PRACE 2.0 for Austria

Document Editors:

A.Univ.Prof. DI Dr. Wolfgang Schreiner
(PRACE Council Delegate)
Johannes Kepler University Linz
Wolfgang.Schreiner@risc.jku.at

Univ.Prof. DI Dr. Gabriele Kotsis
(Vice Rector for Research)
Johannes Kepler University Linz
Gabriele.Kotsis@jku.at

Univ.Prof. Dr. Sabine Schindler
(Vice Rector for Research)
University of Innsbruck
Sabine.Schindler@uibk.ac.at

May 27, 2014

Abstract

PRACE (Partnership for Advanced Computing in Europe) is the premium European infrastructure, research, and training network for large-scale high performance computing. Among 25 European countries, also Austria has been from 2010–2015 member of PRACE and profited from access to its research infrastructure, scientific projects, and training and education events. In 2016–2020, PRACE will enter its next phase "PRACE 2.0". We describe the background of PRACE and its initial phase, the benefits of Austria's further participation in PRACE 2.0, and the contributions that are correspondingly required. By describing a number of projects from various Austrian scientific institutions, we demonstrate how the Austrian scientific landscape will profit from this participation.

Contents

1 PRACE Background

PRACE (Partnership for Advanced Computing in Europe) is an international non-profit association (aisbl) with seat in Brussels. It has 25 member countries whose representative organizations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level [5].

History The members and founders of PRACE have been working together for more than a decade now. Building on EU funded initiatives since 2004 (HPCEUR, HET) and on the first Scientific Case for HPC in Europe, they started the PRACE Preparatory Phase in 2008, which resulted in the founding of PRACE aisbl in April 2010. The four "hosting members" (France, Germany, Italy, and Spain, see below) secured funding for the initial period from 2010 to 2015, while the PRACE Project partners continued to develop the brand and services of PRACE through three FP7-funded Implementation Phase projects. PRACE started with 21 members and grew to 25 by end 2012; several more governments are showing interest. The activities of PRACE are documented in annual reports [10].

Research Infrastructure Researchers and scientists (from both academia and industry) affiliated with PRACE member countries may for the purpose of basic research and development access six leading-edge high performance computing systems via regular calls and a peer-reviewed selection process [4]. These systems are provided and operated by four PRACE "hosting members" (the Barcelona Supercomputing Center BSC representing Spain, the Academic Consortium CINECA representing Italy, the Gauss Supercomputing Center GCS representing Germany, and the Grand Equipement National de Calcul Intensif GENCI representing France) [6]. In pace with the needs of the scientific communities and technical developments, systems deployed by PRACE are continuously updated and upgraded to be at the apex of HPC technology. Additionally, PRACE supports via various implementation projects and regular training activities users and user communities in porting, scaling and optimizing their applications to fully exploit the capabilities of the PRACE systems.

Funding PRACE receives funding from three sources:

- The PRACE HPC systems are funded and operated by the four hosting countries France, Germany, Italy and Spain. Their commitment for the establishment and operation of PRACE systems adds up to €400 million over a five year period (2010—2015).
- All 25 members of PRACE pay an annual fee; some of them provide national HPC resources as additional in-kind contributions.
- The European Commission supports the PRACE Implementation Projects for a total of €67 million under grant agreements RI-261557 (PRACE-1IP, 2010–2012), RI-283493 (PRACE-2IP, 2011–2013) and RI-312763 (PRACE-3IP, 2012–2014). These grants are complemented by a consortium budget of €43 million.

Austria and PRACE Austria is represented in PRACE by the Johannes Kepler University (JKU) Linz; the PRACE membership is currently jointly funded by the budgets of JKU Linz and the University of Innsbruck. Concretely Austria is represented in the PRACE Council (the body that decides on all matters of the association which is composed of one representative from each member) by Wolfgang Schreiner (RISC Institute, JKU Linz) and Michael Krieger (RISC Software); members of the Scientific Steering Committee (responsible for advice and guidance on all matters of a scientific and technical nature) are Christoph Dellago (University of Vienna) and Christian Lang (University of Graz). Information about PRACE relevant to Austrian researchers is available on a central Web page and mailing list [3].

2 PRACE Participation

Countries profit from the participation in PRACE

- by access to its research infrastructure,
- by cooperation in its implementation projects,
- by participation in its education and training activities,

and thus, all in all, by being linked to the *principal pan-European network for high-end computing activities*. These benefits are elaborated below in more detail.

PRACE Research Infrastructure PRACE systems are available to scientists and researchers from PRACE member countries through three forms of access:

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

Multi-year and Project Access are subject to the PRACE peer review process. Leading scientists evaluate the proposals submitted in response to the bi-annual calls [4].

PRACE Implementation Projects In three EU-sponsored implementation projects (PRACE-1IP, PRACE-2IP, and PRACE3-IP) partners have been collaborating to develop a long-term, high-quality infrastructure for European (Tier-0) systems, managing the coordination between the shared portion of the national (Tier-1) HPC resources, and also strengthening the established relationships with industrial users. In particular, the following four activities are central in the current PRACE3-IP [9]:

- *Pre-Commercial Procurement:* Pilot exercise for a joint procurement and joint ownership of innovative HPC prototypes, focusing on high-energy efficiency.
- *Deployment of HPC services for European industry:* Proposes a broad set of services suitable for use by industry, including access to HPC resources, knowledge transfer through application support, training and expertise.
- *Application scaling and support to address major socio-economic challenges:* Tackles major socio-economic challenges and the use of simulation and modeling to deal with them.
- *Training and outreach for growth:* Establishes a broad training and outreach activities specifically designed to engage more user communities, including industry, in the use of HPC systems.

This goal is approached via various networking activities (including dissemination and training), service activities (e.g., supporting applications on Tier-0 and Tier-1 systems), and joint research activities (including development of software prototypes).

PRACE Training and Education PRACE undergoes an extensive education and training effort for effective use of HPC systems by six PRACE Advanced Training Centres (PATC), quarterly seasonal schools, and regular workshops and scientific and industrial seminars throughout Europe. Seasonal Schools target broad HPC audiences, whereas workshops are focused on particular technologies, tools or disciplines or research areas [8].

In 2014, PRACE will organize its first Scientific and Industrial Conference, the first edition of the "PRACE Days", under the motto "HPC for Innovation —- when Science meets Industry". The conference combines the previously separate PRACE Scientific Conferences and PRACE Industrial Seminars and will bring together experts from academia and industry who will present their advancements in HPC-supported science and engineering [7].

