energy* with τ the *temperature*, assuming the heat capacity is equal to one. The boundary condition is a *slip* boundary condition requiring the normal velocity $u \cdot n$ to vanish corresponding to an inpenetrable boundary with zero friction. Below we will consider other boundary conditions including inflow and outflow conditions and non-zero friction. Of course, $\nabla \cdot v = \sum_i v_{i,i}$ denotes the divergence of $v = (v_1, v_2, v_3)$ (and $\nabla w = (w_{,1}, w_{,2}, w_{,3})$ the gradient).

There are five equations in the Euler system (12.1), while the number of unknowns including the pressure is six, and so we need one more equation, which may be a *state equation for a compressible gas* expressing the pressure p as a function of density ρ and temperature τ, e.g. the state equation

$$p = \gamma \rho \tau \tag{12.2}$$

of a *perfect gas*, with here $0 < \gamma < 1$ a *gas constant* (equal to $\frac{c_p}{c_v} - 1$ where c_p the specific heat under constant pressure and c_v that under constant).

For a mono-atomic gas $\gamma = 2/3$. The additional equation may alternatively express that the fluid is *incompressible* in the form $\nabla \cdot u = 0$ in Q. Note that the gas constant γ is here defined as $\gamma = \bar{\gamma} - 1$ with $\bar{\gamma} = \frac{c_p}{c_v}$ the most commonly used gas constant.

The extension of the Euler equations to include viscous forces and heat flow by conduction are referred to as the *Navier–Stokes equations*, which are no longer represent a Hamiltonian system. The Navier–Stokes and Euler equations describe a very rich complex world of fluid dynamics.

The Euler equations (12.1) represents a *one-species* model, which we below will extended to a *many-species* model including chemical reactions with chemical energy adding to the total energy.

The Euler equations represent, up to the gas constant γ, a *parameter-free model*. The determination of parameters such as viscosity and heat conductivity coefficients relevant for complex flows, can be a very difficult (or simply hopeless) task, since the coefficients in general are solution dependent (and the solution depends on the coefficients). In the Euler equations the coefficients are simply put to zero with the motivation that they are small, while their actual values are irrelevant and thus do not have to be determined.

We will find that mean-value outputs are insensitive to the values of viscosity and heat conductivity, once they are small enough, which is reflected in mesh independence in EG2. EG2 thus comes out as an essentially parameter-free model, and we will discover the remarkable (surprising) fact is that EG2 can accurately predict key outputs such as drag and lift of bluff bodies and and total losses in thermodynamical processes.

12.2 Internal Energy Formulation

We shall below use a formulation of the Euler equations in terms of the internal energy e instead of the total energy ϵ, which reads: Find $\hat{u} = (\rho, m, e)$ such that

$$\begin{aligned} \dot{\rho} + \nabla \cdot (\rho u) &= 0 && \text{in } Q, \\ \dot{m}_i + \nabla \cdot (m_i u) + \gamma e_{,i} &= f_i && \text{in } Q, \quad i = 1,2,3, \\ \dot{e} + \nabla \cdot (eu) + \gamma e \nabla \cdot u &= g && \text{in } Q, \\ u \cdot n &= 0 && \text{on } \Gamma \times I, \\ \hat{u}(\cdot, 0) &= \hat{u}^0 && \text{in } \Omega, \end{aligned} \tag{12.3}$$

where we have used that $p = \gamma e$. We will consider (12.3) to express the 1st Law as conservation of mass, momentum and internal energy. Strictly speaking, here only mass is conserved, because of the presence of f in the momentum equation and $\gamma e \nabla \cdot u$ and g in the equation for internal energy, and so conservation of momentum and internal energy is interpreted modulo the effects of these source terms.

We will below write the Euler equations:

$$\begin{aligned} \dot{\rho} + \nabla \cdot (\rho u) &= 0 && \text{in } Q, \\ \dot{m} + \nabla \cdot (mu) + \gamma \nabla e &= f && \text{in } Q, \\ \dot{e} + \nabla \cdot (eu) + \gamma e \nabla \cdot u &= g && \text{in } Q, \\ u \cdot n &= 0 && \text{on } \Gamma \times I, \\ \hat{u}(\cdot, 0) &= \hat{u}^0 && \text{in } \Omega, \end{aligned} \tag{12.4}$$

with $\dot{m} + \nabla \cdot (mu) + \gamma \nabla e = f$ the same as $\dot{m}_i + \nabla \cdot (m_i u) + \gamma e_{,i} = f_i$ for $i = 1, 2, 3$.

12.3 Derivation of the Euler Equations

We now show that the Euler equations (12.1)/(12.3) express conservation of mass, momentum and total/internal energy in the *conservation variables* (ρ, m, e). To this end consider a fixed small volume V in Ω with boundary S. Mass conservation implies that

$$\int_V \dot{\rho}\, dx = \frac{\partial}{\partial t} \int_V \rho\, dx = - \int_S (\rho v) \cdot n\, ds$$

expressing that the rate of increase of total mass in the fixed volume V is equal to the rate of inflow through the boundary S. The Divergence Theorem (see e.g. B&S Vol 3) states that

$$\int_V \nabla \cdot (\rho v)\, dx = \int_S (\rho v) \cdot n\, ds,$$

and we thus conclude that

$$\int_V \dot{\rho}\, dx + \int_V \nabla \cdot (\rho v)\, dx = 0$$

for all volumes V. Assuming that the integrands are continuous, we thus obtain the equation for mass conservation $\dot{\rho} + \nabla \cdot (\rho v) = 0$.

We obtain the differential equation expressing conservation of each component of the momentum m_i similarly, noting that by Newtons second law the rate of change of momentum is given by the corresponding component $-p_{,i}$ of the pressure gradient ∇p with increasing pressure retarding the flow, combined with volume force f_i.

Finally, the equation expressing conservation of total energy ϵ is obtained as above using the Divergence Theorem, noting that the rate of change of the total energy over a volume V convected by the flow, is equal to the work $pu \cdot n$ performed on the boundary of V per unit time step. The equation for the internal energy expresses that the work $p\nabla \cdot u$ by compression/expansion is balanced by heat energy.

12.4 Incompressible Flow

In an incompressible fluid the density ρ does not change if we follow the motion of the fluid particles of the flow. We can express this fact in the differential equation form

$$D_u\rho \equiv \dot{\rho} + u \cdot \nabla\rho = 0$$

where $D_u\rho$ is the *convective derivative* of ρ with respect to the velocity u. We obtain the convective derivative by computing the change in time following the *trajectory* $x(t)$ of a fluid particle satisfying the differential equation $\dot{x}(t) = u(x,t)$. Differentiating $\rho(x(t),t)$ with respect to time, we obtain by the chain rule:

$$\frac{d}{dt}\rho(x(t),t) = (\dot{\rho} + \dot{x} \cdot \nabla\rho)(x(t),t) = D_u\rho(x(t),t).$$

Since mass conservation reads $D_u\rho + \rho\nabla \cdot u = 0$, we conclude that the velocity u in incompressible flow is characterized by the equation

$$\nabla \cdot u = 0 \quad \text{in } Q. \tag{12.5}$$

The Euler equations for incompressible flow thus take the form: Find $\hat{u}$ and p such that

$$\begin{aligned}
\dot{\rho} + \nabla \cdot (\rho u) &= 0 && \text{in } Q,\\
\dot{m} + \nabla \cdot (mu) + \nabla p &= f && \text{in } Q,\\
\nabla \cdot u &= 0 && \text{in } Q,\\
\dot{\epsilon} + \nabla \cdot (\epsilon u + pu) &= 0 && \text{in } Q,\\
u \cdot n &= g && \text{on } \Gamma \times I,\\
\hat{u}(\cdot, 0) &= \hat{u}^0 && \text{in } \Omega,
\end{aligned} \tag{12.6}$$

where the incompressibility condition $\nabla \cdot u = 0$ replaces the equation of state for the pressure p. In this case the energy equation is decoupled from the density and momentum equations; it is possible to solve for (ρ, u, p) from the first three equations and then for the energy ϵ.

If ρ^0 is constant, with $\rho^0 = 1$ say, then the first equation is trivially satisfied with $\rho = 1$, and (u, p) are solvable from the equations

$$\begin{aligned} \dot{u} + \nabla \cdot (uu) + \nabla p &= f \qquad \text{in } Q, \quad i = 1, 2, 3, \\ \nabla \cdot u &= 0 \qquad \text{in } Q, \\ u \cdot n &= 0 \qquad \text{on } \Gamma \times I, \\ u(\cdot, 0) &= u^0 \qquad \text{in } \Omega, \end{aligned} \tag{12.7}$$

which are the usual incompressible Euler equations with constant density and the energy equation left out.

12.5 Continuum and Particle Models

The Euler equations formally represent a *continuum model* with no smallest scale, since there is no smallest scale of the set of real numbers $\mathbb{R}$, and there is no viscosity or heat conduction which could define a smallest scale. It is well known that the Euler equations in general lack exact pointwise solutions, because of the appearance of turbulence and shocks, and our model of thermodynamics is instead EG2, where the Euler equations are solved computationally by a finite element method on a mesh of finite precision of *mesh size* h (variable in space and time).

We may think of the finite element computation as a finite precision computation with a fixed number of digits (e.g. single precision with about 7 digits) instead of computing with real numbers with infinitely many digits with infinite precision (which is impossible). Typical meshes have a mesh size of 10^{-2} on the unit cube with 10^6 mesh points. A gas has about 10^{24} molecules per mole, and thus the values of density, momentum and energy at each mesh point represent mean values of about 10^{18} molecules, thus mean values over incredibly many "fluid particles".

A computational *particle model* of a gas accounting for the position and velocity of each of the 10^{24} particles in each mole, is inconceivable on any kind of thinkable computer. Thus, only some form of continuum model can be used for macroscopic phenomena of fluid flow.

With EG2 we stay within a deterministic framework and only add a restriction of finite precision computation to the formally Hamiltonian Euler equations. A world of thermodynamics governed by Hamiltonian mechanics combined with finite precision computation, follows the laws of mechanics as far as possible taking the finite precision into account, but is not based on any microscopic games of roulette as statistical mechanics. The difference of scientific paradigm is fundamental. We are thus led to a model of the World as a giant *clock with finite precision* as a computer age alternative Laplace's classical clock with infinite precision as well as Boltzmann's micriscopical games of roulette.

In EG2 the mesh size h enters as a parameter which can be given a physical significance as a smallest scale in space and time. We shall discover that mean values of EG2-solutions, or *mean-value outputs*, show little dependence on the mesh size h, and we shall also uncover (some of) the mathematical rationale behind this remarkable feature. This opens the possibility of accurately simulating real phenomena using a coarser mesh size than the physical smallest scale, which is like computing with say 10^6 "super-particles" instead of 10^{24} "real particles", thus making an impossible simulation possible.

12.6 Boltzmann's Equation

Boltzmann starts from a *molecular particle model* of a dilute gas as a very large collection of elastically colliding little spherical particles/molecules according to classical Newtonian mechanics. This model is formally reversible without effects of viscosity, simply because each elastic collision is reversible. From this particle model Boltzmann derives a continuum model from an assumption of *molecular chaos* requiring particles to have statistically independent velocities before collision, in the form of *Boltzmann's equation*:

$$\dot{f} + v \cdot \nabla_x f + F \cdot \nabla_v f = Q(f, f), \qquad (12.8)$$

where $f(x, v, t)$ is the number of gas molecules at the position x moving with velocity v per volume $dxdv$, at time t, F is an applied force, and ∇_x is the gradient with respect to x, ∇_v the gradient with respect to v, and $Q(f, f)$ is Boltzmann's *collision operator* representing the rate of change of $f(x, v, t)$ due to (elastic) molecule collisions. Boltzmann's collision term has a certain dissipative character, from which Boltzmann derived his famous *H-Theorem* stating that $\dot{H} \geq 0$, where

$$H(t) = \int f \log(f) dx dv$$

is Boltzmann's *H-function*. Irreversibility would then be signified by a strictly decreasing H-function, and thus $-H$ could be viewed as a strictly increasing entropy. Boltzmann's equation is deterministic, but it is derived from a statistical assumptiopn of *molecular chaos* requiring the velocities of two molecules about to collide to be statistically independent *before* collision, but not after. The assumption of molecular chaos is what gives the collision term its dissipative character with $H(t)$ strictly decreasing as the gas steadily moves towards its *equilibrium distribution* with minimal H and $Q = 0$.

The motivation of the assumption of molecular chaos is the weak point of Boltzmann's gas kinetics: Statistical independence before collision but not after, obviously introduces a direction of time by direct assumption. The main head-ache of Boltzmann was thus to motivate this assumption, in order not to simply assume what was to be proved, namely time-directionality. To do so he tried various options and finally seemed to converge to the idea that the probability of a macro-state should be related to the number of underlying micro-states, and thus the H-theorem would reflect a tendency of the gas molecules to move from a less probable to a more probable distributions, with the final equilibrium position as the most probable one. To count the number of micro-states underlying a certain macrostate requires (tricky) combinatorics, and this is what makes Boltzmann's statistical mechanics so difficult to understand (for most people). We will come back to this aspect in an account (and resolution) of *Gibb's paradox* exhibiting difficulties of combinatorics in gas kinetics.

We shall below recall that Boltzmann defines the entropy S of a certain macrostate as being proportional to $\log(W)$ where W is the number of corresponding microstates. Boltzmann thus plays with two different definitions of entropy, one statistical in terms of the number of microstates, W and one deterministic in terms of the H-function, which is very confusing to the non-specialist of statistical mechanics.

Did Boltzmann thereby resolve the enigma how irreversibility can arise in a formally reversible Newtonian model like a swarm of elastically colliding particles? Not really, because his basic roulette assumption, also referred to as *molecular chaos*, is asymmetric in time (two particles play roulette *before* collision), and thus introduces viscosity by assumption. Boltzmann thus *assumed* what was to be proved, namely the occurence of effects of viscosity and time asymmetry, and therefore met strong opposition by in particular Loschmidt [33].

12.7 Euler's Equations from Boltzmann's

The Euler equations of fluid mechanics (12.1) can *formally* be derived from Boltzmann's equation of gas kinetics (12.8), by integration over the velocity variable v and defining with M the mass of a molecule,

$$\begin{aligned}\rho(x,t) &= M\int f(x,t,v)\,dv,\\ m(x,t) &= M\int f(x,t,v)v\,dv \\ e(x,t) &= \frac{M}{2}\int f(x,t,v)|v-u|^2\,dv,\end{aligned} \tag{12.9}$$

where as usual $u = m/\rho$. We note in particular that the internal (heat) energy e is defined as a form of (small scale) kinetic energy measuring the standard deviation from the mean velocity u.

12.8 Navier-Stokes Equations

In the Navier-Stokes equations the momentum equation is augmented by a viscous term of the form

$$-\nabla\cdot(\nu\nabla u) - \nabla(\mu\nabla\cdot u), \tag{12.10}$$

where $\nu > 0$ is a *shear viscosity* coefficient and $\mu > 0$ a *bulk viscosity*. The equation for the heat energy is similarly augmented by a heat conduction term of the form $-\nabla\cdot(\kappa\nabla e)$ with $\kappa > 0$ a *heat conductivity*. The determination of correct values of these coefficients in turbulent flow is very complicated, or more precisely in practice impossible, because the coefficients are solution dependent. We stay away from this complications by assuming the coefficients to be *small* and we then effectively put them to zero in the Euler equations, just as Euler did. The mesh-independence of certain mean-value outputs then reflects that the mean-values are insenistive to the absolute size of viscosities and heat conductivity, as long as they are small.

Figure 12.1: The shock wave of a supersonic airplane made visible by condensation

> A theory is the more impressive the greater the simplicity of its premises, the more different kinds of things it relates, and the more extended its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts.(Einstein)

> Nothing in life is certain except death, taxes and the second law of thermodynamics. All three are processes in which useful or accessible forms of some quantity, such as energy or money, are transformed into useless, inaccessible forms of the same quantity. That is not to say that these three processes don't have fringe benefits: taxes pay for roads and schools; the second law of thermodynamics drives cars, computers and metabolism; and death, at the very least, opens up tenured faculty positions. (Seth Lloyd, in *Nature*, 2004)

Chapter 13

Viscosity Solutions to 1d Euler

> The total energy of the universe is constant; the total entropy is continually increasing. (Rudolf Clausius 1865)

> You believe in the God who plays dice, and I in complete law and order in a world which objectively exists, and which I, in a wild speculative way, am tryin to capture. Even the great initial success of Quantum Theory does not make me believe in the fundamental dice-game, although I am well aware that younger collegues interpret this as a consequence of senility. No doubt the day will come when we will see those instictive attitude was the correct one. Some physicists. among them myself, cannot believe that we must abandon, actually and forever, the idea of direct representation of physical reality in space and time; or that we must accept then the view that events in nature are analogous to a game of chance...In any case I am convinced that *He* does not throw dice. (Einstein)

13.1 Regularization of Hamiltonian Systems

We present in this chapter a short-cut to the computational foundation of thermodynamics in the setting of the Euler equations in one space dimension (1d). In particular, we motivate a 2nd Law, which we will below show to be satisfied by EG2 in the full 3d case.

We use the standard approach of *viscous regularization* motivated by the fact that the Euler equations do not admit exact pointwise solutions, because of the inevitable appearance of turbulence/shocks. We will view EG2 solutions as specific regularized solutions, which are computed and thus can be inspected. We shall below in more detail investigate the precise form of the regularization in EG2, and discover that it has interesting features, not only from mathematical and computational, but also from physical point of view.

The basic idea in viscous regularization of a Hamiltonian system described by an equation $H(u) = 0$ over a domain $\Omega \times [0,1]$ in space-time, such as the Euler equations, is to perturb the equation $H(u) = 0$ into

$$H(u_\nu) = \nu \Delta u_\nu \quad \text{in } \Omega \times [0,1],$$

where $\nu > 0$ is a small parameter representing a small (shear) viscosity, and the Laplacian has a regularizing or smoothing effect on the solution.

The presence of the Laplacian (or possibly a higher order regularizing differential operator such as the biLaplacian), makes it possible in some cases to prove the existence of a pointwise solution u_ν to the regularized problem, a *viscosity solution*, by standard techniques of mathematical analysis involving Sobolev and Gronwall inequalities, while the original Hamiltonian system is inaccessible to analysis because the equation $H(u) = 0$ lacks pointwise solutions. For the compressible Euler equations, technical difficulties have hitherto prevented a full proof in the general case, which however is not crucial for the computational foundation since it is based on computed EG2-solutions and not viscosity solutions. We here use viscosity solutions to formally illustrate basic features of EG2-solutions such as the 2nd Law, which we then verify directly for EG2-solutions. EG2 can be viewed as specific viscosity solutions, which are computed and thus do exist.

If the regularized solution u_ν is *smooth* in the sense that Δu_ν is of moderates size, then the perturbation $\nu \Delta u_\nu$ will be small, because ν is small, and thus the regularized solution u_ν will be an approximate pointwise solution of the Hamiltonian system with the Hamiltonian residual $H(u_\nu)$ being small in a pointwise sense. In this case the the perturbation can be said to be *regular*, and is inessential in the sense that already the original problem has a pointwise solution and regularization is not needed.

However, we consider problems where the Hamiltonian residual $H(u_\nu)$ is not small (in fact large) in regions with shocks/turbulence, while $H(u_\nu)$ remains small in a weak norm, so that $\hat{u}_\nu$ still is an approximate solution to the Hamiltonian system, but now only in a weak (but not pointwise) sense. The viscous term $\nu \Delta u$ will thus be pointwise large, which is reflected by the fact that the total dissipation

$$D(u_\nu) = \int_\Omega \nu |\nabla u_\nu|^2 dx$$

is not small (of moderate size). In particular, the regularized solution u_ν is *non-smooth* in the sense that $|\nabla u_\nu|$ and $|\Delta u_\nu|$ are locally very large (of size ν^{-1} and ν^{-2} at shocks and of size $\nu^{-1/2}$ and $\nu^{-3/2}$ in turbulent regions, respectively). In this case the perturbation is *singular*, and is essential in the sense that only the regularized problem has pointwise solutions. We thus consider a Hamiltonian system with singular perturbation.

We understand that $D(u_\nu)$ results from multiplication of $-\nu\Delta u_\nu$ by u_ν and integration (by parts) over Ω. Typically, $D(u_\nu)$ will have a positive limit as ν tends to zero, which expresses an independence of the specific form of the regularization, that is the specific value of ν, with always the term $-\nu\Delta u_\nu$ balancing the non-zero Hamiltonian residual $H(u_\nu)$, with Δu_ν getting larger as ν gets smaller.

We will thus view the appearance of the regularization term as a mathematical formality and we do not seek to connect it to any physical "shear viscosity". This is because the appearance of "shear viscosity" in Hamiltonian systems without viscosity, such as the Euler equations, represents the main mystery of the classical 2nd Law. We thus do not accept the common argument that "there is always some form of (shear) viscosity, which we can model by a Laplacian". The key question is from where such a viscosity comes in a inviscid flow.

We shall see that EG2 offers a new answer to this key question, where the viscosity appears as a loss of kinetic energy because the momentum equation cannot be satisfied pointwise, and not as any form of classical (shear) viscosity. The loss of kinetic energy (which is transformed into heat energy) can be viewed as a "fine" to be paid because the law $H(u) = 0$ is heavily violated pointwise. The fine can take many forms, since there are many possible forms of regularization, while the violation essentially remains the same. We shall see that EG2 penalizes a large residual $H(\hat{u})$, while classical viscous regularization penalizes all large derivates, not only the particular combination of the residual.

EG2 thus has "fine-tuned" penalization with the fine being as close as possible to the violation, like a pencillin with narrow spectrum killing only microbes producing the symptom, which suggests that EG2 can be given a physical significance. On the ohter hand, classical viscous regularization, is more like a broad band penicillin killing both microbes and healthy bacteria, and its physical signicance has remained a mystery.

To sum up, we start from a Hamiltonian system without pointwise solutions (the Euler equations), which we replace by a regularized system with pointwise solutions (by viscous regularization or EG2), which can be viewed as approximate solutions to the original system. We find that certain mean-values of the regularized solutions show little dependence on the specific form of the regularization (the viscosity or the mesh size), and thus can be viewed as stable outputs of approximate solutions to the original system. We first carry out the argmument for viscous regularization and then return below to the real case of EG2 regularization.

13.2 1d Euler

We consider an inviscid perfect gas enclosed in a tube represented by the interval $\Omega = (0,1)$ in space over a time interval $I = (0,1]$ and we assume that $f = 0$ and $g = 0$. The 1d Euler equations expressing the 1st Law as conservation of mass, momentum and internal energy, formally take the form: Find $\hat{u} \equiv (\rho, m, e)$ such that with $v' = \frac{\partial v}{\partial x}$

$$\begin{aligned} R_\rho(\hat{u}) \equiv \dot{\rho} + (\rho u)' &= 0 \quad \text{in } Q, \\ R_m(\hat{u}) \equiv \dot{m} + (mu + p)' &= 0 \quad \text{in } Q, \\ R_e(\hat{u}) \equiv \dot{e} + (eu)' + pu' &= 0 \quad \text{in } Q, \\ u(0,t) = u(1,t) &= 0 \quad t \in I, \\ \hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega, \end{aligned} \tag{13.1}$$

where $p = \gamma e$ with $\gamma > 0$ and $u = \frac{m}{\rho}$, or in short form

$$\begin{aligned} R(\hat{u}) &= 0 \quad \text{in } Q, \\ u(0,t) = u(1,t) &= 0 \quad t \in I, \\ \hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega, \end{aligned} \tag{13.2}$$

where $R = (R_\rho, R_m, R_e)$.

13.3 Formal Reversiblity

The Euler equations (13.1) without regularization are formally *reversible*: Changing the sign of the velocity u and the direction of time (the sign of the time-derivative $\dot{u}$), the Euler equations obviously remain unchanged. This means that if $\hat{u}(t)$ is a solution to the Euler equations in forward time on $[0, T]$ taking the initial value $\hat{u}(0)$ to the final value $\hat{u}(T)$, we obtain a solution in backward time taking $\hat{u}(T)$ back to $\hat{u}(0)$ by reversing the velocity at time $\bar{t}$. Of course we can view this solution as proceeding in forward time by just continuing counting time forward after the velocity reversal.

We conclude that if the Euler equations have a pointwise solution then it can be turned into a perpetuum mobile running for ever without consuming any energy, for ever bouncing back and forth by repeated reversal of the velocity at two given time instances.

13.4 Factual Irreversibility

The trouble with the above argument is that the Euler equations lack pointwise solutions and thus the implication is empty. In contrast viscosity solutions to the regularized Euler equations exist, but these solutions are turbulent with substantial turbulent dissipation and thus are irreversible. Therefore a perpetuum mobile is impossible.

We sum up: The exact solutions which would have been reversible if they had existed, do not exist. The viscosity solutions which do exist, are not reversible. This is the main lesson of this book, and resolves the main open problem of classical thermodynamics: *Loschmidt's paradox* asking how irreversibility can arise in a reversible system.

13.5 Energy Estimates for Viscosity Solutions

We shall now prove that a viscosity solutions of the regularized 1d Euler equations (13.1) is a *dissipative weak solution* of the Euler equations in the sense that its Euler residual is small in a weak sense and it satisfies a 2nd Law expressing an irreversible transfer from kinetic to heat energy in the form of turbulent/shock dissipation. In short we prove that viscosity solutions are dissipative weak solutions of the Euler equations.

We thus consider the following regularized version of (13.1): Find $\hat{u}_{\nu,\mu} \equiv \hat{u} = (\rho, m, e)$ such that

$$\begin{array}{rcl}\dot\rho+(\rho u)' &=& 0 \quad \text{in } Q,\\ \dot m+(mu+p)' &=& (\nu u')'+(\mu p u')' \quad \text{in } Q,\\ \dot e+(eu)'+pu' &=& \nu(u')^2 \quad \text{in } Q,\\ u(0,t)=u(1,t) &=& 0 \quad t\in I,\\ \hat u(\cdot,0) &=& \hat u^0 \quad \text{in } \Omega,\end{array} \tag{13.3}$$

where $p=\gamma e$, and $\nu>0$ and $\mu\geq 0$ are small parameters with ν representing *shear viscosity* and μ a form of *bulk viscosity* with $\mu=0$ if $u'<0$. For simplicity, we here suppress the subindices ν and μ. We here use the balance equation for the internal energy e, modified to account for the contribution to the internal energy from shear viscosity, but without contribution from bulk viscosity, which we consider as a penalty. We observe that only the velocity u is subject to regularization, which gives (as we will see below) the momentum equation a different quality than the balance equations for mass and internal energy, both involving u as a coefficient.

We shall see that it is natural to choose the regularization parameter ν much smaller than μ, and thus the main effect of the regularization comes from the bulk viscosity μ, rather than from the usual shear viscosity ν. We shall see that the bulk viscosity prevents fluid particles from colliding, or more precisely, prevents faster fluid particles to overtake slower particles (along the same streamline), which thus is the main effect of the regularization and not shear viscosity.

