Austrian HPC Meeting 2020

AHPC2020

IST Austria, Klosterneuburg, Austria, February 19–21, 2020

https://ahpc2020.ist.ac.at

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Austrian HPC Meeting 2020 – AHPC2020

Klosterneuburg, February 19-21, 2020

Welcome to the AHPC2020 meeting in Klosterneuburg

From their beginning, the AHPC meetings aimed to discuss all aspects of scientific computing and strategic issues for the future development of HPC in Austria, while bringing together scientists and technicians with a background and interest in supercomputing. In order to achieve these goals, we considered the following aspects when organizing this meeting.

We decided to organize the meeting at the IST Austria campus in Klosterneuburg, instead of a beautiful mountain region in the geographical center of Austria for two main reasons. First, this meeting provides an opportunity to visit IST Austria. Second, it also enables researchers at IST Austria to get involved in the broader HPC community in Austria. Instead of mountains, we provide an opportunity to visit Klosterneuburg Monastery, which is of historical importance to Austria – even nowadays.

The scientific program consists of 50 submitted abstracts, which marks a significant increase compared to previous meetings. There will be a poster session with a complimentary lightning talk (1-minute talk in front of the whole audience). The keynote speakers cover different areas of HPC: Leonid Sazanov will introduce us to the field of "Cryogenic electron microscopy" and its challenges for HPC. Franz Franchetti will address the latest development of optimizing important algorithms like the FFT. Walt Ligon will discuss parallel distributed storage systems. Philippe Notton will tell us about the "European Processor Initiative". Moreover, there will also be an opportunity to publish selected abstracts in a special issue of the MCA Journal dedicated to the AHPC2020 meeting.

In order to extend the reach of this AHPC meeting, we also invited vendors and suppliers of HPC equipment to actively participate in this meeting. Being aware of the different interests, we tried to find a good balance between academic research and commercial approach. With the vendor presentations in the form of an "elevator pitch" (two-minutes-two-slides), I hope we are able to achieve this goal and add some value also for the academic audience of the AHPC meeting.

The organization of such an event and its success is only possible due to support from numerous people. Without mentioning individuals, I want to mention the support and encouragement by several key persons at IST Austria, the support and helpful tips and advice from previous organizers of the AHPC meetings, and the active support by the event office at IST Austria.

Finally, essential parts of such a meeting are, of course, the discussions within and outside of the scientific sessions. Moreover, there are two discussion sessions, one on EuroHPC and one on VSC-5 - the next extension of VSC. Finally, I wish all participants a successful meeting.

Alois Schlögl

Schedule

Day 1: Wednesday, Feb 19th 2020

09:25 - 10:00 *Bustransfer from Railway station Tullnerfeld to IST*

10:00 - 11:00 *Reception*

11:00 - 11:05 Opening

11:10 - 12:00 **Keynote: Franz Franchetti**

12:00 - 13:00 Session S1.1

13:00 - 14:00 *Lunch break*

14:00 - 14:10 Elevator Pitch from Sponsors (2 minutes / 2 Slides)

14:15 - 15:30 Session S1.3

15:30 - 16:00 *Coffee break*

16:00 - 17:40 Session S1.4

18:00 - 20:00 *Dinner - IST Restaurant*

Day 2: Thursday, Feb 20th 2020

08:20 - 8:50 *Bustransfer from Wien-Heiligenstadt to IST*

08:30 - 8:50 *Bustransfer from Klosterneuburg to IST*

09:00 - 10:00 **Keynote: Walter B. Ligon**

10:00 - 10:20 Session S2.1

10:20 - 10:40 Lightning Talks (1 minute / 1 slide per poster)

10:40 - 11:00 *Coffee break*

11:00 - 11:30 Poster Presentations

11:30 - 13:00 Session S2.2

13:00 - 14:00 *Lunch break*

14:00 - 14:30 **Keynote: Leonid Sazanov**

14:30 - 15:10 Session S2.3

15:10 - 15:30 *Coffee break*

15:30 - 16:30 Session S2.4

Bus transfer to Klosterneuburg

17:10 - 18:30 Guided Tour (Stift Klosterneuburg)

18:30 - *Dinner - Stiftskeller Klosterneuburg*

Day 3: Friday, Feb 21th 2020

08:20 - 08:50 *Bustransfer from Wien-Heiligenstadt*

08:30 - 08:50 *Bustransfer from Klosterneuburg*

09:00 - 10:00 **Keynote: Philippe Notton**

10:00 - 10:40 Session S3.1 (including EuroHPC)

10:40 - 11:00 *Coffee break*

11:00 - 12:20 Session S3.2

12:05 - 13:30 *Lunch break*

13:30 - 15:00 Session S3.3 VSC-5: Outlook and Discussion

15:00 - 15:30 *Bustransfer to Railway station Tullnerfeld*

About IST Austria

The Institute of Science and Technology Austria (IST Austria) is an international, multidisciplinary research institution dedicated to basic research in the natural, computer and mathematical sciences. The Institute is located in the city of Klosterneuburg, 18 km from the center of Vienna. As a PhD granting institution, the graduate school at IST Austria educates doctoral students from diverse and international backgrounds with the aim of cultivating world-class research scientists. IST Austria was established jointly by the federal government of Austria and the provincial government of Lower Austria and inaugurated in 2009.

Currently, nearly 700 employees from about 72 countries work at IST Austria. At present, the faculty of the institute consists of 53 professors. Following the implementation of the ambitious development plan, about 90 research groups will be working at IST Austria in a highly modern environment by 2026. To foster a creative and interdisciplinary scientific atmosphere, separating organizational structures, such as departments, are avoided at IST Austria. The scientists are organized into independent research groups, each headed by a Professor or a tenure-track Assistant Professor. The decision to promote an Assistant Professor to Professor with a permanent contract is based entirely on an evaluation of the scientific achievements of the Assistant Professor by international experts. Research excellence and promise are the exclusive hiring criteria for all scientists at IST Austria - from doctoral students to professors. The Institute chooses which fields of science to enter based solely on the availability of outstanding individuals. It will pursue a direction of research only if it can compete with the best in the world.

Contact Information Institute of Science and Technology Austria (IST Austria) Am Campus 1, 3400 Klosterneuburg, Phone: +43 2243 9000

WIFI Access: public-wlan (browser will open)

Catering

Lunches will take place in the IST Cafeteria - each participants will receive a voucher upon registration. Please note, that everything above the voucher value has to be covered by your own money.

Dinner will take place in:

Feb 19th - IST Cafeteria

Feb 20th - Stiftskeller (Klosteneuburg) (optional, in combination with the tour)

Please note on Feb 20th there is a optional Tour and Dinner in downtown Klosterneuburg in the Stift Klosterneuburg (Monastery).

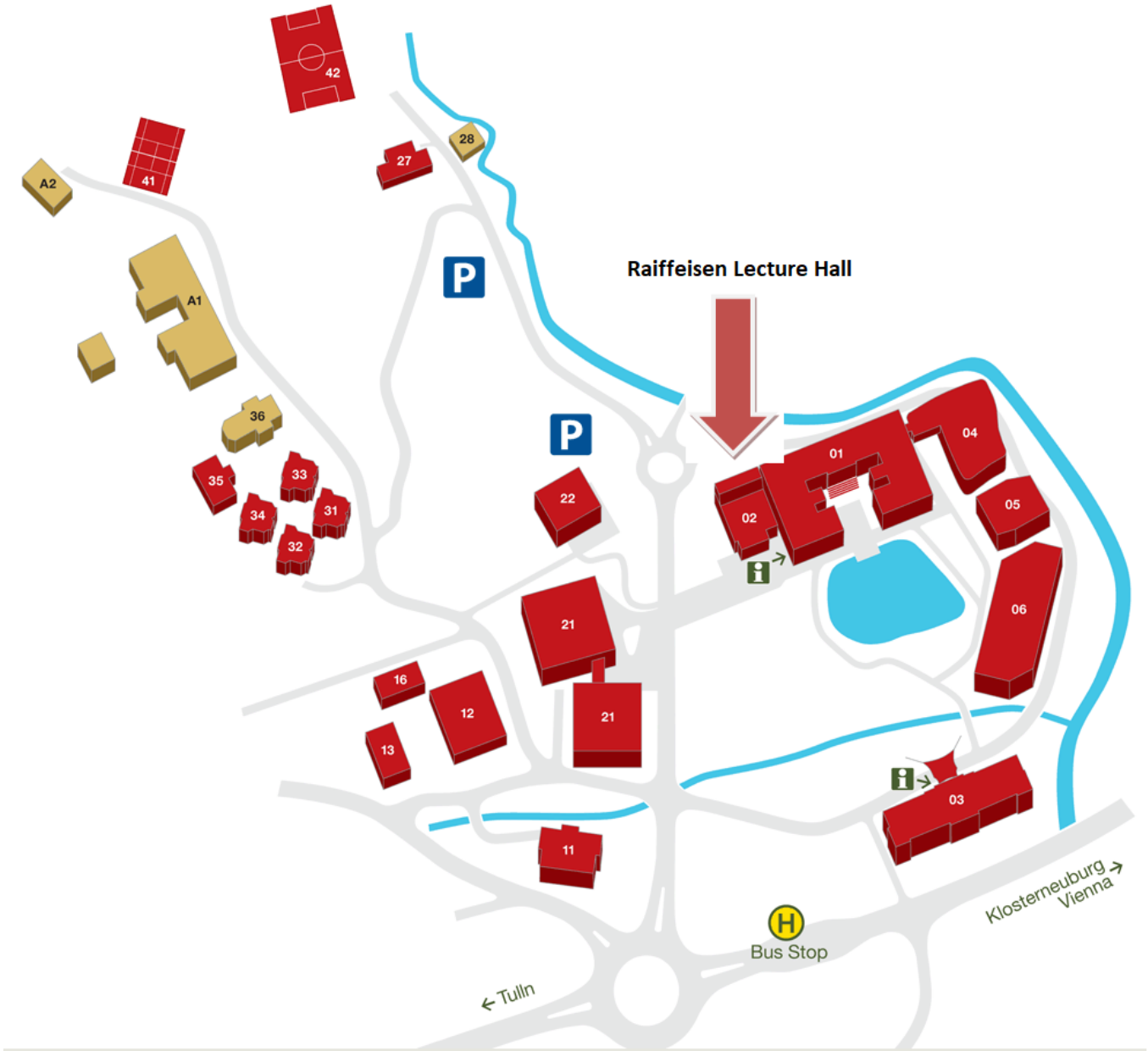
Transport in Vienna

Vienna has efficient public transport consisting of subways (U-Bahn), trams (Straßenbahn) and buses. A single ticket is valid on all means of transport except for the airport (CAT) train. Tickets are bought at the ticket machines located in every subway station and need to be validated by stamping them at the small blue boxes at the entry to the subway platform or inside the trams and buses respectively. Check www.wienerlinien.at for further information.

For going to the airport, you can either take a cab from IST Austria (approx. 45 minutes-1 hour), or go by public transport (shuttle bus or public bus) to U4 Heiligenstadt, take the U4 line to the stop Landstraße-Wien Mitte, and the direct CAT airport train to the airport (altogether approx. 1 1/2 h)

You will be provided with a free IST Austria Shuttle Bus ticket (bus no. 142) in case you need it for your arrival on the first day as well as departure on the last day.

The venue is the Raiffeisen Lecture Hall (Central Building)



Contents

Keynote Talk:

SPIRAL: AI for High Performance Code

Franz Franchetti

Department of Electrical and Computer Engineering, Carnegie Mellon University, Pittsburg, USA

This talk provides a current and comprehensive overview of the SPIRAL system, that has been developed over 20 years at Carnegie Mellon University, and is now available as BSD Open Source System. We show that SPIRAL is a rule based AI system that captures the knowledge of how algorithms, computer architecture, and program transformations are defined and interact. We develop the underlying formal framework to capture computational algorithms, computing platforms, and program transformations of interest, using a unifying mathematical formalism we call operator language (OL). Then we cast the problem of synthesizing highly optimized computational kernels for a given machine as a strongly constrained optimization problem that is solved by a multi-stage rewriting system. Since all rewrite steps are semantics preserving identity operations, our approach allows us to formally prove the equivalence between the kernel specification and the synthesized program. Finally we present a first look at FFTX and SpectralPack. We aim at translating the LAPACK/BLAS approach from the numerical linear algebra world to the N log N/spectral algorithm domain.

References

[1] Franchetti, F., Low, Tze-Meng, Low, Popovici, T., Veras, V., Spampinato, D.G., Johnson, J., Püschel, M., Hoe, J.C., Moura, J. M. F., Extreme Performance Portability, Proceedings of the IEEE, **106**, (2018).

[2] Franchetti, F., Spampinato, D.G., Kulkarni, A., Popovici, T., Low, Tze-Meng, Franusich, M., Canning A., McCorquodale P., Van Straalen, B., Colella P. FFTX and SpectralPack: A First Look, IEEE International Conference on High Performance Computing, Data, and Analytics (HiPC) (2018).

[3] Bolten, M., Franchetti, F., and Kelly, P. H. J., Lengauer C. Mohr, M., Algebraic Description and Automatic Generation of Multigrid Methods in SPIRAL, Concurrency and Computation: Practice and Experience (2017).

CV: Franz Franchetti is Professor in the Department of Electrical and Computer Engineering at Carnegie Mellon University. He received the Dipl.-Ing. (M.Sc.) degree in Technical Mathematics and the Dr. techn. (Ph.D.) degree in Computational Mathematics from the Vienna University of Technology in 2000 and 2003, respectively. Dr. Franchetti's research focuses on automatic performance tuning and program generation for emerging parallel platforms and algorithm/hardware co-synthesis. Within the Spiral effort, his research goal is to enable automatic generation of highly optimized software libraries for important kernel functionality.

NEC SX-Aurora Vector Engine: First Experiences with Quantum Chemistry Applications

Markus Oppel

Institute of Theoretical Chemistry, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria

NEC's SX-Aurora TSUBASA vector engine (VE) is an accelerator card with a newly developed vector processor coupled to high bandwidth memory [1]. Similar to GPUs and FPGAs, the VE is attached to a standard, x86-64 based Linux server (vector host, VH). In contrast to GPUs, programs can execute directly on the VE. The latter is controlled by a daemon running on the VH that provides operation system features and offloads system calls to the VH. Programming can be done using NEC's C/C++ and Fortran compilers, which generate executables for the VE [2].

This presentation reports on porting existing codes from the field of quantum dynamics and quantum chemistry to the new architecture. Most of these codes are written in Fortran and/or C/C++. Performance gains are mainly achieved by using optimized mathematical libraries like BLAS, LAPACK and FFTW3, which are tuned for the architecture of the SX-Aurora.

Fig. 1: NEC SX-Aurora Vector Engine

As a first example, quantum dynamics codes that implement grid based methods to solve the nuclear Schrödinger equation for molecular systems have been ported by recompiling for the SX-Aurora architecture and linking against NEC's numeric library collection. Depending on the problem size, a speed up of 6X to 7X with respect to a Intel Skylake CPU can be observed for symmetric eigenvalue solvers.

