NSC News
2012:2
National Supercomputer Centre at Linköpings universitet

They have arrived

NSC's three new systems have arrived and are currently undergoing acceptance tests. Read further on page 4

Bridging scales in biomodeling

Prof. Aatto Laaksonen develops multi-scale computer modeling methods to tackle the challenging time and length scales in biomodeling.

Read further on page 3

New director at NSC

NSC's new director from first of July, Prof. Patrick Norman, presents himself.

Reed further on page 5

Four and a half years with NSC

This is my last editorial as my directorship ends in June 2012. Thus, I would take the opportunity to look back on these interesting 4 ½ years. First of all, it is amazing to follow the fast developments in the high-performance computing area, and to get NSC keeping up with the challenges and putting our users at the centre of our activities. It is really a vibrant environment and I would like to thank all co-workers at NSC and other SNIC centres and our partners SMHI and Saab. Five years ago, NSC inaugurated the existing computer room, but already early 2013 we will inaugurate the next computer room, which is about four times bigger. This will help to make NSC an attractive host for many future computer systems. Furthermore, the room is prepared for additional expansions with adjacent buildings. On the staff side, we have doubled the number since 2008, and we have also expanded our competences to also include application expertise and system development, apart from the "traditional" system management of computational clusters and large-scale storage. It is with great pleasure that we this spring/summer welcome Krishnaveni Chitrapu, Janos Nagy, Andreas Lindqvist and Fredrik Nyström to NSC. Thanks to our staff expansion, we are now able to help our increasing number of users much better in multiple aspects of high performance computing. In 2010, the strategic e-science initiative SeRC started, which has contributed funding to several application experts. Within SeRC we have close collaborations with our sister centre PDC in Stockholm. Furthermore, we are most grateful to SNIC showing great confidence in NSC by placing their large clusters here. At the time of writing, the first racks of the new flagship cluster Triolith are installed. At the same time, we received SNIC's decision to invest an additional 10 MSEK in a well-needed expansion of NSC's cluster capacity. It is rewarding to see that our collaborations with SMHI and Saab progress prosperously to mutual benefit, most recently with new technical projects and installation of additional cluster systems. I am now passing the baton to Prof. Patrick Norman – our new NSC director from July 2012. I wish him all the best in this position, and I am confident that the next years will be equally fast developing and challenging and that NSC will continue to be at the forefront of Swedish HPC. Finally, I would like to wish all our users, collaborators and skilled staff a well-deserved and rewarding summer vacation.

BENGT PERSSON, NSC DIRECTOR

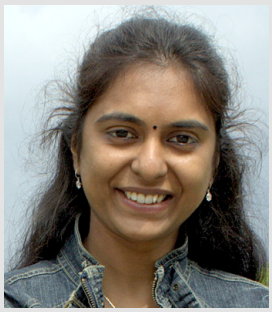
Schrödinger Software Now Available at NSC

After an initial evaluation period, we are pleased to announce that the Schrödinger suite of applications is now available at NSC. We have purchased a one-year license that should give everyone interested in using Schrödinger applications a good chance to do so. The license agreement consists of 30 license tokens and 20 separate Jaguar (incl. pK_a predictor) licenses. Using these licenses at NSC is free for anyone affiliated with a Swedish academic institution. However, the licenses are intended for smaller projects and will only cover a few simultaneous instances of the various Schrödinger applications. Hence, for larger projects with many production jobs the PI may have to complement with personal licenses. Please note that the license owner can easily manage the access to personal licenses placed at NSC using NSC Express.

The current license agreement is for one year, but NSC intends to maintain a Schrödinger license on a longer perspective. However, the details of the license agreement may change depending on both the observed use of the Schrödinger applications and available funding.

If you have any questions regarding getting started with Schrödinger software at NSC, then please don't hesitate to contact support@nsc.liu.se

TORBEN RASMUSSEN, NSC



New staff member

Hi,I moved to Linköping very recently and joined the elite club of NSC in May this year as a Software Developer. I have my Bachelors degree in Computer Science from India and ever since been working in IT Industry for nearly 6 years now. My expertise is in Java, J2EE, web-services, open source frameworks. Earlier, I have been part of Multi National Firms – Hewlett Packard and Infosys Technologies.

At NSC, I am involved with setting up the formal process and development of web Applications and also will be part of dCache development. Working as a System Developer at NSC gives me great opportunity to work with the latest technologies and large scale storage Systems which I am quite enthusiastic about.

