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Research Infrastructures

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PRACE-2IP

PRACE Second Implementation Phase Project

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Final Report on Technical Support for DECI Projects

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[1] http://www.prace-ri.eu
[2] DECI PPR Tool: http://deci-peer-review.cines.fr/login
[3] DECI TTS: https://tts.prace-ri.eu/index.html
[4] http://www.prace-ri.eu/Best-Practice-Guides
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List of Acronyms and Abbreviations

AISBL	Association International Sans But Lucratif (legal form of the PRACE-RI)
AMD	Advanced Micro Devices
API	Application Programming Interface
BSC	Barcelona Supercomputing Center (Spain)
BSCW	Basic Support for Cooperative Work; a web based system that offers shared workspaces
CEA	Commissariat à l'Energie Atomique (represented in PRACE by GENCI, France)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
CINES	Centre Informatique National de l'Enseignement Supérieur (represented in PRACE by GENCI, France)
CPU	Central Processing Unit
CSC	Finnish IT Centre for Science (Finland)

CSCS	The Swiss National Supercomputing Centre (represented in PRACE by ETHZ, Switzerland)
CUDA	Compute Unified Device Architecture (NVIDIA)
DART	DECI Accounting Report Tool; a Java web-start application to retrieve accounting data from computing facilities
DECI	Distributed European Computing Initiative
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.
DNA	DeoxyriboNucleic Acid
DP	Double Precision, usually 64-bit floating point numbers
DPMDB	DECI Project Management Database; a web-based application to view and edit details of DECI proposals and projects
EC	European Community
EPCC	Edinburg Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)
ETHZ	Eidgenössische Technische Hochschule Zuerich, ETH Zurich (Switzerland)
FFT	Fast Fourier Transform
FP	Floating-Point
FPU	Floating-Point Unit
FZJ	Forschungszentrum Jülich (Germany)
GB	Giga (= 2^{30} ~ 10^{9}) Bytes (= 8 bits), also GByte
GCS	Gauss Centre for Supercomputing (Germany)
GENCI	Grand Equipement National de Calcul Intensif (France)
GNU	GNU's not Unix, a free OS
GPGPU	General Purpose GPU
GPU	Graphic Processing Unit
GRNET	Greek Research & Technology Network
HLRS	High Performance Computing Center Stuttgart
HP	Hewlett-Packard
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
IBM	Formerly known as International Business Machines
ICE	(SGI)
ICHEC	Irish Centre for High-End Computing (represented in PRACE by NUI Galway)
IDRIS	Institut du Développement et des Ressources en Informatique Scientifique (represented in PRACE by GENCI, France)
I/O	Input/Output
ISC	International Supercomputing Conference; European equivalent to the US based SC0x conference. Held annually in Germany.
JSC	Jülich Supercomputing Centre (FZJ, Germany)
KTH	Kungliga Tekniska Högskolan (represented in PRACE by SNIC, Sweden)
LQCD	Lattice QCD
LRZ	Leibniz Supercomputing Centre (Garching, Germany)
LU	Lund University, Sweden
MB	Mega (= 2^{20} ~ 10^{6}) Bytes (= 8 bits), also MByte
MB/s	Mega (= 10^{6}) Bytes (= 8 bits) per second, also MByte/s

MKL	Math Kernel Library (Intel)
MPI	Message Passing Interface
NCF	Netherlands Computing Facilities (the Netherlands)
NCSA	National Centre for Supercomputing Applications (Bulgaria)
NUI	National University of Ireland
NUMA	Non-Uniform Memory Access or Architecture
OpenMP	Open Multi-Processing
PCIe	Peripheral Component Interconnect express, also PCI-Express
PDC	Center for High Performance Computing, at KTH (represented in PRACE by SNIC, Sweden)
PI	Principal Investigator
PMO	Project Management Office (PRACE-2IP)
PPR	Project Proposal and Reporting
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE-1IP	First implementation phase of PRACE
PRACE-2IP	Second implementation phase of PRACE
PRACE-3IP	Third implementation phase of PRACE
PRACE-RI	PRACE Research Infrastructure
PSNC	Poznan Supercomputing and Networking Centre (Poland)
QCD	Quantum Chromodynamics
RZG	Rechenzentrum Garching (Garching Computing Centre, of the Max Planck Society, represented in PRACE by GCS, Germany)
SARA	Stichting Academisch Rekencentrum Amsterdam (Netherlands)
SE	Scientific Evaluation
SGI	Silicon Graphics, Inc.
SMP	Symmetric MultiProcessing
SNIC	Swedish National Infrastructure for Computing (Sweden)
SPH	Smoothed Particle Hydrodynamics
STFC	Science and Technology Facilities Council (represented in PRACE by EPSRC, United Kingdom)
SURFSara	Dutch national High Performance Computing & e-Science Support Center
TE	Technical Evaluation
Tier-0	HPC systems hosted by the PRACE RI; the largest European systems
Tier-1	National or topical HPC systems
Tier-2	Regional or campus HPC systems
UHeM	Istanbul Technical University National Center for High Performance Computing (=UYBHM)
UiO	Universitetet i Oslo (represented in PRACE by SIGMA, Norway)
UYBHM	Ulusal Yüksek Başarımlı Hesaplama Merkezi (The National Center for High Performance Computing, Turkey)
UPAT	University of Patras (Greece)
UV	Ultra Violet (SGI)
VSB-TUO	Vysoká škola báňská – Technická univerzita Ostrava (Technical University of Ostrava, Czech Republic)
WCSS	Wroclaw Centre for Networking and Supercomputing (Poland)
WP	Work Package

Executive Summary

This deliverable reports on the technical support provided for DECI (Distributed European Computing Initiative) projects by Task T7.2 of Work Package 7 (WP7) 'Scaling Applications for Tier-0 and Tier-1 Users' in the 2nd year of PRACE-2IP. There were four DECI calls in PRACE-2IP, as shown in the following table. The DECI-11 call has also been launched but implemented in PRACE-3IP. For each accepted DECI project, the resource allocation is one year, unless there was an agreed extension.

DECI Calls	Open Date	Closing Date	Allocation Started Date	Received Proposals	Accepted Projects
DECI-7 (pilot call)	2 May 2011	22 Jun 2011	1 Nov 2011	54	35
DECI-8	2 Nov 2011	10 Jan 2012	1 May 2012	49	33
DECI-9	17 Apr 2012	30 May 2012	1 Nov 2012	45	31
DECI-10	5 Nov 2012	14 Dec 2012	1 May 2013	85	37
DECI-11 (PRACE-3IP)	8 May 2013	10 Jun 2013	1 Nov 2013	119	N/A

Table 1: DECI calls in PRACE-2IP

In the 2nd year of PRACE-2IP, T7.2 continued the support for DECI-7 and DECI-8 projects until both the DECI phases ended. Technical Evaluations (TEs) were provided for the received DECI-9 and DECI-10 proposals and technical support has been provided since the accepted DECI-9 and DECI-10 projects started. By the end of PRACE-2IP, the DECI-9 and DECI-10 projects will be still on going and the DECI support will be continued in PRACE-3IP by subtask T7.1.B in PRACE-3IP.

In the 2nd year of PRACE-2IP, the technical support for DECI projects focused more on the application enabling support, rather than the general projects' progress tracking. The application enabling support was usually provided through 1-6 PMs, including code porting, performance profiling and analysis, optimisation, etc. T7.2 focused on the DECI enabling projects which required more than 1 PM enabling assistance, but also provided the technical support wherever needed by the DECI projects.

Around 20 HPC centers from 17 European countries are involved in T7.2. The task had monthly telcons and parallel sessions at Face-to-Face meetings for the progress tracking and discussions. T7.2 also worked in close collaboration with other PRACE-2IP work packages, especially Work Package 2 (WP2), for the whole DECI process and related work.

Task 7.2 evaluated a total of 233 Proposals and supported 136 projects.

1 Introduction

Task 7.2 'Applications support for DECI projects' is the task in Work Package 7 of PRACE-2IP, which was responsible to provide the technical support for DECI projects. In the 2nd year of PRACE-2IP, T7.2 continued the DECI support and mainly focused on the technical / enabling support for the accepted DECI projects. This deliverable summarised the work done by T7.2 in the 2nd year of PRACE-2IP.

Section 2 gives an overview introduction on the work done by T7.2 in the 2nd year of PRACE-2IP, including Technical Evaluations for the received DECI proposals (Section 2.1), technical support provided for the accepted DECI projects (Section 2.2), the collaborations between T7.2 and WP2 for DECI (Section 2.3), the coordination and progress tracking within T7.2 (Section 2.4), and the DECI support efforts hand-over from PRACE-2IP to PRACE-3IP (Section 2.5).

Section 3 gives further details about the technical support provided for the DECI-7 projects. The enabling reports are provided for a few of DECI-7 projects that required more than 1 PM enabling support. Section 4, Section 5 and Section 6 include the enabling reports for the DECI-8, DECI-9 and DECI-10 enabling projects.

A conclusion is given in Section 0. In Section 0 Annex, a brief report is provided for each DECI project in PRACE-2IP.

2 T7.2 Overview in the 2nd Year of PRACE-2IP

T7.2 continued the technical support for DECI in the 2nd year of PRACE-2IP. This section provides an overview introduction on the work done by T7.2 in M13-M24 of PRACE-2IP.

2.1 Technical Evaluation

T7.2 provided the technical input during the review process for the received DECI proposals. The Technical Evaluations (TEs) started as soon as possible after the DECI calls were closed and the TEs were usually completed within around 2 weeks. Each home site was responsible for the TEs on the received proposals from their own country. In the case that a proposal was from some country which was not involved in PRACE/DECI, a DECI partner site would agree with being the home site for the proposal and was responsible for its TE.

After the TEs, the received DECI proposals were then passed to WP2 for the Scientific Evaluations (SEs). T7.2 was also responsible to update the received proposals information in the DECI Process Management DataBase (DPMDB) for the future usage by WP2 and WP6. The system assignments were completed based on the TEs' results for the final accepted DECI projects.

In the 1st year of PRACE-2IP, T7.2 provided TEs to the DECI-7 and DECI-8 proposals. In the 2nd year of PRACE-2IP, T7.2 provided TEs to 45 received DECI-9 proposals and 85 received DECI-10 proposals. In PRACE-2IP, all TEs were completed using the standard TE form in word version. The online PPR tool [2] for DECI TEs was prepared in PRACE-2IP and has been used since DECI-11 TEs in the PRACE-3IP.

2.2 Technical Support for Accepted DECI Projects

In the 2nd year of PRACE-2IP, T7.2 provided the technical support to the DECI-7, DECI-8, DECI-9, and DECI-10 projects. The technical support by T7.2 mainly includes the following aspects:

2.2.1 *Assistance with system access and initial PI meetings*

At the starting stage of each DECI project, T7.2 helped the DECI users to get access to their assigned Tier-1 systems. The home sites arranged initial meetings with their PIs, to explain all necessary information to the DECI PIs and users, confirm the requirements from the DECI users, and provide assistance where needed. The initial meetings with PIs were face-to-face meetings, telcons, or video conferences, as agreed with the PIs.

The information to be introduced by the home sites at the initial meetings with PIs should mainly include the following aspects:

- Explains the X.509 certificate for users and provides assistance to apply for it.
- Explains the PRACE support system for DECI users (TTS) [3].
- Explains the PRACE Best Practice Guide [4] and PRACE User Documentation [5].
- Explains how to access the assigned Tier-1 systems.
- Explains the PRACE Common Production Environment (PCPE) [6].
- Explains how to obtain the CPU accounting information (DART) [7].
- Informs PIs the final reports and data collection after finalising the DECI projects.
- Reminds the enabling support from T7.2 to DECI users and confirms the efforts needed for the DECI project.

A guide for the DECI support workflow and TODO list for the initial PI meetings has been provided on the T7.2 Wiki page, which was generated and revised based on the 1st year's DECI support experience in PRACE-2IP.

2.2.2 *Application enabling support*

In the 2nd year of PRACE-2IP, T7.2 focused more on the application enabling support for the DECI projects which required porting or enabling assistance from PRACE experts for more than 1 PM efforts. Meanwhile, WP2 was responsible for the general DECI projects progress tracking. If there were any technical issues met, the queries should then be passed from WP2 to T7.2 to get support where needed.

The application enabling support by T7.2 mainly included porting code to the assigned Tier-1 systems, performance benchmarking and analysis, code development (e.g. GPU version implementation), and applications optimisation, etc. The enabling support was usually provided for 1-6 PMs as required in the original DECI proposals, or whenever needed during the DECI projects. Further details of DECI projects' enabling work are reported in the following Section 3.2, 4.2, 5.2 and 6.2. The general information of all DECI project in the 2nd year of PRACE-2IP can be found in the Annex in Section 0.

2.2.3 *Finishing DECI projects and outcomes*

A final report was expected from each PI after the DECI project completed. The final reports should report the work done within DECI, which may be publicised on PRACE webpages, Digest, or Newsletters. In general the PIs' reports were expected to be submitted within 3 months after the DECI projects finishing. In the case that some projects had agreed extensions at the end stage, their reports were expected by the same deadline with others.

When the DECI projects came to the end, the home site should remind the PIs to consume all the assigned resources on time and also remind that the PI's final report as well as any data collection should be completed within 3 months after their project's due date. The PIs' reports have been uploaded to PRACE BSCW after the collection by T7.2.

Besides the collection of final reports from DECI PIs, T7.2 also produced white papers for the DECI projects which required sufficient enabling work provided by T7.2. The white papers aim to introduce more technical details within the DECI projects and share experiences to benefit the DECI users and PRACE experts in the future. For DECI-7, two white papers have been published in July 2013 on the PRACE-RI web site [1] for project "ElmerIce" [8] and "Plank-LFI" [9]. For DECI-8, two white papers for projects "PLANETESIM" [10] and "NAHUJ" [11] have been prepared. The time of this writing undergo the PRACE internal review and approval process; they will be published in September 2013.

2.3 Collaboration with Other Work Packages

Besides providing the Technical Evaluations during the DECI proposal review process, T7.2 worked in close collaboration with other work packages, especially WP2, in the whole DECI process.

The DECI sessions at PRACE-2IP/PRACE-3IP All Hands Meeting in Paris (September 2012) discussed many aspects, including how to improve the collaboration interface between WP2 and T7.2. The following have been agreed and carried out during the 2nd year of PRACE-2IP.

2.3.1 *Technical Evaluations*

It was agreed after the discussion that TEs on the received DECI proposals should be still completed by T7.2. The completed TEs should then be passed to WP2 for the next step Scientific Evaluations (SEs).

2.3.2 *System Assignments*

It was agreed at the PRACE All Hands Meeting in Paris, that the efforts for the system assignments should be moved from WP2 to T7.2. The system assignments should be based on the TEs' results and comments, to assign the most suitable architectures to the accepted DECI projects where possible.

2.3.3 *Reduce Overlap between WP2 and T7.2*

To reduce the overlap of DECI projects management between WP2 and T7.2, it has been agreed that WP2 should be responsible for the general DECI progress tracking and T7.2 should focus on the technical support, i.e. the DECI projects which required more than 1 PM applications enabling support. T7.2 should be responsible for helping the DECI users with getting access to the assigned Tier-1 systems and the initial meetings with PIs at the starting stage of each DECI phase. WP2 should be responsible for the progress tracking of all the ongoing DECI projects. In the case that any issue raised, WP2 should then pass the questions to T7.2 for the technical support.

There was also a WP2/WP7 joint DECI session at the WP7 Face-to-Face meeting in Warsaw (April, 2013). Several topics were discussed by WP2 and T7.2 together, including the allocation scheduling policies across sites, the new submission and evaluation system (PPR tool), and the maintenance and improvement of existing DECI tools (e.g. DPMDB, DART, Workflow portal, etc.). The WP2/WP7 joint DECI session had a very productive discussion to improve the DECI work further. Similar joint DECI sessions are likely to be planned in the future WP7 Face-to-Face meetings.

2.4 Coordination and Progress Tracking

Around 20 HPC centers from 17 European countries are involved in T7.2. To track the progress and provide the opportunities for discussions within the task group, T7.2 had monthly telcons on every 3rd Friday of each month. Besides the monthly telcons, T7.2 also had two discussion sessions at WP7 Face-to-Face meetings in Montpellier (Oct, 2012) and in Warsaw (April, 2013) to review the task progress and discuss the next step work plans.

Several tools were used for the T7.2 work, including:

- BSCW-T7.2 folder: to keep all documents for T7.2 available for PRACE-2IP partners. There are certain folders used for the completed TE forms and the final PIs' reports.
- DPMDB: the database used for the DECI projects information storage and progress tracking. T7.2 was responsible to update the DECI projects information after TEs.
- T7.2 PRACE Wiki: the task internal wiki page where to provide useful information for the T7.2 group, e.g. the terminology within DECI support, task descriptions, work flow, guide for initial meetings with PIs, and certain list of DECI applications requiring GPUs, etc.
- TTS [3]: the query tickets system. DECI users are encouraged to submit queries to the TTS instead of sending to certain persons of DECI sites. This will help to get responses more efficiently and effectively.

2.5 DECI support in PRACE-2IP and PRACE-3IP

In the 2nd year of PRACE-2IP, PRACE-3IP has started in parallel. Both PRACE Implementation Phase projects have the DECI support activities, i.e. T7.2 in PRACE-2IP and T7.1.B in PRACE-3IP. T7.1.B in PRACE-3IP is the subtask which aims to continue providing the technical support for DECI projects after PRACE-2IP ends. To avoid the effort overlap between PRACE-2IP and PRACE-3IP, the following have been agreed and carried out in the 2nd year of PRACE-2IP.

2.5.1 *The starting time of T7.1.B in PRACE-3IP*

During July 2012 – July2013, the main DECI support were provided by T7.2 in PRACE-2IP. T7.1.B in PRACE-3IP will start after PRACE-2IP ends and continue the DECI support. However, to continue the DECI support smoothly from PRACE-2IP to PRACE-3IP, T7.1.B in PRACE-3IP has the joint F2F meetings and telcons with T7.2 in PRACE-2IP together in the 2nd year of PRACE-2IP.

2.5.2 *DECI support effort hand-over from PRACE-2IP to PRACE-3IP*

To avoid effort overlaps, it has been discussed and agreed at the WP7 Face-to-Face meetings in Montpellier (Oct, 2012) and in Warsaw (April, 2013), that the DECI support efforts should have a clear hand-over date to move from PRACE-2IP to PRACE-3IP. The hand-over date was agreed as 1 August 2013, i.e. the DECI support efforts should be counted into PRACE-2IP by the end of July 2013 and from 1 August 2013 all the DECI support efforts should be counted into PRACE-3IP.

Based on the timeline of DECI projects, DECI-7 and DECI-8 should be completed in PRACE-2IP and the support for DECI-9 and DECI-10 which has been started since PRACE-2IP will be continued in PRACE-3IP. All the support for DECI-11 will be counted into PRACE-3IP. The TEs for DECI-11 proposals have been completed in July 2013 by PRACE-3IP.

3 Technical Support for DECI-7 Projects

3.1 DECI-7 Overview

The DECI-7 call (pilot call) was launched before PRACE-2IP started, which was opened on 2 May 2011 and closed on 22 June 2011. 54 proposals were received and 35 proposals accepted. The accepted DECI-7 projects started from 1 November 2011 with duration of one year. Most DECI-7 projects ended at the end of October 2012, unless there were any agreed extensions. The major status of DECI-7 projects has been reported in the 1st year T7.2 deliverable, D7.2.1 "Technical Support for DECI Projects" [12], with many details. The following Section 3.2 mainly includes the updates and finalising of the DECI-7 enabling projects after the reporting in D7.2.1.

In the end of DECI-7, 34 projects completed their runs within the original schedule or within the agreed extensions. One project was cancelled on request from the project. 33 PIs have submitted their final reports and the DECI-7 final reports are available internally on BSCW. Brief reports for all DECI-7 projects are included in the Annex Section 8.1.

3.2 Applications Enabling for DECI-7 Projects (M13-M24)

The following table lists 10 DECI-7 projects which required more than 1 PM enabling support from T7.2. A brief description/update for each DECI-7 enabling project in the 2nd year of PRACE-2IP is given in this section as well.

Home site	Projects	Exec site	Enabling site	Architecture	Enabling
CINES	ElmerIce	SNIC-KTH	CSC	Lindgren (XE6 12C@2.1)	1-3 PMs
CSC	Planck-LFI	CSC	CSC	Louhi XT (XT5 DC@2.3)	1-3 PMs
HLRS	PHOTMAT	CINES, PSNC	PSNC	JADE-Harpertown (Intel Harpertown@3) + SGI UV1000 (Intel Westmere EX@2.67)	1-3 PMs
SNIC-KTH	DiSMuN	SNIC-KTH, SURFSara	SNIC-KTH	Huygens P6 (P6@4.7) + Lindgren (XE6 12C@2.1)	1-3 PMs
SNIC-KTH	MUSIC	IDRIS	IDRIS	BABEL (BGP@0.85)	1 PM
SNIC-KTH	SPIESM	SNIC-KTH	SNIC-KTH	Lindgren (XE6 12C@2.1)	1-3 PMs
RZG	ARTHUS-3	FZJ	RZG	JuRoPA (Intel Nehalem@2.93)	1-2 PMs
RZG	EUTERPE-4	FZJ	RZG	JuRoPA (Intel Nehalem@2.93)	1-2 PMs
RZG	LASIPROD	LRZ	RZG	SuperMig (Intel Westmere EX@2.4)	1-2 PMs
RZG	SMARC	LRZ	RZG	SuperMig (Intel Westmere EX@2.4)	1-2 PMs

Table 2: DECI-7 enabling projects

3.2.1 *ElmerIce*

Due to the DECI-7 time schedule, the major enabling work for ElmerIce has been done in the 1st year of PRACE-2IP. Please refer to D7.2.1 [12] for the detailed description. A white paper for this DECI-7 project has been produced to introduce the technical work done: *"Scaling and Performance Improvements in Elmer/Ice"* [8].

3.2.2 *Planck-LFI*

Due to the DECI-7 time schedule, the major enabling work for Planck-LFI has been done in the 1st year of PRACE-2IP. Please refer to D7.2.1 [12] for the detailed description. A white paper for this DECI-7 project has produced to introduce the technical work done: *"Performance evaluation and data transfer improvements for Planck-LFI data analysis"* [9].

3.2.3 *PHOTMAT*

Accounts and administrative data were prepared by HLRS. The enabling of the software required proper and binary-efficient compilation of the third party application NWCHEM. This was done at PSNC. The system environment there was tuned for specific needs. User level scripts were rewritten.

3.2.4 *DiSMuN*

During the 1st year of PRACE-2IP "Exciting" - one of the two intended codes - was ported to compile on SURFSara's IBM Power 6 machine, Huygens, and recommendations for better compiler flags were given. Accounts and administrative data were prepared by SNIC-KTH. The code ran afterwards fine on Huygens and SNIC-KTH's Cray XE6 machine Lindgren.

The other code needed further in-depth enabling work on optimization and scalability; however the PI changed his decision and the code was not used in the DiSMuN DECI-7 runs and thus not provided to PRACE experts. The enabling of this code is now taken care of within the related follow-up DECI-9 project DifVib.

3.2.5 *MUSIC*

MUSIC (http://software.incf.org/software/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. In this project, MUSIC was benchmarked and tested for its scalability up to hundreds of thousands of cores.

IBM does not support the dynamic gestion of processes, `MPI_COMM_SPAWN` and `MPI_COMM_SPAWN_MULTIPLE` on BG/P. That why the only way to do MPMD program is runs 2 MPI codes, who communicate in a one single `MPI_COMM_WORLD`. We worked first on a simple example to reproduce the problem, the modifications are to suppress arguments on the command line and the environment variable, replace that by a data file for the two applications.

We also made some test using the `MPI_COMM_SPLIT` function in VN, DUAL and SMP mode, in order to reorder the MPI processes of the two programs in a single one.

3.2.6 *SPIESM*

Due to the DECI-7 time schedule, the major enabling work for SPIESM has been done in the 1st year of PRACE-2IP. Please refer to D7.2.1 [12] for the detailed description. No white paper has been written due to the unique nature of part of the software and that the enabling work mainly focused on making the specific auto submit tool ready to install on the execution platform and not so much on optimisation or scalability.

3.2.7 *ARTHUS-3*

For using the computing architecture at the execution site, extensive profiling of the code and optimization of the scaling behaviour has been done with runs up to 12000 cores. Furthermore the I/O performance has been analyzed and optimized for the VERTEX code.