As a second example, the quantum chemistry package OpenMolcas [3] has been ported to the VE. Despite being a rather complex program package consisting of more than 20 modules written in different variants of Fortran, C and C++, adaptation of the configuration files and recompilation of the program package can be easily accomplished. First benchmark calculations show numerically stable results and promising potential performance gains when using simple offloading concepts by running IO intensive parts of the calculations on the x86-64 VH and compute intensive modules on the SX-Aurora VE.

References

[1] NEC SX-Aurora TSUBASA - Vector Engine:
`https://www.nec.com/en/global/solutions/hpc/sx/vector_engine.html`

[2] NEC SX-Aurora TSUBASA Software:
`https://www.nec.com/en/global/solutions/hpc/sx/software.html`

[3] Galván, I. F. et al: OpenMolcas: From Source Code to Insight, J. Chem. Theory Comput. 2019 15, 5925-5964.

Introduction to VSC-4

Jan Zabloudil[a,b]

[a] *VSC Research Center, TU Wien*
[b] *University of Natural Resources and Life Sciences*

The 4th generation Vienna Scientific Cluster system (VSC-4) [1], a cluster based on Lenovo ThinkSystem SD650 servers, has been installed at the Arsenal premises in summer 2019 by the Austrian IT company EDV-Design.

VSC-4, with a total of 38016 CPU-cores and more than 100 TB main memory, was ranked 82th in the June 2019 TOP500 list. The HPL (High Performance Linpack) benchmark has reached a performance (Rmax) of 2.7 PFlop/s, with the theoretical peak performance Rpeak being 3.7 PFlop/s.
The presentation will give an overview of the hardware components of VSC-4 – compute nodes (CPU, memory, etc), network, and cooling concept – and explain the basic usage of the cluster from a user perspective.

Vienna Scientific Cluster, VSC-4

References

[1] `http://vsc.ac.at/systems/vsc-4`

Current Trends in Pharma Research HPC

Dieter Kopecky, Gerald Birringer, and Andreas Bergner

Boehringer Ingelheim RCV Gmbh&Co KG, Dr. Boehringer Gasse 9-11, 1120 Vienna, Austria

Introduction: Drug discovery is a time consuming and expensive process with many small molecules failing in the later stages due to a lack of efficacy or due to toxicity. More complex mechanisms of action and stricter regulation have resulted in a drastic drop in pharmaceutical R&D productivity over the past 60 years [1]. Only 11% of the drug candidates that enter clinical phases make it to approval [2]. As a result, it takes on average Euro 1.9 billion to bring one successful drug to the market. This trend is clearly unsustainable and needs to be urgently addressed, amongst other approaches by leveraging innovative HPC solutions. Some of the current trends within Boehringer Ingelheim (BI) are summarized here.

Flexible Use of Available Resources and Cloud Computing: Big Pharma companies maintain HPC resources in various sites and locations in order to serve the needs of the working groups being located in the respective sites (e.g. computational chemistry, computational biology). These requirements comprise a high number of CPUs and/or GPUs, high IO throughput, enormous amounts of storage capacity, and a significant amount of RAM. In order to deal with varying workloads and correspondingly the need for flexibility and scalability in computing resources, current efforts focus on making all HPC resources available flexibly and independently from location. Cross-site job scheduling, data availability and software license checking pose significant challenges to be tackled. Consequently, moving workloads dynamically and transparently into the cloud, e.g. using AWS resources, in order to cover use cases having resource requirements being significantly beyond on-premise availabilities, and integrating these resources seamlessly into the facilities available for end users is the next logical step in Pharma HPC development.

Machine Learning and Deep Learning: Machine learning & deep learning methods are on the rise in the pharmaceutical business in recent years and are – in particular – also applied in early drug discovery research to virtualize parts of the drug design processes.

These processes can greatly benefit from automatic prediction of various compound properties, such as their activity in relation to target proteins in the human body, and their behavior in terms of absorption, distribution, metabolism and excretion (ADME). At BI, currently 3D convolutional neural networks are being trained to reliably predict activity of input compounds with a selected target protein. For this purpose, the volumetric representation of the molecular electrostatic potential (MEP) of an input compound is calculated using quantum mechanics (QM) as measure for activity of the compound and evaluated whether it represents a reliable classifier.

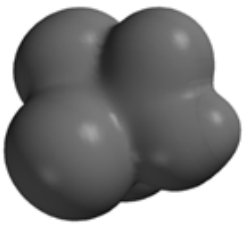


Fig. 1: Surface visualization of MEP

Since the predictive performance of such Machine Learning models is limited by the volume of a single company's data pool being applied as training material, the EU IMI initiative MELLODDY, that BI is part of (`http://www.melloddy.eu`), aims to boost predictive performance by multi-task federated and privacy-preserving Machine Learning across multiple data types and multiple companies' data in a cloud-based AWS environment, fostering containerized computation and distributed ledger technologies. In this way, MELLODDY combines four important trends – Cloud Computing, Deep Learning, extensive use of CPUs, and cross-company cooperation – into a single project.

References

[1] Scannel, J.W., Blanckley, A., and Warrington, B., Nature Reviews Drug Discovery **11**, 191 (2012).

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Performance optimizations for solving the atmospheric tomography problem of extremely large telescopes on real-time hardware

Bernadett Stadler[a], Roberto Biasi[b] and Ronny Ramlau[a]

[a] *Johannes Kepler University Linz* [a]
[b] *Microgate Bolzano, Italy*

Introduction: The new generation of earthbound extremely large telescopes require highly efficient algorithms to achieve an excellent image quality in a large field of view. These systems rely on adaptive optics, a technique where one aims to compensate in real-time the rapidly changing optical distortions in the atmosphere. To achieve such a correction, the deformations of optical wavefronts, emitted by natural or artificial guided stars, are measured via wavefront sensors and, subsequently, corrected using deformable mirrors (DMs). Many of such adaptive optics systems require the reconstruction of the turbulence profile, which is called atmospheric tomography. Assuming a layered model of the atmosphere, the goal of the atmospheric tomography problem is to reconstruct the turbulent layers from wavefront sensor measurements. Mathematically, this problem is ill-posed, i.e., the recovery of the solution from noisy measurements is unstable. Due to the growth of telescope sizes the computational load for this problem is increasing drastically, which makes it a big challenge to meet the real-time requirements. Thus, the collaboration of state-of-the-art real-time hardware with an efficient solver that takes advantage of the available hardware resources is of great importance.

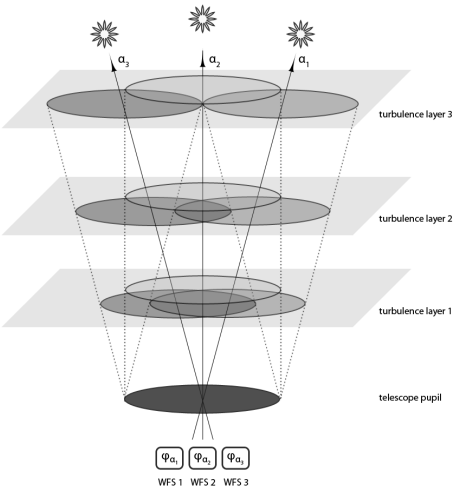

Fig. 1: Atmospheric Tomography.

So far, the standard method for solving the atmospheric tomography problem is the matrix-vector multiplication (MVM) approach. The computational costs of the MVM scales at $\mathcal{O}(n^2)$, where n is the dimension of the adaptive optics system. This dimension is drastically increasing in the next generation of ground-based telescopes, as e.g., for the Extremely Large Telescope (ELT). This telescope is currently built by the European Southern Observatory in the Atacama desert in Chile. When completed, it is planned to become the world's largest optical/near-infrared telescope with a primary mirror of 39 meter.

In this talk, we look at a novel, iterative approach for solving the atmospheric tomography problem called Finite Element Wavelet Hybrid Algorithm (FEWHA) and how it can be adapted to perform best on real-time hardware. In particular, we show the performance of a parallel version of the algorithm on GPU and CPU within the framework of MAORY, an adaptive optics module for the ELT. We conclude our talk with showing the benefits and drawbacks of the MVM method compared to the iterative approach of FEWHA and give a detailed comparison of the two algorithms in terms of computational performance.

References

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Managing a large number of runs of the Lagrangian particle dispersion model FLEXPART on the VSC

Petra Seibert[a], **Anne Philipp**[b]

[a] *Universität für Bodenkultur Wien, Institut für Meteorologie und Klimatologie, Wien*
[b] *Universität Wien, Institut für Meteorologie und Geophysik, und Department für Physik – Aersolphysik, Wien*

FLEXPART is a widely used numerical model for the simulation of atmospheric transport, diffusion, and deposition of trace substances [1]. The two key publications have almost 500 and, respectively, 1000 citations (Web of Science). Basically, the model solves a Langevin (stochastic differential) equation to obtain the trajectories of computational particles, representing fluid motion, under the consideration of turbulence, and additionally tracks trace substance mass or mixing ratio. It requires gridded meteorological fields as produced by weather forecasting models as input. The code and additional information can be found on the FLEXPART community web site [2].

Until version 10, only a scalar version existed. However, as certain applications may require on the order of 10^4 to 10^6 runs with a typical CPU time on the order of 1 h per run, it is appropriate to use HPC infrastructure. The recently released version 10 is able to use MPI parallelisation, which is useful for applications with a large number ($> 10^7$) of computational particles. On one hand, the loops over the computational particles are distributed to parallel processes, and on the other hand, the time-consuming reading and transformation of meteorological input data, required in certain time intervals, is assigned to a separate process.

The first large project with FLEXPART carried out on VSC 1 and 2 was an assessment of risks associated with nuclear power plants in Europe [3]. Some software tools were written in python and bash at this time to efficiently create directory structures and input files, to submit the runs, and to check the status of the runs. In 2018 and 2019, another large application of FLEXPART was (partially) carried out on the VSC, where the origin of certain trace substances (dust particles, black carbon, etc.) measured research aircraft, in-situ stations, and lidars over the Eastern Mediterranean (A-LIFE: Absorbing aerosol layers in a changing climate: aging, lifetime and dynamics). In this case, backward (receptor-oriented) calculations were performed. In order to use the compute nodes efficiently, the tools had to be partially rewritten, so that each job submitted would then spawn a number of FLEXPART runs.

It is expected that in the next years, the VSC infrastructure will be used for a significantly larger number of FLEXPART applications.

References

[1] Pisso, I.; Sollum, E.; Grythe, H.; Kristiansen, N.; Cassiani, M.; Eckhardt, S.; Arnold, D.; Morton, D.; Thompson, R. L.; Groot Zwaaftink, C. D.; Evangeliou, N.; Sodemann, H.; Haimberger, L.; Henne, S.; Brunner, D.; Burkhart, J. F.; Fouilloux, A.; Brioude, J.; Philipp, A.; Seibert, P., Stohl, A., The Lagrangian particle dispersion model FLEXPART version 10.3. Geosci. Model Dev. Discuss., URL:`https://doi.org/10.5194/gmd-2018-333`(2018).

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[3] Seibert, P.; Arnold, Dè.; Arnold, N.; Gufler, K.; Kromp-Kolb, H.; Mraz, G.; Sholly, S., Wenisch, A.: Flexrisk – Flexible tools for assessment of nuclear risk in Europe. Final Report. BOKU-Met Report 23, `http://www.boku.ac.at/met/report/BOKU-Met_Report_23_PRELIMv2_online.pdf` (2013).

Sparse modelling of one- and two-particle response functions

Markus Wallerberger[a,b], Jia Li[b], Anna Kauch[a], Karsten Held[a], and Hiroshi Shinaoka[c]

[a] *Institut für Festkörperphysik, Technische Universität Wien, Austria*
[b] *Department of Physics, University of Michigan, Ann Arbor, United States*
[c] *Department of Physics, Saitama University, Japan*

Efficient *ab-initio* calculations of correlated materials at finite temperature require compact representations of the Green's functions both in imaginary time and Matsubara frequency.

In this talk, we discuss a recently introduced general procedure which generates sparse sampling points in time and frequency from compact orthogonal basis representations, such as Chebyshev polynomials and intermediate representation (IR) basis functions [1]. These sampling points accurately resolve the information contained in the Green's function, and efficient transforms between different representations are formulated with minimal loss of information. As a demonstration, we apply the sparse sampling scheme to diagrammatic GW and GF2 calculations of a hydrogen chain, of noble gas atoms and of a silicon crystal.

We then move on to the two-particle level, where the fundamental object of interest are the two-particle Green's function. Many-body calculations at the two-particle level require a compact representation of two-particle Green's functions. However, the two-particle Green's function has a set of non-trivial discontinuities in imaginary time, or, equivalently, a rich asymptotic structure in frequency.

We will discuss a recently introduced [2] sparse sampling scheme in the Matsubara frequency domain as well as a tensor network representation for two-particle Green's functions, designed to overcome this. The sparse sampling is based on the intermediate representation basis and allows an accurate extraction of the generalized susceptibility from a reduced set of Matsubara frequencies. The tensor network representation provides a system independent way to compress the information carried by two-particle Green's functions. We demonstrate efficiency of the present scheme for calculations of static and dynamic susceptibilities in single- and two-band Hubbard models in the framework of dynamical mean-field theory.

Finally, we will discuss the computation of irreducible quantities in both the one- and two-particle case [2,3].

References

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[3] M. Wallerberger, A. Kauch, K. Held, H. Shinaoka, in preparation.

Free Energy Simulations — Challenges for HPC

Stefan Boresch

Department of Computational Biological Chemistry, Faculty of Chemistry, University of Vienna, Währingerstr. 17, 1090 Vienna, Austria

So-called "alchemical" free energy simulations (FES) can, among other applications, be used to predict binding affinities of ligands. The underlying theory and methods have been known and available for more than thirty years [1]. The central idea is the fundamental tenet of thermodynamics that the free energy is a state function. Thus, rather than having to compute binding affinities directly (which is doable, but tedious), thermodynamic cycles can be used to predict relative binding free energy differences. It is only recently that computational resources have become powerful enough for large scale, practical applications, and this is of high interest for medicinal chemistry and pharmaceutical research, particularly during lead optimization [2,3]. In fact, alchemical FES are becoming a standard technique in this area.

Molecular dynamics (MD) simulations of biomolecules are a classical application of HPC, and many highly optimized codes are routinely run on supercomputing centers. For use of FES as outlined above, speed is particularly critical. Specifically, in order to compete with experimental assays, the calculation of individual binding free energy differences should be accomplished within 24-48 hours. This can be done at affordable cost only if the underlying simulations, typically MD, are fully accelerated by GPUs. FES are challenging in this respect since they require subtle alterations to the MD codes which are detrimental to performance. E.g., a recent re-implementation of alchemical FES for NAMD still is not available on GPUs [4]. Large-scale distributed computation on CPUs is in principle possible, but would quickly become very costly.

A brief overview of the methodology will be given first, outlining the challenges for achieving adequate performance. Past work from my group aimed at overcoming this will be recapitulated. Currently, we are implementing a framework in the context of the charmm-gui web server [5], which permits to exploit the fastest code paths of the MD engine used. The central idea is to reduce multiple alchemical "mutations" to a *common-core*; this is particularly beneficial if a number of related compounds needs to be evaluated [6]. In addition, it will be shown how multiple GPUs can be combined synergistically. The overall challenges of the methodology, accuracy of the force-fields, sampling, and system preparation will be discussed.

