By Charles Day

B y the time you read this column, the Royal Swedish Academy of Sciences will have announced the recipients of this year’s Nobel Prizes in Physiology or Medicine, Physics, and Chemistry. The chances are good that computational science contributed to some of the prize-winning work.

Last year’s physics prize went to Saul Perlmutter, Adam Riess, and Brian Schmidt “for their discovery of the accelerating expansion of the universe through observations of distant supernovae,” to quote the official citation (see www.nobelprize.org/nobel_prizes/physics/laureates/2011/press.html). Using supernovae to gauge cosmic distance requires first finding them, which is a technical and computational challenge. Each galaxy hosts a supernova explosion only once or twice a millennium. To be sure of catching at least one supernova in flagrante delicto, you therefore need to image thousands of galaxies. Of course, you don’t know where exactly to look, so you also need to compare images taken on different nights. What’s more, confirming that a galaxy’s abrupt brightening is due to one of its stars popping off in the right, distance-determining type of supernova entails observing the galaxy right after the explosion—then monitoring it for two months!

Perlmutter and his colleagues built a wide-field imager to monitor thousands of galaxies at a time. They observed patches of sky twice: once just after a new moon and again, about 10 days later, just before the next full moon. Thanks to smart algorithms and fast computers, they could compare the two observations quickly enough to find and validate candidates. Riess and Schmidt used a similar approach.

You could say that computational science was implicitly honored by the 2011 physics Nobel. But in some years, the devisers of algorithms have been explicitly honored. Herbert Hauptman and Jerome Karle won the 1985 chemistry Nobel for Shake-and-Bake, a numerical recipe for solving the phase problem in crystallography. The 1998 chemistry Nobel was awarded for two different computational tools: Walter Kohn’s density functional theory and John Pople’s Gaussian program.

Perhaps the most deeply computational work to earn a Nobel prize so far has been Martinus Veltman’s contribution to elucidating the quantum structure of electroweak interactions, for which he and his former student, Gerard ‘t Hooft, shared the 1999 physics prize. In 1963, faced with solving long, complex equations in quantum field theory, Veltman wrote—in assembly language—the first computer program for manipulating algebraic equations symbolically.

What tours de force of computational science deserve future Nobels? At the top of my list in medicine is the Human Genome Project. However, given Alfred Nobel’s stipulation that no more than three people share a prize, the vast project could miss out.

Particle physics discoveries typically involve Herculean feats of number crunching. The Sudbury Neutrino Observatory’s confirmation in 2001 that neutrinos oscillate in flavor merits a physics prize, a share of which would presumably go to SNO’s director, Art McDonald.

In chemistry, I favor honoring Harvard’s Martin Karplus for pioneering the use of molecular dynamics simulations to elucidate the behavior of proteins and other biomolecules.

By the time you read this column, you’ll know if any of my predictions came true.

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