3.2.8 *EUTERPE-4*

After successful account setup and assistance in connecting to the execution site, no detailed enabling work was any more necessary. Some project-accompanying support has been done during the production phase.

3.2.9 *LASIPROD*

The required software packages Amber and NAMD for the large-scale MD simulations as well as Amber-Tools and VMD for pre- and post-processing and visualization were provided in advance on RZG platforms IBM Power6 and BlueGene/P in order to facilitate the preparation for production runs on the LRZ target machine SuperMIG. The users were assisted with running first test simulations with the MD packages. With this environment, the biological systems to be calculated could be equilibrated. Users were supported with the tests of a larger set of equilibration protocols to identify inaccurate starting models. Basic workflows for the processing chain preprocessing-simulation-postprocessing/visualization were prepared. For the production runs on the LRZ machine, support was provided with the usage of the simulation packages in a different environment.

3.2.10 *SMARC*

For the Tier-1 part of the SMARC project run at LRZ logistics support was given for the execution runs for a subset of parameters for the heating of the solar corona.

4 Technical Support for DECI-8 Projects

4.1 DECI-8 Overview

The DECI-8 call was launched on 2 November 2011 and closed on 10 January 2012. There were 49 proposal received and 33 of them were accepted. The accepted DECI-8 projects started from 1 May 2012 with a length of one year for the project time. Most of the DECI-8 projects completed by the end of April 2013 based on the original time schedule, and the rest DECI-8 projects have also ended with the agreed extensions. The DECI-8 projects' final reports from the PIs are being collection at the time of this deliverable writing. The collected reports are available internally in the BSCW. Brief reports for the DECI-8 projects are enclosed in the Annex Section 8.2.

4.2 Applications Enabling for DECI-8 Projects (M13-M24)

The following table lists 4 DECI-8 projects that required more than 1 PM enabling support. An enabling report for each of these DECI-8 enabling projects is given in this section.

Home site	Projects	Exec site	Enabling site	Architecture	Enabling
CINECA	NAHUJ	CINECA, WCSS	SURFSara	PLX (Intel Westmere EX@2.4) + WCSS Supernova (XEON X5650@2.67)	3-6 PMs
CINES	SMARTWING	ICHEC, WCSS	WCSS	Stokes (Intel Westmere EP@2.67) + WCSS Supernova (XEON X5650@2.67)	2 PMs
IDRIS	MOLED	CSC, ICHEC	CSC, ICHEC, IDRIS	Sisu (Sandy Bridge@2.6) + Stokes (Intel Westmere EP@2.67)	1-3 PMs
SNIC-KTH	PLANETESIM	FZJ, RZG, ICHEC	SNIC-KTH, SNIC-LU, SNIC-Chalmers, ICHEC, RZG	JuRoPA (Intel Nehalem@2.93) + RZG P6 (P6@4.7) / Hydra (Sandy Bridge@2.6) + Stokes (Intel Westmere EP@2.67)	3-6 PMs

Table 3: DECI-8 enabling projects

4.2.1 *NAHUJ*

The enabling work involved porting a legacy 2D fluid dynamics Fortran code to NVIDIA GPUs. Given the complexity of both the code and underlying (custom) numerical method, the natural choice was to use NVIDIA CUDA C to achieve the best performance. This decision is also supported by the maturity of both NVIDIA compiler and profiler, its undisputed power in (small) loop unrolling that the code benefits greatly, and support for C++ templates that were used to optimize inner loops when most of the compute time is spend. Furthermore, NVIDIA CUDA C is freely available for download.

The original code consisted of about a dozen of subroutines in which more than 99% of the runtime is spent, with two consuming ~80% while the remaining ~20% is spread among the rest of the subroutines. Due to Amdahl's law, the only option to achieve over 5x speed-up is to port *all* the hotspots to CUDA; otherwise the speed-up will be limited by the slowest subroutine. In this particular application, after all hotspots have been ported to CUDA the main limitation was due to data transfer over PCIe that had to be done every time-step.

We optimized this part by execution *all* hotspot functions on the GPU. This allowed us to eliminate bulk of the data transfer, and restrict PCIe copies only to the boundary data. This deemed to be necessary due to boundary data is set by a problem-dependent Fortran code, and it will be of great help to the user if the original Fortran code can be used in this step. We

were able to achieve substantial speed-up on NVIDIA K20 when compared to 16 Intel Sandy Bridge cores[1], which we show in Figure 1.

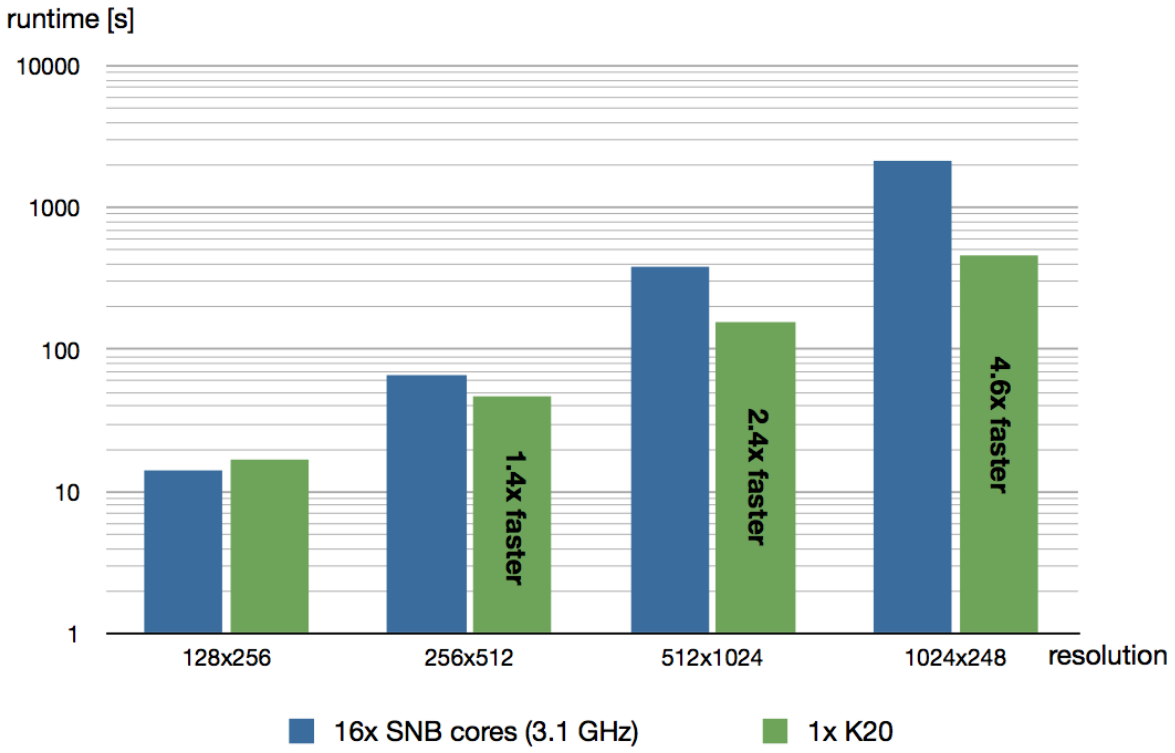

Figure 1: Runtime in seconds of the original code on dual socket (16 cores) Sandy Bridge E5-2687W CPU, and the CUDA port on a single K20s as a function of the problem size (horizontal axis).

A White paper has been produced for the DECI-8 project NAHUJ, which includes more technical details regarding the enabling work done for the project: *"DECI-8: Porting NAHUJ to CUDA"*[11].

4.2.2 *SMARTWING*

WCSS was the exec site for this project. While running jobs on our Supernova system users encountered problems with memory over-allocation and asked for more detailed support. Their application NSMB (Navier-Stokes Multi Block) was consuming too much memory per process, when using MPI, comparing to similar runs on other machines, and exiting due to exceeding the memory limit (23050MB/node), even for one MPI process per node. We performed the code analysis of provided source code, compiled the code and run tests. The source code analysis didn't reveal any obvious weakness or reasons for potential memory leaks. The MPI version of the code was finally compiled with the usage of Intel compiler v12.0.1.107 and OPENMPI v1.4.3 library for the MPI communication. The executable didn't work with the "`mpiexec`" command provided by this OPENMPI version, and we finally used a special version of "`mpiexec`", which also works properly with PBSPro, the queuing system on Supernova. Then we run the test jobs for small and regular test cases, provided by users, to check the correctness of the calculations. The application worked properly for both inputs with the acceptable amount of memory allocated. We tested one-node and multi-node MPI jobs. The memory requirements were quite stable: for the small test: 700MB per MPI process, for the normal test: 1100MB per MPI process. The project PI requested an extension

[1] The application was compiled with Intel Fortran Compiler 13.0.1, with the following flags "`-ipo -O3 -xavx`"

on Supernova, due to a maintenance brake within the DECI-8 allocation period. The access has been prolonged till 3th of July 2013.

4.2.3 *MOLED*

As home site, IDRIS helped MOLED users to access the CSC machines (LOUHI and then SISU) by using `gsissh` command.

From CSC, the applications that were used in the project were already installed on CSC's Cray XT. However, one of the applications (NWChem) didn't work in the simulation case studied. The software itself worked fine, but simulations persistently failed because of memory requirements. Despite a lot of effort, enabling for the Cray XT was stopped in December 2012. The decision was to wait until CSC's new Cray XC30 system is open for customer use in March 2013, and then move the project to there. On the Cray XC30, memory was no longer a problem, but a new problem turned up: NWChem did not yet support the Aries network of the Cray XC30. Therefore additional steps were needed in the build process. Help was obtained from CSCS and PNNL (USA) with this.

4.2.4 *PLANETESIM*

At the application stage, the PI has asked for enabling work regarding his use of Fourier transformation routines and for a modern parallel I/O strategy to be developed into the PENCIL CODE. For the Fourier transformations a replacement of the FFTPACK library with the more modern FFTW library was suggested. On the I/O side the originally deployed I/O strategy of every MPI task writing its own output file was to be change to a parallel I/O strategy. The later would lead to the results being more manageable when the PENCIL CODE is deployed on a large number of cores.

The project profiled the PENCIL CODE using the Scalasca tool using a project relevant benchmark. This work revealed a number of issues, including bottlenecks in the MPI communication, which were not anticipated before the work commenced. It was decided that an improvement of the MPI part of the Fourier transformation would also be attempted by the project.

In the following period the communication routine used by the Fourier transform was updated to use `MPI_Alltoall` within processor subgroups. When studied in isolation this showed a significant performance improvement over the original code. The transformation routines were updated to be able to also use complex data instead of only real data. The project further replaced the FFTPACK library with the FFTW and rearranged the code in the shearing routine to reduce the calls to the exponential. All of these steps showed improvement when the relevant code section implementing the `selfpotential` was studied in isolation.

When studying the performance of the entire application it turned out that the transposition routine using `MPI_Alltoall` would, for reasons still to be understood, damage the performance of other parts of the application, such that the overall performance was poorer. This was observed for two different compilers. However, reverting to the original communication pattern of the transposition routine, modifying the code to transpose complex data and reducing the synchronization resulted in an even larger speed-up of the calculation of the `selfpotential`. Furthermore this would not damage the performance of the other parts of the code. The combined efforts of this part of the project lead to an overall performance improvement of about 8% for the entire application. This work has been publicised to the PENCIL CODE community at their developer meeting in Lund in June 2013.

Further enabling work has been provided to introduce MPI-IO into the PENCIL CODE. This work aims to improve the usability of the code, in particular when deploying a larger number of MPI tasks.

A White paper has been produced as well for the DECI-8 project PLANETESIM, which includes more technical details regarding the enabling work on the parallel Fourier transforms: *"PLANETESIM: Fourier transformations in the Pencil Code"*[10].

5 Technical Support for DECI-9 Projects

5.1 DECI-9 Overview

The DECI-9 call was launched on 17 April 2012 and closed on 30 May 2012. There were 45 proposals received and 31 proposals were accepted. The accepted DECI-9 projects started from 1 November 2012 with a length of one year for the project time, i.e. the due date for the DECI-9 projects will be 31 October 2013. As PRACE-2IP will end on August 2013, the DECI support for DECI-9 projects will be continued in PRACE-3IP by task T7.1.B since 1 August 2013.

Brief reports for the DECI-9 projects are enclosed in the Annex Section 8.3.

5.2 Applications Enabling for DECI-9 Projects

The following table lists 7 DECI-9 projects that required more than 1 PM enabling support in their original proposals. A brief update for each DECI-9 enabling project is given in this section.

Home site	Projects	Exec site	Enabling site	Architecture	Enabling
CSC	Planck-LFI2	CSC	CSC	Sisu (Sandy Bridge@2.6) + Louhi XT (XT5 DC@2.3)	1-3 PMs
EPCC	ESM4OED	EPCC	-	HeCToR XE6 (XE6 16C@2.3)	1-2 PMs
FZJ	TB-Drugs-In_silico	CINECA	CINECA	PLX (Intel Westmere EX@2.4)	1-3 PMs
ICHEC	SPH-WEC	CSCS, NCSA	-	Rosa (XT5 CSCS) + EA ECNIS (BGP@0.85)	1-3 PMs
NCSA	AIMD-PAF	EPCC	NCSA	ICE-Advance (BGQ)	1-2 PMs
SNIC-KTH	DifVib	EPCC, SNIC-KTH	SNIC-KTH	ICE-Advance (BGQ) + Lindgren (XE6 12C@2.1)	6 PMs
GRNET (UPAT)	SPSC	FZJ	GRNET (UPAT)	JuRoPA (Intel Nehalem@2.93)	6 PMs

Table 4: DECI-9 enabling projects

5.2.1 *Planck-LFI2*

There were three points that required a larger amount of support. First, in October 2012, one of the applications (CosmoMC) was configured to use the GSL library. It took some time to realise that none of the GSL versions available on Louhi were compatible with the compiler

that was in use (Intel). The solution was to install a custom version of GSL in the user's application directory.

Second, in December 2012, it turned out that the newest version of CosmoMC required a newer version of the Intel compiler than was available. The solution was to move CosmoMC simulations to the new Cray XC30 once it was available. However, it turned out that CosmoMC cannot be run in hybrid MPI–OpenMP mode. A workaround solution was developed by CSC and Cray, but performance is still not sufficient. MPI–OpenMP computations can be run, though.

Third, in May 2013 one of the applications (LevelS) started to fail although it worked fine in February of the same year. Lot of effort was used to spot the error, first by CSC and later by Cray. The cause of the problem was finally simple: the application was not started with the parallel launcher *aprun*, but with the `"system ()"` command on the compute node. In such a case, the application must be compiled in a different way than it is usually done (see Annex).

5.2.2 *ESM4OED*

As this was an industrial project, where users were not necessarily familiar with the way in which supercomputing facilities are set up, special care was taken to ensure the users were able to work within the PRACE environment. The execution machine, HECToR, was selected specifically because HECToR and EPCC staff have specific expertise in handling industrial projects and also because access to HECToR can be gained without the need for grid certificates which can be difficult for users from industry to obtain. Once the users had obtained their accounts, a telephone meeting was set up where EPCC staff described in detail how the execution environment was set up and examples of scripts used to run the VASP executables on HECToR were provided. Progress was monitored throughout the project life-cycle and the project appears to have been successful so far as a number of publications are forthcoming and the team have submitted a proposal to DECI-11.

5.2.3 *TB-Drugs-In_silico*

Enabling work for compiling the applications and for the establishment of the workflow was envisaged. The home site FZJ and the enabling site CINECA held a phone-conference with the project to discuss the strategies. It turned out that no major enabling was necessary. The project set up its workflow with no additional support from PRACE. Also compiling support for Amber and AUTODOCK was requested by the project; however, both applications were already provided by CINECA staff on the execution-system.

5.2.4 *SPH-WEC*

Although a minimal amount of enabling support was requested for this project, in practice, no actual enabling support was required so far. Support of a non-technical nature was required to transfer time from NCSA to CSCS due to surprisingly poor performance of the application on the BG/Q at NCSA.

5.2.5 *AIMD-PAF*

CP2K software has been compiled for IBM Blue Gene/Q platform. Taking into consideration that CP2K does not provide makefile for the mentioned architecture, work had to be done to solve this problem. The proper IBM Blue Gene/Q XLF90 compiler has been set and linker

options have been selected adequately. The result was CP2K executable able to work in either in MPI or in hybrid MPI/OpenMP mode.

5.2.6 *DifVib*

It was decided right from the start on the two experts best suited to work with the enabling of this project which was considered a logical continuation of the DECI-7 project DiSMuN. The experts were therefore already present at the initial meeting with the PI and their accounts were created as well. Actual enabling work and work plan on enabling the TDEP (Temperature Dependent Effective Potential) code were discussed in several follow-up meetings, some of them being physical.

Although the maximum amount of enabling support was requested for this project, the PI was very secretive on parts of the code which is still under development, which in turn made it difficult for the enabling experts to start with the actual enabling in a speedy way. Thus not the full amount of the initially requested enabling could possibly be delivered. Furthermore the PI also involved further experts partly outside of PRACE to improve the performance of the overall run time in different ways by tuning the usage of the used VASP subroutine.

5.2.7 *SPSC*

For the KMC simulations we have generated a FORTRAN code that has been parallelized via MPI. Using the modules (parastation/mpi2-intel-5.0.26-1) by the local host we have benchmarked our code and we are obtaining almost linear scaling up to 512 processors. We have performed 4 production runs (512 cores, 24h), at different experimental conditions, generating 4 samples with average film thickness of ≈50nm. We increased the number of used processors in the KMC model when modeling systems of larger size, with thickness larger than 100nm and reached the 1024 cores mark. For the second stage we modified the open-source MD simulation program LAMMPS so as to include the Si-H interactions and we asked the local host to install it on the Supercomputer. Since we are simulating large systems (system size> 1.000.000 atoms) the simulations scale very good, obtaining almost linear scaling up to 1024 cores. Using the modified LAMMPS version we have employed MD simulation at the two larger samples of total duration 2ns. This corresponds at 8 runs of 512 cores with duration of 24h in each run. As soon as the resulting surfaces obtain local equilibrium we back-maped to the KMC model the resulting structures so as to further grow the films at 100nm. For the simulations of P3HT we have generated initial structures of high molecular weight for both crystalline and amorphous phase. We are currently finishing the last production runs on the maximum possible system size.

6 Technical Support for DECI-10 Projects

6.1 DECI-10 Overview

The DECI-10 call was launched on 5 November 2012 and closed on 14 December 2012. There were 85 proposal received and 37 of them were accepted. The accepted DECI-10 projects started from 1 May 2013 with a length of 1 year for the project time, i.e. the due date for the DECI-10 projects will be 30 April 2014. The DECI support for DECI-10 projects will be continued in PRACE-3IP by task T7.1.B as of 1 August 2013.

Brief reports for the DECI-10 projects are enclosed in the Annex Section 8.4.

6.2 Applications Enabling for DECI-10 Projects

The following table lists 6 DECI-10 projects that required more than 1 PM enabling support in their original proposals. A brief update for each DECI-10 enabling project is given in this section.

Home site	Projects	Exec site	Enabling site	Architecture	Enabling
CINECA	ERPP	CYFRONET	-	Zeus BigMem (AMD 6276@2.3)	1-3 PMs
FZJ	LargeRB2013	EPCC	-	ICE-Advance (BGQ)	1-3 PMs
ICHEC	APOP20X3	PSNC	-	Cane (Intel Harpertown@2.5)	1-3 PMs
ICHEC	waveclim	CSCS	-	Rosa (XT5 CSCS)	1-3 PMs
SNIC-KTH	DNSTF	EPCC	SURFSara	HeCToR XE6 (XE6 16C@2.3)	2 PMs
RZG	HYDRAD	VSB-TUO	RZG	Anselm (E5-2665-8@2.4)	1-3 PMs

Table 5: DECI-10 enabling projects

6.2.1 *ERPP*

By the time of the deliverable writing, the account for this project has been created for the DECI users and the project is expected to start soon.

6.2.2 *LargeRB2013*

Technically the project has been set-up, but the work on the code itself and production runs will start in September. The enabling requirements will be discussed with the PI, for this a F2F meeting with the PI is planned for mid of September.

6.2.3 *APOP20X3*

Little enabling work is required for this project. Any enabling that may be needed will revolve around compiling of the application.

6.2.4 *waveclim*

Little enabling work is expected to be required as part of this project. If required, enabling support will largely involve ICHEC staff porting and optimising the codebase to the ROSA system at CSCS. If required, this work is expected to be carried out in parallel with production runs assuming a stable and reasonably well performing version is available at an early stage. If necessary, optimization of the MPI and OpenMP sections of the code may be explored to incrementally improve performance. The research group can provide support to this effort by evaluating the validity of results.

6.2.5 *DNSTF*

Administrative and account set-up work was done by the PRACE home site at SNIC-KTH.

During the initial meeting the PI was informed on the possibility and details of available enabling help by PRACE experts. It was discussed that enabling of part of the SLILAB code which is based on the Palabos library package would be of interest in a later stage of the project. After clarifying the detailed desired enabling work together with DNSTF and SNIC-KTH tried first to find interested experts within Sweden.

The enabling work is centered on studying two different aspects:

The first part is concentrated on optimizing the SCLILAB code and improving its MPI OpenMP hybrid parallelization on different system architectures. This would also include simplifying the surface contact tracking for the case of rigid fibres by using the relative geometry of fibres to track the contact between them.

The second part would be to contribute to the multi-layer grid refinement method used to simulate the turbulent channel flow in 3D by adding a new parallel output function which is writing multi-grid data into a paraview compatible format (the Palabos output function is still serial) and by evaluating which of the different interpolation schemes should be preferred.

SURFSara has now volunteered to take over the enabling work and will start by familiarizing with the Palabos library.

6.2.6 *HYDRAD*

The (first-time PRACE) user was assisted with obtaining a certificate from his local RA and with using the certificate for authentication and authorization. The simulation code "nsCouette" was ported by RZG to the platform provided by the execution site. Makefiles and batch scripts were adapted to the VSB software stack, using Intel compilers, MKL and MPI, FFTW3 and parallel HDF5. Together with VSB staff a problem in the installation procedure of the parallel HDF5 library was identified and fixed (see below) which prevented linking hybrid codes (introduced with Intel MPI 4.1.0). Test programs on the VSB cluster were executed in order to ensure proper pinning of MPI tasks and OpenMP threads in the pbs batch environment. This is known in general to be crucial for getting adequate performance for hybrid MPI/OpenMP codes. The performance of the simulation code was assessed by performing a strong-scaling study and by comparing the absolute performance numbers with benchmarks on other systems (RZG cluster *Hydra*). The scalability on nsCouette, which is ultimately limited by the performance of `MPI_Alltoall` could be further improved by selecting a non-default algorithm in the Intel MPI implementation at runtime. Performance on the VSB cluster was eventually found to be within expectations (taking into account differences in Interconnect and CPU).

The parallel HDF5 library is usually linked with the MPI-compiler wrappers which, for Intel MPI leads to a dependency on the plain MPI runtime library (libmpi), or on its multithreaded version (libmpi_mt). Starting with version 4.1.0 of the Intel MPI library, this causes a conflict when trying to link a multithreaded code with the plain-MPI variant of the HDF5 library, or vice versa. Together with Intel, RZG has worked out a patch for the HDF5 installation procedure which simply accounts for using the plain linker (instead of the MPI wrapper) for building HDF5. This makes a *single* HDF5 installation compatible with both, plain MPI and hybrid (MPI + threads) codes.

7 Conclusion

In the 2nd year of PRACE-2IP, task T7.2 continued providing technical support for DECI. Technical Evaluations (TEs) were provided to DECI-9 and DECI-10 for 130 proposals in total. The technical support was provided to all the ongoing DECI projects, including the accepted DECI projects for DECI-7, DECI-8, DECI-9 and DECI-10. A total of 136 projects received support. To improve the collaboration interface between WP2 and task T7.2 and to reduce the effort overlap, it has been agreed and carried out in the 2nd year of PRACE-2IP that T7.2 focused mainly on the applications enabling support for the DECI projects which required more than 1 PM enabling support from PRACE experts. WP2 kept tracking the general DECI projects progress and passed the support requirements to T7.2 whenever the needs were raised.