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[6] Wieder, M., Fleck, M., and Boresch, S., manuscript in preparation.

Atomistic simulations of ion beam implantation of impurity atoms into graphene

Alexander Markevich, Jani Kotakoski, and Toma Susi

Faculty of Physics, University of Vienna, Austria

Ion implantation is a well-established technique for modification of materials properties. It offers a lot of opportunities due to a variety of ion species, wide range of implantation energies and control over the dopant concentration. However, in the case of two-dimensional materials, such as graphene, ion implantation is quite challenging – an ion has to be trapped within a single atomic layer and only ions within a relatively narrow energy range are suitable for embedding of impurity atoms into a 2D lattice [1,2]. The precise choice of ions energy is therefore essential for successful implantation. The suitable energies can be predicted with the use of molecular dynamics (MD) simulations. Density functional theory (DFT) based MD calculations allow to understand details of interactions of an implanted ion with a host lattice and can provide rather precise values for the appropriate implantation energies. Our results show that a large variety of atomic species can be embedded into graphene using low-energy ion irradiation. However, the systematic study for various ions, energies and impact parameters requires thousands of simulations which is computationally too demanding for any *ab initio* method. Classical force-field MD, in turn, lack an accurate description of the breaking and formation of chemical bonds upon incorporation of impurity atoms into the graphene lattice. We plan to develop machine-learning potentials based on the data obtained from DFT-MD simulations. This will allow to create experimentally relevant statistical description of the outcomes of ion irradiation for various atomic species, energies and impact parameters.

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Parallel Adaptive Space-Time Methods for Evolution Equations

Ulrich Langer[a], Andreas Schafelner[b], and Panayot Vassilevski[c,d]

[a] *Institute of Computational Mathematics, Johannes Kepler University*
[b] *DK Computational Mathematics, Johannes Kepler University*
[c] *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, CA*
[d] *Portland State University, OR*

We will present two finite element schemes on completely unstructured simplicial space-time meshes for the numerical solution of evolution equations. In particular, we present a locally stabilized, conforming space-time finite element method [1] to solve parabolic initial-boundary value problems of the form

$$\partial_t u - \mathrm{div}_x(\nu \nabla_x u) = f \text{ in } Q = \Omega \times (0,T),\ u = 0 \text{ on } \Sigma = \partial\Omega \times (0,T),\ \text{and } u = u_0 \text{ on } \Sigma_0 = \Omega \times \{0\}, \quad (1)$$

as well as a constrained first order system least squares (CFOSLS) finite element method [2] that in addition can treat transport problems

$$\partial_t u + \mathrm{div}_x(\boldsymbol{\beta} u) = f \text{ in } Q,\ (\boldsymbol{\beta} u) \cdot \vec{n} = g \text{ on } \Sigma_{in} = \Gamma_{in} \times (0,T),\ \text{and } u = u_0 \text{ on } \Sigma_0, \quad (2)$$

with a prescribed flow field $\boldsymbol{\beta}$. Uniform mesh refinement has a high memory demand, and, moreover, can lead to reduced convergence rates. In order to avoid these problems, we also consider different adaptive procedures. For the CFOSLS method, it is natural to use the localized least squares functional as an indicator for local refinement, whereas for the space-time method, we use error indicators of residual and functional type. Once the elements are marked, we refine them in parallel using bisection.

The huge systems of space-time finite element equations are then solved by means of a Krylov-subspace method like GMRES preconditioned by multigrid. Figure 1 presents convergence rates in the energy norm for the locally stabilized finite element method, comparing uniform and adaptive refinement for different polynomial degrees p, with spatial dimension $d = 3$, i.e. $Q = \Omega \times (0,T) \subset \mathbb{R}^4$. Both uniform and adaptive refinements were performed with 32 nodes, or 1152 cores, on the distributed memory machine `Quartz`[1].

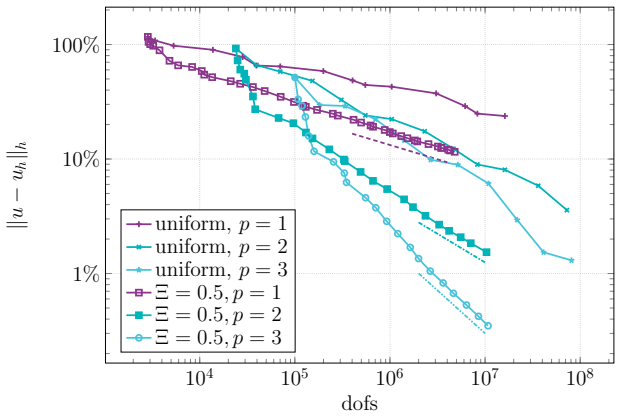

Fig. 1: Convergence rates.

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BiqBin: High-performance computing approach towards NP-hard problems

Janez Povh[a,c], Elisabeth Gaar[a], Nicollo Gusmeroli[b], Timotej Hrga[b], Borut Lužar[c], Angelika Wiegele[b]

[a] *Institute of mathematics, physics and mechanics Ljubljana, Slovenia*
[b] *Alpen-Adria-Universität Klagenfurt, Austria*
[c] *University of Ljubljana, Faculty of mechanical engineering, Slovenia*
[d] *Faculty of information studies in Novo mesto, Novo mesto, Slovenia*

The area of combinatorial optimization studies optimization problems where the feasible set is usually a large discrete set, related with combinatorial objects, and the problems usually fall in the class of NP-hard problems. Integer programming offers several techniques how to solve them (approximately), including branch-and-bound (B&B) algorithm as a classical approach.

We will present how to solve optimization problems, where the objective function non-convex quadratic and the constraints are linear, but the variables are binary (we call them binary quadratic problems). This family of problems includes several well-known optimization problems, like the stable set problem, the max-cut problem, the clustering problem etc.

Our approach is based on B&B algorithm, where all the main ingredients (branching strategy and bounding procedures) are carefully developed using new semidefinite programming relaxations, improved first order methods like ADMM to solve the relaxed problems, new heuristics for finding feasible solutions and new branching strategies to explore the B&B tree. These parts are also carefully parallelized using MPI for the branching part and OpenMP for the bounding part, coupled with Armadillo library for linear algebra operations.

The final result, the solver BiqBin, is written in C++ and is available as free web service running on HPC at University of Ljubljana. Performance optimization for this solver was done at Czech's national supercomputer in Ostrava via PRACE preparatory access. We provide several numerical results which demonstrate that BiqBin is scaling very well and is outperforming the other solvers for binary quadratic problems.

A New Parallel Multi-Step Conjugate Gradient Method for Optimization

Issam A.R. Moghrabi

College of Business Administration, Gulf University for Science and Technology, Kuwait

Conjugate Gradient methods (CG) are a class of methods for solving large unconstrained optimization problems. Their storage requirements are rather minimal compared to other methods as they do not store any matrices. Such methods have been used in a variety of domains to solve nonlinear optimization problems as well as systems nonlinear equations. The methods have proven their effectiveness in applications such as Image restoration using a conjugate gradient-based adaptive filtering and Brain Magnetic Resonance Images Segmentation [29]. While such methods converge in at most n iterations on quadratic functions for exact line searches, they are also used to minimize non-quadratic functions and inexact line searches. In the context of minimizing non-quadratic functions, the methods need to be restarted when certain criteria is met. On the other hand, multi-step methods are secant-like techniques of the quasi-Newton type that, unlike the classical methods, construct nonlinear alternatives to the quantities in the so-called Secant equation. Multi-step methods instead utilize data available from the m most recent iterations and thus create an alternative to the Secant equation with the intention of creating better Hessian approximation that induce faster convergence to the minimizer of the objective function f. The methods, based on reported numerical results published in several research papers related to the subject, have introduced substantial savings in both iteration and function evaluation counts. Encouraged by the successful performance of the methods, we explore in this paper using them in developing a new parallel Conjugate Gradient (CG) algorithm. CG methods gain popularity on big problems and in situations when memory resources are scarce. The numerical experimentations on the new method are encouraging and open venue for further investigation of such techniques to explore their merits in a multitude of applications. The method requires less storage to implement than other known methods. This saving in resources is especially appreciated on large problems and multi processor high performance machines. Other choices for the parameters used in the construction of the search directions are under consideration to determine whether the numerical performance of the method can be improved further. There also remains the issue of developing automatic restart criteria that provides appropriate switching among several options similar to what was done in [1]. The global convergence properties of such methods are also under study.

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Classical and pipelined preconditioned conjugate gradient methods with node-failure resilience

Carlos Pachajoa[a], Markus Levonyak[a], Christina Pacher[a], Jesper Larsson Träff[b] and Wilfried N. Gansterer[a]

[a] *University of Vienna, Faculty of Computer Science*
[b] *TU Wien, Parallel Computing Group*

We present the latest developments in our work on resilience against node failures for classical and pipelined preconditioned conjugate gradient (PCG) methods. Our methods are based on the exact state reconstruction (ESR) approach and exploit the inherent redundancy of the sparse matrix-vector product (SpMV), defining an augmented SpMV that provides the necessary redundancy, at the cost of some communication overhead. If a node failure happens, it is then possible to reconstruct the complete state of the solver as it was before the failure hit, thus enabling it to continue, following the same trajectory of states as an unaffected solver, saving iterations at the cost of a cheap reconstruction operation.

We discuss several improvements over a simple resilient PCG solver, which only has the ability to recover from a single node failure if a spare node is available. In a first instance, we extend the method with the ability to recover from multiple simultaneous node failures [1]. This situation may occur, for example, if a switch fault occurs, affecting several nodes. This approach requires some additional communication between the multiple reconstructing nodes.

Global communication has become a major bottleneck in HPC, and it needs to be reduced to make future exascale machines practical. Pipelined PCG (PPCG) methods address this issue by reducing the amount of global communication required. We also discuss an extension to the ESR approach that can be used in conjunction with PPCG [2], enabling it to resist a node failure while conserving its communication-avoiding property.

The hardware overhead of holding extra spare nodes for being able to recover from (rare) node failures may be unacceptable. Thus, we also discuss an algorithm for recovering from node failures without the use of spare nodes [3]. This is achieved by performing the state reconstruction in one of the surviving nodes, then redistributing the data in the cluster to achieve a balanced load.

All our resilient algorithms are evaluated in terms of their runtime performance, in particular focusing on quantifying the overhead compared to the standard (non-resilient) algorithms. In general, we obtain low overhead and thus very competitive experimental results for all of our methods. With our newly developed framework for resilient PCG-like solvers, we obtain runtimes close to the ones obtained with state-of-the-art libraries, such as PETSc.

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On q-Rising Factorials and the Necessity of Shared Memory Calculations

Ali Kemal Uncu

Johann Radon Institute for Computational and Applied Mathematics,
Austrian Academy of Sciences

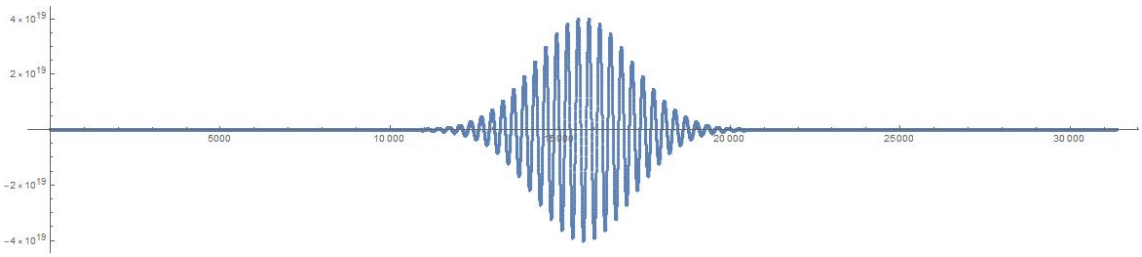
The Euler's Pentagonal Number Theorem,

$$\sum_{k=-\infty}^{\infty}(-1)^k q^{k(3k-1)/2}=\prod_{i=1}^{\infty}(1-q^i)=1-q-q^2+q^5+q^7-q^{12}+\dots,$$

is a world-renowned sum-product identity. The power series coefficients of this series are all 0 or ± 1. This property is not necessarily clear from the product side; moreover, their finite analogs (*q-rising factorials*)

$$(q;q)_n:=\prod_{i=1}^{n}(1-q^i)=\sum_{k=0}^{n(n+1)/2}a_{n,k}\,q^k,$$

do not share this feature for any $n\geq 6$. For example, we plot $(q;q)_{250}$, where every point represent $(k,a_{250,k})$:



Not only the coefficients go beyond ± 1, they grow exponentially. In 1960's, Sudler [3] and Wright [4] studied the growth rate of these maximum absolute coefficients. Recently, the author, joint with Berkovich, [1] found an elementary method of classifying $(q;q)_n$ by their maximum absolute coefficient and became aware that the locations of the maximum absolute coefficients were not known, especially for the cases when n is odd. To that end, we calculated $(q;q)_n$ for all $n\leq 75{,}000$ and conjecturally found that the change in the location of the maximum absolute coefficient show a periodic pattern [2].

The size of the objects, the nature of the problem, and the need for full precision calculations made this problem a computational challenge. Thankfully we had access to the parallel shared memory supercomputer MACH2 at the Johannes Kepler University, where we carried out most of our calculations in a 10 TB capsule of this computer with the invaluable help of the MACH2 team.

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Comparison of a randomized and a deterministic low-rank approximation algorithm

Robert Ernstbrunner, Viktoria Mayer, and Wilfried N. Gansterer

University of Vienna, Faculty of Computer Science

Low-rank approximations of large sparse matrices are important in many scientific applications. We compared a deterministic algorithm for computing a truncated LU factorization with tournament pivoting, proposed by Grigori et al. [1], with the adaptive randomized range finder, proposed by Halko et al. [2]. The latter is a randomized algorithm which computes an approximate basis for the range of the input matrix. Both algorithms are iterative methods for when the numerical rank k is not known.

We developed optimized implementations of both these algorithms in order to evaluate their accuracy and runtime behavior. Moreover, we compared parallelization properties of randomized low-rank approximations to deterministic algorithms by using shared-memory parallelization. For the adaptive randomized range finder, we developed and implemented a blocked version that utilizes sparse embedding matrices to reduce communication. Moreover, we used the Block Classical Gram-Schmidt algorithm in combination with Tall and Skinny QR factorization for orthogonalization, which is known to be communication-optimal.

Since both algorithms are adaptive, the rank k is incremented in each iteration until the desired precision is achieved or the maximum number of iterations has been reached. In each iteration, the magnitude of the rank-increment is determined by the step size. In both algorithms, the step size can be viewed as a tuning parameter. In the truncated LU factorization with tournament pivoting, a smaller step size can exploit more parallelism. In the adaptive randomized range finder, choosing the right step size is important for efficient block orthogonalization.

For the randomized algorithm the runtime can be anticipated well based on the size and the number of nonzeroes of the matrix due to the inevitable use of dense linear algebra, since the resulting low-rank approximation is usually quite dense.

The factors of the deterministic truncated LU factorization are calculated such that they are as sparse as possible, which can give an advantage in terms of memory and storage usage. However, after each iteration the input matrix is updated by removing the portion already approximated so far, which potentially produces fill-in on the matrix used in successive iterations. This can have large impact on the runtime.

