HPC2N Open House with Kebnekaise Celebration

Umeå University, Nov 30, 2017

Sample User Research Projects at HPC2N - Invited Presentations

Capturing Evolution with Computers

Shina Caroline Lynn Kamerlin, *Science for Life Laboratory, Department of Cell and Molecular Biology, Uppsala University*

Abstract: Recent years have seen an explosion of interest in both experimental and computational studies of the evolution of enzyme function [1,2]. In particular, it has been argued that conformational selection plays a major role in allowing old enzymes to acquire new activities [3]. My group and I have performed detailed computational studies of a broad range of catalytically promiscuous enzymes, in order to probe the molecular origins of both their multifunctionality and its implications for their functional evolution [4-7]. These include alkaline phosphatases [4], organophosphate hydrolases [5,6], aldolases [7] and Kemp eliminases, to name a few examples. Based on this work, we present a molecular model for enzyme evolution, highlighting the critical importance of a fine-tuned interplay between enzyme dynamics, electrostatic cooperativity and conformational selection in allowing for the acquisition of new activities, as well as the ability to select more than one possible reaction from a pool of given substrates. We also highlight the role the Kebnekaise has played in facilitating our work, in particular through heavy use of the GPU and (more recently) KNL nodes for large scale simulations of, for example, enzyme evolutionary trajectories.

[1] O. Khersonsky and D. S. Tawfik, *Annu. Rev. Biochem.* **79**, 471 (2010).
[2] A. Pabis, F. Duarte and S. C. L. Kamerlin, *Biochemistry* **55**, 3061 (2016).
[3] N. Tokuriki and D. S. Tawfik, *Science* **324**, 203 (2009).
[4] A. Barrozo, F. Duarte, P. Bauer, A. T. P. Carvalho and S. C. L. Kamerlin, *J. Am. Chem. Soc.* **137**, 9061 (2015).
[5] M. Purg, A. Pabis, F. Baier, N. Tokuriki, C. Jackson and S. C. L. Kamerlin, *Phil. Trans. R. Soc. A* **374**, 20160150 (2016).
[6] D. Blaha-Nelson, D. M. Krüger, K. Szeler, M. Ben-David and S. C. L. Kamerlin, *J. Am. Chem. Soc.* **139**, 1155 (2017).
[7] H. Ma, K. Szeler, S. C. L. Kamerlin and M. Widersten, *Chem. Sci.* **7**, 1415 (2016).

Quantum Modelling of Electron Structure for Materials Properties

Prof. *J. Andreas Larsson*, Chair of Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology

Abstract: I will present how quantum mechanics and the Schrödinger equation of electron structure is connected to materials properties. Everything including structure, hardness, color, and physical properties such as conduction, magnetism and adhesion strength is governed by the electron structure. This provides the fundamental principles for the research at Applied Physics, LTU for exploring new materials for the development of traditional technological applications. I will exemplify this with our efforts to replace metals with conducting carbon nanomaterials. We also look at materials for development of new technologies, which I will present for future devices for data storage, molecular electronics and quantum computers.

Understanding the mechanism of nerve agent antidotes

Anna Linusson, Department of Chemistry, Umeå University

Abstract: Organophosphorus nerve agents interfere with cholinergic signaling by covalently binding to the active site of the essential enzyme acetylcholinesterase (AChE). This inhibition causes an accumulation of the neurotransmitter acetylcholine, potentially leading to overstimulation of the nervous system and death. Current treatments include the use of antidotes that promote the release of functional AChE by an unknown reactivation mechanism. To gain deeper insight into the reactivation mechanism, we use X-ray crystallography and density functional theory (DFT) calculations to study the ternary complex formed between an antidote and AChE inhibited by a nerve agent. Structural studies are hampered by the challenging nature of the system; there are many reacting species involved and the system is dynamic making the electron density maps difficult to interpret. The use of DFT calculations that are integrated into the refinement process, enables an improvement of the analysis of the experimental data and a possibility to validate the resulting structural model. The approach provides new structural insights into the reactivation mechanism that can be implemented both in further mechanistic studies and in future development of improved antidotes.

How the solar wind interacts with the Moon, Mars, Comets, Ceres, Ganymede, Callisto and Exoplanets

Mats Holmström, IRF

Abstract: The solar wind is stream of charged particles from the Sun. Wherever it meets a planet, there will be an interaction with the atmosphere or surface of the object. This will affect the evolution of the atmosphere or surface. We use a hybrid plasma computer model to study such interactions, and compare with observations by our space instruments. The modeling requires access to high performance computing resources, such as Kebnekaise.

Poster Presentations

An auto-tuning framework for a NUMA-aware Hessenberg reduction algorithm
Mahmoud Eljammaly, Lars Karlsson, and Bo Kågström
Abstract: We recently developed a new Hessenberg reduction algorithm. The performance of this algorithm depends greatly on the value chosen for its parameters. The parameters span a huge search space and interact with each other in a way that makes using standard auto-tuning methods impractical. We present an auto-tuning framework for the new algorithm. The framework exposes the underlying subproblems so we can apply standard auto-tuning techniques on them. In addition, the framework's design allows us to apply and test different tuning algorithms easily.