In general, T7.2 completed the DECI technical support as planned, thanks to the great effort of all the DECI sites. As DECI-9 and DECI-10 projects will continue after the PRACE-2IP ends, it has been agreed that T7.1.B of PRACE-3IP will continue supporting DECI-9 and DECI-10 as of 1 August 2013. Joint telcons facilitated the smooth transition.

8 Annex

A brief report for each DECI project in the 2nd year of PRACE-2IP is given in this Annex section. These brief reports are contributed from the DECI home sites and mainly include the basic information about each project, its status, the support provided for the project, and how encountered difficulties were resolved.

8.1 Summary of Technical Support for DECI-7 Projects (M13-M24)

Project Acronym: BlackHoles
Accepted by DECI Call: DECI-7
PRACE Home site: BSC
PRACE Execution site: PSNC
PRACE Enabling sites: none
PRACE Architectures: SGI UV1000
Start enabling: -
Start production: 1-Jan-2012
Project status: Completed
Brief description of project: Black holes dynamics in metric theories of gravity
Types of support work undertaken: Account management, compilation advice on PSNC.
Difficulties encountered and solution: Some unstabilities with the machine at PSNC.

Project Acronym: CatDesign
Accepted by DECI Call: DECI-7
PRACE Home site: BSC
PRACE Execution site: LRZ, PSNC
PRACE Enabling sites: none
PRACE Architectures: Intel cluster, SGI UV1000
Start enabling: -
Start production: 1-Nov-2011
Project status: Completed
Brief description of project: A study of hydrogen properties in order to produce an efficient fuel.
Types of support work undertaken: Account management, compilation of VASP.
Difficulties encountered and solution: Some unstabilities with the machine at PSNC.

Project Acronym: MAESTRO
Accepted by DECI Call: DECI-7
PRACE Home site: CINECA
PRACE Execution site: IDRIS
PRACE Enabling sites: IDRIS
PRACE Architectures: BG/P
Start enabling: 1-Nov-2011
Start production: 1-Apr-2012
Project status: completed
Brief description of project: Study of the stability of the accretion-ejection process and of the jet initial propagation to the onset of non-axisymmetric modes of instability.
Types of support work undertaken: Account creation, scaling tests.
Difficulties encountered and solution: None.

Project Acronym: MIXTUDI

Accepted by DECI Call: DECI-7
PRACE Home site: CINECA
PRACE Execution site: CINECA, FZJ
PRACE Enabling sites: CINECA, FZJ
PRACE Architectures: IBM Power6, Intel Cluster
Start enabling: 1-Nov-2011
Start production: 1-Jan-2012
Project status: completed
Brief description of project: Study of mixing in a fully developed turbulent channel flow.
Types of support work undertaken: Account creation, compilation advice on Cineca Power6.
Difficulties encountered and solution: None.

Project Acronym: PETAHUB
Accepted by DECI Call: DECI-7
PRACE Home site: CINECA
PRACE Execution site: NCSA, SNIC-KTH
PRACE Enabling sites: NCSA, SNIC-KTH
PRACE Architectures: BG/P, CRAY XE6 (Lindgren)
Start enabling: 1-Nov-2011
Start production: 1-May -2012
Project status: completed
Brief description of project: Simulation and Phase diagram of the Hubbard model by quantum Monte Carlo and Petaflop supercomputers.
Types of support work undertaken: Account creation, porting on CRAY.
Difficulties encountered and solution: None.

Project Acronym: SCW
Accepted by DECI Call: DECI-7
PRACE Home site: CINECA
PRACE Execution site: LRZ
PRACE Enabling sites: CINECA, LRZ
PRACE Architectures: Intel Cluster (SuperMig, SuperMuc).
Start enabling: 1-Nov-2011
Start production: 1-Dec-2011
Project status: completed
Brief description of project: Behaviour of supercritical water by means of ab initio Molecular Dynamics simulations.
Types of support work undertaken: Account creation. Performance and scaling analysis of CP2K code on SuperMig.
Difficulties encountered and solution: Initial analysis of the CP2K code on SuperMig demonstrated poorer than expected performance and parallel scaling. In fact, compared with runs using identical input on Cineca's PLX cluster, a hardware architecture similar to that of SuperMig, the maximum performance of PLX was about twice that of SuperMIG and using a third of the cores. In addition, the program gave segmentation faults for some inputs. These problems were resolved by contacting the developers and upgrading the program version on SuperMIG.

Project Acronym: ElmerIce
Accepted by DECI Call: DECI-7
PRACE Home site: CINES

PRACE Execution site: SNIC-KTH
PRACE Enabling sites: CSC
PRACE Architectures: Lindgren
Start enabling: November 2011
Start production: November 2011
Project status: Completed
Brief description of project: Simulation of ice sheets and their impact on sea level rise.
Types of support work undertaken: Implementation of a new block preconditioned solver in the Elmer/Ice code.
Difficulties encountered and solution: None.

Project Acronym: NUWCLAY
Accepted by DECI Call: DECI-7
PRACE Home site: CINES
PRACE Execution site: CINECA
PRACE Enabling sites: none
PRACE Architectures: PLX
Start enabling: none
Start production: June 2012
Project status: Completed
Brief description of project: The research team performed detailed quantitative studies of the energetic, structural, and dynamic aspects of different interaction mechanisms between radionuclides, organic matter, and clay particles in relation to the study of nuclear waste management.
Types of support work undertaken: Porting
Difficulties encountered and solution: Use of grid security certificates has caused difficulties in accessing CINECA.

Project Acronym: Planck-LFI
Accepted by DECI Call: DECI-7
PRACE Home site: CSC
PRACE Execution site: CSC
PRACE Enabling sites: CSC
PRACE Architectures: Cray XT
Start enabling: November 2011
Start production: December 2011
Project status: Completed
Brief description of project: Planck is a satellite mission of the European Space Agency to map the structure of the cosmic microwave background in unprecedented detail. The cosmic microwave background is radiation from the Big Bang, and it shows us the structure of the early universe. This DECI project supported the Planck mission by running the most compute-intensive tasks related to the analysis chain of data from the Low Frequency Instrument (LFI). The project was a follow-up of the DEISA Science Community Support Initiative project Planck. It was a large collaboration of European and American research groups. The number of users was over 20 and they used many different applications. They also transferred a lot of data between CSC and NERSC (USA).
Types of support work undertaken: None in the 2nd year of PRACE-2IP
Difficulties encountered and solution: None

Project Acronym: TanGrin
Accepted by DECI Call: DECI-7

PRACE Home site: CSC
PRACE Execution site: EPCC
PRACE Enabling sites: CSC
PRACE Architectures: Cray XE6
Start enabling: November 2011
Start production: January 2012
Project status: Completed
Brief description of project: This project used the Gromacs molecular dynamics simulation package to unravel how the conformation of the integrin-bound talin depends on its interactions with lipids in a membrane.
Types of support work undertaken: None in the 2nd year of PRACE-2IP
Difficulties encountered and solution: None

Project Acronym: HELIXKINETICS
Accepted by DECI Call: DECI-7
PRACE Home site: EPCC
PRACE Execution site: FZJ, ICHEC
PRACE Enabling sites: EPCC, FZJ, ICHEC
PRACE Architectures: Intel cluster, SGI cluster
Start enabling: 01/11/11
Start production: 01/11/11
Project status: Completed
Brief description of project: This project aims to test the validity of the theoretical models of helix-coil equilibrium and kinetics and determine optimal parameters for such models and to analyse experimental data directly, without needing to invoke a phenomenological model and to investigate whether simulations can explain the differences between the results of different experimental measurements.
Types of support work undertaken: All enabling work had been reported in the previous reporting period.
Difficulties encountered and solution: None.

Project Acronym: HIFLY
Accepted by DECI Call: DECI-7
PRACE Home site: EPCC
PRACE Execution site: EPCC, PSNC
PRACE Enabling sites: EPCC, PSNC
PRACE Architectures: Cray XE6
Start enabling: 01/11/11
Start production: 01/11/11
Project status: Completed
Brief description of project: The aim of this project is the direct numerical simulation of flows occurring in insect and bio-inspired micro-air-vehicle flight.
Types of support work undertaken: All enabling work had been reported in the previous reporting period.
Difficulties encountered and solution: None.

Project Acronym: HYDROGEN-ILs
Accepted by DECI Call: DECI-7
PRACE Home site: EPCC
PRACE Execution site: EPCC, SNIC-KTH

PRACE Enabling sites: EPCC, SNIC-KTH
PRACE Architectures: Cray XE6
Start enabling: 01/11/11
Start production: 01/11/11
Project status: Completed
Brief description of project: This project aims at a microscopic-level understanding of a Ru-catalyzed reaction affording the production of H2 from formic acid in ionic liquids, which is of prime interest in the framework of sustainable energy supply. High-level molecular dynamics simulations will allow the team to explain the key solvation effects occurring in this system and will provide detailed mechanistic information. The results will be of fundamental interest for the understanding of chemical reactivity in ionic solvents and will also be beneficial to experimentalists for optimizing catalytic systems.
Types of support work undertaken: All enabling work had been reported in the previous reporting period.
Difficulties encountered and solution: None.

Project Acronym: HIGHQ2FF
Accepted by DECI Call: DECI-7
PRACE Home site: FZJ
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: -
PRACE Architectures: Lindgren
Start enabling: -
Start production: Nov-11
Project status: Completed
Brief description of project: The nucleon, the hadronic state which makes up most of the observable mass in the universe, has been extensively studied both theoretically as well as experimentally. The internal structure of hadrons is studied by measuring form factors and generalized parton distributions, which can be associated to the charge and magnetization distributions as well as the momentum distribution of quarks and gluons. There have been many studies of these fundamental quantities using state-of-the-art simulations of Quantum Chromodynamics (QCD), the theory of the strong interactions. However, these calculations have been almost entirely restricted to momentum transfers (Q2) up to about 2 GeV2. This is due to the fact that one takes numerically the Fourier transform, which for large momenta becomes very noisy making calculations of the form factors at higher momentum transfers prohibitively expensive. In this project a variation method which has been shown to improve the statistical accuracy of form factors at high Q^2 has been applied.
Types of support work undertaken: The project has been supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ has been in contact with the project over run-time to monitor the status. The final report has been collected after project-end.
Difficulties encountered and solution: No problems occurred.

Project Acronym: NR-NSNS-BHNS
Accepted by DECI Call: DECI-7
PRACE Home site: FZJ
PRACE Execution site: CSC
PRACE Enabling sites: -
PRACE Architectures: Louhi XT
Start enabling: -

Start production: Nov-11
Project status: Completed
Brief description of project: The goal of this project has been to compute gravitational waves (GWs) from the inspiral and collision of binaries involving neutron stars in Einstein's theory of General Relativity (GR). It has become possible to simulate several inspiral orbits and the merger and post-merger phase of compact binaries using the methods of Numerical Relativity (NR) on high performance parallel computers.
These simulations are of interest for the theoretical and technical challenges they represent but more importantly for their use in the larger context of GW detection. In support of the emerging field of GW astronomy, the project intends to compute highly accurate waveforms to investigate specific aspects of the most relevant astrophysical sources. The scientific objective of this proposal is to characterize the GW emission from the quasi-circular inspiral and merger of two binary systems: mixed binary (black hole-neutron star) systems / unequal-mass binary neutron stars.
Types of support work undertaken: The project has been supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ has been in contact with the project over run-time to monitor the status. The final report has been collected after project-end.
Difficulties encountered and solution: No problems occurred.

Project Acronym: DIAVIB
Accepted by DECI Call: DECI-7
PRACE Home site: HLRS
PRACE Execution site: CINECA, SURFSara
PRACE Enabling sites: none
PRACE Architectures: CNE-SP6 (P6@4.7), Huygens P6 (P6@4.7)
Start enabling: -
Start production: Feb 2012
Project status: Completed
Brief description of project: Low dimensional semiconductor systems exhibit several favourable properties that are not present in their bulk counterpart, eg. the optical gap of nanocrystals can be tuned with the charateristic size, however in many cases the size and composition is not exactly known. Recent developments allow the size and shape selected preparation of small diamond nanocrystals (diamondoids). These small diamondlike carbon cages can be considered as building blocks of larger nanodiamonds that have been extensively applied in biological studies where the optical properties are of crucial importance. Theoretical studies can significantly contribute to the underlying mechanisms of the excitation process.

The structure of small diamondoids is known exactly and their absorption spectra have been measured in gas phase close to room temperature. Recently, we have calculated the absorption spectrum by time-dependent density functional theory (TDDFT) with applying a hybrid density functional in the kernel where the hybrid functional was semi-empirical in nature. Later, we also applied a parameter-free quasiparticle correction (GW-method) and the static electron-hole correlation was taken into account by Bethe-Salpeter equation (BSE-method). All these calculations were carried out with frozen coordinates. These results may not even be valid at 0 K due to intrinsic zero-point vibration of atoms. It is well known for example, that in bulk diamond, a zero point renormalization of 0.4 eV occurs for the band gap, thus a direct comparison with the experiment is not straightforward. We found that optical gaps tended to be consequently larger both in TD-DFT and even more in GW+BSE calculations than the measured ones. Since C-C and C-H bonds have strong vibration modes a strong electron-

phonon coupling may shift the onset of absorption significantly that may explain the discrepancy between the experimental and simulation data.

By taking into account the electron-phonon interaction, we will be able to calculate the temperature dependent absorption spectrum close to the optical gap of small nanodiamonds by a parameter-free BSE method. These calculations would reveal how the absorption peaks can shift and broaden as function of the temperature where the spectra were recorded. In that way, direct comparison between the experiment and full ab-initio theory will be possible and it can be considered as a 'horseshoe' test of this methodology, which up to now has been applied mainly to periodic systems. The calculation of temperature dependent absorption spectra with the ab-initio BSE method is extremely demanding. Harnessing the computational capacity of supercomputers allows the usage of the very advanced many-body perturbation theory to real problems with the capability to compare results with experimental findings and previous theoretical results.

Types of support work undertaken: Accounts and administrative data were prepared by HLRS. Assistance in porting the code to Huygens machine was given by SURFSara.
Difficulties encountered and solution: Problems to get certificates for logins and unforeseen problems with the application program owned by the investigators caused some delay to start production. Because of a planned shutdown for replacement by a new machine the system at CINECA could be used till end of May only. These issues caused some additional administrative overhead.

Project Acronym: PHOTMAT
Accepted by DECI Call: DECI-7
PRACE Home site: HLRS
PRACE Execution site: CINES, PSNC
PRACE Enabling sites: none
PRACE Architectures: JADE-Harpertown (Intel Harpertown@3) + SGI UV1000 (Intel Westmere EX@2.67)
Start enabling: -
Start production: December 2011
Project status: Completed
Brief description of project: The project involves the design of fullerene and M- dithiolene-based materials, where M=Ni, Pd etc, for photonic applications. The key parameters for such a design are the nonlinear optical (NLO) properties. The increasing demand for faster data processing, storage and distribution can only be fulfilled by ongoing miniaturisation of the basic electronic devices. The traditional silicon-based technologies used nowadays are approaching intrinsic limits in this respect, and new approaches are needed. Photonic technology, where light is used as information carrier instead of electrons, is considered to offer the answer. An important step towards this goal is the development of new photonic materials with large NLO properties by employing nano-derivatives. Thus, the basic concept on which the project is based, involves the design of novel derivatives for photonic applications, employing fullerenes and metal-dithiolenes as the main building blocks and the solution of several methodological problems, which are of current interest in this area and which are instrumental for the computation of reliable L&NLO properties of the compounds.
Types of support work undertaken: Accounts and administrative data were prepared by HLRS. The enabling of the software required proper and binary-efficient compilation of the third party application NWCHEM. This was done at PSNC. The system environment there was tuned for specific needs. User level scripts were rewritten.
Difficulties encountered and solution: Because of unforeseen technical problems the investigators had serious difficulties to get their programs running at PSNC.

This required a serious amount of additional efforts by HLRS to discuss the problems and find solutions. The project was moved to the cluster architecture instead of SMP SGI, as originally allocated at PSNC. With PSNC agreement, the project has been granted the cluster access until March 2013.

Project Acronym: ViRonSAMs
Accepted by DECI Call: DECI-7
PRACE Home site: HLRS initially and then CSCS
PRACE Execution site: CINECA, CINES
PRACE Enabling sites: none.
PRACE Architectures: iDataPLEX, SGI Altix 8200 ICE
Start enabling: -
Start production: 1 May 2011
Project status: Completed - waiting for the report
Brief description of project: The main scientific question this project aimed to answer was what happens to a virus when it is placed on a surface or alternatively what is the mechanism of virus inactivation on a surface.
Types of support work undertaken: none.
Difficulties encountered and solution: none.

Project Acronym: LGICTAMD
Accepted by DECI Call: DECI-7
PRACE Home site: ICHEC
PRACE Execution site: ICHEC (3M)
PRACE Enabling sites: ICHEC
PRACE Architectures: x86 cluster (Stokes)
Start enabling: project creation date
Start production: 12/2011
Project status: Completed
Brief description of project: MD (user modified NAMD) simulations to study ligand-gated ion-channels.
Types of support work undertaken: To get variant of NAMD working on x86. To evaluate on a GPU-based platform.
Difficulties encountered and solution: Performance was not impressive due to immaturity of GPU port. The x86 version of the application scaled well.

Project Acronym: NANOBIO-2
Accepted by DECI Call: DECI-7
PRACE Home site: ICHEC
PRACE Execution site: CINES (40k) & HLRS (1.96M)
PRACE Enabling sites: no enabling site
PRACE Architectures: x86, (SGI), x86 (Cray)
Start enabling: N/A
Start production: 4/2012
Project status: Completed
Brief description of project: Classical MD simulations with CP2K, LAMMPs, NAMD and Quantum Espresso of the process of biomolecules binding onto metal surfaces.
Types of support work undertaken: Code compilation
Difficulties encountered and solution: Project was successful. All time was burned at HLRS. PI was slow to burn time. Got a Tier-0 allocation at the same time, which took priority. HLRS were asked to allow for an extension, which they kindly granted.

Project Acronym: PICKH
Accepted by DECI Call: DECI-7
PRACE Home site: IDRIS
PRACE Execution site: CINECA
PRACE Enabling sites: CINECA, IDRIS
PRACE Architectures: IBM PLX, IBM BG/Q
Start enabling: 01/12
Start production: 02/12
Project status: Completed
Brief description of project: The interaction between the solar wind and the Earth's magnetosphere is a rich and complex system. From a theoretical point of view, it is a natural laboratory for plasma physics for which in-situ observations are available. From a practical point of view, it is of primary importance for the understanding of Sun-Earth interactions and its implications in term of space weather.

At low latitude, the velocity shear between the magnetosheath and magnetosphere plasma is unstable to the Kelvin-Helmholtz instability. This instability is at first order a fluid instability. However, (i) the magnetosheath and magnetosphere plasma are collision less and (ii) the nonlinear evolution of the Kelvin-Helmholtz instability self-consistently generates gradients at kinetic scales (ion gyro-radius, ion skin depth). That is why a kinetic description of this instability is necessary to fully understand its nonlinear evolution.

2D-3V kinetic plasma simulations of the magnetized Kelvin-Helmholtz instability with application to the Earth magnetopause were performed. The goal is to understand the implications of a kinetic description of this instability.

The Vlasov-Maxwell system is solved through the PIC implicit moment method, which allows studying plasma kinetic effects without the intrinsic limitations of the traditional (explicit) PIC method in terms of spatial resolution. Among the different phenomena of interest, collision less magnetic reconnection spontaneously develops during the non linear evolution of a vortex chain generated by the development of the Kelvin-Helmholtz instability. This local mechanism leads to a global change in the magnetic topology at large scales which is of fundamental importance in understanding the transport properties of the low latitude magnetosphere system.

The project represents today a major challenge in computational plasma physics to be tackled only by means of last generation computers.

Goals:

1. Investigate optimization techniques for Particle-In-Cell implicit moment algorithm to create a high performant implicit PIC code

2. Production runs in 2D-3V configuration for a major cross-scale problem in space plasma research to better understand Sun-Earth interactions.

Types of support work undertaken:
- Code porting to BG architecture.
- Code HDF5 I/O modified and updated to the latest version of HDF5.
- Optimization: filtering and time stepping.
- Kinetic initializations of a magnetized shear flow.
- Two-fluid simulations in preparation of full kinetic simulations.
- Magnetopause challenge: Benchmarking the magnetized Kelvin-Helmholtz instability.
- Using kinetic models to identify the relevant closure in fluid models.
- Kinetic modeling of the nonlinear evolution of the Kelvin-Helmholtz instability.

Difficulties encountered and solution:
- Quite long to obtain the PRACE certificate as the PI was French post-doctoral researcher at K.U. Leuven, Belgium, at the beginning of the project.
- The transition from SP6 to the BG/Q has been eased by using the IBM BG/P (Babel) at IDRIS.

Project Acronym: WESF
Accepted by DECI Call: DECI-7
PRACE Home site: IDRIS
PRACE Execution site: CSC (Louhi XT), RZG (Genius)
PRACE Enabling sites: IDRIS
PRACE Architectures: Cray, IBM BG/P
Start enabling: 11/11
Start production: 01/12
Project status: Completed
Brief description of project: Humidified Gas Turbines promise a significant increase in efficiency compared to the conventional, dry gas turbine cycle. In single cycle applications, efficiencies up to 60% are possible with humidified turbines. Additionally, the steam effectively inhibits the formation of NOx emissions and also allows for operating the gas turbine on biofuels. In order to achieve the high efficiencies, large amounts of steam have to be injected into the combustion chamber. This poses a challenge to the combustor design, since the steam significantly affects the flame stability, and so far, humid gas turbines have usually been investigated with moderate degrees of humidity not higher than 15% to 20%. In the current study, the combustion process is investigated at ultra-wet conditions with steam levels up to 50%.

In this context, Direct Numerical Simulations of two dimensional premixed flames are computed at wet conditions with detailed chemistry. Fundamental combustion properties like turbulent flame speeds, flame stretch and emissions are extracted from these simulations for various temperatures, fuel compositions, degrees of humidity and overall equivalence ratios. The results are compared to new experimental data for prismatic flames. The measurements are conducted on a new rectangular slot burner, using advanced laser diagnostics to gain insight into the flow field, the species concentrations and the temperature distribution. Additional simulations of 2D and 3D stretched flames are also performed with a simplified chemistry model in order to assess the influence of local flame stretch and flame curvature on the measurement results.

This project is conducted in collaboration with the European Advanced Grant GREENEST at the Chair of Experimental Fluid Dynamics at the Technische Universität Berlin, in which a practicle combustor prototype for operation at ultra-wet conditions will be developed during the next 5 years. In the current study WESF, a fundamental understanding of the combustion process at high steam contents will be gained, which is of direct interest for future research on wet combustion. Additionally, the results will provide the required knowledge for further CFD simulations of practical gas turbine combustors.

Types of support work undertaken:
Difficulties encountered and solution:
- Quite long to obtain the PRACE certificate as the PI was French post-doctoral researcher at TU Berlin, Germany.
- Only the cpu hours allocated on the IBM BG/P of RZG have been used because the portability from the RZG to the CSC platforms was not convenient.

Project Acronym: CASiMIR

Accepted by DECI Call: DECI-7
PRACE Home site: LRZ
PRACE Execution site: SURFSara
PRACE Enabling sites: SURFSara
PRACE Architectures: P6@4.7
Start enabling: 2011-10-27
Start production: 2011-11-01
Project status: Completed
Brief description of project: The project "Chemistry of the Atmosphere Simulated with an Earth System Model for the Interpretation of Satellite based Remote sensing observations (CASiMIR)" aims at an improved understanding of the physical and chemical processes, which determine the chemical state of the Earth atmosphere. Particular regions of interest are the polar upper troposphere and stratosphere. Here, the occurrence of polar stratospheric clouds (PSCs) and the heterogeneous chemistry (e.g., chlorine activation) on their particle surfaces are important processes responsible for the spring-time ozone depletion (Antarctic ozone-hole). Despite their importance, these processes are still not understood in detail. New data from satellite based remote sensing instruments promise additional insight in comparison to simulations with state-of-the-art atmospheric chemistry models, which represent the current knowledge about the underlying processes. A direct comparison of observations from satellite with results from model simulations, in particular of short-term and (in time and space) highly variable phenomena, such as PSCs, is, however, not straightforward. The ECHAM/MESSy Atmospheric Chemistry (EMAC) general circulation model has therefore been equipped with a new diagnostic capability: For instruments on sun-synchronous orbiters, the highest possible model data coverage, suitable for point-to-point comparison between satellite observations and model results, is achieved at the lowest possible output storage requirements. This new technique is applied in a series of EMAC model simulations for process studies revealing and assessing the gaps in the current understanding of the chemistry and dynamics in the polar upper troposphere and stratosphere. The simulations include sensitivity studies on the PSC forming process and a simulation with a finer model grid-resolution to optimally represent the horizontal gradients of short-lived, highly variable constituents. The results of the analyses will feed back to the further model development. The project, as detailed process study with a model of high complexity, is ambitious in terms of computational requirements and in particular in terms of data intensity, pushing the usage of resources, which are only available in a computational grid like PRACE, to the limits
Types of support work undertaken: general technical support
Difficulties encountered and solution: none.

