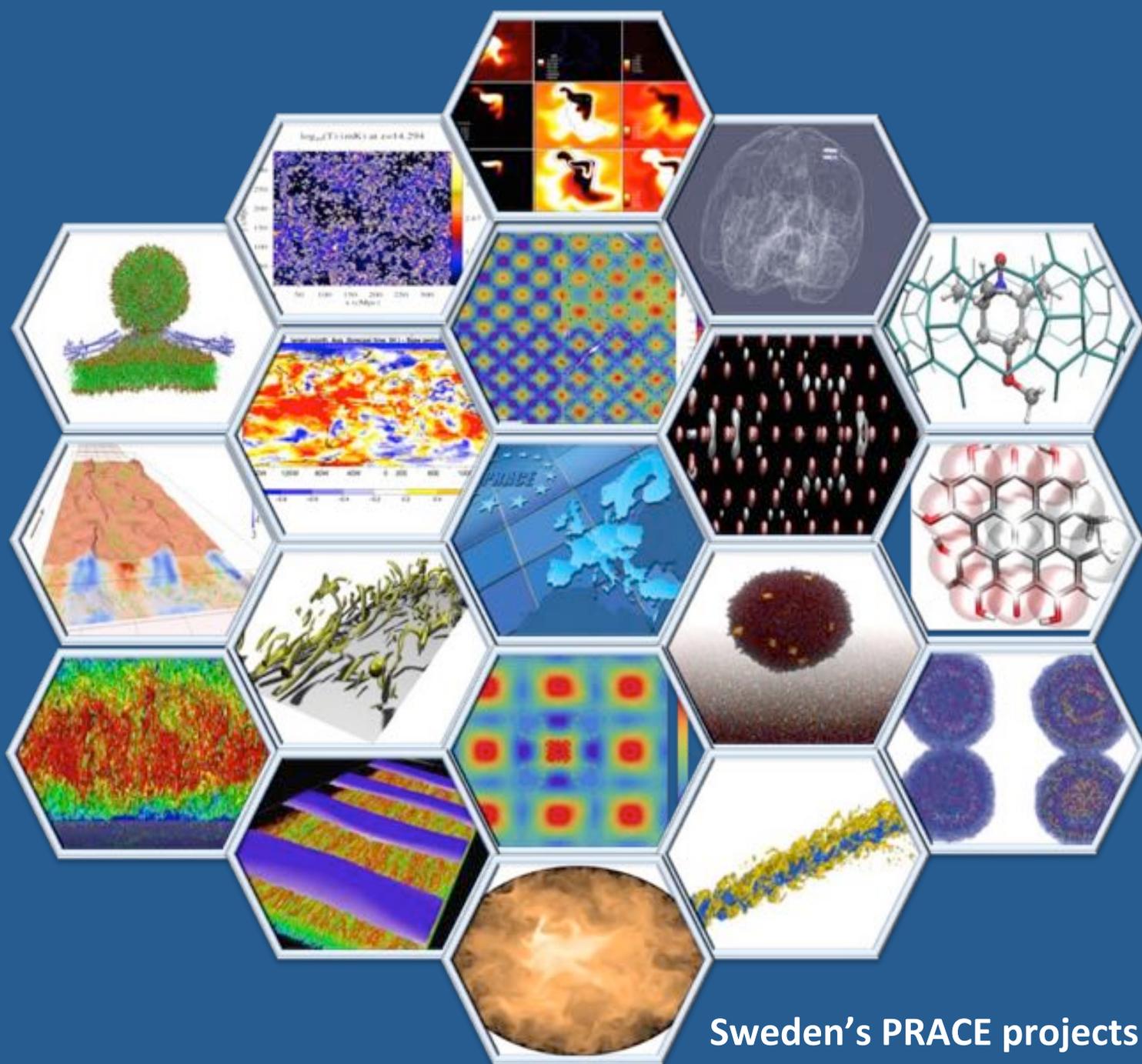




SNIC

SNIC-PRACE DIGEST No.1



Sweden's PRACE projects
2011 - 2014

www.snic.se/international/prace

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EDITORIAL

Swedish researchers are the first within the Nordic countries to receive PRACE awarded compute time

Partnership for Advanced Computing in Europe (PRACE) is offering world class computing and data management resources and services through a peer review process. These are the PRACE Tier-0 systems that were available for access during 2011 - 2014:

- "JUQUEEN", IBM Blue Gene/Q & "JUGENE" IBM Blue Gene/P (GCS@Jülich, Germany),
- "CURIE", Bull Bullx cluster (GENCI@CEA, France),
- "FERMI", IBM Blue Gene/Q (CINECA, Italy),
- "HERMIT" – Cray XE6 (GCS@HLRS, Germany),
- "MareNostrum", IBM System X iDataplex (BSC, Spain),
- "SuperMUC", IBM System X iDataplex (GCS@LRZ, Germany).

PRACE systems are available to scientists and researchers from academia and industry from around the world through three forms of access.

- **Preparatory Access** is intended for preparing proposals for Project Access. Applications are accepted at any time, with a cut-off date every three months.
- **Project Access** is intended for individual researchers and research groups and has duration of one-year.
- **Multi-year Access** is available to major European projects or infrastructures that can benefit from PRACE resources and for which Project Access is not appropriate.

In addition to this, DECI (Distributed European Computing Initiative) is also supported by PRACE. DECI provides cross-national access to European Tier-1 resources (national systems).



PRACE complements the SNIC services by providing access to resources not available nationally (be it because of lack of funding or different national priorities) as well as embedding SNIC in a larger community, providing additional expertise, collaboration stimuli, and policy guidelines.

There are three main objectives for SNIC's participation in PRACE:

- Provide Swedish scientists with access to Europe's largest supercomputers (Tier-0) and the network of large national HPC systems (Tier-1).
- Interface the national HPC infrastructure to the PRACE infrastructure, thereby contributing to the definition of policies, standards and best practices.
- Establish long-term collaborations with (major) European centres to understand and tackle technical, scientific and policy challenges that are inherent to HPC infrastructures.

In the period November 2011 – May 2015, Swedish researchers have received about 245 million CPU hours on Tier-0 in total and about 100 million normalized CPU hours on Tier-1 PRACE systems. Note that the Tier-0 number is a raw sum and is not normalized. For the same period, Sweden committed about 90 million normalized CPU hours to PRACE. These numbers include only projects where Swedish researchers are the principal

investigators (PIs) and do not consider projects where Swedish researchers are collaborators (co-PIs).

Through PRACE, Swedish researchers also received support from PRACE application experts (national and international) to improve their software and prepare it for efficient use of the largest European resources. Swedish researchers received some 45 months of full time support from PRACE HPC experts.

The support provided by PRACE HPC experts also highlighted the lack of appropriate national support and, along with the requirements of the Swedish e-Science initiatives, confirmed the need for an increased investment in SNIC application experts to support Swedish scientists in their use of HPC resources.

The recently published PRACE statistics (<http://www.prace-ri.eu/statistics/>) on the awarded projects and compute time per country show that Sweden takes the 9th place in the countries using PRACE, and the 1st place within the Nordic countries. The awarded compute hours for Sweden are almost identical with those for the Netherlands. This is a clear indication of the maturity and ability of Swedish research to play an important role on the European scene and profit from the existence of a shared European HPC infrastructure. You can find more about PRACE in the last section of this SNIC-PRACE digest.

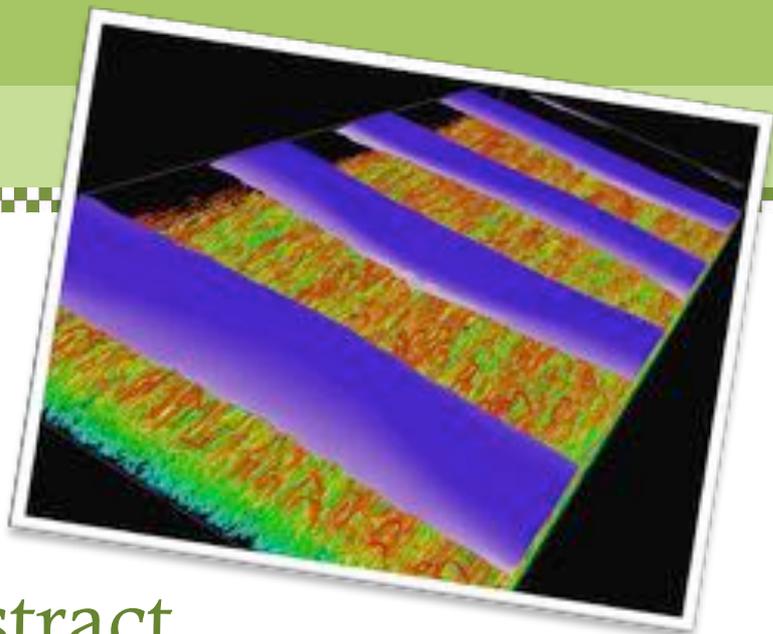
Dr. Lilit Axner SNIC-PRACE coordinator
Prof. Erwin Laure PDC director, Dr. Jacko Koster SNIC director.

REFIT - Rotation effects on flow instabilities and turbulence



Prof. Arne V. Johansson and Dr. Geert Brethouwer

PRACE 2nd Regular Call



PRACE allocation

HPC Center	Jülich Supercomputing Centre (JSC), Germany
Computer System	Jugene
Resource Awarded	46 000 000 core-hours
Start Date	May 2011
Allocation period	1 year
Research Field	Engineering

Abstract

Flows in gas turbines, turbo machinery, pumps, compressors, cyclone separators and other industrial apparatus are often rotating or swirling. They are also usually turbulent since flow rates and thus Reynolds numbers are generally large, meaning that the fluid motions fluctuate in a chaotic and irregular manner in space and time. The induced Coriolis force on the fluid or gas, also occurring when there is a flow over wings, turbine blades and other curved surfaces, causes many intriguing and complex physical phenomena. Coriolis forces, for example, can damp as well as enhance the turbulent fluctuations and influence the mean flow rate. Capturing such effects in engineering turbulence models has so far proved to be elusive and in order to improve and validate those models high quality data of rotating turbulent flows are badly needed.

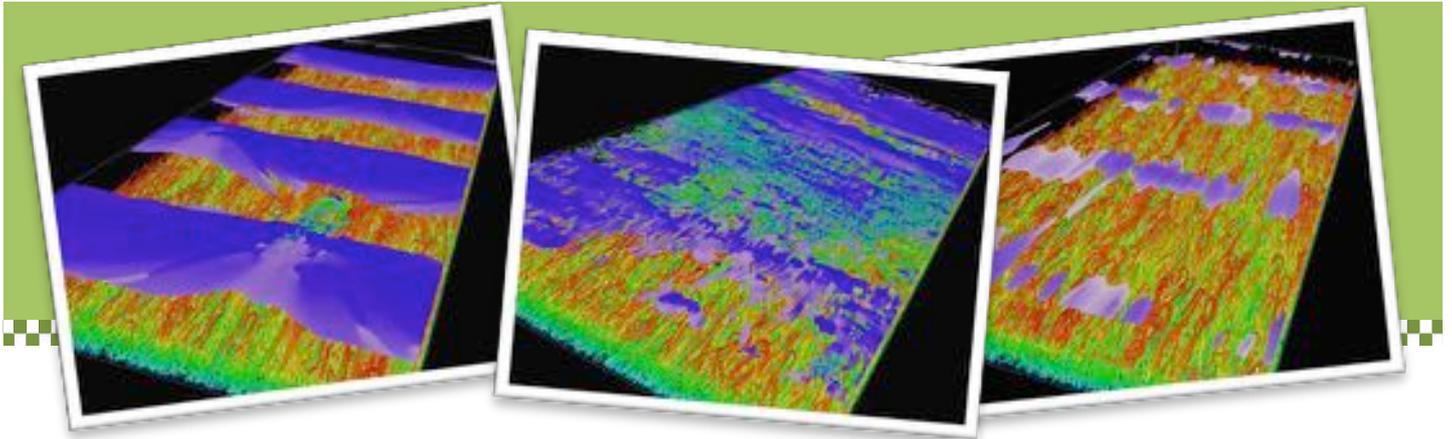
With the resources provided by the PRACE project we were able to perform simulations of rotating turbulent flows at a much higher Reynolds number. Proper simulations of the periodic-like instabilities at high rotation rates and high Re have required especially massive computational resources. The aim of the proposed project was therefore to perform DNS of rotating turbulent channel flow at an order of magnitude higher friction Reynolds number than previously performed DNS.



Project leader: Arne Johansson, KTH Department of Mechanics, Sweden

Collaborators: Dr. Geert Brethouwer, KTH Stockholm, Sweden / Prof. Dan Henningson, KTH Stockholm, Sweden / Prof. Rebecca Lingwood, University of Cambridge, United Kingdom / Prof. Martin Oberlack, Technische Universität Darmstadt, Germany / Dr. Philipp Schlatter, KTH Stockholm, Sweden





Visualization of the growing, unstable plane waves causing the cyclic instabilities in rotating channel flow.

Project Results

Several direct numerical simulations of fully developed turbulent channel flow have been performed. The channel was subject to system rotation about the spanwise axis aligned with the vorticity vector of the mean flow and the rotation rate was varied from zero/moderate to rapid. The Reynolds number based on the bulk mean velocity and channel half-gap width was 31600 and the friction Reynolds number was up to 1500. The domain size was 37.7 long and 10.5 wide in terms of half-gap width in order to capture the so-called very-large scale motions. All spatial and temporal scales of motion of the flow and turbulence governed by the incompressible Navier-Stokes equations were fully resolved with a pseudo-spectral code and resolutions up to 12 billion Fourier modes.

The Reynolds numbers are much larger than in previous studies of rotating channel flow, which makes the new simulations much more relevant for industrial, geophysical and astrophysical flows where high Reynolds numbers are prevailing. Similarly, the domain sizes were much larger than in previous studies. Access to Tier-0 supercomputer facilities has been a prerequisite in order to

reach these high Reynolds numbers and corresponding required high resolutions. Similar Reynolds numbers and rotation rates as in this project are also beyond the potentials of accurate laboratory measurements

An extensive range of flow statistics were computed and many data sets of the complete velocity field were stored for further post processing. The results of the new high-Reynolds number direct numerical simulations of spanwise rotating channel flow show fundamental differences with the previously reported results of lower Reynolds number simulations and uncover some new physical phenomena.

The computed statistical data at higher Reynolds numbers are crucial for the future development and validation of turbulence models for rotating flows needed in the design of industrial devices like turbo machines.

The present flow case offers a rare opportunity to study this dynamics in a well-defined setting, even surpassing the capabilities of experimental studies.

“Access to Tier-0 supercomputer facilities has been a prerequisite in order to reach these high Reynolds numbers and corresponding required high resolutions.”

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Direct numerical simulation of reaction fronts in partially premixed charge compression ignition combustion: structures, dynamics



Prof. Xue-Song Bai

PRACE 4th Regular Call



A sequence of spatial distribution of fuel mass fraction (n-heptane), heat release rate (HR), and CO mass fractions from left to right column, at three instances of time increasing from the top row to bottom row, 0.0317 ms, 0.135 ms, and 0.2 ms.

PRACE allocation

HPC Center	GENCI, CEA, France
Computer System	Curie Thin-Node
Resource Awarded	20 000 000 core-hours
Start Date	May 2012
Allocation period	1 year
Research Field	Engineering

Abstract

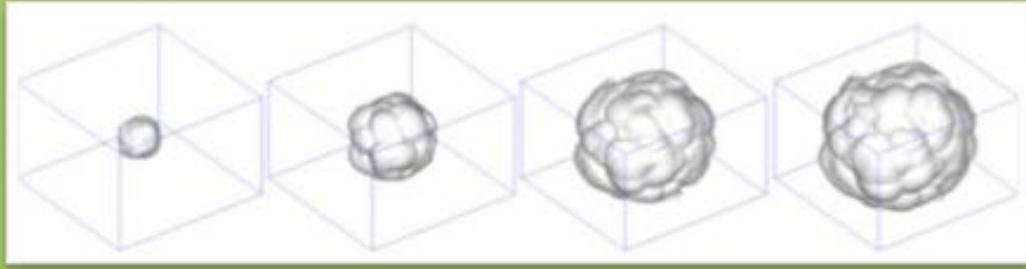
Recent public concerns on global warming due to emissions of the green house gas CO₂, as well as emission of pollutants (soot, NO_x, CO, and unburned hydrocarbons) from fossil fuel combustion, have called for development of improved internal combustion (IC) engines that have high engine efficiency, low emissions of pollutants, and friendly to carbon neutral renewable fuels (e.g. biofuels). The European and world engine industry and research community have spent great effort in developing clean combustion engines using the concept of fuel-lean mixture and low temperature combustion which offers great potential in reducing NO_x (due to low temperature) and soot and unburned hydrocarbon (due to excessive air), and meanwhile achieving high engine efficiency.

The goals of this project were to achieve improved understanding of the physical and chemical processes in overall fuel-lean PCCI processes, and to generate reliable database for validating simulation models for analysis of the class of combustion problems. This led to development of new strategies to achieve controllable low temperature combustion IC-engines, while maintaining high efficiency and low levels of emissions (soot, NO_x, CO and unburned hydrocarbons). Direct numerical simulation (DNS) approach that employs detailed chemistry and transport properties as employed.

Project leader: Xue-Song Bai, Lund University, Sweden

Collaborators: Yu Rixin, Lund University, Sweden/ Henning Carlsson, Lund University, Sweden/ Fan Zhang, Lund University, Sweden/ Rickard Solsjo, Lund University, Sweden.





Temporal evolution of the 3D flame-front in a lean hydrogen/air mixture under spark-assisted homogeneous charge compression ignition (SACI) engine condition at respectively (a) 0.0075 ms, (b) 0.018 ms, (c) 0.0312 ms, and (d) 0.0336 ms after the onset of the spark initiated flame. The flame front is defined as the iso-surface of temperature at 1600K.

Project Results

Three-dimensional direct numerical simulations are performed to study the ignition and reaction front propagation of a primary reference fuel (PRF70, with 30% n-heptane and 70% isooctane) under conditions relevant to partially premixed charge compression ignition (PPC) engines. Detailed transport properties together with a reduced PRF chemical kinetic mechanism are employed in the simulations. The partially premixed charge is prescribed using an initial field that are relevant to fuel injection at two different times. The motion of the piston and hence compression of charge due to piston motion are considered. The simulations are performed on the fine mesh with a spatial resolution of 1.22 micrometers in a cubic domain of 614 micrometers on each side.

The present DNS results indicate that the fuel-rich FRC region will contribute to the emission of CO and soot; hence its size and fuel/air ratio in the region will exert great impact on the emission of these pollutant species. NO are formed mainly due to premixed combustion in the region with stoichiometric mixture and in the LHC region. Thus, the control of CO, soot, and NO emissions

becomes an optimization problem of the mass split between the LHC FRC, and SC regions.

The computations in this project require a large number of processors. The physical relevance of the results obtained using DNS is highly dependent on the numerical resolution employed. In DNS all the physical length and time scales encountered in the flow must be resolved, from the largest (of domain size) to the smallest (Kolmogorov scale). Given the high disparity between the large and small scales, three dimensional fully resolved DNS usually requires more than hundreds of million grid cells and in some case even billions of cells, which cannot be treated within a reasonable time without at least 10000 processors.

The computer demand related to the treatment of chemistry is very high, both in terms of CPU time and memory, which increases the need in performing massively parallel computations. Access to the Tier-0 supercomputer gives us the opportunity to run such high-fidelity simulations.

“Access to the Tier-0 supercomputer gives us the opportunity to run such high-fidelity simulations.”

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3. R. Yu, X.S. Bai, Direct numerical simulation of lean hydrogen/air auto-ignition in a constant volume enclosure, *Combustion and Flame*, vol.160, pp.1706-1716, 2013.
4. F. Zhang, R. Yu, X.S. Bai, Direct numerical simulation of PRF70/air partially premixed combustion under IC engine conditions, *Proceedings of the Combustion Institute*, 35 (2015) 2975–2982.
5. H. Carlsson, R. Yu, X.S. Bai, Flame structure analysis for categorization of lean premixed CH₄/air and H₂/air flames at high Karlovitz numbers: Direct numerical simulation studies, *Proceedings of the Combustion Institute*, 35 (2015) 1425–1432.

HiResClim: High Resolution Climate Modelling

Dr. Ralf Döscher



PRACE 5th Regular Call

PRACE allocation

HPC Center BSC, Spain

Computer System MareNostrum

Resource Awarded 38 000 000 core-hours

Start Date November 2012

Allocation period 1 year

Research Field Earth Science



The number of years simulated on MareNostrum during one period.

Abstract

HiResClim aimed to make major advances in the science of climate change modelling. The key goal was to explore increased climate model resolution aiming to deliver a significant improvement in our ability to simulate key modes of climate and weather variability and thereby provide more reliable estimates of future changes in this variability. To provide credible risk assessment statistics on future change in phenomena such as; extra-tropical and tropical cyclones, heatwaves, droughts and flood events, high climate model resolution is a necessary precondition. In HiResClim we attacked this requirement by utilizing the most advanced HPC systems. Potential applications are improved climate projections and seasonal-to-decadal scale climate predictions.

Approaching the problem of increasing resolution is a scientific and technical challenge, due to the need of physical re-adjustments, revised coupling strategies and performing complex coupled model experiments in so far barely tested set-ups. Experience and improvements gained during this project phase also increases the numerical stability of standard resolution experiments.



