SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures

INFRA-2010-2.3.1 – First Implementation Phase of the European High Performance Computing (HPC) service PRACE

PRACE-1IP

PRACE First Implementation Project

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List of Acronyms and Abbreviations

AISBL	Association internationale sans but lucrative (International association without lucrative purpose)
BoF	Birds of a Feather - an informal discussion session
CCH	Congress Center Hamburg
CPU	Central Processing Unit
EC	European Commission
GÉANT	Collaboration between National Research and Education Networks to build a multi-gigabit pan-European network, managed by DANTE. GÉANT2 is the follow-up as of 2004.
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
ISC	International Supercomputing Conference; European equivalent to the US based SC0x conference. Held annually in Germany.
MD	Molecular Dynamics
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
RI	Research Infrastructure
SSC	Scientific Steering Committee
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1

Executive Summary

PRACE, the Partnership for Advanced Computing in Europe organized the 2012 PRACE Scientific Conferences on June 17, 2012, in Hamburg, Germany in conjunction with International Supercomputing Conference 2012 (ISC'12). This conference continues the successful series of symposia started by DEISA and jointly organized by PRACE and DEISA in 2011 in Helsinki, Finland.

The conference aim was to highlight the scientific achievements that were made possible with PRACE support and to present the HPC opportunities, vision and strategy in Europe. The programme captured interest of a broad audience: scientific users, HPC technology experts and vendors, EC and government representatives, and industry partners. The conference attracted over 230 registrants from 35 countries.

The programme was opened with a presentation on the PRACE perspective by Maria Ramalho, Chairman of the Board of Directors, PRACE AISBL and followed by a European HPC strategy overview by Kostas Glinos, Head of Unit "GÉANT & e-Infrastructure". The scientific part included presentations of results from six projects obtained on PRACE Tier-0 systems and the presentation by the winner of the PRACE Award in 2012.

A high number of members of HPC community used the opportunity to meet colleagues and to exchange ideas during a short PRACE User Forum meeting.

The 2012 PRACE Scientific Conference was very successful both regarding the scientific quality and in strengthening the relations between the European scientific communities.

1 Introduction

The vision of PRACE is to enable and support European global leadership in public and private research and development. PRACE seeks to realize this vision by contributing to the advancement of European competitiveness in industry and research through provisioning of world leading persistent computing and data management resources and services.

Supercomputers enable scientists and engineers to solve today's problems and to develop the new technology for tomorrow's industry, affecting national employment patterns and national wealth. To further stimulate the aim of enabling the academic and industrial research in Europe to develop and use world class HPC, it is important to strengthen contacts with and between scientific communities; in particular those who are involved in helping to develop the very science case on which this effort is based. To this end, the PRACE-1IP project is responsible for organising two scientific conferences during the course of the project.

The first of these, the DEISA PRACE Symposium 2011, was held on April 13–14, 2011 in Helsinki, Finland [2]. The second one, PRACE Scientific Conference 2012 was held on June 17, 2012 in Hamburg, Germany in conjunction with International Supercomputing Conference (ISC'12) [4].

In this report the conference objectives and venue are described first. Next, details of organization and programme of the conference are given. Section 4 enlists all the major communication channels that were used in order to advertise the event and attract targeted audience to participate in the event. Following section provide information on the registration procedure and demographical structure of registrants. Evening networking event, organized jointly with HPC in Asia Workshop, is briefly described. Activities that followed the event are listed, followed by concluding remarks. Finally, abstracts of the scientific presentations are appended to the document as annexes.

2 Objectives and venue

The aim of the PRACE Scientific conference was to present results and highlight advances in large scale simulations obtained on PRACE's Tier-0 resources, as well as to present Europe's vision for HPC by an EC representative and the PRACE director. The programme included the presentation by the winner of the PRACE Award 2012 and a short meeting of the PRACE User Forum which provided an opportunity for users and those considering applying for PRACE resources to discuss issues with the PRACE management and members of the Scientific Steering Committee.

Scientist and researchers from academia and industry were invited to participate, learn from colleagues what can be achieved using PRACE services and indentify opportunities for future PRACE supported projects.