Project Acronym: DisMuN
Accepted by DECI Call: DECI-7
PRACE Home site: SNIC-KTH
PRACE Enabling sites: SNIC-KTH, SURFSara
PRACE Execution site: SURFSara, SNIC-KTH
PRACE Architectures: IBM Power6, Cray XE6
Start enabling: 11/11
Start production: 11/11 (at SNIC-KTH), 03/12 (at SURFSara)
Project status: Completed (80% at SNIC-KTH, 41% at SURFSara)
Brief description of project: This project is aimed at investigating the diffusion processes and spectroscopic properties of multicomponent nitrides using the most fundamental quantum mechanical equations of physics. Since the mixed systems form disordered solid solutions when grown as thin films the stochastic distribution of e. g. Ti and Al atoms in the crystals must be carefully considered which adds a huge complexity and computational challenge to

this project. To investigate atomic diffusion in these materials electronic structure codes are used to calculate the energy barriers needed to be overcome by diffusing species, both inside bulk materials and on top of crystal surfaces. The different local chemical environments in the solid solutions will be studied using a large number of parallel calculations of different paths inside, and on top of, alloy supercells. In order to accurately interpret experimental spectroscopical measurements of nanostructured multicomponent nitrides state-of-the-art modeling scheme will be applied for these properties: the Bethe-Salpeter equation. In this methodology the intricate quantum mechanics of the spectroscopical process is modelled far more accurate then with standard density functional theory methods. Using a clever parallel procedure these difficult equations will be solved to give a solid ground in the understanding of the nanostructure of multicomponent nitrides in collaboration with experimental work.
Types of support work undertaken: During the PRACE Tier-1 Training Workshop in Amsterdam (29 – 30 November 2011) SARA had a hands-on session with the PI of DiSMuN in which SARA assisted the PI in compiling his code "Exciting" on SARA's IBM Power6 machine, Huygens. SARA also provided the PI with some tips on which compiler flags to use for optimizing his code. Accounts were also created by SNIC-KTH and project started its production runs on Cray XE6 machine, Lindgren.
Difficulties encountered and solution: One of the codes needed engaged enabling work; however the PI changed his mind and didn't provide the code to be worked on. The enabling of this code is now instead taken care of within the related follow-up DECI-9 project DifVib.
There were some difficulties with the overlap of persons in the LDAP when DisMuN was still active and DifVib was about to start. Those problems were reported in the TTS and discussed in PRACE operations meetings.

Project Acronym: MUSIC
Accepted by DECI Call: DECI-7
PRACE Home site: SNIC-KTH
PRACE Execution site: IDRIS
PRACE Enabling sites: IDRIS
PRACE Architectures: IBM BG/P
Start enabling: 01/01/2012
Start production: 01/03/2012
Project status: Completed
Brief description of project: MUSIC (http://software.incf.org/software/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. In this project, we will benchmark MUSIC and test its scalability up to hundreds of thousands of cores.
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. A better understanding of neuronal processing may also contribute to computer science and engineering by suggesting novel algorithms and architectures for fault tolerant and energy efficient computing. Simulations of increasingly larger network models are rapidly developing. In principle, we have, already today, the computational capability to simulate significant fractions of the mammalian cortex.
Neuronal network models have been formulated for a great diversity of different simulation tools. The reuse of such models is hampered by the lack of interoperability due to the multitude of languages and simulators used. Also, reimplementation of one model in other software is in practice both time consuming and error prone. Interoperability can be facilitated in several ways. One approach is to provide a model specification in some standardized format which can be understood by many simulation tools. Another approach is to allow different simulation tools to communicate data on-line. The MUSIC project was initiated by the INCF (International Neuroinformatics Coordinating Facility; http://www.incf.org) as a result of the 1st INCF Workshop on Large Scale Modeling of the Nervous System in order to support on-line communication between neuronal simulators and address the interoperability and reusability problems.

Types of support work undertaken:

- IDRIS :

IBM does not support the dynamic gestion of processes, MPI_COMM_SPAWN and MPI_COMM_SPAWN_MULTIPLE on BG/P. That why the only way to do MPMD program is runs 2 MPI codes, who communicate in a one single MPI_COMM_WORLD. We works first on a simple example to reproduce the problem, the modifications are to suppress arguments on the command line and the environment variable, replace that by a data file for the 2 applications. We also made some test using the MPI_COMM_SPLIT function in VN, DUAL and SMP mode, in order ro reorder the MPI processes of the 2 programs in a single one.

Difficulties encountered and solution:

- SNIC-KTH:

One of the users was Russian, so the opening of an account for users that are not citizen of a European Union country requires the authorization of the CNRS Defense Officer. The user sent us all the forms and the account could be created.
Another problem was that the code is a MPMD application and is using the DCMF communication layer on BG/P. That means a none-portability on future other machine like IBM BG/Q.
IBM does not support MPI_COMM_SPAWN and MPI_COMM_SPAWN_MULTIPLE, the dynamic management of MPI processes is not implemented. That why is the only way to do MPMD program running by executing two different codes in one MPI_COMM_WORLD. IDRIS had also a problem with the environment variable passed to each program: it is the same name with different value. The user had to change this in his application, it works only if the name of the environment variable is different for each codes.
The MPMD runs well in SMP mode: the two codes are in a same big MPI_COMM_WORLD which IDRIS split in two sub-communicators, one sub-communicator per application. The SMP mode assumes to have the same number of processes in each sub-communicator; it is not the case in DUAL or VN mode.
The code had basically to be completely rewritten and was only in a running shape late in the project. IDRIS was friendly enough to provide the possibility to have an extension so enough meaningful results could still be produced.

Project Acronym: SIVE-2
Accepted by DECI Call: DECI-7

PRACE Home site: SNIC-KTH
PRACE Execution site: EPCC
PRACE Enabling sites: SNIC-KTH, EPCC
PRACE Architectures: Cray XE6
Start enabling: 11/11
Start production: 11/11
Project status: Completed (113%)
Brief description of project: The group has been developing high-performance simulation methods to analyse membrane fusion and 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, particularly planning to examine how influenza-catalysed fusion is similar to or differs from protein-free fusion.
Types of support work undertaken: Setting up accounts and installing certificates.
Difficulties encountered and solution: It was not really clear to the PI when the allocation expired or how many hours were exactly remaining. EPCC was allowing for a two-week extension so some final runs could be completed.

Project Acronym: SPIESM
Accepted by DECI Call: DECI-7
PRACE Home site: SNIC-KTH
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: SNIC-KTH
PRACE Architectures: Cray XE6
Start enabling: 11/11
Start production: 11/11
Project status: Completed (111%)
Brief description of project: This project contributes to the `Reducing Uncertainty in global Climate Simulations using a Seamless climate prediction system (RUCSS)` project funded by the Spanish Science and Investigation Ministry. In RUCSS the aim is the testing the seamless approach (Palmer et al., 2008) for climate modelling with the EC-Earth Earth System Model (ESM) to constrain the sources of uncertainty in both short-term climate prediction and climate-change projections by increasing the understanding of the climate system. In this project, detailed analysis of climate simulations with different time horizons were carried out using similar metrics to better understand the development of the systematic errors in EC-Earth with the hope of reducing the risk of overconfidence in both climate predictions and long-term projections.
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.
Types of support work undertaken: Accounts created, requested software installed, implemented a configuration of the model with high ocean resolutionwhich was not available at the time of starting the simulations.
Difficulties encountered and solution: There were some difficulties with the installation of the auto submit tool that is specific for this code, however SNIC-KTH successfully managed to install it.

Project Acronym: SIMONA
Accepted by DECI Call: DECI-7
PRACE Home site: PSNC
PRACE Execution site: IDRIS, PSNC, SURFSara
PRACE Enabling sites: PSNC, SURFSara
PRACE Architectures: IBM Power6, IBM BG/P, SGI UV1000

Start enabling: March 2012
Start production: March 2012
Project status: Completed
Brief description of project: Understanding of the underlying microscopic mechanisms is of fundamental importance for bottom-up synthesis of molecules and design of molecular devices. It is crucial to answer unambiguously if the models based on simplified physical assumptions explain the observed phenomena and may predict new expected properties for the properly chosen parameters. The latter can be easier accomplished in a computer experiment than in laboratory.
In the project completed the best quality and up-to-date quantum models are analysed numerically, using the reliable and accurate simulation methods as well as modern high performance computing infrastructure and programming paradigms. The computational tasks and expected results go beyond state-of-the-art in the important field of molecular nanomagnets and are expected to inspire the new syntheses and experiments.
Types of support work undertaken: In the second year PSNC helped with the compilation and tuning of the third party CP2K application on AMD architecture.
Difficulties encountered and solution: none

Project Acronym: ARTHUS-3
Accepted by DECI Call: DECI-7
PRACE Home site: RZG
PRACE Execution site: FZJ
PRACE Enabling sites: RZG
PRACE Architectures: Xeon X5570@2.93
Start enabling: 11/2011
Start production: 01/2012
Project status: Completed
Brief description of project: *Applying Radiation Hydrodynamics to understand Core Collapse supernovae.* Supernova explosions of massive stars are among the most powerful cosmic events. This project runs some of the currently most advanced simulations of the supernova evolution of massive stars and treat the neutrino-matter interactions in the supernova core with unprecedented accuracy. This project moves towards three-dimensional models of core collapse supernovae with detailed neutrino-transport, supplemented by faster two-dimensional simulations to explore variations in parameter space.
Types of support work undertaken: For using the computing architecture at the execution site, extensive profiling of the code and optimization of the scaling behaviour has been done with runs up to 12000 cores. Furthermore the I/O performance has been analyzed and optimized for the VERTEX code.
Difficulties encountered and solution: No difficulties beside the normal enabling work.

Project Acronym: EUTERPE-4
Accepted by DECI Call: DECI-7
PRACE Home site: RZG
PRACE Execution site: FZJ
PRACE Enabling sites: RZG
PRACE Architectures: Xeon X5570
Start enabling: 11/2011
Start production: 12/2011
Project status: Completed
Brief description of project: *Global electromagnetic gyrokinetic simulation in 3D equilibria*. Gyrokinetics as a first principle based theory is well suited to describe the relevant

physics of plasma microinstabilities and related turbulence. An established and flexible method for solving the gyrokinetic system of equations is the simulation via the particle-in-cell (PIC) Monte-Carlo method. For this purpose the EUTERPE code has been developed which solves the gyrokinetic equation globally in arbitrary stellarator geometry including kinetic electrons, and electromagnetic perturbations. The full kinetic treatment of the electrons allows the investigation of trapped electron effects (e.g. TEM) and the inclusion of electromagnetic effects establishes the connection to magnetohydrodynamics (MHD). By using a third species the destabilisation of MHD modes (e.g. TAE, HAE) can also be studied. These developments will make EUTERPE the first code worldwide that is able to simulate global gyrokinetic electromagnetic instabilities in three dimensions.
Types of support work undertaken: After successful account setup and assistance in connecting to the execution site, no detailed enabling work was any more necessary. Some project-accompanying support has been done during the production phase.
Difficulties encountered and solution: No difficulties encountered.

Project Acronym: LASIPROD
Accepted by DECI Call: DECI-7
PRACE Home site: RZG
PRACE Execution site: LRZ
PRACE Enabling sites: RZG
PRACE Architectures: Intel Westmere EX@2.4
Start enabling: 11/2011
Start production: 01/2012
Project status: Completed
Brief description of project: *LArge scale molecular SImulations of PROtein - DNA recognition in the combinatorial control of transcription.* The aim of this project is to reveal the molecular mechanisms of the combinatorial control of gene expression at atomic level of detail. The study is focused on factors relevant for the maintenance of stem cell ability to differentiate in different cell types and for the reprogramming of somatic cells into stem-like cells (induced pluripotent stem cells). Free energy profiles from atomistic molecular dynamics simulations for a set of representative protein-DNA and protein-protein interactions are calculated. These calculations are only attainable on large supercomputers due to the large number of degrees of freedom in the simulated system and the extensive sampling of the conformational space required. This project is performed in close collaboration with experimenters, thus giving the opportunity to readily test the relevance of the findings.
Types of support work undertaken: The required software packages Amber and NAMD for the large-scale MD simulations as well as Amber-Tools and VMD for pre- and post-processing and visualization were provided in advance on RZG platforms IBM Power6 and BlueGene/P in order to facilitate the preparation for production runs on the LRZ target machine SuperMIG. The users were assisted with running first test simulations with the MD packages. With this environment, the biological systems to be calculated could be equilibrated. Users were supported with the tests of a larger set of equilibration protocols to identify inaccurate starting models. Basic workflows for the processing chain preprocessing-simulation-postprocessing/visualization were prepared. For the production runs on the LRZ machine, support was provided with the usage of the simulation packages in a different environment.
Difficulties encountered and solution: No difficulties beside the enabling work were met.

Project Acronym: SMARC
Accepted by DECI Call: DECI-7
PRACE Home site: RZG

PRACE Execution site: LRZ
PRACE Enabling sites: RZG
PRACE Architectures: Intel Westmere EX@2.4
Start enabling: 11/2011
Start production: 04/2012
Project status: Completed
Brief description of project: *Solar Magnetically Active Region Corona.* Cool stars are surrounded by hot coronae, which are heated to some million degrees Kelvin. The heating processes, widely proposed to be related to the stellar magnetic field, lead not only to temperatures in the outer atmosphere well in excess of the stellar surface, but result also in a highly dynamic response of the plasma, inducing flows and waves. The structure and evolution of an active region in the solar corona is studied by this project. So far this modelling has been possible only in simplified setups. The proposed simulation will allow for the first time to model the structure and evolution of a solar active region with a high spatial resolution and at the same time to describe the full extend of the active region.
Types of support work undertaken: For the Tier-1 part of the SMARC project run at LRZ logistics support was given for the execution runs for a subset of parameters for the heating of the solar corona.
Difficulties encountered and solution: No difficulties encountered.

Project Acronym: HRPIPE
Accepted by DECI Call: DECI-7
PRACE Home site: SURFSara
PRACE Execution site: SNIC-KTH
PRACE Enabling sites:
PRACE Architectures:
Start enabling:
Start production: 11/2011
Project status: Completed
Brief description of project: From an engineering point of view turbulent pipe flow is extremely important, because of its wide range of applications. In the case of turbulent pipe flow only a limited number of numerical studies have been carried out, while there is an enormous amount of experimental data for a large range of Reynolds numbers available. There are still many unsolved questions, for instance it is argued that the peak of the axial rms decreases with Reynolds number, while others argued that the peak should increase with Reynolds number. The goal of the present research is to develop a highly accurate numerical model that is able to simulate, by means of DNS, flow with Reynolds numbers in the range of the experiments carried out by (McKeon et al. 2004) and (Morrison et al. 2004).
Types of support work undertaken: none
Difficulties encountered and solution:

Project Acronym: RBflow-2
Accepted by DECI Call: DECI-7
PRACE Home site: SURFSara
PRACE Execution site: RZG, SURFSara
PRACE Enabling sites:
PRACE Architectures:
Start enabling:
Start production: 11/2011
Project status: Completed

Brief description of project: Turbulent flows are abundant in nature. In contrast to a well-established paradigm, recent evidence indicates that several states of fully developed turbulence can coexist. In this project we focus on Rayleigh-Benard and Taylor-Couette flows to understand how these flow states may arise.
Types of support work undertaken: none
Difficulties encountered and solution:

8.2 Summary of Technical Support for DECI-8 Projects (M13-M24)

Project Acronym: CiO2_deg
Accepted by DECI Call: DECI-8
PRACE Home site: BSC
PRACE Execution site: CINES, UHEM
PRACE Enabling sites: none
PRACE Architectures: Harpertown
Start enabling: -
Start production: 1-May-2012
Project status: Completed
Brief description of project: Chlorite degradation by chlorite dismutase enzymes
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: Fulldrug
Accepted by DECI Call: DECI-8
PRACE Home site: BSC
PRACE Execution site: EPCC
PRACE Enabling sites: none
PRACE Architectures: XE6
Start enabling: -
Start production: 1-May-2012
Project status: Completed
Brief description of project: Accurate calculation of drug binding thermodynamics and kinetics
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: LBGLASS
Accepted by DECI Call: DECI-8
PRACE Home site: CINECA
PRACE Execution site: CINECA
PRACE Enabling sites: CINECA
PRACE Architectures: Intel GPU cluster
Start enabling: 1-May-2012
Start production: 1-June-2012
Project status: completed
Brief description of project: Lattice Boltzmann based simulations of flowing soft systems
Types of support work undertaken: Account creation.
Difficulties encountered and solution: None.

Project Acronym: NAHUJ
Accepted by DECI Call: DECI-8

PRACE Home site: CINECA
PRACE Execution site: CINECA, WCSS
PRACE Enabling sites: CINECA, WCSS, SURF_Sara
PRACE Architectures: Intel GPU cluster, HP Cluster, Cluster Supernova@WCSS (Intel Xeon X5650@2.67)
Start enabling: 1-Oct-2012 (June 2012 at WCSS)
Start production: 1-Dec-2012
Project status: completed
Brief description of project: Numerical Analysis of Hydrogen Underexpanded Jets. The aim of this work was the study of the fluid dynamic behavior of underexpanded hydrogen jets by using a High Performance Computing (HPC) methodology. The analysis was carried out by employing a two-dimensional axial symmetric in-house code which is able to take into account real gas effects by employing either Van der Waals or Redlich-Kwong equations of state (EoS). The first aim of this project was to evaluate the influence of real gas effects on hydrogen jets structure. In fact, very recent works have shown the importance to employ real gas equations dealing with highly underexpanded hydrogen jets. A parametric analysis was carried out by varying the injection pressure and temperature, in order to investigate the features of underexpanded jets and real gas effects under different conditions.
Types of support work undertaken:
- CINECA/SURFSara: Porting on GPU using CUDA.
- WCSS: was the exec site for this project and was performing every-day support. The accounts were created on the Supernova cluster based on the PRACE LDAP entries at SURFSara. Users encountered problems with compilation of their software on Supernova cluster. Problems were resolved by enabling other libraries and making changes in the system and user environment, as required by the user's code.
Difficulties encountered and solution:
- CINECA: With the help of experts from SURF_Sara a CUDA version of the code was written and ported on Cineca's GPU cluster (PLX). More details of the porting and the performance enhancements have been reported in a whitepaper.
- WCSS: The project started calculations late, and was not able to use all the awarded core-hours. The solution was to extend the project allocation time till 3rd of June 2013, and this allowed to consume all the allocated time.

Project Acronym: OPTOCHIMEMD
Accepted by DECI Call: DECI-8
PRACE Home site: CINECA
PRACE Execution site: CSCS, SURFSara
PRACE Enabling sites: CSCS, SURFSara
PRACE Architectures: CRAY XE6, Power6 (Huygens)
Start enabling: 1-May-2012
Start production: 1-June-2012
Project status: completed
Brief description of project: MD simulations of engineered light-switched chimeric proteins
Types of support work undertaken: Account creation.
Difficulties encountered and solution: Usage of the resources at SURFSara requires X.509 certificates which the researchers were unable to obtain so in the end the resources here were not used.

Project Acronym: WFNUC
Accepted by DECI Call: DECI-8
PRACE Home site: CINECA

PRACE Execution site: CSCS, RZG
PRACE Enabling sites: CSCS, RZG
PRACE Architectures: CRAY XE6, BG/P
Start enabling: 1-May-2012
Start production: 1-Oct-2012
Project status: completed
Brief description of project: Precision calculations with realistic Wave Functions of NUClei.
Types of support work undertaken: Account creation and general support.
Difficulties encountered and solution: None.

Project Acronym: SMARTWING
Accepted by DECI Call: DECI-8
PRACE Home site: CINES
PRACE Execution site: ICHEC, WCSS
PRACE Enabling sites: WCSS
PRACE Architectures: Cluster Supernova@WCSS (Intel Xeon X5650@2.67)
Start enabling: June 2012 (at WCSS), continued in August and September 2012
Start production: September 2012 (at WCSS)
Project status: Completed
Brief description of project: This project concerned the analysis by numerical simulations of compressible flows or flows with variable density around aerofoils in 2D or 3D. Its aim was to better know the physical mechanisms related to the arising instabilities and the unsteadiness and the transition in flows around obstacles since the very first steps towards turbulence at moderate Reynolds numbers in order to better model these mechanisms at high Reynolds number.
Types of support work undertaken: WCSS was the exec site for this project and was performing every-day support through all the project lifetime. The accounts were created on the Supernova cluster based on the PRACE LDAP entries at SURFSara. Users encountered problems with memory leaks of their code, what required more attention from the site. Besides that there were consultations regarding best practices for submitting jobs on Supernova and parameters.
Difficulties encountered and solution: The project started calculations late, and was not able to use all the awarded core-hours. The solution was to extend the project allocation time till 3rd of June 2013, but due to big underuse it was possible to consume only about 1/3 of the allocated time.

Project Acronym: CYTODYN
Accepted by DECI Call: DECI-8
PRACE Home site: CSC
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: CSC
PRACE Architectures: Cray XE6
Start enabling: May 2012
Start production: May 2012
Project status: Completed
Brief description of project: This project used the NAMD molecular dynamics simulation package to study the cyt bc1 complex in explicit lipid bilayer at physiological salt concentration. The main task of this study was the calculation of the free energy of substrate binding to elucidate substrate bonding modes.
Types of support work undertaken: None in the 2nd year of PRACE-2IP

Difficulties encountered and solution: None

Project Acronym: PARAMETER
Accepted by DECI Call: DECI-8
PRACE Home site: CSC
PRACE Execution site: EPCC
PRACE Enabling sites: CSC, EPCC
PRACE Architectures: Cray XE6
Start enabling: May 2012
Start production: January 2013
Project status: In progress (49%)
Brief description of project: This project applies advanced parameter estimation techniques to quantify the uncertainty of a numerical weather prediction model, and to tune the predictive skill of it by means of algorithmic model parameter estimation. The model under study is Echam5.
Types of support work undertaken: Echam5 was ported to the Cray XE6 of EPCC with help from CSC, EPCC, and NAG.
Difficulties encountered and solution: None

Project Acronym: Photoreception
Accepted by DECI Call: DECI-8
PRACE Home site: CSC (external)
PRACE Execution site: HLRS, LRZ, RZG
PRACE Enabling sites: CSC, HLRS, LRZ, RZG
PRACE Architectures: Intel Xeon clusters
Start enabling: May 2012
Start production: November 2012
Project status: Completed
Brief description of project: This project used the Firefly quantum chemistry package to study light-induced protein dynamics, in order to provide new insight in the molecular basis of vision.
Types of support work undertaken: Firefly was ported to the three execution platforms by the PI and her collaborators. Help was received from the execution sites.
Difficulties encountered and solution: At HLRS the standard maximum walltime limit of jobs was too small for the project. A special batch job queue with longer walltime was set up.

Project Acronym: DrugEffluxMechanism
Accepted by DECI Call: DECI-8
PRACE Home site: CSCS
PRACE Execution site: CSCS
PRACE Enabling sites: none
PRACE Architectures: Cray XE6
Start enabling:
Start production: 19 September 2012
Project status: in progress
Brief description of project: The project focus on simulations of both the P-glycoprotein and Sav1866 protein embedded in a lipid membrane. The purpose is to understand how the proteins interact with its lipid environment to do that the first step of the project involves series of test simulations to identify the optimal lipid configurations. Next it will be to understand the mechanism allowing the substrates to move from the lipid membrane to the core of the transporters。

Types of support work undertaken: none
Difficulties encountered and solution: The project was initially assigned to France (Idris, Babel) because denied a Chinese PhD student involved in this project to have access to the system, the project was hanging for a few months, until CSCS decided to grant its own resources acting both as home and exec sites.

