PRACE 2.0 for Austria

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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 have made a bid in September 2014 [1] which was granted in January 2015.

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: February 4, 2015) 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 (most probably: 4) 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

   - a peak performance of at least 20% higher than the average of the peak performance of the existing PRACE systems (4.2 PFLOPS in 2015, estimated 5.8 PFLOPS in 2016, up to 15 PFLOPS in 2019);
   - of which at least 20% of the annual cycles will be made available to PRACE (amoung to depending on the kind of system used, between 1.5–4.2 billion core hours for 2015).

4. The total cost of ownership (TCO) of Tier-0 resources dedicated to PRACE 2.0 amount to € 60M per year which includes the operating expenses (OPEX) of € 30M per year.

5. All full members share the OPEX based on a percentage that averages the corresponding nation's GDP and the past usage of that system in comparison to all other members; the hosting members will provide their share via the core hours provided to PRACE 2.0 while the other full members provide their share via monetary contributions.

6. The total OPEX budget for PRACE 2.0 is fixed at € 30M per year; an increase in the number of hosting members does not increase the monetary contributions of the other full members (but just leads to a conversion of monetary contributions to contributions of core hours).

7. By these calculations Austria's contribution would amount to 1,09% of the OPEX, i.e. in absolute numbers, € 340 000 per year, over a five year period.

In a nutshell, we thus 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 (including the € 60 000 membership fee)**
>
> **€ 400 000**
>
> **per year for a period of five years (2016–2020).**
>
> **For this investment, Austria gets access to about 4 Tier-0 (European level) HPC systems (with a total performance of about 16 PFLOPS in 2015 up to estimated 60 PFLOPS in 2019); 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 VSC-3 at the Vienna Scientific Cluster [11], has a performance of about 0.584 PFLOPS; this Tier-1 system thus achieves less than 14% performance of a single of the currently available 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.

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Potential PRACE 2.0 Projects

A Multi-Scale Astrophysical Turbulence Simulation

Proposer

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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

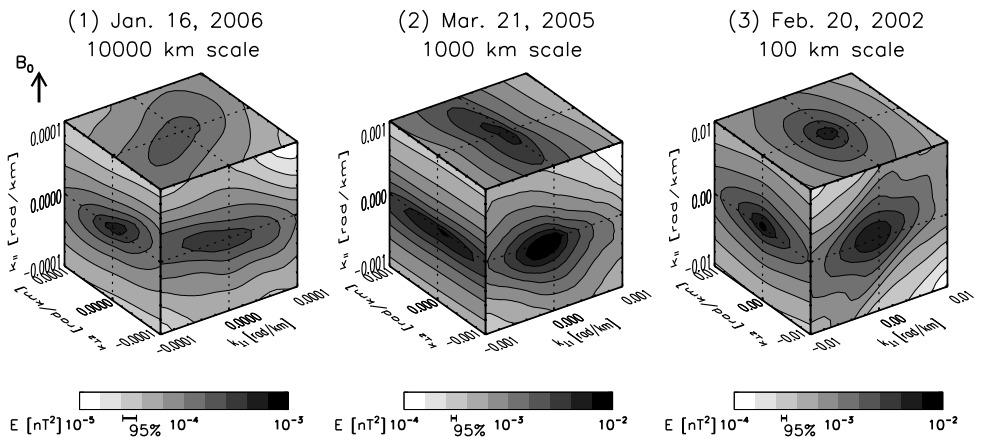

Figure 1: Direct measurement of 3D energy spectra in solar wind plasma on multiple scales, oriented along the direction of a large-scale magnetic field (vertical axis) [9].

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.

