by Svante Littmarck

# Solving Differential Equations

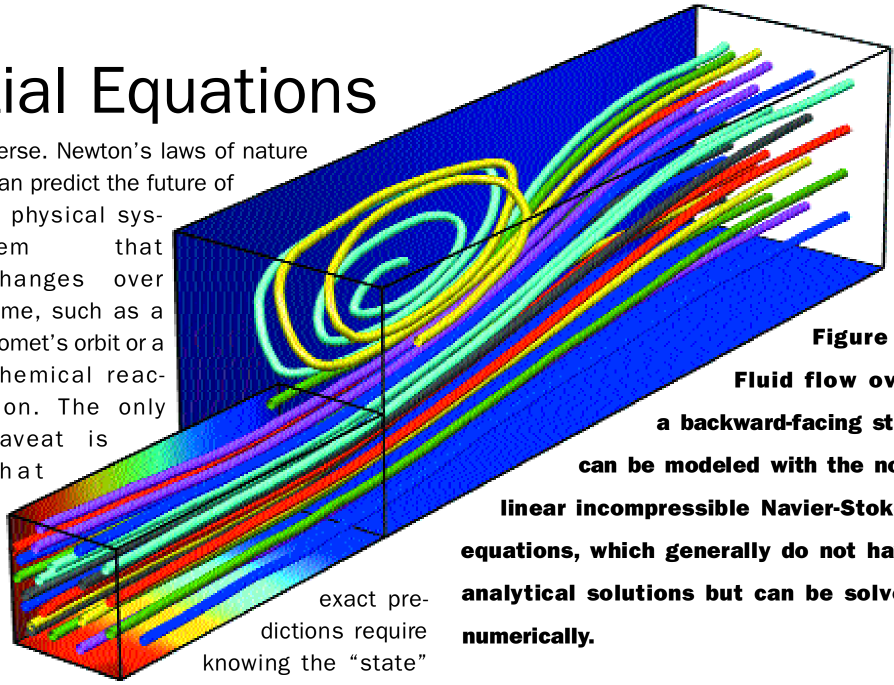

**Figure 1. Fluid flow over a backward-facing step can be modeled with the non-linear incompressible Navier-Stokes equations, which generally do not have analytical solutions but can be solved numerically.**

Mathematical modeling has made significant contributions to scientific progress. From ancient times through the Renaissance, Euclidean geometry provided the framework for all applied mathematics, most notably in surveying, navigation, and astronomy. Unfortunately, geometry expresses eternal—and hence static—relations between shapes. It is, accordingly, graphical and often beautiful, yet it lacks dynamics.

The dynamic feature of mathematical models was not presented until the 17th century, when Isaac Newton and Gottfried Wilhelm von Leibnitz independently developed differential calculus. Its immediate success was in the spectacular creation of Newton's simple models that both reproduced known planetary orbits and predicted the future positions of planets. The motion of celestial bodies was described through the revolutionary invention of a dynamical model, which expressed how changes in velocity are related to positions. Thus, in Leibnitz's words, the model was a set of *differential equations*.

The predictive accuracy of mathematical modeling for celestial mechanics was impressive, and Newton's unrivalled feat changed the contemporary view of the universe. Newton's laws of nature can predict the future of a physical system that changes over time, such as a comet's orbit or a chemical reaction. The only caveat is that exact predictions require knowing the "state" of every physical characteristic with infinite precision.

## Difficult solutions

Differential equations are simple in the sense of having a compact representation, yet the resulting trajectories—a plot of a system's development over time—can be extremely complex (Figure 1). Trajectories may be extraordinarily sensitive to the initial state yet still have some predictable characteristics. Recent research has centered on this subject, as exemplified by the Lorenz differential equations. These equations were developed in 1963 as a crude model for simple meteorology. They addressed problems in which the trajectories always seemed to be on one of two well-determined planes, but it was impossible to predict when and how the orbit—a trajectory plotted in time and space—would shift from one plane to the other.