We shall now prove that $\hat u=\hat u_{\nu,\mu}$ satisfies

$$\|R_m(\hat u)\|_{-1}\leq \frac{\sqrt{\nu}}{\sqrt{\mu}}+\sqrt{\mu}, \tag{13.4}$$

where $\|\cdot\|_{-1}$ denotes the $L_2(I;H^{-1}(J))$-norm, while obviously $R_\rho(\hat u)=0$ and $R_e(\hat u)\geq$ in a pointwise sense in $\Omega\times I$. Further, we shall observe that $\hat u$ satisfies the following 2nd Law:

$$\dot K\leq W-D,\quad \dot E=-W+D,$$

where

$$K=\int_J kdx,\quad E=\int_J edx,\quad W=\int_J pu'dx,\quad D=\int_J \nu(u')^2\,dx>0.$$

Choosing $\mu=\epsilon$ and $\nu=\epsilon^2$, we can assure that $\|R_m(\hat u_{\nu,\mu})\|_{-1}\leq 2\sqrt{\epsilon}$ for any positive ϵ. We shall prove the following result on the existence of *dissipative weak approximate solutions* to the 1d Euler equations:

A viscosity solution $\hat{u}$ of the regularized Euler equations (13.1) satisfies

$$R_\rho(\hat{u}) = 0 \quad \text{in } \Omega \times I, \quad \|R_m(\hat{u})\|_{-1} \leq TOL, \quad R_e(\hat{u}) \geq 0 \quad \text{in } \Omega \times I,$$

where $TOL = \frac{\sqrt{\nu}}{\sqrt{\mu}} + \sqrt{\mu}$, together with the 2nd Law

$$\dot{K} \leq W - D, \quad \dot{E} = -W + D, \quad D > 0. \tag{13.5}$$

We understand that Theorem 13.5 states certain properties of the regularized solution $u_{\nu,\mu}$ in terms of its Euler residuals, without explicitely referring to the regularization, where the 2nd Law compensates for the fact that the momentum residual $R_m(\hat{u})$ is only required to be small in a weak norm, and $R_e(\hat{u})$ is allowed to be pointwise positive. We note that by the 2nd Law (13.5) it follows that

$$\dot{K} + \dot{E} \leq 0 \tag{13.6}$$

stating that the integral (or totality) in space of the total energy ϵ cannot increase.

To make the notion of dissipative weak solution really useful, we have to connect it to *output uniqueness*. We will return to this basic aspect below in the context of EG2, using directly the properties of EG2 without passing through Theorem 13.5. We can thus view Theorem 13.5 as a connection to a classical analytical technique of regularized solutions, which we will not pursue in detail, because what we can compute are EG2 solutions, not classical regularized solutions, and because a EG2 solution can be viewed as a (new) form of regularized solution.

Since the concept of weak solution can be viewed as expressing a form of approximate solution, with an exact solution being a (strong) pointwise solution, we can condense the notation to *dissipative weak solution*. In short, we will thus prove the existence of dissipative weak solutions to the Euler equations and below see that a EG2 solution is a dissipative weak solution.

Proof of Theorem 6.1: The basic technical step is to multiply the momentum equation by u, omitting for simplicity the indices ν and μ, and use the mass balance equation in the form $\frac{u^2}{2}(\dot{\rho} + (\rho u)') = 0$, to get

$$\dot{k} + (ku)' + p'u - \mu(pu')'u - \nu u''u = 0. \tag{13.7}$$

By integration in space it follows that $\dot{K} \leq W - D$, and similarly it follows that $\dot{E} = -W + D$ from the equation for e, which proves the 2nd Law.

Adding next (14.6) to the equation for the internal energy e and integrating in space, gives

$$\dot{K} + \dot{E} + \int_0^1 \mu p(u')^2\, dx = 0,$$

and thus after integration in time

$$K(1) + E(1) + \int_Q \mu p(u')^2\, dxdt = K(0) + E(0). \tag{13.8}$$

We now need to show that $E(1) \geq 0$ (or more generally that $E(t) > 0$ for $t \in I$), and to this end we rewrite the equation for the internal energy as follows:

$$\frac{De}{Dt} + (\gamma + 1)eu' = \nu(u')^2,$$

where $\frac{De}{Dt} = \dot{e} + ue'$ is the material derivative of e following the fluid particles with velocity u. Assuming that $e(x, 0) > 0$ for $0 \leq x \leq 1$, it follows that $e(x, 1) > 0$ for $0 \leq x \leq 1$, and thus $E(1) > 0$. Assuming $K(0) + E(0) = 1$ the energy estimate (14.7) thus shows that

$$\int_Q \mu p(u')^2\, dxdt \leq 1, \tag{13.9}$$

and also that $E(t) \leq 1$ for $t \in I$.

Next, integrating (14.6) in space and time gives

$$K(1) + \int_Q \nu(u')^2 dxdt = \int_Q pu' dxdt - \int_Q \mu p(u')^2 dxdt \leq \frac{1}{\mu}\int_Q pdxdt \leq \frac{1}{\mu},$$

where we used that $\int_Q pdxdt = \gamma \int_Q edxdt \leq \int_I E(t)dt \leq 1$. It follows that

$$\int_Q \nu(u')^2 dxdt \leq \frac{1}{\mu}. \tag{13.10}$$

By standard estimation it follows from (14.8) and (14.9) that

$$\|R_m(\hat{u})\|_{-1} \leq \sqrt{\mu} + \frac{\sqrt{\nu}}{\sqrt{\mu}},$$

and the proof can be completed in an obvious fashion.

13.6 Irreversibility by the 2nd Law

The 2nd Law (13.5) states an irreversible transfer of kinetic energy to heat energy for in the presence of shocks with $D > 0$, which is the generic case. On the other hand, the sign of W is variable and thus the corresponding energy transfer may go in either direction.

13.7 Compression and Expansion

The 2nd Law (13.5) states that there is a transfer of kinetic energy to heat energy if $W < 0$, that is under compression with $u' < 0$, and a transfer from heat to kinetic energy if $W > 0$, that is under expansion with $u' > 0$. As we just remarked, there is a transfer from kinetic to heat energy for solutions with shocks with $D > 0$.

Returning to Joule's experiment, we see by the 2nd Law that contraction back to the original volume from the final rest state in the double volume, is impossible, because the only way the gas can be set into motion is by expansion.

Chapter 14

Viscosity Solutions to 3d Euler

> Everyone knows that heat can produce motion. That it possesses vast motive power no one can doubt, in these days when the steam engine is everywhere so well known. The study of these engines is of great interest, their importance is enormous, their use is continually increasing, and they seem desined to produce a great revolution in the civilized world. (Carnot [7] 1824).

> But maybe that is our mistake: maybe there are no particle positions and velocities, but only waves. It is just that we try to fit the waves to our preconceived ideas of positions and velocities. The resulting mismatch is the cause of the apparent unpredictability.(Stephen Hawking)

> What wanted to say was just this: In the present circumstances the only profession I would choose would be one where earning a living had nothing to do with the search for knowledge". (Einstein's last letter to Born Jan 17 1955 shortly before his death on the 18th of April, probably referring to Born's statistical interpretation of quantum mechanics).

14.1 3d Euler

We now show that the above result for the 1d Euler equations directly extends to 3d. We thus consider the 3d Euler equations for an inviscid perfect gas enclosed in a volume Ω in $\mathbb{R}^3$ with boundary Γ over a time interval $I = (0, 1]$, assuming as above that the applied force $f = 0$: Find $\hat{u} = (\rho, m, e)$ depending on $(x, t) \in Q \equiv \Omega \times I$ such that

$$\begin{aligned} R_\rho(\hat{u}) \equiv \dot{\rho} + \nabla \cdot (\rho u) &= 0 \quad \text{in } Q, \\ R_m(\hat{u}) \equiv \dot{m} + \nabla \cdot (mu) + \nabla p &= 0 \quad \text{in } Q, \\ R_e(\hat{u}) \equiv \dot{e} + \nabla \cdot (eu) + p\nabla \cdot u &= 0 \quad \text{in } Q, \\ u \cdot n &= 0 \quad \text{on } \Gamma \times I \\ \hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega, \end{aligned} \tag{14.1}$$

where $u = \frac{m}{\rho}$ and $p = \gamma e$ with $\gamma > 0$.

14.2 Energy Estimates for Viscosity Solutions

We consider the following regularized version of (14.1): Find $\hat{u}_{\nu,\mu} \equiv \hat{u} = (\rho, m, e)$ such that

$$\begin{aligned} R_\rho(\hat{u}) &= 0 \quad \text{in } Q, \\ R_m(\hat{u}) &= \nabla \cdot (\nu \nabla u) + \nabla(\mu p \nabla \cdot u) \quad \text{in } Q, \\ R_e(\hat{u}) &= \nu |\nabla u|^2 \quad \text{in } Q, \\ u = \frac{\partial u}{\partial n} &= 0 \quad \text{on } \Gamma \times I, \\ \hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega, \end{aligned} \tag{14.2}$$

where $\nu > 0$ is a shear viscocity and $\mu \geq 0$ a bulk viscosity with $\mu = 0$ if $\nabla \cdot u < 0$, and $|\nabla u|^2 = \sum_{i=1}^3 |\nabla u_i|^2$.

As already indicated, the existence of a pointwise solution $\hat{u}_{\nu,\mu}$ to the regularized problem is an open problem of mathematical analysis. However, we only use the regularized problem to formally illustrate basic properties of EG2-solutions, which we prove directly below.

We shall now prove that $\hat{u} = \hat{u}_{\nu,\mu}$ satisfies

$$\|R_m(\hat{u})\|_{-1} \leq \frac{\sqrt{\nu}}{\sqrt{\mu}} + \sqrt{\mu}, \tag{14.3}$$

where $\| \cdot \|_{-1}$ denotes the $L_2(I; H^{-1}(\Omega))$-norm, while we may assume that $R_\rho(\hat{u}) = 0$ and $R_e(\hat{u}) \geq 0$ in a pointwise sense in Q. We shall also find that $\hat{u}$ satisfies the following 2nd Law:

$$\dot{K} \leq W - D, \quad \dot{E} = -W + D,$$

where

$$K = \int_\Omega k\,dx, \quad E = \int_\Omega e\,dx, \quad W = \int_\Omega p\nabla\cdot u\,dx, \quad D = \int_\Omega \nu|\nabla u|^2\,dx.$$

Choosing $\mu = \epsilon$ and $\nu = \epsilon^2$, we can assure that $\|R_m(\hat{u}_{\nu,\mu})\|_{-1} \leq TOL$ for any positive tolerance TOL. We shall thus show the following formal result on the existence of *dissipative weak approximate solutions* to the 3d Euler equations:

A viscosity solution $\hat{u}$ of the regularized Euler equations (14.1) satisfies

$$R_\rho(\hat{u}) = 0 \quad \text{in } \Omega\times I, \quad \|R_m(\hat{u})\|_{-1} \leq TOL, \quad R_e(\hat{u}) \geq 0 \quad \text{in } \Omega\times I,$$

where $TOL = \frac{\sqrt{\nu}}{\sqrt{\mu}} + \sqrt{\mu}$, together with the 2nd Law

$$\dot{K} \leq W - D, \quad \dot{E} = -W + D, \quad D > 0. \tag{14.4}$$

As above, we note that Theorem 13.5 states certain properties of the regularized solution $u_{\nu,\mu}$ in terms of its Euler residuals, without explicitely referring to the regularization, where the 2nd Law compensates for the fact that the momentum residual $R_m(\hat{u})$ is only required to be small in a weak norm, and $R_e(\hat{u})$ is allowed to be pointwise positive. We note that by the 2nd Law it follows that

$$\dot{K} + \dot{E} \leq 0 \tag{14.5}$$

stating that the integral (or totality) in space of the total energy ϵ cannot increase. We shall see below that a EG2 solution is a dissipative weak approximate solution.

Proof of 14.2: The basic technical step is to multiply the momentum equation by u, and use the mass balance equation in the form $\frac{|u|^2}{2}(\dot{\rho}+\nabla\cdot(\rho u) = 0$, to get

$$\dot{k} + \nabla\cdot(ku) + p\nabla\cdot u - \nabla(\mu p\nabla\cdot u) + \nabla\cdot(\nu\nabla u)\cdot u = 0. \tag{14.6}$$

By integration in space it follows that $\dot{K} \leq W - D$, and similarly it follows that $\dot{E} = -W + D$ from the equation for e, which proves the 2nd Law. Adding next (14.6) to the equation for the internal energy e and integrating in space, gives

$$\dot{K} + \dot{E} + \int_\Omega \mu p(\nabla\cdot u)^2\,dx = 0,$$

and thus after integration in time

$$K(1) + E(1) + \int_Q \mu p(\nabla \cdot u)^2 \, dxdt = K(0) + E(0). \tag{14.7}$$

We now need to show that $E(1) \geq 0$ (or more generally that $E(t) > 0$ for $t \in I$), and to this end we rewrite the equation for the internal energy as follows:

$$\frac{De}{Dt} + (\gamma + 1)e\nabla \cdot u = \nu|\nabla u|^2,$$

where $\frac{De}{Dt} = \dot{e} + u \cdot \nabla e$ is the material derivative of e following the fluid particles with velocity u. Assuming that $e(x, 0) > 0$ for $x \in \Omega$, it follows that $e(x, 1) > 0$ for $x \in \Omega$, and thus $E(1) > 0$. Assuming $K(0) + E(0) = 1$ the energy estimate (14.7) thus shows that

$$\int_Q \mu p(\nabla \cdot u)^2 \, dxdt \leq 1, \tag{14.8}$$

and also that $E(t) \leq 1$ for $t \in I$.

Next, integrating (14.6) in space and time gives

$$K(1) + \int_Q \nu|\nabla u|^2 dxdt = \int_Q p\nabla \cdot u dxdt - \int_Q \mu p(\nabla \cdot u)^2 dxdt \leq \frac{1}{\mu} \int_Q pdxdt \leq \frac{1}{\mu},$$

where we used that $\int_Q pdxdt = \gamma \int_Q edxdt \leq \int_I E(t)dt \leq 1$. It follows that

$$\int_Q \nu|\nabla u|^2 dxdt \leq \frac{1}{\mu}. \tag{14.9}$$

By standard estimation it follows from (14.8) and (14.9) that

$$\|R_m(\hat{u})\|_{-1} \leq \sqrt{\mu} + \frac{\sqrt{\nu}}{\sqrt{\mu}},$$

and the proof can be completed in an obvious fashion.

14.3 Irreversibility by the 2nd Law

The 2nd Law (14.4) states an irreversible transfer of kinetic energy to heat energy in the presence of shocks/turbulence with $D > 0$, which is the generic case. On the other hand, the sign of W is variable and thus the corresponding energy transfer may go in either direction.

14.4 Compression and Expansion

The 2nd Law (14.4) states that there is a transfer of kinetic energy to heat energy if $W < 0$, that is under compression with $u' < 0$, and a transfer from heat to kinetic energy if $W > 0$, that is under expansion with $\nabla \cdot u > 0$.

Returning to Joule's experiment, we see by the 2nd Law that contraction back to the original volume from the final rest state in the double volume, is impossible, because the only way the gas can be set into motion is by expansion.

14.5 A 2nd Law witout Entropy

We note that the 2nd Law (14.4) is expressed in terms of the kinetic energy K, the heat enargy E and the work W, and does not involve any concept of entropy S. This relieves us from the task of finding a physical significance of S and a physical justification of a classical 2nd Law of the form $dS \geq 0$. We thus circumvent the main difficulty of classical thermodynamics based on statistical mechanics, while we reach the same goal as statistical mechanics of explaining irreversibility in formally reversible Newtonian mechanics.

Note that since the new 2nd Law is a consequence of the 1st Law and EG2 computation, we can "forget" the 2nd Law: It is automatically satisfied without special attention. This is like 'forgetting" to keep the balance while walking, because is automatically maintained without conscious attention.

Chapter 15

Classical vs New 2nd Law

> It seems to me that the concept of probability is terribly mishandled these days. A probabilistic assertion presupposes the full reality of its subject. No reasonable person would express a conjecture as to whether Caesar rolled a five with his dice at the Rubicon. But the quantum mechanics people sometimes act as if probabilistic statements were to be applied *just* to events whose reality is vague. (Schrödinger to Einstein 1950)
>
> What you cannot speak of, you have to be quite. (Wittgenstein)

15.1 Basics of Classical Thermodynamics

Classical thermodynamics is based on the relation

$$\tau ds = d\tau + pdv, \tag{15.1}$$

where ds represents change of entropy s per unit mass, dv change of volume v and $d\tau$ denotes the change of temperature or internal energy per unit mass τ, combined with a 2nd Law in the form

$$ds \geq 0, \tag{15.2}$$

The rationale behind the 2nd Law in this form was the main mystery of science in the later half of the 19th century, and in an attempt to motivate it on a molecular-mechanistic basis, Boltzmann invented statistical mechanics.

15.2 Entropy of a Perfect Gas

Integrating the classical 2nd Law $\tau ds = d\tau + pdv$ for a perfect gas with $p = \gamma\rho\tau$ and $dv = d(\frac{1}{\rho}) = -\frac{d\rho}{\rho^2}$, we get

$$ds = \frac{d\tau}{\tau} + \frac{p}{\tau}d(\frac{1}{\rho}) = \frac{d\tau}{\tau} - \gamma\frac{d\rho}{\rho},$$

and thus conclude that with $e = \rho\tau$,

$$s = \log(\tau\rho^{-\gamma}) = \log(e\rho^{-(\gamma+1)}), \tag{15.3}$$

up to a constant. Thus, the entropy $s = s(\rho, \tau)$ for a perfect gas is a simple function of the physical quantities ρ and τ (or e) suggesting that s might have a physical significance, because ρ and τ have. Of course, we could get used to a quantity s defined this way, but the basic questions remains:

- What is the physical significance of s?
- Why is $ds \geq 0$?

15.3 Comparing the Classical and New 2nd Law

We have with $D_u = \frac{\partial}{\partial t} + u\cdot\nabla$ the material derivative following fluid particles,

$$\rho D_u s = \frac{\rho}{e}D_u e - (\gamma+1)D_u\rho = \frac{1}{\tau}(D_u e + (\gamma+1)\rho\tau\nabla\cdot u) = \frac{1}{\tau}(D_u e + e\nabla\cdot u + \gamma\rho\tau\nabla\cdot u)$$

since by mass conservation $D_u\rho = -\rho\nabla\cdot u$. It follows that the entropy $S = \rho s$ satisfies

$$\dot{S} + \nabla\cdot(Su) = \rho D_u s = \frac{1}{\tau}(\dot{e} + \nabla\cdot(eu) + p\nabla\cdot u) = \frac{1}{\tau}R_e(\hat{u}) \geq 0, \tag{15.4}$$

where we used the 2nd Law according to Theorem 7.1 in the form $R_e(\hat{u}) \geq 0$. We summarize in A solution $\hat{u}$ of the regularized Euler equations (14.2) satisfies

$$\dot{S} + \nabla\cdot(Su) = \frac{1}{\tau}R_e(\hat{u}) \geq 0 \quad \text{in } Q, \tag{15.5}$$

where $S = \rho\log(\tau\rho^{-\gamma})$.

It is natural to refer to (15.5) as the 2nd Law in classical entropy form, which we may express symbolically as $dS \geq 0$. We have thus shown that that the new 2nd Law effectively includes the classical 2nd Law in the form $dS \geq 0$, without reference to S, only to the physically significant quantities K, E and W.

We thus circumvent what is perceived as the main difficulty of classical thermodynamics and what motivated the introduction of statistical mechanics, namely to give the entropy S a physical meaning and justifying that $dS \geq 0$. We have just seen that we can motivate $dS \geq 0$ by viscous regularization (below by EG2 finite computation) without statistical mechanics, as a consequence of the 2nd Law in the form $R_e(\hat{u}) \geq 0$. The result is that we can motivate the 2nd Law in any of its forms without resort to statistical mechanics.

15.4 Local and Global Forms od the 2nd Law

The 2nd Law (14.4) is expressed in global form, while (15.5) has a pointwise form, and one may ask if the pointwise version is more informative than the global?

Now, the 2nd Law is a consequence of the viscous regularization in the pointwise equations (14.2), which thus can be viewed to contain in pointwise form the origin of the 2nd Law. In particular, the internal energy equation $R_e(\hat{u}) = \nu(\Delta u)^2$ expresses in pointwise form an irreversible transfer of kinetic energy into heat energy.

Whatever form of the 2nd Law we choose, global or poinwise, it will automatically be satisfied by solutions of the regularized problem, and for the main objective of expressing irreversiblity, the global form is sufficient. We hereby follow the device of Ockham that in science you should not worry about what you don't have to worry about. In particular, we do not have to worry about the entropy S and the 2nd Law in the form $dS \geq 0$.

15.5 Boltzmann's Entropy

Boltzmann's great invention is considered to be his definition of the entropy S of a certain *macro-state*, not by (15.3), but instead by the following formula engraved on his grave-stone:

$$S = k \log(W), \tag{15.6}$$

where W is the number of *micro-states* corresponding to the macro-state and $k \approx 10^{-23}$ Joule/Kelvin, is a (very small) constant referred to as *Boltzmann's constant*. Boltzmann thus proposed a probabilistic definition of entropy, where W would be a measure of the probability of the occurence of a certain macro-state, and Boltzmann then motivated the inequality $dS \geq 0$ as a tendency of a to dilute gas to move from less probable to more probable macro-states, or from macro-states with fewer corresponding micro-states to macro-states with a larger number of corresponding micro-states, or from ordered to less ordered states.

Classical thermodynamics thus plays with two different definitions of entropy, the deterministic (15.3), and the statistical (15.6). This is confusing, in particular to the non-specialist, and is the main reason that classical thermodynamics is so difficult to grasp.

We understand that Boltzmann's motivation to give a probabilistic definition of S, was to be able to motivate $dS \geq 0$, by probability. Boltzmann admits that with the probabilistic definition, it is possible that $dS < 0$, although he claims that it is very unlikely to happen. On the other hand, the new 2nd Law shows that $dS < 0$ can never happen.

Again, in the new foundation of thermodynamics including the new 2nd Law, entropy does not appear, and in particular the need of defining entropy using probability does not arise. More precisely, as already pointed out, we show below that the classical 2nd Law $dS \geq 0$ with S defined deterministically by (15.3), is contained in the new 2nd Law, and thus there is no need to resort to cumbersome probabilistic arguments to motivate not even the classical 2nd Law (15.3).

In short, with the new 2nd Law, the main reason to introduce statistical mechanics seems to dissappear. This makes thermodynamics understandable to the many users, who are not specialists of statistical mechanics, to which this book is addressed.

15.6 Extension to Non-Perfect Gases

The 1st Law expressing conservation of mass, momentum and total energy holds for all gases/fluids, but the gas law defining the pressure in terms of the conservation variables in general differs from the law of a perfect gas $p = \gamma\rho\tau$, and the dependence of internal energy E on temperature τ may differ from direct proportionality. As noted above, for a general gas the classical 2nd Law $\tau dS = dE + pdV$ may not define S as a state variable in terms of conservation variables. Further, the statistical mechanics of a general gases is largely unknown. On the other hand, the new 2nd Law without entropy, readily extends to the case of a general gas.

Part IV

Computation

Chapter 16

G2 as Turbulence Model

> For three hundred years science has been dominated by a Newtonian paradigm presenting the World either as a sterile mechanical clock or in a state of degeneration and increasing disorder...It has always seemed paradoxical that a theory based on Newtonian mechanics can lead to chaos just because the number of particles is large, and it is subjectivly decided that their precise motion cannot be observed by humans... In the Newtonian world of necessity, there is no arrow of time. Boltzmann found an arrow hidden in Nature's molecular game of roulette. (Paul Davies in *The Cosmic Blueprint*, 1987)

16.1 EG2 as a Continuum Model

As a model of thermodynamics we start from a *formal continuum model*, in the form of the *Euler equations for an ideal (inviscid) gas/fluid* expressing conservation of mass, momentum and energy as a system of differential equations. We view the Euler equations as a formal model since no procedure for solving the equations is included in merely formulating the equations. A *real model* also includes a constructive (computational) solution procedure. The distinction between formal and real model is absolutely crucial for the Euler equations, since exact pointwise solutions are lacking and thus the formal model has no output, and the real (computational) model will have output and serve as our model of thermodynamics.

To obtain a real model of thermodynamics we apply a residual-stabilized finite element method in the form of EG2 to the Euler equations using a finite element mesh of local mesh size h in space-time. The resulting EG2 model is fed into a computer as a system of algebraic equations, which can be solved to produce a computational solution to the Euler equations on the given mesh.

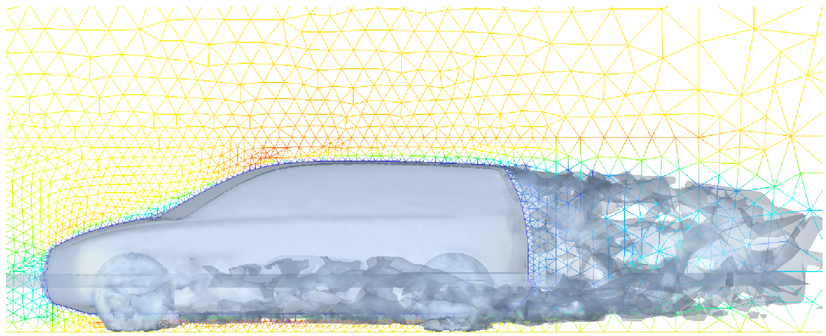

Figure 16.1: Turbulent flow around a car generating drag.

An EG2 solution is a representative of a family of EG2 solutions on different meshes. We are interested in quantitive aspects or *outputs* of EG2 solutions, which converge under mesh refinement referred to as *stable outputs*. We will find that *global mean values* such as *drag* (resistance to motion) and *lift*, are stable outputs and thus are not sensitive to the mesh once sufficiently fine, while pointwise outputs are unstable. We can thus view EG2 as a new form of (real) continuum model for which solutions are computable, while the unsolvable Euler equations represent a formal continuum model without output. It is the combination of the Euler equations with finite precision computation which gives valuable output.

We discover that EG2 solutions of the Euler equations are *turbulent* and have *shocks* reflecting that pointwise solutions are lacking. We find that both turbulence and shocks cause a transfer of large scale kinetic energy into small scale kinetic energy in the form of heat, also referred to as *turbulent dissipation*, which can be viewed as a penalty paid in kinetic energy from pointwise violation of conservation of momemtum.

Note that we do not start from the *Navier-Stokes equations* already containing viscous dissipation *by assumption*, which would be analogous to Boltzmann's assumption of molecular chaos. Effects of viscous dissipation in EG2 arise from an *impossibility* in turbulent flow of achieving a small momentum residual, with the resulting penalty acting *like a viscosity.* The viscous dissipation in turbulent EG2 flow thus can understood as an effect of finite precision computation, while the (true) nature of physical viscosity has shown to be difficult to unmask. Without residual stabilization, computation of EG2 solutions show to be impossible in the presence of turbulence and shocks. With stabilization EG2 solutions can be computed and show to accurately describe thermodynamics including turbulence and shocks.

