# COMPUTATIONAL THERMODYNAMICS

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www.bodysoulmath.org, www.fenics.org, www.icarusmath.com

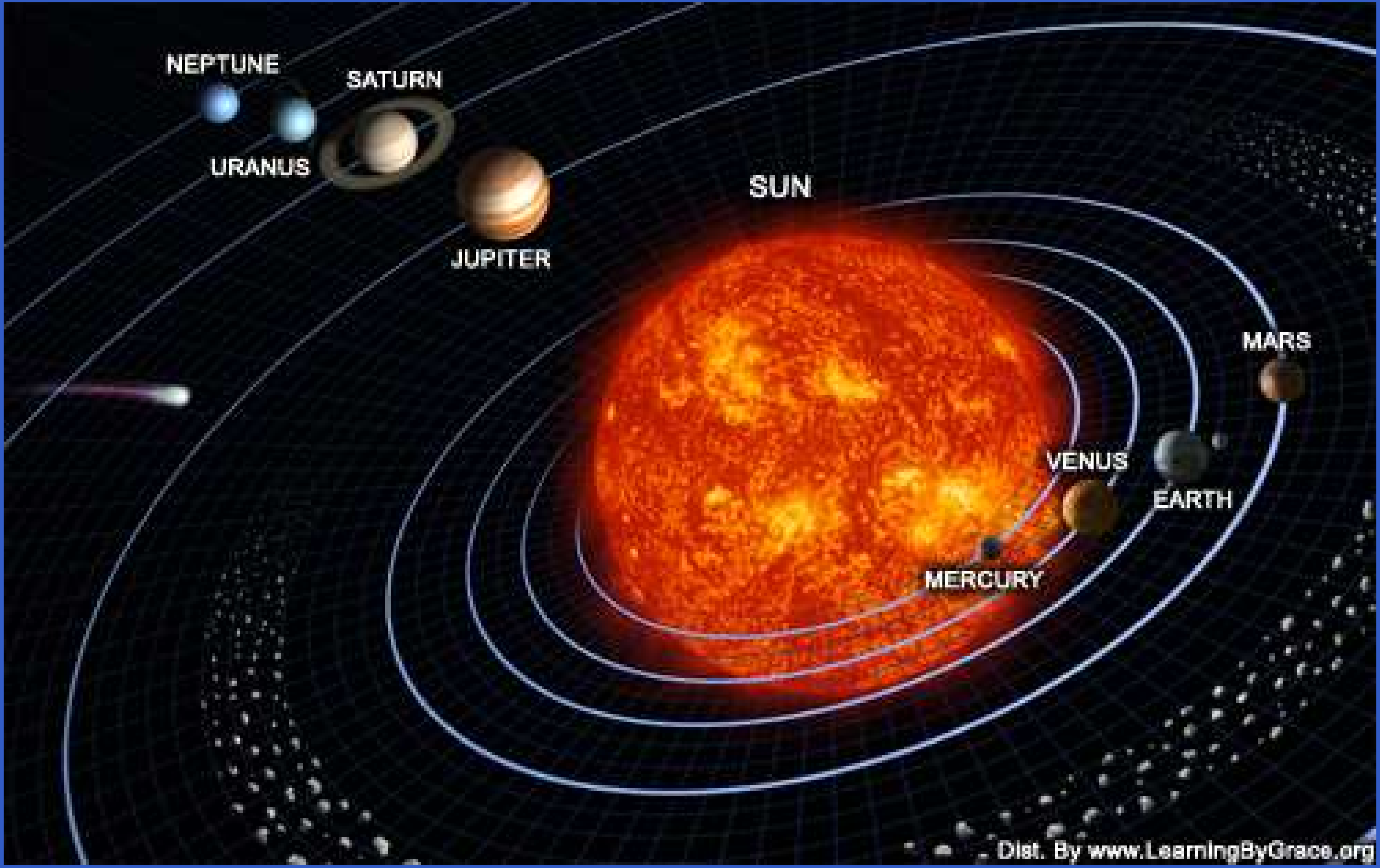
# PERSPECTIVE: Three Periods

- CLASSICAL 1600-1900
- MODERN 1900-2000
- POST-MODERN 2000-
- Where Do We Live?

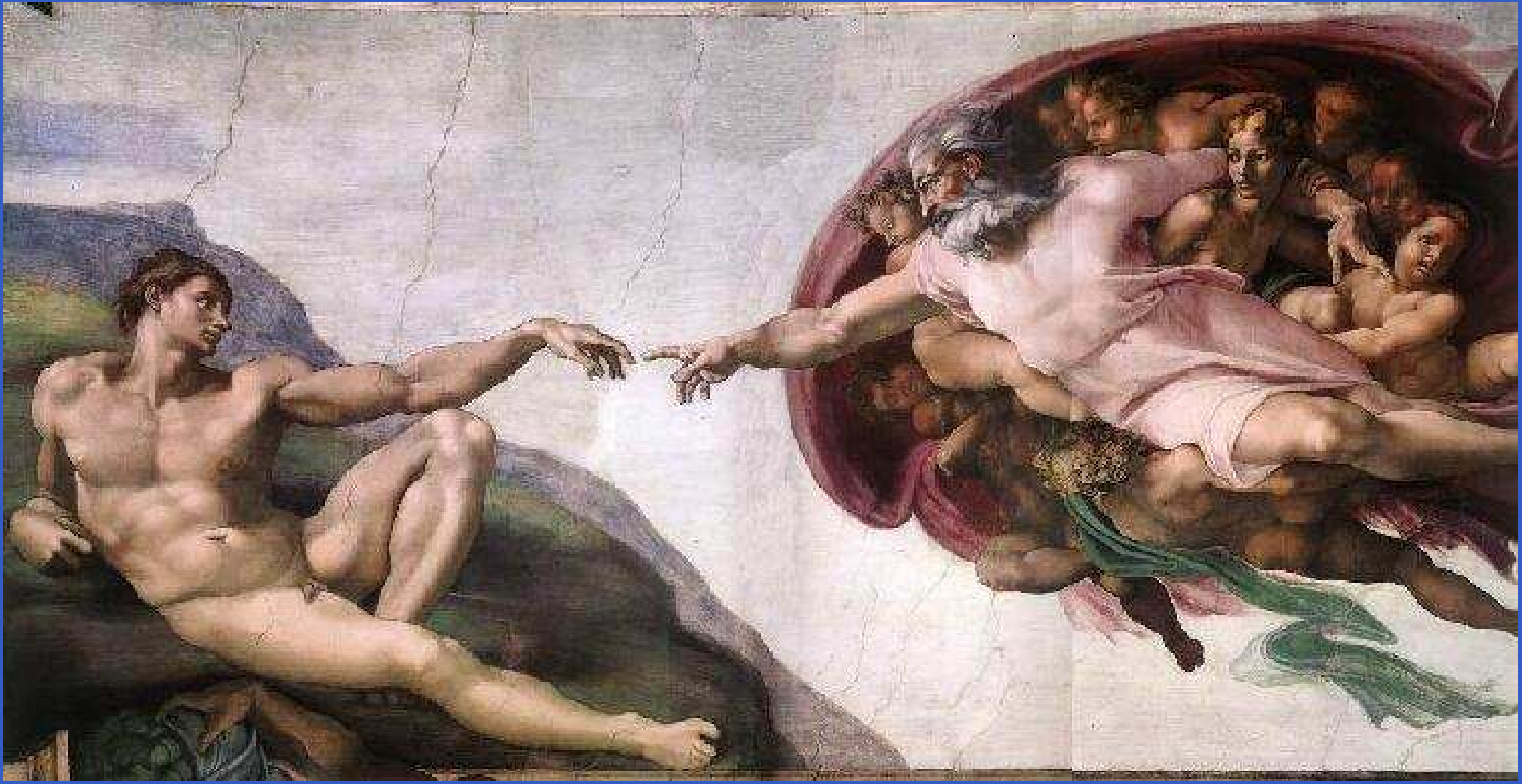
# Classical 1600-1900

- Mathematics: Calculus: Analytical Solution
- Physics: Newtonian Mechanics
- Industrial Society: Mass Production
- Leibniz Newton Euler Lagrange Laplace...
- Main Challenges:
- N-Body, Heat, Wave, ElectroMagnetism

# Solar System



# Local Interaction: Aristotle

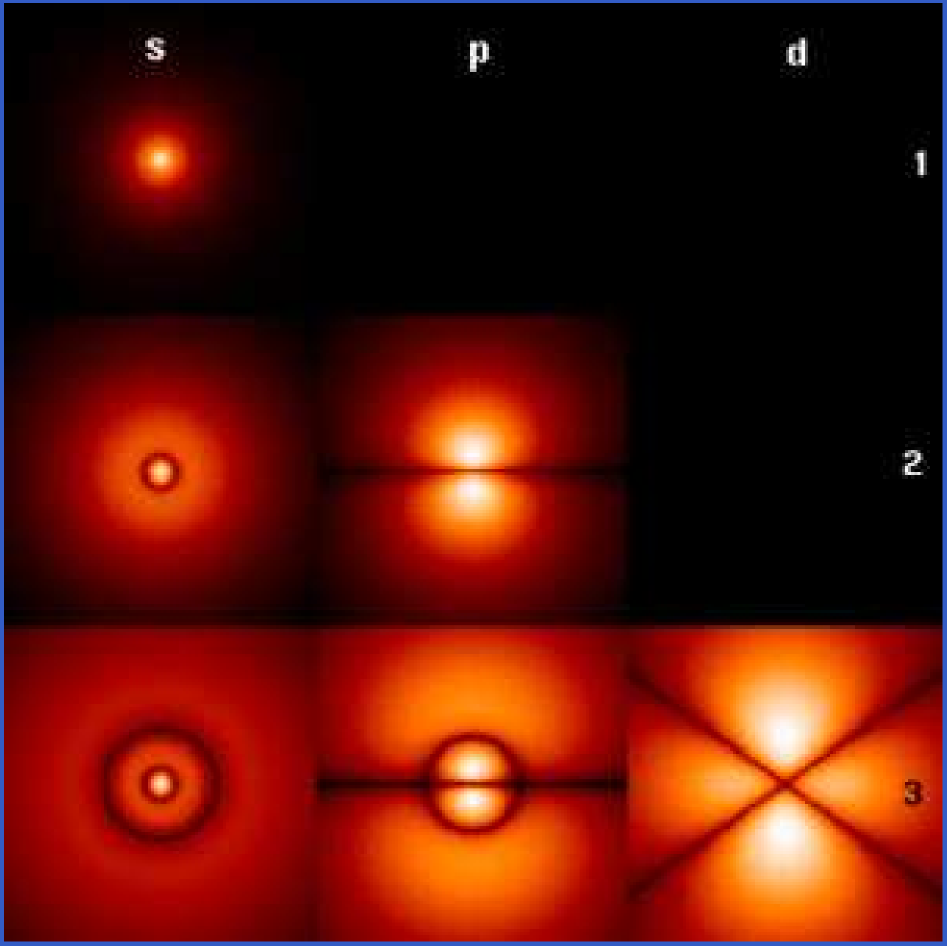


# Action at Distance: Newton

# Modern 1900-2000

- Mathematics: Calculus: Existence of Solution
- Physics: Quantum Mechanics Relativity
- Service Society
- Hilbert Courant von Neumann Lions Lax...
- Main Challenges: Turbulence, Quantum Mech