Project leader: Ralf Döscher, SMHI, Sweden

Collaborators: Laurent Terray, Sophie Valcke, Eric Maisonnave, Christophe Cassou, CERFACS, France / Klaus Wyser, Uwe Fladrich, Swedish Meteorological and Hydrological Institute (SMHI), Sweden / Muhammad Asif, Domingo Manubens, Francisco Doblas-Reyes, Catalan Institute of Climate Sciences, Spain / Chandan Basu, Torgny Faxen, Linköping University, Sweden / Wilco Hazeleger, Richard Bintanja, Camiel Severijns, Royal Netherlands Meteorological Institute (KNMI), Netherlands



Mean SST (K) systematic error for Northern hemisphere summer, one-month lead predictions of EC-Earth3 T255/ORCA1 and T511/ORCA025. The higher resolution case gives improved mean conditions, in particular over the North Atlantic and North Pacific.

After solving initial challenges, HighResClim was able to address the effects of increased model resolution on our predictive capacity with respect to mean climate, monthly-seasonal variability and extremes. As a result, prediction skill for three months ahead give distinctly improved mean conditions, in particular over the key areas of the North Atlantic and North Pacific Ocean (see figure). High resolution gives more realistic turbulent ocean-atmosphere heat fluxes in the western boundary current areas such as the Gulf Stream.

Key ingredients for a skillful prediction are realistic oscillating teleconnection patterns such as the El-Nino Southern Oscillation (ENSO) phenomenon and the North Atlantic Oscillation (NAO). HighResClim finds clear skill improvements with enhanced resolution. The ENSO skill can also be enhanced by a stochastic physics approach in combination with low resolution. In a 10-member ensemble, best prediction skills are achieved by high resolution and no stochastic physics. EC-Earth NAO prediction experiments in high resolution configuration increase anomaly correlations as a quality indicator and beats current advanced operational seasonal prediction systems such as the ECMWF system 4.

For climate prediction two alternative basic setups for initialization (informing the model on the current observed conditions) are possible: full-field initialization as used in the experiments so far, or anomaly initialization. The latter method requires knowledge of the simulated mean climate conditions, thus depends on spin-up and historical simulations. The advantage is seen in the fact that the initial conditions are consistent with the coupled model's preferred mean state (the model's attractor) hence diminishing the model drift towards its own climatological state. Initialization shocks are largely avoided. To establish mean climate conditions, a spin-up of the EC-Earth model in a moderate resolution has been carried out, which in turn formed the base for anomaly-initialized prediction ensembles.

After the end of the HighResClim project, a follow-on project HighResClim 2 (with collaborators from IC3 in Spain as principal investigators) resumed the generation of suitable high-resolution spinups and transient climate simulations. Those are providing the base for forthcoming high-resolution climate prediction experiments on the decadal (10 year) scale started in 2015.

“To provide credible risk assessment statistics on future change in phenomena such as; extra-tropical and tropical cyclones, heatwaves, droughts and flood events, high climate model resolution is a necessary precondition. In HiResClim we attacked this requirement by utilizing the most advanced HPC systems.”

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Simulating the Epoch of Reionization for LOFAR



Prof. Garrelt Mellema

PRACE 5th Regular Call

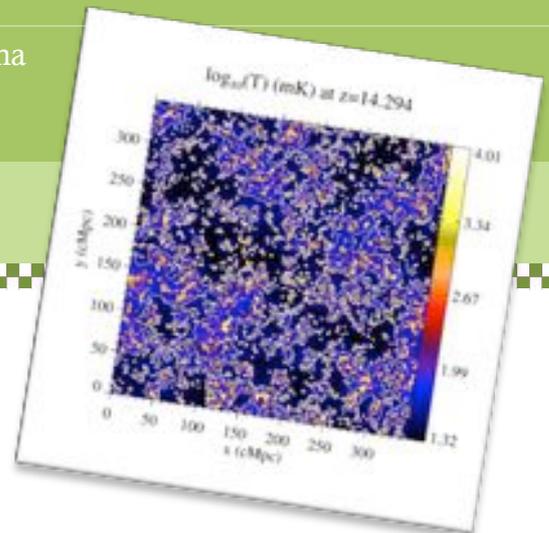


Image showing the temperature (in logarithmic scale) of a slice through the intergalactic medium at a redshift of $z=14.3$. The contour indicates the temperature of the Cosmic Microwave Background radiation at this redshift.

PRACE allocation

HPC Center	GENCI, CEA, France
Computer System	Curie Fat-Node and Curie Thin-Node
Resource Awarded	3 000 000 and 19 000 000 core-hours
Start Date	November 2012
Allocation period	1 year
Research Field	Astrophysics

Abstract

Reionization is believed to be the outcome of the release of ionizing radiation by early galaxies. Due to the complex nature of the reionization process it is best studied through numerical simulations. Such simulations present considerable challenges related to the large dynamic range required and the necessity to perform fast and accurate radiative transfer calculations. The tiny galaxies, which are the dominant contributors of ionizing radiation, must be resolved in volumes large enough to derive their numbers and clustering properties correctly, as both of these strongly impact the corresponding observational signatures. The ionization fronts expanding from all these millions of galaxies into the surrounding neutral medium must then be tracked with a 3D radiative transfer method, which includes the solution of non-equilibrium chemical rate equations. The combination of these requirements makes this problem a formidable computational task.

We propose to perform several simulations with the main goal to simulate, for the very first time the full, very large volume of the Epoch of Reionization (EoR) survey of the European radio interferometer array LOFAR, while at the same time including all essential types of ionizing sources, from normal galaxies to quasars. This structure formation simulation will be used in the LOFAR Epoch of Reionization Key Science Project to construct a large library of reionization simulations on non-PRACE facilities and will be essential in the interpretation of the LOFAR observations.

Project leader: Garrelt Mellema, Stockholm University, Sweden

Collaborators: Ilian Iliev, University of Sussex, United Kingdom / William Watson, University of Sussex, United Kingdom / Saleem Zaroubi, University of Groningen, Netherlands / Alexandros Papageorgiou, University of Groningen, Netherlands / Hannes Jensen, Stockholm University, Sweden / Kai-Yan Lee, Stockholm University, Sweden



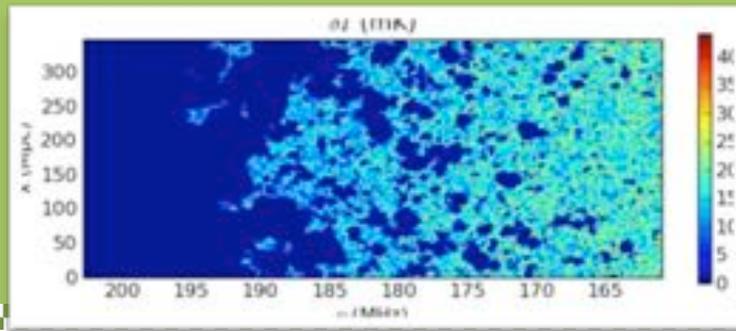


Image showing an observational “slice of sight” of the 21cm signal.

Project Results

Within this project the main aim was to simulate a large cosmological volume of 2.3 billion light years on each side with 8192^3 (550 billion) particles, giving us a smallest halo mass of $10^9 M_0$, and to perform a number of reionization simulations on this volume. As this is one of largest cosmological simulations ever run we first performed a number of smaller n-body simulations to test the code and prepare the subsequent processing of the results. The other purpose of these smaller simulations is to resolve halos of masses, which we would not resolve in the large volume so as to be able to add them as a subgrid model in the large volume.

In this vein we performed three n-body simulations. One of 60 million light years and 3456^3 (41 billion) particles which allows us to resolve halos down to masses of 10^5 solar masses, one of 219 million light years and 1728^3 (5 billion) particles which allows us to resolve halos down to masses of 10^8 solar masses, and one of 1.1 billion light years with the same mass resolution of the planned 2.3 billion light years volume (4000^3 particles). These simulations were all completed, the particle data was gridded, and the halos were extracted using both spherical overdensity and Amiga Halo Finder (AHF). The latter halo finder allows us to determine substructure of the halos as well as the merging history of halos.

We also used this 1.1 billion light years volume to study the early heating of the intergalactic medium by x-ray sources. This simulation was run on the x large nodes of curie and is the first one ever to simulate this process with this high mass resolution. This simulation has currently reached redshift 14.

We have achieved most of our goals: a set of n-body results which allows us to follow the reionization process including all of the possible structures (massive halos and mini-halos) down to at least redshift 9, as well as a set of reionization simulations exploring alternative radiative feedback implementations and an early heating simulation including all the halos down to 10^8 solar masses. These results would have been impossible to achieve without access to Curie.

“We have achieved most of our goals... These results would have been impossible to achieve without access to Curie.”

1. Mellema: *Contributed talk at Synergistic Science with Euclid and the Square Kilometre Array*, 16 – 18 September 2013, Oxford, UK
2. Mellema: *Contributed talk at The Modern Radio Universe 2013*, April 22 - 26, 2013, Bonn, Germany
3. Mellema: *Invited talk at Frontier of Modern Astrophysics*, March 2013, Morelia, Mexico
4. Mellema: *Invited talk at Cosmology for All*, February 2013, Lund, Sweden
5. Iliev: *Invited talk at 'Exascale Computing in Astrophysics' Ascona*, Switzerland, Sept 9-13, 2013
6. Iliev: *Contributed talk at National Astronomy Meeting*, St. Andrews, July 1-5, 2013

High performance adaptive finite element methods for turbulent flow and multiphysics with applications to aerodynamics, aeroacoustics, biomedicine and geophysics



Prof. Johan Hoffman

PRACE 8th Regular Call



PRACE allocation

HPC Center	LRZ, Germany and HLRS, Germany
Computer System	SuperMUC and Hermit
Resource Awarded	10 000 000 and 10 000 000 core-hours
Start Date	March 2014
Allocation period	1 year
Research Field	Mathematics and Computer Sciences

Abstract

This project concerns the development of parallel computational methods for solving turbulent fluid flow problems with focus on industrial applications, such as the aerodynamics of a full aircraft at realistic flight conditions, the sound generated by the turbulent flow past the aircraft during landing and takeoff, the blood flow inside a human heart and geophysical flows. The massive computational cost for resolving all turbulent scales in such problems makes Direct Numerical Simulation of the underlying Navier-Stokes equations impossible. Instead, various approaches based on partial resolution of the flow have been developed, such as Reynolds Averaged Navier-Stokes equations or Large-Eddy simulation (LES). For these methods new questions arise: what is the accuracy of the approximation, how fine scales have to be resolved, and what are the proper boundary conditions? To answer such questions, a number of challenges have to be addressed simultaneously in the fields of fluid mechanics, mathematics, numerical analysis and HPC.

The main focus of the research at The Computational Technology Laboratory (CTL) is the development of high performance, parallel, adaptive algorithms for FEM modeling of turbulent flows and multiphysics, including fluid-structure interaction and aeroacoustics.



Project leader: Dr Johan Hoffman, KTH Royal Institute of Technology, Sweden

Collaborators: Cem Degirmenci, Johan Jansson, Niclas Jansson, Aurelien Larcher, KTH Royal Institute of Technology, Sweden

Project results will be available upon completion of the project period by August 2015 ...

With mesh adaptivity based on "a posteriori" error estimates, efficient parallelization, and the use of unstructured meshes, G2 constitutes a powerful tool in Computational Fluid Dynamics, which can be used to solve time dependent problems efficiently. Of particular interest is the error estimation framework of G2 and, currently, we work to extend the framework to include uncertainty quantification of data and modeling parameters. Within our group, there are a number of projects in various applications areas, where the new adaptive algorithms are being used and developed.

These areas include aerodynamics, aeroacoustics, biomedicine, geophysics and FSI. In the past 3 years, we have obtained significant results in the development of G2. These include: the implementation of a hybrid MPI+PGAS linear algebra backend, which enhanced the performance of the code for larger core counts as compared to the previous MPI implementation; the successful computation of the flow past an extremely complex nose landing gear geometry and the flow past a high-lift device, both as contributions to the second workshop on Benchmark problems for Airframe Noise Computations, BANC-II, proposed and developed by NASA. For the following year, we plan to follow-up these contributions with more detailed, larger computations. In 2013 we were granted the EU FP7 project: "Extensive UNified-domain SimulatiON of the human voice" (EUNISON) for the simulation of the human voice based on our framework. We have also successfully participated in a NASA/Boeing challenge/workshop on simulation of a full aircraft (HiLiftPW-2), and we are invited to submit a paper to the AIAA SciTech 2014 conference based on our results. Our adaptive results were specifically highlighted in the summary by the organizers.

Direct numerical simulation of partially premixed combustion in internal combustion engine relevant conditions

Prof. Xue-Song Bai



PRACE 8th Regular Call



PRACE allocation

HPC Center LRZ, Germany

Computer System SuperMUC

Resource Awarded 26 000 000 core-hours

Start Date March 2014

Allocation period 1 year

Research Field Engineering

Abstract

In the past decade, the European and world engine industry and research community have spent a great effort in developing clean combustion engines using the concept of fuel-lean mixture and low temperature combustion which offers great potential in reducing NO_x (due to low temperature), soot and unburned hydrocarbon (due to excessive air), and meanwhile achieving high engine efficiency. One example is the well-known homogeneous charge compression ignition (HCCI) combustion engine, which operates with excessive air in the cylinder, and produces simultaneously low soot and NO_x. However, HCCI combustion is found to be very sensitive to the flow and mixture conditions prior to the onset of auto-ignition. As a result, HCCI engine is rather difficult to control. At high load (with high temperature and high pressure) engine knock may occur with pressure waves in the cylinder interacting with the reaction fronts, leading to excessive noise and even damage on the cylinder and piston surface. At low load (with lower temperature and pressure) high level emissions of CO and unburned hydrocarbons may occur, which lowers the fuel efficiency and pollutes the environment. Recently, it has been demonstrated experimentally that with partially premixed charge compression ignition, also known as partially premixed combustion (PPC), smoother combustion can be achieved by managing the local fuel/air ratio (thereby the ignition delay time) in an overall lean charge.



Project leader: Xue-Song Bai, Lund University, Sweden

Collaborators: Henning Carlsson, Lund University, Sweden / Vivianne Holmen, Lund University, Sweden / Siyuan Hu, Lund University, Sweden / Rickard Solsjo, Lund University, Sweden / Rixin Yu, Lund University, Sweden

Project results will be available upon completion of the project period by August 2015 ...

There are several technical barriers in applying the PPC concept to practical engines running with overall fuel-lean mixture, low temperature combustion.

For example, it is not known what the optimized partially premixed charge is for a desirable ignition, while at the same time maintaining low emissions. The main difficulty lies in the non-linear behavior of the dominating phenomena and the interaction among them (e.g. chemistry and turbulence). To develop an applicable PPC technology for IC-engine industry, improved understanding of the multiple scale physical and chemical process is necessary. Further, there is a need to develop computational models for simulating the process for the design where a large number of control parameters are to be investigated.

The goals of this project are to achieve improved understanding of the physical and chemical processes in overall fuel-lean PPC processes, and to generate reliable database for validating simulation models for analysis of the class of combustion problems. This shall lead to development of new strategies to achieve controllable low temperature combustion IC-engines, while maintaining high efficiency and low levels of emissions (soot, NO_x, CO and unburned hydrocarbons). Direct numerical simulation (DNS) approach that employs detailed chemistry and transport properties will be used to study the mechanisms responsible for the onset of auto-ignition, and the structures and dynamics of the reaction front propagation in PPC conditions.

Endogenic oil synthesis in Earth interior: ab initio molecular dynamics study



Prof. Anatoly Belonoshko

PRACE 8th Regular Call



PRACE allocation

HPC Center BSC, Spain

Computer System MareNostrum

Resource Awarded 50 000 000 core-hours

Start Date March 2014

Allocation period 1 year

Research Field Earth System Sciences

Abstract

Physics and chemistry of C-O-H fluids at high pressures and temperatures of Earth interior is important in several applications. First, the thermodynamics of these fluids is needed to describe properties of the Earth interior which, in turn, might be important for predicting seismic events. Second, estimating the balance of CO² between atmosphere and Earth interior is impossible without detailed knowledge of thermodynamics of C-O-H fluids. Third, there are indications from experiment that chemical reactions in C-O-H fluids at high P and T might lead to a synthesis of hydrocarbons and heavy alkanes, providing a possibility for formation of oil deposits at the relevant depth. Experimental difficulties in studying C-O-H fluids at high PT are numerous - for example, diffusion of H² is one of them. Therefore, a theoretical approach is a valuable asset in these studies. Presently, we can compute phase and chemical equilibrium using density functional theory and molecular dynamics. When combined together, they represent a powerful tool.

We shall study various components in C-O-H system, systematically collecting data on their equations of state to use for computing, in turn, their Gibbs free energy. Minimization of the Gibbs free energy allows determining chemical composition at equilibrium as soon as thermodynamics of all possible components is available.

Project leader: Prof. Anatoly Belonoshko, The Royal Institute of Technology (KTH), Sweden

Collaborators: Pavel Gavryushkin, V.S. Sobolev Institute of Geology and Mineralogy, Konstantin Litasov, V.S. Sobolev Institute of Geology and Mineralogy, Siberian Branch, RAS, Russian Federation / Tymofiy Lukinov, The Royal Institute of Technology (KTH), Sweden



Project results will be available upon completion of the project period by August 2015 ...

DFT based MD is similar in a way to a high PT experiment, yet without experimental problems. While theoretical approach has its own limitations, they are well known and understood. Thus, we expect that the acquired knowledge of thermodynamics, phase and chemical equilibrium in C-O-H system will be highly reliable. In a way, our simulations are similar to a real experiment - we shall place a certain composition into an experimental box and apply certain pressure and temperature. That will allow us to observe the chemical composition that forms in the 'experimental' chamber. We expect to observe chemical reactions that lead to formation of hydrocarbons and alkanes and describe the range of pressures, temperatures and compositions where these reactions occur. This, in turn, might enable an educated search for the regions in the Earth interior that might contain the products of this reaction. As a spin-off, the acquired knowledge will help us to solve the problem of excessive CO₂ as well as to understand the interior of icy planets and satellites of giant planets.

PRACE4LOFAR



Prof. Garrelt Mellema

PRACE 9th Regular Call

PRACE allocation

HPC Center CEA, France

Computer System Curie Thin-Node

Resource Awarded 19 000 000 core-hours

Start Date September 2014

Allocation period 1 year

Research Field Astrophysics

Abstract

Cosmic reionization is the process that took place 12 billion years ago when the first generations of stars and galaxies formed in the Universe. Ionizing radiation produced by stars and more extreme objects such as black holes, escaped from the galaxies and spread through the medium in between the galaxies. This process transformed this medium from entirely neutral to entirely ionized, which it has remained ever since. Reionization is at the forefront of modern cosmological research. Within the next few years we expect to transform our knowledge about this period through the detection of the redshifted 21cm radio signal from neutral hydrogen during reionization. The European radio interferometer array LOFAR is best placed to make this discovery. However, the discovery of the signal alone will need interpretation in terms of the properties and distribution of the galaxies that caused reionization. This PRACE proposal forms part of the efforts of the LOFAR-EoR Key Science Project and will provide the basic data needed to interpret the observations. We will perform several simulations with the main goal to simulate, for the very first time the full, very large volume of the Epoch of Reionization (EoR) survey of LOFAR, while at the same time including all essential types of ionizing sources, first stars, normal galaxies and quasars. The structure formation data will be provided by an N-body simulation of early structure formation with 6912^3 (330 billion) particles and 2.3 billion light years volume.

Project leader: Prof. Garrelt Mellema, Stockholm University, Sweden

Collaborators: Kyungjin Ahn, Chosun University, Korea, Republic of / Fabian Krause, Saleem Zaroubi, University of Groningen, The Netherlands / Hannes Jensen, Kai Yan Lee, Suman Majumdar, Stockholm University, Sweden / Keri Dixon, Ilian Iliev, Chaichalit Srisawat, David Sullivan, University of Sussex, United Kingdom



Project results will be available upon completion of the project period by August 2015 ...

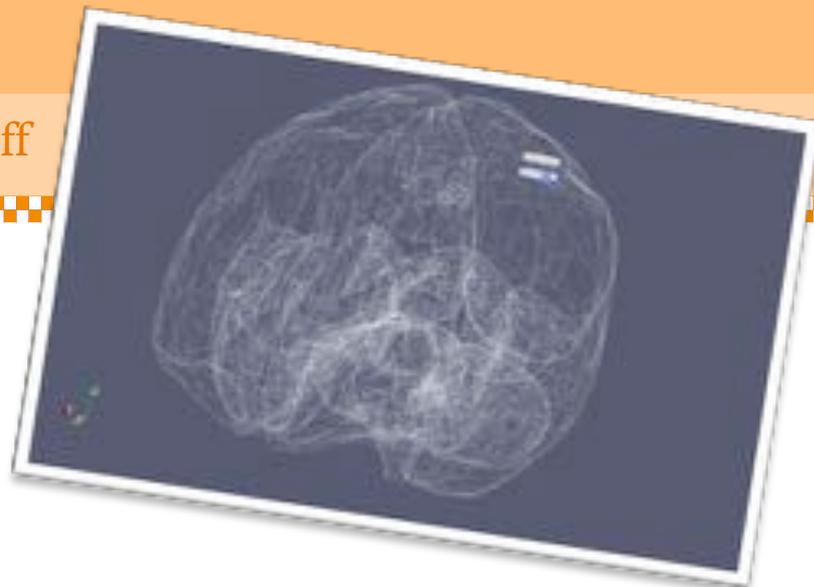
This combination of large volume and high resolution will allow us to study the multi-scale reionization process, including effects which are either spatially very rare (e.g. luminous quasars sources) or for which the characteristic length scales are large (e.g. X-ray sources of photoionization and heating; the soft UV that radiatively pumps the 21-cm line by Lyman-alpha scattering; the H₂-dissociating UV background). We will complement the results from this simulation with results of smaller volumes which allow us to include the effects of structures not resolved in this very large volume. This structure formation simulation will be used in the LOFAR Epoch of Reionization Key Science Project to construct a large library of reionization simulations on non-PRACE facilities on which the interpretation of the LOFAR observations will be based. As part of this proposal we will use the structure formation results to perform reionization simulations, which will address the likely stochastic nature of the sources of reionization, an aspect that to date has not been explored. We will also study the effects from the early rise of the inhomogeneous X-ray background and how much of this background is due to the first stars. The forming early galaxies, and the stars and accreting black holes within them emit copious amounts of radiation in all spectral bands, which in turn affects future star and galaxy formation. There are multiple channels for such feedback, which need to be taken into account, an important one of which are the subtle, but far-reaching effects of X-rays, which strongly modulate the redshifted 21-cm emission and absorption signals at early times.