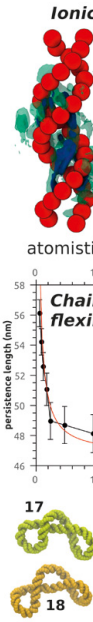
KRISHNAVENI CHITRAPU, NSC

Challenging the time and length scale

Multi-scale computer modeling methods are rapidly developing, constantly expanding and widely used in all disciplines of Science. In Chemistry and Materials Science the goal is to connect particle simulations on atomistic scale with the description and models of macroscopic matter to have a hierarchical "from-bottom-up" methodology to design novel materials with specific properties by starting from its smallest building blocks nuclei, electrons, atoms and molecules. Multi-scale schemes in Biology may one day allow connecting the chain of increasing complexity: Molecules-Organelles-Cells-Tissues-Organs-Organisms. As there is a range of 12–15 orders of magnitude in the length and time scales, it is obviously a highly challenging task to bridge the scales. There are already many computational methods and models applicable on certain intervals of the length and time scales. Combining them together is therefore an obvious strategy to perform multi-scale modeling. Teaching these methods to understand the language used for different physical models so that they can exchange information with each other is the key to multi-scale modeling of this type.

Hierarchical successive coarse-graining (CG) is alternative natural way to extend the length and time scales in computer simulations, by reducing the number of degrees of freedom (details), which are not important on the next more approximate level of molecular description. For example when starting from first-principles simulations with nuclei and electrons and going up to classical (molecular) mechanical simulations the electrons are removed while all atoms are kept. In the next step, the atoms and molecules are made to larger aggregates and treated as single soft particles. The coarse-grained particles have larger masses and softer potentials, allowing use of longer time steps to cover longer time and length scales at the same computational cost. There are several schemes for coarse-graining of molecular systems, such as construction of simple interaction potentials by matching the structures (or forces) between two different resolutions, construction of heterogeneous elastic networks from atomic positions, or using inverse methods based on renormalization theory. Already in 1995 we proposed a method called the "Inverse Monte Carlo" (IMC), based on inversion of radial distribution functions (RDF) to obtain effective pair potentials [1]. It allows us to start from first-principles (ab initio) simulations without any empirical input parameters to obtain an atomistic force field (FF) for conventional classical simulations with Molecular Dynamics, or Monte Carlo. Again in atomistic simulations we can construct a coarse-grained FF where for example the explicit solvent molecules are completely removed but included instead in the effective solvent-mediated potentials [2]. IMC makes it possible to perform truly hierarchical multiscale modeling keeping the full atomistic details for the coarse-grained sites in the more approximate model (schematically shown in Fig.1). The effective pair potentials reproduce accurately the details of the underlying fine-grain model. In other words the IMC creates a model from the results (even experimental) by solving the inverse problem and the solution is proven to be unique between RDFs and pair potentials [3]. Three multi-scale modeling applications are studied at NSC: (i) DNA, (ii) G protein coupled receptors and (iii) Polyamidoamine (PAMAM) dendrimers as drug carrying vehicles penetrating lipid membranes.

For DNA a new class of coarse-grained force fields is constructed using the IMC method where nucleotides (phosphate, sugar and base) are taken as a single interaction site. The beads are linked via a topology of 16 effective solvent-mediated interactions (a more detailed three sites per nucleotide force field is under development). Counter ions interact with the DNA via solvent-mediated effective potentials. The model reproduces the key elastic features of DNA fragments such as persistence length and dependence on the ionic strength while retaining the local ionic atmosphere from underlying all-atom simulations (Fig. 2). The model is used to investigate supercoiling in circular DNA, condensation and packing (Fig. 2). For packing we are implementing a peptide-DNA FF to model the histone core.



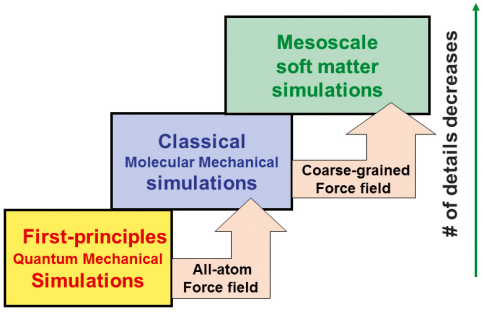


Figure 1: Hierarchical multi-scale modelling – by successive coarse-graining with IMC

New staff member

I joined NSC at the beginning of June, I work with tape libraries and storage systems. I had moved to Linköping from the United Kingdom where I worked as a consultant in Reading, Swansea and London.