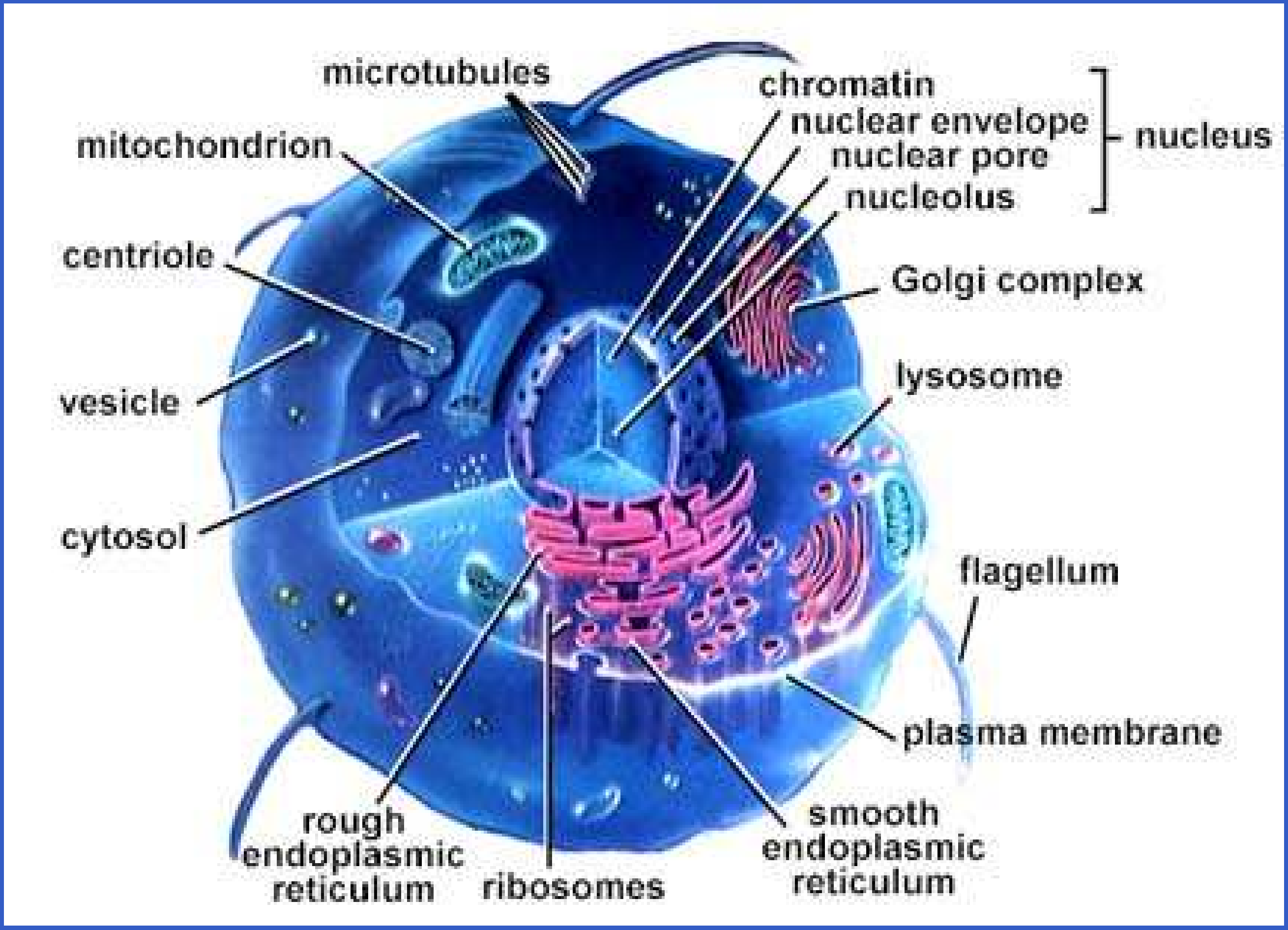
# Schrödinger Equation: Electron Density



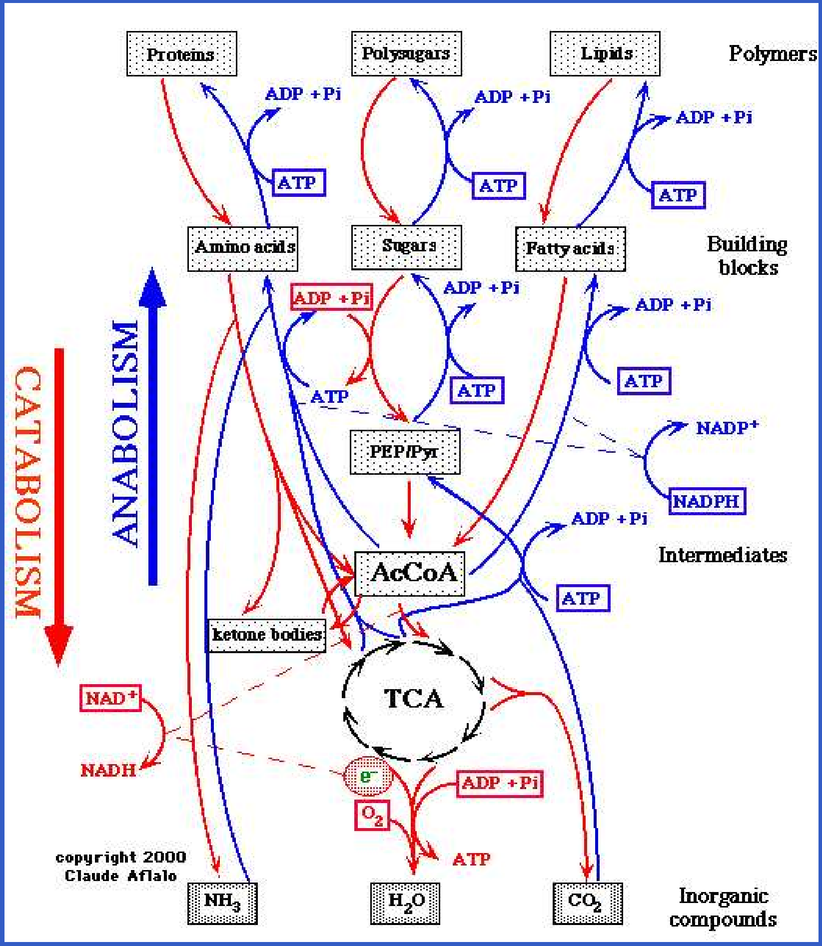
# Post-Modern 2000–

- Mathematics: COMPUTATIONAL CALCULUS
- COMPUTATIONAL SOLUTION
- Physics: Nano-Micro-Bio—Cosmology
- INFORMATION SOCIETY:
- SIMULATION–VIRTUAL REALITY