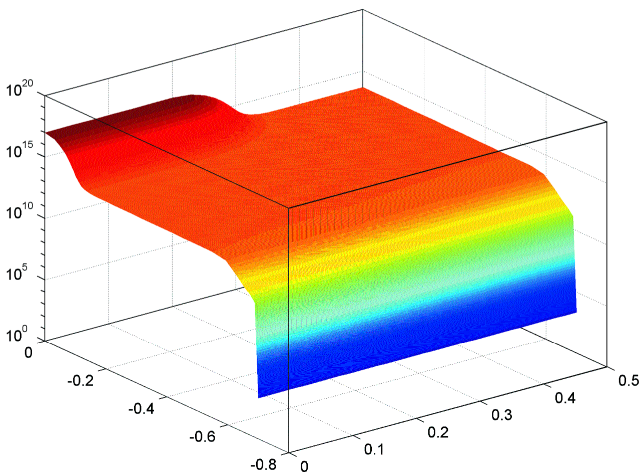


**Figure 2. Hole concentration (on a logarithmic scale) for a semiconductor device model featuring a diode with p- and n-type regions, solved from equations based on charge and field strength.**

Although using numerical methods to predict weather was discussed at the beginning of the last century, reaching today's present prediction accuracy required overcoming many theoretical and practical obstacles. Leibnitz was aware of the power of differential calculus, and he spoke about using machines to carry out such calculations. A recent book, *Computational Differential Equations*, quotes him on this possibility: "Knowing thus the Algorithm of this calculus, which I call Differential Calculus, all differential equations can be solved by a common method…not only addition and subtraction, but also multiplication and division, could be accomplished by a suitably arranged machine."

Creative scientists using clever analytical methods can "solve" simplified versions of differential equations. The resulting formulas yield all the information that we could possibly want for determining, for example, the location of a spacecraft at some future time. Regrettably, there are far too many diverse equations and not enough brilliant minds to solve them all. Leibnitz envisioned a generally applicable way of working with all differential equations, and computing a solution through approximate numerical methods has supplied that technique.

Most of the 19th century was devoted to the construction of large tables—notably of logarithmic and trigonometric functions—for making reliable, faster, and more accurate calculations in navigation and astrono-

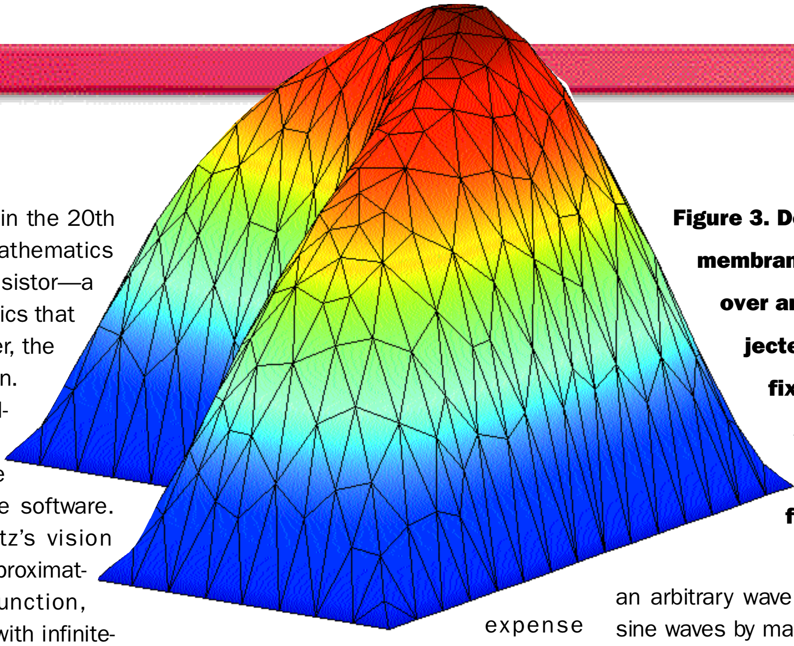

**Figure 3. Deflection of a thin membrane that is stretched over an L-shaped region, subjected to normal loads, and fixed at its perimeter is solved by Poisson's equation and the finite-element method.**

my. This work was superseded in the 20th century not by advances in mathematics but by the invention of the transistor—a breakthrough in solid-state physics that eventually gave us the computer, the machine to fulfill Leibnitz's vision.

What Leibnitz could not realize was that in addition to the theory and the machine, we needed a third component: the software. This missing piece in Leibnitz's vision embodies clever methods of approximating an equation's solution function, which is a continuous function with infinitely many values, and then computing a finite number of values numerically. The methods require detailed attention to preparing numbers for an equation, because using error-prone, brute-force methods to solve problems based on differential equations has time and again proven futile.