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Keynote Talk:

A working tour of OrangeFS

Walter B. Ligon

Clemson University, Clemons, SC, USA

OrangeFS is an open source community constructed parallel file system for Linux based cluster computers. Its primary purpose it to provide high performance file IO for parallel applications on cluster computers. It has various options for networking, storage, user interfaces, caching and security options. The file system can be deployed on something as simple as a linux laptop, up to thousands of nodes in a research cluster. Among its better qualities it is very easy to install, operate, and maintain; it's POSIX user interface is included in Linux 4.8 and up; and it is highly configurable to match different application's IO needs. The software design is highly modular allowing many features and abilities to be changed or added. Thus it is popular as a research vehicle for man projects. This presentation will start with basic definitions and motivations and describe the major features. A few recent project will round out the talk. The presentation will assume basic understanding of HPC and parallel computing from which it will build a better understanding of HPC file IO.

CV: Walter B. Ligon III received his Ph.D. in Computer Science from the Georgia Institute of Technology in 1992 and is currently an Associate Professor of Computer Engineering at Clemson University. For the past 24 years Walt has worked in parallel I/O. Working with a number of national labs Walt and his students developed the Parallel Virtual File System, an open source software system that allows parallel tasks to access data distributed across multiple storage nodes. PVFS has been innovative in a number of areas including its highly modular object-based architecture, distributed metadata, interface features, and avoidance of global synchronization. Walt is currently in the design phase of OrangeFS (PVFS 3.0) which will incorporate a much more widely distributed model for high performance cloud computing. Walt is also working on PXFS, a parallel I/O system for ParalleX that integrates the name space of memory and storage for Exascale computational systems.

VSC-4 Storage

Markus Hickel, Balázs Lengyel

VSC Research Center, TU Wien

As a parallel file system for VSC-4, IBM Spectrum Scale (formerly known as GPFS) was chosen. It will provide user home directories, as well as scratch space similar to the BeeGFS file system used at VSC-3.

The VSC-4 storage system consists of 6 NSD-Servers (Lenovo SR650), 6 storage arrays (Lenovo DE6000H) with expansion enclosures (Lenovo DE600S) and a flash system (IBM 9110). Each NSD-Server is equipped with 256 GByte main memory, 2 Intel Xeon Gold 6148 CPUs and 2 Intel Omni-Path adapters. The storage array and expansion enclosures are each connected via 12 Gb SAS to 2 NSD-Servers redundantly. This ensures continuous operation, in case of a NSD-Server failure or maintenance work. Each storage array and expansion enclosure is equipped with 60×12 TByte HDDs, which adds up to a total of 720 hard drives with a capacity around 6 PByte. The flash system is connected to all NSD-Servers through 16Gb fibre channel and has a capacity of roughly 150 TByte.

We have tried different configurations regarding data consistency, throughput and latency. Rebuild times were also a major factor in our considerations, as well as the designated use for the flash system. Benchmarks are still ongoing with RAID6 and diskpool setups and with meta data on flash or HDDs.

This talk will will provide a short introduction of the Spectrum Scale implementation and the underlying configuration.

Fig. 1: VSC-4 storage drawer

P2.0 Lightning Talk / Poster presentation

Climate Change Simulations at the Kilometer-Scale Resolution

Nikolina Ban[a,b], Roman Brogli[b], Laureline Hentgen[b], Nico Kröner[c], David Leutwyler[d], Christoph Schär[b]

[a] *Department of Atmospheric and Cryospheric Sciences (ACINN), University of Innsbruck, Austria*
[b] *Institute for Atmospheric and Climate Science, ETH Zurich, Switzerland*
[c] *South Pole, Zurich Switzerland*
[d] *MPI Hamburg, Max-Planck-Institute for Meteorology, Hamburg, Germany*

With the recent advancements in the high-performance computing and emerging new supercomputing architectures, it becomes feasible to run high-resolution (kilometer-scale) climate models at continental-scale domains and extended time periods. At such a high resolution, climate models are able to explicitly resolve deep convection (i.e., thunderstorms and rain showers), and thus avoid the use of the convection parameterization - one of the major sources of uncertainties in climate change projections. These are so-called convection-resolving models.

Here we present decade-long convection-resolving climate change simulations at a horizontal resolution of 2.2 km on a computational domain that covers almost entire Europe with 1536x1536x60 grid points. Such computationally demanding simulations have become feasible with a COSMO (Consortium for Small-Scale Modeling) regional weather and climate model version that runs entirely on Graphics Processing Units, and have been performed on Piz Daint at the Swiss National Supercomputing Center.

In this work, we perform two decade-long simulations - one for the present-day climate and one for the future climate. The present-day simulation is driven by ERA-Interim reanalysis, while for the future climate we use Pseudo-Global Warming (PGW) approach. The PGW simulation is driven by ERA-Interim reanalysis modified by the mean annual cycle of climate changes derived from a global climate model.

In this presentation, we compare two different modeling approaches - convection-resolving versus convection-parameterizing (coarse resolution model) - and discuss the effects of it on the simulation of the water cycle and its future changes with the temperature increase [1]. The results show great improvement in the simulation of present-day climate when using convection-resolving model, especially for the simulation of heavy precipitation at sub-daily timescales [2, 3]. Furthermore, differences in the projections of precipitation between the two models are small for mean precipitation, but large for heavy precipitation, especially over complex mountainous terrain like European Alps. We also show that the rate of future intensification of heavy precipitation depends on the investigated region across Europe but are able to reconcile these differences by considering atmospheric temperature changes.

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P2.0 Lightning Talk / Poster presentation

On the sensitivity of convection-permitting climate models simulating precipitation in the Eastern Alpine region

Heimo Truhetz[a]

[a] *Wegener Center for Climate and Global Change, University of Graz, Austria*

This study, recently published in [1], evaluates the representation of precipitation in a set of multi-year convection-permitting sensitivity experiments over the European Alpine region. In the last few years, studies have consistently demonstrated the added value of convection-permitting regional climate models (RCMs) over coarser resolved RCMs with parametrized convection for the representation of precipitation. They allow unprecedented insights in the role of mesoscale processes in the climate system and are hoped to provide more realistic climate change projections. However, their uncertainties due to variations in the models' configurations are still a matter of ongoing research. The present study addresses this issue using a set of hindcast simulations with the model CCLM v5.0 at 0.0275° (3 km) grid spacing, from January 2006 to December 2009. Six configuration parameters are chosen amongst the following categories: parametrization of turbulence, parametrization of microphysics, surface orography, lateral boundary forcing, and driving data. They are tested individually with regards to a reference experiment and evaluated against two high-resolution gridded (1 km grid spacing) observational datasets over Austria, for winter and summer seasons. Also, a simulation with the model WRF v3.7.1, using a similar experimental set up, provides an estimate for the model-dependency of precipitation biases. The added-value regarding coarser resolved (0.11° grid spacing, i.e. 12.5 km grid spacing) CCLM and WRF simulations from the EURO-CORDEX initiative, which were used as driving data, is discussed. In agreement with previous studies, convection-permitting experiments show added-value compared to their driving data regarding precipitation extremes, the height-dependency and the mean diurnal cycle of precipitation in summer. However, CCLM at convection-permitting resolution suffers from a predominant wet bias in mountainous regions in winter, and a dry bias in the eastern Alpine forelands during summer. The latter is related to a significant underestimation of the spatial extent of the precipitation events that cannot be compensated by overestimated intensities as it happens mostly in the mountains. This interplay is insensitive to the parameters tested. In contrast, WRF at convection-permitting resolution largely overestimates precipitation because of too large and too intense precipitation events, though there are improvements in summertime. Using a direct nesting strategy with an operational high-resolution (0.225° grid spacing, i.e. 20 km grid spacing) analysis product from numerical weather prediction as driving data improves seasonal biases in the 3 km CCLM domain, thanks to reduced (enhanced) frontal precipitation in winter (summer), but does not improve the interplay between the spatial extent of precipitation events and their according intensities.

The study was funded by the Austrian Science Fund (FWF) project NHCM-2 (proj.id P24758-N29; `http://nhcm-2.uni-graz.at`).

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P2.0 Lightning Talk / Poster presentation

Matrix-Free Solution of Nonlinear PDEs

Daniel Jodlbauer[a], Ulrich Langer[a], and Thomas Wick[b]

[a] *Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences*
[b] *Institut für Angewandte Mathematik, Leibniz Universität Hannover*

Many of the interesting PDEs are nonlinear, and their efficient solution is still challenging. In this talk we try to provide the building blocks for matrix-free geometric multigrid approaches to tackle such problems.

In particular, we will focus on the problem of fracture propagation in brittle materials. This can be formulated by a phase-field approach, which approximates the originally sharp crack by an auxiliary phase-field variable. The resulting PDE is a nonlinear and coupled system. Furthermore, it has to satisfy an inequality constraint, which is responsible for preventing fractures to heal themselves over time. The variational inequality is handled via a primal-dual active-set algorithm - a kind of semismooth Newton's method.

Within Newton's method, a sequence of linear systems of equations needs to be solved. The classical way of solving these linear equations is to assemble a huge, sparse system matrix and feed it to the selected linear solver, i.e. preconditioned CG, GMRES, or a direct solver.

In the matrix-free framework, one tries to omit the assembling step. This is possible, because iterative solvers (GMG, CG, GMRES, ...) do not require explicit knowledge of the matrix entries, but rather need to know how to form the matrix-vector product. Hence, the strategy for a matrix-free implementation replaces the standard matrix assembling and sparse matrix-vector products by directly assembling the result of the matrix-vector product. Such an approach has the immediate advantage of saving lots memory. By exploiting the special tensor-product structure of the underlying terms, one can even achieve better complexity for the matrix-free setting compared to the standard sparse matrix-vector product. This is particularly true for higher-order elements.

The obvious disadvantage of matrix-free methods is that the matrix entries are not available. This restricts the choice of available solvers and preconditioners. A frequently chosen setup is a geometric multigrid with Jacobi-Chebyshev smoothers. The required diagonal of the matrix can be assembled and stored cheaply.

Furthermore, the implementation is suitable for distributed parallelization (MPI) and vectorized instructions (SIMD). Most of the details are already available in the open-source FEM library deal.II [2]. In this talk, we will address additional challenges resulting from the nonlinear PDE and the variational inequality, in particular on the coarser levels of the multigrid method. The presented strategies provide the building blocks for solving more general nonlinear PDEs.

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P2.0 Lightning Talk / Poster presentation

ASPIDE Project: Perspectives on the Scalabale Monitoring and Auto-tuning

Radu Prodan[a], Vladislav Kashansky[a,b], Dragi Kimovski[a], Prateek Agrawal[a]

[a] *Institute of Information Technology, University of Klagenfurt, Austria*
[b] *School of Electrical Engineering and Computer Science, South Ural State University, Russia*

Introduction

Extreme Data is an incarnation of Big Data concept distinguished by the massive amounts of data that must be queried, communicated and analyzed in (near) real-time by using a very large number of memory/storage elements of both, the converging Cloud and Pre-Exascale computing systems [1]. Notable examples are (1) the raw high energy physics data produced at a rate of hundreds of gigabits-per-second that must be filtered, stored and analyzed in a fault-tolerant fashion, (2) multi-scale brain imaging data analysis and simulations, (3) complex networks data analyses, driven by the social media systems. To handle such amounts of data multi-tiering architectures[1] are introduced, including scheduling systems and distributed storage systems, ranging from in-memory databases to tape libraries. The ASPIDE[2] project [2] is contributing with the definition of a new programming paradigm, APIs, runtime tools and methodologies for expressing data-intensive tasks on the converging large-scale systems, which can pave the way for the exploitation of parallelism policies over the various models of the system architectures, promoting high performance and efficiency, and offering powerful operations and mechanisms for processing extreme data sources at high speed and/or real-time.

Contribution

In this presentation, we will highlight the results achieved by the University of Klagenfurt and partners in frames of the Scalable Monitoring and Auto-tuning workpackage. More specifically we will discuss the Integer Linear Programming (ILP) methods for the monitoring data collection control and practical approach for the selecting monitoring aggregation points, by using the SCIP optimization suite with several variable complexity data gathering policies.

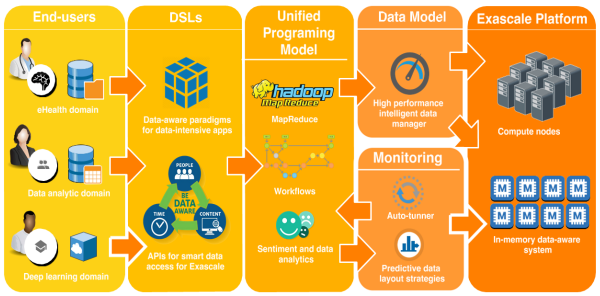

Fig. 1: ASPIDE Project architecture

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Acknowledgement

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[1] HPAC, WLCG
[2] Exascale programing models for extreme data processing

P2.0 Lightning Talk / Poster presentation

Challenges in genomics studies of non-model organisms

Beatriz Vicoso

Institute of Science and Technology Austria, Klosterneuburg, Austria

Recent advances in sequencing technologies have made it possible to perform large genomic studies in virtually any organism. However, working with non-model systems for which no previous genomic resources are available comes with its own set of challenges. We have spent the last years setting up brine shrimp of the genus Artemia as a model for understanding the role of separate sexes in how genomes evolve. I will present examples of the data that we have collected and how we analysed it, and discuss how we have dealt with some of the computing challenges that we faced along the way.

P2.0 Lightning Talk / Poster presentation

The Performance Optimisation and Productivity (POP) HPC Centre of Excellence: Identifying and Finding the Causes of Inefficiency in Parallel Applications

Lubomir Riha[a], Jonathan Boyle[b], Sally Bridgwater[b], Nick Dingle[b], Wadud Miah[b], Jon Gibson[b]

[a] *lubomir.riha@vsb.cz, IT4Innovations, VSB-TU Ostrava, Czech Republic,* [a]
[b] *pop@nag.co.uk, Numerical Algorithms Group Ltd, Oxford, UK*

The POP project [1], a parallel application profiling and optimisation service, successfully completed the first phase of the project which has resulted in more than 125 assessments of parallel HPC applications. The project has just received its second round of funding and this service is free of charge for users based in the EU. This poster will present POP case studies where parallel inefficiency was identified using the POP methodology and open-source profiling tools with recommendations on how to address them. The parallel paradigm, programming languages used, and the type of inefficiencies identified in codes will be presented from the first phase of the project.

The Institute of Physical Metallurgy and Metal Physics of RWTH Aachen University (IMM) develops a code for the simulation of microstructure evolution in polycrystalline materials, called GraGLeS2D. The OpenMP parallel code is designed to run on large SMP machines in the RWTH compute cluster with 16-sockets and up to 2 TB of memory. After a POP performance audit of the code done by POP experts, several performance issues in the code were detected and a performance plan on how these issues could be resolved was set up. To verify the proposed optimization steps, POP experts and the code developer at IMM implemented these steps in close collaboration. After these optimization steps were implemented, a significant performance improvement was achieved. For the hotspot of the application, the convolution region, the speedup going from 1 to 16 sockets is about 15 instead of 6 as it was before the optimization. Overall, the runtime of this region was improved by a factor of more than 10X. So, the proof-of-concept verified that the planned optimizations indeed resulted in significantly better code performance.