Figure 1- Rooms at Radisson Blu Hotel, Hamburg, Germany

This year PRACE Scientific Conference was organized in conjunction with ISC [4], the International Supercomputing Conference, thus maximizing the value for PRACE and ISC'12 attendees. After the end of the sessions, participants of the PRACE Scientific Conference had a chance to enjoy an informal get-together with colleagues participating in the HPC in Asia Workshop organised in parallel by ISC.

Registration of participants was handled by ISC organizers through the official ISC'12 registration form [4]. Participation in the PRACE Day programme on Sunday was free of charge to participants.

The conference took place at the ballroom of Radisson Blu Hotel [6], close to the Congress Center Hamburg [5]. Coffee breaks, lunch and refreshments were included in the conference package.

3 Organization and Programme committees

The organization of the PRACE Scientific Conference was carried out by two teams: An Organization Committee and the Programme Committee.

3.1 Organization

The organization committee was in charge of dissemination and all practicalities regarding the conference. The organization started in June 2011, when the venue and date was selected and the negotiations with ISC organizers started. It was agreed that ISC organizers handle the registration of participants and to advertise the event on the ISC'12 webpage and through ISC regular dissemination channels in addition to the advertisement done by PRACE directly.

The location of the conferences was the Radisson Blu Hotel, due to its proximity to the Congress Center Hamburg [4] (where ISC'12 was held), the availability of a suitable room and an attractive conference package offered by the hotel. The conference took place on the 1st floor of Radisson Blu Hotel in Chicago / Dallas / Philadelphia rooms.

PRACE provided the accommodation and covered travel expenses for invited speakers.

Members of the Organizing Committee were:

- **Tanja Weber** (FZJ) – chair
- **Renata Gimenez** (BSC) – chair deputy
- **Ari Turunen** (CSC)
- **Dietmar Erwin** (FZJ)
- **Danica Stojiljkovic** (IPB)

An email alias was created to reach the organisers: praceday2012-oc@fz-juelich.de.

3.2 Programme

Programme Committee was in charge of identifying and inviting the speakers, and for creating the conference agenda. The PRACE Scientific Steering Committee naturally assumed the role of the Programme Committee. It was chaired by **Richard Kenway**, Chair of PRACE Scientific Steering Committee, who also chaired the Scientific Conference.

It was decided that besides inviting top European scientist to present the major scientific results obtained with support of PRACE, it is of great importance to present the PRACE vision and future plans, as well as the European HPC strategy. Therefore, **Maria Ramalho**, the PRACE AISBL Chairman of the Board of Directors and **Kostas Glinos**, Head of Unit "GÉANT & e-Infrastructure", European Commission, were invited as speakers.

The PRACE award, which is for the fifth time presented during the ISC Opening Session on Monday, June 18, 2012, went to **Yves Ineichen** from Paul Scherrer Institut for the paper titled "A Fast and Scalable Low Dimensional Solver for Charged Particle Dynamics in Large Particle Accelerators" [7] and the presentation of his work was included in the conference programme.

Figure 2 - User Forum Session

The PRACE Scientific Conference 2012 gathered a large number of PRACE current and potential users. It was a great opportunity to hold a short User Forum meeting (Figure 2), chaired by **Turlough Downes**. This short session was intended to give PRACE users an opportunity to discuss their experiences of applying for, and using, PRACE resources. The emphasis was on identifying issues of concern which were common to a number of users. One example of such an issue is the opening of PRACE resources to teams from outside the EU and associated states. The Programme Committee of the User Forum will feed all these concerns directly to the relevant PRACE committees with a view to having them addressed.

The detailed programme is given in Table 1, abstracts of the scientific presentations can be found in Annex 9.1.