Visualization of output from Large-Scale Brain Simulations



Prof. Anders Lansner

PRACE Preparatory 4th cut-off



A wireframe model of a brain signal.

PRACE allocation (type C)

HPC Center FZJ, Germany

Computer System Jugene

Resource Awarded 250 000 core-hours

Start Date May 2012

Allocation period 6 months

Research Field Medicine and Life Sciences

Abstract

This project concerned the development of tools for visualization of output from brain simulations performed on supercomputers. The project had two main parts:

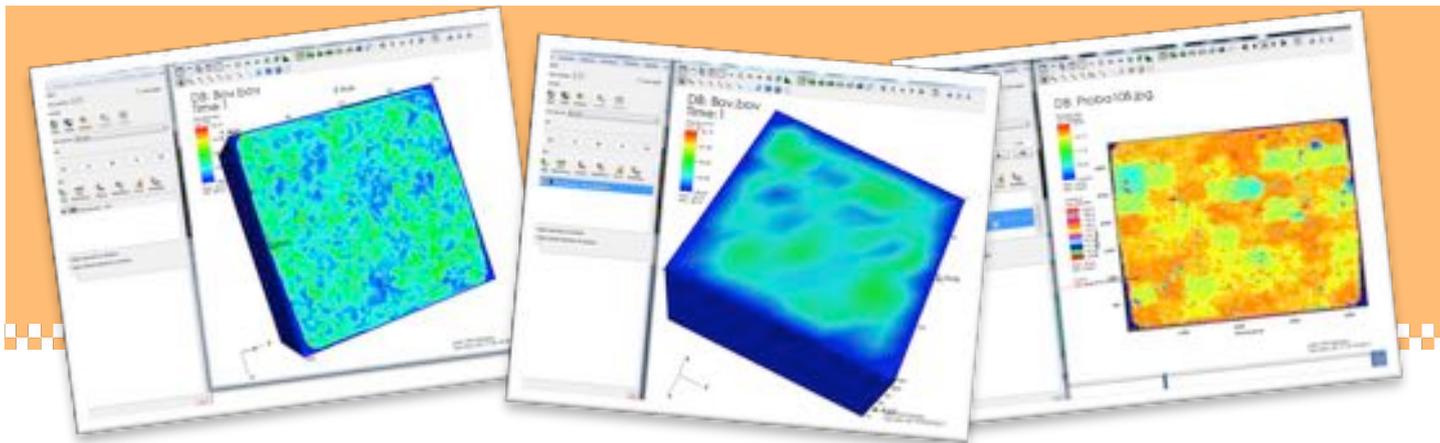
- 1) Creating visualizations using large-scale simulation output from existing neural simulation codes, and
- 2) Making extensions to some of the existing codes to allow interactive runtime (in-situ) visualization.

In 1) simulation data was converted to HDF5 format and split over multiple files. Visualization pipelines were created for different types of visualizations, e.g. voltage and calcium. In 2) by using the VisIt visualization application and its libsim library, the simulation code was instrumented so that VisIt could access simulation data directly. The simulation code was instrumented and tested on different clusters where control of simulation was demonstrated and in-situ visualization of neural unit's and population data was achieved.



Project leader: Anders Lansner, KTH, Computational Biology, Stockholm, Sweden

Collaborators: Simon Benjaminsson, David Silverstein, KTH, Computational Biology, Stockholm, Sweden



Project Results

A regular mesh (201x201 points), received by bilinear interpolation.

We were able to develop a workflow for visualization of network activity of a brain region at both the single neuron and neuronal population levels, together with realtime visualization of simulated network activity. The open source program package VisIt could be used for in-situ visualization and visualization of synthetic cell mesh activity. The tools developed could potentially be of use for researchers to visualize simulations by providing specific files and parameter settings as needed.

One important remaining issue for future work is to test the scalability of the visualization tools developed. The simulation model currently visualized has a relatively modest number of neurons, around 50,000 – 100,000, though during the course of this project we performed simulations with up to 57 million neurons connected by 7 billion synapses. Since the work started from scratch we developed the applications based on HPC enabled components, but time was not enough for extensive tests of scalability. Larger models will be used in the near future, having on the order of 100,000s neurons. For visualizing output from these models the visualization pipelines developed here can in principle be reused, but the larger scale will negatively influence the 3D rendering and data processing capabilities of ParaView. The VisIt package already allows visualization of large-scale system. Its parallel scalability is excellent, especially in the case of multiprocessor/multicore usage and GPU Tesla.

For handling larger models ParaView provides a parallel rendering mode, allowing distributed rendering over multiple rendering nodes, taking advantage of multi-core and multi-GPU hardware. Changes to the HDF5-based data layout might be necessary for this mode, to split up the per-timestep files into several standalone pieces that can be individually read by the render nodes, as this is the way ParaView can most efficiently read in the data in parallel.

Furthermore, the mapping onto the whole brain model can be improved and the visualization of connectivity at the micro- and macroscopic level, including visualization of impulse propagation could be added. But even as it stands now, this preparatory project has provided useful tools to be incorporated in our brain simulation toolkit.

“... But even as it stands now, this preparatory project has provided useful tools to be incorporated in our brain simulation toolkit.”

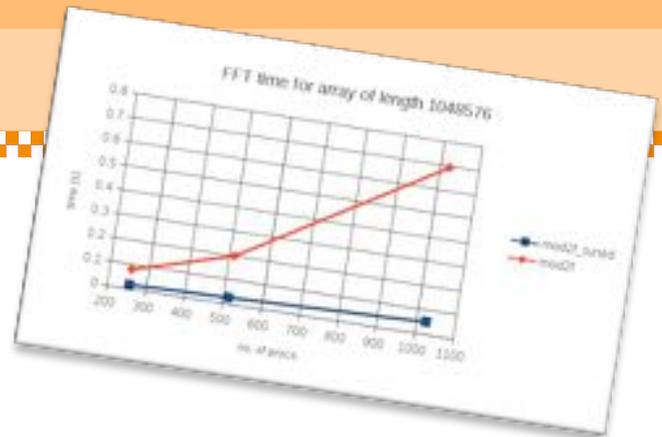
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2. Benjaminsson, S. and Lansner, A. (2011). Extreme Scaling of Brain Simulations. In *Jülich Blue Gene/P Extreme Scaling Workshop 2011*, Mohr, B. and Fring, W. (Eds.), Technical Report FZJ-JSC-IB-2011-02, Forschungszentrum Jülich.
3. Lundqvist, M., Herman, P. and Lansner, A. (2011). Theta and gamma power increases and alpha/beta power decreases with memory load in an attractor network model. *J. Cogn. Neurosci.* 10, 3008-3020.
4. Lundqvist, M., Compte, A. and Lansner, A. (2010). Bistable, Irregular Firing and Population Oscillations in a Modular Attractor Memory Network. *PLoS Comput. Biol.* 6, e1000803.

Automated Network Topology Identification and Topology Aware MPI Collectives

Dr. Chandan Basu



PRACE Preparatory 10th cut-off



PRACE allocation (type B)

HPC Center CEA, France

Computer System Curie Thin-Nodes

Resource Awarded 200 000 core-hours

Start Date November 2012

Allocation period 6 months

Research Field Mathematics and Computer Science

Abstract

Comparison of the scalability of standard MPI_Alltoallv w.r.t. our new optimized Alltoallv

We are trying to develop an efficient runtime system for MPI parallel jobs, focusing on minimizing the communication cost by the effective reassignment of MPI ranks. We also experiment the MPI-I/O performance for the purpose of integrating the new collective design with parallel I/O functionality.

We will collect different network statistics aiming to determine the network topology through statistical clustering of data. We will use this topology information to efficiently map ranks on suitable resources depending on the communication pattern.

Our previous work in PRACE on a synthetic benchmark showed around 40% performance improvement for MPI_Alltoallv performance.

This work is relevant to very wide parallel jobs and testing requires access to large systems.



Project leader: Chandan Basu, Linköping University (Sweden)

Collaborators: Soon-Heum Ko, Johan Raber, Linköping University (Sweden)

Project Results

We use 4 different genetic sequence datasets for parallel I/O experiment: 52KByte, 978KByte, 16MByte, 139MByte. Considering the characteristics of bioinformatics code, global dataset should be stored at each CPU rank.

We have experimented MPI_read function for measuring parallel I/O performance. The idea is to make some ranks to read sequence dataset and broadcast this data to each neighbor. We have experimented on 64 CURIE nodes (1024 CPU cores) by changing the number of I/O-participating ranks. First interesting feature is that the file access through MPI-I/O provides better performance than POSIX-typed I/O in the same condition (MPI_read by a single core, accompanied by the broadcast to all cores). In case of 52K file size, MPI-I/O outperforms the POSIX way by 0.267438 VS 0.312917 after 100 repetitions: 0.299701 VS 0.419340 in 978K; 4.028367 VS 4.746195 in 16M; 31.58357 VS 41.96636 in 139M. The second feature is that MPI-I/O performed best as small ranks participate in I/O operation. In all cases, I/O time keeps going down as the number of I/O ranks reduces and the best performance is achieved when a single core conducts the I/O operation. It is not favorable since parallel I/O should benefit by enabling the concurrent file access from multiple cores at the cost of a sequential file access.

We have found that the topology aware Alltoallv can work much better than normal MPI_Alltoallv especially for small size of data. Our network analysis shows that MPI ranks form high-bandwidth-low-latency-clusters. These clusters can be suitably used in application programs.

The MPI-I/O experiment results that the use of MPI-I/O outperforms the sequential POSIX-type operation in the same condition. An unfavourable characteristic is observed that MPI-I/O performs best when a single core accesses the file. We expect that the further integration of parallel I/O and the current collective design will provide the better performance.

The assigned PRACE system was suitable for our testing. Compilation and running was straightforward. The file system was unstable sometimes.

“ The assigned PRACE system was suitable for our testing.”

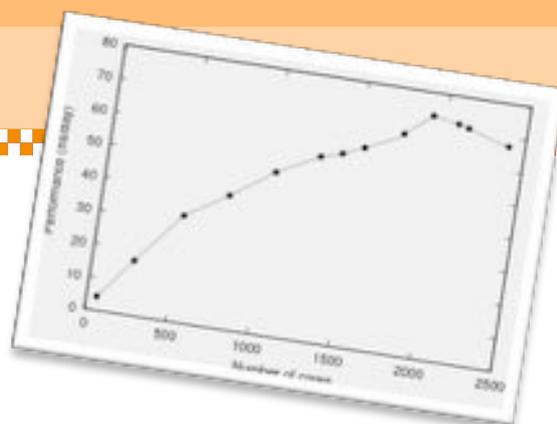
1. Towards Runtime-Clustering and improved Implementations of collective Operations in MPI, *PRACE white paper* 2014
2. Improving MPI communication latency of Euroben kernels, *PRACE white paper* 2013
3. Optimized Collective Algorithm with Automated Runtime MPISub-group Creation, *PRACE white paper* 2013

Dimerization of the beta-2-Adrenegentic Receptor Protein in Different Membrane Environments Studied Through Multiscale Molecular Modeling



Prof. Alexander Lyubartsev

PRACE Preparatory 12th cut-off



PRACE allocation (type A)

HPC Center HLRS, Germany and FZJ, Germany

Computer System Hermit and Juqueen

Resource Awarded 50 000 and 100 000 core-hours

Start Date May 2013

Allocation period 2 months

Research Field Chemistry and Materials

Abstract

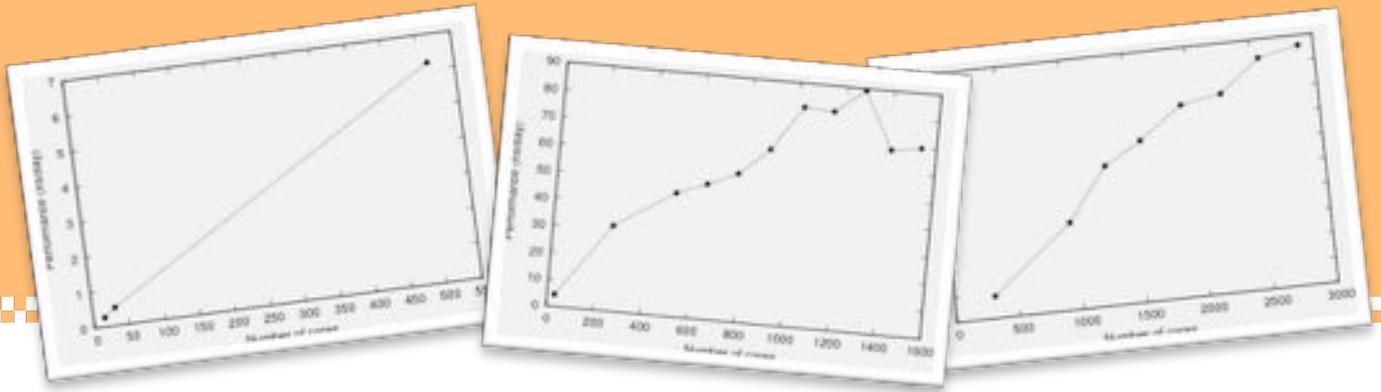
Scaling on Hermit for the largest case

In the humane genome the largest membrane protein family is the G protein-coupled receptors (GPCRs) having roughly one thousand members. These proteins govern cell signaling and are therefore major targets for therapeutic agents. In a recently performed X-ray crystallography study the specific binding of cholesterol to Beta2-AR, a well-characterized GPCR, was found. As it has been speculated that Beta2-AR forms oligomers in biological membranes the closely bound cholesterol is believed to promote these oligomerization processes by increasing the stability of the protein in terms of kinetics and energetics. The actual mechanism for this oligomerization is under debate and the role of cholesterol has not been fully understood. By employing large-scale computer simulations, namely molecular dynamics simulations, on different length and time scales we aim at being able to describe these processes in atomistic resolution. By employing enhanced sampling methods the thermodynamics of the dimerization of Beta2AR can be characterized in a quantitative manner. These calculations have been supplemented by coarse-grained simulations, which allow for systems of larger sizes to be studied under larger time scales. The mentioned simulations have included system sizes ranging from hundreds of thousands of atoms to millions of particles and cover processes from the nanosecond to sub-millisecond time scale. Due to the vast computational resources required for this type of simulations the HPC allocations provided by PRACE are of necessity.



Project leader: Alexander Lyubartsev, Stockholm University, Sweden

Collaborators: Joakim Jambeck, Stockholm University, Sweden



Project Results

Scaling on Juqueen (1) and Hermit (2,3).

The scalability and absolute performance achieved on the HPC resource HERMIT is impressive and indicates that the study proposed is plausible. All tests were performed using all-atomistic models and showed that long (biased) simulations are a possibility. When coarse grained models are used in order to complement the atomistic models it is very likely that even larger time and length scales can be covered using both biased and unbiased simulation techniques in order to answer biologically relevant questions with physical/chemical methods. A number of replicas of one system can also be simulated during one run, which will have a large impact on the statistical sampling of the problems studied and increase the accuracy and reliability of the simulations. The performance follows the expectations making this system a good candidate for the planned study.

On JUQUEEN the total computer time was used due to the poor absolute performance, this facility together with the precompiled version of GROMACS is not an option for the proposed study and hence not all the computer time was used.

With the performance shown and the relevance of the proposed project we plan to apply for a regular PRACE project using the HERMIT HPC facility.

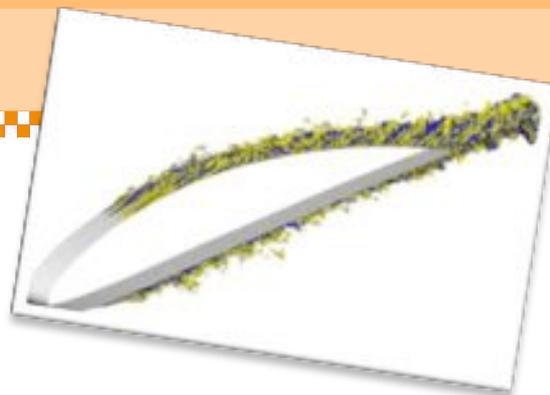
“With the performance shown and the relevance of the proposed project we plan to apply for a regular PRACE project using the HERMIT HPC facility.”

Swept wing simulation in a virtual wind tunnel



Dr. Philipp Schlatter

PRACE Preparatory 15th cut-off



PRACE allocation (type B)

HPC Center	CINECA, Italy; BSC, Spain; CEA, France; HLRS, FZJ, LRZ, Germany;
Computer System	Fermi, MareNostrum, Curie Thin-Nodes, Hermit, Juqueen, SuperMUC
Resource Awarded	250 000, 100 000, 200 000, 50 000, 250 000 and 250 000 core- hours
Start Date	March 2014
Allocation period	6 months
Research Field	Engineering and Energy

Abstract

Flow past a NACA4412 wing.

Flow past an airplane wing in steady and level flight exhibits complex flow phenomena including laminar-turbulent transition, flow separation and turbulence on the wing surface and in the wake of the wing. Additional challenges include understanding how turbulence in the background influences turbulence on the wing and the interaction between transition, turbulence on the wing, and flow separation. Accurate prediction of these processes for engineering design remains a major challenge to this day.

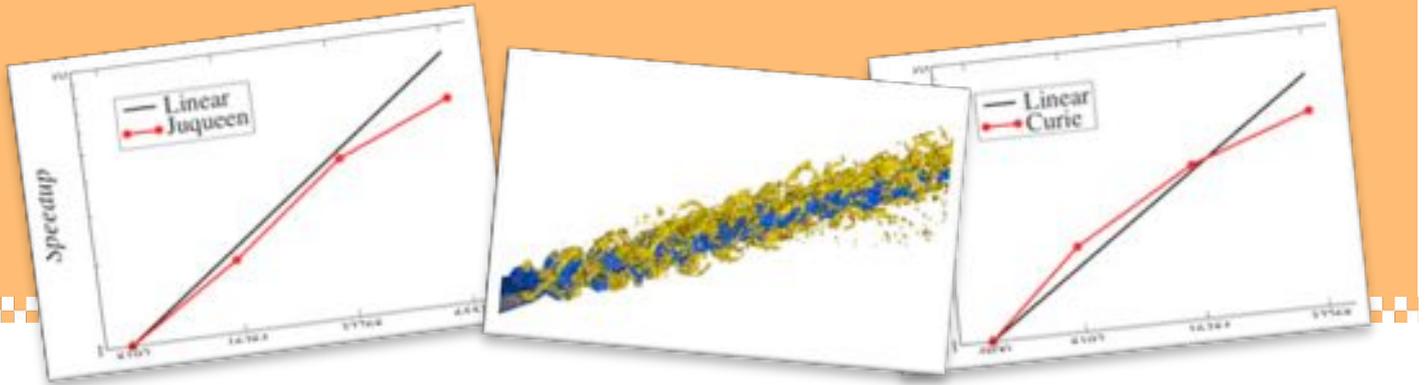
In the present project we extended the state of the art for direct numerical simulation of flow past a swept wing at $Re=O(10^6)$. A Reynolds number of 10^6 is low for an airplane in flight but is a typical value for university-run experimental studies using a wind tunnel. One of the aims of this study is to develop a virtual wind tunnel capable of running cases comparable to what can be done experimentally.

The open source spectral element solver nek5000 has been used for the simulation. Nek5000 combines high spatial accuracy with scalability to over one million ranks. The aim of the preparatory access project is to extend the present methodology from its current capability of simulating flow past the upper half of the wing to a domain covering upstream of the wing, the wing itself and downstream of the wing to capture the full flow from upstream conditions to the wake.

Project leader: Dr Philipp Schlatter; Linné FLOW Centre, Sweden

Collaborators: Dr. Ismaël Bouya, Dr. Matthew de Stadler, Dr. Ardeshir Hanifi, Prof. Dan Henningson, Linné FLOW Centre, Sweden





Project Results

Strong scaling tests for the flat plate test case and the flow past a thick flat plate with rounded leading and trailing edges.