BAND is part of SCM's renowned ADF Modeling Suite, a set of powerful tools used by academic and industrial research chemists, and written in Fortran with MPI parallelisation. After a POP Audit and two Performance Plans, which analysed various components of BAND, a POP Proof of Concept focussed on improving performance of complex matrix multiplications. The earlier work had determined that for multiplication of small matrices the parallel scaling was limited by underperformance of BLAS/PBLAS routines coupled with a large percentage of time within MPI data transfer. The Proof of Concept identified and implemented a range of improvements, which included overlapping computation with communication, improved use of BLAS which doubled the speed of computation, and reorganising the algorithm to reduce the amount of data communicated via MPI. The optimised subroutine showed four times speed up, compared to the original code, on eight 36-core compute nodes.

zCFD by Zenotech is a density based finite volume and Discontinuous Galerkin (DG) computational fluid dynamics (CFD) solver for steady-state or time-dependent flow simulation. It decomposes domains using unstructured meshes. It is written in Python and C++ and parallelised with OpenMP and MPI. An initial Performance Audit using Intel's VTune Amplifier performance profiler identified several areas of potential improvement, which Zenotech went on to address in a POP Proof-of-Concept (PoC) study. As a result of the PoC, zCFD ran 3x faster on a representative input case.

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P2.0 Lightning Talk / Poster presentation

Big data, not astronomical, but genomical: the joint journey from wet-lab to HPC

Boštjan Murovec[a], Leon Deutsch[b], Heribert Insam[c], Hermann Schwärzler[d], Michael Fink[d], Johann Messner[e] and Blaž Stres[b,c,f,g,h]

[a] *Laboratory for Machine Intelligence, Faculty of Electrical Engineering, University of Ljubljana, Slovenia*
[b] *Department of Animal Science, Biotechnical Faculty, University of Ljubljana, Ljubljana, Slovenia*
[c] *Department of Microbiology, Institute of Microbiology, Leopold–Franzens–University, Innsbruck, Austria*
[d] *ZID, Leopold–Franzens–University, Innsbruck, Austria*
[e] *ZID, Johannes–Kepler–University Linz, Austria*
[f] *Center for Clinical Neurophysiology, Faculty of Medicine, University of Ljubljana, Slovenia*
[g] *Institute of Sanitary Engineering, Faculty of Civil and Geodetic Engineering, University of Ljubljana, Slovenia*
[h] *Department for Automation, Biocybernetics and Robotics, Jozef Štefan Institute, Ljubljana, Slovenia*

The Big Data triplet, astronomy, YouTube and Twitter are projected to be severely outcompeted by genomics data in the next 20 years in terms of data acquisition, storage, distribution and analysis. While the former three terms are related to the project capacity, experimental setup diversity and internet infrastructure, the analysis part is one of the key points that are being proven to be critical on a daily basis. The initial steps towards alleviation of the computational problems in the field of the microbial genomics, were taken in 2009, by the introduction of the mothur program [1] within which we helped integrate many of the existing routines and stand–alone programs into a unified platform for massive data quality control, integration, filtration, analysis, statistical evaluation and interpretation in the relevant context of medical and environmental microbiology. The need for a more unified view led us to perform a meta–analysis of datasets relevant for Apple Replant Desease [2] where the need to be able to jointly analyze large sets of data led us to adopt HPC (Mach) at Leopold–Franzens–University and Johannes–Kepler–University. Within this collaboration with HPC administrators and their active help and support was the learning curve overcome at both sides to a production level that enabled us to move from relatively well prepared C++ programs for HPC, to the use of Singularity and the creation of Singularity image type of integrated programs, such as our most recently published program Metagenome–Assembled Genomes Orchestra (MAGO) [3]. MAGO is an open–source software released as a Singularity and Docker container for running it on HPCs and a commodity hardware, and as virtual machine for its use in both research and teaching of genomics and molecular evolution. The introduction of these approaches and the integration of data science into graduate, undergraduate and high–school teaching enables training of the next generations of computational biologists, bioinformaticians, computer scientists and engineers. Currently we are implementing a Singularity integration of state–of–the–art tools from bioBakery branch [`http://huttenhower.sph.harvard.edu/biobakery`] for routine large scale use at HPC Leo3e, Leo4 and Mach2, for researchers and students alike.

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P2.0 Lightning Talk / Poster presentation

Massive parallel and scalable enumeration of minimal metabolic pathways in metabolic networks

Bianca Allegra Buchner[a,b] **and Jürgen Zanghellini**[a,b]

[a] *University of Natural Resources and Life Sciences, Vienna, Austria, EU*
[b] *Austrian Centre of Industrial Biotechnology, Vienna, Austria, EU*

Introduction: The (mathematical) characterization of cellular metabolism by minimal metabolic pathways is a key problem in systems biology. These pathways are also known as elementary flux modes (EFMs). EFMs are minimal sets of reactions that represent unique biological pathways in a metabolic network. In fact, all feasible steady-state phenotypes can be described as a non-negative superposition of elementary pathways. This ability to unbiasedly express the full capabilities of metabolic networks makes EFM analysis a powerful tool. However, the enumeration of unique metabolic pathways in typical genome-scale metabolic models remains currently intractable, as the number of EFMs in a metabolic network explodes combinatorically with its size. This in turn causes an explosion in the memory demand of the current standard algorithm, the double description method (`DDM`), for the enumeration of EFMs.
Methods: However, here we present a fresh take on this old problem: We show that the enumeration of EFMs, contrary to common doctrine, is also possible with reverse search-based methods. Mathematically, the problem of EFM determination is identical with the enumeration of corners and edges in a polyhedron for which two approaches, the `DDM` and the lexicographic reverse search (lrs), have proven particularly useful. We examined and compared two different implementations (`efmtool` [1] and `mplrs` [2]) of these algorithms with respect to their computational performance and their suitability for systems biology applications.
Results: By making use of a parallelized lexicographic reverse search, we show that the EFM enumeration in metabolic networks is almost embarrassingly parallel, strongly scalable and requires negligible memory resources. Thus, EFM enumeration is no longer memory limited, but rather limited by the numbers of available parallel central processing units. We apply `mplrs` to the analysis of a genome-scale metabolic model of *JCVI-syn3.0* [3]. *JCVI-syn3.0* is the first minimal synthetic bacterial cell. We find more than 23 billion elementary flux modes, indicating a surprising metabolic variability despite the cell's minimallity.
Discussion/Conclusion: Although a complete enumeration of EFMs in (large) genome-scale metabolic models remains out of reach, we show that, due to its low memory requirement and the ideal scaling behavior, `mplrs` together with efficient compression methods is an attractive alternative to current standard tools like the `efmtool`. Thus, for the first time an unbiased analysis of alternate optima in flux-balance applications becomes possible in actual research practice.

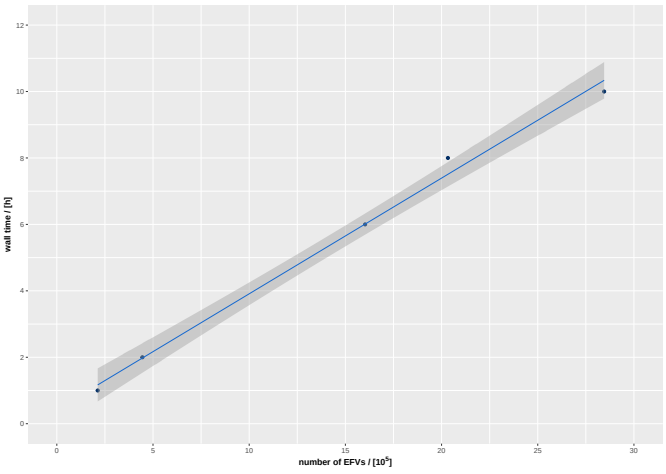

Fig. 1: Analysis of the scaling behavior of the mplrs algorithm as a function of wall time and number of threads taken for an EFM analysis of *JCVI-syn3.0*.

References

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P2.0 Lightning Talk / Poster presentation

Estimating cellular robustness via recursive enumeration of lethal interventions in genome-scale metabolic models

Julian Libiseller-Egger[a,b], Matthias Gerstl[a], Jürgen Zanghellini[a,b]

[a] *Austrian Centre of Industrial Biotechnology, Vienna, Austria*
[b] *University of Natural Resources and Life Sciences, Vienna, Austria*

Robustness is the ability to maintain functionality in spite of perturbations. An accurate quantification, however, remains elusive – especially in biological systems. We address this issue by borrowing ideas developed in safety and reliability engineering and applying them to the study of cellular metabolism.
In analogy to fault tree analysis [1] we count all cut sets (i.e. sets of deleted reactions) up to some fixed cardinality d_0 that disable cellular growth in a metabolic network made up of r reactions in order to quantify its intrinsic probability of failure. To find the total number of these lethal cut sets in a genome-scale metabolic network we first determine all low-cardinality ($d_{\mathrm{MCS}} \leq d_{\mathrm{MCS,\,max}}$) minimal cut sets (MCS; cut sets that are only disruptive if all respective reactions are knocked-out). Then, we enumerate the union of all their supersets with cardinalities $d \leq d_0$ using the inclusion-exclusion principle. Computationally, this means that we need to iterate over the power set of tens of thousands of MCSs and sum up the respective number of lethal higher-cardinality cut sets given by $\binom{r-d}{d_0-d}$.
Our previous implementation [2] already effectively minimized the number of recursions by skipping unions that had been encountered by the algorithm in earlier iterations or that only contained a single extra reaction. However, even on HPC infrastructure the program was not able to regard supersets with cardinalities considerably larger than $d_{\mathrm{MCS,\,max}}$.

Here we present a novel approach capable of handling $d_0 \gg d_{\mathrm{MCS,\,max}}$ for medium-sized networks essentially implementing an inclusion-exclusion approximation using Bonferroni inequalities [3]. We show that increasing d_0 beyond $d_{\mathrm{MCS,\,max}}$ allows for estimating cellular robustness with substantially higher accuracy given the same number of MCS (**Fig. 1**). Equivalently, knowledge of considerably fewer MCS is sufficient to achieve negligible error rates. Since the enumeration of MCS is a computationally expensive MIP problem, this enables us to apply our method to genome-scale models of mammalian cells (e.g. cancer), which have been intractable before.
Biologically, preliminary results of our analysis indicate that structural robustness in microorganisms is not evolutionary selected for, but rather arises as a by-product of the ability to proliferate in multiple growth environments. Results for cancer of various tissue types are pending.

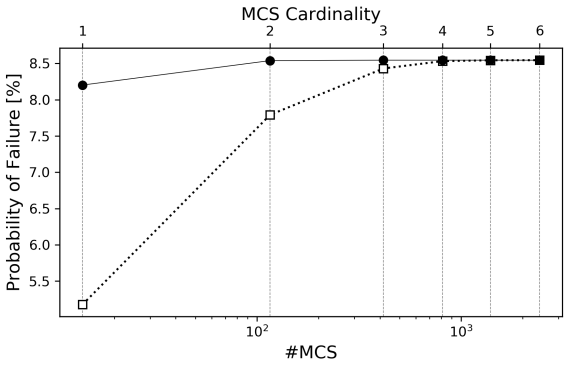

Fig. 1: Probability of failure vs. number of MCS used in calculation and $d_{\mathrm{MCS,\,max}}$ for a model of *E. coli*'s core metabolism ($d_0 = 20$): The previous implementation (empty squares, dotted line) needs to consider MCS with higher cardinalities (which are more numerous) to converge compared to the new approach (filled circles, solid line).

References

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P2.0 Lightning Talk / Poster presentation

Improved Cartesian Topology Mapping in MPI

Markus Lehr, Konrad von Kirchbach

markus.lehr@tuwien.ac.at, konradvonkirchbach@gmail.com
TU Wien, Faculty of Informatics, Institute of Computer Engineering 191-4

Many High Performance Computing (HPC) problems and algorithms are structured as d-dimensional Cartesian grids. Often the desired communication follows some structural patterns, such as stencils. This means that processes communicate with other processes along fixed relative offsets within the given d-dimensional grid. Examples for such patterns can be found in the field of Computer Graphics, such as edge detection filters or in various iterative methods for solving linear systems, such as Jacobi- or Gauss-Seidel stencils.

The Message Passing Interface (MPI) offers some functionality to support such communication, as well as an interface to allow for process remapping, however, current implementations do not leverage these possibilities. Gropp [1] recently presented an overview over some systems and whether they utilize the process remapping features of the `MPI_Cart_create` function. Unfortunately he observed that none of the surveyed systems currently leverage the remapping feature.

In his work, Gropp proposes a mapping algorithm, based on the assumption that communication within a computation-node is faster than between nodes over the network. While his approach of mapping physical processes to vertices in the Cartesian grid yields promising results, it does not take different stencil patterns into consideration nor does it work for heterogeneous node sizes. Furthermore, the quality of Gropp's algorithm depends on the result of a prime factorization and can become arbitrarily bad for some instances.

Lehr's focus is on eliminating the restricted applicability of Gropp's approach, by allowing for heterogeneously sized computation nodes (see Fig. 1 for an example), while still working for different stencils. All three of his presented algorithms work under these conditions and offer bounds wrt. the quality of the solutions. In addition to these algorithms' flexibility, experimental results on our cluster show that for many homogeneous instances, Gropp's algorithm can be outperformed by all three approaches.

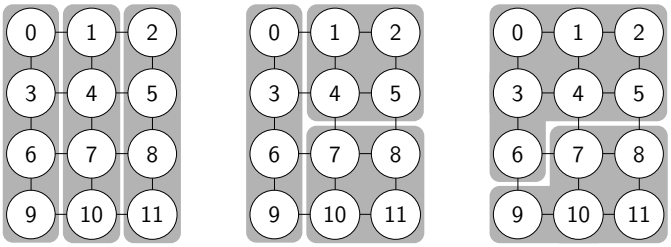

Fig. 1: Three different process assignments on a 3×4 Cartesian grid. Gropp (left) is restricted to equal shaped rectangles; von Kirchbach's (middle) improved partitioning; Lehr's mapping (right) with two different node sizes.

von Kirchbach improves on the idea of Gropp, by explicitly taking the communication pattern into account, while assigning processes to the vertices of the Cartesian grid. By extracting the overall preferred communication pattern along the dimensions, he can recursively bipartition the Cartesian grid such that the communication between partitions and thus between the computation nodes is reduced. He compared his approach with Gropp's algorithm for several instances and communication patterns on a TU-Wien cluster and could show that he can outperform Gropp on average. Figure 1 shows an improved mapping over Gropp's for a 3×4 Cartesian grid.

References

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P2.0 Lightning Talk / Poster presentation

HPC Infrastructure for Cryo-EM at IST Austria

Janos Kiss, Alois Schlögl, and Stefano Elefante

Institute of Science and Technology Austria, Klosterneuburg, Austria

In 2019 at IST Austria two Cryo-EM microscopes have been installed. These have five camera sensors in total, and they generate several TB of high resolution data daily. In addition to the increased demand in storage, our scientists also need intense HPC resources in form of GPU and CPU compute nodes for selecting the particles from the images and performing 3D reconstruction and remote 3D data visualization. Furthermore, based on feedback from real-time preprocessing, the settings for the image acquisition can be adjusted on the fly. Here we present the IT and HPC infrastructure which was built to support our Cryo-EM groups at IST Austria. In the talk we will focus on BeeGFS parallel storage, and its integration into our campus infrastructure. To compare BeeGFS with existing NFS over IPoIB or NFS over RDMA storage, performance metrics will be shown between the different underlying networks and filesystems.