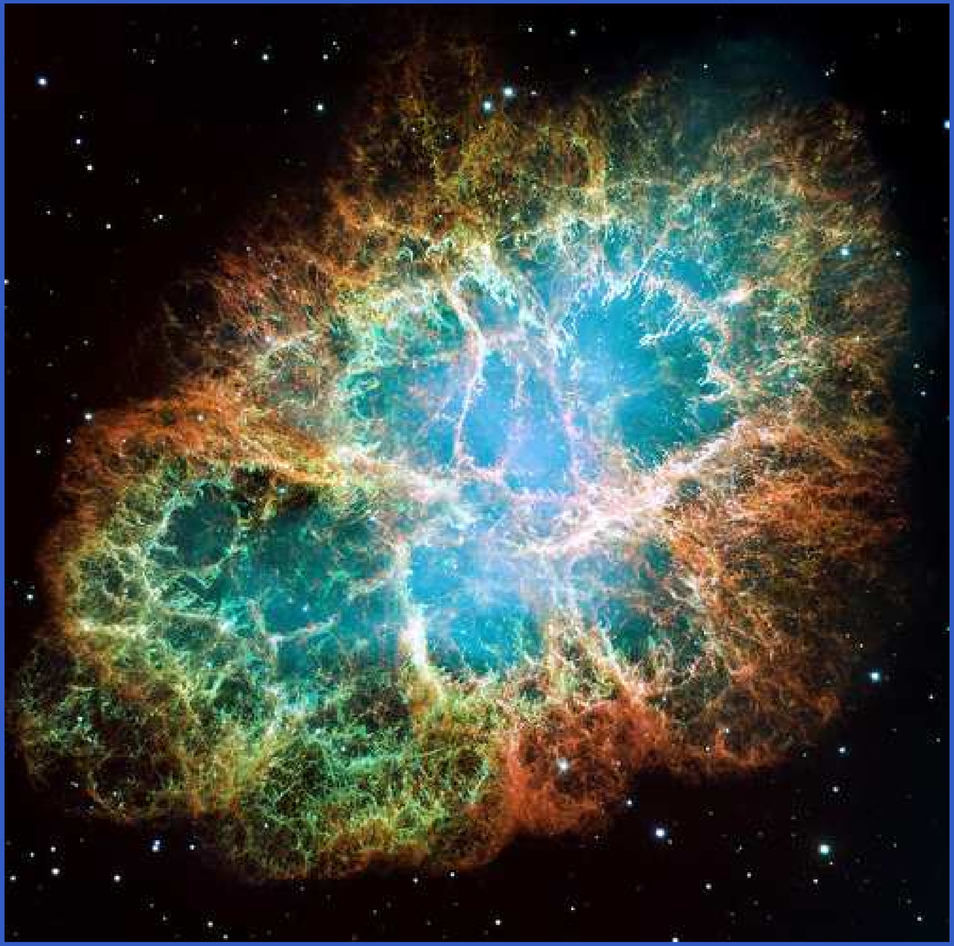
# CHALLENGE: LIFE



# CHALLENGE: LIFE



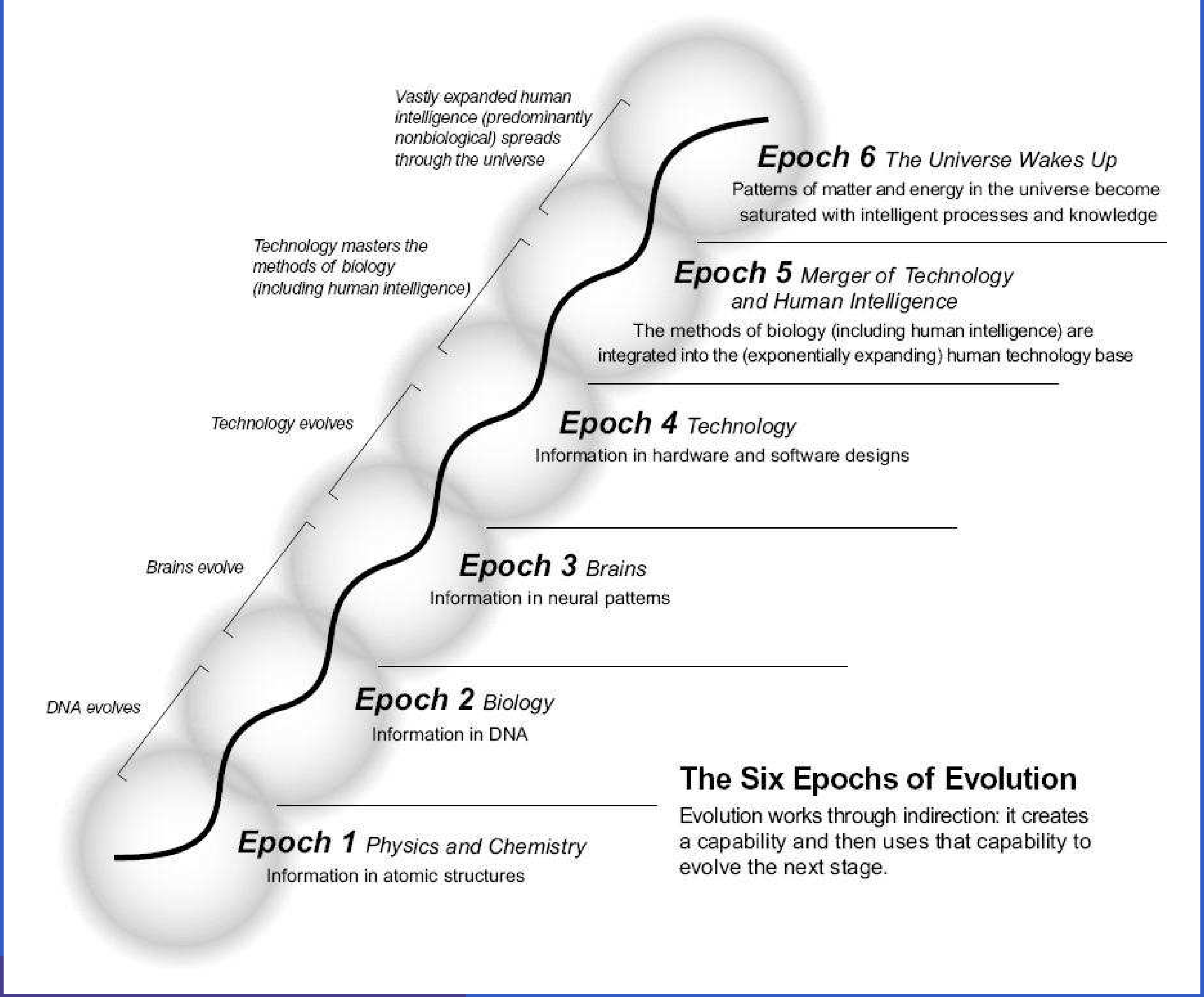
# CHALLENGE: BIG BANG



# Kurzweil: Singularity 2045

- Kurzweil: Synthesizer....
- Moore's law:
- Computational power doubles every 18 months
- DIGITAL SIMULATION
- Computational Technology Blow Up 2045
- Infinite speed of development

# Kurzweil: Epochs of Evolution



# Baudrillard: SIMULATION

- Copy of Reality
- Confusion Simulation–Reality
- Mask of Nonexisting Reality:
- HYPERREALITY
- HyperMarkets

# HYPERREALITY (masking reality)

# Deleuze: SIMULATION

- SIMULATION is REALITY
- REALITY is SIMULATION

# SIMULATION

- Math: COMPUTATIONAL CALCULUS
- Physics: Basic Conservation Laws
- Chemistry-Biology—: Constitutive Laws
- COMPUTATIONAL TECHNOLOGY

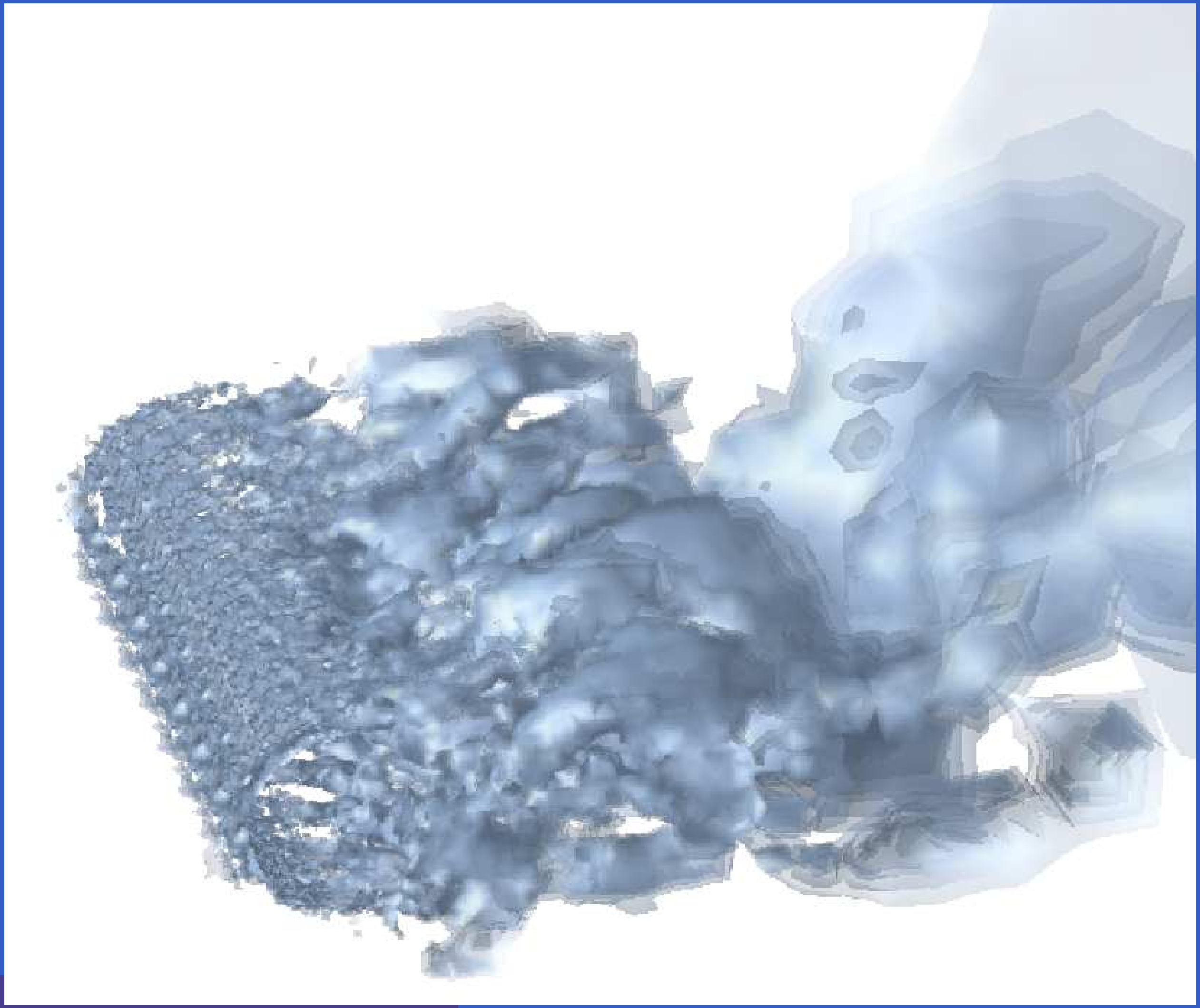
# TEST: THERMODYNAMICS

- DIFFICULT!!
- Why?
- TURBULENCE/SHOCKS!!

# THERMODYNAMICS

- Kinetic Energy $\longrightarrow$ Heat Energy

# CIRCULAR CYLINDER RE$= 3900$



# CLASSICAL THERMODYNAMICS

- DIFFICULT
- 2nd LAW?
- Who can understand and teach?
- Lars Onsager (1903-1976), Nobel Prize 1968
- Ilya Prigogine Nobel Prize 1989
- STATISTICAL MECHANICS
- Microscopic Games of Roulette
- PLANCK: ACT of DESPERATION!

# 1st LAW: EASY

- CONSERVATION of Mass, Momentum, Energy
- EULER EQ PERFECT IDEAL GAS
- UNDERSTANDABLE.

