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Rubin Landau

Discoveries Arising from Computing

Fleeting, off-the-cuff remarks by colleagues, parents and spouses somehow have the ability to stick with you for unreasonably long times. I recall remarks by colleagues to the effect that “if you were any good as a theorist, you would not need to do computing”, and that what we need are “pencil and paper theorists who think about things”. Although I believe that many of these types of remarks, already given too much attention in an earlier sidebar, are just examples of self aggrandizement, they have probably led me to prepare a defense by pondering the question “What important scientific discoveries would not have been possible without computing?” Particularly of interest to me are the original, creative and beautiful developments that make science so interesting. Even though I have now given up trying to make those discoveries myself, the question still interests me, and I present here some thought I have gathered for a talk I gave at a recent Gordon Research Conference.

Some of the first examples I became aware of come from what we now call Nonlinear Science, a field in which many of the discoveries were made computationally and then cleaned up and derived by mathematicians. For example, while the discovery of *solitons* probably should be credited to Russell’s 1834 observations and calculations, I believe it was the numerical studies of Fermi, Ulam and Pastu in 1955, and of Zabusky and Kruskal in 1965 that led to the field’s blooming. Likewise, while Poincaré studied chaos in the 1880s, it seems to me that it was the numerical studies of Lorenz in 1961 that led to the modern progress in the subject.

Probably my most basic example is the field of Lattice Quantum Chromodynamics in which the computation is helping to prove that QCD is not only the first real theory for strong interactions, but also a viable one. Here I believe Ken Wilson deserves the credit for realizing early on that solutions to these complicated and highly nonlinear field equations were possible only via Monte-Carlo simulations. Recent times has seen continuing improvement in the predictions due to both increasing computation power, improved theory, and improved algorithms all developing hand-in-hand.

And while speaking of particle physics, let us not forget the critical place computation and simulation have in particle experiments. Indeed, many of the major experiments at Fermi Lab, CERN, and the Large Hadron Collider are sophisticated and subtle mixes of observation, simulation, reconstruction and analysis that have changed what we mean by “seeing” a particle, as well as changing the way other science are now done. (Need I remind you that the World Wide Web originated at CERN in order to support these collaborations with their huge quantities of multimedia data needing to be handled by scientists all over the world? But that turns the question around into major developments in computing arising from the need to do science, something that nuclear and particle physics has been doing for quite some time.)

One of the recent advances in science that I find most interesting is the integration of the data-intensive computational tools (and people) of particle physics with the Sloan Digital Sky Surveys and digital tools of astronomy. This, when combined with multi-scale and multi-physics simulations (discussed next), seem to have turned what used to be an observational science into an experimental one. As an example, consider the *Supernova on Demand* developments at Lawrence Berkeley Lab. Supernova are very much the standard candle of astronomy and have permitted us to measure the expansion rate of the universe and thereby infer information about the amount of dark energy in the universe. Here computations using a two-point correlation function over tremendous data sets are used to find changes in temporally separated images of selected regions of the sky, and thereby deduce the presence of type 1A supernova. Amazingly, a dozen supernovas have been found while still brightening.

Another example of the application of particle physics computation into astronomy is the Amanda Neutrino Experiment. It employs a detector array for its Cerenkov counter that is three times the size of the Eiffel tower and is buried a mile deep into the ice of Antarctica (the ice is the light source). The volume of data produced is large (15 TB/year), with the data stored and analyzed by using the TerraGrid. This experiment has produced a picture of the very-high energy neutrino sky, which remains a mystery.

As just hinted at, simulations in astronomy have also led to major scientific discoveries. These simulations are fundamentally different from those of QCD in which one solves the equations provided by a single physical description. Many simulations, such as those of galaxy and star formation or complex materials, are Multi-Scale and Multi-Physics models in which the same equations are solved at widely different scales and then (somehow) matched together at the interfaces. These can be thought of as hybrid calculations combining discrete and continuous models, using adaptive, multi-scale grids, and applying stochastic and deterministic algorithms. As you might imagine, it is often very hard to put the disparate pieces together ("What God has joined together let no man put asunder").

While speaking of astronomy, I would be amiss not to mention the simulations and animations of the collision of two black holes. The calculations are challenging and intensive, and predict a shivering of space-time like that of Jell-O that leads to gravitational waves throughout the universe. Observing these gravitational waves is still an unfound holy grail.

Although I fear I tread on thin ice when discussing biology, my foundation is reinforced by using an example cited by Ralph Roskies of PSC in one of his talks. He indicated that the 1993 Noble prize in chemistry was given to Agre for his advances in understanding how aquaporins transmit water, but not other molecules, in both directions through cell walls. Not only did this work employ extensive molecular dynamic simulations to gain that understanding, it also produced an animation of the process and had that animation mentioned by the Noble prize committee (an historical first).

Finally, let me end by noting that the collection of codes and data known as the *Cosmic Simulator* has shown how the scientific ideas first put together in Weinberg's *First Three Minutes* form a robust base for computing the formation of galaxies and the modern universe from the big bag. I call that important. I would be thankful to learn about your examples.