Austrian Participation Since 2011, Austrian researchers have been granted access to the PRACE research infrastructure in the frame of the following projects (joint collaborations with multiple international partners):

- MHD turbulence in the Interstellar Medium: Linking Star Formation and Galaxy Dynamics (Austrian collaborators from University of Vienna),
- Modeling gravitational wave signals from black hole binaries (Austrian collaborators from University of Vienna),
- CAMEL — CArdiac MechanoELectrophysiology (Austrian collaborators from Medical University of Graz).

The rewards granted to these projects amounted to approximately *32.5 million core hours* (which would keep a 1024 core machine busy for 3.5 years) on various of the PRACE high-performance systems.

Various institutions of JKU Linz (ICA, RISC Institute and Software) have participated since 2010 in the three PRACE implementation projects.

- In the former project PRACE-1IP and PRACE-2IP, ICA investigated topics in advanced computer systems design, including parallel systems and acceleration technologies, from hardware to software. The goal was the principled development of system architectures and components that push the boundaries of high performance compute fabrics and simplify their use and programming environment.
- In the current project PRACE-3IP, RISC is engaged in work packages WP 3 (dissemination and outreach), WP 4 (training), WP 7 (application enabling and support). For instance, within WP 7 researchers of RISC have coordinated the project "Multidiscipline Simulations for Aircraft Design" on the coupling of computational fluid dynamics (CFD) code and computational structural mechanics (CSM) code for high-performance simulation systems.

As for training and dissemination activities, the PRACE 2014 Spring School on "Software Engineering for Supercomputers in Research and Industry" was organized in Hagenberg, Austria, from April 15-17 with an international audience of 40 trainees (with 7 of the 12 speakers/trainers and approx. 50% of the trainees from Austria) [2]; similarly Austrian participants have participated at various foreign seasonal schools and training events.

3 PRACE 2.0

PRACE is currently planning the next phase *PRACE 2.0* (2016–2020) of its operation (with PRACE 1.0 representing the initial phase 2010–2015). Part of the preparation of this phase is the elaboration of a proposal for the EU Horizon 2020 call for "e-Infrastructures" (budget: € 82 million) for which the PRACE partner will make a bid in September 2014 [1].

As a major change to the "business model", in PRACE 2.0 the costs for the development of the infrastructure (which was in PRACE 1.0 essentially covered by the four hosting members) will be shared between the hosting members and the general partners. The currently discussed PRACE 2.0 model (status: May 6, 2014) is based on the following principles:

1. An annual fee of € 60 000 of every member will contribute to the general PRACE operation (in addition to European projects in the frame of Horizon 2020).
2. There will be three categories of members:
   a) full members that host Tier 0 systems for PRACE,
   b) full members that do not host such systems, and
   c) associate members

   (see below for the definition of a Tier 0 system).

   Associate members will not contribute to the investment of PRACE 2.0 systems and have no voting rights in the PRACE council. However, they can participate in PRACE 2.0

projects and they will be invited to apply for the use of PRACE 2.0 systems, but with a limit of 1% usage for each of them.

3. The PRACE 2.0 infrastructure will consist of a certain number of "Tier 0 systems" which are broadly defined as

   > *high performance supercomputers that are much more powerful than national machines and could not be afforded by individual countries alone.*

   The general criteria of such a machine are

   - at least 10 PFLOPS performance,
   - about € 50 million hardware investment.

   The total cost of ownership (TCO) over a five year period is estimated to be twice the hardware investment (i.e., it is evenly split between investment and operational costs).

4. Full members contribute to the TCO based on a index that averages the corresponding nation's GDP and the past usage of that system in comparison to all other members. For full members that host PRACE systems, this index is weighted with a factor of 3; for the other full members the weight factor is 1.

   The sum of the weighted indices of full members is currently estimated at 206.4; Austria is assigned an index of about 1.1 which would mean a contribution of about 0.53% to the TCO of the PRACE 2.0 systems.

5. Current estimations for realistic investments run from two to four Tier-0 systems yielding a TCO of about € 200–400 million over a five year period; thus according to above criteria as a full member Austria's total contribution would be € 1–2 million. Austria's yearly contribution to the TCO would be € 200–400 thousand for a period of five years.

Since the discussion among PRACE members is still ongoing, above figures are only preliminary estimations but give a range within which the final figures will most probably reside. In a nutshell, we have the following result:

> **The total cost of Austria's participation in PRACE 2.0 as a full member that does not host a Tier 0 system is in the range of**
>
> **€ 260 000–460 000**
>
> **per year for a period of five years (2016–2020).**
>
> **For this investment, Austria gets access to 2–4 Tier-0 (European level) HPC systems with a total performance of at least 10 PFLOPS each; the amount of access is limited by scientific excellence (as measured in the success in the corresponding project calls) only. Furthermore, Austria is by this investment linked to the premium European research and education network for large scale high performance computing with corresponding profits for its scientific and industrial institutions.**

In comparison, the fastest HPC system in Austria, the soon to be installed VSC-3 at the Vienna Scientific Cluster [11], has a performance of about 0.584 PFLOPS; this Tier-1 system thus achieves less than 6% performance of a single of the planned PRACE 2.0 Tier-0 systems. Access to such European Tier-0 systems (in addition to that of national Tier-1 systems) is for many activities indispensable:

1. Project grants in PRACE 1.0 were typically in the region of about 10–100 million core hours; similar figures can be expected for PRACE 2.0. A typical 50 million core hours grant would occupy the biggest Austrian machine (the VSC-3 with 28 096 cores) busy for 74 days, which makes the execution of such jobs on a Tier-1 system unrealistic.

2. The number of processor cores in a Tier-0 system is an order of magnitude larger than that of a Tier-1 system (the Munich SuperMuc system currently employed in PRACE has more than 155 000 cores). With Tier-0 therefore scalability experiments can be performed in a range that is not possible with Tier-1 systems.

3. The PRACE 2.0 infrastructure provides access to multiple systems with different architectures and performance characteristics. Past experience shows that not all applications perform well on every system; thus access to different systems allows to run a much wider range of applications in an efficient way.

4. The economy of scale of running a Tier-0 system provides several advantages: apart from reducing the general overhead of operation, it allows to bundle a comparatively much larger amount of human expertise with respect to the efficient utilization of a system which can be shared with its users.

As documented in the appendices, there are many Austrian high quality research projects that will profit tremendously from a participation in PRACE 2.0. Taking into account the status of Austria as a research-oriented industrial country and comparing it with other European countries of the same status (Germany has 18,63% GDP among PRACE members and used 20.81% of the PRACE resources in the past), also researchers from Austria (2,14% GDP) will be able to profit from access to a corresponding share of this modern European research infrastructure as well as from being linked to the premium European research and education network in large-scale high performance computing.

References

[1] European Commission. *H2020-EINFRA-2014-2*. 2014. URL: http://ec.europa.eu/research/participants/portal/desktop/en/opportunities/h2020/calls/h2020-einfra-2014-2.html.