Table 1 - Programme of PRACE Scientific Conference 2012

08:30 - 09:00	*Registration at ISC registration desk (Foyer Congress Center Hamburg)*
09:00 - 09:15	**Welcome** *Richard Kenway*, Chair of PRACE Scientific Steering Committee & Conference Chairman
09:15 - 09:45	**PRACE: computing for scientific breakthroughs** *Maria Ramalho*, Chairman of the Board of Directors, PRACE AISBL
09:45 - 10:15	**The European HPC Strategy** *Kostas Glinos*, Head of Unit "GÉANT & e-Infrastructure", European Commission
10:15 - 10:45	*Coffee Break*
10:45 - 11:30	**A Fast and Scalable Low Dimensional Solver for Charged Particle Dynamics in Large Particle Accelerators** *Yves Ineichen*, Paul Scherrer Institut , PRACE Award Winner
11:30 - 12:00	**Excess proton at water/hydrophobic interfaces: A Car-Parrinello MD study** *Paolo Carloni*, German Research School for Simulation Sciences GmbH
12:00 - 12:30	**A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and an in-coming dislocation** *Bing Liu*, Max-Planck-Institut für Eisenforschung
12:30 - 13:30	*Lunch Break*
13:30 - 14:15	**PRACE User Forum with Q&A, Chairman:** *Turlough Downes*
14:15 - 14:45	**Droplet growth by coalescence in turbulent clouds: kinetics, fluctuations, and universality** *Jeremie Bec*, Observatoire de la Côte d'Azur
14:45 - 15:15	**Predictive full-scale fast ignition with PW plasma amplified laser pulses** *Ricardo Fonseca*, Instituto Superior Técnico, Lisbon

15:15 - 15:45	*Coffee Break*
15:45 - 16:15	**Turbulent entrainment due to a plume impinging on a density interface** *Maarten van Reeuwijk*, Imperial College London
16:15 - 16:45	**Ab initio Simulations of Turbulence in Fusion Plasmas** *Frank Jenko*, Max Planck Institute for Plasma Physics
16:45 - 17:00	**Closing Remarks** *Richard Kenway*, Chair of PRACE Scientific Steering Committee & Conference Chairman
17:30 - 18:30	*Networking Event together with ISC'12 HPC in Asia Workshop* *(Foyer - 1st floor)*

4 Dissemination

One of the aims of the conference was to provide an opportunity for PRACE to strengthen its links with HPC initiatives all over the world, to inform about the results achieved with PRACE Tier-0 resources, and to liaise with scientific users in Europe and beyond. The symposium was intended for a broad audience: from scientific users, HPC technology experts and vendors to government and EC representatives and industry partners. This was taken into account when sending out invitations and creating the programme.

4.1 Invitations and publicity

The programme committee was in charge of inviting speakers and User Forum chair to the conference.

Invitations were sent via PRACE dissemination channels to potential participants via email. A press release was made about the event (see more in section 4.2), and the event was also announced in the PRACE newsletters, and event specific pages were created for both PRACE and ISC websites.

The event was free of charge for the participants. A total of 230 participants registered for the event.

4.2 Press releases and Newsletter article

First announcement of PRACE Scientific Conference was published in the "Featured events" article in PRACE Newsletter No.6 from December 2011[8] and a short invitation again in the Newsletter No.8 in June 2012 [9]. More information on conference was published in a press release "PRACE Scientific Conference 2012" published on May 7, 2012 [10]. After the event, the follow-up press release was published on June 26, 2012 which summarized the highlights of the conference. The press releases were also sent to various online HPC magazines, such as Digital Manufacturing Report [14], HPCWire [12] and ISGTW [13]. The press releases were also distributed via the AlphaGalileo [11] service – the world's leading source of European research news – which reaches over more than 7,000 media professionals worldwide.

InsideHPC [15] featured an interview with Maria Ramalho, Chairman of the Board of Directors, PRACE AISBL, titled "PRACE Scientific Conference at ISC'12 to Showcase European HPC", which was published on May 31, 2012.

4.3 Webpages

A dedicated webpage for the conference was created on the official PRACE RI website [3]. It was first published on February 3, 2012 and it was updated with the new information as they were becoming available. The web page contains description of the event, instructions on how to register and a full programme with speakers CVs and photos and abstracts of the presentations. A snapshot of this webpage is shown in Figure 3.

Figure 3 - PRACE Scientific Conference 2012 dedicated webpage on PRACE RI website

As agreed with the ISC'12 organizers, the PRACE Scientific Conference was also advertised on the ISC'12 webpage among the Satellite Events [16] and in the registration page. A snapshot of this webpage is shown in Figure 4.

Figure 4 - PRACE Scientific Conference 2012 dedicated webpage on ISC'12 website

After the conferences all presentations from the event were uploaded to PRACE website [3]. A photo gallery was created and made available on the website. All participants and speakers were informed about the availability of the presentations and photo gallery after the event.