# Classical 2nd LAW

**First Law of Thermodynamics** – *Conservation of Energy*

**Second Law of Thermodynamics** – *It is not possible to create a cyclical heat engine that draws heat from a reservoir without wasting some heat energy.*

**Entropy – is a measure of the disorder in the Universe. It must always increase; local decreases make a bigger mess elsewhere.**

# Classical 2nd LAW

- The 2nd Law cannot be derived from purely mechanical laws. It carries the stamp of the essentially statistical nature of heat. (Bergman in Basic Theories of Physics 1951)
- The total energy of the universe is constant; the total entropy is continually increasing. (Rudolf Clausius 1865)
- PHYSICAL SIGNIFICANCE of ENTROPY??

# HYPER-REALITY

- NON-EXIST EXACT EULER SOL!!
- Reason: TURBULENCE/SHOCKS
- WEAK SOL: NOT STRONG SOL
- APPROX TURBULENT SOL EXIST
- G2: GENERAL GALERKIN
- SIMULATION of NONEXIST EXACT SOL
- DETERMINISTIC NEW 2nd LAW
- ARROW of TIME

# DETERMINISTIC 2nd LAW

- G2 satisfies 2nd LAW AUTOMATICALLY
- PENALTY for not being EXACT
- TURBULENT DISSIPATION
- Kinetic Energy $\longrightarrow$ Heat Energy
- LOSSES
- Cooling of engine
- ARROW of TIME: IRREVERSIBILITY
- DETERMINISTIC: No Statistics!!

# 2nd LAW

- FINITE PRECISION:
- ANALOG or DIGITAL COMPUTATION
- EDGE STABILITY: Not Stable, Not Unstable

# EULER EQUATIONS

- air/water
- in fixed volume $\Omega$ in $\mathbb{R}^3$ with boundary $\Gamma$
- over a time interval $I$
- very small viscosity and heat conductivity
- density $\rho$
- momentum $m = \rho u$
- velocity $u = (u_1, u_2, u_3)$
- total energy $\epsilon$

# Conserv. Mass, Momentum, Energy

Find $\rho$, $m$ and $\epsilon$ such that in $\Omega \times I$

$$\begin{aligned} \dot\rho + \nabla \cdot (\rho u) &= 0 \\ \dot m + \nabla \cdot (m u) + \nabla p &= 0 \\ \dot\epsilon + \nabla \cdot (\epsilon u + p u) &= 0 \\ u \cdot n &= 0 \quad \text{on } \Gamma \times I \end{aligned}$$

inital condition

- $p$ *pressure*, $\dot v = \frac{\partial v}{\partial t}$
- SLIP BC

# Constitutive Equations

- $\epsilon = k + e$ total energy
- $k = \frac{\rho|u|^2}{2}$ *kinetic energy*
- $e = \rho T$ *internal energy*
- $T$ *temperature*.
- $p = (\gamma - 1)\rho T = (\gamma - 1)e$ *perfect gas*
- $\gamma > 1$ *gas constant*, $\gamma = 5/3$ monoatomic gas
- viscosity $\nu = 0$, heat conductivity $\kappa = 0$.

# What is VISCOSITY?

- Nobody knows!!
- kinematic, dynamic, laminar, turbulent,
- molecular, eddy,....??
- solution dependent losses??
- experimental determination??
- ????
- But we know it is small $\nu \leq 10^{-6}$
- Enough!! Euler: $\nu = 0$!!

# Einstein's DREAM

- $\gamma = 5/3$, $\nu = 0$, $\kappa = 0$.
- NO PARAMETER
- Predictive Power??
- YES!!
- The World as Analog Computation
- The World as Digital Computation

# HyperReality of Euler Equations

- NON-EXISTENCE of EXACT SOL: Inf small scales
- COMPUTATIONAL TURBULENT SOL EXIST
- GIVE USEFUL INFO:
- Predict Drag and Lift of Car/Aircraft!!
- (CALCULUS USELESS)
- (COMPUTATIONAL CALCULUS USEFUL)

# NS APPROX EULER

Find $\hat{u} = (\rho, m, \epsilon)$:

$$\begin{aligned} \dot{\rho} + \nabla \cdot (\rho u) &= 0 \\ R_m(\hat{u}) \equiv \dot{m} + \nabla \cdot (mu) + \nabla p &= -\nu \Delta u \\ \dot{\epsilon} + \nabla \cdot (\epsilon u + pu) &= 0 \end{aligned}$$

$$\int R_m(\hat{u})\varphi \, dxdt = \int \nu \nabla u \nabla \varphi \, dxdt = \sqrt{\nu} \|\varphi\|_{H^1}$$

- NS SOL: WEAK APPROX EULER SOL
- $\|R_m(\hat{u})\|_{H^{-1}} \approx \sqrt{\nu}$

# NS APPROX EULER

$$\int (\dot{m}+\nabla\cdot(mu)+\nabla p)\cdot u\,dx = \int \nu|\nabla u|^2 \equiv D(u) \approx 1$$

- $u$ Hölder 1/3
- $D(u) = 0$ if $u$ smoother, but $u$ is not (Onsager)
- NS NOT STRONG APPROX EULER

$$\int (\dot{m} + \nabla \cdot (mu) + \nabla p) \cdot u = \int \nu|\nabla u|^2$$

LARGE $=$ LARGE or LARGE - LARGE =0

# G2 APPROX EULER

- LEAST-SQUARES STABILIZED GALERKIN
- MESH SIZE $h$
- G2 SOL: WEAK APPROX EULER SOL
- $\|R(\hat{u})\|_{H^{-1}} \approx \sqrt{h}$
- $\nu \sim h$
- BOUNDARY LAYERS: $\nu \sim h^2$ (SLIP/FRICTION)

# STABILIZATION $\delta \sim h$

$$(\dot\rho + \nabla\cdot(\rho u), v) + (\delta u\cdot\nabla\rho, u\cdot\nabla v) = 0$$

$$(\dot m + \nabla\cdot(mu) + \nabla p, v) + (\delta u\cdot\nabla m, u\cdot\nabla v) = 0$$

$$(\dot\epsilon + \nabla\cdot(\epsilon u + pu), v) + (\delta u\cdot\nabla\epsilon, u\cdot\nabla v) = 0$$

STABILITY: $v = u$ in MOMENTUM:

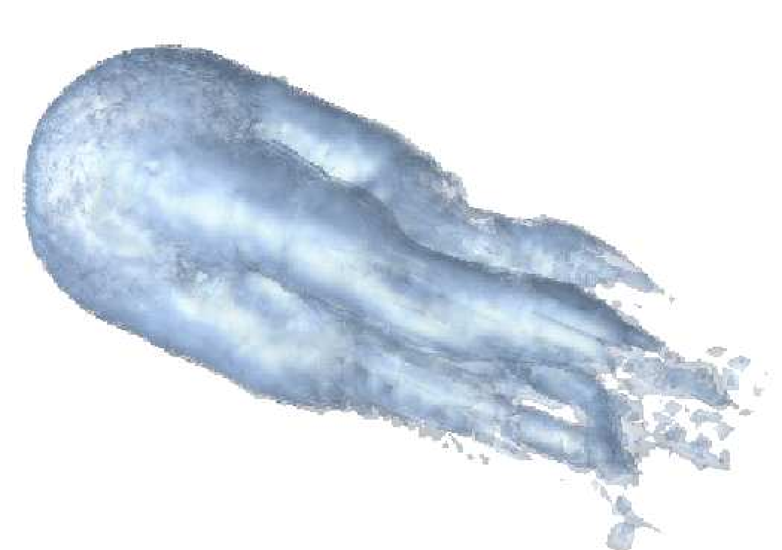
$$D_h(u) = \int h\rho|u\cdot\nabla u|^2 dxdt \quad \text{PENALTY}$$

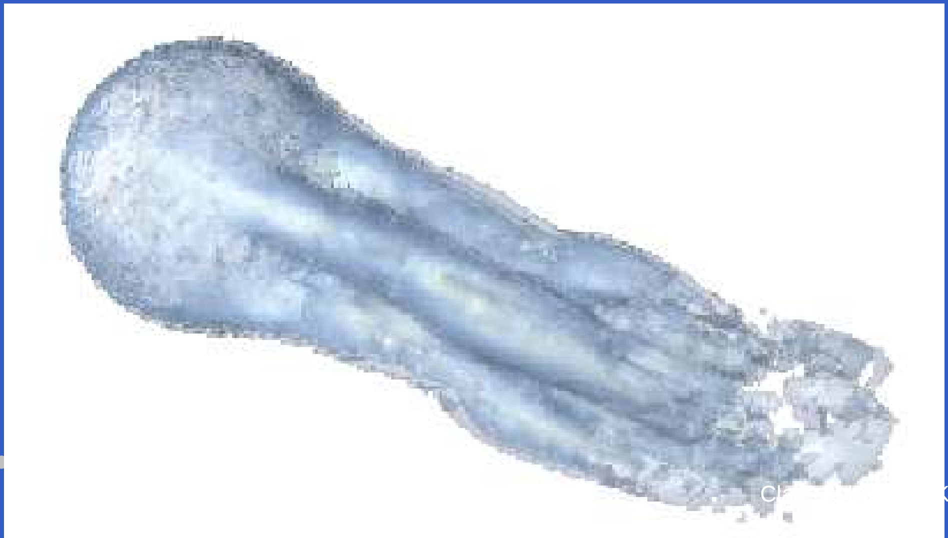
$$D(u) = \int \nu|\nabla u|^2 dx$$

# WEAK UNIQUENESS

- MEAN-VALUE INDEPENDENT of $h$ or $\nu$
- INDEPENDENCE on STABILIZATION
- FOCUS on $R(\hat{u})$ NOT $-\nu\Delta u$
- $R(\hat{u})$ CANNOT BE STRONGLY SMALL!!