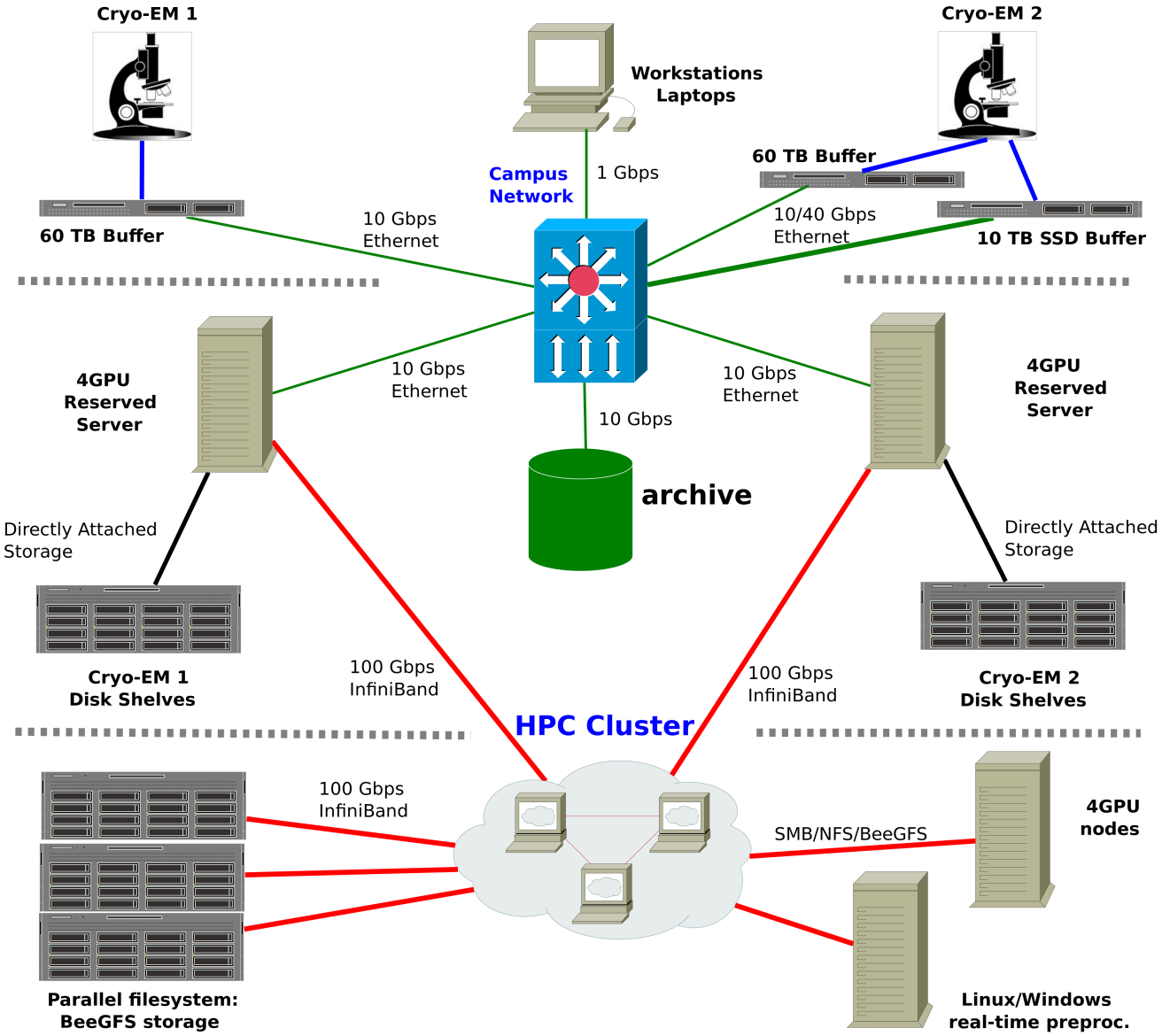

Fig. 1: IT/HPC infrastructure for Cryo-EM data acquisition and analysis at IST Austria.

P2.0 Lightning Talk / Poster presentation

Towards efficient implementation of parquet equations for the 2D Hubbard model: the truncated unity parquet solver

Christian Eckhardt[a,b], Carsten Honerkamp[b], Karsten Held[a], and Anna Kauch[a]

[a] *Institute of Solid State Physics, TU Wien, Vienna, Austria*
[b] *Institute of Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany*

Background: The parquet equations are exact equations that relate one- and two-particle correlation functions in systems of interacting particles. By iterating the equations with a known input called the fully irreducible vertex Λ one can calculate one- and two-particle response functions of the system, such as spectral function or susceptibility. The vertex Λ is in general not known exactly and has to be approximated by its local part or by the Coulomb interaction.

Motivation: The diagrams contributing to different scattering channels (particle-particle, particle-hole and particle-hole transversal) are treated equally, therefore competition between different fluctuations can be reliably studied, e.g. the competition between magnetic, charge and pairing fluctuations that is important for cuprate superconductors. Moreover, the results are obtained through iterative computation of different diagrammatic contributions, which allows for analysis what type of diagrams are important for a given phenomenon and consequently to identify contributions of different electronic processes to e.g. optical conductivitv [1].

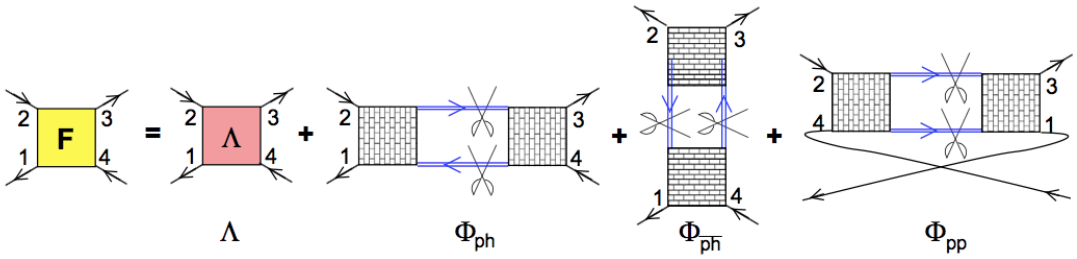

Fig. 1: Diagrammatic visualisation of the parquet decomposition: the connected part of two-particle Green's function contains a vertex F that is composed of diagrams of different types, or in other words belonging to different channels: particle-hole (ph), particle-hole transversal ($\overline{ph}$) and particle-particle (pp).

Challenge: The two-particle functions need to be stored in memory. They depend on energy and momenta of two incoming and two outgoing lines. Even taking into account momentum and energy conservation, it means three momenta and three frequencies for each vertex plus additionally spin and orbital indices. The frequencies are discrete (Matsubara frequencies) and their number depends on the temperature at which we do computations. The size of the vertex for the electronic 2D Hubbard model at room temperature for a momentum grid of 8×8 reaches several TB. The goal is to reach much lower temperature.

Implementations: The direct implementation in momenta and frequencies, the *victory* code [2] uses MPI parallelisation and the memory needed is distributed between the nodes. The disadvantage is the need of massive MPI communication which becomes the bottleneck of the computation. The new TUPS implementation [3] approximates the momentum dependence by using truncated unities. This results in much smaller vertices and removes the communication bottleneck.

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Exploiting Multi-lane Communication in MPI Collectives

Jesper Larsson Träff

TU Wien, Faculty of Informatics, Institute of Computer Engineering 191-4

Many modern HPC systems increase the cumulated node communication bandwidth by offering more than a single network, and/or by having multiple connections to the network, such that the total node bandwidth cannot be saturated by a single processor-core. We call systems with such properties *multi-lane*. An example is the current VSC-3 system (`http://vsc.ac.at`) with dual-socket processors connected to two InfiniBand networks. Important questions for application programmers are a) whether multi-lane capabilities can be exploited at the user-level with MPI communication (point-to-point), and b) whether the MPI collectives can and do take advantage of multi-lane communication.

Simple MPI benchmarks indicate that with full compute nodes, the VSC-3 system can double the node bandwidth when the total amount of data to be sent and received from each node is divided across the MPI processes (p is the number of MPI processes, N the number of nodes, n the number of processes per node, and k the number of processes across which c `MPI_INT`s are divided; average and best time seen are given):

k	n	N	p	c	avg (μs)	min (μs)
1	16	100	1600	160000	20113.76	17813.92
2	16	100	1600	160000	17986.01	17208.10
4	16	100	1600	160000	17874.13	17185.93
8	16	100	1600	160000	17578.57	17155.17
16	16	100	1600	160000	15105.55	8939.98

We give socalled *full-lane* implementations for all regular MPI collectives (broadcast, reduce, allreduce, allgather, etc.) following a common algorithm scheme. Extensive benchmarks indicate that collectives can be implemented to take advantage of multi-lane communication, *and* that many of the collectives in the Intel MPI library *do not*, with significant room for improvement:

BcastLane Implementation					
n	N	p	c	avg (μs)	min (μs)
16	100	1600	16	36.12	22.89
16	100	1600	160	37.78	25.99
16	100	1600	1600	41.01	34.09
16	100	1600	16000	159.20	131.13
16	100	1600	160000	1153.00	987.05
16	100	1600	1600000	15441.33	13645.17
Intel MPI/2018 `MPI_Bcast`					
n	N	p	c	avg	min
16	100	1600	16	23.45	15.02
16	100	1600	160	27.14	20.98
16	100	1600	1600	95.41	61.04
16	100	1600	16000	565.84	535.96
16	100	1600	160000	6917.56	6739.14
16	100	1600	1600000	17362.81	16095.88

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Friction factor scaling and superstructures in pipes: an example of how HPC can help us settle a long standing debate

Jose M. Lopez, Davide Scarselli and Björn Hof

Institute of Science and Technology Austria, Klosterneuburg, Austria

The functional form for the scaling of friction in pipes has been a matter of contention for over a century. The commonly accepted view is that friction follows a logarithmic scaling on the Reynolds number (Re) which is theoretically derived from the so called 'law of the wall'. Experimental evidence however seems to suggest that friction first follows power law behavior and subsequently deviates progressively from this scaling as Re increases. The lack of theoretical backing for the empirical power law, as well as the absence of arguments to explain the subsequent scaling transition, has led to a growing consensus that the power law is simply a good fit of the logarithmic law at low-to-moderate Re. Nevertheless, since the power law and the logarithm differ by less than 2% at these Re, methodological issues have so far prevented from a successful verification of these scalings.

By performing massive parallel simulations of the governing equations based on high order numerical schemes, we could for the first time tackle successfully this problem. I will show that, instead of the presumed logarithmic dependence, the scaling of friction in pipes at low-to-moderate Re precisely follows a power law over nearly two decades in Re, and it only deviates towards the logarithmic scaling at high Re. I will also show that such scaling transition is due to a structural variation of turbulence caused by the advent of large scale motions (also called "superstructures"). These structures modify the dynamics near the wall (in the so-called logarithmic layer), leading to sharper velocity gradients and consequently higher friction.

Finally, I will briefly discuss the software used to carry out the simulations, *nsPipe*, an open source code that I co-develop along with several colleagues from German institutions. I will explain the structure of the code, placing emphasis in the parallelization strategy, and will show the results of performance and scalability tests carried out over a range of different HPC platforms.

Large Eddy Simulation of turbulent channel flow past a wall-mounted cube

Ariane Vieira[1], Hendrik Kuhlmann[1], Johann Waringer[2], Carina Zittra[2], Jan Martini[2], Stephan Handschuh[3], Simon Vitecek[4]

[1] *Institute of Fluid Mechanics and Heat Transfer, TU Wien*
[2] *Department of Limnology and Bio-Oceanography, University of Vienna*
[3] *VetCore Facility for Research, Imaging Unit, University of Veterinary Medicine*
[4] *WasserCluster Lunz*

Embedded LES (ELES) methods have been recently employed to simulate the flow past bluff bodies. In this approach, RANS and LES are combined: LES is employed only in the subregion in which the flow needs to be time-resolved, while RANS is applied elsewhere in the domain. Since LES requires realistic turbulent flow fluctuation at the inlet, a synthetic generation of turbulence should be employed to define interface conditions between the RANS and the LES domain. To apply this strategy to a number of problems, the divergence-free synthetic eddy method (DFSEM) [1] can be used to generate a fully developed inlet condition and it is applied to a benchmark LES simulation of the flow past a wall-mounted cube in a channel. Simulations were carried out using OpenFOAM and a Reynolds number $Re = U_b H/\nu = 4 \times 10^4$, based on the bulk velocity U_b and the cube length H (half the channel height). Two subgrid-scale models were used, the regular k equation (subscript R in fig. 1) and the dynamic k equation (subscript D in fig. 1), as well as three different grids, a coarse (A), a fine (B) and a very fine one (C), with 1.6, 2.5 and 3 million grid points, respectively. The DFSEM was fed by data from an independent auxiliary RANS simulation of same channel flow, but without the cube. The Langtry–Menter SST model was used for the RANS simulation. Average streamwise stress profiles at $x/H = 0.5$ are shown in fig. 1 in the symmetry plane. The results agree well with experimental data [2]. Even the coarse-grid simulation well predicts the overall behavior of the Reynolds stress near the top of the cube in a region of strong flow separation. In fig. 2 turbulent structures are visualised by isosurfaces of Q, showing the horseshoe vortex and the strong vortex shedding from the cube's edges.

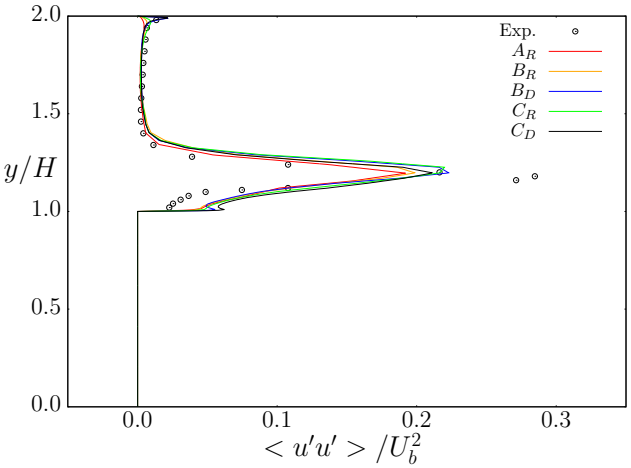

Fig. 1: Average streamwise Reynolds stress at $x/H = 0.5$ in the midplane.