4.4   PRACE Day Bookmark

For the purpose of advertising PRACE Day, a bookmark was produced with "*SAVE THE DATE!*" message on the front, and a calendar for 2012 on the back side with June 17, 2012 circled (Figure 5). This bookmark was distributed at the PRACE booth at ISC'11 (Hamburg) and SC'11 (Seattle), as well as at PRACE trainings and workshops organized in the past year.

Figure 5 - PRACE Day bookmark

4.5   Other dissemination material

All participants received a conference kit which included the conference programme, PRACE folder with brochure and flyer, notepad, pen, PRACE branded monitor cleaner and details on how to access the wireless network that was available at the venue. The conference kit also included the PRACE branded lanyard and PRACE USB-key with digital versions of PRACE Digest 2012 [19], PRACE Newsletter No.8 [9], flyer, brochure, poster, link to PRACE Video [20] and PRACE RI official website [1].

PRACE organized the ISC'12 BoF session "PRACE Future Technologies Evaluation Results" on Tuesday, June 19, 2012, and the programme of this session [17] was also handed out to the participants of the conference.

Figure 6 - PRACE Scientific Conference 2012

At the venue, PRACE generic roll-up were located at the entrance of the conference room and inside the room, on the left side of the screen (Figure 6).

5   Networking event

After the end of the sessions, participants of the PRACE Scientific Conference had a chance to enjoy an informal get-together with colleagues participating in the HPC in Asia Workshop organised in parallel by ISC [18]. The reception took place at Radisson Blu Hotel in a foyer on the first floor (in front of the conference room).

Figure 7 - Networking event: PRACE Scientific Conference 2012 and HPC in Asia Workshop

6 Registration

The participants could register for the conference through ISC'12 registration page (Figure 8). Participation for the PRACE sessions on Sunday, June 17, 2012, was free of charge for all participants and it included lunch and evening networking event.

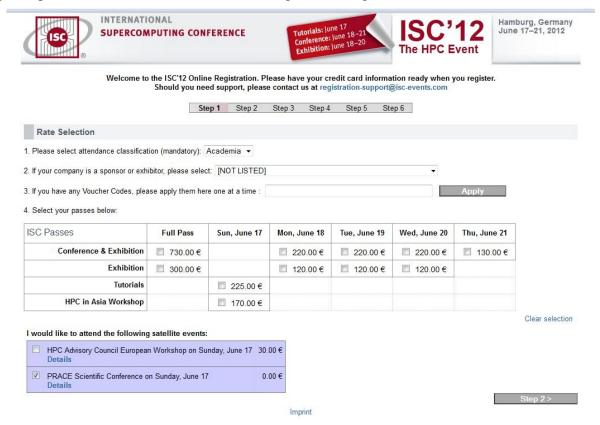**Figure 8 - ISC'12 registration page featuring PRACE Scientific Conference registration**

The PRACE Scientific Conference 2012 attracted 230 registered participants from 35 countries all over the world. This number of participants was limited by the conference room capacity and the registration was closed when this limit was reached. The distribution of participants per country is given in Figure 9.
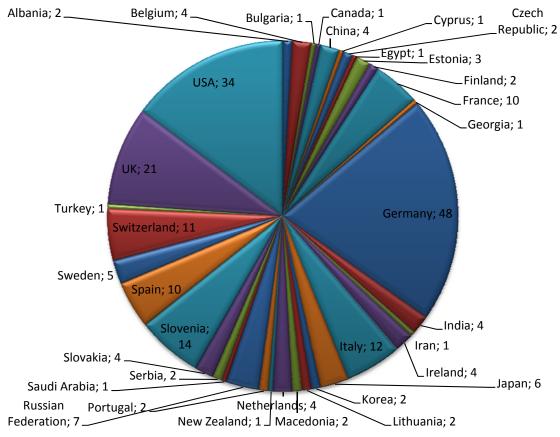
Figure 9 - Distribution of participants per country

7 Post-event activities

All participants were emailed after the event with information about the available online presentations and photo gallery.

A press release about the results and presentations available was published and disseminated after the event. Feature article with pictures will also be published in the coming PRACE newsletter.

8 Conclusions

PRACE Scientific Conference 2012 highlighted selected results obtained on the PRACE Tier-0 systems. This conference continues a good practice of a very successful DEISA and DEISA PRACE Symposium Series that were being held annually in the past seven years. Next PRACE Scientific Conference is planned to be organized again jointly with ISC'13 in Leipzig, Germany.