[2] RISC Institute. *PRACE 2014 Spring School Presentations*. 2014. URL: http://www.risc.jku.at/projects/prace/SpringSchool2014.

[3] RISC Institute. *PRACE in Austria*. 2014. URL: http://www.risc.jku.at/projects/prace.

[4] PRACE Office. *PRACE Call Announcements*. 2014. URL: http://www.prace-ri.eu/Call-Announcements.

[5] PRACE Office. *PRACE Research Infrastructure*. 2014. URL: http://www.prace-ri.eu.

[6] PRACE Office. *PRACE Resources*. 2014. URL: http://www.prace-ri.eu/PRACE-Resources.

[7] PRACE Office. *PRACE Scientific and Industrial Conference 2014*. 2014. URL: http://www.prace-ri.eu/pracedays14.

[8] PRACE Office. *PRACE Training Portal*. 2014. URL: http://www.training.prace-ri.eu/.

[9] PRACE Office. *Third Implementation Phase (PRACE-3IP) Project*. 2014. URL: http://www.prace-project.eu/PRACE-3IP.

[10] Marjolein Oorsprong et al., eds. *PRACE Annual Report 2013*. May 2014. URL: http://www.prace-ri.eu/AR-2013.

[11] Vienna University of Technology. *Vienna Scientific Cluster*. 2014. URL: http://vsc.ac.at/.

Potential PRACE 2.0 Projects

A Multi-Scale Astrophysical Turbulence Simulation

Proposer

Habil. Priv.-Doz. Dr. Yasuhito Narita, Dr. Philippe Bourdin
Institut für Weltraumforschung, Österreichische Akademie der Wissenschaften
Schmiedlstr. 6, 8042 Graz
Email: Philippe.Bourdin@oeaw.ac.at
Web: http://www.IWF.oeaw.ac.at/

Topic

We aim to tackle with the long-standing problem of astrophysical plasma turbulence by performing multi-scale 3D plasma simulation for the first time over a wide range of spatial scales spanning over 4 to 6 orders of magnitude. Plasma turbulence can occur in any stellar-planetary systems in astrophysics. It is the key process to solve the long-standing coronal heating problem; It is an essential ingredient to convert the stellar energy into magnetic field known as dynamo; and it plays an essential role in star-planet formation as turbulence serves as a very effective means to transport mass and angular momentum on short time scales. Without plasma turbulence, the formation and evolution of the Sun and the Earth cannot be explained. In spite of its importance, it is a hard challenge to tackle with plasma turbulence problem in all experimental, observational, and theoretical contexts. Astrophysical plasmas are so hot (reaching to 10^5–10^6 K) yet so dilute (electron number density of the order of 1–10 cm^{-3}) that they cannot be produced and sustained in laboratory experiments. Solar system plasmas such as in near-Earth or interplanetary space are often found to be in a turbulent state. They can be sampled *in situ* by spacecraft observations, yet due to the nature of single spacecraft measurements in space, one cannot distinguish if fluctuations represent temporary evolution or spatial structure passing by the spacecraft. Theoretically, plasma turbulence can be formulated as a competition between splitting eddies (that originate in neutral fluid turbulence) and scattering of electromagnetic waves. Two questions remain unsolved to date, "Which kind of waves are dominant under a condition of hot or cold plasma?", and "What is the effect of large-scale structure or inhomogeneity?".

In multi-spacecraft measurements, energy spectra can be determined experimentally in the full four-dimensional Fourier space spanned by frequencies and wave vectors without assuming any spatio-temporal relations such as frozen-in flow hypothesis (Fig. 1). In order to verify the existing speculations or predictions on dynamics of plasma turbulence, and in order to reproduce the measured turbulence energy spectra, Direct numerical simulation (DNS) serves as the most effective method to advance astrophysical turbulence research.

Previous Work

Various schemes have been developed to study astrophysical turbulence in DNS. They differ in modeling the plasma as described by the equation of motion. Currently, the model types

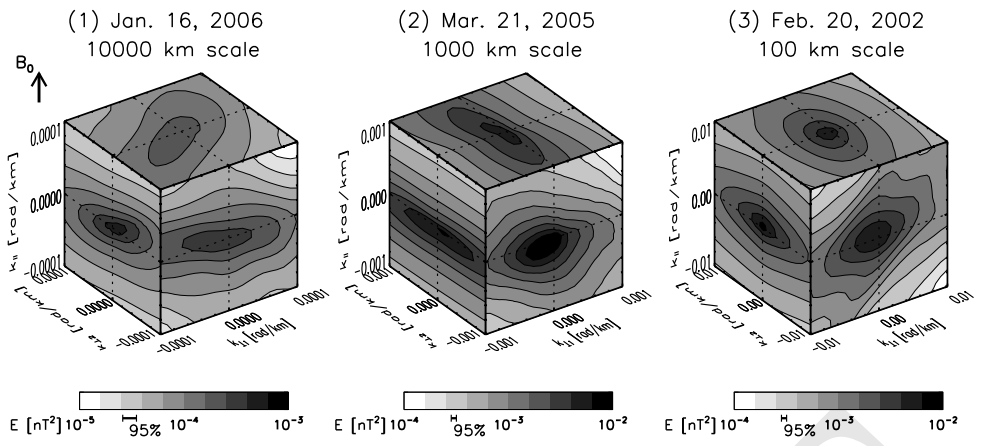

Figure 1: Direct measurement of 3D energy spectra in solar wind plasma on multiple scales, oriented along the direction of a large-scale magnetic field (vertical axis) [9].

can be classified into five groups: single fluid (magnetohydrodynamic picture); multi-fluid; gyro-kinetic [7]; full-particle [10]; and hybrid.

In comparison, single-fluid and multi-fluid models cannot resolve the energy and momentum exchange between ions and electromagnetic fields. Gyro-kinetic models assume an a priori particle motion and electromagnetic fields are axisymmetric around the direction of the large-scale magnetic field, giving only a time-averaged picture of the gyro-motion. Full-particle simulation, under the current computational resource, can only resolve plasma turbulence on a very short time scale as dynamics of individual electrons must be solved. Hence, ion motions are ignored on such short time scales.

At present stage, hybrid models perform best for plasma turbulence studies. But at the same time, these models are computationally expensive, because the individual ion motion needs to be resolved. Therefore, access to high-performance computing on largest scale (Tier-0) is the key for performing cutting-edge science of international level.

Macroscopic plasma simulation

In a macroscopic simulation, plasma is treated as an electrically conducting, magnetized fluid and individual charged particle motions are not resolved. This approximation is particularly useful in studying large-scale behavior of plasma and electromagnetic fields. Various simulation codes have been developed for astrophysical fluid simulation, e.g., ZEUS-3D [5], Pencil Code [4], and Athena [11]. Here, Pencil Code is used i.e. for solving macroscopic plasma turbulence.