Project Acronym: CONTRAR
Accepted by DECI Call: DECI-8
PRACE Home site: EPCC
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: SNIC-KTH
PRACE Architectures: Lindgren (XE6 12C@2.1)
Start enabling: -
Start production: May 2012
Project status: Completed
Brief description of project: First-Principles Calculations on the Conformation Transfer in a Dual-core Molecular Switch.
Types of support work undertaken: general support provided, including account creation, initial PI meetings, etc.
Difficulties encountered and solution: none**.**

Project Acronym: POLARIZABLEFOLDBIND
Accepted by DECI Call: DECI-8
PRACE Home site: EPCC
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: -
PRACE Architectures: Lindgren (XE6 12C@2.1)
Start enabling: -
Start production: May 2012
Project status: Completed
Brief description of project: Simulating Coupled Protein Folding and Nucleic Acid Binding Using a Polarizable Force Field.
Types of support work undertaken: general support provided, including account creation, initial PI meetings, etc.
Difficulties encountered and solution: none.

Project Acronym: TLRSim
Accepted by DECI Call: DECI-8
PRACE Home site: EPCC
PRACE Execution site: CSCS
PRACE Enabling sites: -
PRACE Architectures: Rosa (XT5 CSCS)
Start enabling: -
Start production: May 2012
Project status: Completed
Brief description of project: The Molecular Basis for Ligand Recognition & Signalling in Toll-Like Receptors via Simulation.
Types of support work undertaken: general support provided, including account creation, initial PI meetings, etc.
Difficulties encountered and solution: none.

Project Acronym: POEMatCASP
Accepted by DECI Call: DECI-8
PRACE Home site: HLRS
PRACE Execution site: CINES
PRACE Enabling sites: none
PRACE Architectures: JADE-Harpertown (Intel Harpertown@3)
Start enabling: -
Start production: May 2012
Project status: Completed
Brief description of project: Protein Structure Prediction with Biophysical Models. Proteins are the nanoscale machines of all cellular life. Most proteins fold into a unique three-dimensional structure, determined entirely by their amino acid sequence, in a slow and complicated process that is still not fully understood. Because sequencing techniques are far more efficient than structure resolution, predicting the structure of proteins and their functional complexes is one of the major challenges in the life sciences. Closely related is the investigation of protein-protein interactions as one of the most important mechanism of signalling in biological systems.

After the complete genome of many species has been sequenced, there is a huge gap between the number of known sequences and the number of known structures (factor about 1000). Experimental resolution of protein structures is orders of magnitude more expensive than sequencing and not possible for many interesting proteins at all. Computational methods for protein structure prediction are therefore increasingly used to close this gap, but progress for proteins with low sequence similarity to structure the resolved proteins has been slow.

We have developed and biophysics based atomistic simulation techniques for protein folding and protein structure prediction. Using our biophysical all-atom force fields PFF01/PFF02 and efficient massively parallel simulation techniques (Schug, et al., 2006; Schug and Wenzel, 2006; Verma, et al., 2007) we were able to predict the structure of small proteins (up to about 70 amino acids) solely on the basis of the sequence information. Application of this methodology often has direct applications in the life-sciences: We have applied these techniques in close cooperation with experimental groups to elucidate the genetic origin of some human developmental disorders (Kim, et al., 2010; Kim, et al., 2008; Xu, et al., 2011) and also apply them to design inhibitors for protein-protein interactions(Meliciani, et al., 2009).

In this project were combined these methods with homology modelling techniques and efficient methods for model generation to predict the structure of larger proteins. POEM is one of the few available biophysical simulation prediction methods and therefore well suited for structure prediction of proteins with low homology to known proteins, but this requires massive computational resources that can only be provided by HPC architectures. In this challenging area there has been little progress in established homology-based structure prediction protocols for the last decade. Progress in the development of these methods will be monitored in the blind comparative assessments of protein structure prediction methods (CASP), where we will participate in 2012 using the resources of this project.

Types of support work undertaken: Accounts and administrative data were prepared by HLRS.
Difficulties encountered and solution: Two of the six investigators are not citizens of the European Union. Because of the legal situation in France additional efforts were required to allow access for these two to the system at CINES.

Project Acronym: RCR2CP
Accepted by DECI Call: DECI-8

PRACE Home site: ICHEC
PRACE Execution site: SNIC-KTH (840k)
PRACE Enabling sites: Lindgren Sweden
PRACE Architectures: Cray XE6 system
Start enabling: April 2012
Start production: 8/2012
Project status: Project completed
Brief description of project: Regional Climate Research using a Representative Carbon Pathways Approach. It ran climate predictions to 2100 on the RCP scenarios for Ireland.
Types of support work undertaken: Help compile the software need on Lindgren. Help file transfer.
Difficulties encountered and solution: Main difficultly was the stability of lindgren. They had a severe disk problem. Unfortunately could not do much about that. Second was transfer speed. Input data would take 8-12hrs to copy for one year's run time. Undertook test on connection speed. Found that could get 20 times speed up over sftp to lindgren using scp to dedicated file transfer node.

Project Acronym: SARCEMS
Accepted by DECI Call: DECI-8
PRACE Home site: ICHEC
PRACE Execution site: ICHEC (945k)
PRACE Enabling sites: no enabling site
PRACE Architectures: x86 (Stokes)
Start enabling:
Start production: 8/2012
Project status: In progress (62% burned)
Brief description of project: Studied the active responses of cells to external mechanical stimuli using Abaqus.
Types of support work undertaken: N/A
Difficulties encountered and solution: Stokes was the only system with sufficient Abaqus licenses available – home site and execution site needed to be the same

Project Acronym: TiO2-Interface
Accepted by DECI Call: DECI-8
PRACE Home site: ICHEC
PRACE Execution site: UHEM (2.75)
PRACE Enabling sites: no enabling site
PRACE Architectures: x86
Start enabling:
Start production: 11/2012
Project status: In progress (38% burned)
Brief description of project: Ab initio (VASP) study of Titanium Dioxide Interfaces to engineer photo-catalytic activity in mixed TiO2.
Types of support work undertaken:
Difficulties encountered and solution: Authentication problems. Tyndall are not signed up to a Cert scheme in Ireland. ICHEC got in contact with UHEM to allow for password-based ssh connection which was granted.

Project Acronym: CoMoPro
Accepted by DECI Call: DECI-8
PRACE Home site: IDRIS

PRACE Execution site: RZG (Genius)
PRACE Enabling sites: IDRIS
PRACE Architectures: IBM BG/P
Start enabling: 05/12
Start production: -
Project status: Completed
Brief description of project: Protein motions occurring in the nano- to millisecond time scale are of great relevance to protein function, and a good understanding of protein dynamics is crucial for understanding numerous biophysical processes occurring in these complex systems, such as enzymatic catalysis, molecular recognition, ligand binding, and protein folding. To probe this, we use solid-state NMR spectroscopy, which allows access to site-specific information about biomolecular motions. Different NMR experiments are sensitive to motions from different timescales, allowing us to investigate fast protein dynamics of the order of few nanoseconds to slower dynamics taking place in the miliseconds time scale. Many approaches exist to model dynamics in proteins to explain the NMR experimental data, and in order to validate any of these models a new method must be implemented to confirm the existing results. In particular, the milisecond regime is very challenging to investigate, and methods are not completely established for analyzing and interpreting NMR data recorded for slow motions in proteins. The most unbiased method would be provided by computational approaches, such as performing molecular dynamics calculations on a time scale that would allow us to probe slow motions in proteins. We plan to develop this method, and we will consider two model protein systems, the relatively small immunoglobulinbinding protein G (GB1), and the more complex dimeric 153-residue microcrystalline ZnII-loaded human superoxide dismutase (ZnII-SOD). For these systems, extensive experimental NMR data have recently been acquired in microcrystalline form, and tentatively interpreted in terms of slow local motions. Performing the MD calculations would allow us to confirm this interpretation, and provide a deeper insight into these slow dynamic processes.
Types of support work undertaken:
Difficulties encountered and solution: No consumption for this project. No final scientific report is expected.

Project Acronym: MOLED
Accepted by DECI Call: DECI-8
PRACE Home site: IDRIS
PRACE Execution site: CSC (Louhi, Sisu), ICHEC (Stokes)
PRACE Enabling sites: CSC, ICHEC, IDRIS
PRACE Architectures: Cray, SGI
Start enabling: 05/12
Start production: 05/13
Project status: In progress (10%), extended until the end of August
Brief description of project: Organic light-emitting diodes (OLEDs) are a relatively new technology, which provide a low-cost and potentially high-efficiency alternative to present inorganic lighting and display applications. A typical OLED consists of one layer or a stack of multiple layers of organic semiconducting material sandwiched between two electrodes. Due to the energetic disorder present in organic media, charge carriers are transported by means of hopping between neighbouring molecules and/or segments of polymers. The energetic levels of these hopping sites are disordered and often assumed to be distributed according to a Gaussian density of states.

An OLED works as follows. Electrons and holes are injected in the organic material. They are transported under the influence of an applied bias voltage and their mutual Coulombic interactions either to the opposite collecting electrodes or to each other. Once an electron and

a hole meet each other, they recombine to form a bound electron-hole pair (exciton) which can decay radiatively under the emission of a photon.

Despite the growing commercial success of OLEDs, knowledge of many aspects of their functioning is still fragmental. To increase our theoretical understanding of the transport properties, we integrate several different simulation methods covering one or more length- and/or time-scales. This multi-scale modelling scheme consists of the following steps: 1. By means of coarse-grained Monte Carlo simulations and employing well established atomic force field parameterizations, the morphology of polymers and organic molecules can be simulated. 2. These morphologies are used in density functional theory simulation programs to calculate charge transfer integrals between sites and the energetic landscape 3. The predicted morphologies and the corresponding charge transfer integrals and energetic landscapes are used in a kinetic Monte Carlo program to simulate typical relevant transport properties like the three-dimensional charge carrier current density and recombination statistics.

The described simulation scheme will be used in this project for a multi-scale modelling study of organic devices with tris(8-hydroxyquinolinato)aluminium (Alq3) as an active component. Special focus will be devoted to the influence on charge carrier mobilities of energetic and positional disorder as well as charge density. The work will be extended to model prototypical host:guest systems, where the host is a wide gap molecular semiconductor, such as 4,4′-bis(N-carbazolyl)-1,1′-biphenyl (CBP), N,N′-dicarbazolyl-3,5-benzene (mCP), or Alq3, and where the guest is the well-known triplet emitter fac-tris(2-phenylpyridine) iridium [Ir(ppy)3]. The project requires considerable and varied computational resources, in terms of cpu times, disk space and dynamic memory allocation, which fully justifies application to PRACE.

Types of support work undertaken: ICHEC, CSC: Installation of the needed software (NWCHEM). The applications that were used in the project were already installed on CSC's Cray XT. However, one of the applications (NWChem) didn't work in the simulation case studied. The software itself worked fine, but simulations persistently failed because of memory requirements. Despite a lot of effort, enabling for the Cray XT was stopped in December 2012. The decision was to wait until CSC's new Cray XC30 system is open for customer use in March 2013, and then move the project to there.
Difficulties encountered and solution: Problems in running the NWChem application on CSC's old Cray XT system. The dataset that the PI wants to use was probably too large. The project migrated on their new Cray XC30 in April 2013. On the Cray XC30 of CSC, memory was no longer a problem, but a new problem turned up: NWChem did not yet support the Aries network of the Cray XC30. Therefore additional steps were needed in the build process. Help was received from CSCS and PNNL (USA) with this.

Project Acronym: VIPforVPH
Accepted by DECI Call: DECI-8
PRACE Home site: IDRIS
PRACE Execution site: EPCC (HeCToR XE6)
PRACE Enabling sites: EPCC, IDRIS
PRACE Architectures: Cray
Start enabling: 05/12
Start production: 05/12
Project status: Completed, waiting for the final scientific report
Brief description of project: The Virtual Imaging Platform (VIP) is a project of the French National Research Agency providing an online, open platform to simulate medical images in 4 modalities, namely Magnetic Resonance Imaging (MRI), ultrasound imaging, Positron Emission Tomography (PET), and Computed Tomography (CT). More information about the

project is available at http://www.creatis.insa-lyon.fr/vip. The platform is currently connected to the European Grid Infrastructure to support embarrassingly parallel simulations, but it lacks reliable resources to run parallel codes, in particular MPI.

Therefore, the motivation of project `Virtual Imaging Platform for Virtual Physiological Human` (VIP for VPH) is to offer imaging scientists a convenient mechanism to perform image simulations on PRACE High-Performance Computing (HPC) resources. This will be demonstrated on a 3D+t 512x512x512 simulation of a Magnetic Resonance Imaging acquisition (MRI), and made available for VIP users.

The VIP workflow engine is being interfaced with the Application Hosting Environment (AHE) that can launch jobs on PRACE resources. AHE will be in charge of data transfers, job submission and monitoring to PRACE.
Types of support work undertaken:
Difficulties encountered and solution: No difficulties encountered.

Project Acronym: FFF
Accepted by DECI Call: DECI-8
PRACE Home site: LRZ
PRACE Execution site: CINCECA
PRACE Enabling sites: CINECA
PRACE Architectures: Intel Westmere EX@2.4 + GPU
Start enabling: 2012-04-12
Start production: 2012-05-01
Project status: Completed
Brief description of project: We aim at the development of efficient, reliable and future-proof numerical schemes and software for the parallel solution of partial differential equations (PDEs) arising in industrial and scientific applications. Here, we are especially interested in technical flows including Fluid-Structure interaction, chemical reaction and multiphase flow behaviour which can be found in a wide variety of (multi-) physics problems. In our approach, both numerical and hardware efficiency are addressed simultaneously: On the one hand, the transition of today's computational hardware towards parallel (and heterogeneous) architectures is in progress and therefore all levels of parallelism (vectorisation, parallelism on the core level in multi- and many-core CPUs and accelerator devices like GPUs and finally on the node level within distributed memory clusters) have to be exploited. Algorithms and whole solvers have to be tailored with respect to the target hardware in order to achieve a significant amount of the parallel peak performance. On the other hand, the sole concentration on hardware efficiency does not carry out the whole job (and in some cases may be counter-productive): Numerical efficiency plays a crucial role and itself includes multiple levels that can be optimised. Starting with the overall numerical and algorithmic approach required for the solution of a given domain specific problem (i.e. discretisation of the governing equations in time and space), stabilisation, linearisation of non-linear problems and finally the solution of the linear problems and smoothing therein, all these aspects together with the aforementioned levels of parallelism bear a large amount of interdependencies. In the proposed project, we want to improve our parallel numerical software framework FEATFLOW (www.featflow.de) and augment this powerful simulation toolkit for academic and industrial usage. The planned improvements take both aspects of efficiency into account in order to make it ready for future HPC-architectures: Novel numerical- and physics-components as well as software-techniques for massively parallel (heterogeneous) compute resources are going to be employed that extend the applicability of the package to current and future real-world problems in the field of CFD.
Types of support work undertaken: general technical support

Difficulties encountered and solution: none

Project Acronym: CANONS
Accepted by DECI Call: DECI-8
PRACE Home site: SNIC-KTH
PRACE Execution site: CSCS
PRACE Enabling sites: SNIC-KTH, CSCS
PRACE Architectures: Cray XE6
Start enabling: 05/12
Start production: 05/12
Project status: Completed (19%)

Brief description of project: 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, Gen-IV reactors. The fast neutrons used in Gen-IV reactors damage the structural materials at a rapid pace and therefore materials development is needed. In this project, first principles modelling in the framework of density functional theory have been applied to several different materials in order to study radiation damage and diffusion phenomena. The primary damage in iron has been studied using ab initio molecular dynamics, solute – defect interactions in nano-structured oxide dispersion strengthened (ODS) steels have been characterized, radiation induced segregation in dilute iron alloys has been investigated and noble gas diffusion in nitride fuel matrices has been addressed.
Types of support work undertaken: Account creation, frequent reminders to use the dedicated time. The support network was perceived as very helpful.
Difficulties encountered and solution: Underusage of the dedicated time due to the PI being on six-months paternal leave. Some of the planned alogrithmic developments had to be postponed, but the PI plans to submit new PRACE proposals in the future.

Project Acronym: MBIOMARK
Accepted by DECI Call: DECI-8
PRACE Home site: SNIC-KTH
PRACE Execution site: CSCS
PRACE Enabling sites: CSCS, SNIC-KTH
PRACE Architectures: Cray XE6
Start enabling: 05/12
Start production: 07/12
Project status: Completed (56%)

Brief description of project: Alzheimer□s disease is one of the most prominent cause of the acquired dementia in elderly patients and it affects around 35.6 million people worldwide. The Alzheimer□s disease has a profound impact on 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 people within risk groups. Current options for clinical diagnostics of early stages of the Alzheimer□s disease are very limited and development of novel clinical imaging techniques are highly desirable.
The MBIOMARK research project had the aim to address this problem and focus on the development of the electron paramagnetic resonance (EPR) imaging technique to enable a

methodology for in vivo imaging of early damage to brain tissue cause by Alzheimer□s disease.
Within the project the microscopic factors determining behaviour of nitroxides biomarkers have been investigated using quantum chemistry/molecular mechanics methods. Based on obtained results a new strategy for the design of biomarkers adapt for EPR imaging of amyloid fibrils has been suggested.
The MBIOMARK project has been a highly demanding project computational wise as extensive QM/MM calculations have carried out during the first and third part of this project.
Types of support work undertaken: Parallelization improvements tests of the DALTON program were done within the PRACE community software initiative.
Difficulties encountered and solution: None

Project Acronym: PIPETURB
Accepted by DECI Call: DECI-8
PRACE Home site: SNIC-KTH
PRACE Execution site: EPCC, CSC
PRACE Enabling sites: SNIC-KTH, EPCC
PRACE Architectures: Cray XE6
Start enabling: 05/12
Start production: 07/12
Project status: Completed (130% at EPCC, 91% at CSC)
Brief description of project: The aim of the project was to study fully developed high-Reynolds number turbulent pipe flow through large-scale direct numerical simulations (DNS) resolving all relevant scales of the turbulent flow. These were carried out using the massively parallel DNS code Nek5000, which is based on an accurate and efficient spectral-element discretization. Pipe flow is the case which is easiest realisable in experiments. However, due to numerical difficulties related to the cylindrical coordinates and the corresponding numerical singularity arising along the symmetry line, it was the only canonical flow case that previously had not been thoroughly studied using DNS, as opposed to plane channels and boundary layers. Within PIBETURB large-scale spectral-element DNS of fully developed turbulent pipe flow of an incompressible viscous fluid could now be performed and analysed.
Types of support work undertaken: Setting up accounts and installing certificates.
Difficulties encountered and solution: None**.**

Project Acronym: PLANETESIM
Accepted by DECI Call: DECI-8
PRACE Home site: SNIC-KTH
PRACE Execution site: FZJ, RZG, ICHEC
PRACE Enabling sites: SNIC-KTH, SNIC-LU, SNIC-Chalmers, ICHEC, RZG
PRACE Architectures: JuRoPa, RZG P6 "VIP", Hydra, Stokes
Start enabling: May 2012
Start production: June 2012
Project status: Completed
Brief description of project: The project aims to study the formation of planetesimals by means of high-resolution computer simulations. Planetesimals are km sized objects which constitute an important step in the planet development. However it is currently poorly understood how planetesimals form from dust particles, gas and why there is a discontinuity in the size distribution of the planetesimals in the Kuiper belt for radii around 50 km. The project uses the PENCIL CODE for its numerical work.
Types of support work undertaken: The project profiled the application using the Scalasca tool. Based on this investigation the communications within the parallel Fourier

transformation have been optimised, the FFTPACK library was replaced with the FFTW library and some code re-arrangements have been performed. This work led to an overall performance improvement of about 8% for the entire application. This improvement is on the expected level.
The project also worked on the IO part of the project code. MPI-IO was introduced into the code to improve the usability, in particular when using a larger number of MPI tasks.
Difficulties encountered and solution: When optimising the communications within the parallel Fourier transformation routines, the first attempt using MPI_Alltoall would speed up the Fourier transformation but damage other parts of the application, such that the overall performance was poorer. Reverting to the original code, but removing synchronisation within this part of the code resulted in the expected performance improvement without damaging the overall performance.

Project Acronym: ELORBIC
Accepted by DECI Call: DECI-8
PRACE Home site: PSNC
PRACE Execution site: SURFSara
PRACE Enabling sites: PSNC
PRACE Architectures: IBM Power6
Start enabling: May 2012
Start production: June 2012
Project status: Completed
Brief description of project: Molecular-based metallic clusters and chains behave like individual quantum nanomagnets, displaying quantum phenomena on a macroscopic scale. In view of potential applications of such materials in magnetic storage devices or in envisaged quantum computer processors as well as in the low-temperature refrigerants, the accurate simulation of these complex objects becomes the key issue. The magneto-structural correlations, the role and mechanism of magnetic anisotropy and intrinsic quantum effects following from the geometrical frustration induced by the topological arrangement of spins or particular interactions count among the new challenges for computer simulations. The simulations planned in the project address the quantum phenomenological models which are the most reliable theoretical representatives of the physical molecular-based nanomagnets investigated recently and their reliability from the fundamental microscopic point of view assessed by the well-established first-principle electronic structure calculations.
Types of support work undertaken: Obtaining the user DNs and support in the procedure of obtaining the machine accounts. Some preliminary test-runs have been introduced on the IBM Power6 machine.
Difficulties encountered and solution: None.

Project Acronym: MLMJTAX
Accepted by DECI Call: DECI-8
PRACE Home site: PSNC
PRACE Enabling sites: PSNC
PRACE Execution site: UYBHM
PRACE Architectures: Cluster Intel Nehalem@2.93
Start enabling: 7/2012
Start production: 07/2012
Project status: In progress (85% completed)
Brief description of project: Microtubule stabilizing agents (MSA) interfere with disassembly of microtubules in rapidly dividing cancer cells. Paclitaxel (Taxol®), the complex, diterpenoid natural product and the effective MSA, binds to tubulin in a

stoichiometric ratio and operates by blocking microtubule dissociation into tubulin dimers finally causes apoptosis i.e. programmed cell death. Although the EC structure of paclitaxel on tubulin Zn+2 sheets showed the location of the ligand, the conformation of paclitaxel molecule was not determined with sufficient precision. The estimation of the bioactive conformation indicated two structures: so called T-taxol, proposed by Emory University, Atlanta, GA group and PTX-NY referred to the New York Sony Brook group. In the present project we address computational questions in order to estimate the conformational space (PES) of paclitaxel as well to judge these two proposals of molecular shape. Another purpose of the present work is to precisely determine the possible hydrogen bond patterns, including cooperative enhancement, and to illuminate the weakly recognized aromatic and olefinic fragments orbital interactions because of such information is important to better understand the nature of non-bonding interactions and their effect on final internal energy. Since density functional methods fail to accurately describe weak π-π interactions, the use of second order Møller-Plesset (MP2) or coupled cluster CCSD(T) (SP) is predicted at cc-pVDZ and aug-cc-pVDZ basis set. The stacking bonding, due to London dispersion energy, will be additionally estimated to characterize attractive interaction energies of benzene-benzene and benzene-ethylene complexes of paclitaxel fragments. We hope that the detailed knowledge on paclitaxel binding site regarding its PES led to the development of second-generation taxanes.
Types of support work undertaken: Users were helped with accessing the execution site. General support with obtaining certificates.
Difficulties encountered and solution: n/a

Project Acronym: NELC
Accepted by DECI Call: DECI-8
PRACE Home site: PSNC
PRACE Enabling sites: PSNC, EPCC
PRACE Execution site: EPCC
PRACE Architectures: Cray XE6
Start enabling: 05/2012
Start production: 05/2012
Project status: In progress (95%)
Brief description of project: Advances in quantum theory and high precision computational methods lead to more and more precise predictions of properties for light atoms and molecules. A fundamental goal of such methods is to find precise solutions of the Schrödinger equation. The most precise methods employed to solve the Schrödinger equation are based on the variational principle and take explicitly into account the electron correlations in the construction of a trial wave function. The method of explicitly correlated Gaussian (ECG) functions is one of the best suited to this purpose. It has been widely used for many light atoms and molecules and has proven its ability to supply the benchmark quality results. The goal of this project is a generation of well optimized ECG wave functions for a six-electron molecule (methylidynium, CH+) at the equilibrium distance. This cation is one of the first species discovered in the interstellar space and being essential in formation of carbon hydrates. Our project aims at providing reliable data for solving questions pertaining to astrophysics and for understanding the role of CH in the interstellar chemistry. For that purpose, we plan to employ the ECG method and the massive computations to a large scale deterministic optimization of the energy and wave function according to a well-defined strategy.
Types of support work undertaken: General user support in the first usage and runs on the local LRMS. General support with obtaining certificates.
Difficulties encountered and solution: n/a

Project Acronym: EUTERPE-5
Accepted by DECI Call: DECI-8
PRACE Home site: RZG
PRACE Execution site: FZJ
PRACE Enabling sites: RZG
PRACE Architectures: Intel Nehalem@2.93
Start enabling: 05/2012
Start production: 05/2012
Project status: Completed
Brief description of project: Follow-up project of DECI-7 project EUTERPE-4.
Types of support work undertaken: general support provided, account creation
Difficulties encountered and solution: None.