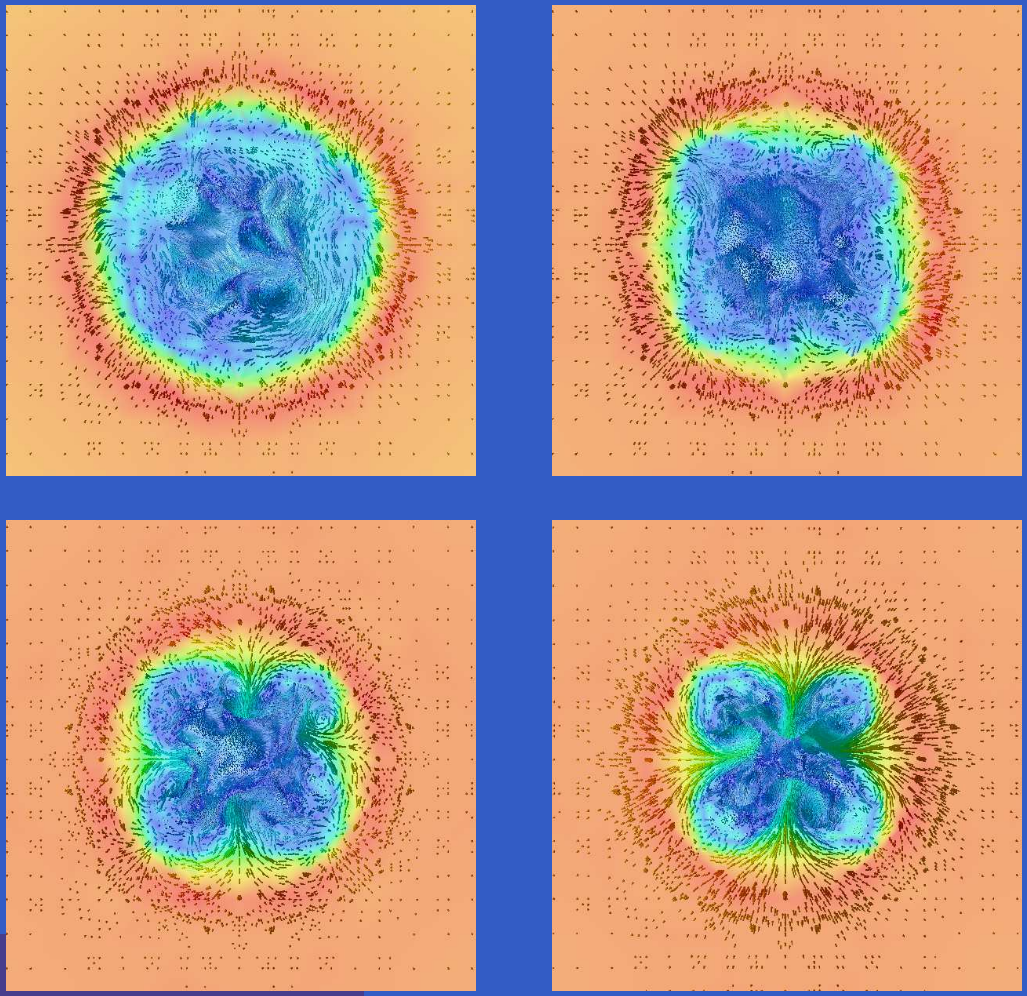
# Drag of Sphere: Vorticity





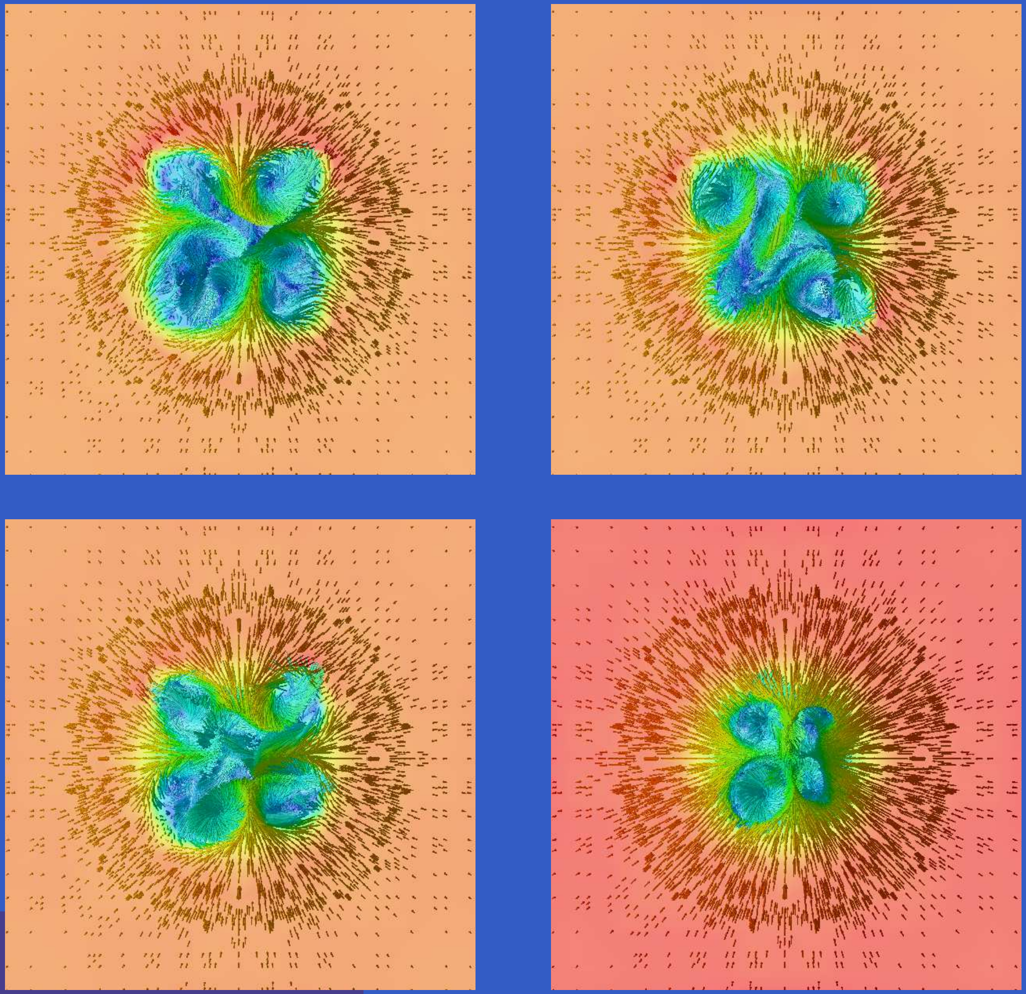
# DRAG CRISIS $c_D = 0.5, 0.3, 0.2, 0.2$

$$\beta = 0.082, 0.032, 0.022, 0.018 \sim \nu^{0.2}$$



# DRAG CRISIS $c_D = 0.2, 0.2, 0.2, 0.1$

$$\beta = 0.013, 0.012, 0.011, 0.0097$$



# Joule-Thompson Experiment

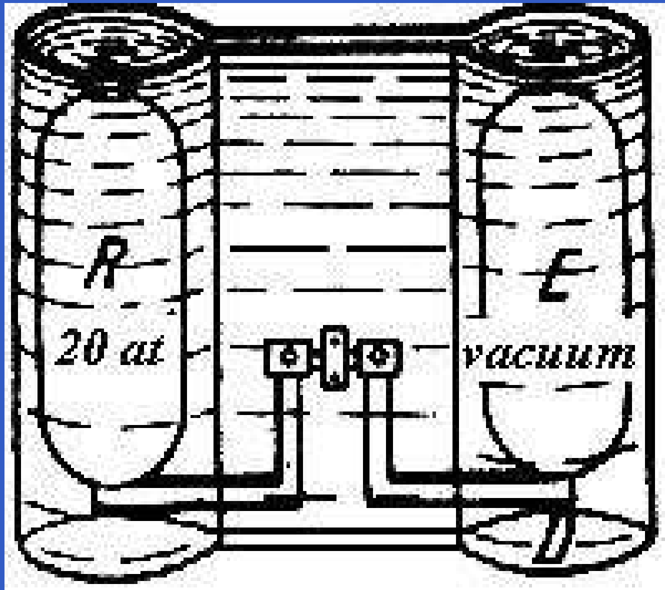
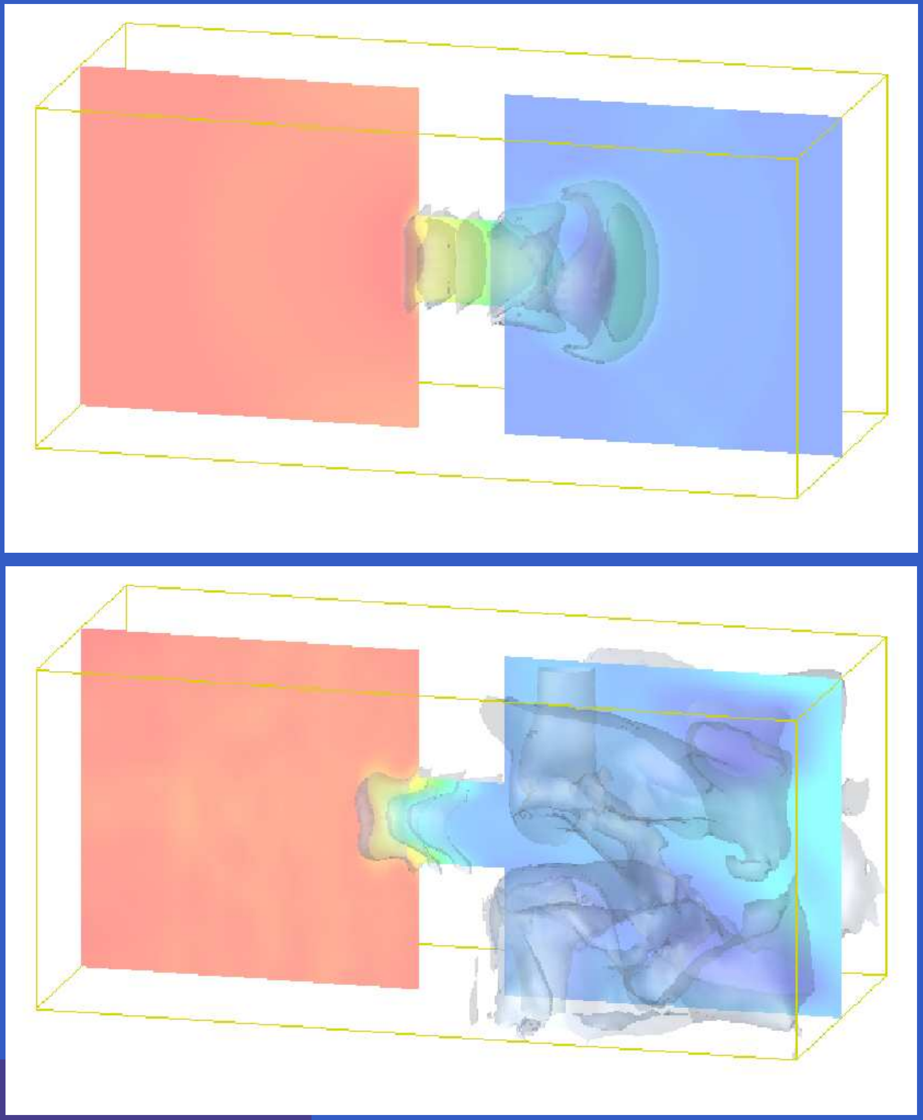