The need for agile and astute computational methods is exemplified in the study of semiconductor devices, where the quantities of interest are the electric field and current. The latter is carried by electrons and their opposite entities, the "holes" in the valence bands of doped silicon. Models consist of the partial differential equations (PDEs) that express the conservation of charge and the relations between fields and concentrations of electrons and holes, from which the voltage-current characteristics of the device are derived. The largest expense of time and effort occurs in the generation and "number crunching" of the numerical solution for the equations. These calculations require that tens of thousands of computational cells, each representing a set of coordinates, be concentrated in the regions where the fields change rapidly. In addition, these fields may well change with applied voltage and so require the generation of a new mesh—an overall picture of a system under specific conditions—for each new voltage step.

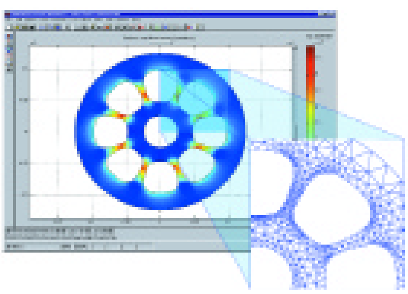

**Figure 4. To solve a plane stress model of a pulley with inertial forces due to rotation and boundary forces of the belt drive, a finite-element mesh on the spokes and holes gives a converged result.**

All of this computation may take billions of arithmetic operations,which now can be done routinely on a personal computer (Figure 2). Although we lack a mathematical proof for the reliability of these methods, computational experience, careful analysis, and comparison with experiments strengthen our confidence in the models and software developed for this application of differential equations.

The obstacle to realizing Leibnitz's vision of solving differential equations by machine is computational efficiency. Growth in computer power has increased exponentially for the past 30 years. It has doubled every 18 months and, thus, increased our problem-solving capacity by a factor of 1 million over three decades (Figure 5). However, contributions have also come from mathematical developments in the numerical methods of differential calculus.

A landmark in numerical analysis occurred in the early 1960s with the invention of the fast Fourier transform (FFT) algorithm by James W. Cooley and John W. Tukey. The FFT cut the time needed to decompose an arbitrary wave train into its constituent sine waves by many orders of magnitude. It changed the perception of what could be accomplished with digital signal processing. The FFT serves as the heart of MPEG (motion picture experts group) and similar schemes for compacting video and sound files onto CDs and transmitting them over the Internet. Electron clouds, clusters of galaxies, and membrane deflection problems are described by the 19th century Poisson PDEs. When used with fast techniques to solve Poisson PDEs, the FFT enables simulations of millions of galaxies, allowing scientists to look at different scenarios for the evolution of the universe in both fast-forward and reverse.

## Finite-element analysis

Finite-element analysis (FEA),an approximation approach to studying continuous physical systems, has evolved in the past 50 years from an ad hoc engineering tool for structural analysis to a sophisticated general purpose method for solving differential equations. There are variants with proven robustness adapted to most important classes of problems, and software packages support all the steps in modeling projects for many applications.

Consider the deflection of a thin membrane stretched over an L-shaped area (Figure 3). The membrane is subject to normal loads and fixed along its perimeter. The first step is to cover the surface with a set of triangles. The approximate shape of the membrane is now a set of plane triangular facets, joined along their edges, like a dome covered with plane tiles. All one must obtain to determine the deflection of the membrane is the heights of the dome at the corners of the triangles. FEA is able to compute the heights that bring the dome closest to the exact deflection shape.

The success of FEA hinges on three key properties:

• It treats complex geometries easily—any domain can be closely approximated by a set of triangles (Figure 4).

• Only a few unknowns appear in each equation. This sparseness makes the numerical solution efficient.

• For greater accuracy, the FEA elements—which include the triangles' geometry and their mathematical functions—can easily be made smaller.

The complete FEA procedure lends itself to computer implementation, which includes generating the elements and equations, computing the solution, and displaying the results. The software was first developed in the form of libraries for the various steps, and you had to adapt these building blocks to your application through Fortran programming. Today, there are large Fortran packages, such as Nastran, for applications in structural analysis, and FEA software, such as FEMLAB, that allows users to tailor a package's capabilities to their needs. Such software does not require special programming, uses standard and intuitive graphical tools, and combines many applications through *multiphysics*, an emerging analytical approach that simultaneously considers all physical characteristics encountered in a real-world problem.