Here we report two sets of strong scaling tests that we have performed using nek5000 (rev. 1010). The case considered is flow past a thick flat plate at $Re=1.2$ million, a simplified model of an airfoil. We want to emphasize that this is a realistic test case and not a toy model problem. Identical performance was obtained on SuperMUC and Curie (they are the same architecture) so we only show data from Curie for scaling. We also show scaling for Juqueen as a demonstration of the general scalability of our code. Note that the tests were performed with regular batch jobs (no dedicated machine).

On Curie (Intel architecture) we used a test case with approximately 2.6 billion grid points. For a small number of cores, the code is known to have close-to-perfect scaling down to about 50,000 grid points per core. For larger core counts, the scaling plot below shows very good scaling (parallel efficiency better than 0.73) if one has $\sim 80,000$ grid points per core. Note that with nek5000, the best performance is achieved for a power of two number of cores (which explains the super-linear behavior), but due to memory restrictions in the code we are limited in the choice of problem size, hence the starting point at 4800 instead of the expected 4096.

On Juqueen (BlueGene architecture) we used a test case with approximately 1 billion grid points. BlueGene has a limitation in terms of memory and computational power per core, but is known to have very good parallel scaling down to as little as 10,000 grid point per core. In the scaling plot above we have parallel efficiency better than 0.68 at $\sim 15,000$ grid points per core (for 65,536 cores).

On both machines we note that when sufficient number of gridpoints per core are present the performance is good. For Curie we require at least 35,000 grid points per processor and on Juqueen we required at least 30,000 grid points per processor. Our expectations were fulfilled and we can run our cases with $> 32,768$ processors. We were able to test the real world performance of a realistic test problem on each of the PRACE machines. We concluded that Curie and SuperMUC are optimal machines to use for our test case in terms of the number of CPU hours per simulation. If we had more hours we could also use any of the other machines. We also determined that some of the other PRACE machines were not ideal due to either smaller system size, slower performance, or long turnaround times for queues. Now we know which PRACE machines we want and have a better estimate of our true costs for a large problem.

“We were able to test the real world performance of a realistic test problem on each of the PRACE machines.”

1. P. Schlatter and R. Örlü. (2010) Assessment of direct numerical simulation data of turbulent boundary layers. *J. Fluid Mech.* 659, pp 116–126.
2. P. Schlatter, J. Malm, G. Brethouwer, A. V. Johansson and D. S. Henningson. (2011) Large-scale simulations of turbulence: HPC and numerical experiments. *In 7th IEEE Conference on e-Science*, pp 319-324.
3. G. K. El Khoury, P. Schlatter, A. Noorani, P. F. Fischer, G. Brethouwer and A. V. Johansson. (2013) Direct numerical simulation of turbulent pipe flows at moderately high Reynolds numbers. *Flow Turbulence Combust.* 91, pp 475-495.
4. S. M. Hosseini, D. Tempelmann, A. Hanifi and D. S. Henningson (2013) Stabilization of a swept-wing boundary layer by distributed roughness elements. *J. Fluid Mech.* 718, pp 1-11.
5. D. Coles and A.J. Wadcock. (1979) Flying-hot-wire study of flow past an NACA 4412 airfoil at maximum lift. *AIAA Journal*, Vol. 17, No. 4, pp. 321-329.

Profiling and Scalability Analysis of Linear Scaling DALTON Code for Large Molecular Simulation of Biological Interest



Dr. Soon-Heum Ko

PRACE Preparatory 15th cut-off

PRACE allocation (type B)

HPC Center CEA, France

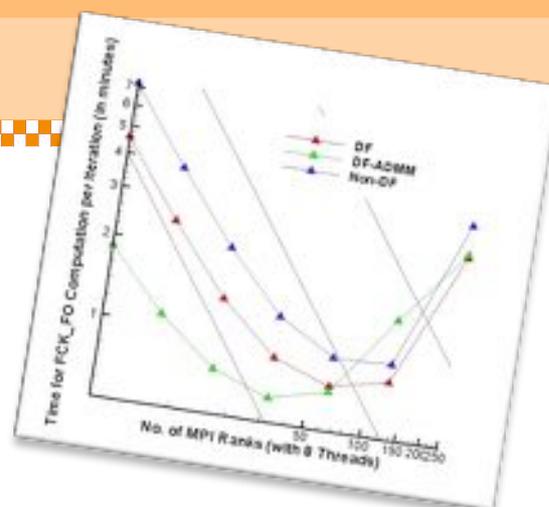
Computer System Curie Thin-Nodes

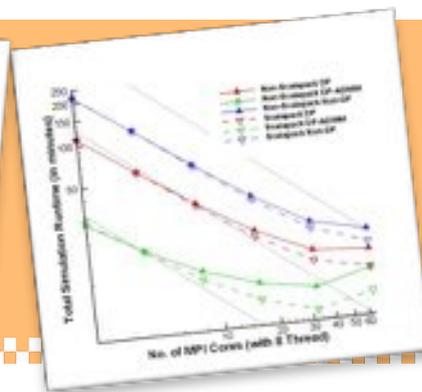
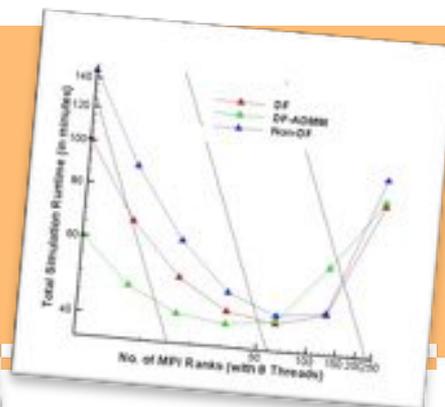
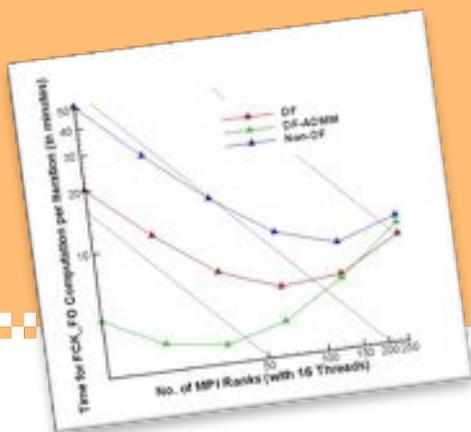
Resource Awarded 200 000 core-hours

Start Date March 2014

Allocation period 6 months

Research Field Chemistry and Materials





Project Results

Elapsed Time at the Single Kohn-Sham Matrix Construction of an Insulin Molecule, total Execution Time for the Titin Molecule Simulation and scalability graph of the hybrid MPI+OpenMP simulation

The parallel performance of the DFT method in LSDALTON code was analyzed through this preparatory access project and an associated PRACE-3IP wp7.1.c project [1]. Findings are as follows:

- The DF and the ADMM schemes proved to contribute much on increasing the performance of the code. In the case of the insulin simulation, the Kohn-Sham matrix construction accelerates by 30 percent with the DF method and 56 percent with the DF-ADMM methods. In terms of the scalability characteristics, the DF scheme provides the same characteristics as the exact Coulombic calculation, while the worse scalability is observed at the DF-ADMM calculation. The current experiment exposes that the simulation time is minimized when the DF-ADMM technique is applied at 256 or 512 CPU cores.
- Large memory consumption is the most important issue in applying the DFT method with DF scheme. The Kohn-Sham matrix and LSDALTON's internal tensor sizes exceed the 32-bit integer boundary in titin and insulin simulations so that the search for a full 64-bit integer-based build environment is necessary. The use of latest Intel compiler with OpenMPI (compiled with 64-bit integer declaration) and Intel MKL's LAPACK/BLAS library was one of successful configurations, which was applied for the current simulation.
- The valinomycin simulation verifies that the performance and scalability improves noticeably by using the ScaLAPACK/PBLAS library. The full support of the 64-bit integer interface will contribute much to improving the performance of a large molecule simulation.
- Scalabilities for current applications were saturated in 1K or 2K cores. We presume that this phenomenon is caused by the small problem size, not by any limitation in implemented algorithms. Molecules' sizes in current simulations stay in the range of O(100) atoms due to the large memory consumption. A lightweight tensor design is mandatory to investigate the scalability of adopted schemes.

It was impressive to see the frequent software updates in the system and the prompt response given by PRACE.

“It was impressive that the reply to my question and request by PRACE were very fast and detailed.”

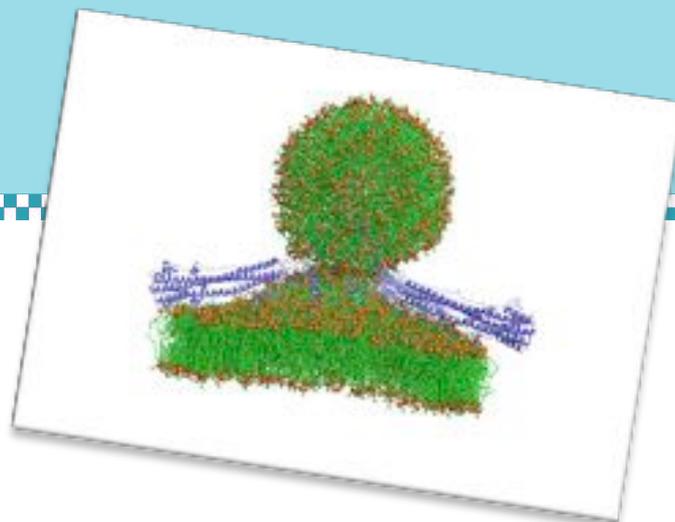
1. Soon-Heum Ko, Simen Reine, Thomas Kjærsgaard, “Enabling Large-Molecule Simulations of Biological Interest through LSDALTON's DFT Method”. *PRACE White Paper*, June 2014.

SIVE-2 - All-atom simulations of influenza viral entry



Prof. Erik Lindahl

PRACE DECI 7th Call



Influenza proteins drive close encounters between membranes.

DECI allocation

HPC Center EPCC, UK

Computer System HeCToR XE6

Resource Awarded 6 250 000 DECI Std. core-hours

Start Date November 2011

Allocation period 1 year

Research Field Life- Sciences

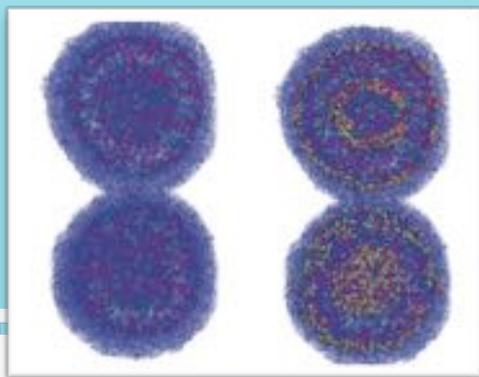
Abstract

Membrane fusion, the process by which neuronal exocytosis and infection by enveloped viruses occur, has been notoriously difficult to characterize at a molecular level. Part of the problem is that the underlying reaction that fusion proteins catalyze is not fully understood. The development of robust predictive models for the mechanism of lipid membrane fusion and its catalysis by viral fusion proteins will greatly aid in the understanding of the underlying physical process and how to effectively target it with antiviral agents. We have been developing high-performance simulation methods to analyze membrane fusion. In our work thus far, we have simulated vesicle fusion at atomic resolution, yielding novel insight into structure and mechanism of fusion intermediates. We are now extending these simulations to generate high-fidelity models of fusion in an experimental model systems, and predict the catalytic mechanism of influenza fusion proteins. In this work, we have simulated a model of the influenza virus interacting with a target membrane. The proteoliposome used to approximate the virus exerts a number of changes on the membrane but, in accordance with recent experimental results, has not yet accomplished fusion in our simulations. Work is ongoing to characterize the metastable pre-fusion states we have thus far simulated, simulate the actual influenza-mediated fusion event, and also characterize the membrane stresses during fusion.



Project leader: Erik Lindahl, Science for Life Laboratory, KTH Royal Institute of Technology

Collaborators: Peter M. Kasson, Departments of Molecular Physiology and Biomedical Engineering, University of Virginia.



Volume rendering of lateral tension in two vesicles prior to fusion. Lipid headgroups were used to define the membrane surface; these are rendered separately.

Project Results

Recent experimental findings have shown that membrane fusion is a stochastic process where fusion times are often not normally distributed—fusion can proceed very quickly or very slowly (Diao 2012). We have observed similar effects in our simulations, with 1-2 fusion trajectories where lipidic intermediates are formed after only ~100-200 ns of simulation and 10+ trajectories where no intermediates have formed after >200-1000 ns of simulation. In these “unproductive” simulations, we nonetheless observe close contact with between membranes. Based on our prior analyses, we believe this is not coincidental: close membrane contact causes a dramatic slowing of membrane and solvent dynamics (Kasson 2011). We are continuing to characterize this effect in our fusion simulations and connect it to the experimental data.

Additionally, we have begun characterizing the membrane stresses that occur during fusion. We have recently published a paper on using our GROMACS software to calculate membrane pressures in a local fashion (Kasson 2013); we are now using this to analyze

membrane stresses in curved fusion intermediates. Preliminary results will be presented at the 2013 Biophysical Society conference. It is hoped that such analyses will yield greater insight into the driving forces behind formation of fusion pores between membranes (and thus influenza viral entry).

The PRACE infrastructure was critical for attaining our goals in this work, as all simulations scaled well to 1500-2000 cores and beyond. Because long simulations are required for slow processes such as membrane fusion but we also required a number of simulation trajectories, we chose 1500 cores for optimum efficiency of utilization. We additionally utilized the infrastructure at KTH for simulation analysis and computation of membrane materials properties during the fusion process. PRACE resources greatly accelerated all these tasks.

“The PRACE infrastructure was critical for attaining our goals in this work....”

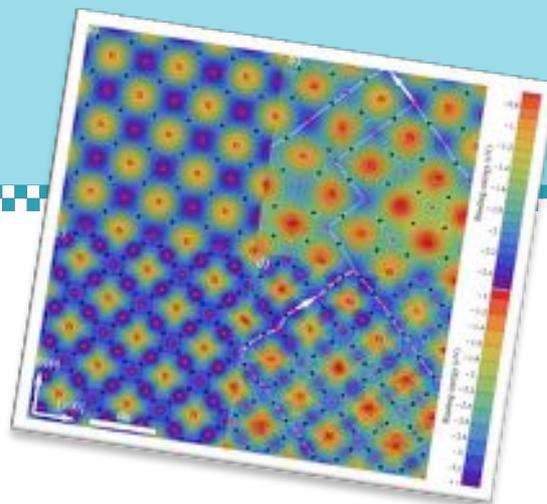
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DiSMuN - Diffusion and spectroscopical properties of multicomponent nitrides



Prof. Igor Abrikosov

PRACE DECI 7th Call



Adsorption energy surface for (a) an Al adatom on TiN(001), (b) an Al adatom on $Ti_{0.5}Al_{0.5}N(001)$, (c) a Ti adatom on TiN(001), and (d) a Ti adatom on $Ti_{0.5}Al_{0.5}N(001)$.

DECI allocation

HPC Center	SurfSARA, The Netherlands and PDC, Sweden
Computer System	Huygens and Lindgren
Resource Awarded	1 578 000 and 2 172 000 DECI Std. core-hours
Start Date	November 2011
Allocation period	1 year
Research Field	Material Science

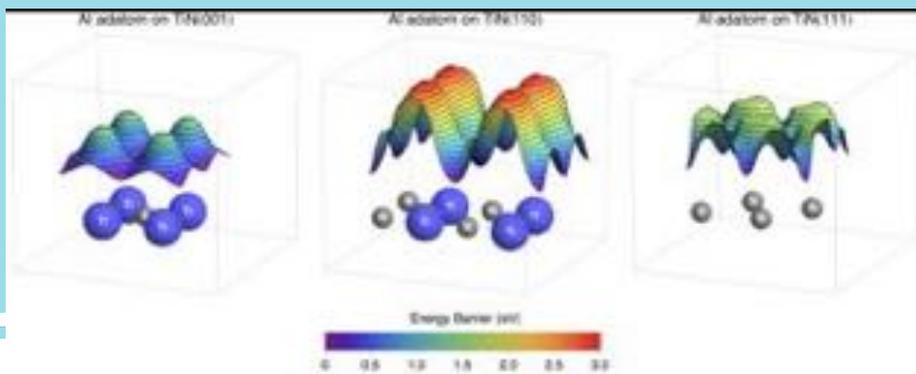
Abstract

Understanding the mobility of adatoms on growing crystal surfaces is crucial for the design of metastable multicomponent nitrides, such as technologically important $Ti_{1-x}Al_xN$. This is so since kinetics rather than thermodynamics govern the phase formation, nano-, and microstructure of physical vapour deposition (PVD) produced coatings [a]. Thermodynamically driven transformations could then be utilised later, e.g. spinodal decomposition induced age-hardening during high temperature cutting tool operations [b]. The energetics and timescales of adatom diffusion is difficult to resolve using experimental techniques and this calls for a quantitative theoretical study utilising supercomputer computations based on the most fundamental physical equations. This type of calculations has previously been employed with success to gain understanding of thin film growth of pure metals [c] and binary compounds [d]. However, for the technologically more relevant pseudo-binary solid solutions, knowledge has been absent. Our DisMuN project is initiating the theoretical study of surface diffusion in disordered multicomponent nitride alloys.



Project leader: Igor A. Abrikosov, Theoretical Physics Division, Department of Physics, Chemistry, and Biology, Linköping University, Sweden

Collaborators: Björn Alling, Weine Olovsson, Lars Hultman, Christopher Tholander, Theoretical Physics Division, Department of Physics, Chemistry, and Biology, Linköping University, Sweden / Claudia Draxl Humboldt-Universität zu Berlin, Physics Department and IRIS, Germany



Project Results

The adsorption potential energy surface for Al adatoms on top of TiN (001), (110), and N-terminated (111) surfaces relative the most favourable binding sites.

Our main focus in this starting year of our investigations has been on the surface diffusion of Ti-, N-, and Al-adatoms on TiN and Ti_{1-x}Al_xN surfaces. This focus is motivated by the large technological importance of this materials together with the high importance surface kinetics is believed to have in deciding phase formation and microstructure development, such as texture, during growth of this type of coatings.

We have used the provided resources to calculate the potential energy surface (PES) of adatom adsorption on pure TiN and disordered Ti_{1-x}Al_xN (001), (110), and (111) surfaces. From these PES we have gained knowledge about preferred binding sites, binding energies, and energy barriers for adatom diffusion on the surfaces. Fig. 1 shows the PES of pure TiN(001) and Ti_{0.5}Al_{0.5}N(001) where the effects of disorder are clearly visible for the alloy surface. Since the diffusion is exponentially related to the barrier heights we observe a drastic reduction of mobilities for Ti adatoms on the disordered surface. We have also gained insight into the difference in mobility of adatoms on the (001), (110), and

(111) surfaces. We have also investigated the difference between the isovalent systems TiN, ZrN, and HfN when it comes surface mobility on the (001) surface.

We have conducted our investigations utilising PRACE resources on the cluster Lindgren at the PDC centre at KTH Sweden as well as the Huygens cluster at the SARA centre in the Netherlands. Thanks to the large allocation we were able to perform a tremendous number of electronic structure calculations using the Vienna Ab-initio Simulation Package, provided and optimised at PDC and SARA by the site administrators. The synthesis of these results are the physically relevant adsorption energy surfaces including: adsorption binding energies and preferred binding sites, diffusion barriers for adatom surface migration, and energy curvatures related to adatom vibrational frequencies. Without PRACE resources, this project would not have been carried out in such a fruitful manner.

“Without PRACE resources, this project would not have been carried out in such a fruitful manner.”

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MUSIC



Dr. Mikael Djurfeldt

PRACE DECI 7th Call

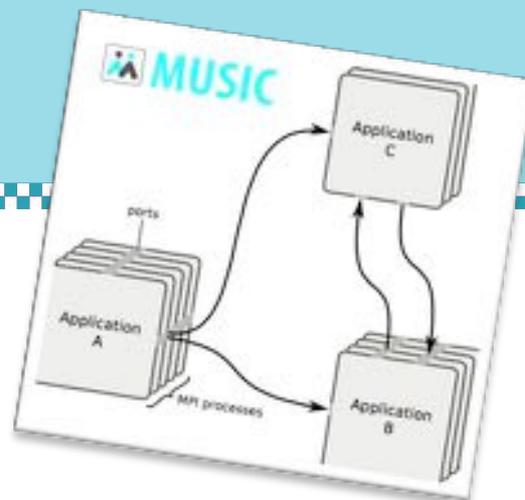


Illustration of a typical multi-simulation using MUSIC. Three applications, A, B, and C, are exchanging data during runtime.

DECI allocation

HPC Center IDRIS, France

Computer System BABEL

Resource Awarded 231 000 DECI Std. core-hours

Start Date November 2011

Allocation period 1 year

Research Field Bio Sciences

Abstract

MUSIC is an API specification that allows for run-time exchange of data between parallel applications in a cluster environment. A pilot implementation was released 2009. MUSIC is designed specifically for interconnecting large scale neuronal network simulators, either with each-other or with other tools.