Project Acronym: LASIPROD-2
Accepted by DECI Call: DECI-8
PRACE Home site: RZG
PRACE Execution site: IDRIS, RZG, SNIC-KTH
PRACE Enabling sites: RZG
PRACE Architectures: BlueGene/P, BlueGene/Q, SandyBridge@2.6, Cray XE6 12C@2.1
Start enabling: 05/2012
Start production: 10/2012
Project status: In progress (60%)
Brief description of project: Follow-up project of DECI-7 project LASIPROD.
Types of support work undertaken: General support provided. Help with the transition of the project from IDRIS to RZG.
Difficulties encountered and solution: The code did run well on BlueGene/P but not on BlueGene/Q. Hence it was moved from the BG/Q Turing from IDRIS to the SandyBridge cluster Hydra at RZG in exchange with another project.

Project Acronym: NanoTherm
Accepted by DECI Call: DECI-8
PRACE Home site: SURFSara
PRACE Execution site: EPCC, SURFSara
PRACE Enabling sites:
PRACE Architectures: Cray, IBM Power6
Start enabling:
Start production: 04/2012
Project status: Waiting for report
Brief description of project: The identification of alternative and renewable sources of energy is one of the most important challenges modern society faces, and has become more urgent and intense in the past few years. One of the most promising technologies is that of thermoelectric (TE) devices, which allow one to transform heat into electrical energy (an alternative energy source) or vice-versa (for refrigeration or heating). Several basic technological problems still need to be solved before thermoelectrics become a competitive energy source. In particular, the efficiency of thermoelectric materials themselves will have to be roughly doubled before cost-effective, large-scale applications can be envisaged. New perspectives on thermoelectrics have been opened recently by their structuring on the nanoscale.
Types of support work undertaken: none
Difficulties encountered and solution:

Project Acronym: TRANSPART
Accepted by DECI Call: DECI-8
PRACE Home site: SURFSara
PRACE Execution site: SNIC-KTH
PRACE Enabling sites:
PRACE Architectures: Cray
Start enabling:
Start production: 05/2012
Project status: Waiting for report
Brief description of project: Traditionally, direct numerical simulations (DNS) of transitional and turbulent flows are performed in simplified computational domains that are characterised by periodic boundary conditions in all three directions. However, real applications in nature and technology often involve the interaction with a solid wall and are thus inhomogeneous is space. Here, we study the flow case of a transitional spatially evolving boundary layer exposed to free-stream turbulence, as typically observed on turbine blades. We focus on the advection of small inertial particles in transitional intermittent flows. Such a computational study based on highly resolved DNS, not yet attempted in the literature, bears many interesting and relevant physical effects due to the growing boundary layer and to the random appearance of regions of laminar and turbulent flows; for instance the non-dimensional number characterising the particle-wall accumulation is gradually changing with the downstream distance. The raw scientific data will be shared with the scientific community (iCFDdatabase, http://cfd.cineca.it).
Types of support work undertaken: none
Difficulties encountered and solution:

8.3 Summary of Technical Support for DECI-9 Projects

Project Acronym: COIMBRALATT
Accepted by DECI Call: DECI-9
PRACE Home site: BSC
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: none
PRACE Architectures: XE6
Start enabling: -
Start production: 01-Jan-2013
Project status: In progress 50%
Brief description of project: Landau gauge propagators and vertices in Lattice QCD
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: ICREIMUTANTS
Accepted by DECI Call: DECI-9
PRACE Home site: BSC
PRACE Execution site: EPCC
PRACE Enabling sites: none
PRACE Architectures: XE6
Start enabling: -
Start production: 1-Nov-2012
Project status: In progress 50%
Brief description of project: Effect of mutations distant from the active site in the nickase activity of I-CreI and related homing endonucleases

Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: SPECBNS
Accepted by DECI Call: DECI-9
PRACE Home site: BSC
PRACE Execution site: RZG
PRACE Enabling sites: none
PRACE Architectures: Intel cluster
Start enabling: -
Start production: 1-Jan-2013
Project status: In progress 50%
Brief description of project: Spin and eccentricity effects on BNS coalescence
Types of support work undertaken: Account management
Difficulties encountered and solution: We helped users to connect to Hydra through a PRACE door node.

Project Acronym: DOPE
Accepted by DECI Call: DECI-9
PRACE Home site: CINECA
PRACE Execution site: CINECA
PRACE Enabling sites: CINECA
PRACE Architectures: Intel-GPU
Start enabling: 1-Nov-2012
Start production: 1-Nov-2012
Project status: In progress (30%)
Brief description of project: Molecular Dynamics simulations of mixed DOPC/DOPE based membrane bilayer.
Types of support work undertaken: Account creation, general usage of CINECA GPU cluster.
Difficulties encountered and solution: None.

Project Acronym: GPCR4D
Accepted by DECI Call: DECI-9
PRACE Home site: CINECA
PRACE Execution site: EPCC
PRACE Enabling sites: EPCC
PRACE Architectures: CRAY XE6
Start enabling:
Start production: 1-Nov-2012
Project status: In progress (100%)
Brief description of project: Large scale molecular dynamics simulations of GPCR proteins in membrane environments: fine tuning the 3D structure for optimal virtual screening campaigns aimed at developing new drugs
Types of support work undertaken: Account creation.
Difficulties encountered and solution: At the time of writing, the team have already used their budget and have requested extra time from EPCC who have agreed to an extra 300K hours.

Project Acronym: iMIG
Accepted by DECI Call: DECI-9

PRACE Home site: CINECA
PRACE Execution site: BSC
PRACE Enabling sites: BSC
PRACE Architectures: Intel GPU cluster
Start enabling: 1-Nov-2012.
Start production: 1-Nov-2012
Project status: In progress (0%)
Brief description of project: The aim of the present project is apply molecular dynamics (MD) techniques to investigate how the different features of chondroitin sulphate (CS) and dermatan sulphate (DS) drive their mechanical properties and in particular their resistance to compression.
Types of support work undertaken: Account creation
Difficulties encountered and solution: The team were hoping to use the software program ACEMD, which is highly optimised for GPU clusters. Unfortunately, due to licensing issues, this program can no longer be used and has had to be replaced with NAMD.

Project Acronym: AuPd-Seg
Accepted by DECI Call: DECI-9
PRACE Home site: CINES
PRACE Execution site: RZG
PRACE Enabling sites: None
PRACE Architectures: Hydra
Start enabling: None
Start production: November 2012
Project status: In progress (81%)
Brief description of project: Study the structure, chemical order and the reactivity of Au-Pd surface nanoparticles under vacuum and in the presence of adsorbates.
Types of support work undertaken: None
Difficulties encountered and solution: None

Project Acronym: FORSQUALL
Accepted by DECI Call: DECI-9
PRACE Home site: CINES
PRACE Execution site: EPCC
PRACE Enabling sites: None
PRACE Architectures: HeCToR
Start enabling: None
Start production: November 2012
Project status: In progress (%)
Brief description of project: Modelling a probabilistic forecast system of squall lines based on a regional ensemble modelling system and state of the art data assimilation techniques that use satellite observation.
Types of support work undertaken: None
Difficulties encountered and solution: None

Project Acronym: IONGATE
Accepted by DECI Call: DECI-9
PRACE Home site: CINES
PRACE Execution site: UIO
PRACE Enabling sites: None
PRACE Architectures: Abel

Start enabling:
Start production: November 2012
Project status: In progress (32%)
Brief description of project: Study of the ion-gating mechanism through atomistic Molecular Dynamics (MD) simulations of pentameric and trimeric Ligand-gated ion channels (LGIC) with an explicit treatment of the solvent and the membrane environment. This study will lead to better understanding of the role of LGICs in the intercellular communications in the brain.
Types of support work undertaken: None
Difficulties encountered and solution: None

Project Acronym: NPR-LQCD
Accepted by DECI Call: DECI-9
PRACE Home site: CINES
PRACE Execution site: CINECA
PRACE Enabling sites: None
PRACE Architectures: PLX
Start enabling: None
Start production: November 2012
Project status: In progress (75%)
Brief description of project: The project goal is to compute renormalization constants for non local fermionic bilinear operators with four dynamical quarks in the sea (Nf=4), involved in the computation of matrix elements used to extract nucleon structure functions. A proper comparison of these matrix elements with experimental values represents both a challenge and an opportunity for lattice QCD (Quantum Chromodynamics).
Types of support work undertaken: None
Difficulties encountered and solution: None

Project Acronym: NMRCONF
Accepted by DECI Call: DECI-9
PRACE Home site: CSC (external)
PRACE Execution site: CSCS
PRACE Enabling sites: CSC, CSCS
PRACE Architectures: Cray XE6
Start enabling: November 2012
Start production: January 2013
Project status: In progress (54%)
Brief description of project: This project uses Gromacs-PLUMED simulations and NMR spectroscopy to describe conformational changes in proteins.
Types of support work undertaken: Users were helped with accessing the execution site and porting their software to there.
Difficulties encountered and solution: None

Project Acronym: CompSym
Accepted by DECI Call: DECI-9
PRACE Home site: CSC
PRACE Execution site: CSCS
PRACE Enabling sites: CSC
PRACE Architectures: Cray XE6
Start enabling: November 2012
Start production: November 2012

Project status: In progress (63%)
Brief description of project: This project uses the Gromacs simulation software to study interaction of drug delivery liposomes with opsonin proteins.
Types of support work undertaken: Users were helped with accessing the execution site.
Difficulties encountered and solution: None

Project Acronym: Planck-LFI2
Accepted by DECI Call: DECI-9
PRACE Home site: CSC
PRACE Execution site: CSC
PRACE Enabling sites: CSC
PRACE Architectures: Cray XT, Cray XC30
Start enabling: November 2012
Start production: November 2012
Project status: In progress (17%)
Brief description of project: Planck is a mission of the European Space Agency (ESA) to map the anisotropies of the cosmic microwave background with the highest accuracy ever achieved. Computational resources for this work were provided through this DECI project.
Types of support work undertaken: The number of users in the project is over 20, which caused in itself a lot of administrative work for PRACE-2IP experts. Typical amount of users in a DECI project is 2–5, so Planck-LFI2 is 4–10 times larger. Most support tasks dealt with porting applications to the Cray XT and Cray XC30 machines of CSC.
Difficulties encountered and solution: There were three things that required a larger amount of support. First, in October 2012, one of the applications (CosmoMC) was configured to use the GSL library. It took some time to realise that none of the GSL versions available on Louhi were compatible with the compiler that was in use (Intel). The solution was to install a custom version of GSL in the user's application directory.

Second, in December 2012, it turned out that the newest version of CosmoMC required a newer version of the Intel compiler than was available. The reason was that the new version of the software was written in Fortran 2008. Using a different compiler collection wasn't an option because they didn't support the application's requirements any better. No further compiler updates were installed on the old system, so the solution was to move CosmoMC simulations to the new Cray XC30 once it was available. The new system had the newest possible compiler collections from all vendors, so the problem was easily solved that way. CSC gave assistance with this in January 2013. In March 2013, a problem turned up: CosmoMC cannot be run in hybrid MPI-OpenMP mode. The parallel launcher, aprun, cannot place threads well into cores if a program is built with the Intel compiler (as it is in this case). In April, a workaround was developed by CSC and Cray, which solved the problem in case of one MPI task per socket (two per node). This means that CosmoMC can be run in hybrid MPI-OpenMP mode, which speeds up the investigators' work. More MPI tasks wouldn't have made the same effect: they only add more statistics, but not make computations faster. Now the CosmoMC computations are run using eight OpenMP threads per one MPI task. According to earlier experience, four threads would perform better, but it cannot be used right now.

Third, in May 2013 one of the applications (LevelS) started to fail although it worked fine in February of the same year. Lot of effort was used to spot the error, first by CSC and later by Cray. The cause of the problem was finally simple: the application was not started with the parallel launcher aprun, but with the "system()" command on the compute node. In such a case, there are three ways to compile the application:

1. load the craype-target-native module before compiling the code;

2. add the -target=native option to the cc, CC, or ftn command; or
3. call the underlying compiler directly (gcc, gfortran, icc, ifort, craycc, crayCC, crayftn).

Project Acronym: LCRR
Accepted by DECI Call: DECI-9
PRACE Home site: CSCS
PRACE Execution site: EPCC and SNIC-KTH
PRACE Enabling sites: none
PRACE Architectures: BG/Q and Cray XE6
Start enabling:
Start production: 1 October 2012
Project status: in progress
Brief description of project: The aim of the proposal is to apply local control theory (LCT) to simulate the manipulation of the photopigment rhodopsin, a transmembrane receptor that is part of the protein family called G protein-coupled receptors (GPCRs). Important for this proposal is that this protein plays a central role in vision, for which the early dynamics are dominated by the cis-trans isomerisation of the retinal chromophore
Types of support work undertaken: none
Difficulties encountered and solution: The project was mainly interested in the allocation on the BG/Q however as of today it is still not clear how much of this resources have been used. In January 2013 the project still had no access to the BG/Q.

Project Acronym: LBSCOM
Accepted by DECI Call: DECI-9
PRACE Home site: EPCC
PRACE Execution site: CSC
PRACE Enabling sites: EPCC, CSC
PRACE Architectures: Cray XE6
Start enabling: 01/11/12
Start production: 01/11/12
Project status: In progress (81%)
Brief description of project: This project involves Lattice Boltzmann Simulation of Soft matter systems such as liquid crystals or DNA.
Types of support work undertaken: Support in getting accounts set up at CSC and advising on the planning of production runs to fit in with the closing of Louhi (Cray XE3) and the starting of Sisu (Cray XC30).
Difficulties encountered and solution: Some delays in getting accounts set up. These were resolved with assistance from CSC.

Project Acronym: ESM4OED
Accepted by DECI Call: DECI-9
PRACE Home site: EPCC
PRACE Execution site: EPCC
PRACE Enabling sites: EPCC
PRACE Architectures: Cray XE6
Start enabling: 01/11/12
Start production: 01/11/12
Project status: In progress (62%)
Brief description of project: This is an industrial project involving the investigation of Self-assembled monolayers (SAMs).

Types of support work undertaken: Support was given in getting the project set up to run VASP on HECToR.
Difficulties encountered and solution: None.

Project Acronym: TB-Drugs-In_silico
Accepted by DECI Call: DECI-9
PRACE Home site: FZJ
PRACE Execution site: CINECA
PRACE Enabling sites: CINECA
PRACE Architectures: PLX
Start enabling: Nov-12
Start production: Dec-12
Project status: In progress (2%)
Brief description of project: Tuberculosis (TB) is one of the most important infectious diseases in the world, for which every year approximately 2 million people die, especially in developing countries. Key point in this project is to perform the Virtual Screening (VS) and further Structure Based Drug Design based on the analysis of predicted protein-drug complex, for this part of the general project, which involves performing Molecular Dynamics and high throughput Docking calculations to perform the VS. It is expected that the successful outcome of the project will provide i) a general strategy for the performance of massive VS projects and more important ii) a short-list of 10-20 small drug like molecules to be tested in-vitro (and in-vivo) for their potential to inhibit the target enzymes (and if possible mycobacterial growth) to be used as new lead compounds for fighting this disease.
Types of support work undertaken: The project is supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ is in contact with the project over run-time to monitor the status. Enabling work for the establishment of the workflow and installation of software was envisaged. This is described in the Applications Enabling section.
Difficulties encountered and solution: No problems occurred.

Project Acronym: MoMoGal
Accepted by DECI Call: DECI-9
PRACE Home site: FZJ
PRACE Execution site: EPCC, UIO
PRACE Enabling sites: -
PRACE Architectures: HeCToR XE6, Abel
Start enabling: -
Start production: Nov-12
Project status: In progress (32%)
Brief description of project: The goal of the project is to implement an improved treatment of the cold interstellar medium, star formation and feedback in cosmological simulations, improving upon previous work in order to produce self-consistent maps of CO, H2 and C+ for massive, high-redshift galaxies. The project will apply new subgrid physics models to two high-resolution simulations of galaxy formation (one quiescent disk, and a merging galaxy pair at $z \geq 2$) capable of resolving the spatial scales characteristic of GMCs. These simulations will be used to make predictions for, and interpret results from, forthcoming ALMA (Atacama Large Millimeter/sub-millimeter Array) observations of massive, high-redshift galaxies.
Types of support work undertaken: The project is supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts

have been distributed to the execution-sites via the PRACE-LDAP. FZJ is in contact with the project over run-time in case of difficulties and to monitor the status.
Difficulties encountered and solution: After project-start it turned out that the execution-system HeCToR had not enough main memory for parts of the production runs. Therefore in collaboration with WP2 a second execution-system has been allocated to the project, which is Abel at UIO.

Project Acronym: Reactive_Ceria
Accepted by DECI Call: DECI-9
PRACE Home site: ICHEC
PRACE Execution site: FZJ (1.5M)
PRACE Enabling sites: no enabling site
PRACE Architectures: x86 (Juropa)
Start enabling:
Start production: 11/2012
Project status: In progress (100% burned)
Brief description of project: Ab initio (VASP) study of new ceria oxidation catalysis and surface doping.
Types of support work undertaken: N/A
Difficulties encountered and solution: not aware of any

Project Acronym: Si_Interfaces
Accepted by DECI Call: DECI-9
PRACE Home site: ICHEC
PRACE Execution site: CINES (2.49M)
PRACE Enabling sites: none
PRACE Architectures: x86 (Jade)
Start enabling:
Start production: 6/2013
Project status: Completed/In progress (%)/Waiting to start
Brief description of project: Ab initio (VASP) project to investigate the interface between amorphous and crystalline silicon in core-shell nanowires on photovoltaic properties.
Types of support work undertaken: none
Difficulties encountered and solution: not aware of any

Project Acronym: SPH-WEC
Accepted by DECI Call: DECI-9
PRACE Home site: ICHEC
PRACE Execution site: CSCS (1.215M) & NCSA (405k)
PRACE Enabling sites: No enabling sites
PRACE Architectures: Cray (ROSA) and BlueGeneQ
Start enabling:
Start production: 11/2012
Project status: In progress (40% burned)
Brief description of project: Modelling of Wave Energy Convertors using computational fluid dynamics and smoothed particle hydrodynamics code.
Types of support work undertaken: none
Difficulties encountered and solution: Transferred time from NCSA to CSCS due to poor scaling on IBM BG/Q

Project Acronym: AIMD-PAF

Accepted by DECI Call: DECI-9
PRACE Home site: NCSA
PRACE Execution site: EPCC
PRACE Enabling sites: NCSA
PRACE Architectures: Blue Gene Q
Start enabling: April 2013
Start production: February 2013
Project status: In progress (40%)
Brief description of project: The biggest problem facing the practical use of hydrogen in fuel-cell powered automobiles is its storage. Hydrogen can be stored in many ways: in gas cylinders, in cryogenic tanks as a liquid or in solid materials – in the form of metal hydrides or adsorbed on high surface area sorbents. The first two methods are conventional technologies with several limitations the most important of which is their low energy efficiencies. Nowadays most of the scientific studies are focused on high surface area sorbents in which hydrogen can be stored by physisorption. The relative weakness of this kind of physical interactions between sorbent and hydrogen can provide reversibility of the process, which is necessary for mobile applications. The goal in hydrogen storage is gravimetric capacity of more than 6% by weight at ambient temperature and pressure, which can be estimated by the surface area and binding energy to hydrogen. Searching for a suitable material for hydrogen storage we used both of the techniques for increasing of enthalpy of adsorption and modelled a system in which two of the carbon atoms in the benzene ring were substituted with boron (Li2C4H6) and added two Li atoms preserving the aromatic nature of the system. The project suggests a modifyed known porous material (PAF-1) suitable for hydrogen storage. It has significant advantage over recently investigated MOF and COF systems, as it is light and has large surface area. The modeled system will be stable on hydrogenation and aggregation of Li atoms. Furthermore, there are no ab-initio calculations for such systems in the literature. That is why we propose performing first principle calculations on the periodic 3D structure of the tunned PAF-1in order to obtain more reliable and actual understanding on the adsorption of hydrogen on porous structures and the stability of the proposed material at different temperatures and pressures.
Types of support work undertaken:
Difficulties encountered and solution: The CP2K does not have makefile for Blue Gene Q. The proper IBM BlueGene/Q XLF90 compiler has been set and linker options have been selected adequately.

Project Acronym: CoStAFuM
Accepted by DECI Call: DECI-9
PRACE Home site: SNIC-KTH
PRACE Execution site: UiO, RZG
PRACE Enabling sites: SNIC-KTH, UiO, RZG
PRACE Architectures: Sandy Bridge
Start enabling: 11/12
Start production: 3/13
Project status: In progress (21% at UiO)
Brief description of project: Computational Studies of Advanced Functional Materials (CoStaFuM) deals with state-of-the-art computational materials science methods applied to advanced functional materials. The project aims to study the (i) correlated electron system, (ii) graphene and molecular-interface systems, (iii) lattice dynamics and (iv) core shell structures and nanoparticles.

These topics will be studied by ab initio density functional theory based methods implemented in codes like VASP and SIESTA. For some appliations, in-house codes such as SCAILD for lattice dynamics and Rspt for dynamical mean field theory will be used.
Types of support work undertaken: Account setup and software install, debugging grid-ftp problems between RZG and the door node at LRZ.
Difficulties encountered and solution: Users were new to certificates and needed some start-up time.
File transfer problems to Hydra could be solved with the support. Still a more flexible data transfer model within PRACE for users who don't have their date already within the PRACE network would be highly desirable.

Project Acronym: DifVib
Accepted by DECI Call: DECI-9
PRACE Home site: SNIC-KTH
PRACE Execution site: SNIC-KTH, EPCC
PRACE Enabling sites: SNIC-LiU, SNIC-UmU, SNIC-KTH, EPCC
PRACE Architectures: Cray XE6
Start enabling: 11/12
Start production: 11/12 at SNIC-KTH
Project status: In progress (65% at SNIC-KTH)
Brief description of project: Transition metal nitrides (TMN), such as TiN and ZrN, are important technological materials owing to their outstanding mechanical, electrical, and corrosive-resistant properties, in combination with applicability in industrial-scale thin film deposition systems. In continuation of the DECI-7 project DiSMuN this project conducts again pioneering theoretical work on the diffusion of adatoms on different crystal surfaces of TiAlN and aims to study aspects of diffusion in nitrides, focusing on TiAlN, ZrAlN and HfAlN. To investigate atomic diffusion in these materials electronic structure codes are used to calculate the energy barriers needed to be overcome by diffusing species, both inside bulk materials and on top of crystal surfaces.
In a second part of the project related to Earth's core structure the project targets completely disordered alloy phases of Fe-Ni and Fe-Ni-Si using special quasirandom structure method in first-principles simulation. This method is based on a new technique developed to study vibrational thermodynamics from first-principles at high pressure and high temperatures. Although the technique is developed from the theoretical point of view, the code of realisation is yet to be finished and the enabling help of PRACE experts is needed in order to obtain greater scalability in parallelization of the applied codes.
Types of support work undertaken: Account creation, several meetings (partly physical) on enabling work.
Difficulties encountered and solution: None.