Before that I had worked as a systems administrator and I was involved with HPC (mostly storage systems, IBM AIX, TSM, Linux and other Unix and non-Unix systems) in various academic/research institutions in the UK, in Australia and in Hungary.

JANOS NAGY, NSC

s in biomodeling

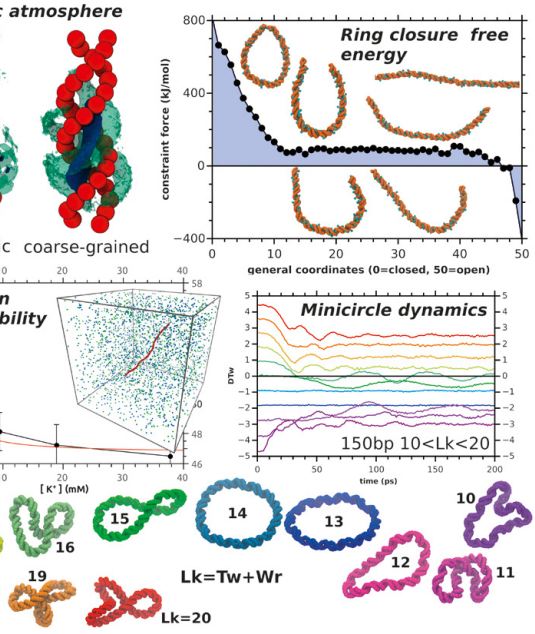


Figure 2

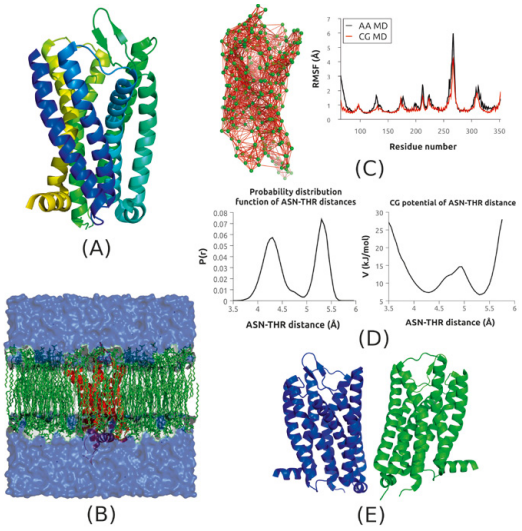


Figure 3

The highly flexible μ opioid receptor (μOR) (Fig. 3A), important in the treatment of acute and chronic pain, is studied embedded in an ion-water-membrane environment for its dynamic characteristics (Fig. 3B). Hierarchical coarse-graining allows computer simulations on a micrometer/microsecond scale. We are systematically developing a family of CG force fields adapted to reproduce the important details from all-atom (AA) MD simulations. The first class of CG Force Field is based on elastic network representations of the μOR (Fig. 3C) to reproduce in AA MD obtained high backbone flexibility of μOR in order to develop a flexible framework operational on microsecond time scale which will improve the currently available docking algorithms. A second class of coarse-grained force fields is developed by using inverse techniques to the all-atom MD simulations. This more sophisticated force field reproduces the multi-well-distributions of structural parameters and will be used to study complex dynamical mechanisms of the μOR like its activation process (Fig. 3D). We also study the aggregation processes of the μOR as many of its biological functions are influenced by its dimerization-state (Fig. 3E). The entire multiscale and multimethod modeling approach brings new important dynamical information about the conformational behavior of μOR and can be connected with its biological function, in order to design and refine novel drugs.