A one day program included nine speakers and a short User Forum meeting, highlighting the major scientific achievements, HPC vision and future opportunities.

The conference had 230 registered participants from 35 countries and represents a promising beginning of a new series of PRACE Scientific Conferences. The aim of strengthening the human network within the scientific community worldwide was fulfilled during the presentations and the joint evening networking event between PRACE and the participants of HPC in Asia Workshop.

9 Annex

9.1   Abstracts of Scientific Presentations

9.1.1 *A Fast and Scalable Low Dimensional Solver for Charged Particle Dynamics in Large Particle Accelerators*

PRACE Award 2012 winning paper
Authors: Yves Ineichen, Andreas Adelmann, Costas Bekas, Alessandro Curioni & Peter Arbenz

Abstract

This paper demonstrates how HPC can be used in real time to tune the operation of particle accelerators, which are invaluable tools for research in the basic and applied sciences, in fields such as materials science, chemistry, the biosciences, particle physics, nuclear physics and medicine. The design, commissioning, and operation of accelerator facilities is a non-trivial task, due to the large number of control parameters and the complex interplay of several conflicting design goals. The team from IBM Research, Paul Scherrer Institute and ETH Zürich achieved strong and weak scalability improvement on BlueGene/P of two orders of magnitude for the most heavily used component of the optimisation framework, which computes the evolving shape of the bunches of particles in the beam. This enables thousands of such calculations to be performed in a matter of minutes, creating close to on-line optimisation capability.

9.1.2 *Excess proton at water/hydrophobic interfaces: A Car-Parrinello MD study*

Project leader: Paolo Carloni, German Research School for Simulation Sciences GmbH, Jülich, Germany

Collaborators: Emiliano Ippoliti, German Research School for Simulation Sciences GmbH, Jülich, Germany / Yana Vereshchaga, German Research School for Simulation Sciences GmbH, Jülich, Germany

Abstract

Recent experimental evidence shows unambiguously that, at room conditions, excess protons are located close to hydrophobic surfaces in liquid mixtures, in contrast to intuitive considerations. Shedding light on structural and energetic facets of this issue is crucial to describe correctly key biochemical processes such as protein folding and ligand/target interactions. So far, approaches have been mostly used classical modeling or empirical quantum-mechanical methods. The latter have suggested that the process is driven by enthalpy, which overcompensates the entropy penalty. First principle study reported so far did not address the energetics of the processes. Here we plan to perform ab initio molecular dynamics of an excess proton in the presence of a water/decane mixture as used experimentally. We plan to calculate the free energy of the process using thermodynamic integration and determine at which distance from the surface it is most probable that the proton localizes.

PRACE Resource awarded: 40 468 480 core-hours

9.1.3 *A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and an in-coming dislocation*

Project leader: Dierk Raabe, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Collaborators: Franz Roters, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany / Bing Liu, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Abstract

Discrete Dislocation Dynamics (DDD) models simulate explicitly the motion, multiplication and interaction of dislocation lines, the carrier of plasticity in crystalline materials, in response to an applied load. This project aims to study the dislocation physics during plastic deformation of metals, focusing on the microstructure evolution (cell structure formation) and the interaction between a low angle grain boundary (LAGB) and an in-coming dislocation.

To simulate the dislocation cell structure formation, both the sample volume and the amount of plastic deformation have to exceed the most computationally expensive simulations (volume: 5 µm on a side; plastic deformation 1.7%) run on Thunder and Blue Gene/L computers at the Lawrence Livermore National Laboratory.

When the wall dislocations and the dislocation loop have the same Burgers vector but on different glide planes (collinear relation), they form a junction with zero Burgers vector (partial annihilation). The collinear dislocation interaction has been reported to be stronger than all other types of dislocation interactions (self interaction, coplanar interaction, interaction leading to non-zero junctions). The finding from our simulations of the interaction between a low angle grain boundary (dislocation wall) and dislocation loops is that: the partial annihilation of wall dislocation and in-coming dislocation loop makes dislocation loop transmission easy and leads to strong interactions at the dislocation wall, and junction formation pins the dislocation loop at the dislocation wall, and strong multiplication events happen outside the dislocation wall region. Both dislocation density and plastic strain increase faster in the junction case than in the collinear case. It is important to further study how the interaction depends on the dislocation spacing of wall dislocations, or in other words the angle of the LAGB. Currently the dislocation spacing is 1000b (b is the magnitude of the Burgers vector), and the use of smaller dislocation spacing (100b) would request the number of DOF to increase 100 times (the number of dislocations x10, and the number of segments per dislocation x10).

