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FRAUNHOFER INSTITUTE FOR ALGORITHMS AND SCIENTIFIC COMPUTING SCAI

1 *Two-phase fluid flow with coupled particle droplets*
© M. Griebel, P. Zaspel
(INS, University of Bonn)

MULTI-GPU ACCELERATED NUMERICAL SIMULATION

Fraunhofer Institute for Algorithms and Scientific Computing SCAI

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Recently Fraunhofer SCAI, in conjunction with the Institute for Numerical Simulation (INS) at the University of Bonn have been selected as one of the first CUDA™ Research Centers in Germany based on the vision, quality and impact of their work. The research is focused on the development of massively paralleled multi-GPU based software packages for numerical simulation in the natural and engineering sciences. Companies benefit from the transfer of knowledge from basic research to practical applications.

Today, numerical simulations are indispensable in industrial production. Examples are the creation of new materials, the modeling of manufacturing process chains, and the simulation of material strength and fluid dynamics. However, these simulations require computing times from hours to days, even on high performance computers. This is why industry and science are very interested to shorten processing times.

The actual fastes high performace clusters are based on acceleration by graphic cards. Computing on graphics cards not only promises an enormous acceleration of numerical simulations. The GPUs also require much less electricity, delivering a much higher performance per watt benefit. For example, the benchmarks calculations with the multi-GPU based high performance fluid dynamics code NaSt3DGPF of the INS show a speedup of 10 to 40 times for a single GPU vs. single conventional CPUs. Moreover, the performance per dollar is two to three times better and Fermi-type GPU exhibit here to be more than two times more power-efficient.

The researchers from INS and SCAI hope to gain similar effects from adapting the software package Tremolo-X for use on multiple graphics cards. Tremolo-X is used for the molecular dynamics of atoms or molecules. This software simulates materials at the nano scale, and therefore

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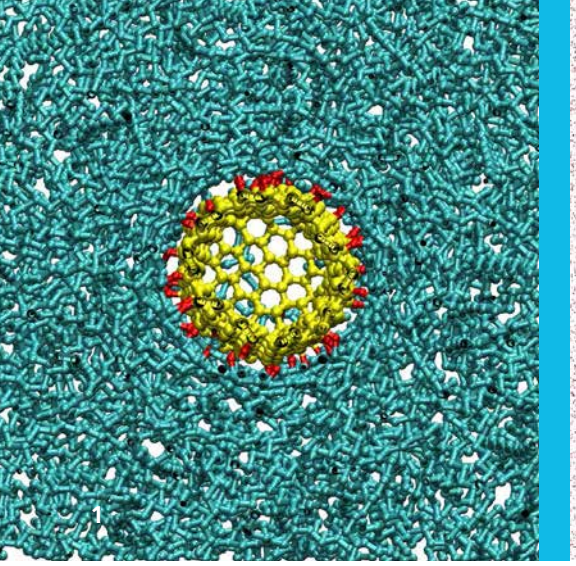

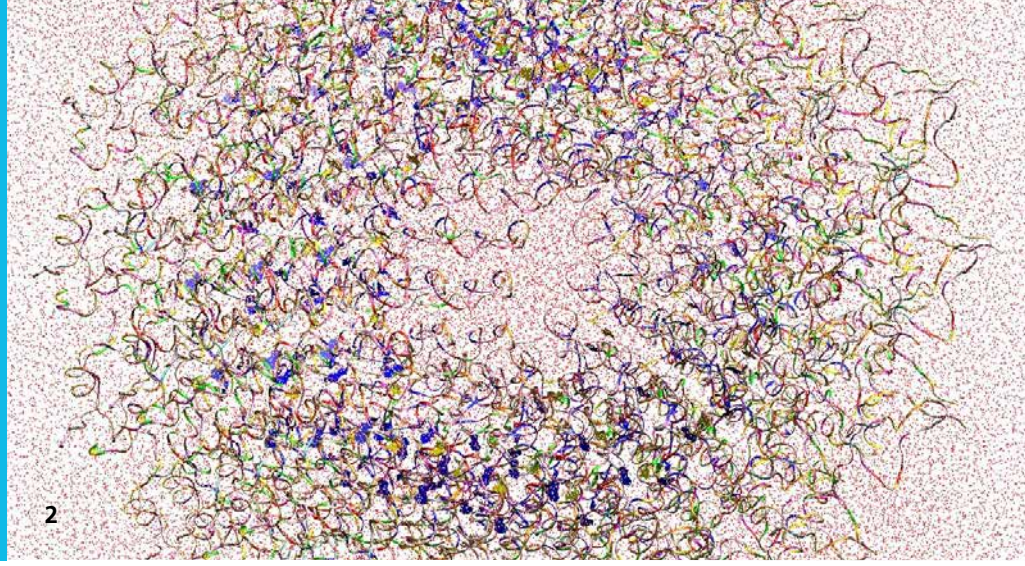

1 *Functionalized C-NT in polyethylene*

2 *Ribbon view of Tobacco Mosaic Virus in water*

TREMOLO X

makes it possible to efficiently design new and innovative materials. Moreover, the research is focused on massively parallel multi-GPU accelerated numerical algorithms in general. E.g. SCAI develops the LAMA library, a numerical library which leverages the performance of heterogeneous hardware architectures in general and GPUs in particular. Furthermore, SCAI is involved in several research projects with the aim of unleashing the power of accelerated computing beyond the community of HPC specialists.

Software package Tremolo-X

Applied research and development at the department »Virtual MaterialDesign« is focused on multiscale modelling and numerical simulation in material science and nanotechnology. An essential basis for designing novel materials is the understanding of their properties on the nanoscale. Molecular dynamics are an important tool for the analysis of a material on that scale. To this end, Fraunhofer SCAI offers Tremolo-X, a massively parallel software package for numerical simulation in molecular dynamics. Here, much emphasis has been placed on the parallel implementation and its efficiency.

Tremolo-X includes an efficient parallel implementation of all potential types commonly used for modeling of systems in the areas material science, nanotechnology and biophysics. Tremolo-X is particularly optimized for parallel application, where it uses tree algorithms for long-range potentials as well as grid algorithms for short- and long-range potentials. In addition, a user-friendly graphical interface is included, which provides an easy set-up and analysis of numerical experiments.

Since the actual fastest high performance clusters are accelerated by graphic cards, essential computation engines of Tremolo-X are actually adapted to multi-GPU based architectures, c.f. the CUDA Research Center located at SCAI and the Institute for Numerical Simulation of the University of Bonn. Here, the research is in particular focused on parallel scalability and efficiency concerning the evaluation of the long-range Coulomb potential, e.g. by FFT and multigrid based methods.

Tremolo-X has been successfully applied within various projects in different fields of applications like nanotechnology, material science, biochemistry and biophysics. For example, it has been employed to predict the mechanical properties of carbon and boron nitride nanotube composite materials, to analyze the nanostructure of cement based materials and study ion channels.