Courses/FEM/modules/science

From Icarus

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Contents

Mathematics, Science and Technology

Theoretical science including

- physics and quantum mechanics
- chemistry
- solid and fluid mechanics
- electromagnetics
- molecular biology
- oceanography, meteorology
- astronomy, cosmology

is based on mathematics and has two basic components:

- modeling: formulate equation
- computation: solve equation.

The mathematical models typically take the form of differential equations expressing basic principles such as

- conservation of mass, momentum and energy
- balance of forces
- constitutive laws such as Hooke's law in elasticity.

The basic areas of science are identified by corresponding basic (non-linear) differential equations:

- physics: Lagrange's equations of motion, Schrödinger' s equation in quantum mechanics
- chemistry: reaction-diffusion-convection equations
- solid mechanics: Navier's elasticity equations
- fluid mechanics: Navier-Stokes equations
- electromagnetics: Maxwell's equations

The classical techniques of solving differential equations are

- analytical formulas expressing solutions in terms of elementary functions
- numerical computation using mechanical calculator or slide rule

where elementary functions such as trigonometric functions are nothing but solutions to simple linear differential equations. However, finding analytical solutions to non-linear differential equations is usually impossible.

In our time the computer opens entirely new possibilities to solve non-linear differential equations by computation, for which a mechanical calculator is too slow. This way human intelligence capapable of formulating differential equations based on principles, can be boosted with the power of the computer capable of solving virtually any non-linear differential equation by brute force computation. The result is a new powerful combination of mind and machine at service to science and technology and education. Principles can be understood and the results of computation can be analyzed and understood according to the famous statement by the (computational) mathematician RichardHamming (http://en.wikipedia.org/wiki/Richard_Hamming) :

- The purpose of computing is insight, not numbers.

A Case Study: Turbulent Flow

To illustrate the above message that mind + computer can do things that was not possible with classical analytical mathematics, we consider the main unsolved problem of classical Newtonian mechanics:

- turbulence.

We know by experience that the flow of a slightly viscous fluid such as water an air usually is turbulent, which means that the flow is irregular and varies quickly in both space and time. In particular, the flow around a vehicle such as an airplane, car, (sailing) boat, is turbulent which causes both

- drag (resistance to motion)
- lift (force perpendicular to direction of motion).

Now fluid flow is described by the Navier-Stokes equations, and by solving the equations it should be possible to predict both tha drag and lift of e.g. the wing of an airplane. This was done already in 1752 by the mathematician d'Alembert, who found analytical solutions to the Euler equations modeling slightly viscous flow in the form of so-called potential solutions. D'Alembert found to his great surprise that the drag (and lift) of a potential solution is zero, suggesting that it should be possible to move through air and water without resistance, in obvious contradiction to all experience. This is

- d'Alembert's paradox: potential flow has zero drag and lift.

Evidently something is wrong with a potential solution, but nobody has been able find what is wrong, until very recently. A resolution of d'Alembert's paradox (http://knol.google.com/k/claes-johnson/dalemberts-paradox/yvfu3xg7d7wt/2#) is presented at Knol (http://knol.google.com/k/knol#) . The eager reader will of course take a look and as a spin-off will be able to understand why it is possible to fly (http://knol.google.com/k/claes-johnson/dalemberts-paradox/yvfu3xg7d7wt/2#H17-Why-It-Is-Possible-to-Fly) , which surprisingly has not been properly understood until very recently.

It is discovered by solving the Euler equations by computation that the potential solution is unstable and under small peturbations develops into a turbulent solution with substantial drag. The potential solution is thus a purely fictitious solution which can never be realized and observed in practice, because small perturbations are always present. D'Alembert's paradox is thus solved by computation as well as the Clay Mathematics Institute (http://www.claymath.org/millennium/)

- One Million Dollar Navier-Stokes Problem (http://knol.google.com/k/claes-johnson/the-clay-navier-stokes-millennium/yvfu3xg7d7wt/14#)

We hope the reader gets the message that computational solution of differential equations opens entirely new possibilities of

- modeling of the real world
- creating new virtual worlds.

The Finite Element Method

The finite element method is a systematic way of discretizing differential equations into a system of algebraic equations which can be solved by a computer by direct Gaussian elimination or by iterative solution using e.g. a steepest descent or Newton method. The finite element method makes it possible to automatize discretization as shown in the FEniCS Project (http://www.fenics.org/wiki/FEniCS_Project) , and thus automatize computational mathematical modeling.

The finite element method is based on the following principles:

- calculus of variation in the form of Galerkin's method
- piecewise polynomial approximation
- error estimation from residuals by duality.

Following the course you will understand these principles and experience the automatization they bring. This is like learning how to create and play music by understanding the principles and pressing the right buttons.

To get more of intro take a look at the web pages of Body and Soul Project (http://www.bodysoulmath.org/) and the book Computational Turbulent Incompressible Flow (http://www.nada.kth.se/~jhoffman/pmwiki /pmwiki.php?n=Main.HomePage) including animations. Intuition based on observation of real and imgained phenomena is very useful, in particular if it is coupled with a mind of principles.