Using Pencil Code, it is possible to produce plasma turbulence on scales of 1'000 km or larger in interplanetary space. It is also a powerful method to reconstruct the 3D plasma and magnetic field structure in solar corona [3]. We obtained fundamental insights into the long-standing coronal heating problem, clarifying the structure formation and plasma transport within a magnetically active region on the Sun [1, 2]. For this work, about 75% of the

computational demand was covered by two PRACE Tier-0 grants, summing to over 15 million CPU-core hours in total on **Curie** and **JuRoPA**.

Microscopic plasma simulation

The AIKEF code (Adaptive Ion-Kinetic, Electron-Fluid) is a state-of-the-art hybrid plasma simulation code [8]. Whenever the plasma dynamics exhibits a fine structure, the mesh size can be adapted in order to resolve this structure. Astrophysical plasmas are dilute and collisionless, so that the particle mean-free-path is comparable to the system size or even larger. Therefore, effects of charge localization can safely be neglected in astrophysical plasma turbulence.

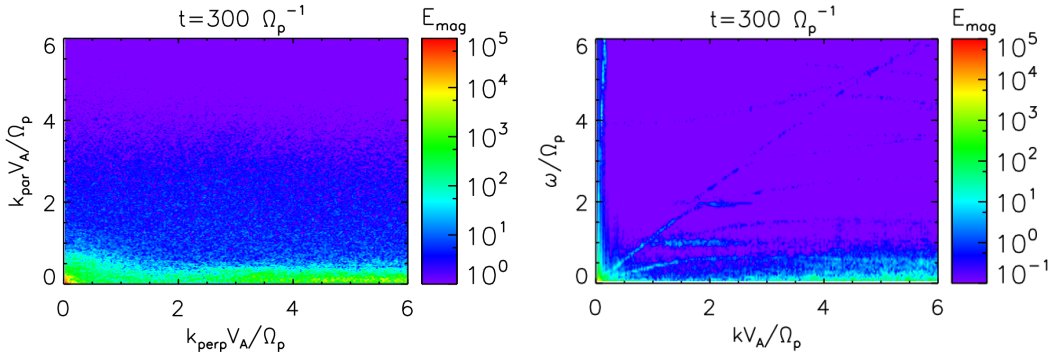

Figure 2: Energy spectra in the 2D wavevector domain (left panel) and as frequency versus wavenumber perpendicular to the mean magnetic field (right panel) produced by AIKEF [6].

Recently, the code has been successfully used to study turbulence in 2D low-beta plasmas [12], and the simulation time was extended to 1'000 ion gyro-periods [6]. In this setting, it was possible to determine the energy spectrum, spanned by the frequencies and two-dimensional wave vectors as a function of time (Fig. 2). For this work, we have been awarded about 1 million CPU-core hours from a Tier-1 call on the supercomputer **JuRoPA**.

Planned PRACE Activites and Infrastructure Access

Multi-scale turbulence evolution. A broad range of spatial resolution and coverage is needed to study astrophysical plasma turbulence. In interplanetary space, turbulence can be found on scales from 100'000 km down to 10 km, expanding over 4 orders of magnitude. We aim to produce astrophysical plasma turbulence over as wide scales as possible. By combining two different plasma simulation codes, we can significantly increase the scale coverage in our turbulence study over 4 to 6 orders of magnitude. Our goal is to obtain information on **3D wave vector anisotropy** and **wave modes** via the energy spectra.

We are able scale our simulation code to up to 8192 CPU cores in parallel and we need to have lowest-possible latency networking between the compute nodes. Typically, we need CPUs with SIMD units for vector computations (such as Intel and AMD processors), equipped

with about 2 GB RAM per CPU core, interconnected with an Infiniband low-latency and high-throughput networking. Our above proposed project would consume about **20 million CPU-hours per year** on such a machine (or about five times more on an **IBM/BlueGene** type of hardware). That requires us to apply for computing time on high-performance computing sites on international (Tier-0) level, because such large projects are not feasible on national (Tier-1) level computing sites. All PRACE Tier-0 systems are capable of performing such a simulation project, except for GPU-based supercomputers than currently still lack the required memory and interconnectivity requirements.

References

[1] Ph.-A. Bourdin. *PhD thesis (Observationally driven 3D MHD model of the solar corona above a magnetically active region)*. uni-edition, Berlin, 2014. ISBN: 978-3-944072-03-6.

[2] Ph.-A. Bourdin, S. Bingert, and H. Peter. "Coronal loops above an Active Region — observation versus model". In: *Publications of the Astronomical Society of Japan* submitted (2014).

[3] Ph.-A. Bourdin, S. Bingert, and H. Peter. "Observationally driven 3D MHD model of the solar corona above an active region". In: *Astronomy and Astrophysics Manuscripts* 555 (July 2013), A123. DOI: 10.1051/0004-6361/201321185.

[4] A. Brandenburg and W. Dobler. "Hydromagnetic turbulence in computer simulations". In: *Comp. Phys. Comm.* 147 (2002), pp. 471–475.

[5] D. A. Clarke. "A Consistent Method of Characteristics for Multidimensional Magneto-hydrodynamics". In: *The Astrophysics Journal* 457 (Jan. 1996), p. 291. DOI: 10.1086/176730.

[6] H. Comişel et al. "Spectral evolution of two-dimensional kinetic plasma turbulence in the wavenumber-frequency domain". In: *Physics of Plasmas* 20 (2013), p. 090701. DOI: 10.1063/1.4820936.

[7] G. G. Howes. "Inertial range turbulence in kinetic plasmas". In: *Physics of Plasmas* 15 (May 2008), p. 055904. DOI: 10.1063/1.2889005.

[8] J. Müller et al. "A.I.K.E.F.: Adaptive hybrid model for space plasma simulations". In: *Computer Physics Communications* 182 (Apr. 2011), pp. 946–966. DOI: 10.1016/j.cpc.2010.12.033.

[9] Y. Narita et al. "Three-dimensional spatial structures of solar wind turbulence from 10 000-km to 100-km scales". In: *Annales Geophysicae* 29 (Oct. 2011), pp. 1731–1738. DOI: 10.5194/angeo-29-1731-2011.

[10] S. Saito et al. "Whistler turbulence: Particle-in-cell simulations". In: *Physics of Plasmas* 15 (2008), p. 102305. DOI: 10.1063/1.2997339.

[11] J. M. Stone et al. "Athena: A New Code for Astrophysical MHD". In: *The Astrophysics Journal Supplement Series* 178 (Sept. 2008), pp. 137–177. DOI: 10.1086/588755. arXiv:0804.0402.

