Contribution ID: **73** Type: **Oral**

Grid computing applications in modeling and simulations of molecular nanomagnets and classical charged particles

Wednesday, 4 March 2009 14:00 (25 minutes)

Physical properties of classical and quantum systems can be obtained using computer simulations, which is of importance in checking the suitability of the theoretical model and prediction of experimental results.
We discuss the use of quantum transfer matrix (QTM) and exact diagonalization (ED) techniques for simulations of quantum systems and the use of the genetic-algorithm (GA) based approach for simulation of classical systems. These methods were exploited using the grid technology.

Impact

To demonstrate the functionality of our approach, we calculated the low temperature torque, specific heat and entropy for the s=3/2 quantum spin system modelling Cr8 molecular ring. To evaluate the scaling of parallel processing, the efficiency and speedup were calculated. Our simulations, based on the QTM technique, scale very well and the efficiency for the shortest runs is 1 up to 1024 processes at which the limit due to the size of our model is reached. The ED scaling is efficient up to about 10 processes, however, for larger molecules the number of exploited processes rapidly increases. Therefore in both cases the scaling is improved when larger systems are considered.
Comparing the calculated ground- and metastable-states to the results obtained by other experimental and theoretical methods (Monte-Carlo, Molecular Dynamic) we were able to find out which of these methods correctly determined the geometric structure and the ground state of the system in particular configurations.

URL for further information

http://kabestan.fizyka.amu.edu.pl/~antekm/egee/

Conclusions and Future Work

We have demonstrated the efficiency of the QTM and ED parallel simulations of the chromium-based molecular rings. Minimal potential energy of the classical system consisting of point-charged particles was calculated using GA. However still some differences between experimental and theoretical results remain.
Thanks to the scientific EGEE grid environment provided by VOCE virtual organisation we could obtain presented results and will be able to simulate even more complicated systems.

Keywords

molecular nanomagnet, quantum transfer matrix, exact diagonalization, genetic algorithm, simulation

Detailed analysis

The thermodynamic quantities and energy structure of the quantum spin systems modelling the chromium-based molecular rings were obtained using QTM and ED technique. The single ion anisotropy and alternation of the nearest neighbour exchange integrals were considered. The parallel processing exploiting MPI library

was employed to speedup the calculations. The self-scheduling scheme and the longest processing time algorithm were used to diagonalise the Hamiltonian matrix by slave processes.
The 2- and 3-dimensional ground-state configurations of the classical point-charge particles were calculated using the GA based approach. The systems consist of a number of particles interacting through the Coulomb and logarithmic potential, trapped by the parabolic conferment potential. The GA approach follows the Holland scenario and finds the global minimum of the potential energy corresponding to the optimal geometrical structure.
The performed tasks are a part of the MAGMANet activity.

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Session Classification: Computational Chemistry

Track Classification: Scientific results obtained using grid technology