ERC Starting Grant ADAPT

Post-doc opening

Parallel algorithms for adaptive molecular dynamics simulations

About the NANO-D research group at INRIA

The NANO-D group, led by Stephane Redon at INRIA, develops novel multiscale, adaptive modeling and simulation methods, which automatically focus computational resources on the most relevant parts of the nanosystems under study. All algorithms developed by the group are gathered into SAMSON, an open-architecture software platform designed by NANO-D (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems, available on SAMSON Connect at https://www.samson-connect.net).

During the twentieth century, the development of macroscopic engineering has been largely stimulated by progress in numerical design and prototyping: cars, planes, boats, and many other manufactured objects are nowadays designed and tested on computers. Digital prototypes have progressively replaced actual ones, and effective computer-aided engineering tools have helped cut costs and reduce production cycles of these macroscopic systems.

The twenty-first century is most likely to see a similar development at the atomic scale. Indeed, the recent years have seen tremendous progress in nanotechnology - in particular in the ability to control matter at the atomic scale. Similar to what has happened with macroscopic engineering, powerful and generic computational tools will be employed to engineer complex nanosystems, through modeling and simulation.

The NANO-D group is funded through ANR grants, an ARC grant, and an ERC Starting Grant (https://team.inria.fr/nano-d/).

Adaptively Restrained Hamiltonians for Computational Nanoscience

The NANO-D group has introduced the theory of Adaptively Restrained (AR) Hamiltonians, to enable adaptive dynamics simulation of particle systems [Artemova and Redon, Physical Review Letters, 2012]. The theory applies to any particle
system, whatever the interaction potential, hence to molecular dynamics simulation of nanosystems.

The AR Hamiltonian is a modified version of the original Hamiltonian, in which the inverse inertia becomes dependent on the particle’s momenta. Under some appropriate conditions (e.g. small momenta), the inverse inertia of the particle system is modified so that some particles’ positions are frozen, although their momenta continue to evolve. During an adaptively restrained simulation, particles thus stop and go repeatedly. Since the calculation of the interaction potential and forces may often be accelerated when some particles’ positions are frozen (using so-called incremental update algorithms, e.g. [Bosson et al. Journal of Computational Chemistry]), AR simulations may be significantly faster than regular simulations, while making it possible to compute statistical properties [Artemova and Redon, Physical Review Letters, 2012]. The figure belows shows how adaptively restrained simulations speed-up collision cascade simulations.

Objectives: Parallel algorithms for adaptive molecular dynamics simulations

The goal of the successful applicant will be to develop adaptive particle simulation algorithms on parallel hardware, i.e. a combination of Graphics Processing Units (GPUs) and multi-core processors. Our adaptive framework should be most appropriate for this task. Indeed, the adaptive integrators have a very similar structure to traditional non-adaptive ones, with supplementary terms for particles that are in the transition regions. Moreover, the algorithms for incremental potential updates will either be generalizations of traditional algorithms for which parallel versions are known, or will rely on our divide-and-conquer decompositions (e.g. partial force tables), which are inherently parallelizable. Besides usual design matters (e.g., designing data structures so that memory accesses are efficient), the design of adaptive parallel algorithms will raise interesting questions of load balance and resource allocation. For example, since CPU-GPU transfer is known to be slow, we will need to set up incremental transfers between the CPU and the GPU to speed up communications.

Desired profile

We are looking for creative, passionate and hard-working individuals with exceptional talent for computer science and mathematics. The successful applicant will have a PhD (or be in the process of obtaining a PhD) in computer science, computational physics or a relevant field, with demonstrated abilities for designing parallel algorithms, preferably in the context of molecular dynamics simulations. Excellent oral, written and interpersonal communication skills are essential (the working language will be English – knowledge of French is a plus).

Requirements

- **Strong** computer science, mathematics and physics background (PhD in computer science, computational physics or a relevant field)
- **Strong** oral, written and interpersonal communication skills (working language is English – knowing French is a plus but is not necessary)
- **Strong** experience of parallel programming (OpenCL, CUDA, OpenMP, MPI, etc.)
- Good knowledge of C++
- Ability to work independently and with a team

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Position and salary

The position is for 18 months and is funded on the ERC Starting Grant project ADAPT. The salary is 2127 Euros net/month.

About Grenoble

Grenoble is the capital city of the French Alps. Combining the urban life-style of southern France with a unique mountain setting, it is ideally situated for outdoor activities. The Grenoble area is today an important centre of industry and science (second largest in France). Dedicated to an ambitious policy in the arts, the city is host to numerous cultural institutions. With 60,000 students (including 6,000 foreign students), Grenoble is the third largest student area in France.

For more information – to apply

Send an email to Stephane Redon (stephane.redon@inria.fr) with a resume.