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On porting low-energy nuclear reaction codes on Grid

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Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

There was always a stringent need for high accuracy nuclear data
due to nuclear
fusion and fission projects, and not only, that have intensified
in the last years
due to new foreseen facilities. The experiments are becoming more
complex, expensive
and lack the power to measure all the required quantities. The
comparison of the
measured and calculated cross sections for nuclear reactions
showed in several
occasions noticeable differences between nuclear computer codes
predictions above the
energy regions with experimental data and also a significant
deviation from unity of
calculated-to-experimental ratio [1], moreover these evaluations
being reported
without estimates of uncertainties. Recent efforts have begun to
address this
uncertainty issue through the generation of covariance files for
nuclear model
calculations [2], a task that requires large scale computations.
It is thus justified
the effort made to improve the actual status of the nuclear
computer codes which in
turn translates in reliable, safer and cost effective modern
facilities [3].

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

Porting the EMPIRE-II [5] nuclear reaction code to computational
GRIDs was done by
integrating it on the GILDA [6] Grid testbed [7] during
ICTP/INFM-Democritos workshop
on "Porting Scientific Applications on Computational GRIDs"[8].
The purpose was to
reduce the time used to systematically evaluate in one run all
reaction channels of
all stable isotopes corresponding to a given element,
and possibly neighboring elements using local and/or regional
parameters [6].
Also a modified version of SCAT-2 [9] nuclear code that searches

“best fit” nuclear optical model parameters was ported to the parallel environment using OpenMPI [10] library, the code being prepared to run on the in the EGEE FUSION VO Grid[9]. The performance tests show that the code is very scalable with the number of processors and thus perfect for the parallel and distributed computational environments.

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possible, point out the experience limitations (both in terms of existing services or missing functionality)

Porting the nuclear-reaction computer code EMPIRE-II to GRID infrastructure and the graphical integration into Genius web portal proved successful. However, there are still remaining issues regarding the MySQL EXFOR experimental database as well as an eventual implementation of a facility for plotting online the calculated results in comparison with the experimental data.
The code SCAT-2 proved to be a highly scalable one, suitable for distributed architectures. It is thus supporting the next step of a concurrent study by taking into account all known experimental elastic-scattering angular distributions for a given isotope/element. The further use of dynamic chunks of data may improve the load balancing on heterogeneous environments, at the cost of the overhead of communication.
The reliability and cost effectiveness of future facilities relies on improved nuclear reaction models as well as faster computer codes and finally the covariance evaluation of nuclear models. In spite of it being a long-standing subject, only recent investigations in this respect have been motivated by the computational power of present computers. This work has showed that it is rather straightforward to integrate actual nuclear computer codes into GRID computational environment for assessment of large data sets. Following the achievement of this goal concurrently and also performing large scale computations with MPI enabled nuclear codes, the related outcome will be firsthand the reduced computational time, and also one of the first steps towards nuclear models uncertainties generation.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

Continuous improvement of a nuclear code is essential for its predicting power and reliability, obviously the most important aspect being the underlying physical models and parameters but another key issue is the computational time performance. This performance is affected by the complexity of the actual physical model which in turn dictates the level of approximations employed to the algorithm used. The simplifications are most of the time satisfactory but with time they become too general for user requirements and tend to restrict the applicability of the algorithm, thus new techniques or models are needed.
Therefore it is desirable to exploit modern hardware and software platforms in order to perform faster and with better precision the necessary calculations and thus improving overall the process of evaluating the nuclear data.
The paper presents the techniques used to improve the performance of low-energy nuclear reaction codes with respect to computational time, namely the porting process of EMPIRE-II and SCAT2MIN nuclear computer codes to grid environment [4], method that provides the highest achievable performance at a reduced cost and a higher security.

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