16.2 Regularization, Finite Precision and Stability

EG2 solutions can be viewed as pointwise solutions to regularized perturbed Euler equations with a specific regularization resulting from least squares residual-based stabilization directly connecting penalty to violation.

We show that EG2 solutions satisfy a 2nd Law, as a consequence of the 1st Law and stabilization. We can view the 2nd Law to express an interplay of *stability* and *finite precision computation* expressing that unstable processes require infinite precision for exact execution, and thus cannot be realized, while stable processes only require finite precision and thus can be realized.

To smash a (very expensive very old) Chinese vase into pieces (e.g. by mistake dropping it on the floor), does not require much of precision, while reversing the process and reassembling all the little pieces would require a very high precision.

Stability is here related to the process output. The result of smashing a vase is a smashed vase and the precise location of the pieces is irrelevant. This allows quick low precision (brutal) smashing: No matter how you smash, the output is a smashed vase. On the other hand, the output of the reverse restoration process is the original vase, and to achieve this result slow high precision (careful) assembly is required. So even if in a pointwise sense both the smashing and the assembly are unstable, the smashing is stable in the sense that the output of a smashed vase can be quickly be achieved with low precision. Reversing the smashing in time would involve quick high-precision assembly, which cannot be done, and thus smashing is an irreversible process. This is the essence of the new 2nd Law in a nutshell illustrating its basic ingredients of (output) stability and finite precision.

If you do not have an expensive Chinese vase to spare, you can instead drop a stone to the ground and notice that it heats up as the (large scale) potential energy of the stone is converted first to (large scale) kinetic energy as the stone falls and picks up speed, and then at impact is converted to (small scale) kinetic energy perceived as heat, cf. Fig 9.3. To get a noticable temperature increase you may have to repeatedly drop the stone. In each drop the total energy is conserved as the large scale potential energy is transformed to small scale kinetic energy in the form of heat energy. Reversal of the process would involve a stone lifting itself by cooling off, a phenomenon nobody has ever observed: The reason is that the precision required to coordinate the small scale heat energy into large scale potential energy cannot be attained in a physical process (while the forward process of dropping the stone does not require much of precision).

We shall find that turbulent flow has a particular form of *output stability* with mean-values being stable and thus computable, while point-values are unstable and thus uncomputable. This is evidenced in *duality-based posteriori error estimation*, where the stability of mean-value outputs of shock/turbulent flow results from *cancellation* in an associated dual problem with *highly oscillating coefficients* reflecting the complexity of turbulent flow. This fits with the observation that the World of thermodynamics is complex and pointwise chaotic, but because of the complexity, mean-value order can develop from pointwise chaos.

The fact that mean-values are stable and computable thus results form the complexity of turbulent flow:

- *Complex (turbulent) structures are stable and thus exist.*
- *Simple (laminar) structures are unstable and thus do not exist.*

This fits with the observation that the existing world of thermodynamics is complex and not simple.

EG2 thermodynamics represents a form of deterministic chaos, where the mechanism is open to inspection and can be used for prediction. Statistical mechanics is based on ad hoc assumption not open to inspection, and is difficult to use for prediction.

We shall see that turbulence/shocks appear as a consequence of an impossibility to satisfy the Euler equations in a pointwise sense: This is like a wave building up when approaching a shore and eventually, when it cannot build up any more, breaks up into a turbulent cascade in which the large scale kinetic energy of the coherent wave is transformed into small scale incoherent heat energy, in an obviously irreversible process.

The aspect of sharpening or increasing gradients in a wave building up, which preceeds the resolution into a turbulent cascade, is a fundamental aspect of the stability of irreversible processes and closely couples to finite precision: It is the finite precision which sets a limit to the sharpening and ultimately forces the process to choose the only option available in an impossible situation: turbulent dissipation.

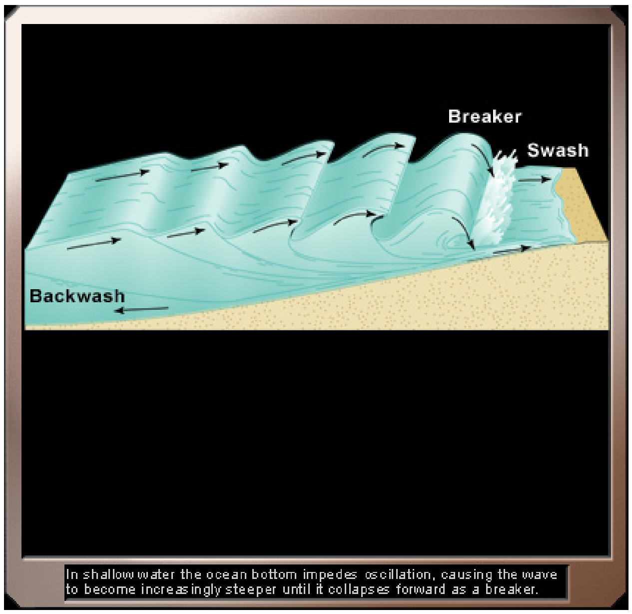

Figure 16.2: The irreversible process of a breaking wave illustrates the 2nd Law.

16.3 Finite Precision vs Uncertainty

The idea that the World performs some form of analog finite precision computation when evolving from one time instant to the next, may seem new (and repugnant) to physicists. But this is not necessary, since the pillars of modern physics, statistical mechanics and quantum mechanics, both involve *uncertainty* of microscopics, which can be viewed as a form of finite precision. Thus, both finite precision computation in the form of EG2 and statistical/quantum mechanics involve an essential aspect of modern physics of *imprecision of microscopics*. An advantage of finite precision computation is that no data on statistical distributions is required, only deterministic data.

16.4 Internal Energy or Heat Energy

Heat energy is also referred to as *internal energy*. The new 2nd Law expresses a transfer of kinetic energy into internal energy. The irreversibility of this process means that kinetic energy once converted to "internal" energy, cannot be retrieved and thus is "lost": The energy has been locked in "internally". We shall understand below that this is because small kinetic (internal) energy cannot be coordinated (because of finite precision) in a reversed process of recovering large scale kinetic energy. Thus the term "internal" seems to capture the physics in a suggestive metaphor.

We shall see that the new 2nd Law in a way is not new, since it is so completely basic and results from an energy balance obtained by the basic operation of multiplication of the momentum equation by the velocity combined with the finite precision computation of EG2 as a specific form of regularization. Yet the new 2nd Law is non-standard and thus (surprisingly so), in fact in a certain sense is new, in particular when seen as an interplay of stability and finite precision. A basic observation is that generically $D > 0$ because of the presence of turbulence/shocks in all inviscid flow, except trivial flow with constant velocity.

The novelty of the new 2nd Law thus can (and hopefully will) be debated, since it is so completely basic, but it is undeniable that it can replace the classical 2nd Law without any reference to entropy, and is a consequence of the 1st Law and certain finite precision computation, which appears to be genuinely new and open to a simplification of the difficult subject of classical thermodynamics.

16.5 Maxwell's Demon and Separation

Mixing can be done quickly with low precision (brutally), while *unmixing/separation* must be done with high precision and thus must be slow, if at all feasible. Compare quickly mixing milk into your coffee with a spoon with the impossible reversed process. Quick (brutal) mixing is irreversible. But what about slow mixing, is it also irreversible? Is slow unmixing possible?

This connects to *Maxwell's Demon* who is supposed to separate/unmix slow gas molecules from fast ones through a gate allowing only fast molecules to pass. Because all fast molecules would have to pass through the gate, one by one, the separation would have to be slow, since the molecules would only present themselves by some natural process at the gate and could not be quickly forced through the gate by the Demon. Maxwell's Demon could thus be expexted to reverse slow mixing but not fast mixing.

Now, does Maxwell's Demon exist? Are there processes of slow unmixing/separation? Yes, in Nature there are two basic processes of slow unmixing: *sedimentation* in geology and *osmosis* in biology, both contradicting the popular science version of 2nd Law stating that "everything has a tendency to disperse", which we met above.

In sedimentation in the sea, gravitation makes certain particles fall to the bottom quicker than others, which (very slowly) produces layers of different material. In osmosis a solvent like water moves through a semi-permeable membrane from a solute of small concentration to a solute of higher concentration. Osmosis is the mechanism through which a tree can suck up water from the ground all the way to the top of the tree, and thus separate water out of the ground into the cells.

Unmixing/separation is a form of *sorting*. We know that *digital sorting* can be made quickly with high precision by computers, but is quick analog sorting possible? Yes, a high speed *separator* can do the job essentially by a process of sedimentation driven by strong inertial forces from quick rotation. But biology has not developed high speed separators, which make many biological processes irreversible. And a high speed separator does not exactly reverse a process of mixing.

We understand that separation of a substance out of a mixture with other substances, involves *identification* and *transport* of the substance. This can be performed quickly in digital form, if the process is digitized, but in analog form only slowly, by processes like sedimentation or osmosis.

16.6 Mixing-Unmixing vs Precision

We note that a process of mixing

(m1) decreases macroscopic difference,

(m2) increases microscopic difference,

while a process of unmixing

(u1) increases macroscopic difference,

(u2) decreases microscopic difference.

We understand that both (m1) and (m2) and also (u1) may be performed with low precision, while (u2) requires high precision on microscopic scales for identification and separation, which in analog form cannot be quick. Thus quick mixing cannot be reversed.

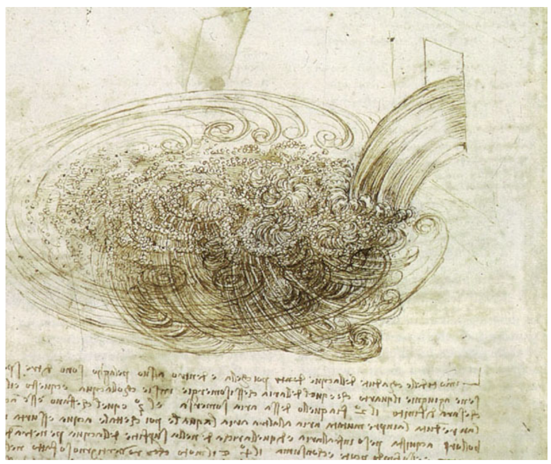

Figure 16.3: Emergence of organized structures in turbulent flow according to Leonardo da Vinci.

> The second law of thermodynamics is, without a doubt, one of the most perfect laws in physics. Any reproducible violation of it, however small, would bring the discoverer great riches as well as a trip to Stockholm. The world's energy problems would be solved at one stroke. It is not possible to find any other law (except, perhaps, for super selection rules such as charge conservation) for which a proposed violation would bring more skepticism than this one. Not even Maxwell's laws of electricity or Newton's law of gravitation are so sacrosanct, for each has measurable corrections coming from quantum effects or general relativity. The law has caught the attention of poets and philosophers and has been called t he greatest scientific achievement of the nineteenth century. Engels disliked it, for it supported opposition to Dialectical Materialism, while Pope Pius XII regarded

it as proving the existence of a higher being. (Bazarov in *Thermodynamics*, 1964)

There is at present in the material world a universal tendency to the dissipation of mechanical energy. — We have the sober scientific certainty that the heavens and earth shall "wax old as doth a garment." — Although mechanical energy is indestructible, there is a universal tendency to its dissipation, which produces throughout the system a gradual augmentation and diffusion of heat, cessation of motion and exhaustion of the potential energy of the material Universe. — Any restoration of mechanical energy, without more than an equivalent of dissipation, is impossible in inanimate material processes, and is probably never effected by means of organized matter, either endowed with vegetable life, or subjected to the will of an animated creature. — Nothing can be more fatal to progress than a too confident reliance on mathematical symbols; for the student is only too apt to take the easier course, and consider the formula not the fact as the physical reality. — I have no satisfaction in formulas unless I feel their numerical magnitude. (Lord Kelvin)

Chapter 17

EG2

> The 2nd Law cannot be derived from purely mechanical laws. It carries the stamp of the essentially statistical nature of heat. (Bergmann [1])
>
> Therefore I feel that the Heisenberg-Bohr (Copenhagen) statistical interpretation of quantum mechanics is dead. (Zeh [44])
>
> If a scientist says that something is possible he is almost certainly right, but if he says that it is impossible he is probably wrong. (Arthur C. Clarke)

17.1 Introduction

We refer to [20] for a detailed presentation of EG2 for the incompressible Euler equations. The extension to the compressible Euler equations has the principal form: Find $\hat{u} \in V_h$ such that

$$((R(\hat{u}), \hat{v})) + ((hR(\hat{u}), R'(\hat{u}, \hat{v}))) = 0 \quad \text{for } \hat{v} \in V_h \tag{17.1}$$

where V_h is a space-time finite element space on a mesh with mesh size h, $((\cdot, \cdot))$ denotes space-time L_2 scalar products, and $R'(\hat{u}, \hat{v})$ is a linearization of the Euler residual $R(\hat{u})$ at $\hat{u}$ such that $R'(\hat{u}, \hat{u}) = R(\hat{u})$, which leads to residual least squares stabilization through the positive penalty term $((hR(\hat{u}), R(\hat{u}))$ obtained choosing $\hat{v} = \hat{u}$.

In the actual implementation of EG2 on cG(1)cG(1)-form stated below, the stabilization has a reduced form involving only some of the terms summing to the residual. The rationale is that the stabilization has an effect when the residual is large pointwise, and then stabilizing one term of the residual suffices. A residual-based *shock-capturing* stabilization with viscosity coefficient $\sim h^2|R(\hat{u})|$ is also used, which eliminates (small) oscillations at shocks, but shock-capturing alone is not sufficient.

The 2nd Law satisfied by EG2 shows that the stabilization effectively concerns one term of the momentum equation, and not the mass and energy equations. The motivation is that since the momentum equation will not be pointwise (strongly) small, only weakly small, a stabilization is required because the the balance of kinetic energy results from multiplication of the momentum equation by the velocity and this operation is not stable under weak convergence to zero of the momentum residual. On the other hand, the mass and energy equations are not similarly multiplied by density and energy, and thus do not need (the same form) of stabilization.

17.2 EG2 in cG(1)cg(1) Form

EG2 in cG(1)cG(1)-form for the Euler equations (14.1) is a time-stepping method defined by find $\hat{u} = (\rho, m, e) \in V_h$ such that for all $(\bar{\rho}, \bar{u}, \bar{e}) \in W_h$

$$\begin{aligned} ((R_\rho(\hat{u}), \bar{\rho})) + ((\delta u \cdot \nabla \rho, u \cdot \nabla \bar{\rho})) &= 0, \\ ((R_m(\hat{u}), \bar{u})) + ((\delta u \cdot \nabla m, u \cdot \nabla \bar{u})) &= 0, \\ ((R_e(\hat{u}), \bar{e})) + ((\delta u \cdot \nabla e, u \cdot \nabla \bar{e})) &= ((d_h, \bar{e})), \end{aligned} \tag{17.2}$$

where

$$d_h = \sum_{i=1}^{3} \delta \rho (u \cdot \nabla u_i)^2, \tag{17.3}$$

and V_h is a trial space of continuous piecewise linear functions on a space-time mesh of size h satisfying the initial condition $\hat{u}(0) = \hat{u}^0$ with $u \in V_h$ defined by nodal interpolation of $\frac{m}{\rho}$, and W_h is a corresponding test space of function which are continuous piecewise linear in space and piecewise constant in time, all functions satisfying the boundary condition $u \cdot n = 0$ at the nodes on Γ. The space-time mesh is organized into space-time slabs between discrete time levels, and the velocity in the stabilization terms is averaged over each time step. Further, $((\cdot, \cdot))$ denotes relevant $L_2(Q)$ scalar products. Finally, the least squares stabilization weight $\delta = \frac{ch}{|u|}$ with $c \approx 0.5$, and *shock-capturing viscosity* with viscosity coffecient $\nu_i \sim h^2|R_i(\hat{u})|^2$, $i = \rho, m, e$, is also added to each equation separately, which eliminates the small oscillations occuring at shocks with only least squares stabilization. For small densities (almost vacuum), the velocity is computed by $u = \frac{m}{\rho+\epsilon}$ with $\epsilon > 0$ suitably small.

EG2 (17.2) combines a weak satisfaction of the Euler equations with a weighted least squares control of (a part of) the momentum residual $R_m(\hat{u})$ and represents a midway between the Scylla of weak solution and Carybdis of least squares strong solution. The form of the stabilization terms in the density and energy equations secures exact global conservation since the stabilization terms vanish with $\bar{\rho} = \bar{e} \equiv 1$. Notice that choosing $\bar{\rho} = \rho$ (mean-value over time step) gives a bound on $\int_Q \delta(u \cdot \nabla\rho)^2 dxdt$ in terms of $\int_Q \rho^2 \nabla \cdot u dxdt$, with a similar control of e.

Notice that EG2 as expressed in (17.2) has a remarkable simplicity, as compared to finite difference methods based on diagonalization of the full system together with Riemann solvers, and also compared to stabilized finite element methods using diagonalization of the full linearized operator. In (17.2) each scalar convection equation is stabilized separately without diagonalization. In particular, the net numerical dissipation d_h has a contribution from each separate momentum/velocity component, but there is no net numerical dissipation in mass and internal energy.

17.3 The 2nd Law for EG2

Choosing $\bar{u}$ in the momentum equation as the time average of u over the time step, and subtracting the mass equation with $\bar{\rho} = I_h(\frac{|u|^2}{2})$, where $I_h(\frac{|u|^2}{2})$ is a nodal interpolant of $\frac{|u|^2}{2}$, we obtain

$$\dot{K} = W - D_h, \tag{17.4}$$

where

$$D_h = \int_Q d_h \, dxdt, \tag{17.5}$$

modulo the additive term

$$I = |((R_\rho, \frac{|u|^2}{2} - I_h(\frac{|u|^2}{2})))|$$

which by super-approximation as in [20] can be estimated as follows,

$$I \leq C\|h^2 R_\rho(\hat{u})|\nabla u|^2\|_0,$$

where $\|\cdot\|_0$ is the $L_2(Q)$-norm and $C \sim 1$ is an interpolation constant. Assuming $|R_\rho(\hat{u})| \sim h^{-1/2}$ and $|\nabla u| \sim h^{-1/2}$, we obtain $I \sim \sqrt{h}$, indicating that I is a small perturbation, which in computation can be checked a posteriori. Finally choosing in the equation for internal energy $\bar{e} = 1$, we obtain

$$\dot{E} = -W + D_h,$$

and we thus obtain the following 2nd Law for EG2 (modulo a $\sqrt{h}$ correction)

$$\dot{K} = W - D_h, \quad \dot{E} = -W + D_h. \tag{17.6}$$

For solutions with turbulence/shocks, $D_h >> 0$ expressing a substantial irreversible transfer of kinetic energy into heat energy, just as above for regularized solutions. We note that in EG2 only the momentum equation is subject to viscous regularization, since D_h expresses a penalty on the term $u \cdot \nabla u_i$ appearing in the momentum residual. A turbulent solution is identified by $D_h \sim 1$ under mesh refinement.

17.4 The Stabilization in EG2

We have seen that the stabilization in EG2 is expressed by the dissipative term $D_h \sim 1$ which can be viewed as a weighted least squares control of the term $\rho u \cdot \nabla u_i$ in the momentum residual. The rationale is that least squares control of a part of a residual which is large, effectively may give control of the entire residual, and thus EG2 gives a least squares control of the momentum residual. But the EG2 stabilization does not correspond to an ad hoc viscosity, as in classical regularization, but to a form of penalty arising because Euler residuals of turbulent/shock solutions *cannot* be pointwise small.

In particular the dissipative mechanism of EG2 does not correspond to a shear viscosity acting in all directions, as in standard ad hoc regularization, but rather to a form of bulk viscosity in the form of *streamline diffusion* preventing fluid particles from colliding while allowing strong shear, connecting to the *streamline diffusion method* presented in [11].

Chapter 18

Output Wellposedness by Duality

In love all the contradiction of existence merge themselves and are lost. Only in love are unity and duality not at variance. Love must be one and two at the same time. Only love is motion and rest in one. (Rabindranath Tagore, Literature Nobel Prize 1913)

Those who have talked of "chance" are the inheritors of antique superstition and ignorance...whose minds have never been illuminated by a ray of scientific thought. (T. H. Huxley)

18.1 A Posteriori Error Estimation

Consider a mean-value output $M(\hat{u})$ in the form of a space-time integral

$$M(\hat{u}) = ((\hat{u}, \hat{\psi})) \tag{18.1}$$

defined by a smooth (positive) weight function $\hat{\psi}$ with $\|\psi\|_0 = 1$, where as above $\|\cdot\|_0$ is the $L_2(Q)$-norm. Let $\hat{u}$ and $\hat{w}$ be two EG2 solutions on two meshes with joint maximal meshsize h. By the mean-value theorem their residual difference can be expressed as

$$R(\hat{u}) - R(\hat{w}) = R'(\hat{u}, \hat{w}) \cdot (\hat{u} - \hat{w}),$$

where $R'(\hat{u}, \hat{w})$ is a linearization of $R(\cdot)$. Letting $\hat{\varphi}$ be the solution of the dual linearized equation

$$R'^{\top} \hat{\varphi} = \hat{\psi}, \tag{18.2}$$

where $\top$ denotes transpose, we obtain the following basic *output error representation*:

$$M(\hat{u}) - M(\hat{w}) = ((\hat{u} - \hat{w}, R'^{\top}\hat{\varphi})) = ((R(\hat{u}) - R(\hat{w}), \hat{\varphi})). \tag{18.3}$$

We can thus estimate the output error in terms of the residuals as follows:

$$|M(\hat{u}) - M(\hat{w}| \leq S(\|R(\hat{u})\|_{-1} + (\|R(\hat{w})\|_{-1}) \tag{18.4}$$

or alteratively, using also *Galerkin orthogonality* as in [20]

$$|M(\hat{u}) - M(\hat{w}| \leq S(\|hR(\hat{u})\|_0 + (\|hR(\hat{w})\|_0), \tag{18.5}$$

where

$$S = S(\hat{u}, \hat{w}) = \|\hat{\varphi}\|_1 \tag{18.6}$$

with $\|\cdot\|_1$ the $H^1(Q)$-norm.

For a given output $M(\hat{u})$, we choose an error tolerance TOL and define a G2-solution $\hat{u}$ to be *wellposed* up to the tolerance TOL, if

$$S\|hR(\hat{u})\|_0 \leq TOL/2, \tag{18.7}$$

where $S = S(\hat{u}, \hat{u})$. Given two wellposed G2 solutions $\hat{u}$ and $\hat{w}$, we may expect

$$|M(\hat{u}) - M(\hat{w}| \leq TOL, \tag{18.8}$$

up to a variation of the corresponding stability factors, which can be computed a posteriori. A solution which is not wellposed with respect to some tolerance of interest, is said to be *illposed*.

Turbulence is characterized by

$$D_h \sim \|\sqrt{h}R(\hat{u})\|_0 \sim 1 \tag{18.9}$$

under mesh refinement. We may thus expect an output $M(\hat{u})$ to be *wellposed* up to the tolerance TOL if

$$S(\hat{u}, \hat{u}) \lesssim \frac{TOL}{2\sqrt{h}}. \tag{18.10}$$

A wellposed output can be uniquely computed up to a tolerance TOL of interest, but an illposed cannot.

Computational results, some of which is presented below and more on the book web page [**?**], show that indeed $\|hR(\hat{u})\|_0 \sim \sqrt{h}$ conformiing (18.9), and that the corresponding stability factors $S(\hat{u}, \hat{u})$ for global mean-values such as drag, lift and total turbulent dissipation, can satisfy (18.10) for toleralnces TOL of interest. In short, global mean-value outputs can be wellposed, and thus represent stable computable emergent aspects of turbulent flow.

Chapter 19

Linearized Equations and Acoustics

De Broglie, the creator of wave mechanics, accepted the results of quantum mechanics just as Schrödinger did, but not the statistical interpretation. (Born in the Born-Einstein Letters)

19.1 Linearization

Consider a solution $\hat{u} = (\rho, m, e)$ of the Euler equations:

$$\begin{aligned}
\dot{\rho} + \nabla \cdot (\rho u) = \dot{\rho} + \nabla \cdot m &= 0 \quad \text{in } Q, \\
\dot{m} + \nabla \cdot (mu) + \gamma \nabla e &= f \quad \text{in } Q, \\
\dot{e} + \nabla \cdot (eu) + \gamma e \nabla \cdot u &= g \quad \text{in } Q, \\
u \cdot n &= 0 \quad \text{on } \Gamma \times I \\
\hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega,
\end{aligned} \tag{19.1}$$

where $u = \frac{m}{\rho}$. The corresponding *linearized Euler equations*, linearized at $\hat{u}$, take the following form in $\underline{\hat{u}} = (\underline{\rho}, \underline{m}, \underline{e})$ representing a perturbation of $\hat{u}$ with corresponding perturbation of data, with $\underline{u}$ defined by $\underline{m} = \underline{\rho} u + \rho \underline{u}$:

$$\begin{aligned}
\dot{\underline{\rho}} + \nabla \cdot (\underline{\rho} u) + \nabla \cdot (\rho \underline{u}) = \dot{\underline{\rho}} + \nabla \cdot \underline{m} &= 0 \quad \text{in } Q, \\
\dot{\underline{m}} + \nabla \cdot (\underline{m} u) + \nabla \cdot (m \underline{u}) + \gamma \nabla \underline{e} &= \underline{f} \quad \text{in } Q, \\
\dot{\underline{e}} + \nabla \cdot (\underline{e} u) + \nabla \cdot (e \underline{u}) + \gamma \underline{e} \nabla \cdot u + \gamma e \nabla \cdot \underline{u} &= \underline{g} \quad \text{in } Q, \\
\underline{u} \cdot n &= 0 \quad \text{on } \Gamma \times I, \\
\underline{\hat{u}}(\cdot, 0) &= \underline{\hat{u}}^0 \quad \text{in } \Omega,
\end{aligned} \tag{19.2}$$

or alternatively with $Dw = \dot{w} + u \cdot \nabla w$ the u-convective derivative:

$$\begin{aligned} D\underline{\rho} + \underline{\rho}\nabla \cdot u + \nabla \cdot (\rho\underline{u}) &= 0 \quad \text{in } Q, \\ D\underline{m} + \underline{m}\nabla \cdot u + \nabla \cdot (m\underline{u}) + \gamma\nabla\underline{e} &= \underline{f} \quad \text{in } Q, \\ D\underline{e} + \underline{u} \cdot \nabla e + (\gamma+1)\underline{e}\nabla \cdot u + (\gamma+1)e\nabla \cdot \underline{u} &= \underline{g} \quad \text{in } Q, \\ \underline{u} \cdot n &= 0 \quad \text{on } \Gamma \times I \\ \underline{\hat{u}}(\cdot, 0) &= \underline{\hat{u}}^0 \quad \text{in } \Omega. \end{aligned} \tag{19.3}$$

This is a linear convection-reaction system with coefficients depending on the base flow $\hat{u}$ and the stability properties of this system govern the perturbation growth.