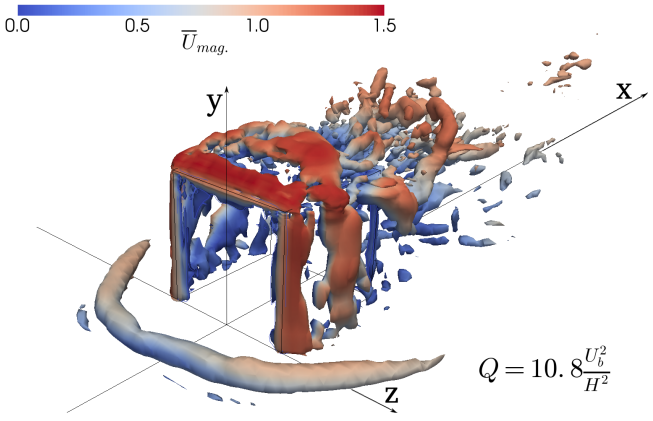

Fig. 2: Global turbulent structure visualized by isosurfaces of $Q = 10.8 U_b^2/H^2$ (Q-criterion).

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Investigation of the apical flow field under left ventricular assist device support

Ghodrati, M.[a,b], Maurer, A. [a,b], Schlöglhofer, T.[a,b,c], Khienwad, T.[a], Moscato, F.[a,b], Zonta, F.[c], Gross C.[a,b,d], Aigner, P.[a,b], Schima, H.[a,b,d]

[a] *Center for Medical Physics and Biomedical Engineering, Medical University of Vienna, Austria,* [a]
[b] *Ludwig Boltzmann Institute for Cardiovascular Research, Vienna, Austria*
[c] *Institute of Fluid Dynamics and Heat Transfer, Technical University of Vienna, Austria*
[d] *Department for Cardiac Surgery, Medical University of Vienna, Austria*

The use of Left Ventricular Assist Devices (LVAD) as a treatment method for heart failure patients has been steadily increasing; however, pathological studies showed presence of thrombi around the HVAD inflow cannula (IC) in more than 95% of patients after device explantation. Flow fields around the IC might trigger thrombus formation and require further investigation. In this study the flow dynamics parameters were evaluated for different patient geometries.

The left ventricular (LV) models of two LVAD patients were obtained by image segmentation of computed tomographic images. The LV volumes of patient 1 (P1) and patient 2 (P2) were 264 cm^3 and 114 cm^3 with the IC angle of 20° and 26° from the mitral-IC tip axis. Transient Computational Fluid Dynamics (CFD) simulations were performed using the laminar model with the pulsatile flow at the mitral annulus over five cardiac cycles. The region of the interest (ROI) was defined from the cannula tip to the wall of the LV apex. Mean velocity magnitude and blood stagnation areas at the ROI (volume with mean velocity <5mm/s) as well as the Wall Shear Stress (WSS) at the IC surface were calculated.

Higher apical velocities were seen for the patient with large LV (mean velocity P1: 1.1, P2: 0.2 cm/s). Larger stagnation volumes were observed for the patient with small LV (P1: 0.4, P2: 1.9 cm 3). Lower shear stresses at the cannula surface were seen for the patient with small LV (P1: 0.09, P2: 0.02 Pa) leading to an attachment of stagnant blood to the whole IC surface.

Flow fields around an LVAD cannula can be influenced by many parameters such as LV size and IC angle. Careful consideration of influencing parameters is essential to get reliable evaluations of the apical flow field and its connection to apical thrombus formation.

araDeepopsis: A Transfer Learning Approach to Plant Phenotyping

Patrick Hüther, Niklas Schandry and Claude Becker

Gregor Mendel Institute of Molecular Plant Biology
Austrian Academy of Sciences
Vienna BioCenter, 1030 Vienna, Austria

In the field of plant biology, the advent of new sequencing technologies has led to a plethora of plant genome resources available to the scientific community. While panels such as 1001-Genomes project [1] in *Arabidopsis thaliana* or the 3000-Rice-Genomes project provide extensive genotype information, a severe bottleneck currently is to collect high-throughput phenotype measurements. A major challenge lies in maximizing the accuracy of such measurements, while at the same time retaining as many data points as possible, in order to faithfully relate phenotype and genotype. Existing methods for (semi-)automated plant phenotyping are often image-based and have limitations when it comes to throughput, scalability, or robustness towards changes in conditions during image acquisition. As these methods often rely on color channel information, they are very sensitive to changes in illumination, plant color, or background configuration.

Here, we present *araDeepopsis*, an open-source tool that allows robust and versatile measurement of phenotypic traits from image data using a transfer learning approach. *araDeepopsis* is built upon the publicly available convolutional neural network (CNN) DeepLabv3+ [2] implemented in tensorflow and is able to efficiently assess plant phenotypes by semantic image segmentation. Efficient training of such a model however requires substantial compute resources and is heavily dependent on the availability of Graphics Processing Units (GPUs). Using the CLIP Batch environment, a novel SLURM cluster available at the Vienna BioCenter, we trained the model asynchronously by implementing between graph-replication across 4 GPU nodes with NVIDIA Tesla V100 GPUs per node, which enabled time-efficient training for 65.000 iterations.

We show how the deep learning model, in combination with scikit-image [3], can extract biologically relevant phenotypic traits from images, independent of phenotyping platform, background, plant health and developmental stage. For *Arabidopsis thaliana* rosettes, *araDeepopsis* reached a segmentation accuracy of 97% measured as mean intersection over Union (mIoU) after training on only 300 manually annotated images. Because of its open-source character and robust training on small training sets, users can expand *araDeepopsis* to their preferred plant species or phenotype with little time investment or prior knowledge.

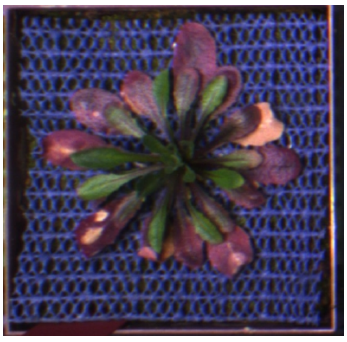

Fig. 1: Plant phenotype.

Fig. 2: CNN prediction

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Keynote Talk:

Cryo-EM of membrane-embedded molecular machines

Leonid Sazanov

Institute of Science and Technology Austria, 3400 Klosterneuberg, Austria

Membrane proteins are responsible for many fundamental cellular processes including the transport of ions and metabolites, energy conversion and signal transduction. Many of these proteins work as molecular machines, employing large-scale motions to perform their function. We are interested in the structure and function of such machines, mainly from the domain of bioenergetics (i.e. biological energy conversion, such as in respiration and photosynthesis).

Respiratory chain of mitochondria and bacteria, responsible for most of energy production in the cell, comprises a series of molecular machines (complexes I-V) working in concert to produce ATP (universal biological energy carrier). Recently we have determined the first atomic structures of complex I [1], complex V [2] and transhydrogenase [3] (regulator of mitochondria) using new cryo-electron microscopy methods. Each new structure brings a lot of surprises, showing nature's ingenuity in efficiently implementing different pathways necessary for life.

Previously we performed data collection at various facilities around Europe, but this year IST inaugurated the installation of the latest top-of-the-range electron microscopes, including Titan Krios, allowing in house data collection and significantly increasing our throughput. These microscopes can produce several terabytes of data per day, creating challenges for data storage, access and backup. On average each cryo-EM research group requires 200 TB of fast access data and about the same amount for archiving. We use single particle data analysis in order to calculate high resolution density maps, allowing us to build atomic models. This workflow requires constant and fast access to many processing nodes, mostly about 4 GPU cards-based but in some cases requiring 200-300 CPUs per job as well. I will discuss our experience in implementing these data intensive cryo-EM workflows on IST Austria high performance computing cluster.

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CV: Leonid Sazanov is a Professor leading the research group "Structural Biology of Membrane Protein Complexes" at the Institute of Science and Technology Austria. He uses cryo-electron microscopy and X-ray crystallography to study structure and mechanism of membrane-embedded molecular machines from the domain of bioenergetics. His group solved the first atomic structures of bacterial and mammalian respiratory complex I, V/A-type ATPase and proton-translocating transhydrogenase. Leonid was born in Belarus, studied Biophysics at Belarus State University, obtained PhD in Biophysics from Moscow State University in Russia, and performed research in UK at the University of Birmingham, Imperial College London and MRC Laboratory of Molecular Biology in Cambridge. Since 2000 he was a group leader in the MRC Mitochondrial Biology Unit in Cambridge and came to IST in 2015. Leonid is a member of EMBO (European Molecular Biology Organisation) and a Fellow of the Royal Society.

cryoSPARC (Live) on HPC systems

Ümit Seren, Erich Birngruber, Petar Jager and Klaus Rembart

Vienna Bio Center (VBC)

In 2017, the Nobel Prize for chemistry was awarded to Jacques Dubochet, Joachim Frank and Richard Henderson "for developing cryo-electron microscopy (cryo-EM) for the high-resolution structure determination of biomolecules in solution". Cryo-EM is a state of the art electron microscopy (EM) technique applied on samples cooled to cryogenic temperatures and has a lot of potential in drug discovery.

Low Dose Transmission Electron Microscopes (TEM) used in cryo-EM produce terabytes of low contrast and noisy two-dimensional (2D) images. To reconstruct 3D structures, various computational image processing techniques have to be applied [1]. The image analysis requires significant computational resources and can be accelerated using modern Graphics processing units (GPUs), which represents a good fit for modern HPC systems. However, most researchers working in the field of cryo-EM are not computer science experts. In recent years, the cryo-EM community has developed user friendly software tools (EMAN2, Relion, cryoSPARC) to help researchers carry out the image processing using HPC systems.

One of these software tools is cryoSPARC/cryoSPARC Live [2], an integrated platform to power high-throughput single particle cryo-EM workflows. According to its own mission statement, cryoSPARC is a user friendly web-based platform that requires no computational expertise from the user side and integrates well with any computational hardware ranging from workstations, servers to clusters.

We will demonstrate how we have integrated cryoSPARC into our SLURM based CLIP batch environment (CBE) at the Vienna Biocenter and replaced the various custom and manually managed setups on user workstations. The presentation will focus on the good and bad parts of the software stack as well as the challenges in the integration with the SLURM cluster, user authentication and filesystem access. We will also demonstrate our automated system to deploy cryoSPARC and cryoSPARC Live and onboard new users. Furthermore, we outline potential improvements to the software that would ease the integration with a batch scheduling system in the future.

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HPC usage in cryo-electron tomography

Florian Fäßler, Martin Obr, Florian K. M. Schur

Institute of Science and Technology Austria, Klosterneuburg, Austria

We aim for a quantitative and qualitative structural description of selected biological specimens (virus structures and the ultrastructure of the cellular actin cytoskeleton) using cryo-electron tomography (cryo-ET) and image processing methods. In the standard cryo-ET workflow, the specimen is tilted within the electron microscope across a specified range (-60 to 60 degree) and projection images are acquired every other degree with a direct electron detector. The resulting tilt-series then has to be carefully aligned in order to reconstruct a 3D representation (a tomogram) of the imaged objects via a weighted back-projection algorithm. Features of interest within tomograms can then be quantitively analyzed via segmentation, followed by subsequent modeling of their spatial distribution. Manual segmentation of a single tomogram can take several days and is thus a major bottleneck within the workflow. To overcome this, we have integrated a convolutional neural network (CNN) approach to facilitate the annotation of features. Alternatively, subtomogram averaging allows us to obtain higher-resolution structures of specific proteins within a tomographic data set. For this, boxes containing identical features are extracted, aligned and averaged to generate a coulomb potential density map of the protein of interest. Challenges in this workflow are manifold (i.e. low signal-to-noise ratio, large data sets, no established pipeline) and includes different computational resources, which are most efficiently provided in a HPC environment:

1) Data acquisition and pre-processing: Our direct electron detector in normal counting mode produces 24-megapixel images and is read out at 10 fps. Projection images need to be subsequently processed and cleaned. During and after tomogram reconstruction, subtomogram extraction, modeling, etc. smaller computational steps are required to be performed in parallel for the whole data set.

2) Tomogram reconstruction: During the reconstruction of tomograms several TBs of temporary data (with individual files reaching up to 160 GBs) are created. Cluster storage and individual nodes require sufficient memory. These steps are performed in parallel for all data and can require up to 60 CPUs.

3) Template matching: Analysis of a down-sampled tomogram (to reduce file size and search space) to detect features of interest via template matching requires roughly 48 hours on 4 CPUs. Data sets can contain more than 100 tomograms and need to be processed in parallel.

4) Subtomogram averaging: This includes a 6-dimensional search (3 rotations and 3 translations) to achieve correlation between subvolumes that need to be averaged, a step for which efficient parallel GPU computing can be employed.

5) CNN assisted segmentation: The 3-dimensionality of our data requires the neural network approach to take the information of several Z-layer into account, which scales with the requirement of available GPU memory.

6) Data visualization: To allow several users to simultaneously process data and the visual inspection of 3D volumes, a dedicated visualization node using VirtualGL is employed. This avoids extensive data transfer from the HPC storage to individual workstations.

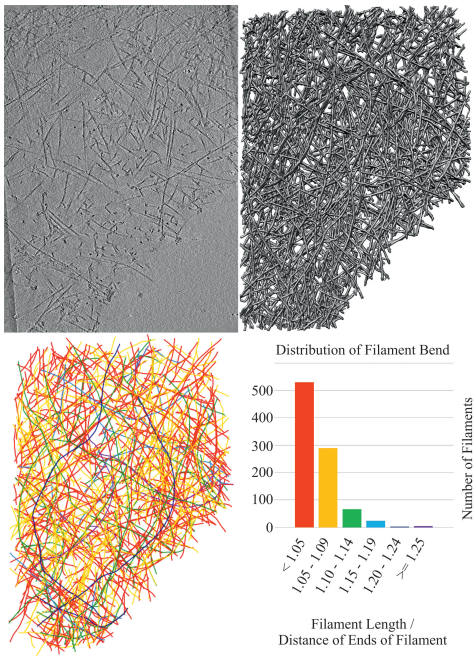

Figure 1: Example data from cryo-ET of cellular samples: Slice through a tomogram of a branched actin network. Actin density has been segmented via a neural network approach. Filaments have been sorted and annotated according to their overall bend.

Celerity — High-Level Distributed Accelerator C++ Programming

Philipp Gschwandtner, Philip Salzmann, Peter Thoman, and Thomas Fahringer

University of Innsbruck, Austria

Reflecting recent developments in HPC, end-users such as domain scientists are turning to design, develop, and run their applications on heterogeneous clusters in order to tackle growing application workloads and exploit the performance potential offered by accelerators. Evidence is provided by the fact that more than half of the current top 50 supercomputers worldwide are equipped with accelerators of some sort. However, there is a lack of programming models featuring a separation of concerns, yet retaining the flexibility required to support multiple domains. It is our belief that domain scientists should be shielded from the complexities of modern heterogeneous hardware architectures, but not be constrained to pre-determined use cases of specific domains.

For this reason we present Celerity, a combined API and task-based runtime system for programming distributed-memory GPU-based HPC hardware platforms. Celerity seeks to provide the means to scale C++ applications to distributed-memory accelerator clusters with relative ease by leveraging the SYCL domain-specific embedded language. At its core, Celerity allows users to transparently execute parallel kernels over dense 1-, 2- and 3-dimensional buffers on an arbitrary number of GPUs.