Project Acronym: HydFoEn
Accepted by DECI Call: DECI-9
PRACE Home site: SNIC-KTH
PRACE Execution site: UHEM
PRACE Enabling sites: SNIC-KTH, UHEM
PRACE Architectures: Intel Nehalem
Start enabling: 11/12
Start production: 02/13
Project status: In progress
Brief description of project: Our energy-hungry world has become increasingly depending on new methods to store and convert energy for new, environmentally friendly modes of

transportation and electrical energy generation as well as for portable electronics. Hydrogen would be ideal as a synthetic fuel for transport vehicles because it is lightweight, highly abundant and its oxidation product (water) is environmentally benign. However, the storage of hydrogen remains a problem and hinders the highly desirable development in this direction. The project on hydrogen storage materials for energy applications deals with studying the interaction of hydrogen with novel materials having multiple length scales such as clusters, nano-particles, nano-tubes, multi-layers, and crystalline bulk. The materials include light metal hydrides such as alkali-alanates and boro-hydrides and Metal organic frameworks. Due to the light weight of these materials, the gravimetric density of hydrogen is higher than that in the inter-metallic hydrides. Although these materials are regarded as potential candidates for a new generation of hydrogen storage materials and are critical to a new hydrogen economy, very little fundamental understanding is available about the nature and strength of hydrogen bonding, the influence of catalysts on the uptake and release of hydrogen and the effect of nanostructuring on the thermodynamics of hydrogen.
This project aims at providing this fundamental understanding by carrying out first principles calculations based on density functional theory.
Types of support work undertaken: Accounts created, providing GAUSSIAN 09 and VASP 5
Difficulties encountered and solution: Certificate login was perceived as complicated. PI didn't even try to login before February this year.

Project Acronym: GanDaLF
Accepted by DECI Call: DECI-9
PRACE Home site: RZG
PRACE Execution site: UIO
PRACE Enabling sites: RZG
PRACE Architectures: Sandy Bridge@2.6
Start enabling: 11/2012
Start production: 03/2013
Project status: In progress (10%)
Brief description of project: *Galaxies and Dark- and Luminous-matter Feedback: the origin of cosmic structures and the effects of feedback processes during cosmological evolution.* The starting point of any investigation on the origins of cosmic structures and feedback mechanisms is the detailed calculation of the most relevant physical processes, i.e. gravity, hydrodynamics, chemistry evolution, and radiative transfer. Then, higher-order complications can derive from molecular evolution at early times, metal production in stellar cores, metal pollution of the cosmic medium, turbulence, establishment of large-scale magnetic fields, cosmic rays, tidal torques, and angular momentum acquisition. All these phenomena should take place and interact with each other during the growth of cosmological structures. The main difficulties in properly following such processes at early and late cosmological times are related to their high non-linearity. In this project, numerical Nbody, hydrodynamic, chemistry, radiative simulations taking into account all the aforementioned processes are run to understand cosmic structure formation. This allows to provide the scientific community with a set of complete, selfconsistent, but computationally expensive, state-of-the-art simulations, which will be a fundamental tool to better understand the build-up of the observed cosmic structure and the role played by the various physical processes during cosmological evolution.
Types of support work undertaken: General support provided, account creation, contact with PI and execution site to solve some software problems and problems with certificates.
Difficulties encountered and solution: None.

Project Acronym: PTACRB

Accepted by DECI Call: DECI-9
PRACE Home site: RZG
PRACE Execution site: ICHEC
PRACE Enabling sites: RZG
PRACE Architectures: Intel Westmere EP@2.67
Start enabling: 11/2012
Start production: 12/2012
Project status: In progress (66%)
Brief description of project: *Identifying Proton Pathways in a Multi-Drug-Resistance Membrane Transporter by EVB-MD Simulations.* The emergence of multi-drug resistance in pathogenic bacteria is a threat to human health on a global scale. Resistance is in part conferred by an array of proteins in the bacterial membranes whose function is to remove a variety of toxic compounds from the cell interior - for example, man-made antibiotics. Multi-drug resistance transporters have been identified in several membrane protein subfamilies. For example, the main drug-efflux pump in *Escherichia coli*, termed AcrB, is a member of the so-called RND family. Importantly, to power this complex mechanism AcrB harvests the energy stored in the membrane in the form of an electrochemical gradient of H+. With a systematic series of umbrella-sampling molecular dynamics simulations, the potential of mean force associated with H+ movement is calculated. To simulate the dynamics of the permeating H+, the most up-to-date implementation of the Multi-State Empirical Valence Bond method is used in combination with the CHARMM molecular-mechanics force field. In sum, the project will employ state-of-the-art methods to reveal a level of mechanistic insight not yet attained for any H+-driven membrane transporter, and in particular the multi-drug resistance efflux pump AcrB. These investigations will be carried out in parallel with novel experimental work, both at the functional and structural levels.
Types of support work undertaken: General support provided, account creation.
Difficulties encountered and solution: None.

Project Acronym: SPSC
Accepted by DECI Call: DECI-9
PRACE Home site: GRNET (UPAT)
PRACE Execution site: FZJ Europa
PRACE Enabling sites: GRNET (UPAT)
PRACE Architectures: Intel (No GPU)
Start enabling: 01/11/2012
Start production: 01/02/2013
Project status: In progress (80%)
Brief description of project: The project aims in modeling at the atomistic scale micro-crystalline silicon (μc-Si) thin films and poly(3-Hexylthiophene) (P3HT). The simulation of μc-Si will be performed in two stages. Initially films will grow using our Kinetic Monte Carlo (KMC) scheme until they reach a thickness in the order of several tens on nanometers. At the second stage the resulting films will be subjected to an atomistic simulation study to restore the atomistic details lost or ignored in the KMC model. Succesive loops of KMC and atomistic MD (the atomistic model will be backmapped to the KMC) will allow us to generate films in the order of hundreds of nanometers. For the simulation of the P3HT at first, we aim to *separately* study the crystalline and amorphous phase of these systems by conducting detailed atomistic molecular dynamics (MD) simulations with relatively large systems (100000 atoms) with molecular lengths corresponding to approximately 60 thiophene rings. The scope behind these simulations is to generate fully relaxed structures for both phases (crystalline and amorphous) characterized by realistic density and conformational properties, and low potential energy over a wide range of temperatures. At a second stage, we intend to

extend the simulations to larger crystal dimensions and higher MWs of Rr-P3HT. To this, we will initially design and implement an atomistic parallel-tempering Monte Carlo (MC) algorithm combined initially with a crude molecular model capable of simulating realistically the semi-crystalline nature of the system (corresponding to the development of both crystalline and amorphous regions in the material).
Types of support work undertaken: For the KMC simulations we have generated a FORTRAN code which has been parallelized via MPI. Using the modules (parastation/mpi2-intel-5.0.26-1) by the local host we have benchmarked our code and we are obtaining almost linear scaling in using up to 512 processors. We have performed 4 production runs (512 cores, 24h), at different experimental conditions, generating 4 samples with average film thickness of ≈50nm. We increased the number of used processors in the KMC model when modeling systems of larger size, with thickness larger than 100nm and reached the 1024 cores mark. For the second stage we modified the open-source MD simulation program LAMMPS so as to include the Si-H interactions and we asked the local host to install it on the Supercomputer. Since we are simulating large systems (system size> 1.000.000 atoms) the simulations scale very good, obtaining almost linear scaling up to 1024 cores. Using the modified LAMMPS version we have employed MD simulation at the two larger samples of total duration 2ns. This corresponds at 8 runs of 512 cores with duration of 24h in each run. As soon as the resulting surfaces obtain local equilibrium we back-maped to the KMC model the resulting structures so as to further grow the films at 100nm. For the simulations of P3HT we have generated initial structures of high molecular weight for both crystalline and amorphous phase. We are currently finishing the last production runs on the maximun possible system size.
Difficulties encountered and solution:

Project Acronym: HiSSor
Accepted by DECI Call: DECI-9
PRACE Home site: UHeM
PRACE Execution site: RZG, EPCC
PRACE Enabling sites:
PRACE Architectures: SandyBridge cluster @RZG, BG/Q @EPCC
Start enabling:
Start production: January 2013 for RZG, May 2013 for EPCC
Project status: In progress (6%)
Brief description of project: Scientists are working on design and implementation of new hybrid algorithm and solver for large sparse linear systems. they focus on scalable direct solvers. They design a new parallel algorithm HybridSuperLU 1.0 for large scale server systems containing fat nodes. HybridSuperLU 1.0 is utilizing the MPI+OpenMP hybrid programming approach. They plan to compare the effectiveness of the hybrid algorithm with the state of the art sparse direct solvers MUMPS, Pardiso and SuperLU_DIST Version 3.1.
Types of support work undertaken: Enabling accounts, installation programs.
Difficulties encountered and solution:

Project Acronym: MPI-FETI
Accepted by DECI Call: DECI-9
PRACE Home site: VSB-TUO
PRACE Execution site: EPCC
PRACE Enabling sites: VSB-TUO
PRACE Architectures: Cray XE6 “HeCToR“
Start enabling:
Start production: 5. 12. 2012

Project status: In progress (4%)
Brief description of project: Massively parallel implementation of Total-FETI algorithms

FETI methods are very successful for the solution of large scale engineering problems. The reason is that duality reduces large primal problem to smaller dual, relatively well conditioned strictly convex iteratively solved quadratic programming problem. Total-FETI-1 (TFETI-1) simplifies the inversion of stiffness matrices of subdomains by using Lagrange multipliers not only for gluing the subdomains along the auxiliary interfaces, but also for the enforcement of the Dirichlet boundary conditions.

Our research deals with parallel implementations of TFETI-1 algorithm for problems in non-linear and contact mechanics using PETSc and Trilinos frameworks. The main goal of our research is to develop new generation of algorithms for efficient solution of very large and complex problems in engineering on upcoming multi-petascale systems. Current experiments show that our codes scale up to thousands of cores and the main goal of the proposed project is their performance analysis, comparison and optimization on large scale parallel architectures to further improve the scalability up to tens of thousands of cores and hundreds of millions of unknowns. The performance of the codes will be tested on the solution of huge real world or model problems. For the performance analysis and optimization we are going to use some established performance analysis tools like Scalasca.

Some of the bottlenecks of the TFETI-1 codes are already known. The natural effort to reduce the computational and memory requirements for subdomain problems' solution decomposing domain into large number of subdomains (thus reducing the local primal dimension) leads to increase of the dual and null space dimension. This affects the time needed for the coarse problem solution and natural coarse space matrix-vector multiplication appearing in the application of orthogonal projectors, the reconstruction of the primal solution from the dual one etc. However there is a lot of space for an optimization. For example the coarse problem can be solved in many ways - directly using the Cholesky factorization, iteratively using the conjugate gradient method, using the explicit inverse computation, or this problem can be even eliminated through the natural coarse space matrix orthonormalization using Gram-Schmidt process. All these approaches can be performed either sequentially by master process, or in parallel on each of processes.

Thus the objectives of the proposed project are to analyze an impact of various data distribution on the algorithm performance, to implement various parallelization of TFETI-1 coarse problem solution and to compare these approaches as well as to compare the implementations in PETSc and Trilinos frameworks. These frameworks should be good choice for interfacing of implemented codes to existing engineering codes for their application to solution of real world problems.

Types of support work undertaken: General support with obtaining certificates.
Difficulties encountered and solution: None.

Project Acronym: NPT_MC
Accepted by DECI Call: DECI-9
PRACE Home site: VSB-TUO
PRACE Execution site: UHeM
PRACE Enabling sites: VSB-TUO
PRACE Architectures: x86 cluster “Karadeniz”
Start enabling:
Start production: 10. 12. 2012
Project status: In progress (20%)

Brief description of project: Molecular clusters – non zero pressure Monte Carlo simulations. The project is focused on the modelling of thermodynamic and structural properties of small clusters consisting of several through tens of water molecules. More specifically, classical Monte Carlo methods enhanced with the parallel-tempering scheme and two-dimensional multiple histograms will be used to calculate enthalpies, heat capacities, and selected structural parameters of water clusters containing 17 – 22 molecules (a size region within which a transition from the all-molecules-on-the-surface structures to one-molecule-in-center structures takes place) with the main emphasis on the phase changes in this clusters. A full pressure-temperature phase diagrams will be obtained. In addition, selected larger clusters (up to 50 molecules) will also be studied to get a deeper insight into temperature and pressure induced structural transformations and their evolution with cluster size. In last two decades, a lot of theoretical studies on thermodynamic properties have been published. However, the studies almost exclusively focus on constant volume – constant energy (NVE) or constant volume – constant temperature (NVT) calculations, and only a few papers describe molecular clusters at non-zero pressures. The main goal of the present project is to fill this gap.

For the modelling of water clusters under non-zero pressures, we will use the parallel tempering Monte Carlo algorithm, originally developed for the NVT and NVE statistical ensembles and later modified for the NPT ensemble. A classical thermodynamic Monte Carlo simulation performed for a given temperature/energy and volume/pressure employs Markov's chains and is, thus, inherently a serial process. Calculations performed for different temperatures/energies and volumes/pressures can be, on the other hand, straightforwardly parallelized. For example, a parallel tempering approach has been recently proposed for the NVT ensemble, which significantly accelerates convergence by simulating a bunch of systems at different temperatures in parallel and occasionally exchanging information (configurations) between different systems. Later on, parallel tempering approach has been extended to the NPT ensemble. In that case, hundreds of systems are simulated at different temperatures and pressures in parallel and exchanges of configurations and volumes between randomly selected systems take place periodically. This computationally demanding algorithm is predestined for an MPI parallelization when, ideally, each system is simulated on its own core. As a result, one obtains the values of measured thermodynamic parameters for all the temperatures and pressures included at once.

In addition, thermodynamic properties depending on cluster configurations through the internal energy and volume (like the enthalpy or the heat capacity) will be calculated using multiple histogram methods, originally developed for the NVT ensemble and recently extended to the NPT ensemble in our group. Two dimensional, energy-volume histograms pre-calculated for each simulated system form an input to this algorithm and, as a result, classical two-dimensional density of states is obtained as a function of volume and energy. From the density of states, one can simply obtain the value of the thermodynamic quantity at an arbitrary temperature and pressure by a computationally cheap two-dimensional integration. If this integration is repeated for a sufficiently dense grid of temperatures and pressures, one obtains a smooth dependence of the calculated parameter on the temperature and pressure.

Types of support work undertaken: General support with obtaining certificates and login procedures. Support with job submitting/scheduling/monitoring at exec site.
Difficulties encountered and solution:

- Problems with limits on queues in exec site's scheduler (too small to allow to run PI jobs). Solved/reconfigured with staff from exec site.
- Inability to access the exec system at all for four months after exec site's change in network topology (joining PRACE internal network). Still in progress - TTS tickets, coordination with PRACE operations, exec site staff. So far no result.

8.4 Summary of Technical Support for DECI-10 Projects

Project Acronym: AIDMP
Accepted by DECI Call: DECI-10
PRACE Home site: BSC
PRACE Execution site: FZJ
PRACE Enabling sites: none
PRACE Architectures: Nehalem
Start enabling: -
Start production: 01-Jun-2013
Project status: In progress 10%
Brief description of project: Ab-initio design of mutant proteins
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: fplb
Accepted by DECI Call: DECI-10
PRACE Home site: BSC
PRACE Execution site: WCSS
PRACE Enabling sites:
PRACE Architectures: Supernova (XEON X5650@2.67)
Start enabling: June 2013 (WCSS)
Start production: 1 June 2013 (WCSS)
Project status: In progress (10%)
Brief description of project: Interaction of a homologous series of fluorescent probes with different lipid bilayers
Types of support work undertaken:
- BSC: Account management
- WCSS: as the exec-site and is performing every-day support. The accounts were created on the Supernova cluster based on the PRACE LDAP entries at SURFSara. The users were assisted and consulted with the best practices for running jobs on Supernova using the code GROMACS. Some issues with jobs configurations were analyzed and resolved.
Difficulties encountered and solution: None.

Project Acronym: Novel_Anticoagulants
Accepted by DECI Call: DECI-10
PRACE Home site: BSC
PRACE Execution site: CINECA
PRACE Enabling sites: none
PRACE Architectures: GPU Cluster
Start enabling: -
Start production: 01-Jun-2013
Project status: In progress 10%
Brief description of project: Discovery of Novel Anticoagulants
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: SPAITAC
Accepted by DECI Call: DECI-10
PRACE Home site: BSC
PRACE Execution site: EPCC

PRACE Enabling sites: none
PRACE Architectures: XE6
Start enabling: -
Start production: 01-Jun-2013
Project status: In progress 10%
Brief description of project: Seasonal Prediction of the Arctic Ice and Tropical Atlantic Cyclones
Types of support work undertaken: Account management
Difficulties encountered and solution: None

Project Acronym: ERPP
Accepted by DECI Call: DECI-10
PRACE Home site: CINECA
PRACE Execution site: CYFRONET
PRACE Enabling sites: CYFRONET
PRACE Architectures:
Start enabling: 1-Jun-2013
Start production: 1-Jun-2013
Project status: Waiting to start.
Brief description of project: Exact Regularized Point Particle Method for the momentum coupling in particle-laden turbulent flows
Types of support work undertaken: Account creation.
Difficulties encountered and solution: None so far.

Project Acronym: MOTUS
Accepted by DECI Call: DECI-10
PRACE Home site: CINECA
PRACE Execution site: ICM
PRACE Enabling sites: ICM
PRACE Architectures:
Start enabling: 1-Jun-2013
Start production: 1-Jun-2013
Project status: Waiting to start
Brief description of project: A High-Resolution Modelling Study of the Turkish Straits System Utilizing HPC
Types of support work undertaken: Account creation.
Difficulties encountered and solution: None so far.

Project Acronym: CONVDYN13
Accepted by DECI Call: DECI-10
PRACE Home site: CSC
PRACE Execution site: RZG
PRACE Enabling sites: CSC
PRACE Architectures: Intel Xeon cluster
Start enabling: May 2013
Start production:
Project status: Waiting to start
Brief description of project: This project uses the Pencil software to study convection-driven dynamos in rapidly rotating late-type stars. An example of such a star is the Sun during its first billion years.
Types of support work undertaken: Users were helped with accessing the execution site.

Difficulties encountered and solution: None

Project Acronym: HIV1-GSL
Accepted by DECI Call: DECI-10
PRACE Home site: CSC
PRACE Execution site: EPCC
PRACE Enabling sites: CSC
PRACE Architectures: Cray XE6
Start enabling: May 2013
Start production: May 2013
Project status: In progress (10%)
Brief description of project: This project uses the Gromacs software to study functional roles of glycosphingolipids in modulating entry of human immunodeficiency virus type 1 (HIV-1) into host cell. In addition to the role of glycosphingolipids as facilitators of HIV infection, some of them can act as a natural resistance factor for HIV prevention.
Types of support work undertaken: Users were helped with accessing the execution site.
Difficulties encountered and solution: None

Project Acronym: HyVaMPI
Accepted by DECI Call: DECI-10
PRACE Home site: CSC
PRACE Execution site: UiO
PRACE Enabling sites: CSC
PRACE Architectures: Intel Xeon cluster
Start enabling: May 2013
Start production:
Project status: Waiting to start
Brief description of project: This project uses a novel plasma code, Vlasiator, to study plasma dynamics in the Earth's space environment. The aim is too facilitate the future numerical forecast of space weather, which affect spacecraft and space-based technological solutions for positioning and communications.
Types of support work undertaken: Users were helped with accessing the execution site.
Difficulties encountered and solution: None

Project Acronym: NANODROPS
Accepted by DECI Call: DECI-10
PRACE Home site: CSC (external)
PRACE Execution site: EPCC
PRACE Enabling sites: CSC
PRACE Architectures: Cray XE6
Start enabling: May 2013
Start production:
Project status: Waiting to start
Brief description of project: This project uses molecular dynamics (Gromacs software) and dissipative particle dynamics (own DPD code) to study the interaction of triglycerides and nanoparticles with lipid biomembranes.
Types of support work undertaken: Users were helped with accessing the execution site.
Difficulties encountered and solution: None

Project Acronym: Dissipative_Phenomena
Accepted by DECI Call: DECI-10

PRACE Home site: EPCC
PRACE Execution site: EPCC
PRACE Enabling sites: -
PRACE Architectures: ICE-Advance (BGQ)
Start enabling: -
Start production: -
Project status: in progress (0%, just started)
Brief description of project: Dissipative phenomena on Local Group dwarf galaxies. The purpose is this study is to investigate the interplay between environment and internal processes in the star formation history of dwarf galaxies neighbouring a hosting system. In particular the goal is to explore the environmental effects on the formation and evolution of dwarf galaxies in relation with the properties of the hosting environment.
Types of support work undertaken: general support so far, including account creation, initial meeting with PI.
Difficulties encountered and solution: none.

Project Acronym: GalChem
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: SURFSara
PRACE Enabling sites: EPCC, SURFSara
PRACE Architectures: Bullx SandyBridge
Start enabling: 01/05/13
Start production: 01/05/13
Project status: In progress (0 %)
Brief description of project: The project is to run Milky Way-type simulations with a view to running more realistic Milky Way simulations.
Types of support work undertaken: Assistance with using gsissh to access the machine at SURFSara.
Difficulties encountered and solution: Some delays in access via gsissh but underway now.

Project Acronym: Galsim
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: CSC
PRACE Enabling sites: EPCC, CSC
PRACE Architectures: Cray XC30
Start enabling: 01/05/13
Start production: 01/05/13
Project status: Waiting to start
Brief description of project: Understanding the formation and clustering properties of galaxies using N-body simulations
Types of support work undertaken: Only assistance in getting accounts so far
Difficulties encountered and solution: Some delays in PI getting hold of a grid certificate. These are not yet resolved.

Project Acronym: HIGHERFLY
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: EPCC
PRACE Enabling sites: EPCC

PRACE Architectures: Cray XE6
Start enabling: 01/05/13
Start production: 01/05/13
Project status: In progress (0 %)
Brief description of project: The project aim is to perform high-fidelity fluid-structure interaction simulations of insect and bio-inspired micro-air-vehicle flight. This is a follow-on project from the DECI-7 HIFLY project.
Types of support work undertaken: This project follows on from a previous DECI project and require no assistance to continue running.
Difficulties encountered and solution: None.

Project Acronym: InterDef
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: SURFSara
PRACE Enabling sites: -
PRACE Architectures: Cartesius
Start enabling: -
Start production: -
Project status: in progress (0%, just started)
Brief description of project: Interface defects. This project will focus on computational modeling of mechanisms underpinning formation and performance of resistive random access memory (ReRAM).
Types of support work undertaken: general support provided, i.e. account creation, initial telcon with PI.
Difficulties encountered and solution: Cartesius was not yet available when the DECI-10 projects started. The PI was aware with the situation and has got the access as soon as Cartesius is available for access.

Project Acronym: JOSEFINA
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: -
PRACE Architectures: Lindgren (XE6 12C@2.1)
Start enabling: -
Start production: May 2013
Project status: in progress (~1%)
Brief description of project: Jet nOiSe intEraction with Fuselage in INstalled configuration.
Types of support work undertaken: general support provided, i.e. account creation, initial meeting with PI, help with system access.
Difficulties encountered and solution: The PI had several questions regarding the assigned Tier-1 system access and the support was provided by both home site and exec site.

Project Acronym: WISER
Accepted by DECI Call: DECI-10
PRACE Home site: EPCC
PRACE Execution site: STFC
PRACE Enabling sites: EPCC, STFC
PRACE Architectures: IBM BG/Q
Start enabling: 01/05/13

Start production: 01/05/13
Project status: In progress (0 %)
Brief description of project: This project deals with weather / climate change using the NCAR WRF (Weather Research and Forecasting) model.
Types of support work undertaken: Discussions are on going about the transfer of this project from an Early Access BG/Q project to a run fully under DECI.
Difficulties encountered and solution: Some difficulties in getting the code up and running. This is in progress.

Project Acronym: INPHARMA
Accepted by DECI Call: DECI-10
PRACE Home site: FZJ
PRACE Execution site: EPCC
PRACE Enabling sites: -
PRACE Architectures: HeCToR XE6
Start enabling: -
Start production: May-13
Project status: In progress (4%)
Brief description of project: Protein-ligand docking is an important computational tool in structure based drug design. It allows for rapid prediction of the binding orientation of small molecules to a target protein. The presence of a reliable protein-ligand model facilitates systematic optimization of lead compounds to high affinity drug candidates. However, current docking protocols suffer from a low success rate due to deficiencies in the ranking of the ensemble of docking orientations (referred to as docking modes). Moreover, the inability to properly account for protein flexibility inflicts additional challenge to obtain a reliable model for arbitrary protein ligand pairs.
This project aims at combining a fully flexible model of the target protein by MD simulations with INPHARMA-guided rescoring of docking modes to overcome docking deficiencies in scenarios where structural data is limited. Specifically, when (i) only an apo structure is available, or (ii) when the structural data derives from a low quality homology model. The project extends its research to new target proteins including G-protein coupled receptors (GPCRs) and cyclin-dependent kinase 2 (CDK2) -- both being of major pharmaceutical interest. While experimental data is currently being collected for sets of ligands in our lab, there is the need of extensive computational power to employ MD simulations of the relevant targets for subsequent INPHARMA-guided ensemble docking.
Types of support work undertaken: The project is supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ is in contact with the project over run-time to monitor the status.
Difficulties encountered and solution: No problems occurred.