19.2 Wave Equation

Let $\hat{u}$ be a constant ground state with velocity $u = 0$ and temperature $\tau = 1$. If τ is not subject to perturbation, so that $\underline{e} = \underline{\rho}$, then (19.2) reduces to (leaving out initial and boundary conditions):

$$\begin{aligned} \dot{\underline{\rho}} + \nabla \cdot \underline{m} &= 0 \quad \text{in } Q, \\ \dot{\underline{m}} + \gamma\nabla\underline{\rho} &= \underline{f} \quad \text{in } Q, \end{aligned} \tag{19.4}$$

which leads to the *wave equation* for the density perturbation, assuming $\nabla \cdot \underline{f} = 0$:

$$\ddot{\underline{\rho}} - \gamma\Delta\underline{\rho} = 0 \quad \text{in } Q. \tag{19.5}$$

Small density-pressure variations at constant temperature around a constant ground state thus obeys the linear wave equation with wave speed $c = \sqrt{\gamma}$.

Allowing a non-zero velocity of the ground state, but still constant unit temperaure, the linearized equations reduce to (assuming $\underline{e} = 0$):

$$\begin{aligned} \dot{\underline{\rho}} + \nabla \cdot \underline{m} &= 0 \quad \text{in } Q, \\ \dot{\underline{m}} + 2\nabla \cdot (\underline{m}u) - \nabla \cdot (\underline{\rho}uu) + \gamma\nabla\underline{\rho} &= \underline{f} \quad \text{in } Q, \end{aligned} \tag{19.6}$$

which is a generalized wave equation with contributions from convection with velocity u.

19.3 Acoustics

Acoustics concerns propagation of (usually small) density-pressure variations in a fluid. Acoustics simulation can be based on (i) directly solving the Euler equations for the full state (ground state plus perturbation), or (ii) solving the Euler equations for the ground state followed by solution of the linearized Euler equations for the perturbation with the ground state given. We just saw that the simplest model for acoustics is the wave equation (19.5) as a basic case of (b). In general, (ii) may be expected to give higher accuracy at the expense of solving both the Euler and linearized Euler equations.

The wave equation can be used for progagation of sound waves in in a fluid at rest, but for the generation of sound in e.g. human speech or musical instruments, fluid-structure interaction is used, which requires the Euler equations for the (usually turbulent) flow and an elasticity model for the structure (e.g, vocal chords).

19.4 Linearized Stability

The nature of the linearized system (19.2) depends on the ground state and ranges from its simplest incarnation in the form of the wave equation (19.5) for a constant ground state, to a highly complex problem for a turbulent ground state. Below we analyze the linearized problem for a shocks and rarefaction waves in a model case, and in [20] we discuss the case of turbulent incompressible flow. For now, we only observe that the equation for $\underline{\rho}$ contains the term $\underline{\rho}\nabla \cdot u$, and the same for $\underline{m}$ and $\underline{e}$, which indicates exponential perturbation growth along particle paths under compression with $\nabla \cdot u < 0$, which occurs when a compression shock is forming.

Chapter 20

Dual Linearized Problem

> Those who do not understand the nature of sin and virtue are attached to duality; they wander around deluded. (Sri Guru Granth Sahib)

Formally multiplying the linearized equation (19.2) by the dual variable $\hat{\varphi} = (\rho_d, \varphi, e_d)$ and integrating by parts and varying $\underline{\hat{u}}$, we obtain the following dual problem

$$\begin{array}{rcl} -\dot{\rho}_d + \sum_j u \cdot \nabla\varphi_j u_j + \frac{e}{\rho} u \cdot \nabla e_d + \frac{\gamma}{\rho} u \cdot \nabla(e e_d) &=& \psi_\rho, \\ -\dot{\varphi} - u \cdot \nabla\varphi - \sum_i u_i \nabla\varphi_i - \nabla\rho_d - \frac{e}{\rho}\nabla e_d - \frac{\gamma}{\rho}\nabla(e e_d) &=& \psi, \\ -\dot{e}_d - u \cdot \nabla e_d + \gamma\nabla \cdot u e_d - \gamma\nabla\cdot\varphi &=& \psi_e, \end{array} \tag{20.1}$$

where the data $\hat{\psi} = (\psi_\rho, \psi, \psi_e)$ defines the output. We check by writing the Euler equations alternatively in the variables $\hat{u} = (\rho, u, e)$:

$$\begin{array}{rcl} \dot{\rho} + \nabla\cdot(\rho u) &=& 0, \\ \dot{\rho} u + \rho\dot{u} + \nabla\cdot(\rho u u) + \gamma\nabla e &=& f, \\ \dot{e} + \nabla\cdot(e u) + \gamma e \nabla\cdot u &=& g, \end{array} \tag{20.2}$$

with corresponding dual linearized problem in $\hat{\varphi} = (\rho_d, \varphi, e_d)$:

$$\begin{array}{rcl} -\dot{\rho}_d - u\cdot\nabla\rho_d - u\cdot\dot{\varphi} - \sum_i u_i u\cdot\nabla\varphi_i &=& \psi_\rho, \\ -\rho\dot{\varphi} - \rho u\cdot\nabla\varphi - \rho\nabla\rho_d - e\nabla e_d - \gamma\nabla(e e_d) - \rho\sum_i u_i\nabla\varphi_i &=& \psi, \\ -\dot{e}_d - u\cdot\nabla e_d + \gamma\nabla\cdot u e_d - \gamma\nabla\cdot\varphi &=& \psi_e, \end{array}$$

which by eliminating $\dot{\varphi}$ from the first equation using the second gives

$$\begin{array}{rcl} -\dot{\rho}_d + \sum_j u \cdot \nabla\varphi_j u_j + \frac{e}{\rho} u \cdot \nabla e_d + \frac{\gamma}{\rho} u \cdot \nabla(e e_d) &=& \psi_\rho, \\ -\dot{\varphi} - u \cdot \nabla\varphi - \sum_i u_i \nabla\varphi_i - \nabla\rho_d - \frac{e}{\rho}\nabla e_d - \frac{\gamma}{\rho}\nabla(e e_d) &=& \psi, \\ -\dot{e}_d - u \cdot \nabla e_d + \gamma\nabla \cdot u e_d - \gamma\nabla\cdot\varphi &=& \psi_e, \end{array}$$

which is the same as (20.1) with a properly modified right hand side.

The dual problem (20.1) is solved backward in time on $[0, T]$ with e.g. $\hat{\varphi}(\cdot, T) = 0$, for simplicity with stabilization by artificial diffusion of size h in each equation instead of least squares stabilization. The crucial stability factor is defined by $S = \|\varphi\|_{H^1(Q)}/\|\psi\|_{L_2(Q)}$, which bounds the error in the output $(\hat{u}, \psi)_Q$ by $S\|hR(\hat{u})\|_{L_2(Q)}$.

Chapter 21

EG2 as a Model of Physics

Die Welt ist alles, was der Fall ist. (Wittgenstein)

21.1 A Dissipative Mechanism

We propose to view EG2 as a real model of thermodynamics with output, as compared to the Euler equations, which represent a formal model without output. We have seen that the least squares stabilization introduces a specific form of viscosity and that an EG2 solution $\hat{u}$ has Euler momentum residual $R_m(\hat{u})$ typically satisfying

$$\|R_m(\hat{u})\|_{-1} \sim \sqrt{h}, \quad \|R_m(\hat{u})\|_0 \sim \frac{1}{\sqrt{h}}. \tag{21.1}$$

Roughly speaking this means that local mean-values of the Euler momentum residual $R_m(\hat{u})$ are small, and that point-values not too large. Momentum balance is thus (heavily) violated locally and then penalized by a viscous dissipative mechanism consuming kinetic energy, while momentum balance is satisfied in a local mean value sense. Turbulence creates violent kinetics violating momentum balance locally, and is countered by a dissipative mechanism on kinetic energy curbing the violation. EG2 flow thus is out of momentum balance in a pointwise sense but in balance in a mean-value sense. It is thus possible to interprete EG2 in physical terms as a dissipative mechanism compensating local imbalance of momentum.

The reason EG2 cannot satisfy pointwise momentum balance is that the Euler equations lack pointwise solutions. Facing the impossibility of pointwise solution, EG2 reacts by producing an approximate solution in which some of the kinetic energy by turbulent/shock dissipation. The total dissipation shows to be a stable output under vanishing mesh size and occurs mainly on the finest scale of the mesh. The turbulent/shock dissipation thus is "smart" and does not act on coarser scales.

The key here is to realize that the dissipative stabilization is (i) necessary, (ii) substantial, (iii) irreversible, (iii) not a numerical artifact which can be diminished by increasing the precision. The key new fact behind (i)-(iv) is the non-existence of pointwise solutions to the Euler equations. Note that (iii) reflects the well-known difficulty of getting a refund of a fine which has been paid.

21.2 From Exact to Computational Solutions

The nonexistence of (stable) pointwise solutions to the Euler equations upsets classical mathematics: With nonexistent exact solutions, the attention has to move to existing approximate solutions, and thus the computational aspect takes the lead before analytical mathematics. This suggests an entire shift of paradigm, which we can now only vaguely imagine.

The non-existence of pointwise solutions to the Euler equations, which may be viewed as a failure of mathematics, in fact may be turned around into an advantage from a computational point of view: If there were an exact solution, one could always ask for more precision in computing this solution requiring finer resolution and higher computational cost, but if there is no exact solution, then we could be relieved from this demand beyond a certain point. A key feature in this situation is that the absolute size of the fine scales no longer are important, and this could save computational work. In turbulence this means that mean value outputs may be computed on meshes which do not resolve the turbulent vortices to their actual physical scale.

In order for a Hamiltonian system to develop turbulence, it has to be rich enough in degrees of freedom. In particular, the incompressible or compressible Euler equations in less than three space dimensions are not rich enough, even if the mesh is very fine. On the other hand, turbulence invariably develops in three dimensions once the mesh is fine enough. Our experience with turbulent solutions of the incompresible Navier-Stokes equations indicates that a mesh with 100.000 mesh points in space may suffice in simple geometries, while in more complex geometries millions, but not billions, of mesh points may be needed.

21.3 Imperfect Nature and Mathematics?

How shall be interprete that the Euler equations do not have pointwise solutions? Does this express an imperfection of both mathematics and physics? We can make a parallel with the squareroot of two $\sqrt{2}$, which is the length of the diagonal in a square with side length 1. We know that the Pythagoreans discovered that $\sqrt{2}$ is not a rational number. This knowledge had to be kept secret, since it indicated an imperfection in the creation by God formed as relations between natural numbers according the basic belief of the Pythagoreans. Eventually this unsolvable conflict ruined their philosophical school and gave room for the Euclidean school based on geometry instead of natural numbers. Civilization did not recover until Descartes resurrected numbers and gave geometry an algebraic form, which opened for Calculus and the scientific revolution.

But how is the Pythagorean paradox of non-existence of $\sqrt{2}$ as a rational number handled today? Well, we know that the accepted mathematical solution since Cantor and Dedekind is to extend the rational numbers to the real numbers, some of which like $\sqrt{2}$ are called irrational, and which can only be described approximately using rational numbers. We may say that this solution in fact is a kind of non-solution, since it acknowledges the fact that the equation $x^2 = 2$ cannot be solved exacly using rational numbers, and since the existence of irrational numbers (as infinite decimal expansions or Cauchy sequences of rational numbers) has a different nature than the existence of natural numbers or rational numbers. The non-existence is thus handled by expanding the solution concept until existence can be assured.

We handle the non-existence of pointwise solutions to the Euler equations similarly, that is, by extending the solution concept to approximate solution in a weak sense combined with some control of pointwise residuals. Doing so we necessarily introduce a dissipation causing irreversibility. In this case, the non-existence of solutions thus has a cost: irreversibility. In the perfect World, pointwise solutions would exist, but this World cannot be constructed neither mathematically nor physically, and in a constructible World necessarily there will exist irreversible phenomena as a consequence of the non-existence of pointwise solutions. The non-existence of pointwise solution reflects the development of complex solutions with small scales, and thus the non-existence also relects a complexity of the constructible World. The perfect World would lack this complexity, so in addition to being non-existent it would also probably be pretty non-interesting. The World we live in thus does not seem to be perfect, but it surely is complex and interesting.

An imperfect World of mathematics and physics, where equations cannot be solved exactly or laws of physics cannot be exactly satisfied, is unthinkable to the classical mathematician and physicist, but nevertheless seems "to be the case" in Wittengenstein's words. The perfect World "is not the case" and thus can be only marginal of interest.

The contradiction of a non-existing perfect World, and an existing imperfect World, has been met by statistical mechanics and quantum mechanics based on microscopical games of Roulette. We propose to resolve the contradiction instead by finite precision computation, because it is simpler and more useful.

21.4 Idealism and Materialism

From philosophical point of view, we may say that the traditional paradigm of both mathematics and physics is Platonistic in the sense that it assumes the existence of an Ideal World, where equations/laws are satisfied exactly. We may say that this is an Ideal World of infinities because exact satisfaction of e.g. the equation $x^2 = 2$ requires infinitely many decimals. This is the mathematical Ideal World of Cantor, which represents a formalist/logicist school. In strong opposition to this school of infinities, is Brouwer's constructivist school, which only deals with mathematicial objects that can be constructed or computed in a finite number of steps. In the constructivists Constructible World, the set of natural numbers does not exist as a completed mathematical object as in Cantors Ideal World, but only as a never-ending project where always a next natural number can be constructed if needed, which follows the suggestions of e.g. Aristotle and Gauss. The Constructible World is finitary and thus inherently computational, while Cantors Ideal World is non-finitary and non-computational.

Figure 21.1: Cantor and Brouwer.

Chapter 22

Thermodynamics of Reactive Flow

> To every action there is always opposed an equal reaction: or, the mutual actions of two bodies upon each other are always equal, and directed to contrary parts. (Newton's 3rd Law)

> President Bush gave his first-ever presidential radio address in both English and Spanish. Reaction was mixed, however, as people were trying to figure out which one was which. (Dennis Miller)

22.1 Reactive Euler Equations

We now generalize the Euler equations (12.1) to a *mixture* of N gas species, undergoing M chemical reactions: We seek the *species densities* $\rho_1, ..., \rho_N$, the *mixture momentum* $m = \rho u$ with $u = (u_1, u_2, u_3)$ the *mixture velocity* and $\rho = \sum_i \rho_i$ the *mixture density*, and the *mixture internal energy* e satisfying

$$\begin{array}{rcll} \dot{\rho}_i + \nabla \cdot (\rho_i u) & = & s_i, & \text{in } Q, \quad i = 1, ..., N, \\ \dot{m} + \nabla \cdot (mu) + \nabla p & = & f & \text{in } Q, \\ \dot{e} + \nabla \cdot (eu) + p \nabla \cdot u & = & \sum_i s_i r_i & \text{in } Q, \\ u \cdot n & = & 0 & \text{on } \Gamma \times I, \\ \hat{u}(\cdot, 0) & = & \hat{u}^0 & \text{in } \Omega, \end{array} \tag{22.1}$$

where s_i is the net reaction rate of species i from all the reactions, and we assume the following constitutive relations

$$e = \sum_{i=1}^{N} \rho_i r_i + \rho\tau$$

with τ the *mixture temperature* and r_i the *heat of formation* of species i, together with a *mixture pressure* p given as the sum of the partial pressures from the different species:

$$p = C\tau \sum_i \frac{\rho_i}{W_i}.$$

where W_i is the molecular weight of species i and C a positive constant. Evidently, we assume here that the species velocities are all equal to the mixture velocity and that all species take on the mixture temperature.

22.2 Reaction Rates

We assume that the reaction rate s_i of species i is given by an *Arrhenius law* of the form

$$s_i = W_i \sum_{k=1}^{M} (\nu''_{i,k} - \nu'_{i,k}) B_k T^{\alpha_k} e^{-\frac{E_{\alpha,k}}{RT}} \prod_{j=1}^{N} (\frac{X_j p}{RT})^{\nu'_{j,k}},$$

where the ν are stochiometric coefficients, R is the gas cosntant, the B_k are reaction constants, $E_{\alpha,k}$ is an activation energy, and

$$X_i = \frac{\frac{\rho_i}{\rho W_i}}{\sum_j \frac{\rho_j}{\rho W_j}}$$

is the mole fraction of species i.

22.3 The 2nd Law for Reactive Euler

The new 2nd Law takes the form:

$$\dot{K} = W - D, \tag{22.2}$$

$$\dot{E} = -W + D + \sum_i s_i r_i, \tag{22.3}$$

where $D \geq 0$ is the turbulent dissipation, and

$$k = \frac{\rho |u|^2}{2}, \quad K = \int_\Omega k\, dx, \quad E = \int_\Omega e\, dx, \quad W = \int_\Omega p\nabla \cdot u\, dx.$$

The 2nd Law shows irreversibility of turbulent mixing and heating, while the chemical reactions as such, are reversible.

22.4 Simulation of Combustion

Chapter 23

Loschmidt's and Gibbs' Paradoxes

> How wonderful that we have met with a paradox. Now we have some hope of making progress.
> (Nils Bohr)

> There is apparently a contradiction between the law of increasing entropy and the principles of Newtonian mechanics, since the latter do not recognize any difference between past and future times. This is the so-called reversibility paradox (Umkehreinwand) which was advanced as an objection to Boltzmann's theory by Loschmidt 1876-77. (Translators foreword to Lectures on Gas Theory by Boltzmann).

> Neither Herr Boltzmann nor Herr Planck has given a definition of W... Usually W is put equal to the number of complexions. In order to calculate W, one needs a *complete* (molecular-mechanical) theory of the system under consideration. Therefore it is dubious whether the Boltzmann principle has any meaning without a *complete* molecular-mechanical theory or some other theory which describes the elementary processes (and such a theory is missing). (Einstein)

23.1 Scientific Paradoxes

We now present new resolutions of *Loschmidt's paradox* on irreversibility in reversible Hamiltonian systems and *Gibbs' paradox* on inextensivity of

Boltzmann's entropy. We first give some give some general comments on the role of paradoxes in science.

The above citation by the physicist Nils Bohr illustrates the role of a *paradox* in the development of a physical theory, as a striking formulation of a contradiction within the theory, or between a prediction of the theory and a factual observation. Scientific progress can be made by showing that the contradiction is only *apparent*, thus improving the understanding of the meaning of a theory remaining correct, or that the contradiction is *real*, thus showing that the theory is not correct and thereby opening for a new better theory to be developed. A theory predicting that an apple let free to fall, will stay where it is, will be contradicted by Newton's observation that the apple falls to the ground, and thus will have to be abandoned.

The first known paradoxes were formulated by Zeno of Elea (490-430 BC) on the (still) puzzling nature of motion: Zeno asked e.g. how it can be that a flying arrow, which at each instant looks just the same as a motionless arrow, can be moving? Modern physics harbors many unresolved paradoxes including the wave-particle duality of quantum mechanics and time dilation of special relativity.

Since an unresolved paradox is a deadly threat to a theory, it has to be resolved by showing that the contradiction is only apparent and not real, "at any price, no matter how high that might be..." from the above citation of the famous physicist Max Planck facing in 1900 the paradox of the ultra-violet catastrophy in the classical theory of black-body radiation.

If a paradox cannot be resolved by showing that the contradiction is only apparent and not real, it can be *covered up* by presenting new information. When asked where the tortoises can be seen, which according to a certain (ancient) theory support the Earth, the cover up would be to claim that they are invisible (but still there).

In Loschmidt's paradox formulated in 1876 [33], mathematics of Hamiltonian systems (with zero viscosity) predicts that time reversal and a perpetuum mobile is possible. But everybody (except possibly a physics specialist) knows that time is always moving forward and that a perpetuum mobile is impossible, even though ultimately the World is based on Hamiltonian (quantum) mechanics.

In Gibbs' paradox formulated in 1875, statistical mechanics predicts that removing a membrane separating two volumes of equal gases at rest in the same state (same density, temperature and pressure), will result in a significant increase of entropy. But everybody (except a statistical mechanics specialist) understands that removing (or inserting) a membrane in such a situation changes nothing.

23.2 Cover Up

The cover up of Loschmidt's paradox by Boltzmann [4] is to introduce statistical mechanics based on microscopic games of roulette. Statistical mechanics poses difficulties of *falsification* required by Popper in a scientific theory, since the validity of Boltzmann's basic microscopic assumption of statistical independence in a gas with each mole consisting of $6 \cdot 10^{23}$ molecules, seems to be beyond the possibility of any kind of conceivable experiment or mathematics; only indirect evidence in the form of macroscopic observations seem to be possible, which is far from enough. In fact, it is known that Boltzmann's assumption can only be (nearly) true in the very special case of a very dilute gas with rare collisions, and the derivation of Boltzmann equations for more general situations seems to pose unsurmountable problems.

The cover up of Gibbs' paradox by Gibbs' himself [**?**], is to change the counting of microstates underlying Boltzmann's definition of entropy in statistical mechanics, to give no change of entropy for equal gases, but retaining a substantial entropy change as soon as the two gases differ slightly. We will below argue that such a discontinuous change is not scientifically convincing, and present a different resolution based on computational turbulence avoiding tricky statistics.

23.3 Resolution of Loschmidt's Paradox

We have seen that the Euler equations are formally reversible but in reality are irreversible, because pointwise solutions to the Euler equations are non-existing. The irreversiblity arises because pointwise conservation of momentum is impossible to achieve, while the flow cannot cease to exist. The only way out is to violate momentum balance and pay a penalty in the form of turbulent dissipation with an irreversible transfer from kinetic to heat energy.

In other words, pointwsie solutions of the Euler equations would have been reversible had they only existed, but they do not exist, and the weak dissipative solutions which do exist are irreversible and thus define an Arrow of time.

More generally, Hamiltonian systems sufficiently complex to allow turbulence, have an Arrow of time defined without any reference to a concepts of entropy and statistical mechanics.

23.4 Gibbs' Paradox

On Boltzmann's tombstone the famous formula

$$S = k\log(W) \tag{23.1}$$

is engraved, where k is Boltzmann's constant ($k \approx 10^{-23}$ joules/kelvin) and W denotes the probability of a certain state representing the number of "complexions" or "microstates" corresponding to a "macrostate". Increasing entropy would then reflect that Nature would tend to move from less probable to more probable states or towards states with more complexions. However, the crucial questions *why* and *how* Nature would seek to always increase entropy, was left without any answer.

The definition $S = k\log(W)$ is different from the classical expression $S = S = \log\tau\rho^{-\gamma} = \log(\tau V^\gamma)$ derived above, which illustrates some of confusion surrounding the classical concept of entropy in classical thermodynamics.

Boltzmann's statistical mechanics poses serious difficulties from scientific point of view and paradoxes line up. One of them is *Gibbs' paradox* [?] illustrating the difficulty of defining entropy by counting micro-states: Consider a volume V divided by a membrane into two equal volumes $V/2$ filled with two different types of gas at rest with the same density and temperature. Remove the membrane and let both gases expand to the double volume and come to rest in a mixed state. Gibbs recalls that according to Boltzmann the entropy of each gas would then increase by the factor $\gamma(\log(V)-\log(V/2)) = \gamma\log(2)$, since for constant temperature $S = \gamma\log(V)$ with V the volume of the gas. The entropy of the system would then also increase by a $\gamma\log(2)$ factor.

Gibbs then compares with the case with the gases being of the same type in which case removal of a membrane would change nothing and in particular the entropy should not change, in contrast to the above case. In other words, the entropy should be *extensive* in the sense that the entropy of a gas over a volume V should be equal to the sum of the entropies over two volumes $V/2$. To achieve this, Gibbs suggested to change the counting of microstates in the case of equal gases, taking into account permutations of equal molecules, but was then faced with a paradoxical discontinuos behavior of the entropy: No change for the same type of gas, and a log(2) change as soon as the types of gas differ only the slightest.

23.5 New Resolution of Gibbs'Paradox

With our experience from the Joule-Thomson experiment, we can easily resolve this paradox. It suffices to note that an initial pressure difference resulting from different state equations for two types of gas in the two volumes, would drive a process towards equal pressure in the full volume, with the associated turbulent dissipation (entropy production) being small if the initial pressure difference is small, that is, if the type of gas is nearly the same. In particular, for equal gases nothing would happen and there would be no sudden entropy jump under a slight change of gas, as in Gibbs' resolution by recounting microstates.

We understand that the Gibbs'paradox results from Boltzmann's idea to define entropy by counting microstates, and thus is (one of many) indications that statistical mechanics creates more problems than it solves, and from scientific point of view therefore is questionable.

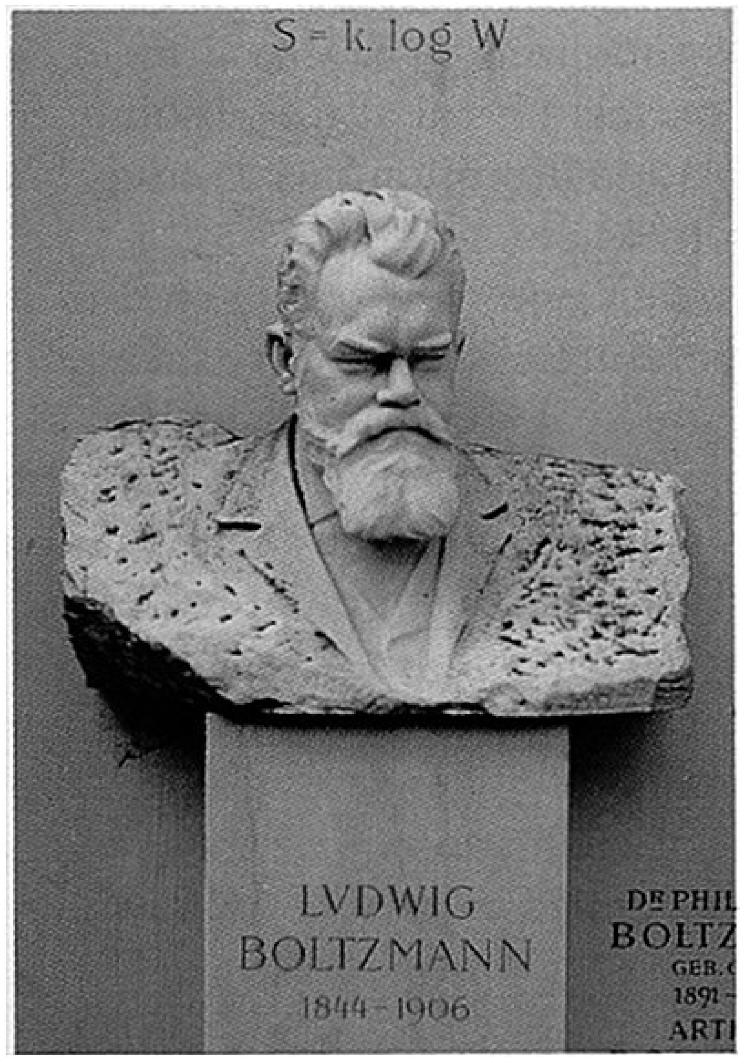

Figure 23.1: Boltzmann's tombstone with $S = k\log(W)$.