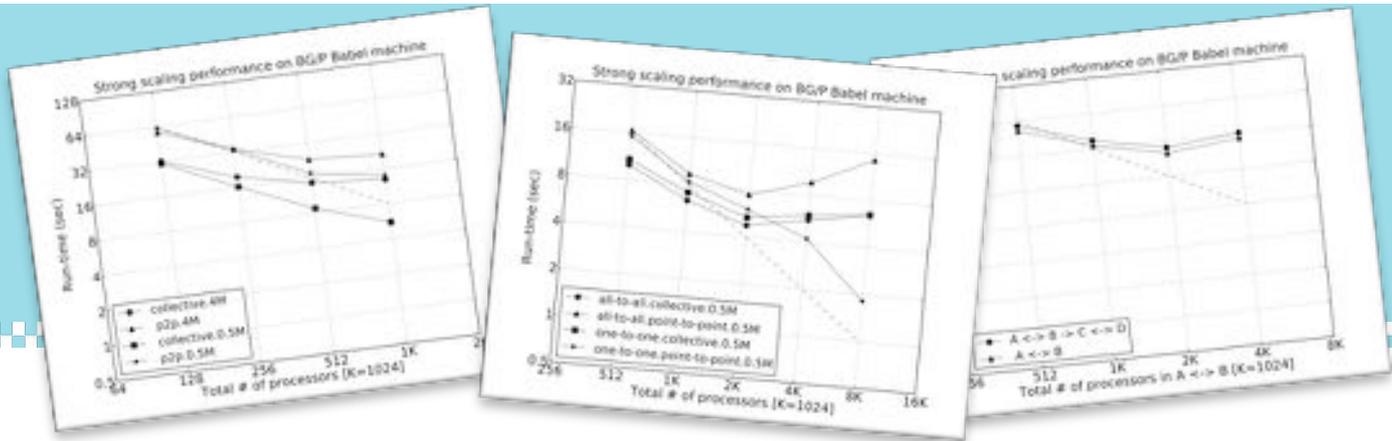
The primary objective of MUSIC is to support multi-simulations where each participating application itself is a parallel simulator with the capacity to produce and/or consume massive amounts of data. Applications publish named MUSIC input and output ports. A specification file lists the applications participating in a multi-simulation and also specifies how ports are connected. The current version of the API supports transfer of time-stamped events, multi-dimensional time series and text messages. The API encourages modularity in that an application does not need to have knowledge about the multi-simulation in which it participates.

Large scale neuronal network models and simulations have become important tools in the study of the brain and the mind. Such models work as platforms for integrating knowledge from many sources of data. They help to elucidate how information processing occurs in the healthy brain, while perturbations to the models can provide insights into the mechanistic causes of diseases such as Parkinson's disease, drug addiction and epilepsy.

Project leader: Mikael Djurfeldt, PDC and CSC, KTH, 100 44 Stockholm, Sweden, and INCF, KI, Stockholm

Collaborators: Ekaterina Brocke, INCF, KI, Stockholm, Sweden and CSC, KTH, 100 44 Stockholm, Sweden / Markus Diesmann, INM, FZJ, Jülich, Germany





Project Results

Comparison of scaling of two communication algorithms (point-to-point, collective) for two network connectivity structures (all-to-all-like, one-to-one-like)

The MUSIC library is implemented in C++ and on top of the MPI API. It also depends on the standard template library (STL). The code base consists of approximately 30000 lines of code and has a modular architecture. Standard object orienting techniques and design patterns are used to model concepts such as a parser, configuration, communication ports, and connections to other applications, event routers and a scheduler. Layout of application data is abstracted through memory efficient index and data map objects. Configuration, setup and initialization of MUSIC data structures is made in a distinct phase governed by a dedicated setup object which is deallocated before the start of a multi-simulation. The setup phase involves negotiation among ranks regarding data layout, topology of communication and communication timing parameters. MUSIC has two user-configurable communication algorithms. One is based on point-to-point MPI calls. The other is based on collective communication through MPI_Allgatherv.

Through this project, we have been able to test and benchmark MUSIC on an IBM BlueGene/P

supercomputer (IDRIS/Babel). This has allowed us to find and fix several bugs and make other improvements.

The access to PRACE resources allowed us to identify scaling problems related both to the point-to-point algorithm and the collective algorithm. The point-to-point algorithm causes large memory consumption for higher number of ranks (16K cores and upwards). Although we achieved a better performance for this algorithm during the project, we also need to analyze the communication pattern and causes of scaling problems to greater depth. The collective algorithm is currently based on MPI_Allgatherv, which inherently scales poorly for larger number of ranks. In a future project, we want to explore the use of alternative communication primitives which could either include one-sided communication or architecture-specific API:s such as DCMF.

“The access to PRACE resources allowed us to identify scaling problems related both to the point-to-point algorithm and the collective algorithm.”

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SPIESM - Seasonal prediction improvement with an Earth System Model

Dr. Colin Jones



PRACE DECI 7th Call



DECI allocation

HPC Center PDC, Sweden

Computer System Lindgren

Resource Awarded 3 750 000 DECI St. core-hours

Start Date November 2011

Allocation period 1 year

Research Field Earth Sciences

Example of the monitoring interface for a prediction experiment in Autosubmit.

Abstract

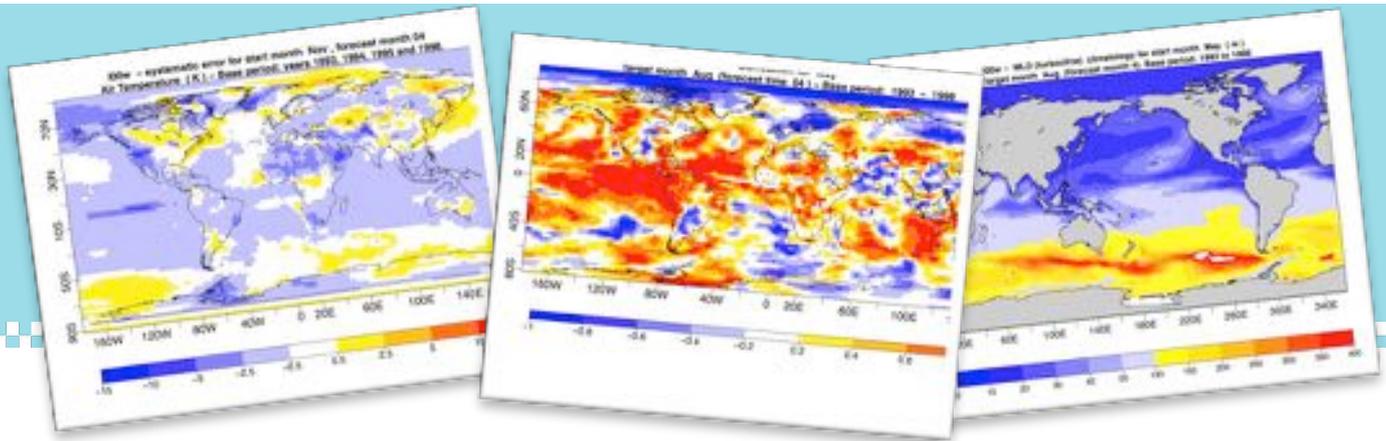
The SPIESM project investigates to which extent improvements in the resolution in climate model simulations, an aspect of climate modelling that requires substantial increases in computing resources, benefits the quality of the climate information produced in a climate forecasting context. Preliminary results suggest that the increase in ocean resolution not only reduces the systematic error, but also increases the forecast quality of the climate predictions.

The EC-Earth Earth System Model (<http://eearth.knmi.nl>) is the tool selected to perform the investigation. Apart from a large number of scaling experiments, to optimize the use of the model on the HPC, a substantial amount of time was required to adapt the standard way of performing climate prediction experiments with EC-Earth to the PDC running environment. Each forecast was run for four months into the future. Two sets of re-forecasts were carried out: one with the low-resolution version of the ocean, ORCA1 (about one degree horizontal resolution), and another one with the high-resolution configuration, ORCA025 (0.25° resolution). The experiments were carried out using the Autosubmit tool (Donners et al., 2012), developed at IC3, that allows launching and monitoring EC-Earth experiments remotely in a transparent way for the user.



Project leader: Colin Jones, Swedish Meteorological and Hydrological Institute (SMHI), Rossby Centre, Norrköping, Sweden

Collaborators: Prof. Francisco Doblas-Reyes and Dr. Virginie Guemas, Institut Català de Ciències del Clima, Climate Forecasting Unit (CFU), Barcelona, Spain / Dr. Laurent Brodeau, Stockholm University, Department of Meteorology (MISU), Stockholm, Sweden / Dr. Uwe Fladrich, and Dr. Klaus Wyser, Swedish Meteorological and Hydrological Institute (SMHI), Rossby Centre, Norrköping, Sweden



Project Results

Different errors from the near-surface air temperature in May and November months.

The analysis of the experiment is work in progress. Data from the May start dates for the years 1993-1998 and for 1993-1995 plus 1998 from the November start dates have been used in this report.

ERA-interim (Dee et al., 2011), for atmospheric variables, and the Extended Reconstructed Sea Surface Temperature (ERSST) version 3.b (Smith et al., 2008) for SST were used to assess the forecast quality of the experiments.

The systematic error of a number of atmospheric variables was computed as the difference between estimates of the model and the observed climatologies. The model climatology was computed for all members together using the per-pair method (García-Serrano and Doblas-Reyes, 2012). The general features of the bias are similar in both experiments, with reduced bias with higher resolution in the tropical Pacific and the Arctic. For the May start dates, the increase in resolution results in decreased bias in the North Atlantic and the west of Australia.

The results presented in this report suggest that the

increase of resolution of the ocean model within our forecast system leads to a reduced systematic error in most regions. This results in a better definition of the oceanic features and to some noticeable improvements in the forecast fields and associated diagnostics. A positive result is that the additional information introduced by the finer model grid is transferred to the rest of the coupled system and its impacts have been perceived in the performance of the atmospheric fields.

The wealth of information of these experiments deserves a deeper analysis of their results, which we will pursue further.

It would have been extremely difficult to perform this work without the computing time granted by PRACE given the substantial amount of resources required not only to perform this type of simulations, but also to install an efficient version of the forecast system on a new platform and to implement a configuration of the model, the one with high ocean resolution, that was not available at the time of starting the simulations.

“It would have been extremely difficult to perform this work without the computing time granted by PRACE ...”

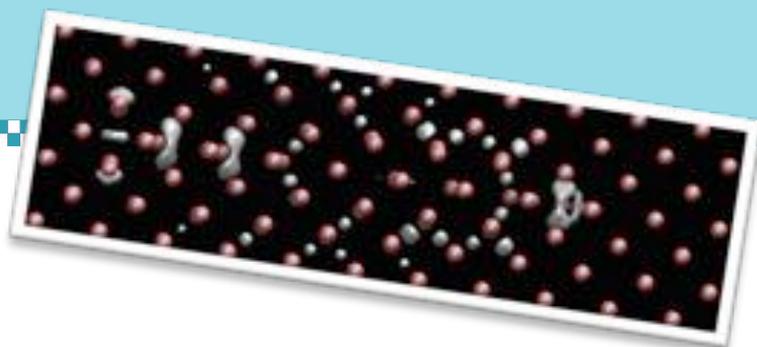
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CANONS - Comprehensive Ab initio studies of Nitride and Oxide fuels and Nuclear Structural materials

Dr. Pär Olsson



PRACE DECI 8th Call



DECI allocation

HPC Center CSCS, Switzerland

Computer System Rosa

Resource Awarded 3 125 000 DECI St. core-hours

Start Date May 2012

Allocation period 1 year

Research Field Material Sciences

A snapshot of the electronic charge density difference of a channelling defect in iron, travelling to the right.

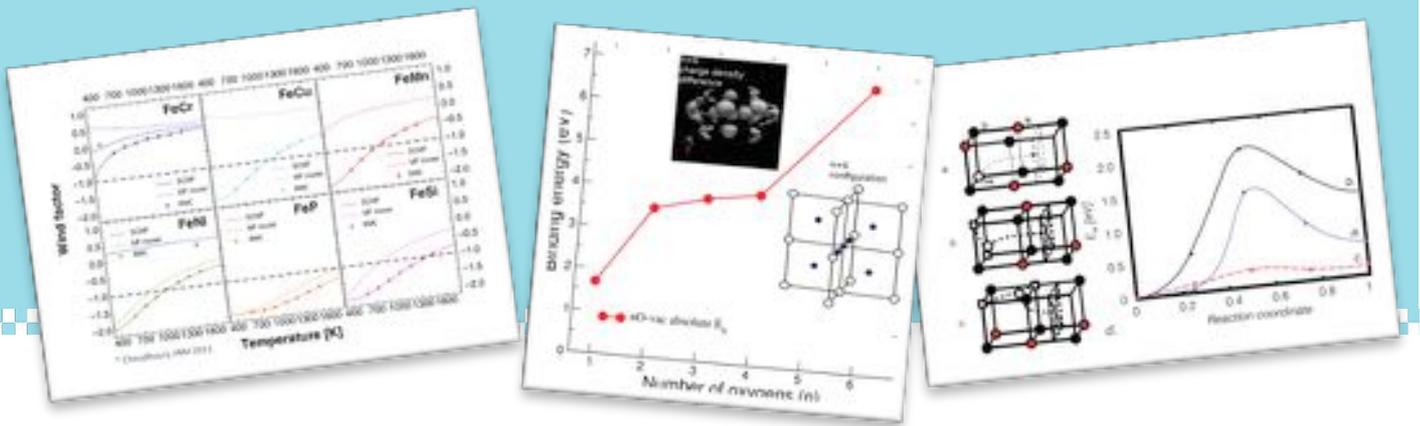
Abstract

For future generation nuclear power plants, fission or fusion based, the need for improved fuels and structural materials is crucial. The use of nuclear power is associated with several major problems: the handling of the long-lived radioactive waste, the limited resources of U-235 and the safety and integrity of the structural materials. These issues are addressed by the development of advanced reactor types, GenIV reactors, in which Am and Pu are transmuted, thereby decreasing the effective half-life of the waste, and at the same time fissile fuel is generated from natural uranium (U-238). This is achieved by the use of non-moderated (fast) neutrons in the fission process, and so-called fast reactors have been used on an experimental scale for decades. A fundamental challenge connected to the use of fast neutrons is the damage induced in various parts of the reactor. Much effort has been put into experimental studies and modeling of radiation damage since its discovery about 50 years ago. In contrast, the fundamental mechanisms of radiation damage in typical fuel matrices, like uranium-oxide or, more importantly, in innovative fuels like metal-nitride matrices, are not well understood. In the current project, we use first-principles electronic structure calculations to study the structural and thermal properties of radiation induced defects in ceramic fuels, and their interaction with transmutation gas atoms like He and Xe.



Project leader: Dr. Pär Olsson KTH Royal Institute of Technology, Reactor Physics, Stockholm, Sweden

Collaborators: Antoine Claisse, Luca Messina, Merja Pukari, Nils Sandberg, Janne Wallenius, KTH Royal Institute of Technology, Reactor Physics, Stockholm, Sweden



Project Results

The *ab initio* predicted vacancy wind for six dilute binary iron alloys, the binding energy of nO-vacancy clusters and The migration paths in ZrN for releasing a He atom

The direction averaged TDE is used in basically all phenomenological radiation damage models as a material constant. The TDE for iron has previous only been estimated using semi-empirical interaction models and only a few experimental data points exist for high symmetry directions. Molecular dynamics density functional theory in the Born-Oppenheimer approximation (BO-DFT) was here applied in order to determine the TDE from first principles in iron – the first *ab initio* dynamic displacement simulation in a metal. The BO-DFT results agree strikingly well with experiments for the available high-symmetry directions and predict a 25% lower average TDE than the reference value.

It is the continuation of an earlier study that showed that in the absence of a supersaturation of vacancies, the oxide particles can nucleate, but only in planar, 2D, configurations. These have never been observed experimentally, and the current study shows that the presence of vacancies can stabilize small coherent spherical oxide clusters.

A key result, showing the importance of taking a large number of interactions into account, and of applying correct diffusion models. The vacancy wind, which determines if solutes are dragged by vacancies ($G < -1$) or not, as a function of temperature, is shown for six dilute binary alloys. Comparing with previous calculations using simpler diffusion models, show the importance of using a correct scheme.

Actinide bearing zirconium nitride is a proposed fuel for certain lead cooled Gen-IV reactor concepts. Recent irradiation experiments showed large variation in the relative release of the different noble gases. Helium escaped and the heavier gases stayed in the fuel. The diffusion mechanisms for these processes were recently elucidated and an *ab initio* study of the diffusion coefficients for self-diffusion and noble gas diffusion in ZrN is under way.

“The PRACE resource Rosa at CSCS in Switzerland was used for this project. The support network was very helpful.”

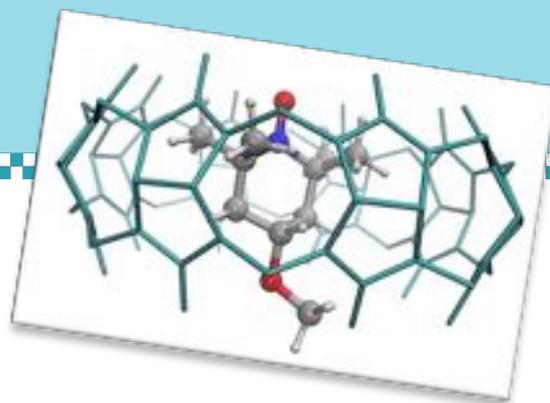
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3. L. Messina, Z. Chang, P. Olsson, *Nucl. Instr. Meth. Phys. Res. B* 303 (2013) 28–32.
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MBIOMARK - Multifunctional biomarkers for electron paramagnetic resonance imaging



Dr. Zilvinas Rinkevicius

PRACE DECI 8th Call



DECI allocation

HPC Center CSCS, Switzerland

Computer System Monte Rosa

Resource Awarded 1 875 000 DECI St. core-hours

Start Date May 2012

Allocation period 1 year

Research Field Material Sciences

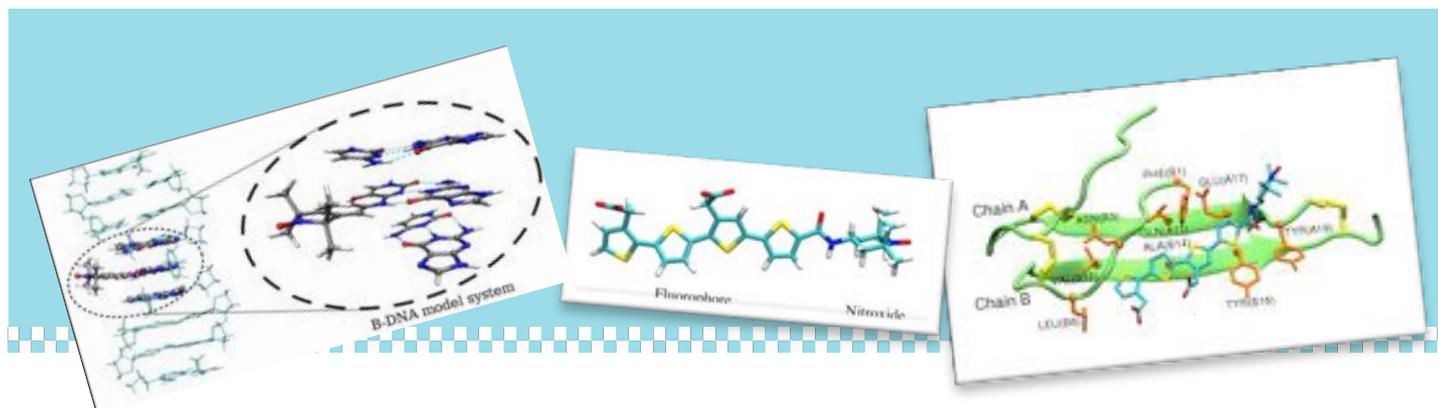
Prototypical nitroxide encapsulated in cucurbituril.

Abstract

Alzheimer's disease is one of the most prominent causes of the acquired dementia in elderly patients and it affects around 35.6 million people worldwide. In Sweden among the 160 thousands with dementia around 45% have been diagnosed with Alzheimer's disease. The Alzheimer's disease have the profound impact on the patients and their families and the overall impact of this disease on the whole society is expected to increase in the future with the population aging in Europe. Early diagnostics of the Alzheimer's disease is essential for efficient treatment of this disease and efficient screening of the people within risk groups. Unfortunately, currently options for clinical diagnostics of early stages of the Alzheimer's disease is very limited and development of novel clinical imaging techniques are highly desirable. Present research project aims to address this problem and focuses on the development of the electron paramagnetic resonance imaging technique, which is promising methodology for in vivo imaging of early damage to brain tissue cause by Alzheimer's disease. Within this project we aim to develop novel fluorescent spin labels, which are employed as the contrast agents in the electron paramagnetic resonance imaging, using the state of the art molecular modeling tools.



Project leader: Dr. Zilvinas Rinkevicius, KTH, School of Biotechnology, Stockholm, Sweden



Project Results

Nitroxide biomarker inside DNA model system, Multifunctional biomarker consisting of nitroxide moiety, linker and fluorophore, and Multifunctional biomarker bound to amyloid fibril model system.

The MBIOMARK project has investigated several problems relevant to the design of multifunctional biomarkers for EPR imaging of amyloid fibrils using quantum chemistry methods. More specifically, this project addressed the following unresolved issues: a) encapsulation effects on the magnetic properties of nitroxides in aqueous solution, b) p-stacking effects on the electronic structure and magnetic properties of biomarkers, consisting of nitroxide fused with a conjugated binding anchor, and c) amyloid fibril binding effects on the magnetic properties of multifunctional “nitroxide-linker-fluorophore”-type biomarkers.

During the course of the MBIOMARK project we investigated various aspects affecting the computational design of nitroxide-based biomarkers for EPR imaging applications. We expect that further in silico design techniques, similar to those used in this project, will become applicable to other types of biomarkers in the near future, provided that the computational power of HPC systems keep growing at the current rate.