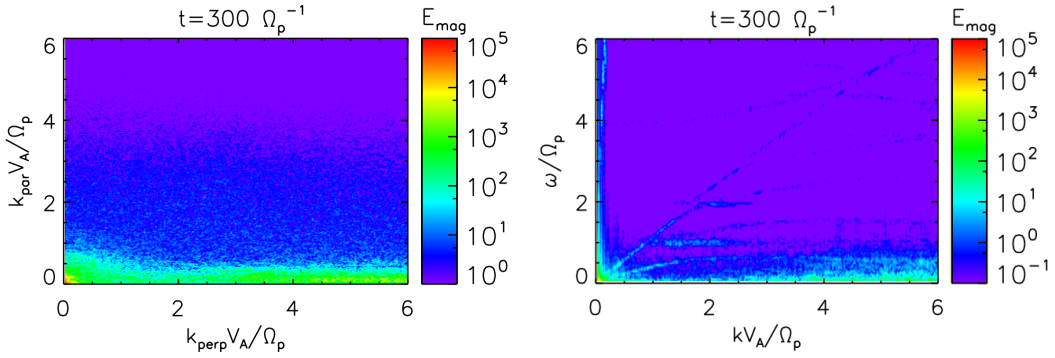

Figure 2: Energy spectra in the 2D wavevector domain (left panel) and as frequency versus wavenumber perpendicular to the mean magnetic field (right panel) produced by AIKEF [6].

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.

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B First-Principle Investigation of the Lattice Vibrations in Garnet Solid Solutions Including Anharmonic Analysis

Proposer

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Topic

Lattice vibrations are the main physical reason for the macroscopically measurable heat capacity, C_p, that is an important thermodynamic property of a solid. When C_p of solid solutions is plotted as a function of composition, it often deviates from linear behaviour at low temperatures. The resulting excess heat capacities are of vibrational and/or non-lattice (e.g., magnetic and electronic) origin. Excess vibrational entropies may be in the order of the configurational entropy and may have thus large effects on phase stability calculations (for a review of the vibrational entropy in solid solutions, see e.g., [9, 6]).

Considerable excess vibrational entropies have been demonstrated for the pyrope (py, $Mg_3Al_2Si_3O_{12}$) - grossular (gr, $Ca_3Al_2Si_3O_{12}$) garnet solid solution using calorimetric techniques [7, 5]. So far, the thermodynamics of this in the Earth Sciences important binary has been investigated theoretically only by means of static lattice energy calculations based on empirical pair potentials [8], but not by ab initio methods. We have studied the excess heat capacity of py - gr garnets by performing DFT calculations using CASTEP [4] as implemented in the Materials Studio software (Accelrys®). This work is a continuation of already published work on Ag-Pd, Cu-Zn alloys [1, 3] and the alkali feldspar solid solution [2]. The lattice dynamics calculations were done using the High Performance Computing system DOPPLER at the Department of Computer Sciences, Salzburg University. They were performed on 160 cores within the linear response approximation (quasi-harmonic) implemented in CASTEP using the interpolation approach and lasted around 22 days per job. As a result of these ab-initio calculations it turned out that the agreement between calculated and measured excess heat capacities is unsatisfactory. One likely reason for this discrepancy is that anharmonicity cannot be taken into account by using the linear response approximation.

Planned PRACE Activites and Infrastructure Access

In the future, we want to restudy the excess heat capacity of py - gro garnet by using the finite displacements method as an alternative approach. An advantage of this method is that it is also possible to investigate phonon anharmonicity by increasing the amplitude of the

displacements. This, however, requires considerably larger computational effort and it is not possible to get results in reasonable time using the DOPPLER HPC cluster in Salzburg as has been shown by test calculations that we have done.

We, thus, plan to apply for getting access to the Tier 0 computer in order to do these calculations intended to study phonon anharmonicity in the py - gr solid solution. As the major scientific result of the planned lattice dynamics calculations, we expect to be able to quantify for the first time, using ab initio calculations, the role of anharmonicity in the lattice dynamics of solids.

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C Modeling and Simulation of Epidemic Type Processes

Proposer

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Topic

In order to improve our chances to control an epidemic outbreak, we need proper models which describe the spread of a disease in a population. Institutes, governments, and scientists all over the world work intensively on forecasting systems to be well prepared if an unknown disease appears. In recent years a huge amount of theoretical and experimental study has been conducted on this topic. While theoretical analysis provides important and sometimes even counter intuitive insights into the behavior of an epidemic (e.g. [3, 5]), in an experimental study one can take many different settings and parameters [9, 8] into account, which usually cannot be considered simultaneously in a mathematical framework. The goal of this project is to analyze a new dynamic model for the spread of epidemics. One of our objectives is to find the right parameters, which lead to realistic settings. Therefore, we investigate a general simulation environment, in which the different parameters can easily be adjusted to real world observations. A second objective is to evaluate similarities between countermeasure approaches in our model and the real world. We use empirical data for the comparison. Our tool is agent-based, i.e., the individuals (or groups of them) are modeled by agents interacting with each other. The environment we consider approximates the geography of different countries in Europe, in which agents may travel between cities.