Part V

Model Analysis

Chapter 24

Burgers Equation

> Some physicists. among them myself, cannot believe that we must abandon, actually and forever, the idea of direct representation of physical reality in space and time; or that we must accept then the view that events in nature are analogous to a game of chance. (Einstein 1954)

24.1 A Model of the Euler Equations

As an instructive model of the Euler equations exhibiting basic aspects of *shock waves* and *rarefaction waves*, we consider the following *scalar conservation law*, referred to as *Burgers equation*: Find the scalar function $u = u(x, t)$ such that

$$\begin{aligned} \dot{u} + (f(u))' &= 0 \quad \text{in } Q, \\ u(\cdot, 0) &= u^0, \end{aligned} \tag{24.1}$$

where $f(u) = u^2/2$, $Q \equiv \mathbb{R} \times I$ with $I = (0, T]$, and we assume that the initial data $u^0(x)$ vanishes for large $|x|$.

Burgers equation takes the pointwise form $\dot{u} + uu' = 0$ for a differentiable pointwise solution u, which expresses that $u(x, t)$ is constant with values $u^0(\bar{x})$ along straight lines $x = st + \bar{x}$ with slope $s = u^0(\bar{x})$), that is, along *characteristics* defined by $\frac{dx}{dt} = u(x, t)$ with $x(0) = \bar{x}$.

If $u^0(x)$ is increasing with increasing x and is smooth, then there is a pointwise solution $u(t, x)$ for all time given by the simple recipe

$$u(x, t) = u^0(\bar{x}) \quad \text{for } x = u^0(\bar{x})t + \bar{x}. \tag{24.2}$$

However, if the initial data $u^0(x)$ somewhere is strictly decreasing, which of course will always be the case if $u^0(x)$ vanishes for large $|x|$, then characteristics will cross in finite time with different values and the solution formula gives conflicting function values, which can be interpreted as *breakdown* of the pointwise solution. The result is that there is no differentiable function $u(x,t)$ satisfying Burger's equation $\dot{u} + uu' = 0$ pointwise. We shall see that this corresponds to the occurence of *shocks*, which are represented by *discontinuous* functions, which satisfy the differential equation in a weak sense, and in a pointwise sense only away from discontinuities or jumps.

What to do with an equation without pointwise solution? Of course, we regularize and consider instead the *viscous/regularized Burgers equation*:

$$\begin{aligned} \dot{u} + uu' - \nu u'' &= 0 \quad \text{in } Q, \\ u(\cdot, 0) &= u^0, \end{aligned} \tag{24.3}$$

with $\nu > 0$ a small viscosity. This problem can be solved uniquely in a pointwise sense for all initial data, and as above the solution can be viewed as an approximate weak solution to the original inviscid Burgers equation satisfying a 2nd Law of the form

$$\dot{K}(u;t) = -D_\nu(u;t) \quad \text{for } t \in I, \tag{24.4}$$

where

$$K(u;t) = \int_{\mathbb{R}} \frac{u(x,t)^2}{2}\, dx, \quad D_\nu(u;t) = \int_{\mathbb{R}} \nu (u'(x,t))^2\, dx. \tag{24.5}$$

The 2nd Law follows by multiplication of the viscous Burgers' equation by u and integration (by parts) with respect to x.

To give a perspective we now briefly recall the basics of the mathematical theory for conservation laws developed in the 1950s motivated by the Euler equations of compressible flow, in the model setting of Burgers equation. The basic idea is to introduce the concept of *weak solution* allowing discontinuous solutions, and complement by a 2nd Law. We shall see that the 2nd Law singles out *physical shocks*, which are discontinuous weak solutions satisfying the 2nd Law, from *non-physical shocks* which are discontinuous weak solutions violating the 2nd Law.

We also present an alternative approach to single out physical shocks based on a stability analysis showing that a a physical shock is stable and represents a an observable physical phenomenon (like the "bang" from a supersonic airplane), while a non-physical shock is unstable and thus does not represent any observable physical phenomenon.

Burgers equation is formally reversible: If $u(x,t)$ is a pointwise solution in forward time on $[0,T]$, so is $-u(x,T-t)$ in reverse time. Burgers equation thus is formally reversible system, but in reality is irreversible, as a consequence of the non-existence of stable pointwise solutions. We thus use Burgers equation to illustrate that a World governed by the formally reversible Euler equations, is an irreversible World, that is a world with an Arrow of time.

24.2 Weak Solutions

A possibly discontinuous function $u(x,t)$ is said to be a *weak solution to Burgers' equation* if

$$\int_{\mathbb{R}\times\mathbb{R}_+}(-u\dot{\varphi} - f(u)\varphi')dx\,dt - \int_{\mathbb{R}} u^0(x)\varphi(x,0)\,dx = 0 \qquad (24.6)$$

for all differentiable test functions φ such that $\varphi(x,t)$ vanishes for large (x,t), assuming here $I=(0,\infty)$. This equation is obtained from (24.1) by multiplication by φ and integration by parts, shifting the derivatives onto φ, thus allowing u to be discontinuous.

24.3 The Rankine-Huginiot Condition

A discontinuous function $u(x,t)$ defined by $u(x,t) = u_+$ if $x > st$ and $u(x,t) = u_-$ if $x < st$, where u_+ and u_- are two constant states and s is a constant, corresponding to a discontinuity propagating with speed s, is a weak solution to Burgers' equation if the shock speed satisfies the *Rankine-Hugoniot condition*

$$s = \frac{[f(u)]}{[u]}, \qquad (24.7)$$

where $[u] = u_+ - u_-$ and $[f(u)] = f(u_+) - f(u_-)$. With $f(u) = u^2/2$ as in Burgers' equation, we have

$$s = (u_+ + u_-)/2. \qquad (24.8)$$

The Rankine-Hugoniot condition expresses the conservation law (Burgers' equation) in weak form for a piecewise constant discontinuous solution candidate u.

24.4 Rarefaction wave

The solution to Burgers equation with the *increasing* discontinuous initial data $u^0(x) = 0$ for $x < 0$, and $u^0(x) = 1$ for $x > 0$, is a *rarefaction wave* given by

$$\begin{aligned} u(x,t) &= 0 \quad \text{for} \quad x < 0, \\ u(x,t) &= \tfrac{x}{t} \quad \text{for} \quad 0 \le \tfrac{x}{t} \le 1, \\ u(x,t) &= 1 \quad \text{for} \quad 1 < \tfrac{x}{t}. \end{aligned} \tag{24.9}$$

This is a continuous function for $t > 0$ which satisfies (24.1) pointwise for $t > 0$ off the lines $x = 0$ and $x = t$ and can be viewed as a pointwise solution (since it is continuous and piecewise differentiable). In a rarefaction wave, an initial discontinuity separating two constant states develops into a continuous linear transition from one state to the other of width t in space, corresponding to "fan-like" level curves in space-time as shown in Fig. 24.1.

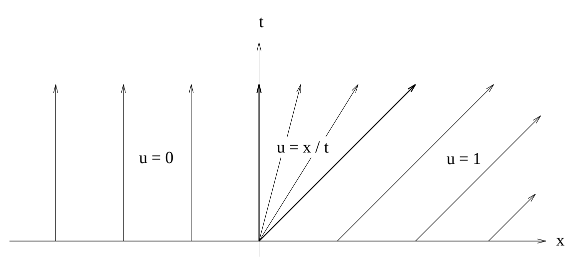

Figure 24.1: Characteristics of a rarefaction wave.

24.5 Shock

The solution with decreasing discontinuous initial data $u^0(x) = 1$ for $x < 0$, and $u^0(x) = 0$ for $x > 0$, is a discontinuous *shock wave* moving with speed $\frac{1}{2}$:

$$\begin{aligned} u(x,t) &= 1 \quad \text{for} \quad x < \tfrac{t}{2}, \\ u(x,t) &= 0 \quad \text{for} \quad x > \tfrac{t}{2}, \end{aligned} \tag{24.10}$$

as shown in Fig 24.2. We shall motivate that this is a *physical shock* satifying a 2nd Law.

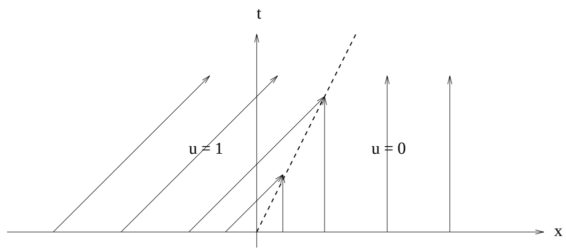

Figure 24.2: Characteristics of a shock

24.6 Weak solutions may be non-unique

The rarefaction wave initial data $u^0(x) = 0$ for $x < 0$ and $u^0(x) = 1$ for $x > 0$, also admits the alternative discontinuous weak solution

$$\begin{aligned} u(x,t) &= 0 \quad \text{for} \quad x < \tfrac{t}{2}, \\ u(x,t) &= 1 \quad \text{for} \quad x > \tfrac{t}{2}, \end{aligned} \tag{24.11}$$

corresponding to a discontinuity $\{x,t) : x = st\}$ moving with speed $s = \frac{1}{2}$. This solution is obviously different from the rarefaction wave solution (24.9), which since it is a pointwise solution, also is a weak solution. Thus, we have in this case two different weak solutions, and thus we have an example of *non-uniqueness of weak solutions.* We shall see that the discontinuos solution (24.11) violates the 2nd Law and thus is a *non-physical shock solution.* The physical solution in this case is the rarefaction wave (which satisfies the 2nd Law with equality).

24.7 The 2nd Law for Burgers Equation

We now check if (24.11) satisfies the appropriate form of the 2nd Law (24.4) restricting space to $-1 \leq x \leq 1$ and time to $0 \leq t \leq 1$ assuming the boundary conditions $u(-1,t) = 0$ and $u(1,t) = 1$. In this setting, we obtain by multiplication of the viscous Burgers equation with u and integrating by parts and using the sign of the viscous term, the following form of the 2nd Law

$$-D_\nu(u;t) = \dot{K}(u;t) + \int_{-1}^{1} (\frac{u^3}{3})' = \dot{K}(u;t) + \frac{1}{3} \tag{24.12}$$

But for (24.11) we have $\dot{K} = -\frac{1}{2}\frac{d}{dt}\frac{t}{2} = -\frac{1}{4}$, which violates (24.12).

Changing to the boundary conditions to $u(-1,t) = 1$ and $u(1,t) = 0$, the 2nd Law changes to

$$-D_\nu(u;t) = \dot{K}(u;t) + \int_{-1}^{1} (\frac{u^3}{3})' = \dot{K}(u,t) - \frac{1}{3}, \tag{24.13}$$

which is satisfied by (24.10) since now $\dot{K} = \frac{1}{2}\frac{d}{dt}\frac{t}{2} = \frac{1}{4} < \frac{1}{3}$.

We conclude that a discontinuous function $u(x,t)$ with the constant states u_- for $x < st$ and u_+ for $x > st$ corresponds to a physical shock solution with shock speed $(u_- + u_+)/2$ if $u_- > u_+$, and to a non-physical shock if $u_- < u_+$.

We furher see that a shock dissipates substantial kinetic energy into heat since for a viscous profile of width ν joining two states u_- and u_+

$$D_\nu(u;t) \equiv \int_{\mathbb{R}} \nu(u')^2\, dx \approx (u_- - u_+)^2 \tag{24.14}$$

for small ν.

24.8 Burning Books

The 2nd Law states that the characteristics of a physical shock “converge into” the shock, corresponding to $u_- > u_+$. For the unphysical shock solutin corresponding to the rarefaction initial data with $u_- < u_+$, the characteristics appear to “emerge from” the discontinuity. The 2nd Law thus allows information (features of the solution) to be “destroyed” (in a shock with converging characteristics), but not “created out of nothing” (in an unphysical rarefaction with diverging characteristics). This connects to the essence of irreversibility: Burning books can readily be done without any sophistication, while recovering the original text from the ashes is impossible.

24.9 Stability of a Rarefaction Wave

We shall now see that the 2nd Law can be replaced by a stability analysis in its main mission to distingush physical shocks from unphysical shocks. This reflects the fact that a stable process can be physically realized and observed, while an unstable process will have no permanence and thus will be very difficult (or impossible) to realize.

The stability of a solution $u(x,t)$ is governed by the linearized equation

$$\dot{w} + (uw)' = 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_+ \tag{24.15}$$

where w represents a (small) perturbation (tending to zero for $|x|$ tending to infinity), and the solution u acts as a given coefficient. The growth properties of the solution w of the linearized equation determines the stability: If w grows quickly in time, then the solution u is unstable, and if w stays bounded, then u is stable. Of course, stability connects to finite precision: the level of the perturbation represents the precision.

We first consider the case of a rarefaction wave given by (24.9). Multiplying by w and integrating in space, we obtain by a simple computation using the fact that $u'(x,t) = 1/t$ for $0 \leq x \leq t$ and $u'(x,t) = 0$ else,

$$\frac{d}{dt}\int_{\mathbb{R}} w^2(x,t)\,dx + \int_0^t w^2(x,t)\frac{1}{t}\,dx = 0, \quad \text{for } t > 0,$$

from which follows that

$$\int_{\mathbb{R}} w^2(x,t)\,dx \leq \int_{\mathbb{R}} w^2(x,0)\,dx \quad \text{for } t > 0. \tag{24.16}$$

This inequality shows that the L_2-norm in space of a perturbation from initial data does not grow with time, which proves stability of a rarefaction wave. Note that this argument builds on the fact that the rarefaction wave $u(x,t)$ is increasing in x so that u' is non-negative.

24.10 Stability of Shock

The stability proof used above to prove stability of a rarefaction wave, does not work the same way for a shock, since in this case $u(x,t)$ is decreasing with x. In fact a shock does not satisfy an L_2 stability estimate of the form (24.16). However, one can prove instead an L_1-bound of the form

$$\int_{\mathbb{R}} |w(x,t)|\,dx \leq \int_{\mathbb{R}} |w(x,0)|\,dx \quad \text{for } t > 0. \tag{24.17}$$

This follows by multiplying (24.15) by $sgn(w) = +1$ if $w > 0$ and -1 if $w < 0$, to get by integration by parts:

$$\frac{d}{dt}\int_{\mathbb{R}} |w(x,t)|\,dx + (u_- - u_+)|w(\frac{t}{2},t)| = 0, \tag{24.18}$$

and using the fact that for a shock $u_+ < u_-$. Moreover, we will below with a different type of stability estimate show that a shock is stable from computational G2 point of view, Thus, a shock is a stable phenomenon from both physical and computational point of view.

24.11 Instability of Non-Physical Shock

We saw above that the rarefaction wave solution is stable, and we now study the stability of the alternative weak solution (24.11). By the same argument as used to prove (24.18) we obtain

$$\frac{d}{dt}\int_{\mathbb{R}} |w(x,t)|\,dx = (u_+ - u_-)|w(\frac{t}{2},t)|, \tag{24.19}$$

where now $u_+ > u_-$. In this case, $\int_{\mathbb{R}} |w(x,t)|\,dx$ can grow arbitrarily fast, since the positive right hand side in (24.19) in no way can be controled by the left hand side. We thus conclude that an unphysical shock is unstable.

24.12 2nd Law = Stability + Finite Precision

We thus have two methods to single out physical shocks, one based on stability, and the other based on the 2nd Law. This shows that ultimately the 2nd Law expresses a stability condition, reflecting that Nature only can realize phenomena which are properly stable, in its analog finite precision computation. We thus may view the 2nd Law to express a combination of stability and finite precision.

24.13 A Traffic Model

The equation (24.1) with $f(u) = u(1-u)$ models the flow of cars along a highway represented by the x-axis with $0 \leq u \leq 1$ the car density and $0 \leq v = (1-u) \leq 1$ the car velocity as a function of density: Sparse cars ($u \approx 0$) move fast ($v \approx 1$) and packed cars ($u = 1$) stand still ($v = 0$). The equation (24.1) then expresses conservation of mass in the sense that there are no side roads through which cars can enter or exit (and they cannot simply disappear into the sky).

We understand that if $u(x,t)$ is increasing in x so that the car density increases in the direction of motion, then the car velocity will be decreasing in the direction of motion which means that faster cars behind will approach slower cars ahead. But the x-axis is a one-lane street and does not allow a faster car to overtake a slower car, and so eventually faster cars will have to break in order to not run into slower cars ahead, that is, the law $v = (1-u)$ will have to be violated and thus the conservation law (24.1) cannot be satisfied pointwise. In the inviscid equation (24.1) this will correspond to the appearence of a shock. The corresponding regularized equation takes the form

$$\dot{u} + ((u(1-u))' - \nu u'' = 0,$$

which we formally can write as

$$\dot{u} + (uv)' = 0$$

with the modified velocity law

$$v = (1 - u - \frac{\nu}{u}u'),$$

with the effect that in the dangerous case of increasing density ($u' > 0$), faster cars will be slowed down more than slower cars and collisions from behind will thus be avoided.

In this model the shock corresponds to the well-known situation when an inexperienced driver suddenly steps on the brake to avoid collision into a cue, which in the regularized problem corresponds to the smoother action of an experienced driver slowing down because the car density is larger ahead than behind.

24.14 Non-Existence Exact Euler Solutions

We have seen that the inviscid Burgers equation has discontinuous shock solutions, which can be viewed as weak solutions satisfying a 2nd Law. One can thus speak about a shock solution as an exact weak solution of Burgers equation satisfying a 2nd Law, and this solution is the limit of regularized solutions as the viscosity tends to zero. The goal of the classical mathematical analysis of conservation laws based on regularization, is to establish a corresponding result for the Euler equations: The goal is thus to prove the existence of a function satisfying the Euler equations in a weak sense together with a 2nd Law, as a limit of regularized solutions.

However, this goal has not been reached, and we have good reasons to believe that it cannot be reached. This is because of the appearence of turbulent solutions to the regularized Euler equations which do not seem have a limit in the form of a function. It is thus not meaningful to speak about exact solutions to the Euler equations, because such objects do not exist, but we may speak about regularized solutions because they do exist and we may view such solutions as approximate solutions to the Euler equations.

With this perspective it is reasonable to view a shock solution not as is usual as an exact weak solution to the Euler equations, but rather to view a viscous shock solution, an exact solution to the regularized Euler equations, as an approximate solution to the Euler equations. Thus only strong pointwise solutions could deserve the title of “exact solution”; a weak solution which is not a strong solution like a shock, could only be an approximate solution. This may seem to differ from the common way of looking at weak solutions of differential equations, as functions satisfying the differential equation “weakly exactly”, but this is not completely natural since the notion of “weakly” has an element of “inexactly” built in. Only a strong pointwise solution can be an exact solution. I somebody offers you to buy an unknown painting by van Gogh, which you are only allowed to inspect from a distance of 10 meters, you may get suspicious and refrain from a deal.

Chapter 25

BurgersG2

> But maybe that is our mistake: maybe there are no particle positions and velocities, but only waves. It is just that we try to fit the waves to our preconceived ideas of positions and velocities. The resulting mismatch is the cause of the apparent unpredictability. (Stephen Hawking 1988)

25.1 Introduction

We will now consider G2 applied to Burgers' equation as a simple version of EG2. We recall that G2 is Galerkin's finite element method combined with a weighted least-squares control of the residual. G2 is based on piecewise polynomial approximation in space-time and offers spectrum of computational methods depending on the choice of the space-time mesh, as presented in detail in [11, 20]. G2 uses piecewise polynomials which are continuous in space and possibly discontinuous in time. These variants are referred to as cG(p)cG(q) or cG(p)dG(q) with cG(p) referring to continuous piecewise approximation of degree p in space, and cG(q)/dG(q) referring to continuous/discontinuous approxiamtion in time of degree q. G2 is *Eulerian* if the space-time mesh oriented along the space and time coordinate axis, is *Lagrangean* if the space-time mesh is oriented along particle paths in space-time, and *Arbitrary Lagrangean-Eulerian* or *ALE* if the space-time mesh is oriented according to some other feature such as space-time gradients of the solution. Lagrangean variants are also referred to as *characteristic Galerkin*, and Eulerian variants as *streamline diffusion methods.*

In all these variants the space-time mesh is usually organized in space-time slabs between discrete time levels, and G2 then gives a time-stepping method allowing the solution to be computed form one time level to the next progessing in time. The space mesh may be changed across the discrete time levels to avoid mesh distortion and allow mesh adaption. In dG(q) the approximation is discontinuous in time and the space mesh may vary from one slab to the next. If the space mesh is changed across a discrete time level in cG(q), then a projection from the previous mesh to the new mesh is performed. The projection is built into the Galerkin method through a jump term corresponding to a L_2 projection. The discrete solution between the discrete time levels may be viewed as an approximate *transport* step, and the whole process may be viewed as a method of the basic form *projection-transport*.

The traditional finite difference methods are of Eulerian type with the first order Lax-Friedrichs' scheme from the 50s as a prototype on conservation form and with artificial viscosity proportional to the mesh size. The next generation of classical schemes originates from Godunov's method in 1d, which is of the form projection-transport with piecewise constant (discontinuous) approximation and a Riemann solver for the transport step. The multi-dimensional finite volume schemes developed in recent decades, use discontinuous polynomial approximation with numerical fluxes often constructed using 1d Riemann solvers. All these methods may alternatively be viewed as particular G2 methods.

25.2 Semi-Discrete G2 for Burgers Equation

For the purpose of analysis displaying essential aspects, we consider a *semi-discrete* G2 method for Burgers equation with cG(1) discretization in space. Full discretization with cG(q) or dG(q) in time can be analyzed similarly. Let then for a given mesh on $\mathbb{R}$ with mesh size h, V_h be the set of continuous functions $v(x,t)$ which for $t \in I = [0,T]$ are piecewise linear in x on the mesh. The simplest version of semidiscrete G2 takes the form: Find $U \in V_h$ such that

$$((R(U), v)) + ((hU', v')) = 0 \quad \forall v \in V_h, \tag{25.1}$$

where $R(U) = \dot{U} + UU'$ is the Burgers residual, $((v,w)) = \int_Q vw\,dxdt$ with $Q = \mathbb{R} \times I$ and $U(x,0) \in V_h$ interpolates $u^0(x)$. This is equivalent to a system of ordinary differential equations in time. We have here replaced residual stabilization by (hU', v'), and we thus consider a Galerkin method in space for a viscous Burgers equation with viscosity $\nu = h$.

25.3 Basic Energy Estimate as 2nd Law

Choosing $v = U$ in (25.1), we obtain by integration by parts over $\mathbb{R}$ the following direct analog of (24.4):

$$\dot{K}(U;t) = -D_h(U;t), \quad \text{for } t \in I.$$

In the presence of shocks, $D_h(U;t)$ will be substantial and thus U' will at shocks be large ($\sim h^{-1}$).

25.4 A Posteriori Error Estimation by Duality

We shall now prove we the following a posteriori error estimate, where u is the solution of the viscous Burgers equation with $\nu = h$:

$$\|u - U\|_Q \leq S\|hR(U)\|_Q, \tag{25.2}$$

where $\|\cdot\|_Q$ is the $L_2(Q)$-norm and

$$S = \frac{\|h\varphi''\|_Q}{\|e\|_Q}, \tag{25.3}$$

is a stability factor defined by the solution φ of the following linearized dual problem:

$$\begin{aligned} -\dot{\varphi} - a\varphi' - h\varphi'' &= e, && \text{in } Q,\\ \varphi(x,t) &\to 0, && x \to \pm\infty, t \in I,\\ \varphi(x,T) &= 0, && x \in \mathbb{R}, \end{aligned} \tag{25.4}$$

where $a = (u + U)/2$. We notice that the dual problem has a viscous term with viscsoity coefficient h.

To prove the a posteriori error estimate (25.2) we multiply (25.4) by $u - U$ and integrate in space and time to get the error representation

$$\|u - U\|_Q^2 = ((R(U), \varphi)) + ((hU', \varphi')).$$

We then use the Galerkin orthogonality (25.1) with $v = \Phi \in V_h$ an interpolant of the dual solution φ, to get

$$\|u - U\|_Q^2 = ((R(U), \varphi - \Phi)) + ((hU', \varphi' - \Phi')),$$

which combined with an interpolation error bound of the form

$$\|\varphi - \Phi\|_Q + \|h(\varphi' - \Phi')\|_Q \leq C_i \|h^2 \varphi''\|_Q,$$

where C_i is an interpolation constant, shows that

$$\|u - U\|_Q^2 \leq C_i \|hR(U)\|_Q \|h\varphi''\|_Q,$$

where $R(U)$ has been augmented by the contribution $\|hU'\|_Q$, which proves (25.2), setting $C_i = 1$ for simplicity.

By the basic energy stability estimate, we have

$$\|hU'\|_Q \leq \sqrt{h} \quad \text{if } \|u^0\|_{\mathbb{R}} = 1,$$

suggesting the same estimate for $\|hR(U)\|_Q$, which of course is checked a posteriori, and thus we expect

$$\|u - U\|_Q \leq S\sqrt{h}. \tag{25.5}$$

We shall now prove that for a shock $S \sim 1$, which shows that a shock is computable with G2, with a $L_2(Q)$ error of size $\sqrt{h}$, which is optimal from approximation point of view (if we consider the exact solution u to be discontinuous) and U is continuous in x on the mesh.

25.5 Stability Estimate for a Shock

We shall now investigate the stability properties of the dual problem (25.4) and seek to bound $h\varphi''$ in terms of the right hand side e. For simplicity we linearize at the exact solution $u(x,t)$ (instead of the mean value $(u + U)/2$) and thus consider the dual problem

$$\begin{aligned} -\dot{\varphi} - u\varphi' - h\varphi'' &= e, \qquad \text{in } Q, \\ \varphi(\cdot, T) &= 0. \end{aligned} \tag{25.6}$$

The stability properties are largely determined by the sign of u', which reflects the change of the direction u of the characteristics. If $u' \leq 0$, then the characteristics converge with increasing t, which typically occurs in the case of a shock. If $u' \geq 0$, then the characteristics diverge, which typically occurs in the case of a rarefaction. If u' is bounded below by a moderate constant, e.g. $u' \geq 0$, then we may estimate $\|\varphi\|_{L_\infty(L_2(\mathbb{R}))}$ and $\|\sqrt{h}\varphi'\|_Q$ in terms of a moderate constant times $\|e\|_Q$, which we refer to as *weak stability*. If u' is bounded above by a moderate constant, e.g. $u' \leq 0$, then we may estimate $\|h\varphi''\|_Q$ in terms of a moderate constant times $\|e\|_Q$, which we refer to as *strong stability*, because we estimate second derivatives of φ, cf. (25.3). These estimates are proved by multiplying by φ and $-h\varphi''$, respectively, bringing in the positive stabilizing terms $\frac{1}{2}u'\varphi^2$ and $-\frac{1}{2}hu'(\varphi')^2$, respectively.