[12] D. Verscharen et al. “Kinetic cascade beyond magnetohydrodynamics of solar wind turbulence in two-dimensional hybrid simulations”. In: *Physics of Plasmas* 19.2 (Feb. 2012), p. 022305. DOI: 10.1063/1.3682960. arXiv:1201.2784.

B Synthesis of Microscopic Models for the Design of Improved Multiphase Flow Systems

Proposer

Univ.-Prof. DI Dr. Johannes G. Khinast, Ass.Prof. DI Dr. Stefan Radl
Institute for Process and Particle Engineering (IPPT)
Graz University of Technology
Inffeldgasse 13/III, 8010 Graz
Email: khinast@tugraz.at, radl@tugraz.at
Web: http://ippt.tugraz.at

Topic

Understanding the flow behavior of disperse multiphase systems, i.e., fluid or solid particles dispersed in a continuous fluid phase, is of key importance in various scientific disciplines, such as medicine (e.g., blood flow) or chemical engineering (e.g., particle separation or mixing). In addition to flow, often the transport of dissolved species (e.g., oxygen dissolved in our blood), as well as chemical reactions are critical factors that impact the overall system dynamics.

Unfortunately, there are significant gaps in our current understanding of these multiphase flow systems, and questions like:

- *How fast do particles exchange heat and mass with the surrounding fluid?*
- *How should we operate a chemical reactor such that the output of the desired product is a maximum ?* , or
- *How can we separate, or mix, spherical and non-spherical particles in a suspension most efficient?*

still require tedious experimental studies, or excessive computer simulations. Indeed, the above questions have been addressed by many researchers, with the conclusion that a so-called *Multiscale modeling strategy* is the most promising approach. Such a strategy aims on connecting the *micro scale* (i.e., that of individual particles), the *meso scale* (i.e., that of an ensemble of particles), and the *macro scale* (i.e., that of the largest scales, i.e., a chemical reactor). [27, 2]. The proposed project focusses on the smallest scales, for which still elementary models are missing, especially for (i) reactive systems, as well as (ii) systems made up by irregular non-spherical particles, and (iii) systems with complex particle-particle interaction forces. Connection of scales will be realized by filtering high-fidelity simulation data, subsequent data analysis, and model synthesis.

Previous Work

Bubble Swarms and Reactive Mass Transfer at Dynamic Interfaces This project (duration 2008-2011, FWF-funded) focussed on the simulation of mass transfer and (bio-)chemical reactions in bubbly flows. The work consisted of (i) model and code development, (ii) application of the models to study various multiphase systems, and to (iii) experimentally confirm selected simulation results [12, 9, 16, 10, 11, 14, 15, 3].

Infrastructure Used: ccluster.tugraz.at (cluster with ca. 90 CPUs, hosted by TU Graz).

Code Used: In-house FORTRAN code coupled to PETSC (http://www.mcs.anl.gov/petsc/).

Accelerated Multiphase Flow Predictions This project (duration 2010-2012, FWF-funded) developed a code for the simulations of cohesive gas-particle systems on graphic processing units (GPUs). The work consisted of (i) code development, (ii) development of data filtering routines, and (iii) model development to accelerate multiphase flow predictions using a so-called "filtered" simulation approach. [7, 19, 8, 23]

Infrastructure Used: GPU-Workstations and GPU-Servers (hosted by the IPPT and TU Graz)

Codes Used: In-house GPU code *r2d2* (using CUDA programming languange), as well as OpenFOAM (http://www.openfoam.com/).

Comprehensive Investigation of Wet Powder Blending This project (duration 2012-2015, FWF-funded) is currently on the way to simulate liquid transport in flowing granular materials. The work consists of (i) development of a numerical strategy to simulate wet agglomerates, (ii) experimental validation, (iii) apply the methodology to relevant systems, and (iv) couple the numerical strategy to simulations on the next larger scale. [18, 21, 22, 17, 6].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: OpenFOAM (http://www.openfoam.com/), LIGGGHTS and CFDEM (http://www.cfdem.com/).

aiBAT - advanced industrial-scale Bioreactor Analysis Tool This project (duration 2013-2016, FFG-funded) focusses on the development of an improved tool to optimize large-scale reactors for the anti-infectives production. The project connects to previous work that focussed on the development of a Lattice-Boltzmann code to simulate multiphase stirred tank bio-reactors. [26, 24, 25].

Infrastructure Used: dcluster.tugraz.at (a cluster with ca. 1900 CPUs, hosted by TU Graz, sponsored by NAWI Graz) and a local GPU-Servers (hosted by the IPPT and TU Graz)

Codes Used: Latticle-Boltzmann Code (FORTRAN using MPI for parallelization, as well as CUDA GPU code).

FLIPPR - Future Lignin and Pulp Processing Research This project (duration 2013-2017, FFG-funded) is currently ongoing, with a consortium consisting of key players in the Austrian pulp and paper industry, as well as three academic partners (http://www.flippr.at/). The IPPT is focussing on fibre fractionation technology, for which simulations are used to better understand the flow and motion of suspended particles. Specifically, the IPPT (i) is currently developing a fibre model, as well as (ii) is performing simulation of flow in (structured) channels to understand the separation process. The work connects to previous work on flow in micro-channels [29, 28].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: LIGGGHTS and CFDEM (http://www.cfdem.com/).

NanoSim - A Multi-scale Simulation-Based Design Platform This project (duration 2014-2017, EU FP7-funded) is currently ongoing under the lead of Stiftelsen SINTEF (Norway, http://www.sintef.no/NanoSim/. The IPPT is leading the second-largest Work Package in the project (i.e., Lagrangian Modelling), which aims on developing two new open-source libraries to (i) simulate mass transfer and reactions on a sub-particle scale, as well as to (ii) filter data of high-fidelity simulations on various scales and using various codes. The work connects to previous work at our institute, which focussed on the development of particle-scale models for catalyst preparation, combustion and gas-cleaning processes [4, 30, 5], as well as direct numerical simulation of reactive flows and data filtering [16, 8, 13].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: LIGGGHTS and CFDEM (http://www.cfdem.com/), as well as the in-house developments *PaScal* and *C3PO*.

Planned PRACE Activites and Infrastructure Access

The IPPT is planning to contribute to PRACE 2.0 by writing proposals for preparatory access within (A) the ongoing NanoSim project, as well as (B) a possible follow-up project focussing on three-phase flow systems.