Topology optimization of microwave components with minimum size control
Emadeldeen Hassan, Eddie Wadbro, Linus Hägg, Daniel Noreland, and Martin Berggren
Abstract: This poster presents a density-based topology optimization approach to design microwave components. In essence, the problem is to optimize the placement of a metallic material inside a given design domain in order to maximize the performance of such components. The underlying optimization problem shows a strong self-penalization towards binary solutions, which entails mesh-dependent designs that generally exhibit poor performance. To address the self-penalization issue as well as to obtain minimum size control of the resulting designs, we develop a filtering approach. The objective function gradient is derived based on the FDTD discretization of Maxwell's equations and is expressed in terms of field solutions of the original problem and associated adjoint field problems. We solve both the original problem and the adjoint problem by using Kebnekaise's GPU nodes. The resulting designs perform very well, and one design case is verified experimentally.

Atomistic Simulations of Smectite Hydration PROCESSES
Michael Holmboe
Combined experimental and computational investigations are steadily becoming more and more popular, as advances in the computational techniques expand both time and spatial scales as well as type of properties that can be examined by in silico experiments (molecular simulation). In particular, classical molecular dynamics (MD) simulations have emerged as a useful tool for obtaining detailed insights into the structure, dynamics and thermodynamics of various geochemical systems, which often constitute complex and highly anisotropic molecular environments. Using MD simulations this research investigates several water-loading dependent properties and the overall hydration energetics of montmorillonite (MMT), which is a swelling smectite clay mineral and true natural nano-particle with a wide range of industrial applications. This mainly because MMT has an extreme surface area of approx. 750m2/g and high capacity for water-uptake and cation retention, making it an attractive candidate for many high-level radioactive waste disposal concepts in Sweden, Finland and other countries.

Anion exclusion in hydrated clay nanopores studied by molecular dynamics simulations
Michael Holmboe, Ian C. Bourg, Christophe Tournassat
Abstract: Due to smectites extreme surface area and high capacity for water uptake and sorption capacity towards cationic solutes, smectite-rich clays are considered for geological storage of high-level nuclear waste in Sweden, Finland and many other countries. Because of the permanent and structural negative charge of the smectite clay particles, anionic solutes such as chloride, iodide and sulfate, are partially repelled from the smectite surfaces due to the so-called anion-exclusion effect, causing non-trivial diffusion behavior of anions in compacted smectite clays. This research aims to quantify and give a molecular scale understanding of the anion-exclusion effect in the smectite clay mineral Montmorillonite (MMT), hindering chloride entry into the clay interlayer nanopores.

Parallel computations of matrix permanents
P. H. Lundow and K. Markström
Abstract: The matrix permanent, a close relative of the more common determinant, is notoriously difficult to compute. Unlike the determinant the best known algorithm is exponential. We have implemented this to exploit both MPI and OpenMP capabilities. Using this implementation we computed the permanent of a 54x54-matrix on Kebnekaise using its 400 nodes for 9 hours (11 core years). This beat a previous record of computing it for a 48x48-matrix.

Profiling Tools for Analysis of HPC Applications

Pedro Ojeda-May and Jerry Eriksson

Abstract: Efficiency of HPC applications is limited, among other factors, by process communications and memory usage which are difficult to
monitor through manual instrumentation. Thus, effective tools to monitor these features as well as individual threads behavior are required. Although there are several Profiling Tools available to analyze the performance of applications, the current trend is to use manual instrumentation according to a recent survey conducted on several Centers of Excellence (CoEs). In this work, we will explore the most relevant features of three Profiling Tools, namely, Extrae/Paraver, SCALASCA/Score-P, and Intel VTune and their usage to analyze modern Scientific software such as GROMACS and CHARMM. The goal of the project is to attract the interest of the developers community to explore the available tools in Kebnekaise and in general to HPC clusters.

Blocked and Robust solution of triangular systems

Carl Christian Kjelgaard Mikkelsen and Lars Karlsson

Abstract: We consider the problem of computing a scaling α such that the solution x of the scaled linear system $Tx = \alpha b$ can be computed without exceeding an overflow threshold Ω. Here T is a non-singular upper triangular matrix and b is a single vector, and Ω is less than the largest representable number. This problem is central to the computation of eigenvectors from Schur forms. We show how to protect individual arithmetic operations against overflow and we present a robust scalar algorithm for the complete problem. Our algorithm is very similar to xLATRS in LAPACK. We explain why it is impractical to parallelize these algorithms. We then derive a robust blocked algorithm which can be executed in parallel using a task-based run-time system such as StarPU. The parallel overhead is increased marginally compared with regular blocked backward substitution.

Rheology of sickled-cell-blood by GPU computing

Dhrubaditya Mitra and Anton Ljungdahl

Abstract: Sickle-cell anemia is a genetic disease. The individuals suffering from this disease have an abnormal haemoglobin(Hb). If the Red Blood Cells (RBCs) of such individuals are starved off oxygen the abnormal haemoglobin precipitates out to form a solid core. While flowing through capillaries such RBCs get stuck and block the capillary giving rise to the classical case of vaso-occlusion. We want to study this phenomenon by computation. We are going to use a finite-difference code for fluid flow with an added viscoelastic solid objects in it. The code would be parallelised in GPUs with the rolling-cache algorithm.

A Task-Based Algorithm for Reordering the Eigenvalues of a Matrix in Real Schur Form

Mirko Myllykoski

Abstract: A task-based parallel algorithm for reordering the eigenvalues of a matrix in real Schur form is presented. The algorithm is realized on top of the StarPU runtime system. Only the aspects which are relevant for shared memory machines are discussed here, but the implementation can be configured to run on distributed memory machines as well. Computational experiments indicate that the new algorithm is between 1.5 and 6.6 times faster than a state of the art MPI-based implementation found in ScaLAPACK. The overhead and the core idle time are shown to be negligible with the exception of the smallest matrices and highest core counts.