THE MATHEMATISATION OF SCIENCE

LUIS A. CAFFARELLI

I was asked to make a short presentation on trends and directions in mathematics.

Mathematics has become a vast subject, with different techniques and scientific values. Even in a confined area like fluid dynamics, the same subject, say the Navier-Stokes equation, has a different connotation for different research groups (compressible versus incompressible, formation of singularities, zero viscosity limits, etc.)

I have chosen therefore to:

a) Stay very close to my area of expertise, non-linear analysis, partial differential equations and applied mathematics, where I could better present the issues.

b) More than a determined aspect or evolution of a theory, to discuss several examples of a trend that I feel will have enormous importance in my area of mathematics, as well as in our relation to the rest of the sciences.

The main theme of my examples will be that science and engineering are requiring the development of very sophisticated mathematical theories.

The enormous computational capabilities that are becoming available year after year have allowed scientists not only to look at more detailed models of existing physical phenomena, but also to be able to simulate complex materials and processes to optimize their design properties.

The first area I would like to discuss concerns mathematical development in image treatment (storage, enhancing, and compression). For simplicity, a black and white image simply means to provide a function (the grey scale) that may be piecewise smooth with sharp transitions, or dotted with very fine dots, or blurred and imprecise. Nevertheless, the eye has a special ability in grouping the essential features of it and reconstructing out of it a familiar image. The first development that I would like to discuss is the theory of wavelets, which has to do with a way of extracting from a picture its detail up to a given level, and allowing us to reconstruct it (see Pictures 1, 2, and 3 Brushlets).

In trying to do so, there are two conflicting interests, very common in physics and mathematics sciences: size and oscillation, i.e. the choice between intensity and contrast.

Mathematically, this means having to choose between an approximation that averages in space, or one that averages in frequencies.

Averaging in space (a finite element discretization, for instance) will lose the detail in the oscillations; averaging in frequencies loses the local spatial detail. The representation of a function as a superposition of sines and cosines (the computation of the Fourier coefficients) depends globally on the function, although it attempts to represent it pointwise.

The compromise solution has been the development of wavelet theory. Wavelets are *bases* families of elementary profiles for decomposing function, intensity in our case, that are localized simultaneously in space and frequency.

In fact, they are *telescopic* both in space and frequencies, in the sense that they are:

a) Layered in space. There is a layer of size one, one of size 1/2, 1/4, 1/8, etc.

b) Layered in frequencies: they are mostly concentrated between frequencies 1 and 2, 2 and 4, 4 and 8, etc. (In fact they can all be constructed by translating and diadically shrinking a single profile, the wavelet) (Picture 4).

Wavelet theory has found deep applications not only in image compression but also in fluid dynamics, as well as classic harmonic analysis.

The other mathematical tool developed due to the needs of image treatment concerns geometric deformation and evolution.

In the same way that wavelets address an issue of multiple scales, geometric deformations address an issue of multiple models (Pictures 5 and 6: plane and geometric picture).

The issue is: given a blurred or a spotted, noisy image, how can it be grouped in order to make it a recognizable object. The idea, a classic one, borrowed from phase transition theory, is to assign to every configuration an energy that combines its closeness to the given, disorganized image and its degree of "organization". (For instance, if it is a curve enveloping a region, its length.)

Next, one lets the configuration "flow" towards its energy minimum. For instance, a curve will evolve trying to minimize a combination of its



Picture 1 – 8:1 Compression



Picture 2 – 16:1 Compression



Picture 3 - 128:1 Compression

Pictures 1, 2, 3 – Brushlet Pictures. Yale Wavelet Computational Group. http://www.math.yale.edu:80/YCM







Picture 4.



Picture 5 – Results for a very noisy image, with the initial curve not surrounding the objects. Top: u_0 and the contour. Bottom: the piece-wise constant approximation of u_0 .