(A) NanoSim - Probing the Scalability of COSI The newly development libraries *PaScal*, as well as *C3PO* will be integrated into the first fully open-source co-simulation platform *COSI*, which bill be based on CFDEM http://www.cfdem.com/ to simulate reactive fluid-particle systems. Preparatory access to PRACE would enable benchmarking of *COSI* beyond the current resources available at TU Graz or VSC. Specifically, we would like to assess the scalability of the platform that performs a coupled integration at three length and time scales: (i) integration of the Navier-Stokes equations to model fluid flow, (ii) solution of Newton's equation of motion to describe particle motion, as well as (iii) solution of heat and mass particles of reacting porous particles. Clearly, these simulations are extremely demanding, and an optimal (i) domain decomposition,

as well as (ii) parallelization of the individual integrators for each sub problem is key. Despite individual parts of COSI have demonstrated excellent scalability on PRACE Tier-0 systems (see the recently published OpenFOAM [1] benchmark), or other HPC systems (e.g., see http://lammps.sandia.gov/bench.html), the coupling of individual components of COSI is still a bottleneck, and is currently untested beyond 128 CPUs. We are planning to run COSI on up to ca. 5k cores to identify bottlenecks in message passing, as well as to fine-tune the domain-decomposition and parallelization strategy used in COSI. Also, the performance of data filtering operations across multiple CPUs to be developed needs to be assessed. Finally, the computationally costly modelling of certain particle properties (e.g., non-sphericity, or cohesive forces) will be attempted. Acceptable scalability of COSI would enable studies of reactive particulate systems with a meaningful size, such that models on the next level (characterized by larger length and time scales) can be developed. Currently model development is clearly limited to unreactive systems and several model assumptions, that might be unrealistic in some situations (e.g., in case heat conduction within individual particles is limiting, or cohesive particle-particle interaction forces exist). PRACE 2.0 could help in removing some of these model assumptions, and lead to a break-through in the modelling of realistic reactive particulate systems involving non-spherical, cohesive, or porous particles that undergo fast chemical reactions.

Infrastructure Required: Preparatory access to a PRACE system to allow parallel computation on up to 5k CPUs. In case scalability is demonstrated, a follow-up request for project access will be prepared.

(B) Three-Phase Simulations of Gas-Particle-Solid Systems Our previous projects clearly identified that effects of (i) suspended particles in bubbly flows [20], as well as (ii) liquid droplets in a gas-particle suspension are extremely hard to model [6]. Consequently, often an over-simplified simulation approach to study these three-phase systems must be chosen. Within the ongoing project "Comprehensive Investigation of Wet Powder Blending", we have already developed the basic methodology to directly simulate three-phase systems. Unfortunately, these direct simulations are limited to a few particles, which is clearly too small to derive closures for certain phenomena that required tracking of (at least) a few thousand particles. Within this future project we will run the developed code on a larger cluster to assess scalability, as well as push the limit on the maximal system size that can be simulated in order to gather meaningful data on, e.g., clustering phenomena observed in wet granular flows, or attachment of suspended particles to gas bubbles.

Infrastructure Required: Preparatory access to a PRACE system to allow parallel computation on up to 5k CPUs. In case scalability is demonstrated, a follow-up request for project access will be prepared.

References

[1] Massimiliano Culpo. *Partnership for Advanced Computing in Europe Current Bottlenecks in the Scalability of OpenFOAM on Massively Parallel Clusters*. URL: http://www.prace-project.eu/IMG/pdf/Current_Bottlenecks_in_the_Scalability_of_OpenFOAM_on_Massively_Parallel_Clusters.pdf.

[2] Niels G. Deen, M von Sint Annaland, and J A M Kuipers. "Multi-scale modeling of dispersed gas–liquid two-phase flow". In: *Chemical Engineering Science* 59.8-9 (May 2004), pp. 1853–1861. ISSN: 00092509. DOI: 10.1016/j.ces.2004.01.038. URL: http://linkinghub.elsevier.com/retrieve/pii/S0009250904000971.

[3] Michael C. Gruber, Stefan Radl, and Johannes G. Khinast. "Coalescence and Break-Up in Bubble Columns: Euler-Lagrange Simulations Using a Stochastic Approach". In: *Chemie Ingenieur Technik* 85.7 (July 2013), pp. 1118–1130. ISSN: 0009286X. DOI: 10.1002/cite.201300024. URL: http://doi.wiley.com/10.1002/cite.201300024.

[4] Azzeddine Lekhal, Benjamin J. Glasser, and Johannes G. Khinast. "Impact of drying on the catalyst profile in supported impregnation catalysts". In: *Chemical Engineering Science* 56.15 (Aug. 2001), pp. 4473–4487. URL: ISI:000170877800002.

[5] Xue Liu, Johannes G. Khinast, and Benjamin J. Glasser. "Drying of supported catalysts for low melting point precursors: Impact of metal loading and drying methods on the metal distribution". In: *Chemical Engineering Science* 79 (Sept. 2012), pp. 187–199. ISSN: 00092509. DOI: 10.1016/j.ces.2012.05.046. URL: http://linkinghub.elsevier.com/retrieve/pii/S0009250912003272.

[6] Mohan, Bhageshvar et al. "Regimes of Liquid Transport through Sheared Beds of Inertial Smooth Particles". In: *Powder Technology (accepted)* (2014).

[7] Charles Radeke, Stefan Radl, and Johannes G. Khinast. "Granular Flows - Showing Size Effects by Using High-Performance Simulations on GPUs". In: Multi-Scale Modelling Symposium. Melbourne, Australia: CSIRO Australia, 2009.

[8] Stefan Radl, Matthew Girardi, and Sankaran Sundaresan. "Effective Drag Law for Parcel-Based Approaches - What Can We Learn from CFD-DEM?" In: *ECCOMAS 2012*. Ed. by J Eberhardsteiner. Eccomas. Vienna, Austria, 2012.

[9] Stefan Radl and Johannes G. Khinast. "Flow and Mass Transfer of Fully Resolved Bubbles in Non-Newtonian Fluids". In: *AIChE Journal* 53.7 (2007), pp. 1861–1878. DOI: 10.1002/aic.

[10] Stefan Radl and Johannes G. Khinast. "Multiphase Flow and Mixing in Dilute Bubble Swarms". In: *AIChE Journal* 56.9 (2010), pp. 2421–2445. DOI: 10.1002/aic.

[11] Stefan Radl and Johannes G. Khinast. "Multiphase Flow and Mixing in Dilute Bubble Swarms". In: 56.9 (2010), pp. 2421–2445. DOI: 10.1002/aic.

[12] Stefan Radl and Johannes G. Khinast. "Prediction of Mass Transfer Coefficients in Non-Newtonian Fermentation Media Using First-Principles Methods". In: *Biotechnology and bioengineering* 97.5 (2007), pp. 1329–1334. DOI: 10.1002/bit.

[13] Stefan Radl and Sankaran Sundaresan. “A Drag Model for Filtered Euler-Lagrange Simulations of Clustered Gas-Particle Suspensions”. In: *Chemical Engineering Science (submitted)* (2014).