PAMAM dendrimers (branched polymers) can be used as nano-devices for

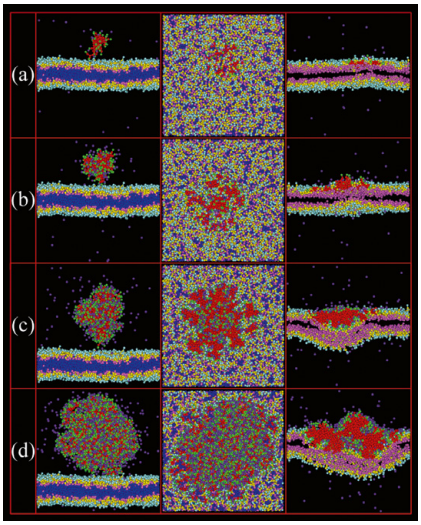


Figure 4

nonviral gene delivery and antitumor therapeutics. Among the important issues to study using computational methods are how these charged star-like polymers interact with zwitterionic head groups of cell membranes (the walls of living cells) and how we can control the dendrimer–membrane complexes during the delivery including the penetration through the cell wall. A multiscale simulation study is performed based on successive coarse-graining of atomistic models. However, charged soft particle systems are very difficult to model as charges inside soft particles can come too close. After implementing ENUF, a new linearly (Nlog(N)) scaling robust Ewald summation method, based on non-uniform FFTs [4] in our Dissipative Particle Dynamics simulation code we are able to accurately study the highly complex PAMAM dendrimers and dimyristoylphosphatidylcholine lipid interactions using mutually consistent CG models The PAMAM model describes correctly the conformational behavior

Three new systems

All three new systems, Skywalker for Saab, Krypton for SMHI and Triolith for NSC's academic users are now under acceptance testing. The first, Skywalker, arrived on May 28 and the last, phase one of Triolith on June 14. We hope to allow "test pilots" on Triolith phase one from week 27. The system should be close to production already at that stage but interrupts may be more frequent and the user experience less smooth than on a normal NSC system even though NSC will do its best. Normal production is planed to start a few weeks later. Projects with large scale SNIC time allocated on Neolith will have their allocations moved to the much faster system Triolith. NSC currently plan to power off half of Neolith on September 15 in order to allow for the installation of Triolith phase two to start. Users in projects that will have their allocation moved are strongly advised to become test pilots and start the migration from Neolith to Triolith as soon as possible to be ready by that date. Please, send an e-mail to support@nsc.liu.se if you would like to become a test pilot on Triolith.

PETER MÜNGER, NSC

of the dendrimers while the DMPC model gives a proper surface tension for the membrane. In our simulations (as well as in experiments) the PAMAM dendrimers penetrate the lipid membrane. The cavity forming in membranes is influenced by increasing the dendrimer concentration which enhances the permeability [5]. Higher generation dendrimers (with longer branches) can more easily disrupt the membrane introducing pores on the surface. Higher generation dendrimers undergo a conformational transition from planar to spherical (Fig. 4). Inside the spherical structure they can transport drugs.

All the calculations are carried out by Aymeric Naômé, Mathieu Fossepre and Yonglei Wang, PhD students in Aatto Laaksonen's group.

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Aatto Laaksonen is Professor in Physical Chemistry at Stockholm University. He has been using NSC resources three decades from the days NSC bought the first supercomputer in Sweden, a Cray 1S.

Patrick Norman – NSC's new director

NSC has installed a new director in terms of Prof. Patrick Norman with a background in theoretical chemistry. He describes his background starting with an anecdote from his PhD defense dissertation at Linköping University in 1998.

At the end of my PhD defense dissertation I was asked to identify a Fortran punch card. The punch card had become outdated before my entering the field of scientific computing but stories had been told by my supervisor about the fatal consequences of dropping your box of cards on the way to the computer hall so I did recognize it and passed the exam question. Many of the calculations in my thesis titled "Nonlinear Optical Properties of Fullerenes, Oligomers, and Solutions" were instead carried out by means of an IBM RS/6000 computer with 64 MB of RAM and an impressive hard disk capacity of 2 GB. What more could one ask for?

After my PhD defense, I completed post doctoral studies on relativistic quantum chemistry at the University of Southern Denmark, Odense, and molecular vibrations at the University of Ottawa, Canada. I returned to Computational Physics at IFM and took part in an FOI lead project aimed at the construction of solid-state glass materials for sensor protection against laser damage. The design of chromophores responsible for the desired eye-safe optical power limiting require a detailed understanding of linear and nonlinear light-matter interactions and involved, in our case, heavy-atom induced spin-forbidden transitions as a key component. This project spurred a series of methodological and software developments and most of these efforts were incorporated into two quantum chemistry programs of Scandinavian origin namely Dalton and Dirac. But the successes of scientific software simulations depend critically not only on good algorithms but also top-performing computers. Our simulation work became all the more realistic after gaining access to the Monolith cluster at NSC. Imagine a computer with around 400 processors and 2GB of RAM per node. What more could one ask for?

