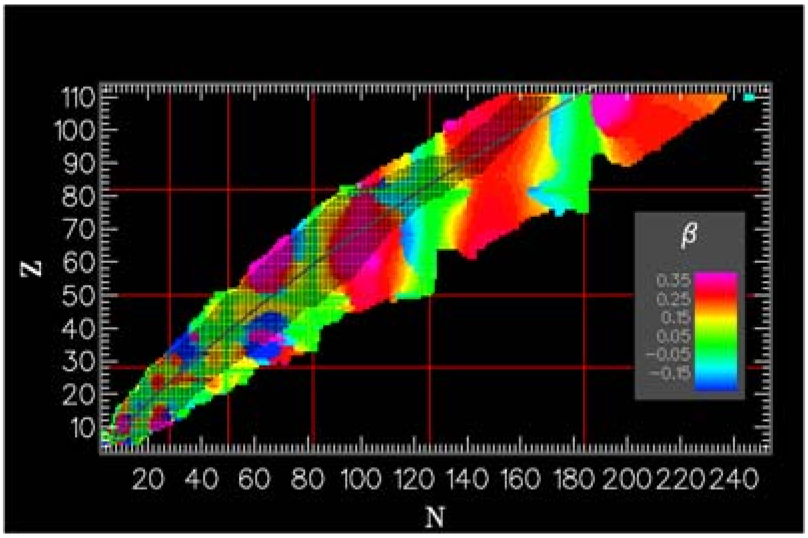
Determining the masses of nuclei by high-performance computing using TERA

Knowledge of the properties of atomic nuclei is essential for improving our understanding of the various processes involved in stellar nuclear synthesis and for understanding the abundance of the various elements which make up the current universe. This knowledge is also required to improve use of new types of experimental and industrial equipment which make use of many radioactive nuclei. Since we do not have any experimental information for the majority of nuclei, the required properties can only be predicted by adopting theoretical approaches. The problem is therefore difficult to solve, since not only is the interaction which ensures the cohesion of neutrons and protons within the nucleus incompletely understood, but also an exact resolution of the n-body problem is impossible because we are interested in systems containing more than 10 nucleons.
To reduce these limitations, physicists specialising in nuclear structure use effective interactions and approximate-solution techniques from the n-body problem, to try and accurately reproduce experimental information relating to nuclei which are stable or nearly stable. Among these interactions, the so-called Gogny force which was developed nearly 30 years ago exhibits the peculiarity of allowing the nucleons from a nucleus to interact at a distance. While this special characteristic has made this force renown, it has also limited its application to a reduced number of nuclei, since use of this force requires significant calculation time in comparison to simpler interactions.
The development of new computing resources has now made possible a systematic study of all the nuclei likely to exist. The overall predictive potential of the Gogny force has therefore been confirmed. However some of its limitations have also been underlined, the main one of these being an insufficient description of the binding energies of the nuclei, which decrease as one moves away from the stability minimum.

The physical challenge

This involves improving the main weakness while conserving the good properties which have already been validated by several decades of in-depth study. The main difficulty in this task resides in the amplitude of the range of variations in the interaction parameters. The problem is doubled by a time constraint on the calculation which negates the idea of automatic optimisation of the parameters within a reasonable time period. The optimisation process has therefore been divided into several interacting, iterative steps. Indeed, theoretical calculation of the mass of a nucleus involves several terms. Certain dominant terms can be systematically calculated during the optimisation process whereas other corrective terms can only be determined occasionally. These corrective terms are therefore assumed, during the first phase, to be independent of the interaction and are only recalculated once significant progress has been made using the dominant terms, in order to achieve a new coherence.
The outcome of such a project was only achievable using the large number of processors that are offered by supercomputers. In our approach, we must calculate the masses of several hundred nuclei independently from each other by using meshes in which the nodes are independent. In total around 70,000 computation points need to be considered which requires some 250 processors over a period of one week, and this for each integrally tested interaction. Using the TERA-10 computer, we have been able to test 25 interactions in a coherent manner having used around 1 million hours of computation time (i.e. around a century) over a period of six months.



Quadrapole moment of the nuclei, a function of the number of neutrons, N, and the number of protons, Z, calculated using Hartree-Fock-Bogoliubov formalism with the Gogny interaction

The result

We have developed an interaction which responds to our requirements since the standard deviation obtained between the theoretical and experimental binding energies for 2149 known masses is 798 keV. This compares well with the best approaches available in the field and constitutes a significant advance in comparison to the greater variation of 2 MeV provided by the initial set of parameters. The preliminary analyses carried out with this new interaction do not reveal major degradation of the other properties with regard to the initial interaction. This work has now been published (Physical Review Letters 102, 242501 (2009)).