We now give the details in the case of a shock with $u' \leq 0$, where we assume u is differentiable with a very large negative x-derivative close to the shock. We indicate the general nature of the characteristics of the dual problem in Fig 25.5. We shall prove that the solution φ of (25.6) satisfies

$$\|h\varphi''\|_Q + \|\dot{\varphi} + u\varphi'\|_Q + \sup_{0<t<T} \|h^{1/2}\varphi'(\cdot,t)\|_R \leq 3\|e\|_Q. \tag{25.7}$$

To see this we multiply the first equation in (25.6) by $-h\varphi''$, integrating by parts with respect to x, and integrating in time over (τ, T) with $0 < \tau < T$, we get with $Q_\tau = \mathbb{R} \times (\tau, T)$

$$\begin{aligned} &\tfrac{1}{2}\int_{\mathbb{R}} h\left(\varphi'(\cdot,\tau)\right)^2 dx + \int_{Q_\tau} \left(h\varphi''\right)^2\, dxdt + \int_{Q_\tau} \tfrac{1}{2}\left(uh\left(\varphi'\right)^2\right)'\, dxdt \\ &\leq \tfrac{1}{2}\int_{Q_\tau} \left(hu'\left(\varphi'\right)^2 + e^2 + \left(h\varphi''\right)^2\right)\, \mathrm{d}x\mathrm{d}t, \end{aligned} \tag{25.8}$$

which proves the desired result stating that $S \sim 1$ for a shock.

As comparison, let us now attempt to derive a weak stability estimate for (25.6) in the case u is a shock. Multiplication by φ and integration over Q_τ gives

$$\begin{aligned} &\tfrac{1}{2}\int_R \varphi^2(x,\tau)\, dx + h\int_{Q_\tau} \left(\varphi'(x,t)\right)^2\, dxdt \\ &= -\tfrac{1}{2}\int_{Q_\tau} u'\varphi^2(x,t)\, dx + \int_R e(x,t)\varphi(x,t)\, dx. \end{aligned}$$

Since u' is large negative in the case of a shock, we have large positive term of the right hand side, and using a Gronwall inequality would results in a very large stability factor. On the other hand, we show below weak stability for a rarefaction wave with $u' \geq 0$, reflecting the above stability result for the perturbation equation.

Summing up, we see that for a shock, the linearized dual problem statisfies a strong stability estimate with a stability factor of moderat size, while a

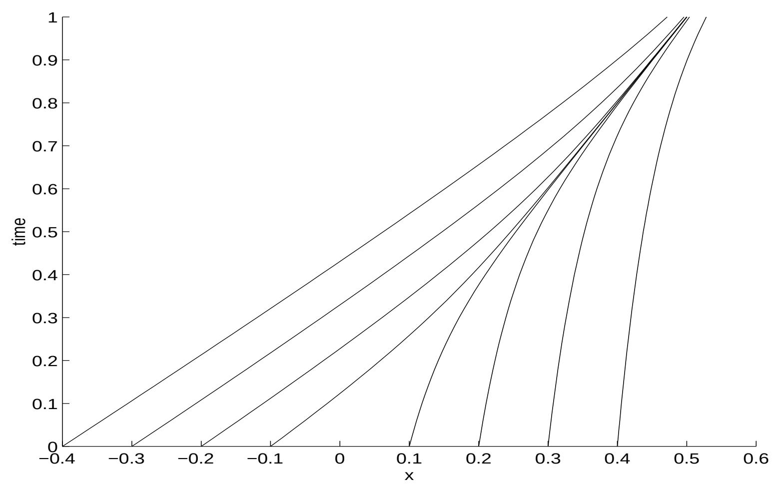

Figure 25.1: Characteristics of the dual problem for a regularized shock solution.

corresponding weak stability estimate appears to have a very large stability factor. These stability features may be understood in a qualitative sense, by pondering the directionality of the characteristics and the nature of the L_2-norm.

25.6 Stability Estimates for a Rarefaction Wave

We now consider the linearized dual Burgers' equation (25.6), linearized at the exact solution $u(x,t) = x/t$, corresponding to a rarefaction wave. Multiplying now (25.6) by $-ht\varphi''$, and using standard manipulations, we obtain the following weighted norm strong stability estimate for $0 < \tau < T$,

$$\|\tau^{1/2}h^{1/2}\varphi'\| + \|\omega h\varphi''\|_{Q_\tau} \leq \|\omega e\|_{Q_\tau}, \tag{25.9}$$

where $\omega(t) = t^{1/2}$ acts as a weight.

A weighted norm analog of the a posteriori error estimate (25.2) takes the form

$$\|\omega^{-1}e\|_{Q_N} \leq S_\omega\|\omega^{-1}hR(U)\|_{Q_N} \tag{25.10}$$

with S_ω defined by the direct weighted norm analog of (25.3). The estimate (25.9) then shows that $S_\omega \sim 1$, and thus a rarefaction wave solution is computable in the weighted norm with computational work corresponding to interpolation. Note that the presence of the weight $t^{-1/2}$ will force more stringent demands on the mesh for t close to zero, which will force an accurate resolution of the initial phase of the rarefaction. This is intuitively reasonable and corresponds to the fact that an initial error in the computation of a rarefaction will get amplified as time goes, because characteristics diverge forward in time. On the other hand, in the case of a shock, an initial error may be eliminated at later times, because of converging characteristics, Thus, a rarefaction is more delicate to compute than a shock, which we will see in the computational results we now present.

25.7 Dual Solution and Stability Factors

We display below G2 computations of a combination of a rarefaction wave and a shock using the cG(1)dG(0)- method on a uniform space mesh with $h = 10^{-3}$ and time step 10^{-4} taken from [3]. We plot the computed solution at t=0, t=0.3 , t=0.8, t=1 in Fig 25.2. We see that the initial discontinuity develops into a rarefaction and that a shock is formed for $t \approx 0.5$.

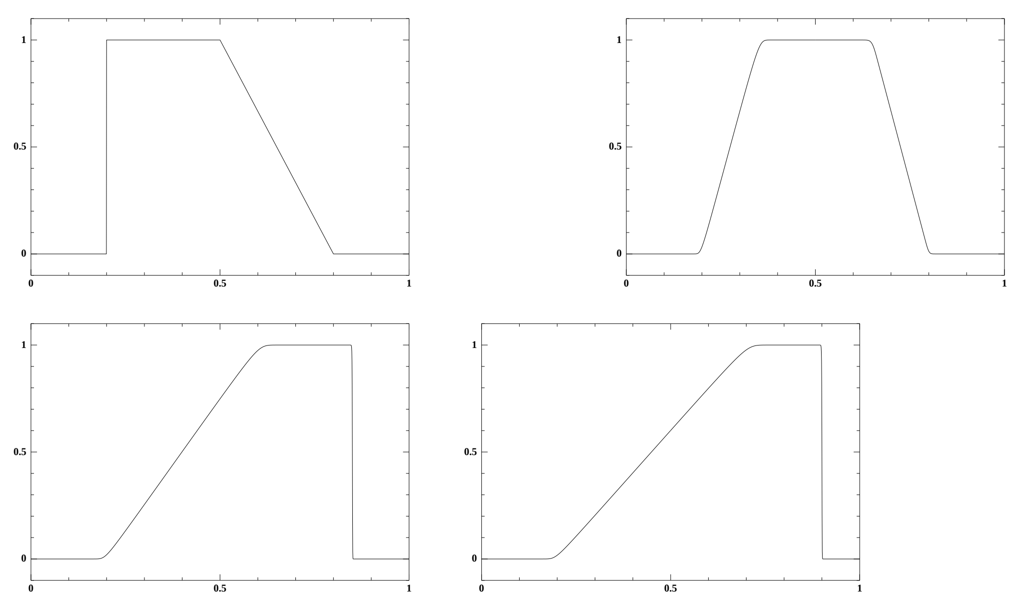

Figure 25.2: A combined rarefaction and shock wave

We solve the dual problem using the following different approximations of the coefficient $a = (u + U)/2$ and the error e, with $\bar{u}$ the analytical, inviscid solution, and $U(h)$ the finite element solution on a mesh of size h: (i) $a = (\bar{u} + U(h))$ and $e = \bar{u} - U(h)$, (ii) $a = U(h)$ and $e = \bar{u} - U(h)$, (iii) $a = (U(h/4) + U(h))/2$ and $e = U(h/4) - U(h)$. We plot the corresponding dual solutions φ at the same time levels as above, but in revers e order (t=1, t=0.8, t=0.3 , t=0) in Fig 25.7. We also plot in Fig. 25.4 the corresponding

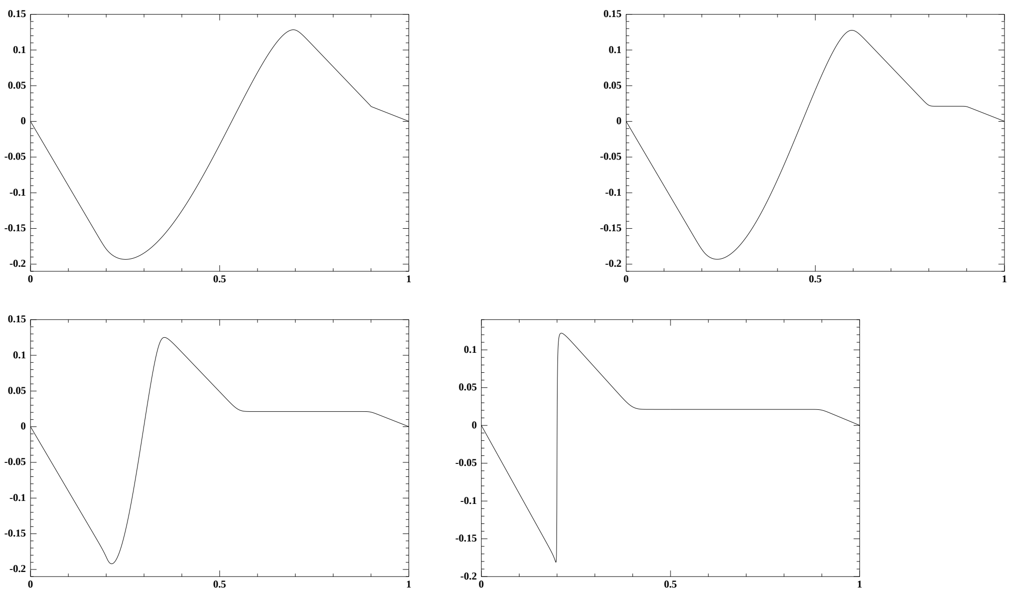

Figure 25.3: Dual solution in reverse time.

second derivatives φ''. We note the change of $|\varphi''|$, which may be viewed as a weight in the a posteriori error estimate, from being large close to the shock at final time towards being large close to the initial discontinuity at $(x, t) = (0.2, 0)$ initiating the rarefaction. We see that that it is the data from the rarefaction at final time which generates the large values of φ'' at $t = 0$, and not those from the shock. This indicates that a rarefaction is more delicate to compute than a shock.

We plot in Fig. 25.5 the strong stability factor S defined by (25.3) for (i)-(iii) and $h = 0.0001$, $h = 0.00005$, $h = 0.00001$. We see that $S \sim 1$, which shows that the Burgers' solution consisting of a rarefaction and shock wave is computable in $L_2(Q_N)$ with work comparable to interpolation.

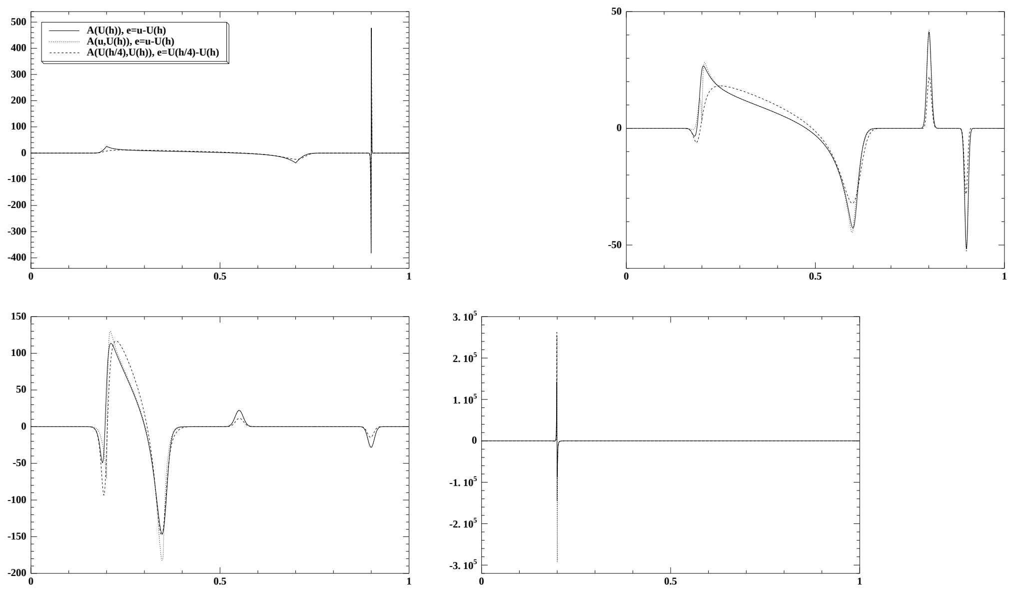

Figure 25.4: Second deriatives of the dual solution in reverse time

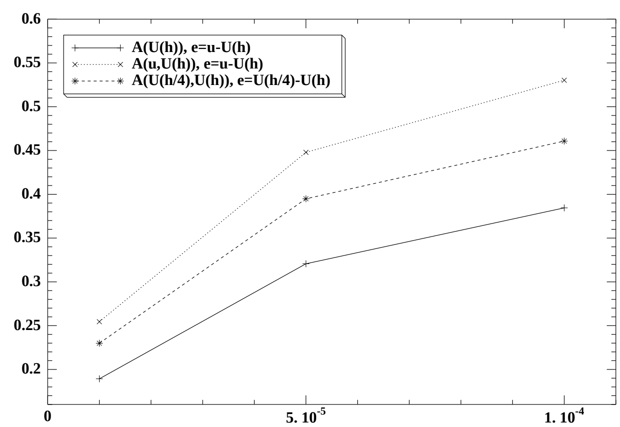

Figure 25.5: Strong stability factor for different h

25.8 Turbulent Bluff Body Flow

We show EG2 flow with shocks around a sphere and cylinder in Figs. 25.6 and 25.8. This section will be extended with turbulent/shock flow around a cube and sphere.

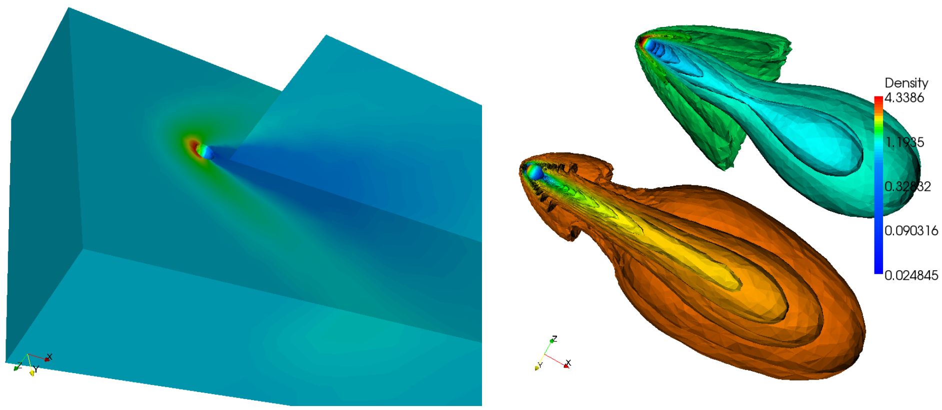

Figure 25.6: Flow around a sphere

25.9 Turbulent Flow in Heat Engines and Refrigerators

This section will contain EG2 simulations of diffuser flow with gas expanding under cooling while getting heated by turbulence, with the objective of computing losses and efficiency.

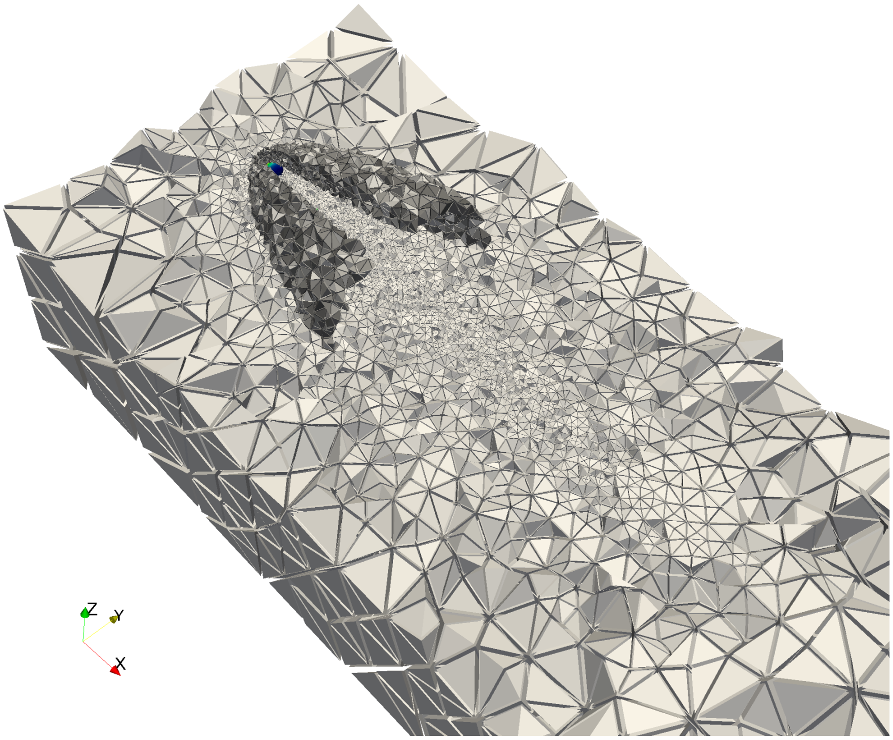

Figure 25.7: Mesh around a sphere

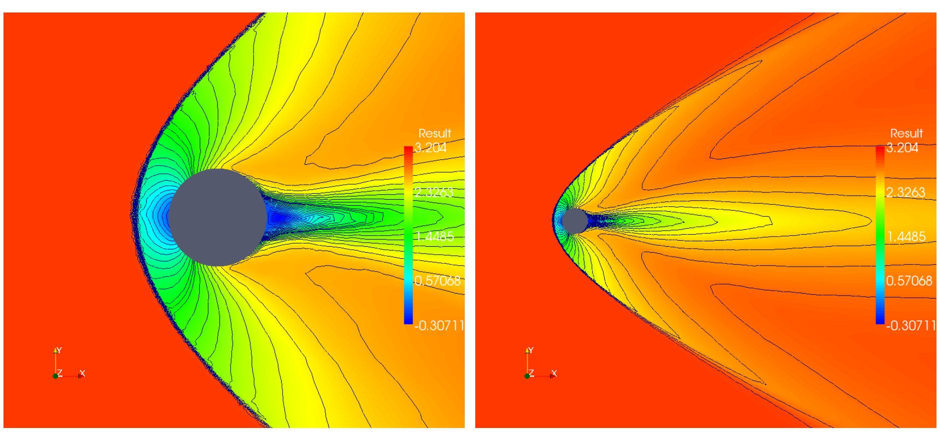

Figure 25.8: Section of 2d flow around a cylinder

Chapter 26

Supersonic Flow around a sphere

Experimental data for compressible flow around a sphere for different Mach numbers and Reynolds numbers are available over the number of publications starting from the 18th century. A review article by Miller & Bailey [**?**] studies the experiments of the 18th and 19th centuries for different Mach numbers $0.2 \leq M \leq 2.0$ at $Re \approx 10^7$. The analyses in the mentioned article show that the experimental data obtained three centuries ago are in good agreement to the modern data.

Sphere measurements obtained by [**?**] and [**?**] show that regardless of the diameter size of the sphere, the drag coefficient increases rapidly in the transonic region and for $M \geq 1.6$ and $Re \geq 10^5$ it stays to be constant with further increases in Reynolds number. Experimental analyses in [**?**] and earlier in [**?**] show that the drag coefficient slowly decreases when the Mach number increases above $M \geq 2$ for the flow with $Re \gtrapprox 10^6$. We leave a complete discussion for different Mach numbers for future research, but in this paper we present results for only one Mach number, in order to see if the G2 solution gives a correct result according to the experiment.

We use Algorithm **??** for the supersonic flow around a sphere with diameter $d = 0.074$ at Mach number $M = 2$. For this Mach number the flow characterized by a detached three dimensional bow shock wave in front of the sphere and is in a mixed subsonic and supersonic flow behind the sonic line $M = 1$. Here the pressure drag at the stagnation point is high compared to the subsonic case. An attached shock wave develops in the rear of the sphere, which is also counted as a substantial source of the pressure drag. Therefore, the area for the pressure stagnation point and attached shock waves should be resolved by computation for the correct drag coefficient. We observe from the results that the adaptive G2 method tries to resolve these regions.

We present the results from the simulation in Table 26.1. 10% of the largest cells are refined during the adaptive algorithm. We start with an initial coarse mesh, which has 9 720 vertices and 53 312 cells, which reaches 168 820 vertices and 918 605 cells after 9th adaptive iteration. The error bound of the drag coefficient $\sum_{n,K} \eta_n^K$ converge by the mesh refinement, as the drag coefficient approximately stays around the experimental data $C_{dp} \approx 1$. In Figure 26.3 the drag coefficients are plotted after each adaptive iterations.

We plot the solution of the adaptive algorithm in Figure 26.1 after eight refinements. The right column of the figure shows the primal solutions and the left column presents the corresponding dual solutions. The magnitude of the dual solution is high in the areas with the significant contribution to the pressure drag force. The plot of the primal pressure shows that already in eight adaptive step the pressure structures are close to be resolved.

In Figure 26.2 we present the initial coarse mesh and the mesh after nine adaptive refinements. After each refinement the boundary nodes, which appear from the Rivara algorithm are projected to the surface of the sphere. Also, we notice that similar to the 2D result, the algorithm focuses to resolve the pressure stagnation point, area of the sonic line and attached shock wave, which is expected since they are the main source of pressure drag. With ad hoc refinement, for instance residual based or gradient based adaptation, the region with strong shocks are well resolved. However, we notice that the duality based adaptive algorithm does not resolve a propagating bow shock and other strong discontinuities, it only refines the areas with the largest error contribution. Consequently, it significantly decreases the computational cost of the drag force computation.

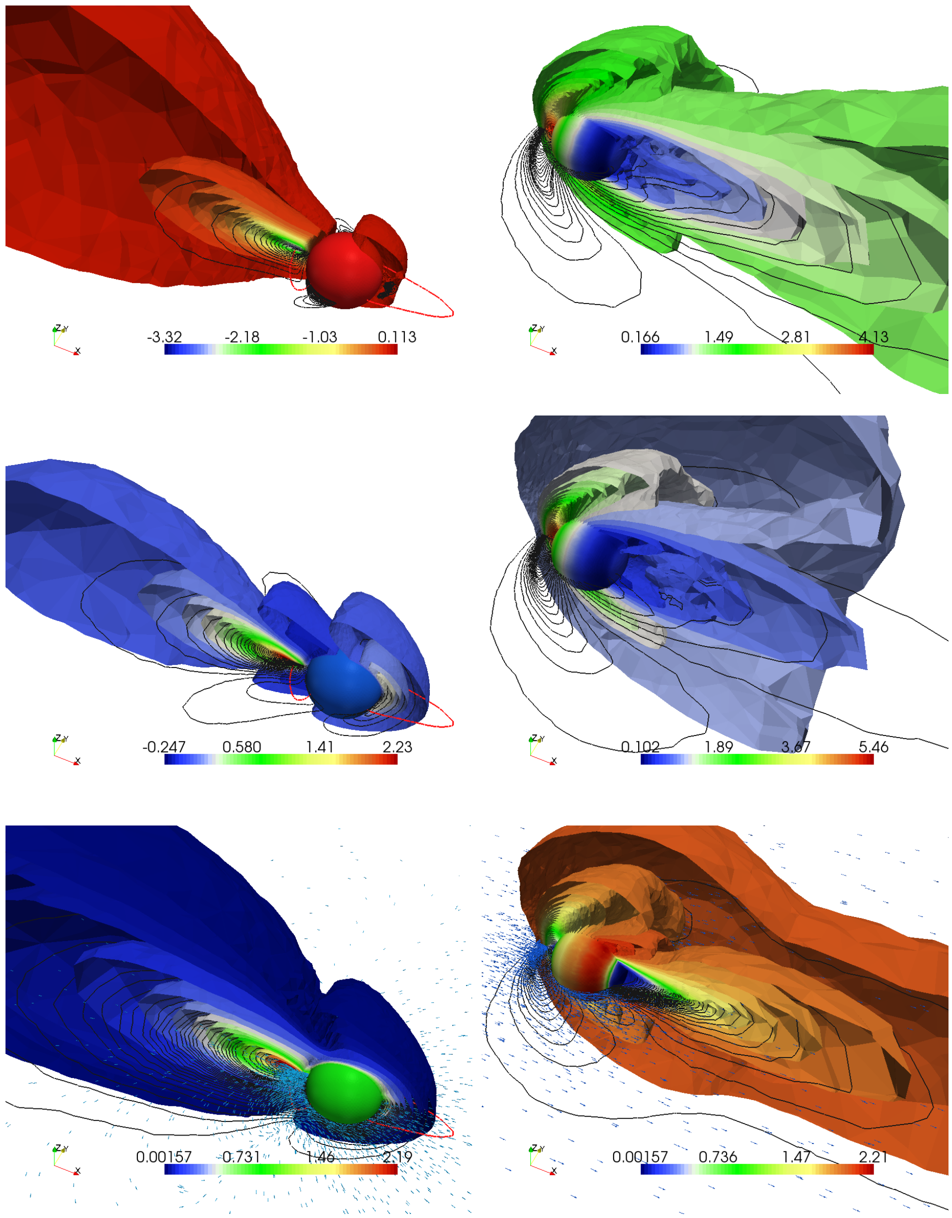

Figure 26.1: Supersonic flow around a sphere: the dual solution at time $t = 0$ of density *(top-left)*, pressure *(middle-left)* and magnitude of velocity *(bottom-left)*; the primal solution at time $t = 0.5$ of density *(top-right)*, pressure *(middle-right)* and magnitude of velocity *(bottom-right)*. The contours are plotted in the collormap. The sonic line in red is plotted together with the dual solution.