Fig. 358 Concerning overflowing experiment of Joule (Scientific Papers). *R* contains at first air compressed to 20 atm, *E* is initially a vacuum, *D* the tube

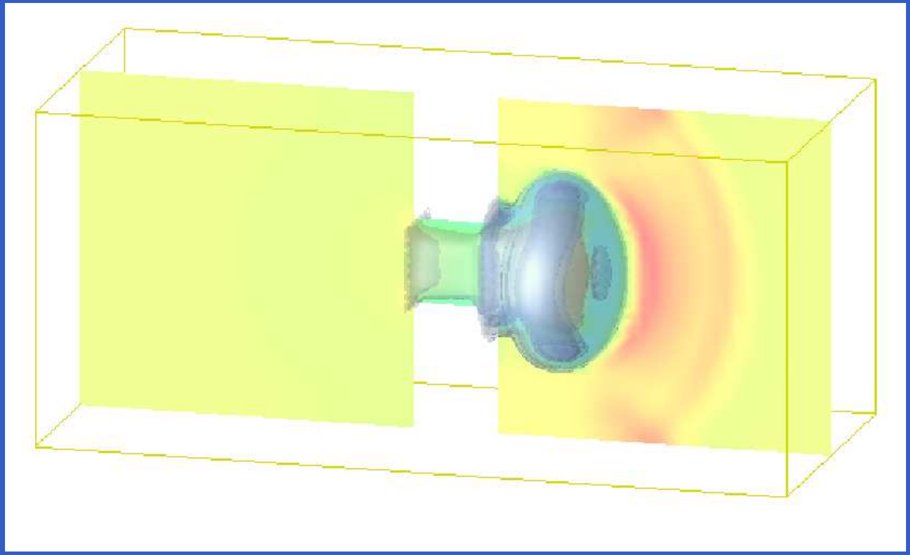
# JOULE'S EXPECTATION

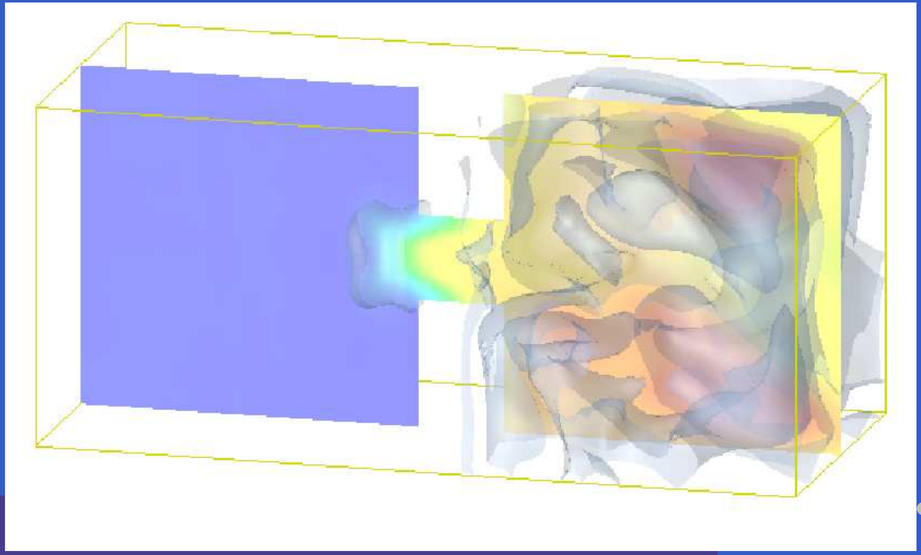
- $T = 1$ in both chambers
- High Pressure/Density in 1
- Gas expands from 1 into 2.
- Kinetic energy $K$ increases
- Temperature $T$ drops $< 1$
- Finally $T =?$