Our model incorporates both intra- and inter-city movement. We model the inter-city movement using a complete graph $G = (V, E)$. In this graph, each $c \in V$ corresponds to a city of the given country. However, depending on the size, not every city is contained in V. The population is represented by $n = \sum_{c \in V} n_c$ agents, with n_c being the number of agents assigned to c proportional to its real world population. Furthermore, each city contains a number of so called *cells* described below. Agents may move independently from one cell to another or travel to another city in each step. Each city $c \in V$ is assigned an attractiveness d_c proportional to its population size (w.r.t. the whole population). Note, afterwards d_c does not change anymore. Let $A_{i,s,t}$ be the event that agent i travels from city s to t. Let further p be the probability that an agent decides to travel at all, and let $dist(s,t)$ be the Euclidean distance between cities s and t. Then, the probability that event $A_{i,s,t}$ occurs is given by

$$Pr(A_{i,s,t}) = p \cdot \frac{d_t \cdot dist^{-1}(s,t)}{\sum_{(s,j) \in E} d_j \cdot dist^{-1}(s,j)}.$$

Thus, the probability for an agent entering a specific city is governed by the distance to the city, its population size as well as the current position of the considered agent.

Since our model incorporates intra-city movement as well, each $c \in V$ is a clique of cells on its own. These cliques are defined by $G_c = (V_c, E_c)$ with kn_c being the size of V_c (recall that n_c is the number of agents assigned to city c). Note, k is a normalizing constant, which does not affect the amount of agents but the amount of cells only. The nodes $v \in V_c$ are the *cells* described above. The cells represent locations within a city an agent can visit. Each cell may contain agents (individuals), depending on the cells so called *attractiveness*. The *attractiveness* d of a cell v is chosen randomly with probability proportional to $1/d^\alpha$, where $\alpha > 2$ is a constant depending on the simulation run [10]. In each step, if an agent decides not to visit another city, then it moves to a cell according to the distribution of the attractiveness' among the cells. In order to determine the movement between the cells we are going to run a number of experiments combined with real world data obtained from telecommunication companies.

Previous Work

Modeling epidemics Two of the most popular directions are the so called agent-based and structured meta-population-based approach, respectively (cf. [1, 7]). Both models have their advantages and weaknesses. The main idea of the meta-population approach is to model whole regions, e.g. georeferenced census areas around airport hubs [4], and connect them by a mobility network. Then, within these regions the spread of epidemics is analyzed by using the well known mean field theory. The agent-based approach models individuals with agents in order to simulate their behavior. The main issue of the agent-based approach is the huge amount of computational capacity needed to simulate huge cities, continents or even the world itself [1]. This limitation can be attenuated by reducing the number of agents, which then entails a decreasing accuracy of the simulation.

In the meta-population approach the simulation costs are lower, sacrificing accuracy and some kind of noncollectable data. To combine the advantages of both systems, hybrid environments were implemented (e.g. [2]). The main idea of such systems is to use an agent-based approach at the beginning of the simulation up to some point where a suitable amount of agents is infected. Then, the system switches to a meta-population-based approach. Certainly, such a system combines the high accuracy of the agent-based simulations at the beginning of the procedure with the faster simulation speed of the meta-population-based approach at stages in which both systems may provide similar predictions. Here, the situation to switch between both approaches (in both directions) is defined by a threshold describing a specific amount of infected agents. However, for certain epidemics this adjustment may be difficult or even not feasible at all.

In the past, we have described the inter-city movement by a simple model, in which the agents move between the cells according to the attractiveness of these cells, independently [5, 6]. However, this approach does not model the reality, since there are several dependencies between movements of individuals and locations.

Infrastructure Used: To simulate an epidemic process in a large European country - such

as the Federal Republic of Germany - building on the simple model described above, we utilized approximately 500 cores of a parallel machine simultaneously, and had a memory requirement of 2,5 TB in total. Each of the cores was a 2.3 GHz AMD Opteron. Note that we have not taken into account any dependency between the movement of the agents.