Differential equations

Science is based on modeling reality, mainly with differential equations (http://en.wikipedia.org/wiki/Differential_equation) .

Precondition

No precondition needed.

Theory

Partial differential equations

An abstract form:

$$A(u(x)) = f, \quad x \in \Omega$$

where:

- $u(x)$ is the unknown **solution**

- A is a **differential operator**.
- Ω is the **domain**, i.e. $\Omega = [0,1]$.
- f is a given **source term**.
- typically the x is dropped, i.e. $u = u(x)$

Initial value problem
  $u(x_0) = g$
  Here x is typically a "time" variable.
Boundary value problem
  $u(x) = g, \quad x \in \Gamma$
  Here x is typically a "space" variable.
Initial boundary value problem
  Can have both at the same time.

Residual

We define the **residual** function $R(U)$ as:

$$R(U) = A(U) - f$$

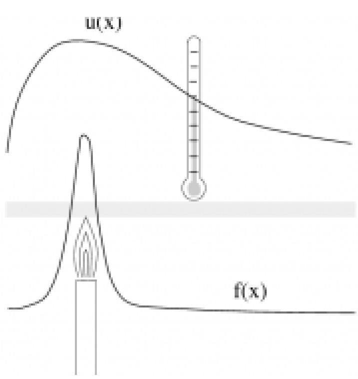
We can thus define an **equation** as computing an object u such that:

$$R(u) = 0$$

Poisson's equation

A model for stationary heat conduction

We model heat conduction a thin heat-conducting wire occupying the interval $[0,1]$ that is heated by a *heat source* of intensity $f(x)$.



We are interested in the stationary distribution of the temperature $u(x)$ in the wire. We let $q(x)$ denote the heat flux in the direction of the positive x-axis in the wire at $0 < x < 1$. Conservation of energy in a stationary case requires that the net heat flux through the endpoints of an arbitrary sub-interval (x_1, x_2) of $(0,1)$ be equal to the heat produced in (x_1, x_2) per unit time:

$$q(x_2) - q(x_1) = \int_{x_1}^{x_2} f(x)\,dx.$$

By the Fundamental Theorem of Calculus,

$$q(x_2) - q(x_1) = \int_{x_1}^{x_2} q'(x)\,dx,$$

from which we conclude that

$$\int_{x_1}^{x_2} q'(x)\,dx = \int_{x_1}^{x_2} f(x)\,dx.$$

Since x_1 and x_2 are arbitrary, assuming that the integrands are continuous, we conclude that

$$q'(x) = f(x) \quad \text{for } 0 < x < 1,$$

which expresses conservation of energy in differential equation form. We need an additional equation that relates the heat flux q to the temperature gradient (derivative) u' called a *constitutive equation*. The simplest constitutive equation for heat flow is *Fourier's law*:

$$q(x) = -a(x)u'(x),$$

which states that heat flows from warm regions to cold regions at a rate proportional to the temperature gradient $u'(x)$. The constant of proportionality is the *coefficient of heat conductivity* $a(x)$, which we assume to be a positive function in $[0,1]$. Combining energy conservation and Fourier's law gives the *stationary heat equation* in one dimension:

$$-(a(x)u'(x))' = f(x) \quad \text{for } 0 < x < 1.$$

To define a solution u uniquely, the differential equation is complemented by *boundary conditions* imposed at the boundaries $x = 0$ and $x = 1$. A common example is the homogeneous *Dirichlet* conditions $u(0) = u(1) = 0$, corresponding to keeping the temperature zero at the endpoints of the wire. The result is a *two-point boundary value problem*:

$$-(au')' = f, \quad x \in (0,1)$$
$$u(0) = u(1) = 0$$

The boundary condition $u(0) = 0$ may be replaced by $-a(0)u'(0) = q(0) = 0$, corresponding to prescribing zero heat flux, or insulating the wire, at $x = 0$. Later, we also consider non-homogeneous boundary conditions of the from $u(0) = u_0$ or $q(0) = g$ where u_0 and g may be different from zero.

Software

Familiarize yourself the software tools and the computer environment for the course.

Postcondition

You should now be familiar with:

- why it's important to be able to solve differential equations
- the notation for differential equations
- some basic differential equations used in science:
  - Poisson's equation
  - The convection equation
  - The wave equation
- boundary conditions (Dirichlet, Neumann, Robin)

Exercises

CDE 6.7:

Determine the solution u of the stationary heat equation with $a(x) = 1$ by symbolic computation by hand in the case $f(x) = 1$ and $f(x) = x$.

Examination

1.1.

Investigate a different science domain (**elasticity**, **fluid flow** or **electromagnetism**) and make your own derivation of Poisson's equation (in 1D or 2D) for that domain using appropriate simplifications. Discuss the physical interpretation of boundary conditions.

1.2.

Solve Poisson's equation in 2D using FEniCS with data of your choice. Specify homogenous Neumann boundary conditions on one part of the boundary and homogenous Dirichlet boundary conditions on another part of the domain. Plot the results.