Picture 6 - An Active Contour Model without Edges

Pictures 5, 6 – Chan, Tony F. and Luminita A. Vese. "Active Contours without Edges." *IEEE Transactions on Image Processing.*

length and the intensity it encloses. When one tries to do that, singularities arise, and as the structure of the "approximate" configuration deteriorates, it is necessary to go to a higher model. For instance, a "field theory model" that adds "artificial viscosity" or diffusivity to the surface movement, to resolve the singularities.

For computational purposes we have thus a *multi-model* theory, where in areas of "normal" evolutions we use simpler geometric evolution, but couple them with higher complexity models to resolve singularities in the flow. The issue is, of course, when to use each model and how to couple them.

The issue of matching different models is a very important one; we will see another example later.

Next, there are two examples that come from continuous mechanics and one is multiscale, the other is multi-model.

The multi-scale concerns homogenization (see Pictures 7 and 8). Typical examples of homogenization are composite materials, or flows through layered rock formations.

Fluid or gas through a porous media, for instance, can be studied at several scales: at a few centimeters scale, the structure of the pore and the capillary properties of the fluid enter into consideration. At a few meters important factors are soil layers, large cracks, etc.

The interest, though, centers mainly on trying to simulate reservoirs at kilometer scales.

One must, therefore, model the interplay of each of the scales. At a kilometer scale, for instance, flow laws are much simpler, but the parameters (effective constants) or the non-linearities in these laws depend heavily on the small-scale behavior. Homogenization appears in many areas: elasticity, crack propagation, etc; and involves very sophisticated tools of non-linear analysis and probability theory.

The last example comes independently both from aerospace engineering and semiconductor design. In terms of aerospace engineering, a typical example of the problem can be described as follows: a jet fired in an atmosphere of very low density goes from a very compressed regime to a very low density one in a length of a few meters.

According to its local density or density gradient there are several classical models of gas dynamics.

The continuous model, where densities are relatively high and shocks are weak, assumes that the gas moves locally in a coherent fashion, that is, there is locally a bulk velocity, one of our unknowns responsible for the flow.



Picture 7 – The centers of the 2000 fibers in 15 crossections 50 μ m apart. All these centers are depicted in the figure which shows the movement of the fibers in the z-direction.



Picture 8 - Model problem for a unidirectional composite.

Pictures 7, 8 – Babuska, Ivo, Borje Andersson, Paul J. Smith, and Klas Levin. "Damage analysis of fiber composites." *Computer methods in applied mechanics and engineering*. 172 (1999) 27-77.

For lower densities, when particles spend a non-negligible time traveling before hitting each other, there are transport models where at each point in space there is a density of particles having a given velocity vector (so now, your ambient space is position and velocity) and colliding laws are prescribed.

Finally, there is always a basic computational model, called the Montecarlo simulation: just give a bunch of particles, with initial position and velocity, prescribe a "bouncing" law and see how they evolve by following each one of them (Picture 9).

This is, of course, the closest model to the "truth", but computationally very restrictive, so the issue is to use it only in those regimes where previous approximations fail.

How to match these three models is a central issue in continuum mechanics, since obviously the Montecarlo method is a simple fundamental way of modeling from granular dynamics to charged particle flows in semiconductor devices, but one would like to (correctly) transform it into transport or continuum approximations whenever possible.

The mathematical issue is, then, as density increases, what is the simplest proper transport model corresponding to a "bouncing" law, and further for higher local densities, the simplest proper continuum (hydrodynamic) model corresponding to the transport one. And, of course, how to couple different regimes (Pictures 9, 10, and 11, see p. I).



Direct Simulation Monte Carlo method (DSMC)

Pictures 9, 10, 11 – Roveda, Roberto, David B. Goldstein, and Philip L. Varghese. "A combined Discrete Velocity/Particle Based Numerical Approach for Continuum/Rarefied Flows." AIAA Paper 97-1006, Reno, NV, January 1997, (see p. I).

LUIS A. CAFFARELLI



Ι