The MBIOMARK project has been a highly demanding project in terms of computational resources as extensive QM/MM calculations have been carried out during the first and third parts of this project. These computations would have not been possible without the generous time allocation from PRACE. Furthermore, apart from enabling us to carry out computational investigations of nitroxide-based biomarkers, the access to PRACE resource (Cray XE6 supercomputer Monte Rosa, Swiss National Supercomputing Centre, Switzerland) allowed us to test parallelization improvements in the DALTON program developed in conjunction with the ScalaLife FP7 project (www.scalalife.eu) and the PRACE community software initiative, in which we participated as DALTON program developers.

The main technical challenge for more effective usage of PRACE HPC resources for in silico design of biomarkers is the development of an automated management system for computational processes.

“These computations would have not been possible without the generous time allocation from PRACE”

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2. B. Frecus, Z. Rinkevicius and H. Ågren, “p-Stacking effects on the EPR parameters of a prototypical DNA spin label”, *Phys. Chem. Chem. Phys.*, 2013,15, 10466-10471.

PIPETURB - Large scale simulation of turbulent pipe flow



Dr. Philipp Schlatter

PRACE DECI 8th Call



DECI allocation

HPC Center	CSC, Finland and EPCC, UK
Computer System	Louhi and HeCToR
Resource Awarded	2 312 500 and 3 937 500 DECI St. core-hours
Start Date	May 2012
Allocation period	1 year
Research Field	Engineering

Visualization of the turbulent flow in cross-plane of the pipe

Abstract

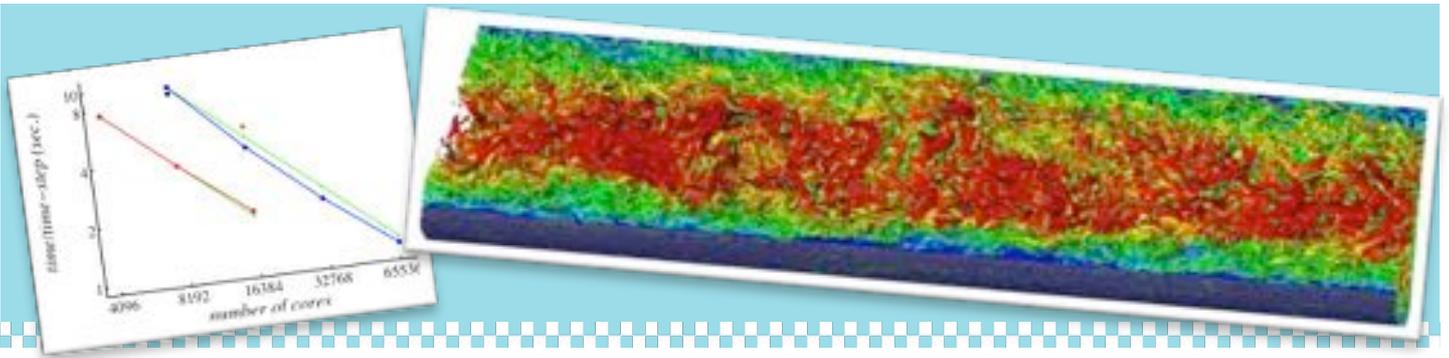
The flow of fluids in pipes with circular cross-sections is frequently encountered in a variety of environmental, technical and even biological applications. Typical examples of pipe flows can be found in urban drainage systems, transport of natural gas or oil in the energy sector, or the flow of blood in veins and arteries. Most fluid flows observed in nature are indeed turbulent. Of particular importance in flows delimited by solid walls is the near-wall region in which a large fraction of the drag stems from velocity fluctuations in a thin boundary layer adjacent to surfaces. Near-wall turbulence structures in wall-bounded shear flows primarily scale in terms of the so-called viscous length scale, which might be very small as Reynolds number is increased. However, according to recent experimental studies, very large-scale motions with lengths of $5R$ up to $20R$ are found in fully developed turbulent pipe flow (R being the radius). These large-scale structures are very energetic and active. Large-scale motions thus play an important role in the dynamics of turbulent pipe flows.

The aim is to study fully developed high-Reynolds number turbulent pipe flow through direct numerical simulations (DNS). DNS attempts to resolve all relevant scales of the turbulent flow. These will be carried out using the massively parallel DNS code available at KTH Mechanics, nek5000, which is based on an accurate and efficient spectral-element discretization



Project leader: Dr. Philipp Schlatter, KTH, Department of Mechanics, Stockholm, Sweden

Collaborators: Dr. Geert Brethouwer, Dr. George El Khoury, Prof. Arne V. Johansson, KTH, Department of Mechanics, Stockholm, Sweden / Prof. Elisabetta De Angelis and Prof. Alessandro Talamelli, Università di Bologna, CI RI Aeronautica, Bologna, Italy / Dr. Paul Fischer, Argonne National Laboratories, Mathematics and Computer Science, Argonne, USA



Project Results

Parallel scaling (strong scaling) of the Nek5000 code on the HeCToR, Triolith and Lindgren and the Three-dimensional visualization of the turbulence structures in the simulation of pipe flow.

A wide variety of flow statistics like single-point and two-point statistics and spectra have been computed and visualizations have been generated. For the first time, we could prove with numerical simulations that near-wall turbulent flows at higher Reynolds numbers have a practically perfect similarity in these three canonical cases. This similarity pertains to all statistics, i.e. low- and higher order statistics of the flow and turbulence and spectra pointing out that near-wall turbulence is only little affected by the outer flow geometry and has a high degree of universality. This conclusion is of practical and fundamental importance, and shows that it should be feasible to develop a universally applicable near-wall turbulence model for e.g. industrial applications.

The employed spectral-element code showed a practically perfect linear scaling up to 65 536 cores on these systems, as shown above. Due to the DECI project and the high performance on the used systems we could carry out large-scale massively parallel simulations of turbulent pipe flow, and understand the scaling behavior of our method for real production cases.

Such simulations would not have been possible without DECI. Furthermore, the availability of these computing hours and the corresponding results allowed us to further develop and optimize our code, in particular related to the computation of turbulence statistics. During the work with PRACE infrastructure, we implemented, validated and employed a new way of calculating complete Reynolds stress budgets from DNS, using a sequence of tensor rotations and interpolation steps. All data could be obtained with spectral accuracy.

The infrastructure offered by PRACE enabled us in this project to carry out a large-scale simulation of a flow case with a high fundamental and practical importance. In general, we anticipate that also in the future PRACE will play an essential role in fundamental studies of flow processes and will make it possible to address essential problems found in industrial, biological and environmental flows.

“The infrastructure offered by PRACE enabled us in this project to carry out a large-scale simulation of a flow case with a high fundamental and practical importance.”

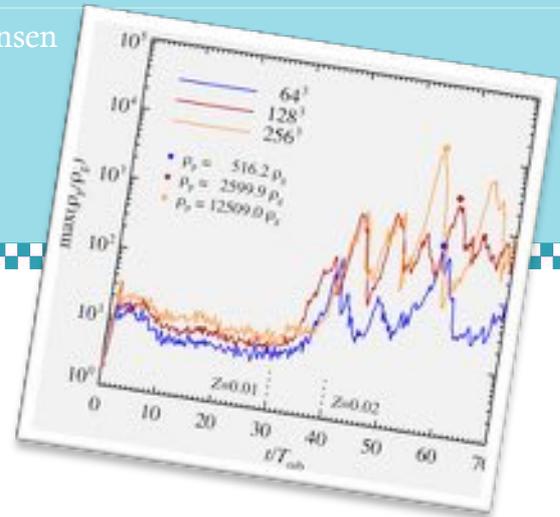
1. El Khoury, G. K., Schlatter, P., Noorani, A., Fischer, P. F., Brethouwer, G. & Johansson, A. V. Direct numerical simulation of turbulent pipe flow at moderately high Reynolds numbers. *Flow Turbul. Combust.* DOI 10.1007/s10494-013-9482-8 (2013).
2. Schlatter, P. & El Khoury, G. K. Turbulent flow in pipes, *PDC Newsletter*, No:1 (2012)
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5. El Khoury, G. K., Schlatter, P., Noorani, A., Brethouwer, G. & Johansson, A. V. Large-scale simulations of turbulent pipe flows. *The 9th European Fluid mechanics Conference (EFMC-9)*, Rome-Italy, June 9-13 (2012).

PLANETESIM - Towards an initial mass function of planetesimals



Dr. Anders Johansen

PRACE DECI 8th Call



The maximum particle density as a function of time, for three different resolutions

DECI allocation

HPC Center FZJ, Germany,
ICHEC, Ireland and
RZG, Germany

Computer System JuRoPa, Stokes and
VIP/HYDRA

Resource Awarded 3 472 030,
1 860 016 and
868 008 DECI St.
core-hours

Start Date May 2012

Allocation period 1 year

Research Field Astro Sciences

Abstract

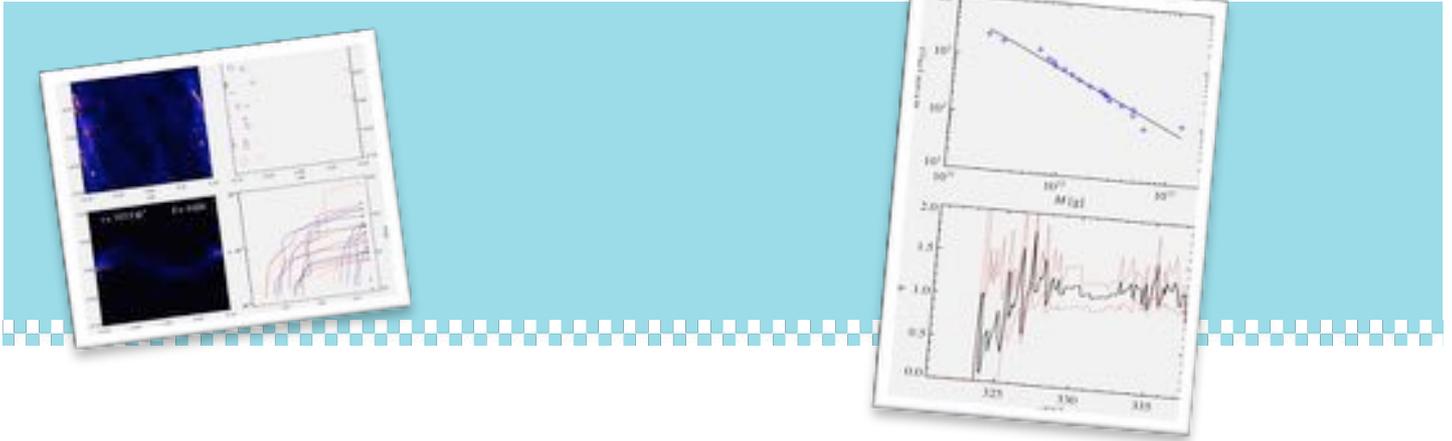
The planets of the solar system and the exoplanets - planets that orbit stars other than the sun - are a fascinating research area. Fuelled by new detection methods that find more and more planets around other stars, satellite missions to other planets, moons and asteroids in our solar system, and the ever-growing power of supercomputers, planet research is in rapid development and enjoys lots of interest from the broad public. Supercomputer simulations performed by members of our group have identified a surprising phenomenon that allows growth from pebbles to planetesimals: pebble-sized particles concentrate in dense filaments that protect them from gas drag, in a process related to why bicycle riders and migrating geese travel in groups. The densities of pebbles get so high that gravity takes over and leads to gravitational collapse to form planetesimals.

The aim of this research project is to use high-resolution computer simulations to understand the birth sizes of planetesimals. The asteroid belt between Mars and Jupiter and the Kuiper belt beyond Neptune are examples of planetesimal belts left over from the planet formation process. The largest asteroids and Kuiper belt objects have sizes that are similar to the largest planetesimals that form in the computer simulations, but an important feature of both these populations is that the size distribution of the planetesimals show a break around 50 km in radius. This has been dubbed the missing intermediate-sized planetesimals problem.

Project leader: Anders Johansen, Lund University, Department of Astronomy and Theoretical Physics, Lund, Sweden

Collaborators: Mordecai-Mark Mac Low, American Museum of Natural History, New York, USA / Melvyn B. Davies, Ross Church and Michiel Lambrechts, Department of Astronomy and Theoretical Physics, Lund, Sweden





Project Results

This figure shows the column density of pebbles in a protoplanetary disc and the size distribution of newly born planetesimals in high-resolution simulations.

We have simulated dust dynamics in protoplanetary discs at high resolution with 256^3 grid cells and 19.2 million particles. This is twice the resolution that was obtained in previous papers. We measured the maximum concentration of solid particles moving in the turbulent gas. The maximum concentration is approximately four times higher than previous simulations at 128^3 grid cells, confirming a trend that was already confirmed at lower resolution. This way we can obtain extremely high local particle densities and thus potentially form planetesimals, which are much smaller than at high resolution.

We have also run simulations including the self-gravity of the particles. For this purpose we have developed a sink particle module into the Pencil Code, in order to reduce the particle number once bound planetesimals have formed. We have tested this algorithm at many PRACE platforms and at very high resolution. The planetesimals that form are from 50 to 250 km in radius. The lower size is much smaller than what we observed at lower resolution and this confirms the original aim of the project to be able to resolve smaller planetesimals at higher

resolution.

We can now proceed to measure the size distribution of the newly born planetesimals. The mass distribution follows rather closely $dN/dM = K M^{-1}$. Thus the number is dominated by the smallest planetesimals. The mass, on the other hand, is dominated by the largest planetesimals.

Our simulations were run on JUROPA, VIP, HYDRA and STOKES. Some simulations were run over several platforms after copying the latest data snapshot of the code. Data transfer was rather smooth, except for access to and from STOKES, which was often very slow. However, this seemed to have improved recently.

“We have tested this algorithm at many PRACE platforms and at very high resolution.”

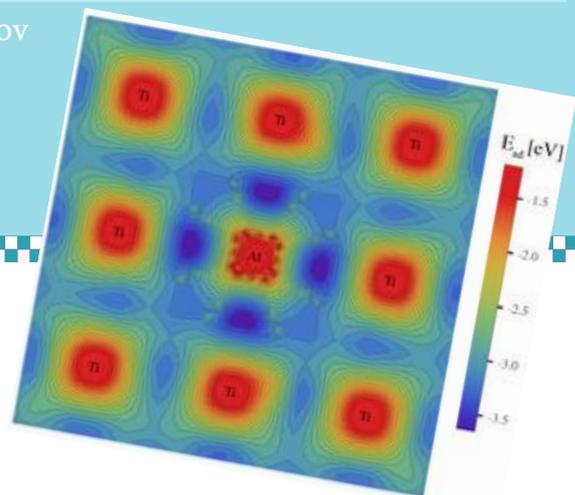
1. Johansen A., Youdin A., & Lithwick Y., Adding particle collisions to the formation of asteroids and Kuiper belt objects via streaming instabilities, *Astronomy and Astrophysics* (2012)
2. Johansen A., Youdin A., & Mac Low M.-M., Particle clumping and planetesimal formation depend strongly on metallicity, *The Astrophysical Journal*, vol. 704, p. L75-L79, 2009

DifVib - Diffusion and spectroscopical properties of multicomponent nitrides



Prof. Igor Abrikosov

PRACE DECI 9th Call



DECI allocation

HPC Center	EPCC, UK and PDC, Sweden
Computer System	ICE-Advance and Lindgren
Resource Awarded	3 125 000 and 3 125 000 DECI Std. core-hours
Start Date	November 2012
Allocation period	1 year
Research Field	Material Science

The binding energy landscape of a Ti adatom on the TiN(001) surface with a Al_{Ti} surface atom present

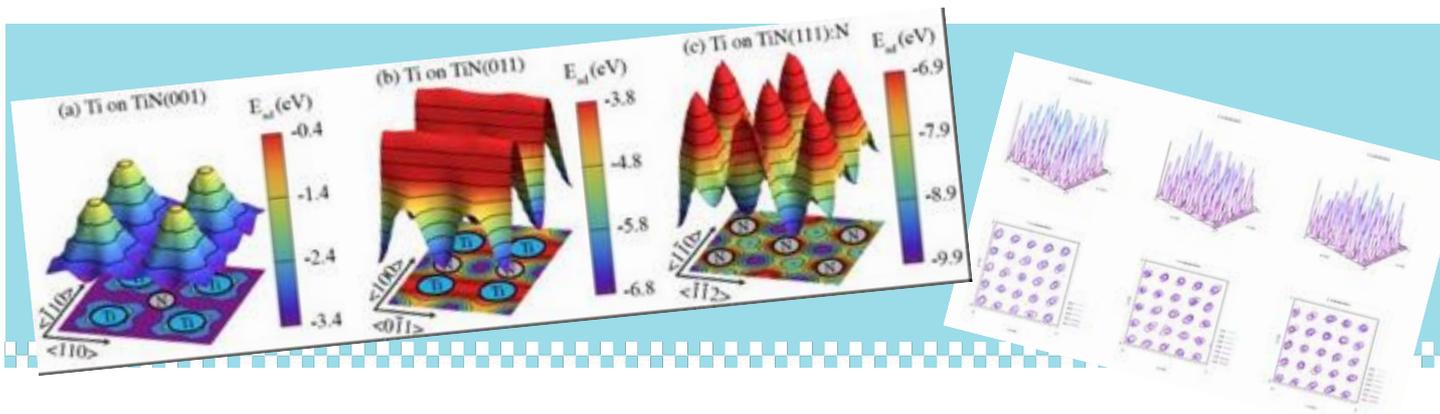
Abstract

Understanding the mobility of adatoms on growing crystal surfaces is crucial for the design of metastable multicomponent nitrides, such as technologically important $Ti_{1-x}Al_xN$. This is so since kinetics rather than thermodynamics govern the phase formation, nano-, and microstructure of physical vapour deposition (PVD) produced coatings [a]. Thermodynamically driven transformations could then be utilised later, e.g. spinodal decomposition induced age-hardening during high temperature cutting tool operations [b]. The energetics and timescales of adatom diffusion is difficult to resolve using experimental techniques and this calls for a quantitative theoretical study utilising supercomputer computations based on the most fundamental physical equations. This type of calculations has previously been employed with success to gain understanding of thin film growth of pure metals [c] and binary compounds [d]. However, for the technologically more relevant pseudo-binary solid solutions, knowledge has been absent. Our DisMuN project is initiating the theoretical study of surface diffusion in disordered multicomponent nitride alloys.



Project leader: Igor A. Abrikosov, Theoretical Physics Division, Department of Physics, Chemistry, and Biology, Linköping University, Sweden

Collaborators: Björn Alling, Olle Hellman, Igor Mosyagin, Lars Hultman, Christopher Tholander, Theoretical Physics Division, Department of Physics, Chemistry, and Biology, Linköping University, Sweden / Prof. Leonid Dubrovinsky, Universität Bayreuth, Bayerisches Geoinstitut, Bayreuth, Germany



Project Results

The binding energy landscape for Ti adatoms on the 001, 011, and 111 surfaces of TiN and Projections of probability densities of bccFe at 4700K and 350 GPa, 5x5x5 Supercell (125 atoms).

Our massive Density functional calculations using the VASP code have revealed the qualitatively different adatom mobility on the 001, 011, and 111 surfaces of all three nitrides. We have also been able to identify distinct differences between the TiN and the two other nitrides both in terms of which position that serve as stable binding sites for Ti/Zr/Hf adatoms, and in values of the activation energy barriers.

Most interestingly we have been able to identify the effect of Al surface impurities on the adatom migration on the different surfaces. In particular Ti adatoms on the TiN(001) and Al adatoms on the TiN(111) surfaces are influenced by such impurities.

With the help of PRACE computational scientists, we were able to pack our MD simulations in VASP in such way that it uses its internal subroutine. This allows for better scaling and proper benchmarking. We used these scaling results to apply for PRACE Tier-0 application with this part of the project (the decision would be announced on the 4th of March). Scientifically wise, we

estimated the stability region of pure Fe in bcc, hcp and fcc phases under mentioned conditions.

This project was carried out on PDC Lindgren system at Royal Institute of Technology, Stockholm, Sweden.

PRACE experts helped us to prepare our codes for Tier-0 application, in particular, PRACE experts helped us to collect benchmarking and scaling information, choose which machine to apply for, and provided technical guidance during the writing of the application. During this collaboration we also developed a set of tools to monitor an ongoing simulation. These tools are currently being tested and scheduled for future use.

“PRACE experts helped us to prepare our codes for Tier-0 application”

1. C. Thollander, B. Alling, F. Tasnádi, J. E. Greene, and L. Hultman, Effect of Al surface atoms on Ti, Al, and N adatom dynamics on TiN(001), (011), and (111) surfaces, *In final preparation*.