[14] Stefan Radl, Daniele Suzzi, and Johannes G. Khinast. “Fast Reactions in Bubbly Flows: Film Model and Micromixing Effects”. In: *Industrial & Engineering Chemistry Research* 49.21 (Nov. 2010), pp. 10715–10729. ISSN: 0888-5885. DOI: 10.1021/ie100539g. URL: http://pubs.acs.org/doi/abs/10.1021/ie100539g.

[15] Stefan Radl, Daniele Suzzi, and Johannes G. Khinast. “Fast Reactions in Bubbly Flows: Film Model and Micromixing Effects”. In: *Industrial & Engineering Chemistry Research* 49.21 (Nov. 2010), pp. 10715–10729. DOI: 10.1021/ie100539g.

[16] Stefan Radl et al. “DNS-based prediction of the selectivity of fast multiphase reactions: Hydrogenation of nitroarenes”. In: *Chemical Engineering Science* 63.12 (June 2008), pp. 3279–3291. ISSN: 00092509. DOI: 10.1016/j.ces.2008.03.025. URL: http://apps.isiknowledge.com/full_record.do?product=UA\&search_mode=GeneralSearch\&qid=1\&SID=3BMMnMl5n@7D9lmEDpm\&page=1\&doc=2\&colname=WOS.

[17] Stefan Radl et al. “Flow and mixing of granular material over a single blade”. In: *Powder Technology* 226 (Apr. 2012), pp. 199–212. ISSN: 00325910. DOI: 10.1016/j.powtec.2012.04.042. URL: http://linkinghub.elsevier.com/retrieve/pii/S0032591012002847.

[18] Stefan Radl et al. “Mixing Characteristics of Wet Granular Matter in a Bladed Mixer”. In: *Powder Technology* 200.3 (2010), pp. 171–189. URL: ISI:000277719700010.

[19] Stefan Radl et al. “Parcel-Based Approach for the Simulation of Gas-Particle Flows”. In: *8th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries*. June. Trondheim, Norway: SINTEF/NTNU Trondheim, 2011, 124 (1–10).

[20] Jodi a. Raffensberger, Benjamin J. Glasser, and Johannes G. Khinast. “Analysis of heterogeneously catalyzed reactions close to bubbles”. In: *AIChE Journal* 51.5 (May 2005), pp. 1482–1496. ISSN: 0001-1541. DOI: 10.1002/aic.10445. URL: http://doi.wiley.com/10.1002/aic.10445.

[21] Muhammad Shafiq Siraj et al. “Effect of blade angle and particle size on powder mixing performance in a rectangular box”. In: *Powder Technology* 211.1 (July 2011), pp. 100–113. ISSN: 00325910. DOI: 10.1016/j.powtec.2011.04.004. URL: http://linkinghub.elsevier.com/retrieve/pii/S0032591011001719.

[22] Muhammad Shafiq Siraj et al. “Effect of blade angle and particle size on powder mixing performance in a rectangular box”. In: *Powder Technology* 211.1 (July 2011), pp. 100–113. ISSN: 00325910. DOI: 10.1016/j.powtec.2011.04.004. URL: http://linkinghub.elsevier.com/retrieve/pii/S0032591011001719.

[23] Sankaran Sundaresan et al. “Coarse-Grained Models for Momentum, Energy and Species Transport in Gas-Particle Flows”. In: *Fluidization XIV*. Vol. 1. 2013.

[24] Radompon Sungkorn. “Euler – Lagrange Modeling of a Gas – Liquid Stirred Reactor with Consideration of Bubble Breakage and Coalescence”. In: *AIChE Journal* in press.0 (2011), pp. 1–15. DOI: 10.1002/aic.

[25] Radompon Sungkorn. “Euler-Lagrange Modeling of Dispersed Gas-Liquid Reactors”. PhD Thesis. Graz University of Technology, 2011.

[26] Radompon Sungkorn, Jos J Derksen, and Johannes G. Khinast. “Modeling of turbulent gas-liquid bubbly flows using stochastic Lagrangian model and lattice-Boltzmann scheme”. In: *Chemical Engineering Science* 66.12 (Mar. 2011), pp. 2745–2757. ISSN: 00092509. DOI: 10.1016/j.ces.2011.03.032. URL: http://linkinghub.elsevier.com/retrieve/pii/S0009250911001989.

[27] M A Van der Hoef et al. “Numerical Simulation of Dense Gas-Solid Fluidized Beds: A Multiscale Modeling Strategy”. In: *Annual Review of Fluid Mechanics* 40 (Jan. 2008), pp. 47–70. ISSN: 0066-4189. DOI: 10.1146/annurev.fluid.40.111406.102130. URL: http://arjournals.annualreviews.org/doi/abs/10.1146/annurev.fluid.40.111406.102130.

[28] Daniele Vigolo, Stefan Radl, and Howard a Stone. “Unexpected trapping of particles at a T junction.” In: *Proceedings of the National Academy of Sciences of the United States of America* (Mar. 2014). ISSN: 1091-6490. DOI: 10.1073/pnas.1321585111. URL: http://www.ncbi.nlm.nih.gov/pubmed/24639547.

[29] Daniele Vigolo et al. “An experimental and theoretical investigation of particle – wall impacts in a T-junction”. In: *Journal of Fluid Mechanics* 727 (2013), pp. 236–255.

[30] Johann C Wurzenberger et al. “Thermal Conversion of Biomass : Comprehensive Reactor and Particle Modeling”. In: 48.10 (2002).

C Structure Prediction and Modeling of Conformational Transitions of Biological Macromolecules and Dye Aggregates

Proposer

Univ. Prof. Dr. Thomas Renger
Dr. Marcel Schmidt am Busch
DI Christian Friedl
Institute of Theoretical Physics
Johannes Kepler University Linz
Altenberger Straße 69, 4040 Linz
Email: thomas.renger@jku.at
Web: http://www.jku.at/itp/content/e61104

Topic

A prerequisite for the understanding of structure-function relationships of macromolecules is the information about the atomic structure of these molecules. In the case of biological macromolecules, e.g. proteins, crystallographic information is often available, which, however, can provide only a subset of the physiologically relevant structures, in particular, if the physiological function of the protein involves large scale conformational transitions. In order to resolve the latter additional techniques are required. One way is to link a donor and an acceptor dye molecule at two critical positions of the macromolecule and to measure the energy transfer efficiency between the donor and acceptor, after optical excitation of the donor. From this energy transfer efficiency the distance between the donor and acceptor molecules, and thereby the conformation of the macromolecule, may be inferred. Besides the large scale conformational transitions of the protein there is much faster conformational dynamics of the attached dye molecules in their local binding sites in the protein, which has to be taken into account for an estimation of the energy transfer efficiency, by performing an orientational average of the rate constant.

