Personnel: J. Terasaki, J. Engel

References: J. Terasaki and J. Engel, in preparation

About the graphics: The graph on top plots transition in strength in an isoscalar dipole channel vs. excitation energy. The large line near zero energy represents motion of the nucleus as a whole (center-of-mass motion) rather than an internal excitation. The facts that this motion occurs so close to its exact value (0 MeV) and that a correction to remove admixtures of center-of-mass motion from the internal excitations make so little difference imply that the calculation is extremely accurate.

The picture at the bottom is the remnant of stellar explosion supernova 1987A. It was taken by the Hubble Space Telescope in 1994.

What has been accomplished: QRPAdef is now complete and we are finishing a preliminary examination of vibrations in heavy nuclei. We have received 10,000,000 CPU hours on the supercomputer Kraken at ORNL for a systematic study of 2+ vibrations in rare-earth nuclei. This will test the ability of modern energy functionals to describe excitations.

Methods and resources used: QRPAdef constructs and diagonalizes the Skyrme QRPA Hamiltonian in the A,B matrix representation in axially symmetric nuclei. The starting point is an HFB calculation in a axially symmetric "box" with the radial coordinate rho running from 0 to 10 or 20 fm, and the coordinate z from -10 or -20 fm to +10 or +20 fm. Next, the code constructs the QRPA Hamiltonian in the basis of canonical
2-quasiparticle states, up to high energy, by evaluating a large number of two-dimensional integrals. It then diagonalizes the resulting large matrix to obtain excited-state energies and wave functions, and evaluates the matrix elements of transition operators between the ground state and those excited states.

The code is parallelized and has been tested on the two of the fastest parallel supercomputers in the country: Kraken and Jaguar (both located at Oak Ridge National Laboratory). It runs on more than 10,000 processors simultaneously.

Impact: The study of vibrations will tell us both about deformed nuclear excitations and the ability of density-functional theory (DFT) to describe them. (There are reasons to think that DFT will work better in deformed nuclei than in spherical ones, but also reasons to doubt its prospects.) When applied, within the next year, to beta decay, QRPAdef will help us understand the creation of heavy nuclei . The location and workings of this process (the "r" process) is one of the most important problems in physics.