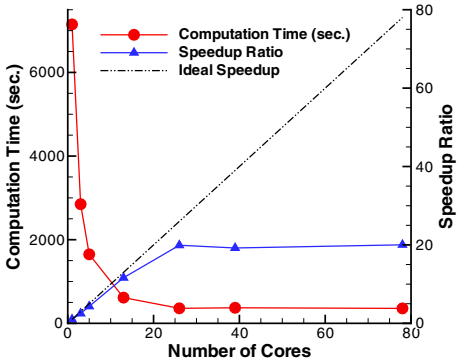
In 2003 I was recruited to NSC in the capacity of application expert, a position which I held for about five great years. The years were great because I could tap into the vast knowledge bank of the supercomputer experts at the same time as I to some degree could control the software platform for my scientific ambitions. It may even have occured that one or two processor benchmark tests coincided with a simulation of concern to an ongoing project. I had the benefit of being a small but proud part of the complex procedure of replacing one cluster with another, which eventually lead to the inauguration of Neolith, before returning full time to research as a VR Researcher (rådsforskare). In recent work, we have focused particularly on to the development of time-dependent response theories for electronic resonance spectroscopies, such as UV/vis and X-ray absorption and circular dichroism spectroscopies.

One question was posed twice in the above but it will find no answer here or elsewhere. I can just conclude by saying that algorithms and computer hardware will forever improve and widen the scope of scientific applications, and I am excited to be right in the middle of this development.

PATRICK NORMAN, NSC

Parallelisation Support of a Large Eddy Simulation Code

NSC have started to provide code parallelization support to prominent Swedish domain scientists. Scientists can expect to be able to increase their problem sizes and reduce the computational time for their applications by this service. This high-end collaboration between NSC and scientists will strengthen the international competitiveness of top-ranked Swedish scientists and increase NSC's contribution to Swedish academia.



Prof. Lars Davidson's LES (Large Eddy Simulation) fluid dynamics code has been chosen as a pilot project for this code parallelization service. This code solves the incompressible Navier-Stokes equations by solving the decoupled velocity field (convection-diffusion equation) and pressure field (pressure Poisson equation) iteratively. The convection-diffusion solver use a conventional 3- dimensional structured stencil, while the pressure Poisson solver applies a multi-grid method and stores the multi-level data in a 1-dimensional array. Minor changes was made on the baseline code for the imposed generic boundary condition, effective memory allocation, and the wall-distance function for turbulence computation. Mesh partitioner and communicators are implemented for parallel execution. A structured multi-block partitioner provides a load balanced decomposition at a sufficient multi-grid level. Communication functions are incorporated for structured 3-dimensional domains and the 1-dimensional multi-grid implementation. These implementations are made generic and therefor direct applicable to any mesh-based solver.

Parallel performance has been measured for a 3-dimensional flow simulation. The problem size was limited to roughly 2.4 million mesh points due to the memory allocation limit for the sequential code. As presented in Figure 1, the speed-up ratio is linear (with around 90% parallel efficiency) at small number of cores and it is maintained around 20 for higher number of cores. The linear range as well as the maximum speed-up ratio improves for larger problem domains. We also observe that algorithmic changes in the time evolution scheme and reduction of the imposed boundary condition in the baseline code will improve the parallel performance with retained convergence criteria. This will be the next main objective.

This high-end user support provides the opportunity of possessing well-tuned application codes to domain scientists. It will accelerate the production of high-quality scientific researches. Meanwhile, this cooperation requires the sufficient number of application experts in individual scientific domain who is capable of dedicating this long-term service. It necessitates more financial support for incrementing application experts on various scientific domains.

SOON-HEUM ("JEFF") KO, NSC

Parallel Programming Support

SNIC now has a number of application experts in computational science and parallel programming that are available to help you with your code development projects. They can, for example, help you with debugging, profiling, and tracing, as well as, simpler optimization, parallelization or code porting tasks. An application expert will devote up to 10 full workdays to a request, which will be handled when time is available on a best effort basis.

If you think that your project requires more than 10 workdays worth of assistance, then please submit your request anyway, so an application expert can make an assessment of how much work the requested assistance will be. This assessment can then be used for further discussions regarding setting up a more long-term application expert commitment to the project.

Any researcher affiliated with a Swedish university institution (incl. Ph.D. project students) can submit a request for parallel programming support. Please submit your request to application-support@snic.se.

For more information, please see http://docs.snic.se/wiki/support

TORBEN RASMUSSEN, NSC

Linköping University

National Supercomputer Centre, Linköpings universitet, 581 83 Linköping, Sweden
Tel: +46 (0) 13-28 26 18, fax: +46 (0) 13-28 25 35, e-mail: info@nsc.liu.se
www.nsc.liu.se

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