Discrete or Continuous?

At the beginning of April I attended the SIAM Conference on Uncertainty Quantification in Raleigh, North Carolina. UQ is a rapidly growing field at the interface of statistics and computational science, and this was SIAM’s first meeting on the subject. A new journal is starting up, too, the SIAM/ASA Journal on Uncertainty Quantification, joint with the American Statistical Association.

In the old days, science had no choice but to make extreme simplifications. Just the right concepts would be found to compress the complexity of our world, leading to great advances. What’s happening lately, bewilderingly, is that our computers are becoming so fast and their storage capabilities so vast that extreme simplification is becoming a choice rather than a necessity. Science can be multiscale and it can be stochastic, when we wish. A process that used to be modeled deterministically by the heat equation may now be simulated by a random cloud of particles. An answer that used to be a single number may now be a statistical distribution. The aim of UQ is to develop the best ways to compute with such enhanced information.

In his talk on the final day of the conference, Clint Dawson of UT Austin showed a memorable movie. Dawson’s group does large-scale simulations of hurricane storm surges in the Gulf of Mexico, and this particular movie showed a simulation of Hurricane Katrina’s assault on the Louisiana coastline in 2005. You could see the water surging up on shore as Katrina approached, flooding many miles inland.

I found myself thinking about the interplay of discrete and continuous that enables us to watch a scientific output like this.

You could start at the bottom, with the fundamental laws of physics, particularly Schrödinger’s equation, a deterministic equation for the evolution of quantum state functions. At this fundamental level, the Gulf of Mexico is a continuum.

But we would never apply Schrödinger’s equation on an oceanic scale. Everything we care about is a matter of bouncing molecules in classical interactions. At this level, the Gulf is discrete, a stochastic system of about $10^{44}$ particles.

But molecules are irrelevant too for science across hundreds of kilometres. To an oceanographer, the Gulf is a continuum again, with molecules giving way to abstractions like pressure and velocity governed by the partial differential equations of fluid mechanics. This is the starting point of Dawson’s computation, which makes use of the shallow-water equations.

How does he solve the PDEs? He discretizes them by finite elements on a grid of $10^{10}$ nodes. This number is large, though it is nowhere near $10^{44}$, and has nothing to do with the molecular discretization.

After $10^9$ timesteps on $10^3$ processors, out comes the solution: the flow field, a continuum once more.

What does Dawson do with the flow field? He discretizes it to render it as a movie on the computer screen. This entails conversion of the water depth function at each moment of time to $10^6$ colored pixels.

These pixels are, of course, a discretization of a continuous image to be presented to our eyes, which detect the continuum, not the pixels.

How does an eye do its detection? Well, here the system is discrete again. The light from the movie strikes the cones of the retina, $10^9$ of them. The cones send signals to the brain, which processes the data.

And that’s where our final perception of Katrina comes from. In the end we perceive a continuously moving storm, with no awareness of water molecules, finite element nodes, graphics pixels, or retinal cones—not to mention finite element timesteps, movie-rendering timesteps, or floating-point arithmetic!

The last nine paragraphs took us through nine alternating levels: continuous, discrete, continuous, discrete, continuous, discrete, continuous, discrete, continuous. One could hardly say which level represents the “truth,” though there is an interesting tendency for concepts to be continuous and their hardware implementations discrete.

In the old days, research mainly had to concentrate on one piece at a time. Now, it is getting less simple. We are glimpsing a kind of science in which we can afford to relax the boundaries, and UQ is part of this. How do uncertainties at the molecular level propagate through the equations of fluid mechanics and their numerical discretizations, and how should those uncertainties be blended with the quite different ones associated with imperfect resolution of the topography of the Gulf and inexact wind speed measurements? Which should we try to quantify, and which should we ignore? The new world is exciting, but also unnerving for a person like me trained in a notion of science as relentless simplification.

In the world of materials, new tools are bridging the gap from engineering to physics, and we call the result nanotechnology. In the world of computation, we saw in Raleigh how new computers may bridge analogous gaps. As graphics pioneer Alvy Ray Smith proposed in the 1970s, “Reality is 80 million polygons per frame.”