Another way to predict conformational transitions of proteins is by computer simulations. Often, however, physiologically relevant conformational transitions occur on a microsecond to millisecond timescale, whereas standard molecular dynamics simulations of proteins with a couple of 10000 atoms are only performed in the submicrosecond range. One way to reach longer timescales is to carry out a normal mode analysis of the macromolecule and to use the low-frequency normal modes to create a steering potential to accelerate the molecular dynamics simulations. The strength of this artificial potential, depends on the computational resources that one has available. The weaker the potential, the more realistic will be the simulation of the conformational transition. In this project, we plan to use the PRACE facilities in order to model conformational transitions of the translocon protein, which are investigated in the framework of the *Doctoral College Nanocell: Nano-Analytics of Cellular Systems: From molecular dynamics, recognition and organization to membrane transport and mobility*

in collaboration with the experimental group of Peter Pohl (Biophysics, JKU Linz), that will perform the optical FRET (Förster resonance energy transfer) experiments, which we will analyze. In addition, it is planned to perform a direct calculation of the conformational transition by a combination of normal mode analysis and molecular dynamics simulations.

A second class of systems that shall be investigated with the PRACE facilities are artificial dye aggregates, which self-assemble in polar solvents. These aggregates exhibit a dramatic change of the optical properties, when compared to those of the isolated dye molecules in solution. In particular, narrow bands with giant oscillator strengths may appear. These changes can be understood by taking into account a delocalization of excitation energy between the dye molecules in the aggregate. Depending on chemical details of the dye molecules and the preparation technique, dye aggregates with very different optical properties can be obtained. Unfortunately, however, there is no crystal structure available for these aggregates. The only structural information comes from cryo-transmission electron microscopy, which can, however, only give a rough estimate of the aggregates dimension but no molecular details. Here, we plan to obtain the missing structural information from computer simulations using fragmentation quantum chemical techniques. In the latter, large molecular systems can be studied by only considering one part (a fragment) of the macromolecule explicitly by a single high-level ab initio calculation including the remaining fragments as a classical environment, and in the end combining the calculations on the different fragments in a way that allows to obtain the properties of the whole macromolecule. Since calculations on different fragments can be done on independent compute nodes this type of calculation is well suited for the massively parallel computers of the PRACE project. This project will be carried out in collaboration with Hans von Berlepsch (Freie Universität Berlin), who performed cryo-transmission electron microscopy on these aggregates in solution and measured their optical spectra. Using the quantum chemical calculations described above, we plan to optimize the molecular structure and to parameterize the Hamiltonian of the aggregates in order to calculate the optical spectra and compare with experiment.

Previous Work

We have developed theory and calculation schemes for the description of excitation energy transfer and optical spectra of biological macromolecules, in particular photosynthetic pigment-protein complexes (references to our original publications are given in two recent reviews on this topic [5, 3]). Using a combination of quantum chemical/ electrostatic and normal mode calculations the Hamiltonian of these macromolecules can be parameterized. We have developed methods for all three classes of parameters which concern (i) the local transition energies of the pigments in their binding site in the protein, (ii) the excitation energy transfer coupling between pigments and (iii) the spectral density of the exciton-vibrational coupling [4], which describes how quantities (i) and (ii) fluctuate due to the vibrational dynamics of the protein. These parameters enter a dynamic theory of excitation energy transfer and optical spectra that is also developed in our group [5, 3].

So far, the local computational resources at JKU were sufficient for our purposes. The most demanding numerical simulation so far was a normal mode analysis of a pigment-protein complex with 60000 degrees of freedom. The PRACE facilities will allow us to combine our

previously established techniques with molecular dynamics simulations, in order to include the effect of anharmonic motion and conformational transitions on one hand. On the other hand, these facilities will allow us to approach also systems with not so well defined structures, like the self-assembled J-aggregates.

Planned PRACE Activites and Infrastructure Access

Conformational transitions of the translocon protein To predict conformational transitions of the translocon protein we plan to perform molecular dynamics (MD) simulations using the program NAMD [2]. NAMD was designed for high-performance simulations of large biomolecules and scales to hundreds of cores for simulations for intermediate sized proteins and beyond 200000 cores for the largest simulations. These calculations will allow us to directly calculate the conformational dynamics of translocon on one hand, and to analyze the optical FRET experiments on the other hand. For the present translocon protein we plan to include an explicitly modeled lipid membrane and aqueous environment in the MD simulation. To reach physiologically relevant time scales (microseconds) for this 50000 atom system, about 5 million CPU hours are needed.

Structure prediction of J-Aggregates We plan to use the ab initio quantum chemistry program GAMESS to refine the structure of a TTBC aggregate, tabulate the pairwise interactions between molecules of the aggregate and calculate optical excitations of individual molecules in the aggregate. GAMESS includes the Fragment Molecular Orbital method (FMO) [1] which permits quantum chemistry methods to be applied to very large systems by dividing the computation into small fragments. The calculations will provide a chemically reasonable molecular structure as well as optical spectra which can be directly compared to experiments. In order to obtain accurate results for the aggregate geometry a sufficiently large basis set should be used in the quantum chemical calculations. The FMO method in GAMESS has been implemented in such a way as to include coarse-grained parallelism among different compute nodes (for the calculation of the contribution of every fragment to the total energy) and fine-grained parallelism (for high-level quantum chemistry on each fragment) among the cores of each node. This method scales perfectly on tens of thousands of cores. A minimum of 5 million CPU hours would be needed for this project.

In summary, we would like to apply for 10 million CPU hours including both subprojects.

References

[1] Mark S. Gordon et al. “Fragmentation Methods: A Route to Accurate Calculations on Large Systems”. In: *Chem. Rev.* 112.1 (2012), pp. 632–672. DOI: 10.1021/cr200093j.

[2] James C. Phillips et al. “Scalable molecular dynamics with NAMD”. In: *J. Comput. Chem.* 26.16 (2005), pp. 1781–1802. DOI: 10.1002/jcc.20289.

[3] Thomas Renger and Frank Müh. “Understanding photosynthetic light-harvesting: a bottom up theoretical approach”. In: *Phys. Chem. Chem. Phys.* 15.10 (2013), pp. 3348–3371. DOI: 10.1039/C3CP43439G.

[4] Thomas Renger et al. “Normal Mode Analysis of the Spectral Density of the Fenna-Matthews-Olson Light-Harvesting Protein: How the Protein Dissipates the Excess Energy of Excitons”. In: *J. Phys. Chem. B* 116.50 (2012), pp. 14565–14580. DOI: 10.1021/jp3094935.

[5] Thomas Renger et al. “Structure-based modeling of energy transfer in photosynthesis”. In: *Photosynth. Res.* 116.2-3 (2013), pp. 367–388. DOI: 10.1007/s11120-013-9893-3.