Planned PRACE Activites and Infrastructure Access

Realistic models for the spread of epidemics In our project, we first analyze the movement of individuals in a large urban area. For this, we utilize empirical data from telecommunication companies, in order to find a correct distribution for the movement of individuals between the cells covered by antennas. Furthermore, we will study the distribution of the communities occuring within one antenna cell, as well as the movement of individuals from one community to another. We will also focus on the dependencies between these movements. To find the right model for these dynamic processes, we need to run extensive simulations on a parallel machine, which is far beyond the resources offered by a national center for high performance computing. Once a proper model for the dynamical movement of individuals is found, extensive computations are needed to simulate the spread of epidemics on a national scale. The number of agents modeling the individuals as well as the huge amount of cells contained in a city requires again extremly powerful parallel machines.

Infrastructure Required: To run the extensive simulations required by our project, we need more than 10.000 cores to be deployed simultaneously. Additionally, our memory requirements will exceed 5 TB. The simulations can only be completed if a fast connection is guaranteed between the computing nodes. All these needs together can only be obtained on one of the Tier 0 machines of the PRACE initiative in Europe.

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

Proposer

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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.

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

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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.

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F Simulation of Thermomechanical Deformations in NC Milling

Proposer

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Topic

In this project fictitious domain methods based on finite element approaches are developed to simulate thermo-mechanical processes in the NC milling. The project is currently supported by the DFG within the Priority Program 1480 for the "Modelling, Simulation and Compensation of Thermal Effects for Complex Machining Processes".

In the roughing process of the NC milling, a significant amount of heat is induced into a work piece due to the conversion of energy during the chip formation process. This results in global thermo-mechanical deformations that remain present in the subsequent finishing process and may consequently cause a strong deviation of the work piece surface from its designed shape after cooling down. Thus, critical manufacturing tolerances may be exceeded.

The major aim of this project is to simulate the heat input and the thermo-mechanically caused deformations during the NC milling process for geometrically complex shapes, to allow for predictions on possible deviations between the designed and the produced shape, even before the first actual NC milling. This is achieved through the development of a hybrid simulation system composed from an efficient finite element system to compute thermo-mechanically caused deformations of a workpiece and from a simulation system for the NC milling process. The coupling of the milling simulation and the finite element system is accomplished via a state-dependent mesh refinement/adjustment for the workpiece that permits the modeling of heat and material removal as well as heat input due to the constantly changing contact situation between the workpiece and the milling tool. The computation of cutting forces accounts amongst others also for the changing contact situation implied by the heat induced deformations of the workpiece.

The deformations are modeled by the equations of linear thermo-elasticity that are here discretized via the Crank Nicolson scheme in time and, in particular, via a higher-order fictitious domain method in space. The continuous (deformation dependent) material removal implied by the NC milling process causes a continuously changing domain of possibly complex geometry. To model that changing domain, state-dependent mesh refinements are pursued using interface representation algorithms such as the marching cubes algorithm along with corresponding volume meshes on an adaptively refined axis-parallel hexahedron mesh. These meshes are utilized in the fictitious domain method using (coarse-scale) hexahedrons from the

mesh refinement history for the definition of the higher-order Ansatz spaces and using any further refinement of these hexahedrons as sub-meshes. The latter allow for an appropriate definition of a characteristic function for the state-dependent domain of the milled work piece and may hence serve for quadrature purposes in the discretized equations of linear thermo-elasticity. For the definition of the Ansatz spaces, standard higher-order tensor product finite element shape functions based upon integrated Legendre polynomials are multiplied with the state-dependent characteristic function for the domain. Possible multi-level hanging nodes and varying polynomial degrees in the chosen mesh for the Ansatz spaces are efficiently handled with so called connectivity matrices.

Previous Work

Simulation of moderate test cases Within the Priority Program 1480 rather moderate test cases have been pursued to compare and verify the results of actual NC milling processes with those obtained from the simulation. These test cases are reduced to sections of work pieces and the corresponding relevant milling paths. The results showed excellent conformance and hence applicability of the simulation software [2, 1, 3].

Infrastructure Used: The computations are currently pursued on nodes of the Doppler-Cluster of the University of Salzburg. This cluster has 33 nodes and more than 1200 cores in total with storage of 2-8 GB per core.