Additionally, we would like to study the (average) migration velocity of a clean and solitary LAGB in contrast to the (messy) case when concurrent activity of numerous dislocation loops destroys the neat boundary structure. Both cases are investigated under the same applied stress. Experimental observations suggest a massive reduction in the migration rate in the latter case. Likely, the generation of low-mobility junctions slows down a disrupted boundary. The messy case (dislocation wall with massively-tangled dense dislocation network) needs the computational capability of the Blue Gene/P.

PRACE Resource awarded: 15 600 000 core-hours

9.1.4 *Droplet growth by coalescence in turbulent clouds: kinetics, fluctuations, and universality*

Project leader: Jeremie Bec, Observatoire de la Côte d'Azur, Nice, France

Collaborators: Holger Homann, Observatoire de la Côte d'Azur, Nice, France / Samriddhi Sankar Ray, Observatoire de la Côte d'Azur, Nice, France / Rainer Grauer, Ruhr-University Bochum, Bochum, Germany

Abstract

Warm clouds are constituted of small water droplets that do not follow exactly the turbulent airflow but have inertia. They thus react with some delay to the fluid motion and feel gravity, so that they distribute non-uniformly in space and can have very large velocity differences. Consequently the rate of collision and growth by coalescence of such droplets cannot be predicted by simple arguments and the timescales of precipitation are often under-estimated. Our objective is to investigate this issue by a direct numerical simulation of coalescing particles that are passively transported by a homogeneous isotropic turbulent flow.

While atmospheric scientists attach importance to account simultaneously for all processes to be as much realistic as possible, the proposed approach simplifies the main mechanisms to obtain a better handling of fundamental questions. The novelty of the intended work originates in extending and adapting to the problem of rain formation the statistical physics tools developed for Lagrangian turbulence. The main ingredient of such approaches is the statistical Lagrangian formalism developed during the last decade, which consists in reformulating transport and mixing problems in terms of averages along particle paths. The key task is then to estimate the cumulative weights of fluctuations along trajectories or to determine the probability of the events giving a dominating contribution to the statistics. This method has two advantages: first, it is well adapted for dealing with systems that are far from equilibrium, and second, it allows controlling the history of individual particle paths. The problem of estimating time scale of rain formation in warm clouds requires tools that cope with these two difficulties.

In order to accompany and validate such analytical modelings, we will perform state-of-the-art numerical simulations of a cloud portion. For being ensured that the airflow turbulence is sufficiently developed, we plan to integrate the fluid phase on a 2048^3 periodic grid with a high-accuracy pseudo-spectral solver. To match particle loading encountered in strato-cumulus, one billion particles will be seeded in the flow with an initial size distribution that mimics observations and which will be centered around a typical radius equal to one twentieth of the dissipative Kolmogorov scale. The system will then be evolved using an efficient collision detection algorithm and performing particle mergers that conserve mass and momentum. The simulation will be evolved for at least fifty large-scale turnover time to obtain a typical size of particle that has increased by at least one order of magnitude. The objective is to measure timescales for the growth of droplets and to highlight universal properties of the size distribution in the large-time asymptotics. Such measurements will confirm or refute the validity of predictions from standard mean-field kinetic models.

PRACE Resource awarded: 50 000 000 core-hours

9.1.5 *Predictive full-scale fast ignition with PW plasma amplified laser pulses*

Project leader: Luis O. Silva, Instituto Superior Técnico, Lisbon, Portugal

Collaborators: Warren Mori, University of California Los Angeles, Los Angeles, United States / Raoul Trines, Rutherford Appleton Laboratory, Didcot, UK / Frederico Fiuza, Instituto Superior Técnico, Lisbon, Portugal / Ricardo Fonseca, Instituto Superior Técnico, Lisbon, Portugal