# Density at two times

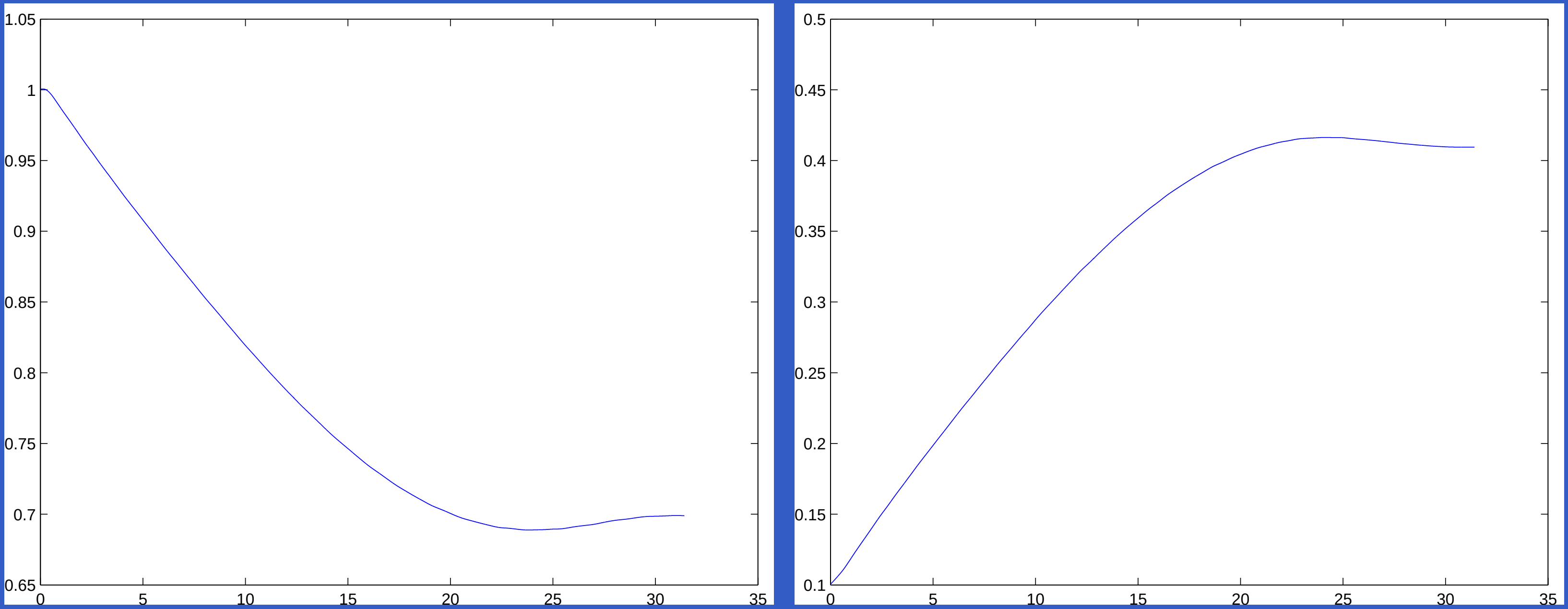


# Temperature at two times

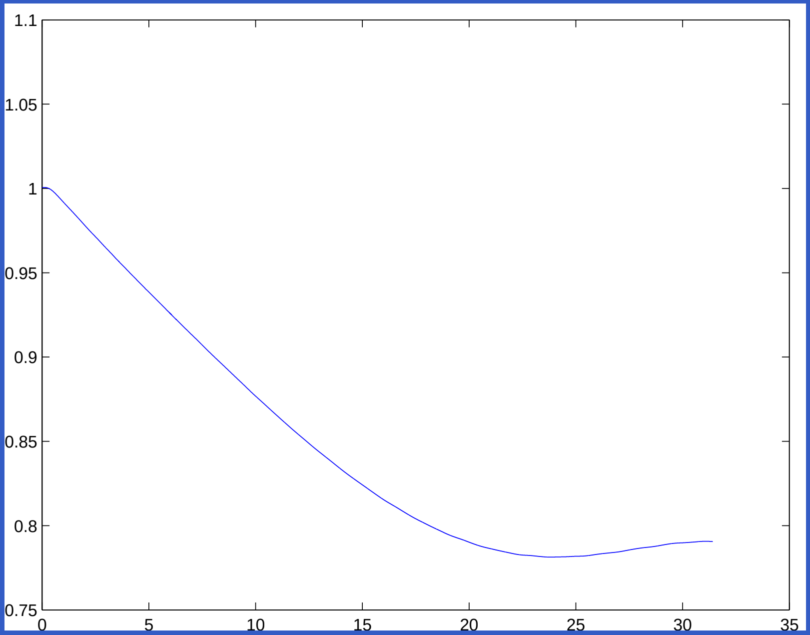


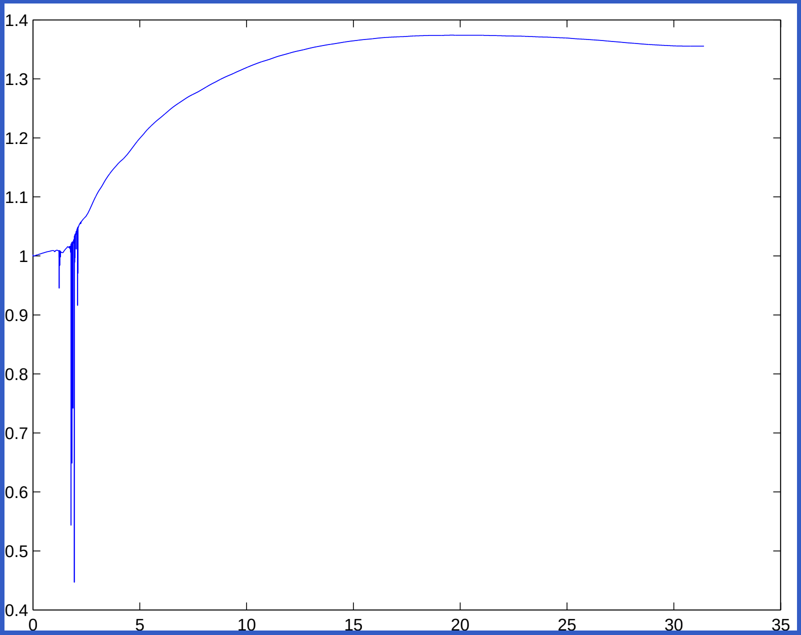


# Average Density in Left/Right Chamber

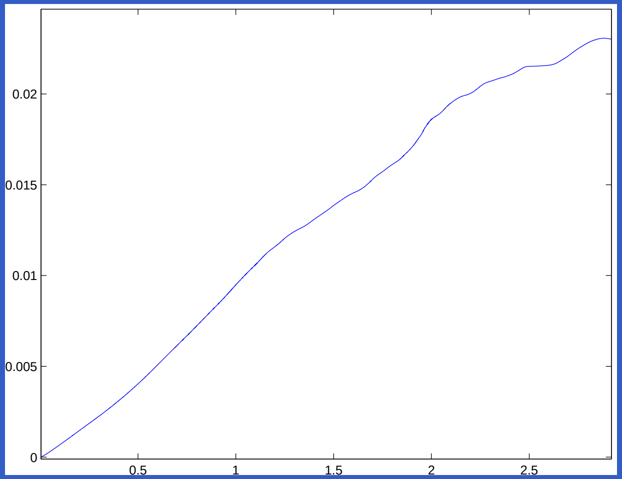


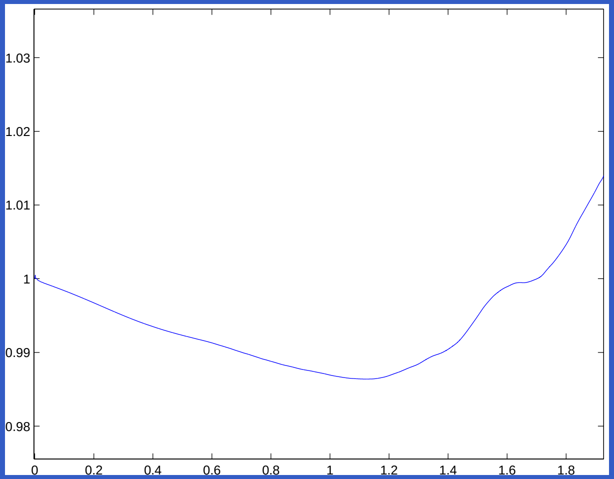
# Average Temp Left/Right

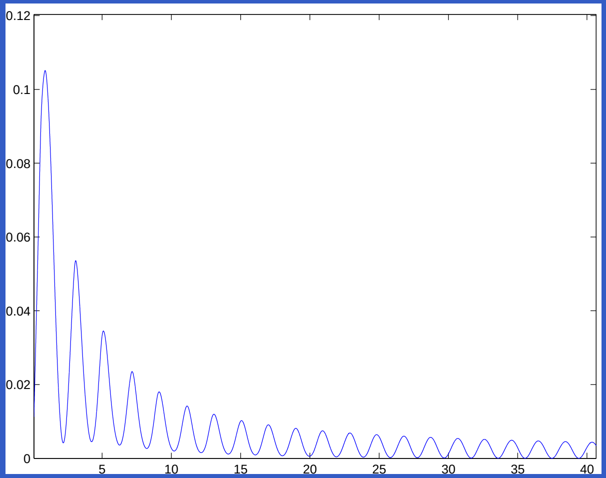


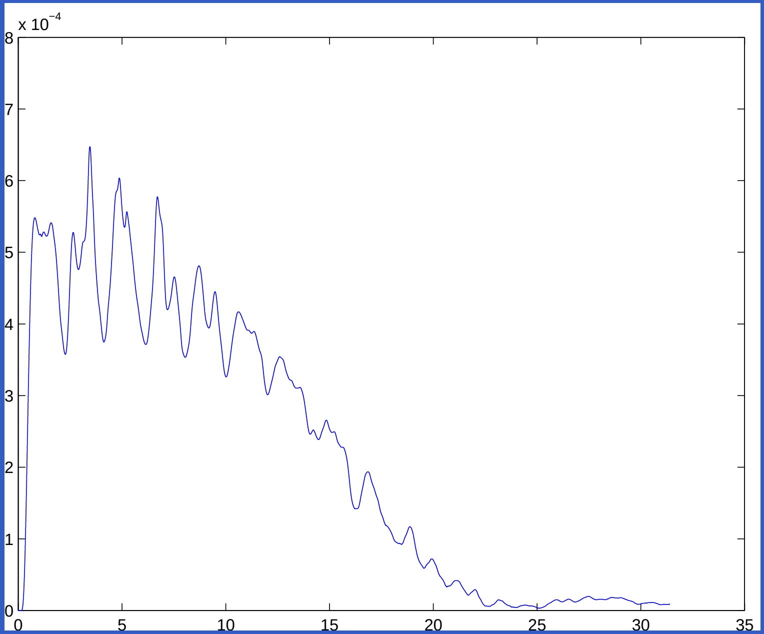
# Average kinetic and heat energy

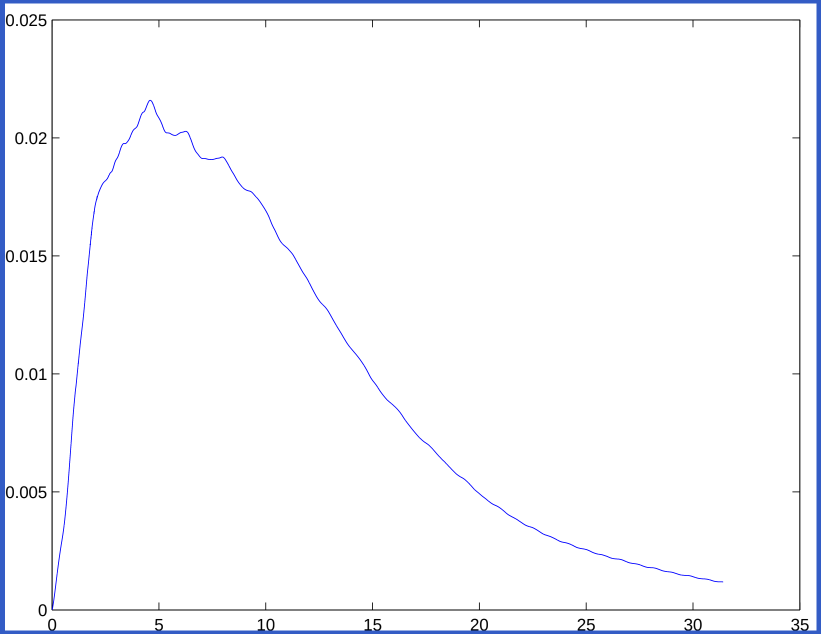


# Average Kinetic Energy Left/Right



# Irreversibility

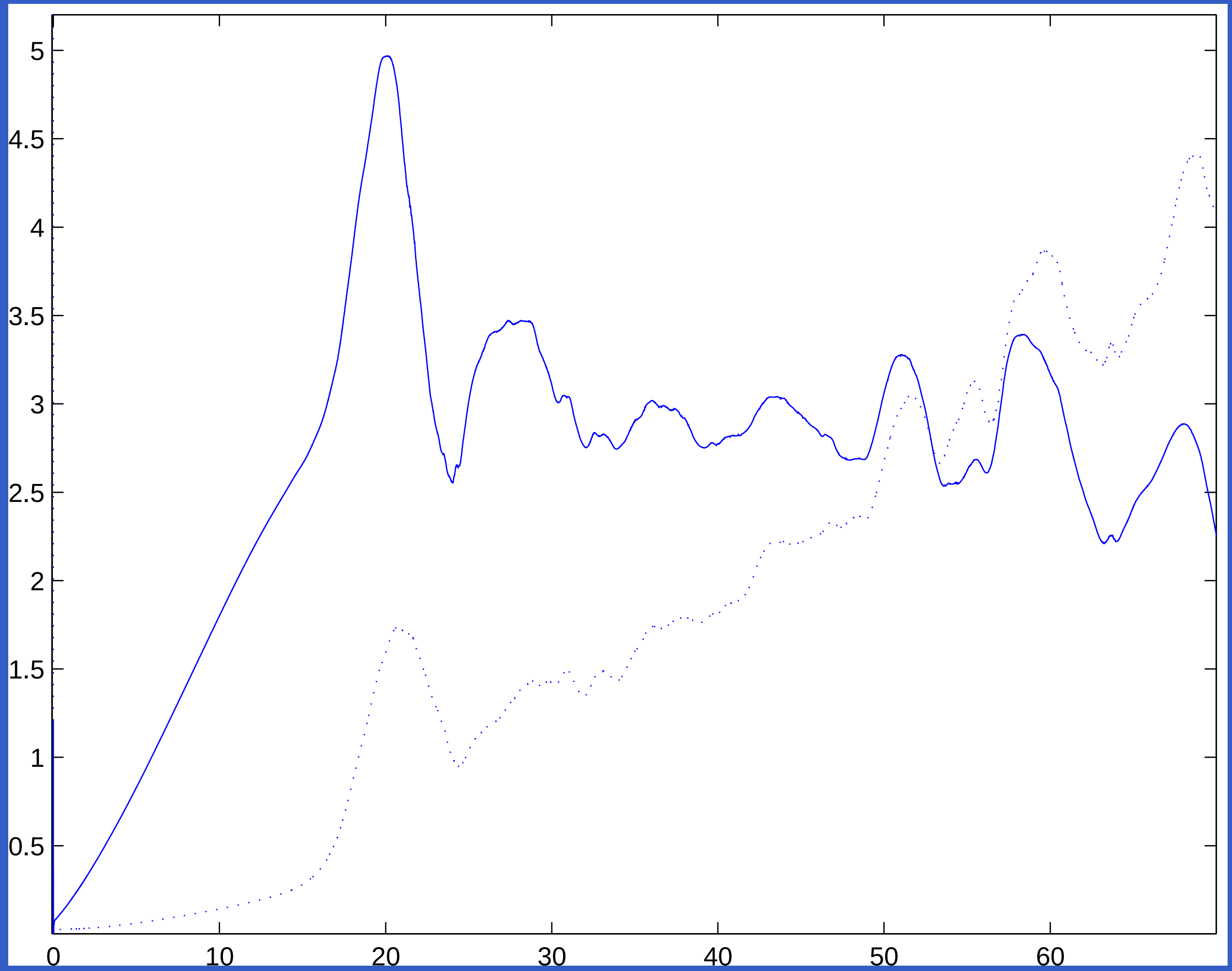
- Kinetic energy increases under expansion.
- No tendency of gas to return to Chamber 1 (compression)
- Gas expands by itself but does not compress by itself.
- Compression produces heat: cooling: lost energy.