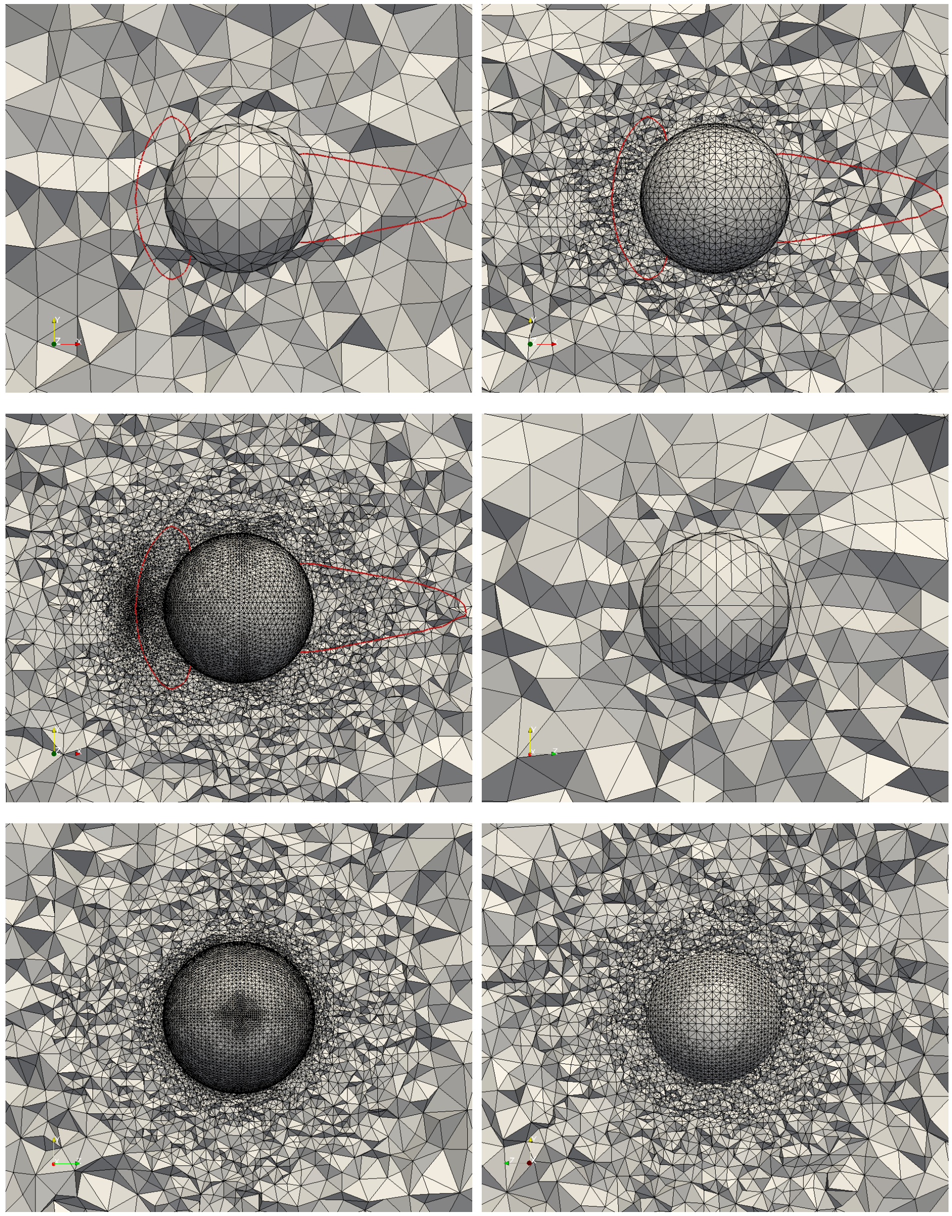

Figure 26.2: Supersonic flow around a sphere: the (x, y) - view of the mesh for the initial mesh *(top-left)*, four times *(top-right)* and nine times *(middle-left)* adaptive refinement according to the drag force together, the sonic line is plotted in red, (y, z) - view of the mesh for $x = x_s$ of the initial mesh *(middle-right)*, where x_s - is x coordinate of the center of sphere, the finest mesh close to the stagnation point of pressure $x = x_s - d/2$ *(below-left)*, and the finest mesh at $x = x_s + 0.02$ from back *(below-right)*

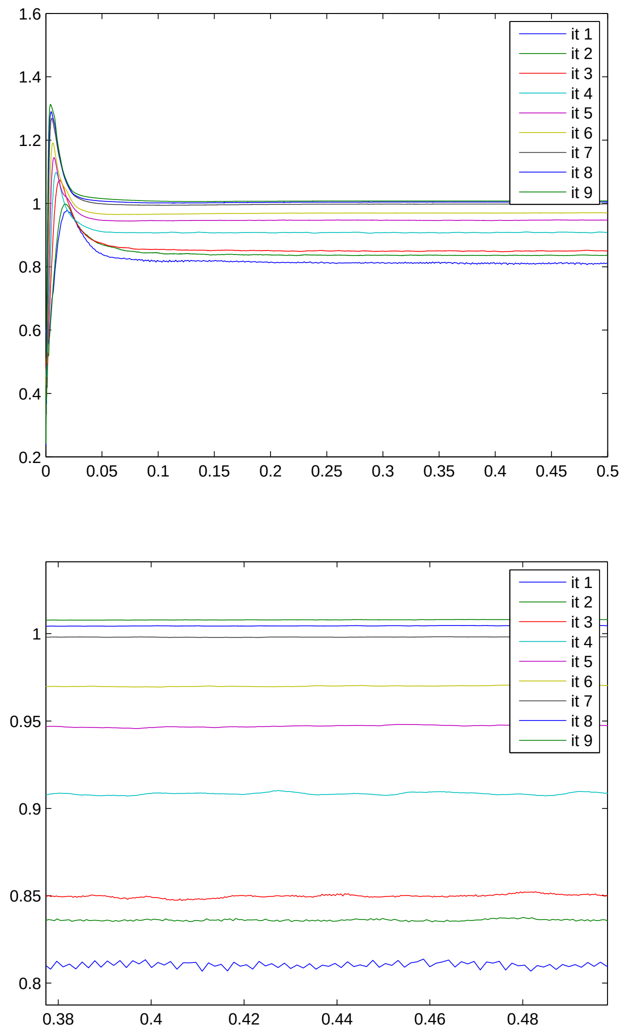

Figure 26.3: Supersonic flow around a sphere: the drag coefficient C_{dp} in different adaptive iterations.

Table 26.1: The convergence history of the drag coefficient. Here $\bar{C}_{dp}$ is a mean value of C_{dp} over the time interval $[t-\epsilon_t, t]$, where ϵ_t is a small number, and $\sum_{n,K} \eta_n^K$ denotes a sum of error indicators.

#iter	#vertices	#cells	S	$\bar{C}_{dp}$	$\sum_{n,K} \eta_n^K$
0	9720	53312	0.8218	0.8115	1.5018
1	17405	94572	0.9571	0.8360	1.3096
2	22915	124884	1.1586	0.8502	1.0234
3	29686	160313	1.4233	0.9085	0.8651
4	39328	212637	1.6683	0.9474	0.7352
5	51746	280031	1.8440	0.9705	0.6236
6	69418	376144	2.0050	0.9873	0.5429
7	93696	508209	2.0538	0.9982	0.4532
8	126012	685079	2.1038	1.0046	0.3844
9	168820	918605	2.0541	1.0081	0.3199

Part VI

Applications

Chapter 27

Carnot Heat Engine

> No heat engine can be more efficient than a Carnot engine with efficiency $1 - \frac{\tau_c}{\tau_h}$, when operating between two temperatures τ_h and $\tau_c < \tau_h$. (Carnot 1824)

27.1 Introduction

We now pass on to basic applications including *heat engines*, *heat pumps* and *refrigerators*, which are cyclic thermodynamics processes sharing essential aspects. A main issue is the *losses* caused by turbulence/shocks, which determine the *efficiency* of the device. We show that EG2 allows simulatation of real processes including accurate computation of losses and efficiency.

We start recalling the theoretical analysis the ideal *Carnot heat engine* and the *Carnot heat pump* offered by classical thermodynamics, and then pass on to EG2 simulation and analysis of real engines, pumps and refrigerators.

27.2 Heat Engines

A *heat engine* is a cyclic thermodynamic process converting heat energy to useful mechanical work. The *efficiency* of a heat engine is the quotient between the useful mechanical work and the heat energy supplied. Carnot claimed that no heat engine operating between two temperatures $\tau_h = \tau_{hot}$ and $\tau_c = \tau_{cold} < \tau_h$, can have an efficiency exceeding $1 - \frac{\tau_c}{\tau_h}$. A heat engine with small temperature difference with $\frac{\tau_c}{\tau_h} \approx 1$, thus would be very inefficient.

To show this Carnot assumed that a *heat engine* is a cyclic thermodynamic process of a perfect gas connecting four states 1-4 through the following consecutive sub-processess:

(12) isothermal expansion absorbing heat at τ_h from a recervoir,

(23) adiabatic expansion to temperature $\tau_c < \tau_h$,

(34) isothermal compression delivering heat at τ_c to a recervoir,

(41) adiabatic compression to temperature τ_h,

where (ij) is the process leading from state i to state j. We recall that *adiabatic* means that there is no exchange of heat with the surrounding reservoirs, and *isothermal* that the temperature stays constant. Carnot defined a *Carnot heat engine* to be an *ideal reversible* heat engine operating without losses. Any real heat engine would be subject to losses and thus, by definition, would be less efficient than a Carnot heat engine.

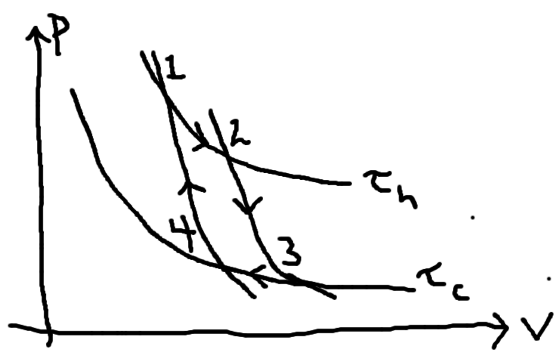

Figure 27.1: Carnot heat engine cycle.

27.3 Classical Efficiency of a Carnot Heat Engine

We now recall the classical analyis showing that the efficiency of a Carnot heat engine is $1 - \frac{\tau_c}{\tau_h}$. It is based on energy balance in the form $dQ = d\tau + pdV = dE + dW$, where dQ is supplied heat energy, $d\tau$ change of internal energy, dV change of volume V and dW change of work W. We note that in process 12 and 23 work is done *by* the process ($dV > 0$) and in step 34 and 41 *on* the process ($dV < 0$). Noting that $dQ = 0$ in process 23 and 41, we obtain integrating $d\tau + pdV = 0$,

$$W_{23} = \int_2^3 pdV = \tau_h - \tau_c = -\int_4^1 pdV = -W_{41},$$

where W_{ij} is the work in process ij. Further, recalling the state equation of a perfect gas $pV = (\gamma - 1)\tau$, we get integrating $0 = \frac{d\tau}{\tau} + (\gamma - 1)\frac{dV}{V}$ over the processes 23 and 41,

$$(\gamma - 1)\log(\frac{V_3}{V_2}) = -\log(\frac{\tau_c}{\tau_h}) = -(\gamma - 1)\log(\frac{V_1}{V_4}), \qquad (27.1)$$

where V_i is the volume of state i. Further, since $d\tau = 0$ in process 12 and 34

$$W_{12} = Q_{12}, \quad W_{34} = Q_{34},$$

where Q_{ij} is the heat energy absorbed/released in process ij. Using that $p = (\gamma - 1)\tau_h/V$ in process 12, we have

$$W_{12} = \int_1^2 pdv = (\gamma - 1)\tau_h \int_1^2 \frac{dV}{V} = (\gamma - 1)\tau_h \log(\frac{V_2}{V_1}),$$

and similarly

$$W_{34} = (\gamma - 1)\tau_c \log(\frac{V_4}{V_3}).$$

We conclude since by (27.1), $\log(\frac{V_2}{V_1}) = \log(\frac{V_3}{V_4})$

$$\frac{-W_{34}}{W_{12}} = \frac{\tau_c}{\tau_h}.$$

Thus the efficiency η_e of a Carnot heat engine, the quotient of performed work and used energy, is given by

$$\eta_e = \frac{W_{12} + W_{23} + W_{34} + W_{41}}{Q_{12}} = \frac{W_{12} + W_{34}}{W_{12}} = 1 - \frac{\tau_c}{\tau_h},$$

as announced. The argument is based on an energy balance in the form $0 = d\tau + pdV = d\tau + dW$ in the adiabatic processes 23 and 34, and in the form $dQ = dW$ in the isothermal processes 12 and 34. Apparently we have assumed that there is no loss in any these processes: A Carnot engine is a heat engine without losses.

In a realization of the above cyclic process 1-4 the flow will be partly turbulent, in which case both $W_{12} > 0$ and $W_{34} < 0$ can only decrease. It follows that no heat engine based on the cyclic process 1-4 can be more efficient than a Carnot engine. A Carnot engine is really the best heat engine of the form 1-4. But of course, the real issue is the efficiency of a real heat engine, to which we return below.

Chapter 28

Carnot Heat Pump

> No heat pump can be more efficient than a Carnot heat pump with efficiency $\tau_h/(\tau_h - \tau_c)$ operating between two temperatures τ_h and $\tau_c < \tau_h$. (Carnot)

28.1 Classical Efficiency of a Carnot Heat Pump

Running a Carnot heat engine in reverse, we get a *Carnot heat pump* absorbing energy from a heat recervoir at low temperature and delivering heat energy to a recervoir at higher temperature $\tau_h > \tau_c$ at the expense of mechanical work, consisting of the following processes:

(21) isothermal compression delivering heat energy at τ_h to a recervoir,

(14) adiabatic expansion to temperature τ_c,

(43) isothermal expansion absorbing heat energy at τ_c from a recervoir,

(32) adiabatic compression to temperature τ_h,

where now in step 21 and 32 work is done on the process and the work in step 32 and 14 as above sums to zero. The efficiency η_p of Carnot heat pump is commonly measured by the quotient of delivered heat energy $-Q_{21}$ divided by the total work W supplied

$$\eta_p = \frac{-Q_{21}}{W} = \frac{Q_{12}}{W} = \frac{1}{\eta_e}. \tag{28.1}$$

A Carnot heat pump is an ideal heat pump without losses, while in a real heat pump the inevitable turbulence/shocks in the expansion steps 14 and 43 would increase the temperature and thus reduce the heat absorption in step 43, thus reducing Q_{43} and then also $-Q_{21}$ and the efficiency.

Carnot's analysis captured in (28.1) suggests that a lousy heat engine would be an excellent heat pump (and vice versa). Of course, reality does not work this way, because of the inevitable losses from turbulence. Thus, Carnot's analysis at best only gives a very rough idea of the efficiency of a heat engine or heat pump. We observe the obvious fact that even if the efficiency of a Carnot heat pump working with a small temperature drop would seem to be formidable according to classical analysis, it would tend to give a small output $-Q_{12}$ in absolute terms.

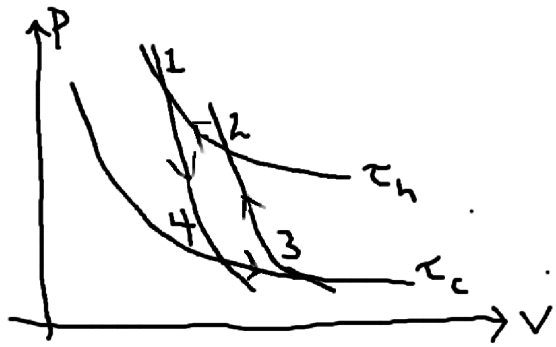

Figure 28.1: Carnot heat pump.

Chapter 29

Real Heat Engines

29.1 EG2 Model of Real Heat Engine

We simulate by EG2 a real heat engine operating through the same cycle of steps as the Carnot heat engine. We find that each step involves a certain loss due to turbulence/shocks and the total loss determines the efficiency as compared to a Carnot engine.

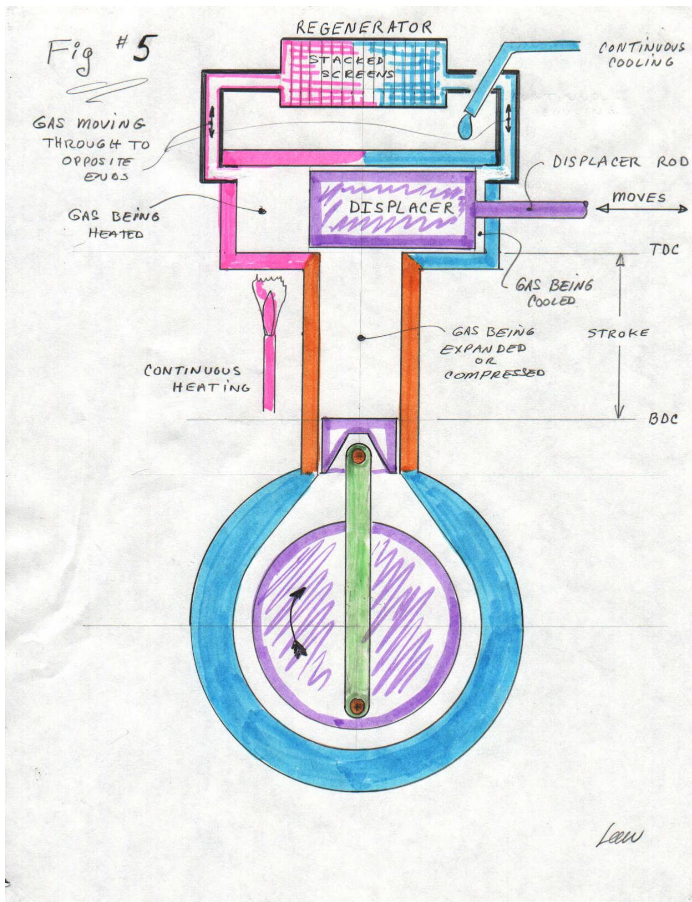

Figure 29.1: A heat engine prototype

Chapter 30

Real Heat Pumps

30.1 Increasing Efficiency by Phase Transition

To increase the efficiency of a heat pump, the cycle may be formed to contain a *changes of phase* from fluid to gas phase (*evaporation*) in the expansion step 43 and from ghas phase to fluid phase (*condensation*) in step 21. The *latent heat* being released during condensation and absorbed during the vaporization increase both Q_{43} and $-Q_{21}$ without increasing W, and thus increases efficiency.

30.2 EG2 Model of Real Heat Pump

We simulate a simple heat pump consisting of two chambers 1 and 2 connected with a channel as in Joule's experiment. We assume the fluid moves back and forth between the two chambers being in liquid phase in chamber 1 at pressure $p > p_c$ and in gas phase in chamber 2 at pressure $p < p_c$, with p_c the condensation/vaporization pressure, in the following cyclic process:

1. Open the valve in the channel and let the fluid at temperature T_h and pressure $p > p_c$ in chamber 1 expand into chamber 2 while evaporating into the gas phase at pressure $p < p_c$ under temperture drop below T_c in chamber 2. Close the valve.

2. Let chamber 2 absorb heat from a surrounding reservoir at temperature T_c.

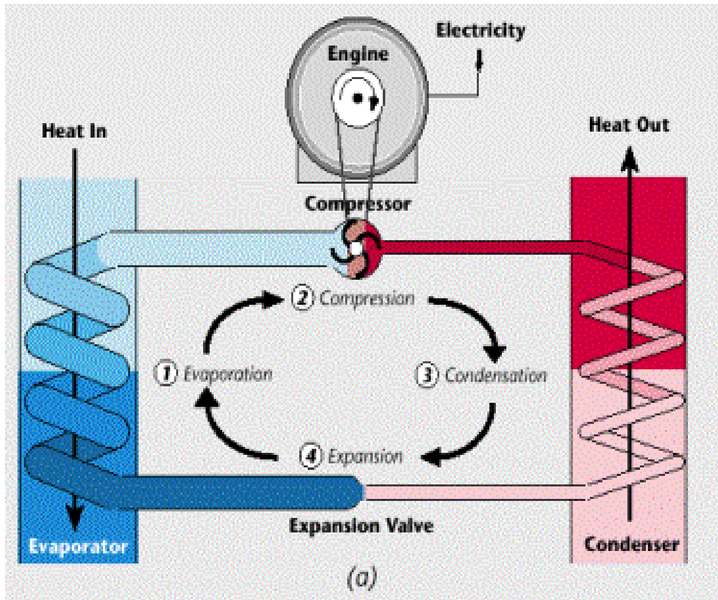

Figure 30.1: Principle of a heat pump.

3. Open the valve and start a compressor in the channel forcing the gas to move from chamber 2 into chamber 1, while changing to fluid phase under release of heat, to reach a temperture above T_h in chamber 1. Close the valve and stop the compressor.

4. Let the chamber 2 supply heat to a surrounding reservoir at temperture T_h, and go back to 1.

The heat consumed for evaporation and heat released by condensation is modeled by defining the internal energy e to be

$$e = \rho(T \pm \Delta H) \tag{30.1}$$

where ΔH is a constant heat of formation, or change of enthalpy H, the plus-sign is used if $p > p_c$, the minus-sign if $p < p_c$, and p_c is the pressure at which condensation and evaporation takes place. For simplicity we assume that p_c does not depend on temperature.

We model the cyclic process by the one-fluid compressible Euler equations with internal energy given by (30.1), the heat release in chamber 2 and the heat absorbtion in chamber 2 by suitable source terms in the energy equation, and the compression in the channel by a volume force in the momentum equation. We compute the efficiency η_p as defined above.

Chapter 31

Refrigerators

> The final aim of all science is to resolve itself into mechanics. (Helmholtz)
>
> The orbit of the electron obeys no law....All is caprice, the calculable world has become incalculable....superstitions have risen from the dead and cast down the mighty from their seats and put paper crowns on presumptious fools. (Bernard Shaw in *Too True to be Good*)

31.1 Importance of Cooling

Without refrigerators, modern society and urban life, would be very complicated, if not impossible. The traditional method for storing food by cooling in countries with a Winter season, used well into the middle of the 19th century, was to store ice harvested in the Winter, typically under thick layers of saw dust, to use it over the Summer season. To cool a multi-million city this way would require enormous installations.

31.2 The Compressor Refrigerator

A refrigerator is a form of heat pump, absorbing heat energy from a reservoir at low temperature (the inside of the refrigerator) and delivering heat energy to a reservoir at higher temperature (to the surrounding room). The above analysis directly applies and the maximal Carnot efficiency is given by

$$\eta_r = \frac{Q_{43}}{W} = \frac{1}{\eta_e}. \tag{31.1}$$

A refrigerator would suffer losses in the expansion steps 14 and 43 increasing the temperature and reducing the heat absorption in process 43, thus reducing Q_{43} and the efficiency.

A regular refrigerator uses a compressor for the condensation from gas to fluid phase. A compressor is a mechanical device with a rotating fan powered by electricity, which causes a certain noise.

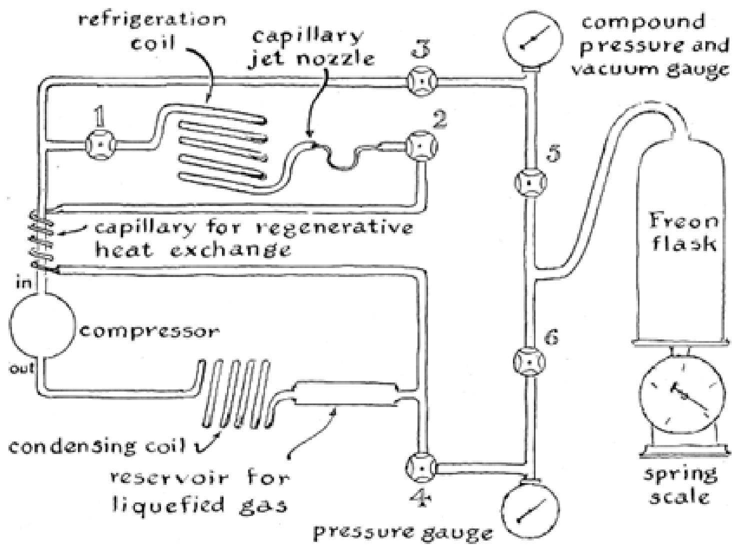

Figure 31.1: Principle of a compressor refrigerator

31.3 Absorption Refrigerator of Platen/Munters

An absorption refrigerator uses a different method that requires no moving parts (thus reducing noise) and is powered only by heat. By supplying heat you thus generate cold, which is apparent contradiction with the 2nd Law in Clausius form stating that heat can only "spontaneously"go from hot to cold. Typically, it uses three substances: ammonia, hydrogen gas, and water. Normally, ammonia is a gas at room temperature (with a boiling point of -33C), but the system is pressurized to the point that the ammonia is a liquid at room temperature.

We cite from Wikipedia: *The cooling cycle starts at the evaporator, where liquefied anhydrous ammonia enters. (Anhydrous means there is no water in the ammonia, which is critical for exploiting its sub-zero boiling point.) The "evaporator" contains another gas (in this case, hydrogen), whose presence lowers the partial pressure of the ammonia in that part of the system. The total pressure in the system is still the same, but now not all of the pressure is being exerted by ammonia, as much of it is due to the pressure of the hydrogen. Ammonia doesn't react with hydrogen - the hydrogen is there solely to take up space - creating a void that still has the same pressure as the rest of the system, but not in the form of ammonia. Per Dalton's law, the ammonia behaves only in response to the proportion of the pressure represented by the ammonia, as if there was a vacuum and the hydrogen wasn't there. Because a substance's boiling point changes with pressure, the lowered partial pressure of ammonia changes the ammonia's boiling point, bringing it low enough that it can now boil below room temperature, as though it wasn't under the pressure of the system in the first place. When it boils, it takes some heat away with it from the evaporator - which produces the "cold" desired in the refrigerator.*

The next step is getting the liquid ammonia back, as now it's a gas and mixed with hydrogen. Getting the hydrogen away is simple, and this is where the "absorber" comes in. Ammonia readily mixes with water, and hydrogen does not. The absorber is simply a downhill flow of tubes in which the mixture of gases flows in contact with water being dripped from above. Once the water reaches the bottom, it's thoroughly mixed with the ammonia, and the hydrogen stays still (though it can flow freely back to the evaporator).

At this point, the ammonia is a liquid mixed with water and still not usable for refrigeration, as the mixture won't boil at a low enough temperature to be a worthwhile refrigerant. It's now necessary to separate the ammonia from the water. This is where the heat from the flame comes in. When the right amount of heat is applied to the mixture, the ammonia bubbles out. This phase is called the "generator". The ammonia isn't quite dry yet - the bubbles contain gas but they're made of water, so the pipe twists and turns and contains a few minor obstacles that pop the bubbles so the gas can move on. The water that results from the bubbles isn't bad - it takes care of another need, and that is the circulation of water through the previous absorption step. Because that water has risen a bit while it was bubbling upwards, the flow of that water falling back down due to gravity can be used for this purpose. The maze that makes the ammonia gas go one way and the bubble water go the other is called the "separator".

The next step is the condenser. The condenser is a sort of heat sink or heat exchanger that cools the hot ammonia gas back down to room temperature. Because of the pressure and the purity of the gas (there is no hydrogen here), the ammonia condenses back into a liquid, and at that point, it's suitable as a refrigerant and the cycle starts over again.

The absorption refrigerator was invented by Baltzar von Platen and Carl Munters in 1922, while they were still students at the Royal Institute of Technology in Stockholm, Sweden. Commercial production began in 1923 by the newly formed company AB Arctic, which was bought by Electrolux in 1925.