In the relatively short time that researchers have used FEA for solving PDEs, it has become apparent that the analysis system lends itself to solving problems in a wide range of disciplines. A few examples of models include:

• electromagnetics models, such as those used to examine the effect of changing magnet sizes or materials in the windings of an electric motor.

• fluid-dynamics models, whose uses include investigating heat flow in a room or airflow around a prototype vehicle.

• geophysics models, whose uses include studying the potential flow of fluid in a rock fracture.

• heat transfer models, which are used to investigate such things as the heat distribution in a radioactive rod.

• semiconductor device models, such as those used for computing the current versus voltage characteristic curves of new devices.

• acoustics models, whose uses include examining the source of a humming sound coming from electrical machinery.

• finance models, such as those used to study the Black-Scholes equation for predicting the value of a stock option.

• chemical-reaction models, such as those used to understand the operation of a three-way catalytic converter in an automobile. These models are able to simultaneously transform unburned hydrocarbons, carbon monoxide, and nitrogen oxides from the exhaust into carbon dioxide, nitrogen, and water.

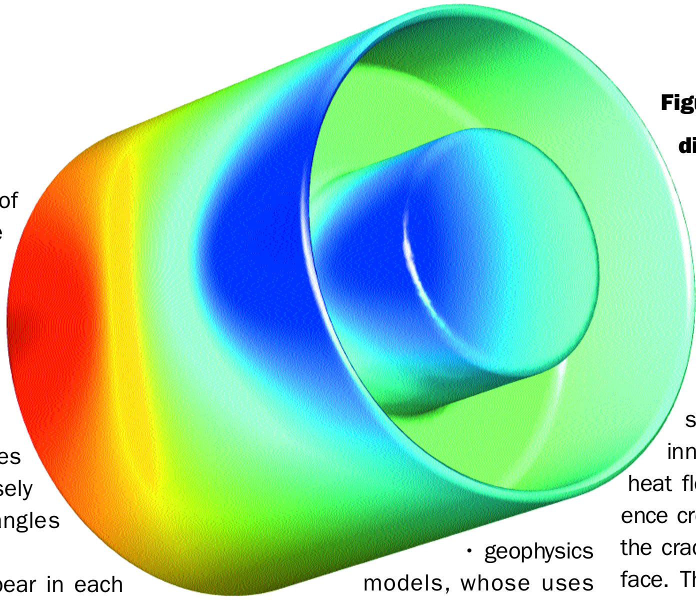

**Figure 5. This model of a high-voltage disconnector was created with finite-element analysis software on a PC more powerful than the supercomputers of the 1980s.**

## Multiphysics problems

Although such modeling problems are interesting, they do not account for all physical phenomena for one key reason: in nature, it is not unusual for several physical phenomena to occur in the same local region and for all of them to interact. Indeed, these physical processes often affect the outcome of each other in a complex fashion. Problems that exhibit this kind of behavior fall under the heading of multiphysics.

As an example of multiphysics, consider a model that calculates the stresses in a cracked heat-exchange tube such as you might find in a pulp mill. Because these tubes must resist corrosion from very different chemicals on the inside and outside, they are made of two concentric layers of different stainless steels. A crack in the joint between the inner and outer tubes severely impedes heat flow. The resulting temperature difference creates thermal stresses, which cause the crack to propagate along the tube interface. The tube eventually deforms, and the cracked surfaces separate. Immediately, you can see that this problem involves both structural mechanics and heat transfer considerations.

## The future

Today, it is easy to solve PDEs on a personal computer, and it appears that we are close to realizing Leibnitz's vision. As usual, expectations grow with achievements, and during the next few years the wide accessibility of PDE modeling will have a noticeable impact on science and engineering. Graduates of engineering schools will take such tools for granted and will concentrate on the truly creative processes of design and development. Turnaround times for what-if simulations will be shortened, increasing the number of design ideas that can be assessed and, therefore, allowing all aspects of a design to be studied.

## For further reading

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Hairer, E.; Norsett, S.; Wanner, G. *Solving Ordinary Differential Equations* I; Springer-Verlag: New York, 1987; 480 pp.

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## B I O G R A P H Y

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