# EG2: EULER G2

- STABILIZATION PENALTY: $D(u) = \int hR^2 dx$
- $h$ mesh size, $R(u)$ Residual $\approx h^{-1/2} >> 1$
- $D(u)$ NOT SMALL $\approx 1$: TURBULENCE
- $10^7$ meshpoints for COMPLEX GEOM
- output error $\leq S\|hR\|_{L2} < 1$, S Stability factor
- NO VISCOUS BOUNDARY LAYER
- $10^{18}$ for DNS: IMPOSSIBLE USELESS

# SECRET of FLYING

# LIFT DRAG vs ANGLE of ATTACK



# EG2 BREAKTHROUGH

- NO VISCOUS BOUNDARY LAYER
- $10^7$ meshpoints for COMPLEX GEOM
- OUTPUT ERROR $\leq S\|hR\|_{L2} < 1$,
- S Stability factor

# 2nd Law for EG2

MULT of MOMENTUM by $u$ gives:

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

- $D > 0$ NOT SMALL $=$ TURBULENCE
- $K(t)$ (total) KINETIC energy at time $t$
- $E(t)$ (total) HEAT energy
- $W = \int_\Omega p \nabla \cdot u \, dx$ WORK rate
- $W > / < 0$ under EXPANSION/COMPRESSION
- $W = 0$ incompressible flow

# ESSENCE of THERMODYNAMICS

- $\dot{K} = W - D, \quad \dot{E} = -W + D$
- Transfer of kinetic energy $K$ to heat energy $E$
- Irreversibility Arrow of Time
- $K$ grows by expansion ONLY
- $E$ grows by compression
- Entropy: NO ROLE
- NOBODY knows what Entropy is (Neumann)
- G2 THERMODYN: Understandable $+$ Useful
- COMPUTATIONAL CALCULUS!!

# PENDULUM

$$\dot{v} = -u, \quad \dot{u} = v$$

$$\frac{d}{dt}(\frac{v^2}{2}) = -uv, \frac{d}{dt}(\frac{u^2}{2}) = uv,$$

$$\dot{K} = W, \quad \dot{E} = -W, \quad W = -uv$$

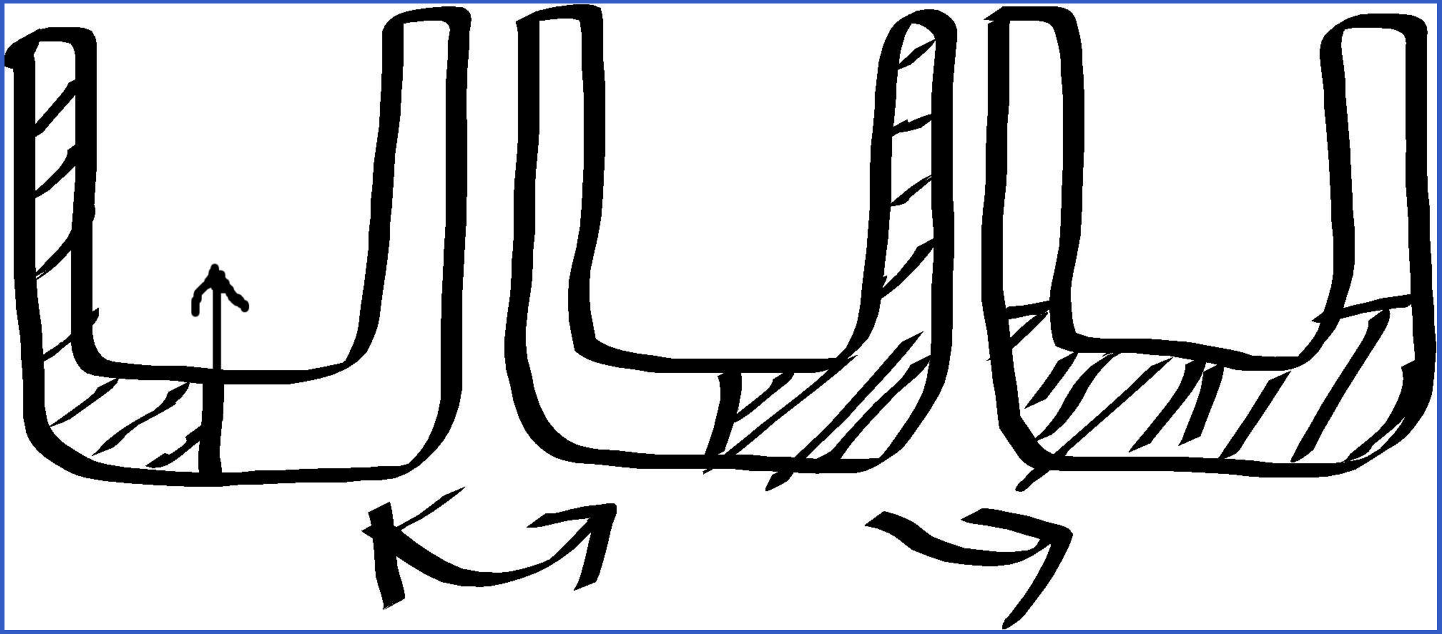
- $K$ kinetic energy, $E$ potential energy
- $W$ work rate, $D = 0$: reversible
- Oscillation: kinetic–potential energy
- Thermodyn $=$ Oscill: kinetic–heat energy

# JOULE EXPERIMENT

- $T = 1$ in both chambers
- Gas expands from 1 into 2.
- Kinetic energy $K$ increases
- Temperature $T$ drops $< 1$
- Turbulence develops in 2
- Kinetic energy transforms into heat energy
- Temperature increases
- Final state $T = 1$ in both chambers.
- Simple Clear: Dynamics: No Mystery

# SHEEP

# U-GLASS



# Boltzmann: Statistical Mechanics?

- Entropy/disorder increases
- More disorder in bigger volume
- Small probability that gas will return.
- Difficult Unclear: No Dynamics: Mystery

# CLAY $1 MILLION PRIZE

- EXISTENCE:APPROX TURB EULER SOL
- NON-EXISTENCE: EXACT EULER SOL
- APPROX: WEAK LERAY INCOMPRESS NS SOL OR G2
- SAME FOR COMPRESS EULER (NEW)
- WEAK UNIQUENESS: OUTPUT ERROR CONTROL
- ANY REGULARIZATION!!
- NONTRIVIAL SOL of PRIZE PROBLEM??

# SOCIETY of FINITE PRECISION

- FLAG FLAT in PERFECT SOCIETY

# TURBULENCE

- Analytical Turbulence: IMPOSSIBLE
- Computational Turbulence: POSSIBLE

# Computational Calculus vs Calculus?

- Mathematicians: MINOR Modification
- BUT MAJOR CHANGE!!
- Calculus: DIFFICULT
- Computational Calculus: EASY!!
- Calculus: IMPOSSIBLE to Teach
- Computational Calculus: POSSIBLE!!

# CHINA CHALLENGE

- China: 400.000 Engineers/year
- Europe: Tradition
- Math Education stable for 100 years:
- Calculus–Classical–Analytical
- REFORM: COMPUTATIONAL CALCULUS
- COMPUTATIONAL TECHNOLOGY
- Start: First Day of First Year

# INVESTMENTS

- CALCULUS 1700-2000: 300 years!!
- FLUID DYNAMICS: DNS Impossible!!
- RESISTANCE to REFORM!!

# BODY&SOUL: www.bodysoulmath.org

Solve

$$\dot{u} = f(u)$$

- Derivative, integral, lin alg, Gauss, Stokes
- Compute general ODE
- Compute general PDE: Poisson, heat, wave, convection, Maxwell
- Compute Euler/Navier-Stokes, Schrödinger...
- Turbulence...Computer Games...

# BOOKS

- Vol 1: Derivatives and Geometry in $\mathbb{R}^3$ 2003
- Vol 2: Integrals and Geometry in $\mathbb{R}^n$ 2003
- Vol 3: Calculus in Several Dimensions 2003
- Vol 4: Comp Turbulent Incompress Flow 2007
- Vol 5: Computational Thermodynamics 2007
- Vol 6. The Arrow of Time 2007
- Vol 7: Many-Minds Relativity 2000
- Vol 8: Many-Minds Quantum Mechanics 2008
- Vol 9: Comp Solid Mech 2008....Vol 10...

# FENICS: AUTOMATION of CC

- G2 General PDE
- FEniCS Form Compiler
- Adaptivity–Duality
- A Posteriori Error Control
- Optimization- Control
- www.fenics.org

# ICARUS: www.icarusmath.com

- Web version of BODY&SOUL
- Computer Game = CC
- DEMO: Crash Course Thermodynamics

# COMPUTER GAMES

- $\dot{u} = f(u)$
- Interactive Model
- Input: Data
- Output: Solution
- CONTROL
- Stimulate Students: Active Learning

# SUMMARY

- COMPUTATIONAL CALCULUS
- COMPLEX MODELING: TURBULENCE
- HYPERREALITY: SIMULATION
- KNOWLEDGE SOCIETY
- REFORM? WHEN?