31.4 Simulation of Compressor Refrigerator

Chapter 32

Cosmology

According to the *Perfect Cosmological Principle*, the Universe on a large scale looks the same everywhere and at all times. (Fred Hoyle)

The thermodynamic properties of self-gravitating systems are still unclear...The tendency of increasing granularity with time (in a self-gravitating system), so important to the structure and development of the Universe, seems to represent a fundamental principle. (Paul Davies [10])

GRAVITATION: The universal property of all material objects to attract each other.
GRAVITON: A hypothetical particle which, when passing to and fro in virtual form bewteen two masses, in large numbers, is thought to mediate the gravitational attraction between them. (Guillemin [16])

32.1 Euler's Equations with Gravitation

The Euler equations including gravitational forces from the mass distribution can be viewed as a basic (non-relativistic) *cosmological model*. We thus consider an inviscid perfect gas enclosed in a volume Ω in $\mathbb{R}^3$ with boundary Γ (or the whole of $\mathbb{R}^3$), over a time interval $I = (0, 1]$, assuming that the gas is subject to a gravitational force $\nabla\varphi$, where φ is a *gravitational potential* coupled (at each time instant) to the mass distribution ρ through Poisson's equation $\Delta\varphi = \rho$ with (for simplicity) $\varphi = 0$ on Γ. This is a *self-gravitating system* since the gravitational force depends on the mass-distribution

Replacing ρ by $\Delta\varphi$, we are led to the following version of Euler's equations with gravitation: Find $\hat{u} = (\varphi, m, e)$ depending on $(x,t) \in Q \equiv \Omega \times I$ such that

$$\begin{aligned} \Delta\dot{\varphi} + \nabla \cdot m &= 0 \quad \text{in } Q, \\ \dot{m} + \nabla \cdot (mu) + \nabla p - \rho\nabla\varphi &= 0 \quad \text{in } Q, \\ \dot{e} + \nabla \cdot (eu) + p\nabla \cdot u &= 0 \quad \text{in } Q, \\ u \cdot n &= 0 \quad \text{on } \Gamma \times I \\ \varphi &= 0 \quad \text{on } \Gamma \times I \\ \hat{u}(\cdot, 0) &= \hat{u}^0 \quad \text{in } \Omega, \end{aligned} \tag{32.1}$$

where $u = \frac{m}{\Delta\varphi}$, $p = (\gamma - 1)e$ with $\gamma > 1$, and we normalize the gravitational constant to unity.

32.2 The Hen and the Egg

An interesting aspect of this model with the gravitational potential φ as a primary variable and the mass distribution ρ as a derived quantity, is that it does not include *action at distance* in the same way as the conventional model with φ derived from ρ through Poisson's equation $\Delta\varphi = \rho$. Instead we have to deal with the new equation $\Delta\dot{\varphi} + \nabla \cdot m = 0$, still containing the Laplacian.

Considering the equation $\Delta\varphi = \rho$ as defining φ in terms of ρ or vice versa, of course connects to which comes first: the egg or the hen.

Choosing (in an exam for example) to explain either how a hen can lay an egg or how an egg can develop into a hen, you may go for the first option as appearing to be (somewhat) simpler to deal with. The idea would be that it would be advantageous to choose the more complex object of the potential/hen rather than the simpler mass/egg, as the primary unknown which will come out by solving the equations, (by some form of computation). Thus the more complex object, the potential/hen will be "created by computation" in front of our eyes, thus relieving us from *explaining* how a mass/egg can create a potential/hen. But doing so we have to deal with the equation $\Delta\dot{\varphi} + \nabla \cdot m = 0$ expressing "mass conservation" in a non-standard form, which admittedly seems to involve action at distance if we rewrite it in the form. $\dot{\varphi} + (\Delta)^{-1}\nabla \cdot m = 0$ for the purpose of explicitly updating φ by time-stepping. What can we do to allow time-stepping without inverting the Laplacian?

32.3 Perturbed Mass Conservation

Well, we may consider to perturb the equation for mass conservation $\Delta\dot{\varphi} + \nabla \cdot m = 0$ into:

$$\kappa\ddot{\varphi} - \Delta\dot{\varphi} - \nabla \cdot m = 0$$

with κ a small positive constant, now allowing time stepping without inverting the Laplacian. Of course, you could regularize the equation $\Delta\varphi = \rho$ similarly into $\kappa\dot{\varphi} - \Delta\varphi = \rho$ keeping mass conservation in the standard form $\dot{\rho} + \nabla \cdot (\rho u) = 0$. In any case, (32.1) with φ instead of ρ and a perturbed equation for mass conservation, is a model without action at distance.

32.4 Gravitons?

Solving Poisson's equation $\Delta\varphi = \rho$ equation for the gravitational potential φ in terms of the density ρ, reflect that (somehow) a mass distribution "creates" its own gravitational field (seemingly infinitely fast). The physics of this creation of a hen out of an egg in the form of a gravitational potential/force from a mass distribution, is unknown: A conjecture is that the gravitational field is established through an *exchange* of certain hypothetical particles called *"gravitons"*. But no gravitons have been detected despite intense search.

The reverse question is how a hen can lay an egg or how a gravitational potential can "create" a mass. A potential with a sharp peak of the form $\frac{1}{4\pi|x-\bar{x}|}$, would then represent a unit mass at position $\bar{x}$. In this perspective a tendency of "mass lumping" from very small initial density variations, is to be expected from the fact that application of the Laplacian may enhances variations and thus create positive and negative peaks/masses out of nothing, with masses of different equal signs attracting each other and masses with different signs repelleing each other. Our Universe with positive masses would thus have a twin Universe with negative masses.

In this model, it is thus the gravitational potential φ, which is given initially and which evolves in time (together with momentum and energy) and from which the mass density ρ is generated by $\Delta\varphi = \rho$ in a local "creation process". We here avoid action at distance and we also get a hint to the possible nature of all the "dark mass" seemingly required to account for the observed gravitational forces on cosmic scales, as mollified potential peaks not strong enough to "create visible mass", but yet having gradients and exerting gravitational forces.

32.5 The 2nd Law with Gravitation

The 2nd Law with gravitation takes the form

$$\dot{K} = W - D + P, \quad \dot{E} = -W + D, \quad D > 0, \tag{32.2}$$

where

$$P = -\int_\Omega \rho \nabla\varphi \cdot u \, dx = +\int_\Omega \varphi \nabla \cdot m \, dx = -\int_\Omega \varphi \dot{\rho} \, dx = \dot{\Phi},$$
$$\Phi = -\frac{1}{2}\int_\Omega \varphi \Delta\varphi \, dx = \frac{1}{2}\int_\Omega |\nabla\varphi|^2 \, dx.$$

By summation, we have

$$\frac{d}{dt}(K + E - \Phi) = 0$$

stating that the total energy, the sum of kinetic, heat and gravitational energy $K + E - \Phi$, is conserved.

32.6 Irreversibility and Heat Death

A natural scenario is to start with a hot compressed gas at rest, which is let free to expand in a *Big Bang* with $W - D - P > 0$ setting the gas in motion until $W - D - P < 0$ and $K = 0$, whereupon the gas contracts by gravitation back to a hot compressed state in a *Big Crunch* allowing the process to start all over with a new Big Bang.

In each cycle of this process some kinetic energy would irreversibly be transformed into heat energy, which ultimately could lead to a stationary state with $W = D$ and $P = 0$, a *heat death*. But the whole process may have many cycles....and so there may have been Worlds and intelligent cultures including thermodynamics even before the Big Bang of the World we happen to live in...

32.7 EG2 Simulations of a Self-Gravitating Gas

We give below some results from G2 solutions of (32.1) showing the development mass granularity from uniform mass distributions under expansion.

Figure 32.1: Cosmology theories

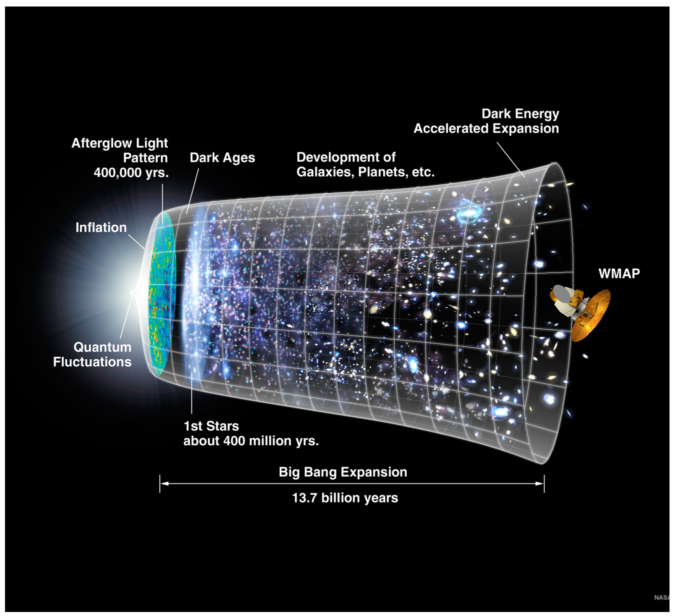

Figure 32.2: Big Bang expansion

Chapter 33

Information

> The fundamental problem of communication is that of reproducing at one point either exactly or approximately a message selected at another point. (Shannon in [40], 1948)

> You should call it entropy for two reasons; in the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, no one knows what entropy really is, so in a debate you will always have an advantage. (von Neumann to Shannon)

33.1 Introduction

Information theory was created by Shannon [40] in the 1940s borrowing the concept of entropy from thermodynamics. We now explore if the new foundation of thermodynamics presented may open to a new approach to information theory. We thus consider a model of *information flow* in the form of the Euler equations for a variable density incompressible fluid flow with the distribution in space of *mass density* representing information like a message, image or movie, which is being transported or *communicated* from one location to another by the fluid flow. The key question is what aspects of the information which can be communicated to what precision. We expect to see fine details of an image being distorted or destroyed by the communication, while gross features may remain unaltered. We introduce a measure of *irrecoverable loss of information*, which couples to increase of entropy in the classical setting, which corresponds to information which cannot be retrieved.

We thus distinguish between *recoverable information*, which can be recovered from a distorted image by some form of image processing, and *irrecoverable information* which cannot be recovered by image processing.

33.2 Entropy vs Loss of Information

In Shannon's information theory the notion of entropy is used to measure the randomness or complexity of the information to be communicated, with random complex information requiring more work to communicate than organized simple information. Shannon's entropy thus is a measure of the work to communicate certain information, assuming that the communication itself does not distort the information. In this setting information is coded into a digital representation, which is communicated without loss of any digits and then is decoded after reception. The main question then concerns the number of digits required to represent the information, which directly couples to the work of accurate communication of the digits. In Shannon's theory the digital coding in general introduces a certain loss of information, with more loss for complex information, while the communication of the digital representation is assumed to be without loss. Shannon's entropy thus may be viewed as a measure of loss of information arising from the digital representation but not from the communication.

Our notion of entropy is a bit different and measures the *total loss of information* taking into account not only the loss from digital representation, but also from the communication process itself. In our setting, the digital representation of the information as a mass density, is a finite element approximation on a mesh of certain mesh size h, which can be viewed as generalized Fourier or wavelet representation, and the communication is realized through a finite element solution of the Euler equations. The mesh size h directly couples to the work required for the communication.

The main aspects influencing the total loss of information, and thus the error in the communication, relate to (a) the complexity of the information and (b) the complexity of the communication process, where (b) can be viewed as a measure of the distortion from the communication process. We identify the following basic cases:

(i) simple information and simple communication,

(ii) complex information and simple communication,

(iii) simple information and complex communication,

(iv) complex information and complex communication.

We will see that in (i) the loss of information typically is small, in case (ii) and (iii) it is of medium size, and in case (iv) it is large. We will see that (i) requires little work (h is not small), (ii) and (iii) require medium work and (iv) large work (h small), for the same accuracy. We shall see that if the communication is partly *turbulent*, which is the generic case, then the loss of information cannot be made arbitrarily small by decreasing h, relecting that the turbulent dissipation has a non-zero limit as h tends to zero.

33.3 A Model Problem

As a simple model of communication, we consider the following 1d transport equation:

$$\begin{aligned} \dot\rho + \rho' &= 0 \quad \text{for } 0 < x < 1\,, 0 < t \leq 2, \\ \rho(x,0) &= 0 \quad \text{for } 0 < x < 1 \end{aligned} \tag{33.1}$$

where $\dot\rho = \frac{\partial\rho}{\partial t}$, $\rho' = \frac{\partial\rho}{\partial x}$, and $\rho(0,t) = \rho^-(t)$ with $0 \leq t \leq 1$ represents an input signal and $\rho^+(t) = \rho(1,t)$ with $1 \leq t \leq 2$ the corresponding output signal. Since the solution to the convection equation is given by $\rho(x,t) = \rho(0,t-x)$ for $t \geq x$, we simply have $\rho^+(t) = \rho(1,t) = \rho(0,t-1) = \rho^-(t-1)$ for $1 \leq t \leq 2$, that is, the output signal is equal to the input signal with a unit time delay.

Let now ρ_h be a finite element computational solution of the convection problem representing a realization of the communication from input to output with a certain imprecision due to the numerics. More precisely, let $\rho_h \in V_h$ be a cG(1)-solution determined by

$$((\dot\rho_h + \rho_h', v)) + (\rho(0,\cdot) - \rho^-, v(0,\cdot)) + ((h\rho_h', v')) = 0, \quad \text{for all } v \in V_h, \tag{33.2}$$

where V_h is the set of continuous piecewise linear functions on a space-time mesh of $Q = [0,1] \times [0,2]$ with mesh size h, $((v,w)) = \int_Q vw\,dxdt$ and $(v,w) = \int_0^1 vw\,dx$. Here, the first two terms come out of Galerkin's cG(1)-method and boil down to a centered difference scheme on a regular mesh and the the third term is a stabilizing artifical viscosity term. More generally, we may apply the G2 (General Galerkin) method with a residual-based artificial viscosity.

We observe observe the reverse communication process taking ρ^+ to ρ^-, would read: Find $\rho \in V_h$ such that

$$((v, -\dot{\rho}_h - \rho_h')) + (\rho(1,\cdot) - \rho^+, v(1,\cdot)) + ((h\rho_h', v')) = 0, \quad \text{for all } v \in V_h,$$

where $(v,w) = \int_1^2 vw\,dx$. This means that neglecting the viscous terms, we could retrieve ρ_h^- exactly from ρ_h^+ by time stepping backwards in time. In contrast, we cannot "undo" the effect of the viscous term in a process from ρ_h^- to ρ_h^+, since time stepping backwards with the artificial viscosity present would just add more diffusion to the process.

To study the resulting output error in the communication from ρ^- to ρ^+, let $\psi(t)$ with $1 \le t \le 2$ be a given weight function, and let $\varphi(x,t)$ solve the dual problem

$$\begin{aligned} -\dot{\varphi} - \varphi' &= 0 \quad \text{for } 0 < x < 1\,, 0 < t \le 2, \\ \varphi(x,2) &= 0 \quad \text{for } 0 < x < 1, \\ \varphi(1,t) &= \psi(t) \quad \text{for } 1 < t < 2. \end{aligned} \tag{33.3}$$

Multiplying the dual equation by $e = \rho - \rho_h$, integrating by parts and using (33.2) assuming $\rho_h(0,\cdot) = \rho^-$, we obtain the following error representation:

$$E_h \equiv \int_1^2 (\rho^+ - \rho_h(1,\cdot))\psi dt = \int_1^2 e(1,t)\psi(t)\,dt = ((R(\rho_h), \varphi - \varphi_h)) + ((h\rho_h', \varphi_h')),$$

where $R(v) = \dot{v} + v'$, and $\varphi_h \in V_h$ is a finite element approximation φ.

It is now natural to define $I = (R(\rho_h), \varphi - \varphi_h))$ to represent a *recoverable* error, and $II = ((h\rho_h', \varphi_h'))$ an *irrecoverable* error. In particular, choosing φ_h to be a cG(1)-approximation, we can make the I vanish, which may be viewed as retrieving ρ^- by backwards time stepping. With this motivation we now focus on the irrecoverable part II of the error, neglecting here the recoverable part I, and thus consider the error representation

$$E_h \approx ((h\rho_h', \varphi_h')). \tag{33.4}$$

We can now rephraze the above basic cases as follows: (i) ρ_h and φ_h smooth, (ii) ρ_h smooth and φ_h non-smooth , (iii) ρ_h non-smooth and φ_h smooth, and (iv) ρ_h non-smooth and φ_h non-smooth. We will then typically have in case (i): $E_h \approx h$, in cases (ii) and (iii): $E_h \approx \sqrt{h}$ and in case (iv): $E_h \approx 1$. We may refer to (i) and (ii) as laminar cases and (iii) and (iv) as turbulent cases. With a smooth φ, we measure the output error in a weak mean value sense, and with a non-smooth φ_h we measure the error in a more pointwise sense. We see that in the case of non-smooth ρ_h, only mean-value outputs can be meaningful.

Viewing entropy as a measure of loss of information, we may say that (i) has small entropy production or little loss of information, (ii) and (iii) has medium entropy production and loss of information while (iv) has massive entropy production and loss of information.

33.4 Simulations in Model Problem

33.5 Euler's Equations

We now generalize to the Euler equations for a variable density incompressible fluid over a time interval $I = (0, T)$, in a cylinder $\Omega = \{x = (x_1, x_2, x_3) = (x_1, \bar{x}) : 0 \leq x_1 \leq L, |\bar{x}| \leq R\}$ of length L and radius R, with boundary Γ with outward unit normal n, take the form: Find the *density* $\rho(x, t)$, the *flow velocity* $u(x, t)$ and *pressure* $p(x, t)$, such that

$$
\begin{aligned}
\dot{\rho} + \nabla \cdot (\rho u) = 0 \quad & \text{in } \Omega \times I, \\
\dot{u} + u \cdot \nabla u + \frac{\nabla p}{\rho} = 0 \quad & \text{in } \Omega \times I, \\
\nabla \cdot u = 0 \quad & \text{in } \Omega \times I, \\
u \cdot n = u^- \quad & \text{on } \Gamma^- \times I, \\
\rho = \rho^- \quad & \text{on } \Gamma^- \times I, \\
\rho(\cdot, 0) = \rho^0,\ u(\cdot, 0) = u^0 \quad & \text{in } \Omega,
\end{aligned}
\tag{33.5}
$$

where the fluid enters Ω through $\Gamma^- = \{x \in \Gamma : x_1 = 0\}$ with a given inflow velocity $u \cdot n = g < 0$ and leaves through $\Gamma^+ = \{x \in \Gamma : x_1 = L\}$ with $u \cdot n > 0$, and $u \cdot n = 0$ on the remaining (inpenetrable) part of the boundary. Here $\rho(0, \cdot, \cdot) = \rho^-$ represents a given input signal, or rather movie, consisting of a sequence of time dependent 2d images $\rho^-(\cdot, t)$ with $t \in I$, defined on the cylinder cross section $\omega = \{\bar{x} : |\bar{x}| \leq R\}$, which is transported by the flow through the channel to an output movie $\rho^+(\cdot, t) = \rho(L, \cdot, t)$ for t in a relevant interval. The communication thus concerns the transformation of ρ^- to ρ^+. The basic problem concerns the *distortion* $d = \rho^+ - \rho^-$, which measures the *accuracy* of the communication.

It is natural to assume that $\rho = \bar{\rho} + \tilde{\rho}$ where $\bar{\rho}$ is a constant given "background" and $\tilde{\rho}$ contains the information of interest. Replacing ρ by $\bar{\rho}$ the second equation (momentum equation) takes the form $\dot{u} + u \cdot \nabla u + \nabla \bar{p} = 0$ with the modified pressure $\bar{p} = p/\bar{\rho}$. This decouples ρ from the last two equations, which determine $(u, \bar{p})$ as a solution to the (unit density) incompressible Euler equations. In this case, ρ thus can be determined from the first equation alone, which with $(u, \bar{p})$ given is a linear convection equation. For simplicity we consider this decoupled situation below, in which the image itself is not influencing the flow, and thus is transported "passively".

The solution $(u, \bar{p})$ to the (unit density) incompressible Euler equations in general is (partly) *turbulent* with a complex flow velocity u, and thus the image $\rho(\cdot, t)$ in general is convected in a (partly) complex convection field with a corresponding distortion. For short time also a *laminar* smooth flow velocity u is possible. Thus the image can be convected by a laminar or turbulent flow velocity, with vastly different distortion effects.

33.6 Finite Precision Euler Solution: G2

We solve the Euler equations (33.5) using as above a stabilized cG(1)-method on a finite element mesh in space-time with mesh size $h(x, t)$, and denote the finite element solution by $\hat{u}_h = (\rho_h, u_h, p_h)$ with output ρ_h^+. We will compare with a non-distorted output $\rho^+ = \rho^-$ convected by a constant velocity field $\bar{u}(x, t) = (\bar{u}_1, 0, 0)$, where $\bar{u}_1$ is a representative inflow velocity. We will thus as a measure of the distortion, use the mean value

$$E_h = \int_\omega (\rho^- - \rho_h^+)\psi \, d\bar{x} \, dt. \tag{33.6}$$

where $\psi(\bar{x}, t)$ is a weight function.

33.7 Error Estimation by Duality

As in the model problem, we may assume that (see [20] for details)

$$E_h \approx ((h\nabla \rho_h, \nabla \varphi_h)),$$

where $((v,w)) = \int_0^T \int_\Omega vw\,dx\,dt$, and φ_h is an approximate solution of the dual problem

$$-\dot{\varphi} - u_h \cdot \nabla\varphi = 0 \quad \text{in } \Omega \times I,$$

$$\varphi(L,\cdot,\cdot) = \psi \quad \text{in } \omega \times I,$$

,

$$\varphi(\cdot,T) = 0 \quad \text{in } \Omega,$$

,

33.8 Laminar and Turbulent Communication

As in the model problem, E_h depends both on $\nabla\rho_h$ and $\nabla\varphi_h$. If u is turbulent, then E_h may be small if ψ is smooth with large support, corresponding to a gross feature of interest. If u is laminar, then E_h may be small also for a small feature of interest.

33.9 The 2nd Law

The basic energy balance for ρ_h reflecting the structure of the stabilized cG(1) method, reads:

$$\int_{I^+}\int_\omega \rho_h(L,\bar{x},t)^2\,dx\,dt + D(\rho_h) = \int_{I^-}\int_\omega \rho_h(0,\bar{x},t)^2\,dx\,dt$$

where

$$D(u_h;\rho_h) = \int_0^T \int_\Omega h|\nabla\rho_h|^2\,dx\,dt,$$

and I^- and I^+ are relevant time intervals for input and output, respectively. As above, $D(u_h;\rho_h)$ represents an *irrecoverable loss of information.* Reversing the process letting ρ_h convect backwards in time starting from $\rho_h(\cdot,T)$, we have an analogous energy balance with a new dissipation term of positive sign, showing that the initial data $\rho(\cdot,0)$ cannot be fully recovered.

33.10 Dissipation of Information

As a rough measure of the amount of irrecoverable information we may use the *total dissipation of information*:

$$D_h = \int_0^T \int_\Omega h|\nabla \rho_h|^2 \, dx \, dt.$$

33.11 Simulations

We consider communication in cylindrical channels of different length. If the channel is short enough, then the flow may stay laminar all along the channel and the image suffer little distortion, while if the flow gets turbulent, then the image may get more distorted. Because of boundary layer effects the distortion will usually be bigger close to the boundary.

We also study the effects of different obstructions in the channel perturbing the flow, modeling a communication system with bottle-necks.

Figure 33.1: Flow of information at New York Stock Exchange

Chapter 34

Traffic Flow

> I think the idea of getting out of a traffic jam and getting out of work each week and going and doing all this stuff would be really exhausting.(Paul McCarthy)

34.1 A Model of Traffic Flow

We return to the simple traffic model which we considered above as a variant of Burgers equation: Find the density $\rho(x,t)$ and the velocity $u(x,t)$ such that

$$\begin{aligned} \dot{\rho} + (u\rho)' = 0 \quad \text{for } x \in \mathbb{R},\, t > 0, \\ \rho(x,0) = \rho^0(x) \quad \text{for } x \in \mathbb{R}, \end{aligned} \tag{34.1}$$

combined with the constitutive law $u = (1-\rho)$, assuming $0 \leq \rho^(x) \leq 1$ for $x \in \mathbb{R}$.

34.2 Shocks and Congestions

We have seen that a shock corresponds to the abrupt changes of density and velocity encountered when the end of que of packed cars at rest is propagating in the opposite direction to the direction of the traffic.

34.3 Rarefactions and Traffic Lights

A rarefaction solution corresponds to the situation when at a traffic light turning green, the cars gradually accelerate one after the other. A nonphysical shock solution corresponds to the familiar situation when the driver in the first car at the traffic light, does not notice the light turning green, with the instability of this situation being illustrated by the fact that a slight "honk" usually will alert the driver to get going and allowing the rarefaction to develop. Instead of a honk a little bit of viscosity will get the car going.

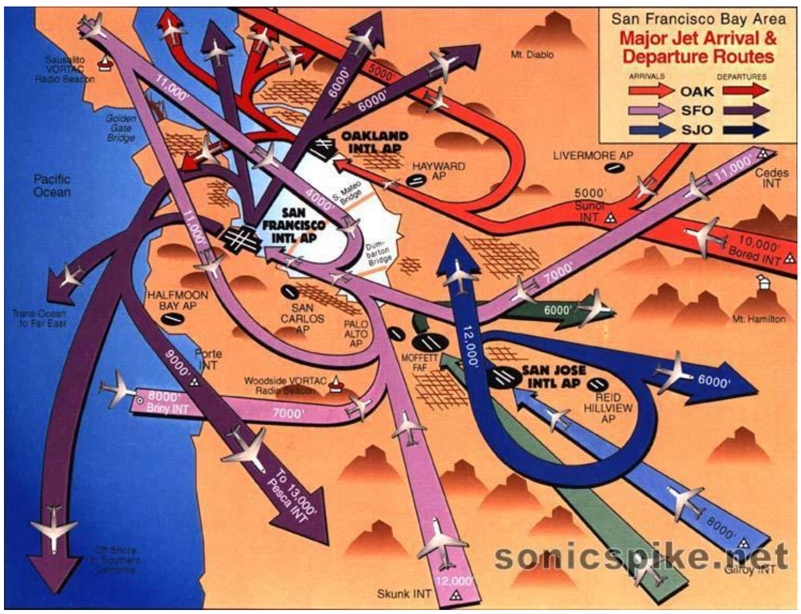

Figure 34.1: Traffic flow in the Bay Area

Chapter 35

Economy

> As every individual, therefore, endeavours as much as he can both to employ his capital in the support of domestic industry, and so to direct that industry that its produce may be of the greatest value; every individual necessarily labours to render the annual value of society as great as he can. He generally, indeed, neither intends to promote the public interest, nor knows how much he is promoting it. By preferring the support of domestic to that of foreign industry, he intends only his own security; and by directing that industry in such a manner as its produce may be of the greatest value, he intends only his own gain, and he is in this, as in many other cases, led by an invisible hand to promote an end which was no part of his intention. Nor is it always the worse for the society that it was no part of it. By pursuing his own interest he frequently promotes that of society more effectually than when he really intends to promote it. I have never known much good done by those who affected to trade for the public good. It is an affectation, indeed, not very common among merchants, and very few words need be employed in dissuading them from it. (Adam Smith)

35.1 A Flow Model

We model an economy as a form of of reactive flow in a network.

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