Planned PRACE Activites and Infrastructure Access

Simulation of realistic construction components with large size For the simulation of the NC milling process of large construction components as required, for instance, in the airplane industry, the mesh generation for an appropriate modelling of the actual geometry of the continuously changing workpiece as well as the update and solution of the resulting systems of equations imply a huge amount of computational work which has to be done with a massively parallelized finite element code. The aim is to simulate the production of realistic construction components with large sizes and complex surface geometries. For this purposes, extremely complex NC milling paths have to be simulated leading to extensive computational work which can only be appropriately handled on high performance computing environments as provided in PRACE.

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G Quantum Monte Carlo for Electronic Structure

Proposer

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Topic

Many problems in applied material science, such as hydrogen storage in energy research, photovoltaics, surface chemistry, or the design of semiconductor quantum dots, require quantitative understanding of the electronic structure. However, solving the many-body Schrödinger equation for many electrons is all but trivial because of the Coulomb interaction between electrons. Numerous methods have been developed to tackle this problem, from highly accurate ones (e.g. configuration interaction, coupled cluster) that scale poorly with system size (but there are efforts to improve this bottle-neck), to more phenomenological ones such as the widely used density function theory (DFT) that scale favorably. We refer to all the above methods as the classical methods of electronic structure calculations. They have been refined, tuned and specialized over more than have a century. A method that uses a completely different approach, but in principle boasts good size scaling and is highly accurate, is quantum Monte Carlo (QMC) and, for fermions such as electrons, in particular diffusion Monte Carlo (DMC).[**grossmanJCP02**] In QMC one tries to avoid approximations that reduce the many-electron problem to a few-body problem (e.g. to a one-electron problem in case of DFT), but instead devised a Monte Carlo random walk that simulates all electrons in the system. Clearly, this is computationally more demanding than phenomenological methods such as DFT, but Monte Carlo methods have a natural tendency to run efficiently on highly parallel computer architectures and indeed it is has been demonstrated to scale well up to hundred of thousands of computing cores, employing standard techniques based on OpenMP and MPI. Unlike the classical electronic structure methods, QMC is still not very widely adopted in the material sciences, therefore (or because) there are very few out-of-the-box packages for QMC. The freely available open source code "Casino"[**casino**] is probably the most evolved package in the QMC field.

In this project, we will use the Casino code as starting point to investigate the interactions between large molecules and between molecules and surfaces. Knowing such interactions is essential before e.g. studying the dynamics by means of molecular dynamics (MD) simulations. Very often, MD simulations of complex molecules are done with purely phenomenological, parametrized force fields rather than forces based on electronic structure calculations. QMC provides the means to obtain accurate interactions. The most immediate interest are weak dispersive interactions of adsorbates, but we plan to extend our area of interest as we go.

Previous Work

QMC for bosonic helium Various Monte Carlo techniques (DMC, but also path integral Monte Carlo) have been used by us in the past to simulate superfluid helium-4, in particular helium nanodroplets doped with molecular chromophores.[**zillichJCP05**] The experimental technique of helium nanodroplet isolation spectroscopy is used to take spectra of single molecules at sub-Kelvin temperatures, or of well-characterized clusters of atoms of molecules. We have obtained computational results for many experiments, such as rotational coupling between chromophore and helium and formation of exciplexes (bound states of excited atoms with helium atoms).

Infrastructure Used: supercomputing resources at the JKU (lilli, alex, mach).

Planned PRACE Activities and Infrastructure Access

QMC calculation of interactions In our work we often encounter the problem that interactions between molecules and surfaces are not known accurately. For example water flow through carbon nanotubes (CNT) depends crucially on the H_2O-CNT interaction. The study of the filling of CNTs with water, and the type of flow that is possible, as function of diameter, partial charges, or when the CNT is functionalized with other molecules has been a very active field for more than a decade since the seminal paper by Hummer et al.[**hummer**]. However, the molecular dynamics studies almost exclusively employ very crude phenomenological models, typically a simple Lennard-Jones interaction. We plan to use the Casino code to calculate accurate interaction potentials for large systems such as, but not limited to, the water-CNT system. Simple biological nanochannels in cell membranes could be the next step.

Despite their favorable scaling with system size compared to accurate classical electronic structure methods, QMC is still computationally very demanding, but at least scales well on massively parallel architectures, see above. Therefore the Prace Tier-0 infrastructure is well suited for QMC simulations. We estimate that 1e6 CPU hours will be sufficient in the first stage of our planned investigate of substrate interactions.