2. O. Hellman, P. Steneteg, I. A. Abrikosov, and S. I. Simak, Temperature dependent effective potential method for accurate free energy calculations of solids, *Phys. Rev. B* 87, 104111 (2013) [DOI: 10.1103/PhysRevB.87.104111]

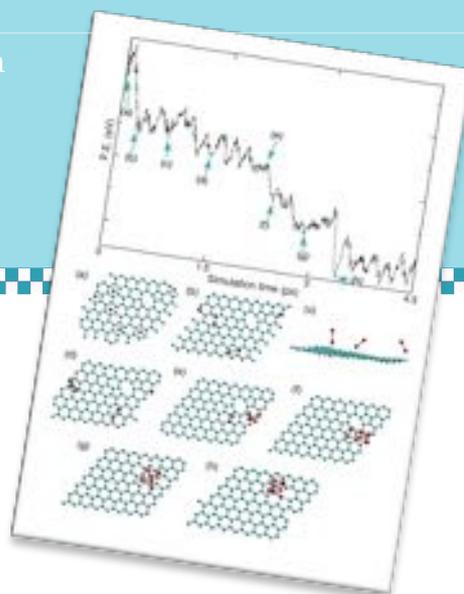
3. O. Hellman, I. Abrikosov, Temperature-dependent effective third-order interatomic force constants from first principles, *Phys. Rev. B* 88, 144301 (2013) [DOI: 10.1103/PhysRevB.88.144301]

CoStAFuM - Diffusion and spectroscopical properties of multicomponent nitrides



Prof. Olle Eriksson

PRACE DECI 9th Call



Potential energy (P.E.) landscape as a function of simulation time.

DECI allocation

HPC Center RZG, Germany and UiO, Norway

Computer System Hydra and Abel

Resource Awarded 1 937 522 and 7 750 086 DECI Std. core-hours

Start Date November 2012

Allocation period 1 year

Research Field Material Science

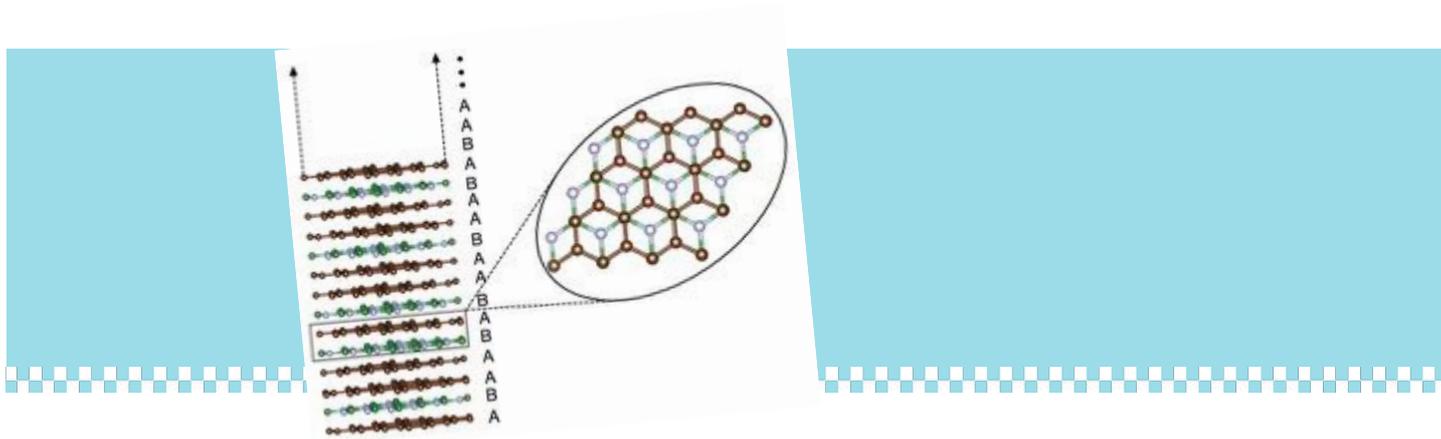
Abstract

This proposal deals with state-of-the-art computational materials science methods applied to advanced functional materials. We aim to study the following topics, (i) correlated electron system, (ii) graphene and molecular interface systems, (iii) lattice dynamics and (iv) core shell structures and nanoparticles. All these topics will be studied by ab initio density functional theory based methods implemented in codes like VASP and SIESTA. For some applications, in-house codes such as SCAILD for lattice dynamics, RSPT for dynamical mean field theory will be used.



Project leader: Olle Eriksson, Department of Physics and Astronomy, Uppsala University, Sweden

Collaborators: Dr. Biplab Sanyal, Department of Physics and Astronomy, Uppsala University, Sweden



Project Results

Schematic representation of quasi-periodic stacking of graphene and h-BN. Inset shows schematic representation of Bernal stacking, which is used to form these structures.

In this work, we have studied the chemical and magnetic interactions of Fen ; $n=1-6$ clusters with vacancy defects (monovacancy to correlated vacancies with six missing C atoms) in a graphene sheet by ab-initio density functional calculations. It is found that the vacancy formation energies are lowered in presence of Fe, indicating an easier destruction of the graphene sheet. Our ab initio molecular dynamics simulations show that (i) Fe adatoms form clusters and (ii) mobile Fe clusters get strongly chemisorbed at defect sites.

Advancement towards opening a band gap paved the way to make two-dimensional heterostructures with graphene and hexagonal boron nitride (h-BN). An alternate arrangement of graphene and h-BN layers in a three dimensional stacking can tune the band gaps of these composites depending on the position of B and N atoms with respect to C atoms of graphene. Symmetry breaking at the Dirac point leads to an opening of a band gap. In this study, we have explored a unique possibility of arranging graphene and h-BN atomic layers in a quasiperiodic Fibonacci sequence to study the possibilities

of controlling electronic properties of these heterostructures. Our density functional calculations combined with van der Waals corrections reveal that these quasi-periodic heterostructures are more stable than normal periodic stacking of monolayers of graphene and h-BN. Moreover, for certain arrangements of atomic layers, sizeable band gaps can be obtained.

We have mainly used Abel super computing facility from PRACE DECI tier-1 site Norway (SIGMA). We have also used PRACE middleware 'globus toolkit' for generation of proxies, login to the PRACE platform and data transfer. All the calculations were done very smoothly without any interruption from the PRACE nodes.

“All the calculations were done very smoothly without any interruption from the PRACE nodes.”

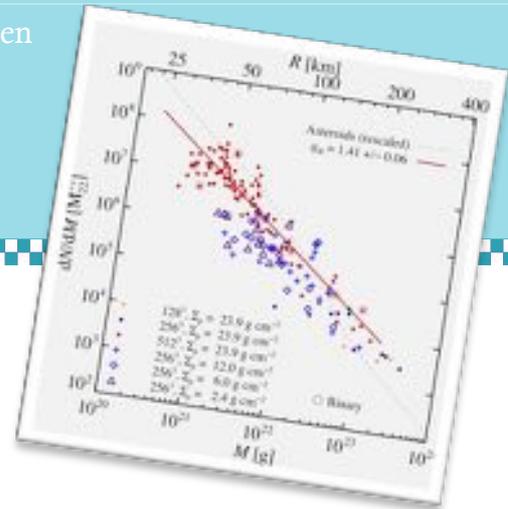
1. Magnetism of Fe clusters (Fen ; $n \leq 6$) chemisorbed on vacancy defects in graphene; S. Haldar, B. S. Pujari, S. Bhandary *et. al. In manuscript.*
2. Electronic structure of graphene/h-BN heterostructures in a quasi-periodic Fibonacci sequence; S. Bhandary, S. Haldar *et. al. In manuscript.*
3. Temperature-driven transition of the magnetic dipole moment in magnetite; D. Schmitz *et. al. Submitted to Phys. Rev. B*

PLANETESIM-2 - Towards an initial mass function of planetesimals



Dr. Anders Johansen

PRACE DECI 10th Call



DECI allocation

HPC Center FZJ, Germany

Computer System JuRoPa

Resource Awarded 7 500 000 DECI St. core-hours

Start Date May 2013

Allocation period 1 year

Research Field Astro Sciences

Birth size distribution of planetesimals forming by the streaming instability in 25-cm-sized particles

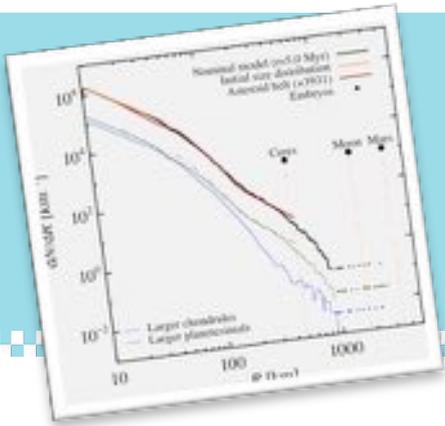
Abstract

The aim of this research project is to use high-resolution computer simulations to understand the birth sizes of planetesimals. The asteroid belt between Mars and Jupiter and the Kuiper belt beyond Neptune are examples of planetesimal belts left over from the planet formation process. The largest asteroids and Kuiper belt objects have sizes that are similar to the largest planetesimals that form in the computer simulations, but an important feature of both these populations is that the size distribution of the planetesimals show a break around 50 km in radius. This has been dubbed the missing intermediate-sized planetesimals problem. Previously we have in our computer simulations only been able to form the largest planetesimals (with radii of 150-1500 km) from overdense filaments of pebbles. Small planetesimals form from small-scale particle overdensities and hence it requires very high-resolution simulations to model their formation. The computational resources granted by PRACE in May 2012 has allowed us to run for the first time 256^3 simulations of planetesimal formation on some of Europe's most powerful supercomputers. This work is making good progress and has already produced exciting preliminary results.



Project leader: Anders Johansen, Lund University, Department of Astronomy and Theoretical Physics, Box 43, 22100 Lund, Sweden

Collaborators: Mordecai-Mark Mac Low, American Museum of Natural History, New York, USA / Pedro Lacerda, Max Planck Institute for Solar System Research, Göttingen, Germany / Martin Bizzarro, Centre for Star and Planet Formation, University of Copenhagen, Denmark.



The size distribution of asteroids after accreting chondrules for 5 Myr.

Project Results

PLANETESIM-2 aimed specifically at updating the measurements of the initial mass function of planetesimals with 512³ simulations to see the shape of the size distribution down to 25 km in radius.

We find that the sizes of the largest planetesimals which form in the simulations, typically 200-300 km in radius, are relatively independent of the grid resolution. Higher resolution allows consecutively smaller planetesimals to form alongside these large planetesimals, reaching sizes down to 25 km at 512³. The size distribution dN/dM can be fitted with a power law, yielding a fitted coefficient of approximately -1.4. This size distribution has most of the mass in the few largest bodies, while the planetesimal number is dominated by the smallest bodies in the distribution.

The size distribution is not in agreement with the size distribution of asteroids, which displays a bump at 60 km in radius. There is no sign of this bump in the planetesimals formed in the simulations. This result is interesting and shows that additional processes are needed

to change the size distribution after the formation of the planetesimals. Fragments of asteroids land on Earth as meteorites, and some meteorites contain up to 80% of their mass in mm-sized chondrules (crystallised silicate droplets). We have developed a numerical model of how the size distribution of planetesimals changes if the planetesimals are allowed to accrete such chondrules over millions of years. The resulting size distribution matches the observed size distribution of asteroids very well. Therefore we propose that asteroid seeds had initial sizes from 10 to 50 km in radius and then grew up to 500 km in radius (Ceres) by accretion of chondrules over 5 million years.

Our simulations were run on JUROPA. This was a continuation of simulations already performed at JUROPA, so their execution was smooth.

“Our simulations were run on JUROPA. This was a continuation of simulations already performed at JUROPA, so their execution was smooth.”

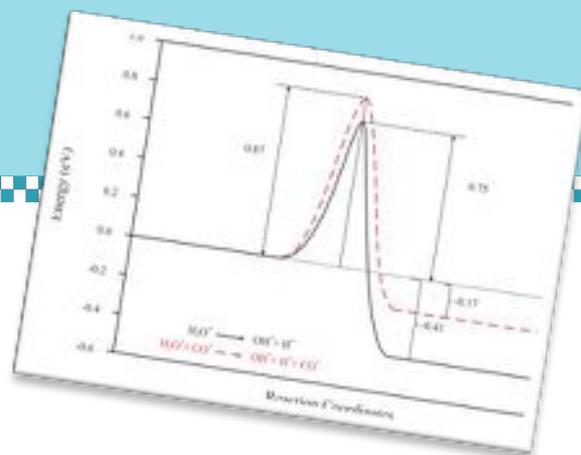
1. Johansen, Mac Low, Lacerda, & Bizzarro (2014, submitted)
2. Yang C.-C., & Johansen A. On the feeding zone of planetesimal formation by the streaming instability, *The Astrophysical Journal*, vol. 792, 88 (10 p.) 2014
3. Johansen A., Blum J., Tanaka H., Ormel C., Bizzarro M., & Rickman H., The multifaceted planetesimal formation process, *In Protostars and Planets VI*, University of Arizona Press, 2014

MEGAREACT - Metal catalysed gasification reactions

Prof. Kim Bolton



PRACE DECI 10th Call



Reaction profiles for water dissociation over Ni (111) with and without co-adsorbed CO

DECI allocation

HPC Center UiO, Norway

Computer System Abel

Resource Awarded 750 000 DECI St. core-hours

Start Date May 2013

Allocation period 1 year

Research Field Materials Science

Abstract

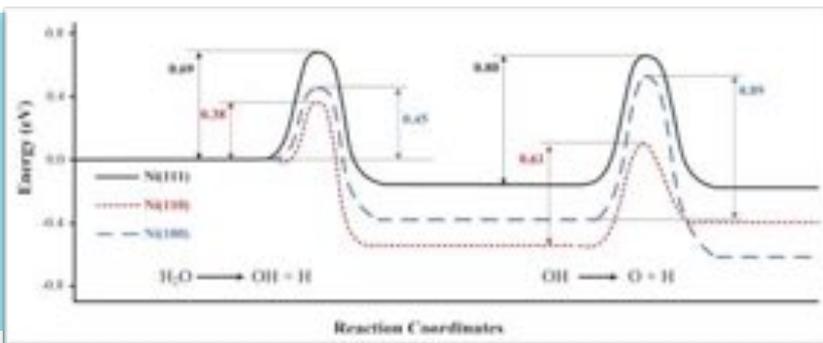
Gasification, the conversion of carbonaceous material to a gaseous product with an employable heating value, is one of the most important and effective production methods of energy carriers employed toward sustainable development. Making use of quantum mechanics simulation tools, mechanisms of reactions during the metal catalysed gasification process are investigated. In particular, we obtain reactant and transition state energies and frequencies that are used to obtain the reaction barriers and Arrhenius pre-exponentials of the elementary reactions on a transition metal catalyst surface. These data will subsequently be used in kinetic modelling of the entire reaction. The first reaction that was studied was the water gas shift (WGS) reaction, which is important in almost all gasification reactions.



Project leader: Kim Bolton, University of Borås, School of Engineering, Borås, Sweden

Collaborators: Abas Mohsenzadeh Syouki, University of Borås, School of Engineering, Borås, Sweden





Reaction profiles for the water dissociation over Ni(111) (solid black line), Ni(110) (short-dashed red line) and Ni(100).

Project Results

The calculations were performed using the Vienna ab initio simulation package (VASP) implementing spin polarized DFT. Transition states were located using the climbing image-nudged elastic band (CI-NEB) method.

One of the subprojects studied the effect of carbon monoxide co-adsorption on the dissociation of water on the Ni(111) surface. The structures of the adsorbed water molecule and of the transition state are changed by the presence of the CO molecule. The changes in structures and vibrational frequencies lead to a reaction energy that is 0.17 eV less exothermic in the presence of the CO, and an activation barrier that is 0.12 eV larger in the presence of the CO. At 463 K the water dissociation rate constant is an order of magnitude smaller in the presence of the CO. This reveals that far fewer water molecules will dissociate in the presence of CO under reaction conditions that are typical for the water-gas-shift reaction.

This work was granted access to the HPC resources of Abel (Oslo, Norway) made available within the Distributed European Computing Initiative by the

PRACE-2IP, receiving funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement no. RI-283493.

This project would have been difficult to perform without having access to the highly parallelized VASP program in combination with extensive computer hardware resources. Therefore the proper time allocation from PRACE significantly increased the impact of our research.

The future plan is to investigate more complex industrial processes such as steam methane reforming over a variety of catalytic surfaces. The understanding gained from these studies will, together with experimental investigations, lead to improved catalysts and reaction conditions.

“Therefore the proper time allocation from PRACE significantly increased the impact of our research.”

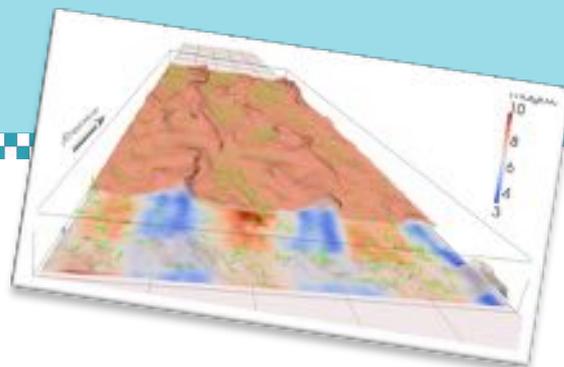
1. Mohsenzadeh, A., et al., The Effect of Carbon Monoxide Co-Adsorption on Ni-Catalysed Water Dissociation. International journal of molecular sciences, *Int. J. Mol. Sci.* 2013, 14(12), 23301-23314; doi:10.3390/ijms141223301
2. Mohsenzadeh, A., K. Bolton, and T. Richards, DFT study of the adsorption and dissociation of water on Ni (111), Ni (110) and Ni (100) surfaces. *Surface Science*, 2014, Volume 627, Pages 1–10; doi:10.1016/j.susc.2014.04.006
3. Mohsenzadeh, A., K. Bolton, and T. Richards, Oxidation and dissociation of formyl on Ni(111), Ni(110) and Ni(100) surfaces: A comparative density functional theory study. *Topics in Catalysis*
4. Mohsenzadeh, A., K. Bolton, and T. Richards, A density functional theory study of hydrocarbon combustion and synthesis on Ni surfaces, *J. Mol. Model.*

DNSTF: Simulation of finite-size fibres in turbulent channel flow



Prof. Gustav Amberg

PRACE DECI 10th Call



DECI allocation

HPC Center EPCC, UK

Computer System HeCToR, Archer

Resource Awarded 8 437 500 DECI St. core-hours

Start Date May 2013

Allocation period 1 year

Research Field Engineering

Three-dimensional view, fibre length $L^+ = 9.6$, $v_f = 0.43\%$. The fibres shown here are fibres with a distance to the wall less than $1.5L$.

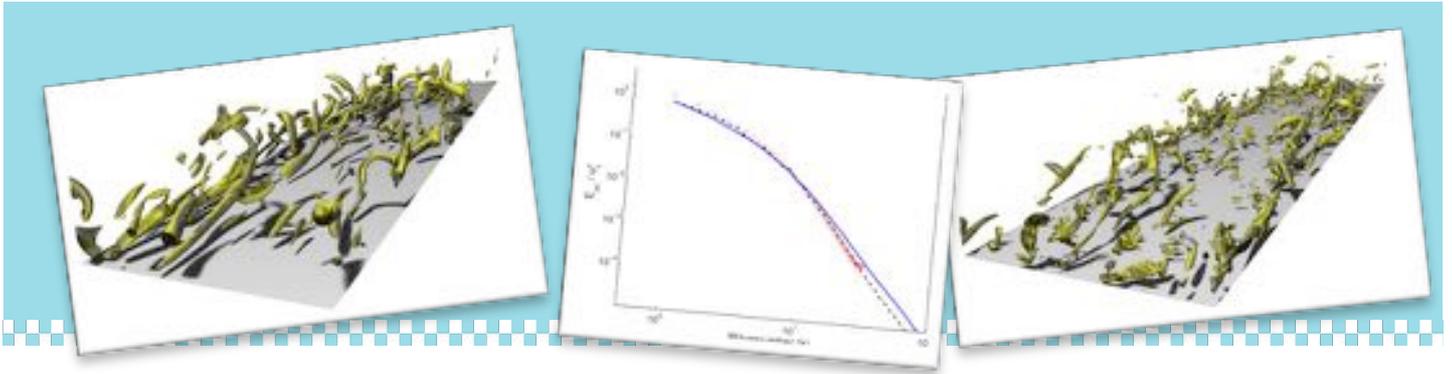
Abstract

Using the lattice Boltzmann method, the group at the Mechanics department – Royal institute of Technology – Sweden, performed direct numerical simulation of the dynamical behavior of almost neutrally buoyant finite-size rigid fibres in turbulent channel flow. The time evolution of the fibre orientation and translational and rotational motions in a statistically steady channel flow is obtained for different fibre lengths. The turbulent flow is modeled by an entropy lattice Boltzmann method and the interaction between fibres and carrier fluid is modeled through an external boundary force method. Direct contact and lubrication force models for fibre-fibre interactions and fibre-wall interaction are used to allow for a full four-way interaction. The project also developed a new code (named SLILAB), using a hybrid parallel approach for the multi phase flow simulation.



Project leader: Gustav Amberg, Department of Mechanics, Royal Institute of Technology, Stockholm, Sweden

Collaborators: Minh Do-Quang, Department of Mechanics, Royal Institute of Technology, Stockholm, Sweden



The iso-surface of the second invariant $Q = 0.45$ of ∇u for (left) the case without fibres and (right) case with fibres. Comparison between the streamwise one-dimensional spectra of the streamwise velocity fluctuation of single phase flow and suspension flow at location $y^+ = 19$

Project Results

The fibres are introduced into the fully developed turbulent single-phase flow at time t_0 with an initial translational velocity and angular velocity equal to the fluid velocities found at the location of each fibre. Statistics were collected after the flow and suspension had reached a statically steady state. All cases were run in the same computational domain ($8 \times 2.28 \times 28$ in the streamwise, spanwise, and wall-normal directions, respectively) and same resolution $\Delta^+ = 2$. The volume fraction of fibres is $\nu_f = 0.11\%$ up to 0.44% and density ratio between fibre (ρ_f) and fluid (ρ_l) is $\rho_r = 1.0$ or 1.2 . The density ratio $\rho_r = 1.2$ is chosen to mimic cellulose fibres in water. In our model the gravity is not included. Therefore, the density ratio only influences inertial dynamics, and not fibre settling.