Abstract

Fusion energy is regarded as a possible long-term energy solution for humanity, capable of providing the energy resources to drive economic growth and social development. Fast ignition is one of the most promising and exciting inertial confinement fusion schemes to improve the viability of inertial fusion energy as a practical energy source. Even if up to now experiments have been limited to laser energies still far from ideal conditions for ignition and simulations, which are extremely complex due to the different temporal and spatial scales involved, have been limited to reduced scales/simplified models, in the very near future we expect transformative results as novel laser systems are now coming online, with the National Ignition Facility and, in the near future, the ESFRI roadmap project HiPER (High Power laser Energy Research), reaching the conditions required for ignition. In this proposal, and using massively parallel simulations, we aim to perform, for the first time with realistic target properties (e.g. density, temperature, dimensions) and the correct simulation dimensionality, and with realistic ultra-intense laser pulses obtained from Raman amplification, self-consistent fast ignition simulations including all the relevant microphysics/particle dynamics, taking advantage of the novel hybrid model incorporated into the state-of-the-art relativistic particle-in-cell massively parallel code OSIRIS, with the goal of identifying possible paths to demonstrate fast ignition as an efficient scheme for inertial fusion energy.

PRACE Resource awarded: 31 000 000 core-hours

9.1.6   *Turbulent entrainment due to a plume impinging on a density interface*

Project leader: Maarten van Reeuwijk, Imperial College London, London, UK

Collaborators: Harm Jonker, Delft University of Technology, Delft, The Netherlands / Gary Hunt, Imperial College London, London, UK

Abstract

The entrainment of fluid across density interfaces is a fundamental physical process with applications throughout the natural sciences and engineering. This process is of importance in density stratified environments which are subject to regions of localized turbulence. For example, in oceanic and atmospheric contexts, turbulent entrainment has a bearing on the rate of deepening of oceanic and atmospheric mixed layers, respectively. This then has a direct impact on the concentration of pollutants released in the atmosphere or trapped in a mixed layer in the ocean. As entrainment involves a transport of fluid between layers, it has widespread applications in water-air quality problems. However, despite its significance, existing entrainment laws, which couple an entrainment velocity to a turbulence intensity and density contrast between the layers, are subject to very significant uncertainties and currently there is no consensus in the literature regarding which is correct or the most appropriate. With laboratory measurements of entrainment rates in identical apparatus varying by orders of magnitude, this then presents the scientific community with real concerns and throws into question many models and modeling approaches which rely on a specification of such entrainment rates. This proposal aims to pin down the entrainment law for localized turbulent patches using direct numerical simulation (DNS).

An improved entrainment law for localized turbulent patches will enable enhanced predictive capability. One pertinent example is the low-energy design of ventilation in buildings. Here, the turbulent entrainment across a thermal interface - an interface separating a cool lower region in a room from the warmer upper region - as is typically induced by a thermal plume rising from localized heat sources, is an extremely important mechanism as it plays a significant role in determining the temperature distribution in the room and thus, the comfort of occupants. Optimization of the energy-efficiency in a ventilated building is only possible if the simplified models typically used to provide design guidance are accurate.

PRACE Resource awarded: 30 000 000 core-hours

9.1.7   *Ab initio Simulations of Turbulence in Fusion Plasmas*

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Abstract

The world-wide demand of electricity is projected to increase by about a factor of six throughout the 21st century. At the same time, the use of fossil fuels will have to be reduced. At present, we still have no silver bullet which can be used to close this gap. Fusion energy is an attractive option in this context, and high-performance simulations play a key role for its further development. The present project represents an important contribution to the European effort to employ Petascale (and later Exascale) computing for fusion energy applications. Its main goal is to use the latest version of the plasma turbulence code GENE to perform a number of millenium-type simulations which are closely linked to the international flagship fusion experiment ITER - one of the most challenging scientific projects to date and currently under construction in Southern France. The first target is to perform the first physically comprehensive simulations of the ASDEX Upgrade tokamak at Garching, presently one of the world's leading fusion devices and conceptually very similar to ITER, although about four time smaller in the linear dimensions. The second question to be addressed is the dependence of the turbulent transport on the system size. Given that ITER is expected to benefit from the fact that it will be significantly larger than all existing fusion devices, this is a key issue to ensure the project's success. Since the theoretical understanding of it is still far from complete, these simulations will provide very valuable insights.

PRACE Resource awarded: 50 000 000 core-hours