Project Acronym: LargeRB2013
Accepted by DECI Call: DECI-10
PRACE Home site: FZJ
PRACE Execution site: EPCC
PRACE Enabling sites: FZJ
PRACE Architectures: ICE-Advance
Start enabling: Sep-13
Start production: Sep-13
Project status: Waiting to start

Brief description of project: Many turbulent flows in nature and technology are driven by sustained temperature differences. Applications range from cooling devices of chips to convection in the Earth and the Sun. Turbulent Rayleigh-Bénard convection (RBC) is the paradigm for all these convective phenomena because it can be studied in a controlled manner, but it still has enough complexity to contain the key features of convective turbulence in the examples just mentioned.
This project study will provide new insights of the turbulent transport processes which have remained vague until now. As such, the proposed research will be transformational in the domain of fluid dynamics, with potential relevance for natural and technological applications.
Types of support work undertaken: The project is supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ is in contact with the project over run-time to monitor the status.
Enabling work for the project is envisaged and will be started in September 2013 as described in the Applications Enabling section.
Difficulties encountered and solution: No problems occurred.

Project Acronym: MoDSS
Accepted by DECI Call: DECI-10
PRACE Home site: FZJ
PRACE Execution site: RZG
PRACE Enabling sites: -
PRACE Architectures: Hydra
Start enabling: -
Start production: May-13
Project status: In setup
Brief description of project: Trisiloxane surfactants are widely used in various products such as paints, inks, and herbicides because of their capacity to enable "superspreading," the greatly enhanced spreading of aqueous solutions on hydrophobic surfaces. As these surfactants are toxic and chemically unstable, alternative superspreading agents are eagerly desired, which is why the re have been numerous studies in the last 20 years in academia and industry with the aim of uncovering the mechanisms that facilitate the ultra-rapid spreading. Since experimental setups are unable to resolve fully the processes occurring on the molecular scale, the driving mechanisms of superspreading have not yet been completely identified, leading to the existence of competing theories.
The project will perform large-scale Molecular Dynamics simulations of trisiloxane surfactant-laden water droplets on various surfaces. These simulations will clarify open questions on the fundamental behavior of trisiloxane surfactants in solutions and the various interfaces involved in the process and in this way contribute to the understanding of superspreading and the development of alternative environmentally friendly superspreading agents.
Types of support work undertaken: The project is supported technically. Accounts have been created at the home site to provide access to the PRACE infrastructure. The accounts have been distributed to the execution-site via the PRACE-LDAP. FZJ is in contact with the project over run-time to monitor the status.
Difficulties encountered and solution: No problems occurred.

Project Acronym: APOP20X3
Accepted by DECI Call: DECI-10
PRACE Home site: ICHEC
PRACE Execution site: PSNC (1.564M)

PRACE Enabling sites: none
PRACE Architectures: x86/GPGPU
Start enabling:
Start production:
Project status: Setup ongoing
Brief description of project: MD (AMBER+GPGPU) simulation of proteins-ligand complexes involved in apoptosis (XIAP and Survivin).
Types of support work undertaken: none
Difficulties encountered and solution: not aware of any

Project Acronym: RODCS
Accepted by DECI Call: DECI-10
PRACE Home site: ICHEC
PRACE Execution site: CSCS (3.75M)
PRACE Enabling sites: none
PRACE Architectures: Cray
Start enabling:
Start production: No calculations have run to date
Project status: In progress (0%) (Just started)
Brief description of project: Ab initio or QM (VASP) calculations to study the reactivity on doped ceria surfaces.
Types of support work undertaken: N/A
Difficulties encountered and solution: none

Project Acronym: waveclim
Accepted by DECI Call: DECI-10
PRACE Home site: ICHEC
PRACE Execution site: CSCS (2.295M)
PRACE Enabling sites: none
PRACE Architectures:
Start enabling:
Start production: 6/2013
Project status: In progress. Just started. Already burning time
Brief description of project: Nearshore wave climate analysis for the West coat of Ireland using WAVEWATCH III v3.14.
Types of support work undertaken: NA
Difficulties encountered and solution: none

Project Acronym: CELESTE
Accepted by DECI Call: DECI-10
PRACE Home site: ICM
PRACE Execution site: CSCS
PRACE Enabling sites: -
PRACE Architectures: Rosa (XT5 CSCS)
Start enabling: -
Start production: -
Project status: Waiting to start
Brief description of project: Cosmo-Eulag semi-operational testing. It is proposed to perform routine testing of the next generation dynamical core for European high resolution (1 km and better) regional weather prediction. The focus is to provide robust and efficient solver for atmospheric flows over complicated topography of Alps that also poses basic conservative

properties. To date, the new EULAG dynamical core of COSMO Consortium for Small Scale Modelling weather forecasting framework has been extensively tested in a range of idealized and semi-realistic experiments. Currently, COSMO runs a project CELO aiming at operationalization of the EULAG dynamical core. The weather forecasting framework of COSMO with EULAG dynamical core will be run daily in close-to-operational configuration to test its robustness and forecast quality. This aims at acceleration of the process of operationalization of the new dynamical core and expedited provision of next generation of weather prediction framework. On the scientific side, the proposal bases on exceptionally powerful and well established EULAG model developed at the National Center of Atmospheric Research in Boulder, CO, USA and the successful COSMO operational weather prediction model.
Types of support work undertaken: No report from ICM.
Difficulties encountered and solution: No report from ICM.

Project Acronym: DNSTF
Accepted by DECI Call: DECI-10
PRACE Home site: SNIC-KTH
PRACE Execution site: EPCC
PRACE Enabling sites: SURFSara
PRACE Architectures:
Start enabling: 05/13 (08/13)
Start production:
Project status: In progress
Brief description of project: The goal of this project is to adapt a numerical model of the dynamical behaviour of finite size fibres in high Reynolds number, turbulent flow. The chosen approach is to start from direct numerical simulations for both turbulent flow and to resolve the flow around individual fibres. The turbulent flow is modelled by an entropy lattice Boltzmann method and the interaction between fibres and carrier fluid is modelled through an external boundary force method (EBF). Direct contact and lubrication force models for fibre-fibre interactions and fibre-wall interaction are taken into account to allow for a full four-way interaction. This model will allow to study the influence of wall effects and interaction effects on turbulent flow.
Types of support work undertaken: Creating accounts, assigning exec
Difficulties encountered and solution: None yet

Project Acronym: LipoSim
Accepted by DECI Call: DECI-10
PRACE Home site: SNIC-KTH
PRACE Execution site: SNIC-KTH
PRACE Enabling sites: SNIC-KTH
PRACE Architectures: Cray XE6
Start enabling: 05/13
Start production: 06/13
Project status: In progress (24%)
Brief description of project: This project employs massively parallel computations in order to simulate drug delivery from a drug loaded liposomes into a cellular plasma membrane. The use of PRACE facilities enables us to understand at a detailed atomic 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. We focus in this landmark study on different compounds aimed for cancer therapy, with the aim to thereby have established a system to be used in the study of a wide range of other

compounds in the future, in order to better optimize conditions for their usage in connection with lipid vesicles for drug delivery. Deeper insight into these processes will also 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.
Types of support work undertaken: Creating and reactivating old accounts.
Difficulties encountered and solution: One person had two different accounts which needed to be unified in a non-standard procedure where competences and responsibility where not clearly defined. However SNIC-KTH managed this task in the end.

Project Acronym: MEGAREACT
Accepted by DECI Call: DECI-10
PRACE Home site: SNIC-KTH
PRACE Execution site: UiO
PRACE Enabling sites: UiO, SNIC-KTH
PRACE Architectures: Sandy Bridge
Start enabling: 05/13
Start production: 06/13
Project status: In progress (? %)
Brief description of project: 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, this project aims to 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 will be studied is the water gas shift (WGS) reaction, which is important in almost all gasification reactions.
Types of support work undertaken: Account set-up and gsi-ssh debugging and advice
Difficulties encountered and solution: One of the users was using a certificate that was not listed in his entry in the LDAP. Told user to use the certificate which was entered in the LDAP instead.

Project Acronym: PLANETESIM-2
Accepted by DECI Call: DECI-10
PRACE Home site: SNIC-KTH
PRACE Execution site: FZJ
PRACE Enabling sites: SNIC-LU
PRACE Architectures: Intel Nehalem
Start enabling: 05/13
Start production: 05/13
Project status: In progress (56%)
Brief description of project: 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 a re 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.

This project is a follow-up to the corresponding DECI-8 project and will push the resultion up to 512^3 which will allow us to determine the initial mass function of planetesimals down to 30 km in radius and thus to compare critically to the observed properties of the Kuiper belt and the asteroid belt.
Types of support work undertaken: Assigning compute time
Difficulties encountered and solution: None

Project Acronym: HYDRAD
Accepted by DECI Call: DECI-10
PRACE Home site: RZG
PRACE Execution site: VSB-TUO
PRACE Enabling sites: RZG
PRACE Architectures: E5-2665-8@2.4
Start enabling: 05/2013
Start production: 07/2013
Project status: Enabling completed, production in progress
Brief description of project: *Hydrodynamic stability of rotating flows in accretion disks*
The origin of turbulence in accretion discs has been debated for many decades. In order for matter to accrete, angular momentum has to be transported outward and as molecular viscosity is too small a turbulent viscosity has been put forward to explain observable accretion rates. The velocity profiles of discs (Keplerien profiles) are centrifugally stable and therefore a different instability mechanism is required for turbulence to arise. While in hot discs turbulence can arise through the magnetorotational instability, cooler discs lack sufficient ionization and it is unclear how turbulence sets in. In analogy to pipe and other shear flows it has often been argued that turbulence in disc flows could also be triggered by perturbations of finite amplitude. State-of-the-art laboratory experiments by different groups yield contradictory results and call for a numerical investigation. Here we perform numerical simulations to clarify if such a subcritical instability mechanism may be responsible for turbulence in Keplerian flows at high Reynolds numbers.
Types of support work undertaken: The (first-time PRACE) user was assisted with obtaining a certificate from his local RA and with using the certificate for authentication and authorization. The simulation code “nsCouette” was ported by RZG to the platform provided by the execution site. Makefiles and batch scripts were adapted to the VSB software stack, using Intel compilers, MKL and MPI, FFTW3 and parallel HDF5. Together with VSB staff a problem in the installation procedure of the parallel HDF5 library was identified and fixed (see below) which prevented linking hybrid codes (introduced with Intel MPI 4.1.0). Test programs on the VSB cluster were executed in order to ensure proper pinning of MPI tasks and OpenMP threads in the pbs batch environment. This is known in general to be crucial for getting adequate performance for hybrid MPI/OpenMP codes. The performance of the simulation code was assessed by performing a strong-scaling study and by comparing the absolute performance numbers with benchmarks on other systems (RZG cluster *Hydra*). The scalability on nsCouette, which is ultimately limited by the performance of MPI_Alltoall could be further improved by selecting a non-default algorithm in the Intel MPI implementation at runtime. Performance on the VSB cluster was eventually found to be within expectations (taking into account differences in Interconnect and CPU).
Difficulties encountered and solution: No major difficulties were encountered. The VSB machine just became operational in June 2013. Thanks to excellent support by VSB staff all start-up problems could be resolved smoothly.
Technical issues: The parallel HDF5 library is usually linked with the MPI-compiler wrappers which, for Intel MPI leads to a dependency on the plain MPI runtime library (libmpi), or on its multithreaded version (libmpi_mt). Starting with version 4.1.0 of the Intel

MPI library, this causes a conflict when trying to link a multithreaded code with the plain-MPI variant of the HDF5 library, or vice versa. Together with Intel, RZG has worked out a patch for the HDF5 installation procedure which simply accounts for using the plain linker (instead of the MPI wrapper) for building HDF5. This makes a *single* HDF5 installation compatible with both, plain MPI and hybrid (MPI + threads) codes.

Project Acronym: PTACRB-2
Accepted by DECI Call: DECI-10
PRACE Home site: RZG
PRACE Execution site: ICHEC, CYFRONET
PRACE Enabling sites: RZG
PRACE Architectures: Intel Westmere EP@2.67, AMD 6276@2.3
Start enabling: 05/2013
Start production: 07/2013
Project status: In progress
Brief description of project: Follow-up project of DECI-9 project PTACRB.
Types of support work undertaken: General support. Account creation.
Difficulties encountered and solution: Moving the project from ICHEC, which was the execution site for the predecessor project in DECI-9 to CYFRONET was not convenient for the PI, hence part of the compute time was moved from CYFRONET to ICHEC to facilitate the continuity of the two follow-up projects PTACRB (DECI-9) and PTACRB-2 (DECI-10).

Project Acronym: DIVI
Accepted by DECI Call: DECI-10
PRACE Home site: SURFSara
PRACE Execution site: ICHEC
PRACE Enabling sites:
PRACE Architectures: SandyBridge@2.6
Start enabling:
Start production: 05/2013
Project status: In progress (1%)
Brief description of project: Culgi is a technical consulting company in the area of chemical informatics and modelling in materials and life sciences. One of its main activities is the development, distribution and support of the Chemistry Unified Language Interface (CULGI). As a result of our vast experience with industrial and academic partners, in various field as chemicals, pharmaceuticals, aerospace, petroleum, we started to develop a novel protocol to automatically fragment and parameterize any chemical component for further use in simple, rapid particle based simulations. The DECI-10 programme, by the extensive computational resources offered, will enable the creation of a representative database of molecular fragments with known physico-chemical properties and interaction parameters calculated using Monte Carlo techniques, quantum mechanics, thermodynamics information and optimisation techniques.
Types of support work undertaken: none
Difficulties encountered and solution:

Project Acronym: SCostS
Accepted by DECI Call: DECI-10
PRACE Home site: SURFSara
PRACE Execution site: CSC
PRACE Enabling sites:

PRACE Architectures: Cray
Start enabling:
Start production: 05/2013
Project status: In progress (5%)
Brief description of project: Understanding the influence of steps and kinks on reactivity is of great importance in catalysis. Most catalytically important systems are composed of nanoparticles which consist mostly of surfaces with a varying defect density. Due to computation costs most DFT simulations however only focus on either simple high symmetry facets or on very short terraces. Increasing availability of HPC resources makes it possible to simulate systems with longer terraces. This allows for clear seperation between the effects of the step area and the previously studied highly symmetric terraces. The main aim here is to study the non-linear effect that steps and defects have on the water structure on an important catalytic surface, i.e. platinum.
Types of support work undertaken: none
Difficulties encountered and solution:

Project Acronym: TheoMoMuLaM
Accepted by DECI Call: DECI-10
PRACE Home site: SURFSara
PRACE Execution site: UiO
PRACE Enabling sites:
PRACE Architectures:
Start enabling:
Start production: 05/2013
Project status: In progress (1%)
Brief description of project: The research project TheoMoMuLaM goal is to explore from first-principles new exotic properties at layer interfaces of oxides and fluorides. The group will use density functional theory calculations and effective Hamiltonian techniques to design new optimised materials.
Oxide-based materials have gained a lot of attention in the last two decades due to their promising properties for technological applications. More interesting is the recent discovery of the apparition of totally new exotic phenomena at surfaces and interfaces of oxides.
Types of support work undertaken: none
Difficulties encountered and solution:

Project Acronym: GREENLIGNITE
Accepted by DECI Call: DECI-10
PRACE Home site: UHeM
PRACE Execution site: UHeM
PRACE Enabling sites: -
PRACE Architectures: Nehalem Cluster
Start enabling:
Start production: Not started yet
Project status: Waiting to start
Brief description of project: Major consumers of the world's energy resources today are in dire need of secure and affordable energy solutions. While oil reserves are dwindling, coal reserves, are still abundant globally. Hence, coal is the major source of electrical power today but coal burning has been also a major source of pollution due to various challenges, which need to be overcome before coal can be used as a sustainable source of energy. Initiatives such as clean coal technologies can pave the way to environmental sustainability, and create a new and improved image for coal-based energy while the technology is evolving for energy

production from renewables. Coal gasification is considered one of the critical technologies for clean energy in the near future as it can provide an opportunity to meet the ever-increasing energy demands of the both developed and developing countries across the world in an environmentally sustainable manner. Despite its potential, this technology has been met with resistance mainly due to the uncertainties in the economic viability and the environmental impact of the process. To help address these issues, high-resolution computer simulations are being proposed to provide information to industrial stakeholders to address these uncertainties. The overall performance of coal gasifier is directly linked to a few key operating parameters. Coal feed rate, reaction kinetics, solids and syngas re-circulation rates are key factors in the daily operation of the gasifier. The production of polluting species in the exit syngas, low energy content of the syngas, locally high temperatures, and un-reacted coal are some of the problems linked to these factors, which are quite difficult to understand and quantify without the aid of high resolution simulations for large scale operation. The proposed project intends to employ a validated computational fluid dynamics models for reacting multiphase flows in fluidized beds and gasifiers to investigate several of these important design parameters and their interactions specifically for Turkish lignite and biomass based feedstock.
Types of support work undertaken: Accounting
Difficulties encountered and solution: There were some difficulties about definition of execsite. Finally, UHeM is assigned as execsite. Communitation with PI has been done and installation procedure will start in a short time.

Project Acronym: WIND-FORECAST
Accepted by DECI Call: DECI-10
PRACE Home site: UHeM
PRACE Execution site: CYFRONET
PRACE Enabling sites: -
PRACE Architectures:
Start enabling: -
Start production:
Project status: Waiting to start
Brief description of project: In this project, we aim at development of a multi-scale multi-physics atmospheric flow simulation tool for short-to-medium term wind power forecasts at wind farms. Wind power forecasts are very valuable for daily and day-ahead operations of power generation and utility companies. Numerical simulations of atmospheric flows from meso-scale down to turbine scale might help these companies in forecasting power from wind turbines over a range of time scales. However, there are few challenges for development of such an operational tool. First, there are hardly any single numerical simulation tool that can simulate the range of scales exist in this problem altogether. Therefore, integration of few models, each one developed for simulation of certain range of scales, is needed in order to accurately handle this problem. Second, each of these tools and their aggregate simulation capability should be validated against existing measurement data which require interrogating and analysing 4D simulation data (i.e. mean wind speed data). In this project, we propose a work plan for step-by-step development of such an operational forecasting tool as well as investigating its validation and uncertainty quantification using state-of-the-art statistical and measurement techniques.
Types of support work undertaken: Enabling accounts
Difficulties encountered and solution:

Project Acronym: EXC-XMCD
Accepted by DECI Call: DECI-10

PRACE Home site: VSB-TUO
PRACE Execution site: PSNC
PRACE Enabling sites: VSB-TUO
PRACE Architectures: SGI UV (x86 cc-NUMA) "Chimera"
Start enabling:
Start production:
Project status: Waiting to start
Brief description of project: The excitonic effects on X-ray circular and linear dichroism at 2p edges. The understanding of the X-ray magnetic circular/linear dichroism (XMCD/XMLD) in metals and magnetic insulating materials has advanced tremendously in last years [Stoehr and Siegmann 2006, Antonov 2007, 2008]. The basic advantage of the XMCD is the ability to estimate the orbital and spin moments based on the sum rules in ferromagnetic materials (Thole 1992, Carra 1993). There are not any such sum rules in XMLD, however this technique (using effect that is quadratic in magnetization) has the advantage over XMCD to detect antiferromagnetic materials (v.d. Laan 1998). With the help of the first- principles (ab initio) calculations the origins of both effects, XMCD and XMLD, were revealed to large extent in the case of transition metals in recent decades (Kunes 2003). However, for oxide systems and/or early d-metals the structures of the XMCD/XMLD spectra are much more complex, often reasonably well modeled by "multiplet theory" codes, i.e. codes which are not parameter free, but not in a such good agreement as if the spectra were modeled by pure quantum mechanics codes, e.g. using density functional theory (DFT) parameter free technique. Following deficiencies may originate from the improper description of many-body effects, particularly from quasiparticle electron-hole: missing satellite peaks at high(low) energy side of 3d transition atoms in pure metals and insulating compounds, incorrect branching ratio of the X-ray absorption spectra (XAS) at 2p edges (L 3/L2), and fine-structure features (oscillations) of XMCD/XMLD in the magnetic insulating materials. To some extent these experimentally observed features can be resembled using multiplet calculations that strongly depend on number of empirical parameters. Here, we would like to identify for the first time the role of the excitonic effects on the XAS, XMCD, XMLD of magnetic solids with different electron screening (magnetic metals and insulators) with ferro-(XMCD) and antiferro-(XMLD) ordering. We will widen the existing knowledge of XAS of nonmagnetic solids (Laskowski 2012) by use of developed Bethe-Salpeter (BSE) equations (Onida 2002) and by further investigations of selected magnetic metallic (3d transition metals) and insulating or half-metallic materials, e.g. NiO, CrO2, respectively. We will continue in further development of the code and hence we intend to determine the magnitude of the quadruple contributions with respect to the dipolar contributions of the simulated spectra using BSE technique, as found in some materials (Rueff 2004). Our approach is at the atomistic level using first-principles (quantum mechanics) calculations and therefore no empirical parameters for such calculations are required. The only inputs needed are atomic number of constituents and some structural information, e.g. body-centered cubic structure in the case of Fe. However, computational demand to perform BSE calculations is about 3 orders of magnitude higher than for the independent single particle approximation for the same structure and material.
Types of support work undertaken: General support with obtaining certificates and login procedures.
Difficulties encountered and solution: Difficulties to obtain certificate for one investigator (Polish living in Austria moving back to Poland). Waited for accounts creation at exec site 2.5 months.

Project Acronym: TransMem
Accepted by DECI Call: DECI-10

PRACE Home site: VSB-TUO
PRACE Execution site: SURFSara
PRACE Enabling sites: VSB-TUO
PRACE Architectures: x86 cluster "Cartesius"
Start enabling:
Start production:
Project status: Waiting to start
Brief description of project: Translocation of Biomolecules Across Cell Membranes. Cell penetrating peptides have drawn considerable attention recently, thanks to their ability to cross phospholipid membranes and deliver various molecular cargos, such as nucleic acids, proteins, quantum dots, and various drugs, inside the cells. A crucial structural requirements for an effective penetration of a peptide through the phospholipid bilayer is the presence of multiple guanidinium cations, which are present in the side chains of arginines. Confocal microscopy and flow cytometry techniques have demonstrated that oligoarginines containing six or more amino acids internalize into the membrane more efficiently than equally long lysine oligomers. However, the molecular mechanism of penetration into and translocation across the phospholiúpid bilayer of these peptides is poorly understood. Among the possible mechanistic explanations inverse micelle formation, electroporation, endocytosis, and anion mediated energy-independent diffusion through the membrane could be considered. Nevertheless, none of these mechanisms is able to fully rationalize the difference in membrane permeability of arginine containing peptides and those containing the other cationic amino acids, i.e., lysines. Within the present proposal we aim at clarifying the molecular mechanisms of membrane permeabilities of different cationic peptides of varying length and composition. We will explore the ability of guanidinium cationic groups present in arginine containing peptides (but not of ammonium groups in oligolysines) to pair via like-charge ion pairing and consequences thereof on membrane permeation. Homo- ion pairing of guanidinium cations is one of the driving forces for oligoarginine aggregation in water. and at the lipid bilayers, as shown by our previous all-atom molecular dynamics simulations. By a combination of all-atom and coarse-grained molecular simulations we will ask and aim to answer the following question: Does the higher charge density of membrane adsorbed oligoarginine aggregates, in comparison to single oligoarginines or oligolysines, play a decisive role in the ability to penetrate across the cellular membrane? Succesfully answering this question by means of extensive simulations will allow us to suggest a plausible and experimentally testable molecular mechanism of translocation of cell penetrating peptides across the cellular membrane. This will have direct consequences for devising new strategies of drug delivery into cells.
Types of support work undertaken: Help with obtaining certificates for the traveling investigators (see below), coordination with Czech certificate issuing organization (CESNET).
Difficulties encountered and solution: Difficulties to obtain certificates (Polish moving between Czech rep. Poland and Nordics, a Croatian moving between Czech rep., Croatia and Nordics). Waited for installation of the new system at exec site and production level of PRACE services (e. g. login with GSI-SSH). Coordinated with staff from exec site.