The newly developed SLILAB code will clearly benefit the whole community by enabling solutions for the four-ways coupling between fluid and nonspherical particles. It might also benefit the scientific computing community working with the hybrid method of MPI/OpenMP.

The result presented will clearly have a broad impact in the turbulence two phase flow community as the large number of resolved particles rise up on the demand of the statistics and the reality problems.

Currently, a new setup for higher Reynolds numbers is being tested with the new optimization hybrid MPI/OpenMP methods. With the development of the new method, we hope to soon be able to present a high-resolution result of the finite-size fibres in turbulent channel flow.

“The newly developed SLILAB code will clearly benefit the whole community by enabling solutions for the four-ways coupling between fluid and nonspherical particles.”

1. Do-Quang, M., Amberg, G., Brethouwer, G., Johansson, A. Simulation of finite-size fibres in turbulent channel flow, *Physical Review E*, **89**, 013006 (2014).
2. E. Gaburov, M. Do-Quang, L. Axner, OpenMP parallelization of Slilab code, *submitted to www.prace-ri.eu* (2014).

LIPOSIM: Large scale simulations of liposomes as drug carriers



Prof. Leif A. Eriksson

PRACE DECI 10th Call



DECI allocation

HPC Center PDC, Sweden

CG model of liposome and bilayer system (waters excluded for clarity)

Computer System Lindgren

Resource Awarded 8 750 000 DECI St. core-hours

Start Date May 2013

Allocation period 1 year

Research Field Materials Science

Abstract

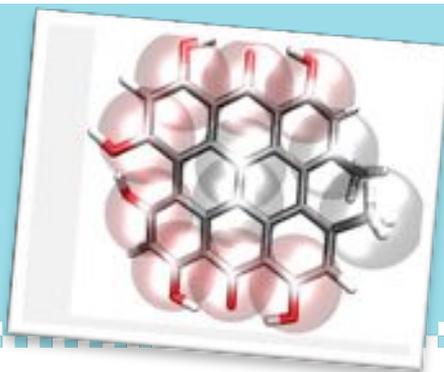
An attempt was made to use massively parallel computations in order to simulate drug delivery from drug-loaded liposomes into a cellular plasma membrane. The aim was to understand at a detailed atomistic level, how different lipid mixtures, drug concentrations and sizes of the liposome or micelle based carriers influence the ability of these to actually bring the drug molecules to their intended targets. Deeper insight into these processes will eventually allow researchers to design new molecules that better dissolve into and transfer between liposome and cell, or that are able to diffuse out of the liposome as response to small variations in the local environment.

Based on initial benchmark calculations, our aim was to perform the computations using more than 1,000 computer nodes in parallel, with each system corresponding to approximately 10,000,000 atoms. The work was carried out in collaboration between researchers at the universities of Stockholm and Gothenburg.



Project leader: Leif A. Eriksson, Department of Chemistry and Molecular Biology, University of Gothenburg, Sweden

Collaborators: Emma S.E. Eriksson, University of Gothenburg, Sweden / Joakim Jämbeck, Aatto Laaksonen and Alexander Lyubartsev, Stockholm University, Sweden



Model of atomistic and CG hypericin

Project Results

The project plan was to start from the point at which the liposome and the membrane have been equilibrated, where after the simulation would be continued by adding a weak force to push the liposome closer to the membrane, in order for the liposome to approach the membrane and to initiate the fusion process. The simulation would be set to run for 500 ns and generate the liposome at a distance of 0.5-1.0 nm from the membrane. At this point, four separate simulations without force would be performed, starting from different conformations from the final part of the previous simulation. These simulations would be 2.5-5.0 μ s each. If spontaneous fusion of the liposome with the membrane was observed in any of these simulations, two additional 2.5-5.0 μ s simulations would be performed to ensure that the fusion could be reproduced. The simulations would then be repeated using higher hypericin concentration in order to elucidate the effects of higher amounts of the drug. In addition a CG membrane with high cholesterol content will also be developed, and same type of simulations performed. These simulations would then be followed by umbrella sampling (US) simulations of the fusion process in order to generate reliable potential of mean force (PMF) data. The same simulations were also planned for the 'empty' system and using 5ALA loaded

liposomes. Of the above, a first benchmarking study of the full Liposome + membrane bilayer system was conducted, using up to 2500 cores. These simulations showed a very good scaling, and that using 1000 cores we could obtain approximately 500 ns simulation time per day. Smaller systems were also constructed, consisting of a bilayer fragment interacting with a bilayer fragment, in order to explore details of the very initial steps of the fusion process.

The simulations planned for, for which only the initial benchmarking was successfully performed, used the GROMACS programme combined with the MARTINI force field. Allocation was given on the 'Lindgren' Cray XE6 cluster at the center for parallel computing (PDC), KTH, Sweden, on which the software was already successfully implemented. No further programming, compilation or optimization was necessary.

Simulations of this magnitude would not be possible without the use of such facilities.

The benchmarking study, on up to 2500 cores, showed that these large-scale simulations are indeed possible, and scale very well.

“Simulations of this magnitude would not be possible without the use of such facilities.”

1. E.S.E. Eriksson and L.A. Eriksson, *J Chem Theory Comput*, **2011**, *7*, 560-574.
2. J.P.M. Jämbeck, E.S.E. Eriksson, A. Lyubartsev, A. Laaksonen and L.A. Eriksson, *J. Chem. Theory Comput.* **2014**, *10*, 5-13.

Interesting Statistics

Benefits of Swedish researchers from PRACE

The primary objectives for SNIC's participation in PRACE are to assist Swedish scientists to apply for access to and make efficient use of Europe's largest supercomputers (Tier-0) and the network of large national HPC systems (Tier-1).

Each call for access to PRACE Tier-0 and Tier-1 systems published by PRACE is distributed to all principal investigators (PIs) of large allocations on the SNIC compute resources. In addition, the largest users of the SNIC resources are approached directly to identify their interest in applying for access to the PRACE resources. Users that have the potential to become large users are approached as well.

In the period November 2011 - May 2015, Swedish researchers have received about 245 million CPU¹ hours in total on Tier-0 systems and about 100 million normalized CPU hours on Tier-1 systems. In the same period, Sweden committed about 90 million normalized CPU hours to PRACE. These numbers include only projects where Swedish researchers are the principal investigators (PIs) and do not consider projects where Swedish researchers are collaborators (co-PIs).

So far, eight applications with a Swedish project leader have been accepted for Tier-0 access. Successful applications with Swedish collaborators are not listed here.

PRACE TIER-0 REGULAR ACCESS WITH SWEDISH PROJECT LEADER

TIER-0 Call N (From-To)	PI	Discipline	University	Machine (Exec site, Country)	CPU hours (million)
Tier-0 Call 2 (2011/05 - 2012/05)	Arne Johansson	Mechanical Engineering	KTH	JUGENE	46
Tier-0 Call 4 (2012/05 - 2013/05)	Xue-Song Bai	Engineering and Energy	LU	CURIE TN	20
Tier-0 Call 5 (2012/11 - 2013/11)	Colin Jones	Climate	SMHI/SU	MareNostrum	38
Tier-0 Call 5 (2012/11 - 2013/11)	Garrelt Mellema	Astrophysics	SU	CURIE	22
Tier-0 Call 8 (2014/05 - 2015/05)	Xue-Song Bai	Engineering and Energy	LU	SuperMUC	26
Tier-0 Call 8 (2014/05 - 2015/05)	Johan Hoffman	Mechanical Engineering	KTH	HERMIT and SuperMUC	20
Tier-0 Call 8 (2014/05 - 2015/05)	Anatoly Belonoshko	Theoretical Physics	KTH	MareNostrum	50
Tier-0 Call 9 (2014/09 - 2015/09)	Garrelt Mellema	Astrophysics	SU	CURIE	19
Total (million CPU hours):					241

i) Note: this number is a raw sum and is not normalized

PRACE TIER-0 PREPARATORY ACCESS WITH SWEDISH PROJECT LEADER and CO-LEADER

Preparatory access is intended for testing and developing codes in order to prepare applications for PRACE Tier-0 project access.

The following types of Preparatory access are available:

- Preparatory access type A; Code scalability tests with maximum allocation period of two months
- Preparatory access type B; Code development and optimisation with maximum allocation period of six months
- Preparatory access type C; Code development and optimisation with the support of PRACE experts with maximum allocation period of six months

Tier-0 Prep Cut-off N	Date	Type of access	PI/co-PI	Name	Institution	Discipline	Machine (Exec site, Country)	CPU hours
Tier-0 Prep 4th	2011-05-01	A	Co-PI	Mellema Garrelt	SU	Astrophysics	CURIE	50000
				Axel Brandenburg, Piyali Chatterjee, Gustavo Guerrero, Dhruvaditya Mitra			CURIE	
Tier-0 Prep 4th	2011-05-02	C	Co-PI		Nordita	Astrophysics		200000
Tier-0 Prep 4th	2011-05-03	C	PI	Anders Lansner	KTH	Life Science	JUGENE	250000
Tier-0 Prep 8th	2012-03-01	A	Co-PI	Tobias Berg	ANSYS Sweden AB	Material	HERMIT	50000
Tier-0 Prep 8th	2012-03-01	B	PI	Sven Öberg	UmU	Material	CURIE and HERMIT	150000
Tier-0 Prep 10th	2012-09-01	B	PI	Chandan Basu	LiU	Computer science	CURIE	200000
				Axel Brandenburg, Jorn Warnecke			HERMIT	
Tier-0 Prep 11th	2012-12-01	A	Co-PI		Nordita	Astrophysics		50000
				Alexander Lyubartsev	SU	Material	HERMIT and JUQUEEN	150000
Tier-0 Prep 12th	2013-03-01	B	Co-PI	Jan Dufek	KTH	Energy	JUQUEEN	250000
Tier-0 Prep 12th	2013-03-01	C	Co-PI	Pär Strand	Chalmers	Plasma physics	JUQUEEN and SuperMUC, JUQUEEN and FERMI	500000
Tier-0 Prep 12th	2013-03-01	C	Co-PI	Rossen Apostolov	KTH	Life science	FERMI	500000
						Computer science	CURIE	
Tier-0 Prep 15th	2013-12-01	B	PI	Soon-Heum Ko	LiU	Mechanical Engineering	All Tier-0 systems	200000
Tier-0 Prep 15th	2013-12-01	B	PI	Philipp Schlatter	KTH			1100000
Tier-0 Prep 16th	2014-03-01	B	Co-PI	Jan Dufek	KTH	Energy	SuperMUC	250000
Total:								3900000

PRACE TIER-1 DECI PROJECTS WITH SWEDISH PROJECT LEADER

DECI N	Project	PI	Discipline	Institution	Exec site(s)	Allocation	
						DECI Std hours	CRAY XE6 hours
DECI7	SIVE-2	Lindahl, Erik	Bio Science	KTH	EPCC	6250000	5000000
DECI7	DiSMuN	Abrikosov, Igor	Material Science	LiU	PDC, SARA	3750000	3000000
DECI7	MUSIC	Djurfeldt, Mikael	Bio Science	KTH	IDRIS	231000	184800
DECI7	SPIESM	Colin Johns	Earth Science	SU	PDC	3750000	3000000
DECI8	CANONS	Pär Olsson	Material Science	KTH	CSCS	3125000	2500000
DECI8	MBIOMARK	Zilvinas Rinkevicius	Material Science	KTH	CSCS	1875000	1500000
DECI8	Pipeturb	Philipp Schlatter	Mechanical Engineering	KTH	CSC, EPCC	6250000	5000000
DECI8	Planetesim	Anders Johansen	Astro Science	LU	RZG, FZJ and ICHEC	6200054	4960043
DECI9	CoStAFuM	Olle Eriksson	Material Science	UU	NTNU, RZG	9687608	7750086
DECI9	DifVib	Abrikosov, Igor	Material Science	LiU	PDC, EPCC	6250000	5000000
DECI9	HydFoEn	Rajeev Ahuja	Material Science	UU	UHEM	2501125	2000900
DECI10	PLANETESIM-2	Anders Johansen	Astro Science	LU	FZJ	7500000	6000000
DECI10	DNSTF	Gustav Amberg	Mechanical Engineering	KTH	EPCC	8437500	6750000
DECI10	LipoSim	Leif A. Eriksson	Material Science	GU	PDC	8750000	7000000
DECI10	MEGAREACT	Kim Bolton	Material Science	HB	UIO	750000	600000
DECI11 (on-going)	FLOCS	Philipp Schlatter	Mechanical Engineering	KTH	EPCC	12500000	10000000
DECI11 (on-going)	GSTP	Hans Nordman	Plasma & Particle Physics	Chalmers	FZJ	5000000	4000000
DECI12 (on-going)	FENICS	Johan Hoffman	Mechanical Engineering	KTH	PDC	1250000	1000000
DECI12 on-going)	DNSTF2	Gustav Amberg	Mechanical Engineering	KTH	CSC	6250000	5000000
DECI12 on-going)	ParaWEM	Gunilla Efraimsson	Aerodynamics	KTH	EPCC	3750000	3000000
DECI12 on-going)	VFEH	Deliang Chen	Earth Science	GU	EPCC	500000	400000
DECI12 on-going)	EXODUS	Biplab Sanial	Material Science	UU	Cyfronet, Castorc	3750000	3000000
Total						100307287	74245830

Through the same PRACE calls Swedish researchers also received support from PRACE application experts (either locally or nationally) to improve their scientific software and prepare it for the next level future supercomputing systems. In the period November 2011 - May 2015 Swedish researchers received up to 45 months full-time support from PRACE HPC experts. This is a crucial investment for Swedish research and development to remain in tact with the rapid evolution of HPC technologies. The activities within PRACE helped to clearly identify the need for HPC knowledge in different scientific disciplines and highlighted the fact that Swedish researchers have a great need for assistance from HPC experts.

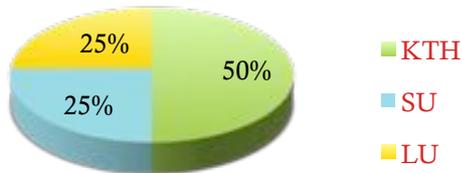
The interest from researchers in applying for access to PRACE resources depends on several factors:

1. Their interest in using resources that are of a scale larger (Tier-0) or a different architecture (Tier-1) than those that are available in Sweden.
2. The size of the allocations that are granted on the national systems: the smaller the allocations that are granted on the national level (for example relative to the request), the more researchers may be tempted to investigate possibilities for getting additional allocations elsewhere, for example through collaborators in other countries or by applying for access to PRACE resources.

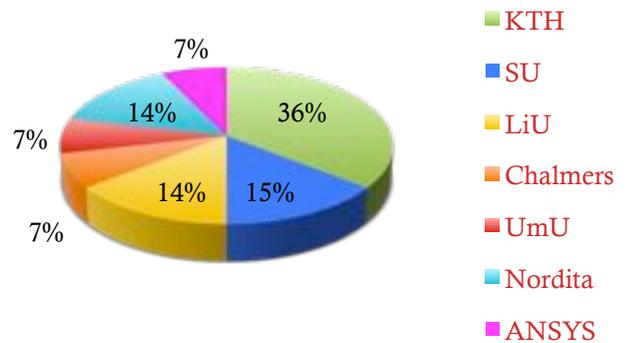
Finally, researchers also get interested to apply for access to PRACE resources when they see the possibility to get support from (local/national) application experts to help them prepare the software applications.

In Summary

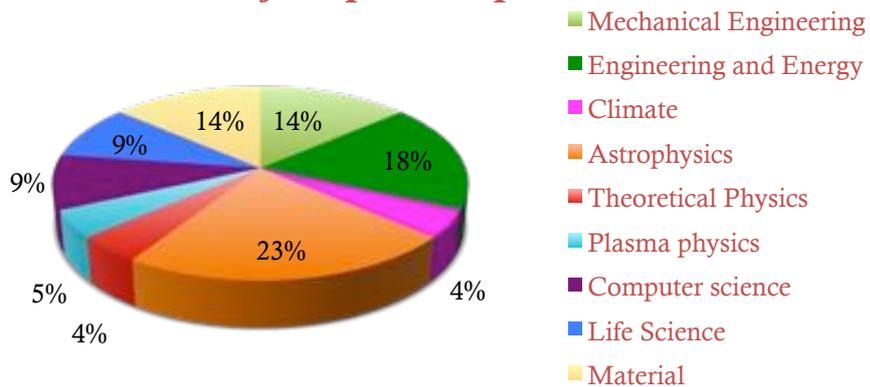
Awarded Number of Tier-0 Projects per University in %



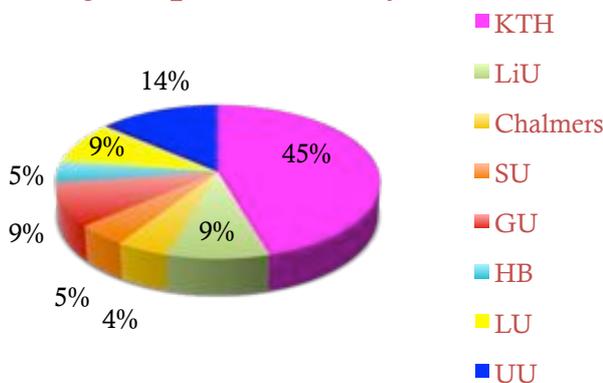
Awarded Number of Tier-0 Preparatory Projects per University in %



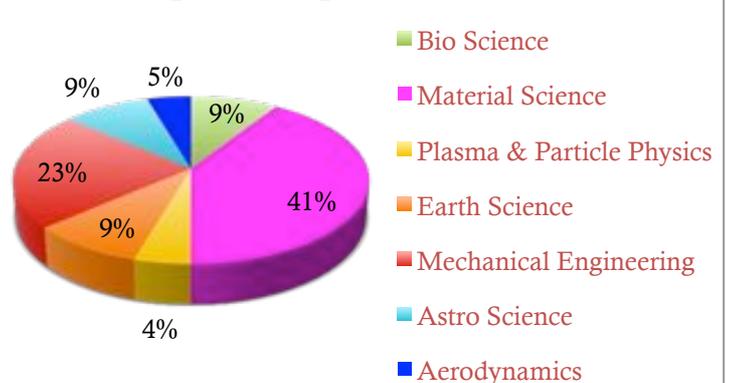
Awarded Number of Tier-0 & Preparatory Projects per Discipline in %



Awarded Number of DECI Projects per University in %



Awarded Number of DECI Projects per Discipline in %



In Summary

Achievements in Science: Six large allocations were granted on the PRACE Tier-0 resources for projects with Swedish Principle Investigators (PIs). In addition, there have been projects with Swedish collaborators that have been granted allocations on Tier-0 resources. 22 projects with Swedish PI were granted access to Tier-1 resources. These Tier-0 and Tier-1 projects not only provided Swedish scientists with access to more and different resources than are available nationally but also helped fostering and establishing collaboration between Swedish research groups and their European peers. (Many of the projects are collaborative in nature, involving researchers from across Europe.)

Achievements in HPC Collaboration: SNIC participated in the PRACE-1IP, PRACE-2IP and PRACE-3IP projects. The participation in these projects allowed staff at the participating SNIC centres to collaborate with other centres in Europe concerning the definition, study, development and deployment of HPC-relevant policy, applications, technologies and services. The PRACE projects have been very successful in creating a pool of resources and competence in which SNIC staff can participate and increase knowledge. (Such a pool is not available in Sweden or even the Nordic countries.) SNIC itself would not have initiated the service- and research-oriented activities to the level that they are carried out within the projects, primarily due to insufficient critical mass in staffing and funding.

Considerable knowledge has been obtained from establishing communication and collaboration between SNIC staff and staff at other data centres, from having access to a wide range of hardware architectures (e.g., for application scaling and for early access to new technologies), and from understanding HPC infrastructure in other countries (e.g., organization and implementation). This knowledge is of immediate use at several levels, e.g., (i) to the further development and structuring of the Swedish national HPC infrastructure, (ii) to individual SNIC centres and (iii) to individual staff members at the SNIC centres.

Achievements in providing Tier-1 services: The PRACE-xIP projects implement the Tier-1 service (also known as DECI). Sweden participates in the Tier-1 service by allocating ca. 10% of the available capacity on the Cray XE6 (Lindgren) at KTH to successful PRACE Tier-1 proposals. The Distributed European Computing Initiative (DECI) enables users to apply for access and use Tier-1 systems within PRACE. The Tier-1 service requires the deployment of the PRACE Common Production Environment and adequate user support.

SNIC participated in the first call for Tier-1 access that was organized by PRACE (DECI-7), which started November 2011, and has participated in DECI-7 to DECI-12.

So far, circa 15 whitepapers and 2 best practice guides were produced or contributed to by the participating SNIC centres. All centres have contributed to multiple deliverables. See for example:

<http://www.prace-ri.eu/white-papers>

<http://www.prace-ri.eu/Best-Practice-Guide-Cray-XE-XC-HTML>

<http://www.prace-ri.eu/Best-Practice-Guide-Intel-Xeon-Phi-HTML?lang=en>

<http://www.prace-ri.eu/ueabs>



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