By providing information about the logical and spatial buffer access behavior of kernels, users enable the Celerity runtime system to automatically split work across multiple GPUs. Encoded in an execution graph, correctness of the distributed program is ensured by tracking kernel data dependencies and issuing data transfers when required. This flexible design facilitates the effective utilization of hardware resources without the need for manual scheduling.

```
celerity::distr_queue queue;

celerity::buffer<float, 2> buf_a(in_a,sycl::range<2>(512, 512));
celerity::buffer<float, 2> buf_b(in_b,sycl::range<2>(512, 512));
celerity::buffer<float, 2> buf_c(sycl::range<2>(512, 512));

queue.submit([=](celerity::handler& cgh) {
  auto one_to_one = celerity::access::one_to_one<2>();
  auto r_a = buf_a.get_access<acc::read>(cgh, one_to_one);
  auto r_b = buf_b.get_access<acc::read>(cgh, one_to_one);
  auto w_c = buf_c.get_access<acc::write>(cgh, one_to_one);
  cgh.parallel_for<class MyMatrixAdd>(sycl::range<2>(512, 512),
    [=](sycl::item<2> itm) {
      w_c[itm] = r_a[itm] + r_b[itm];
    });
});
```

Fig. 1: A simple matrix addition using the Celerity API.

To further increase productivity, Celerity provides an easy-to-use API intended to offer frequently-encountered higher-order parallel programming patterns such as reductions, stencils and parallel I/O. We believe this programming model enables domain scientists to express their applications on a high level of abstraction while retaining the performance benefits offered by accelerator-specific distributed-memory implementations. A fully-functional prototype implementation was developed at UIBK and is currently used for porting domain science applications to accelerator clusters. This talk describes the Celerity programming model and presents first results produced by our framework. Additionally, the way Celerity facilitates hurdle-free porting of existing SYCL applications to distributed memory clusters will be outlined.

References

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A Multilevel Algorithm for Hierarchical Process Mapping

Marcelo Fonseca Faraj[a] **and Christian Schulz**[a]

[a] *University of Vienna, Faculty of Computer Science, Vienna, Austria*

As high-performance computing (HPC) systems expand their processing power, there is also a growth regarding number of components, level of parallelism, sophistication of the topology, and complexity to be programmed efficiently. A practical assumption in HPC is that the cores are distributed within a hierarchical topology with fixed cost per exchanged message inside each level of the hierarchy. In particular, each exchanged message is relatively cheap if the communicating cores share the same processor, but it is more and more expensive as the lowest hierarchy level shared by both cores is higher and higher.

Regarding parallel and distributed algorithms, the assignment of processes to physical cores in an HPC system should address two important parameters: (i) imbalance of work between cores; (ii) total cost of communication between cores. The general process mapping problem (GPMP) gives a convenient theoretical description for this assignment. GPMP receives as input a communication graph, a description of the topology, and an allowed imbalance. Nodes represent processes and their weights represent respective running times, edges represent messages and their weights represent respective lengths. Furthermore, the allowed imbalance represents the exceeding running time any core can have in comparison with the average running time by core. The objective of GPMP is to assign each node to a single core respecting the imbalance constraint in order to minimize the total communication cost between cores.

There are two most common approaches to solve GPMP. The *two-phase* approach [1] consists of two consecutive steps: (i) partition the processes among an amount of blocks equal to the number of available cores, respecting the imbalance, in order to minimize the total edge-cut [2]; (ii) perform a one-to-one process mapping to assign each block to a unique core in order to minimize the communication costs. On the other hand, the *integrated* approach consists of tackling GPMP directly, i.e. not decomposed into independent sub-problems.

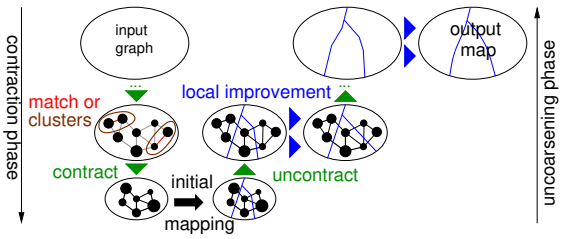

Fig. 1: Multilevel scheme used to solve GPMP.

We engineered all the details of a novel multilevel algorithm to solve GPMP in an integrated way. The general structure of our algorithm is outlined in Fig. 1, and includes: (i) a recursive construction of initial solutions based on bisections throughout the hierarchy of processors; (ii) contraction-uncontraction schemes based on matching or clustering, depending on the type of input graph; (iii) high quality refinement methods such as label propagation, quotient graph refinement, and very localized local searches; (iv) a compressed structure to efficiently compute processor distances without storing a distance matrix; and (v) a sophisticated memory scheme to keep delta-gain updates in order to avoid recomputations of the objective function. After the implementation, we performed a large set of experiments. Preliminary results indicate that our approach produces solutions with higher quality than competing algorithms for all tested instances. For instance, it outperforms Scotch [3] with objective function gains around 60%.

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Coping with Software Complexity: Using the Spack HPC Software Package Manager

Michael Fink

University of Innsbruck, IT Services (ZID)

Installing and maintaining HPC software for a growing and increasingly diverse and demanding user community has become a taxing burden for HPC support teams, calling for automation of software installation to the largest possible extent.

Among various alternatives, Lawrence Livermore's open source *Spack* software package manager [1, 2] is rapidly gaining popularity in HPC sites worldwide. Since its initial release in 2014, the number of software packages supported by Spack has increased to over 3700, to a large extent thanks to contributions by Spack's growing user community.

Spack will, for any requested piece of supported software and for all of its prerequisites, automatically download sources, build and install the program, and create environment module files. Software may be built and installed side by side in differing versions and variants, using various compiler toolchains, MPI implementations, and arbitrary combinations or inclusion/exclusion of individual dependencies. Software packages are described in a highly abstracted manner by Python scripts, resorting on standard methods where possible while allowing explicit handling of special cases where necessary.

Spack not only allows software administrators and users to comfortably deploy and access software on HPC clusters, but it also provides a useful means to automatically install software into containers.

In my talk, I will give a brief overview of functionality and use of Spack and report on first experiences, challenges, and usability questions at the University of Innsbruck HPC systems [3] from the perspective of both software administrators and users.

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Apache Spark is here to stay

Giovanna Roda[a], Lukas Linauer[a], Dieter Kvasnicka[a,b]

[a] *TU Wien, TU.it*
[b] *VSC Research Center*

Spark began as a research project at the UC Berkeley in 2009 and was released to the open source the following year [2]. The aim was to improve and exceed the *MapReduce* computing engine while maintaining its benefits: scalability and fault-tolerance.

MapReduce is a programming paradigm and framework designed to process massive amounts of data on a distributed computing architecture based on a split-apply-combine strategy. While at its core are the customary *mapper* and *reducer* functions from functional programming (similar to the MPI *scatter* and *reduce* operations), MapReduce refers to the whole system responsible of partitioning the input data, scheduling task execution on a cluster and handling failures [1].

One of the main performance bottlenecks of MapReduce is the mapper's output being written to disk. In addition to that, every data transformation requires a new job, which may become costly for complex pipelines. Spark addresses these issues with its fundamental data abstraction: the RDD (Resilient Distributed Dataset).

RDDs are immutable, partitioned collections of records that can be operated on in parallel. Lazy evaluation, as well as in-memory processing of RDDs, are the core features of Spark, that enable it to outperform MapReduce by orders of magnitude.

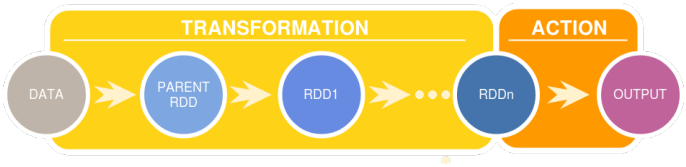

Fig.1: RDD: transformations are evaluated lazily, i.e. they won't be executed until an action is performed.

Born within the Apache Hadoop ecosystem with its standard resource manager YARN (Yet Another Resource Negotiator), Spark can also be deployed as standalone on any cluster, including Kubernetes- and Slurm-managed clusters.

Is Apache Spark here to stay? Spark is a general-purpose tool for distributed computing and thanks to its SQL and Dataframe APIs, as well as libraries for Graph computations and Machine Learning, it is popular among data scientists. Additionally, scientific fields such as bioinformatics, high energy physics, and geosciences increasingly rely on the use of Spark.

Spark is available on the Little Big Data cluster at the TU Wien in a Hadoop environment (864 cores with hyper-threading, `http://lbd.zserv.tuwien.ac.at`), as well as on the High Performance clusters of the Vienna Scientific Cluster (≈ 50000 cores, `http://vsc.ac.at`), where a standalone Spark cluster can readily be launched by a Slurm script that takes care of allocating the necessary resources.

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Keynote Talk:

How Europe is preparing its core solution for Exascale machines and global sovereign, advanced computing platform.

Philippe Notton[a,b]

[a] *European Processor Initiative*
[b] *SiPearl*

Out of the three offers submitted for the European Union's call for proposals, the bid from the consortium coordinated by Bull (Atos Group) - the European Processor Initiative (EPI) - was chosen to design, maintain and implement the roadmap for developing a new generation of high-performance, low-power microprocessors for:

- The high performance computing market and especially supercomputers to support their transition to exascale,
- The autonomous mobility and artificial intelligence markets.

With a total budget of over €120m, the EPI project, which started up on December 1, 2018, will be active through to December 2021. It is currently made up of 27 members, research institutes, universities and supercomputing centres, as well as IT, electronics and automotive specialists.

The European Processor Initiative, laying the foundations for SiPearl, is it's industrial hand.

Philippe Notton will present EPI genesis, scope and progress and how SiPearl will convert EPI from research to production.

CV: Philippe Notton is General Manager of the European Processor Initiative and CEO of SiPearl, the fabless company designing the main EU processor. He received a Dipl. Ing. In Electrical engineering and Signal Processing from Supelec (France, 1993) and an Exec. MBA from Essec (France, 2008) and Mannheim (Germany, 2008). Philippe has more than 20 years of experience in semiconductor including multiple senior exec roles in MStar Semiconductor Taiwan and ST Microelectronics.

Building a national HPC system in Slovenia

Miran ULBIN, Zoran REN

Faculty of Mechanical Engineering, University of Maribor, Maribor, Slovenia

The EU has launched EuroHPC Joint Undertaking initiative plan to build an exa-scale HPC by 2025 [1]. A representative peta-scale HPC system with approx. 10 PFLOP/s computing capability will be built in Maribor, Slovenia, in a concerted effort by the end of 2020. The aim is to establish a national HPC system by own design with low maintenance and power consumption costs. A small prototype HPC system of about 240 TFLOP/s computing capability was first built at the University of Maribor in 2019 to test various combinations of computing nodes and components as well as software solutions. The aim of this effort was to determine the best combinations, which will be integrated into a primary supercomputer built next in year 2020. The architecture of prototype HPC system is unique, built from the off-the-shelf state-of-the-art components, and is operating using the open source system software. The throughput of the latest Infiniband and Ethernet interconnect solutions is of a particular interest due to its significant influence on the architecture of the primary HPC system. The presentation is first focused on architecture of the prototype HPC system consisting of 82 heterogeneous nodes based on double AMD Epyc and Intel Xeon SCL processors in combination with GPU nodes [2], with discussion of possible variations of interconnect configurations. Network configuration of the primary HPC system with approximately 600 computing and GPU accelerated nodes and about 40 PB storage system and its fast connection to the prototype HPC system will be discussed next. Possibilities of open source software for operating, provisioning and maintaining the system, as well as development of several solutions for flexibility and security options for user access [3] will be given in conclusion.

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EuroHPC – Opportunities for the Austrian Scientific Community

Christoph Dellago

Faculty of Physics, University of Vienna

EuroHPC is an initiative of the EU and several European countries, including Austria, with the objective to create a world-class supercomputer ecosystem in Europe. Within this initiative, 1 billion Euro will be invested to install three pre-exascale systems and two exascale systems by 2022/23, to be used by the public and private sector primarily for research purposes. In this presentation, I will give an overview of EuroHPC, paying particular attention to the opportunities arising for the Austrian scientific community. In particular, a national competence center for HPC will be created in Austria, co-funded by the EU and the Austrian government, to support Austrian scientists in making use of the EuroHPC resources. Furthermore, Austria is a member of the Leonardo-Consortium, led by CINECA in Bologna, Italy, which will host one of the three European pre-exascale systems. I will report on the current status of the Austrian effort within EuroHPC and outline future plans.

CyVerse Austria - Computational infrastructure and data management for BioTechMed Graz: services and outlook

Konrad Lang[a], Sarah Stryeck[a], Manfred Stepponat[a], Ursula Winkler[b], David Bodruzic[b], Slave Trajanoski[c], Michael Fladischer[c], David Garcia de Marina Llorente[d], Stefanie Lindstaedt[a,d]

[a] *Graz University of Technology*
[b] *University of Graz*
[c] *Medical University of Graz*
[d] *KNOW-CENTER GmbH Research Center for Data-Driven Business & Big Data Analytics*

CyVerse Austria (CAT) is an extensible platform deployed within the frame of BioTechMed-Graz [1] in order to support life science researchers at Graz University of Technology, University of Graz and Medical University of Graz in data management and complex bioinformatic analyses. CAT is a powerful infrastructure providing data storage, management of HPC resources and APIs, but it also enables usage of existing storage solutions and utilization of available HPC clusters [2,3].

Cyberinfrastructure (also known as CI or computational infrastructure) provides solutions to the challenges of large-scale computational science. In analogy to physical infrastructures such as laboratories making it possible to collect data, the hardware, software, and people that comprise cyberinfrastructure make it possible to store, share, and analyze data. Using cyberinfrastructure, teams of researchers can attempt to answer questions that previously were unapproachable because the computational requirements were too large or too complex.

The infrastructure of CAT includes:

- A data storage facility with the possibility to integrate existing storage facilities
- An interactive, web-based, analytical platform
- Web authentication and security services to allow the usage of existing authentication solutions
- Support for scaling computational algorithms to run on HPCs, also by using existing HPC resources
- Publication of data by issuing persistent identifiers, e.g. Digital Object identifiers (DOI)

CyVerse was originally created by the National Science Foundation in 2008 with the name iPlant Collaborative. From its inception, iPlant quickly grew into a mature organization providing powerful resources and offering scientific and technical support services to researchers nationally and internationally. In 2015, iPlant was rebranded to CyVerse to emphasize an expanded mission to serve all life sciences. In the last years the applicability of CyVerse for other disciplines (e.g. social sciences) has been proven.

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ACOnet - High Performance Networking for R&E in Austria

Christian Panigl

University of Vienna, Austria

ACOnet (www.aco.net) is Austria's National Research and Education Network (NREN) interconnecting science, research & education institutions on the national level and internationally through GÉANT (www.geant.org). In 2017/2018 the ACOnet backbone topology has been redesigned to better support national collaborations between the regions. The next backbone renewal is already due in 2022, therefore feedback and planning input is welcome also from the HPC and research community.

Within its service portfolio, ACOnet also enables its participating institutions to make use of the GÉANT IaaS Cloud Services Framework contracts and of the upcoming OCRE (www.ocre-project.eu) service portfolio.

This talk will give a brief overview of these new opportunities.

Interactive applications on HPC systems

Erich Birngruber, Petar Jager, Klaus Rembart, Ümit Seren

Vienna Biocenter (VBC)

Exploratory data analysis has increased the demand for interactive tools. In the same way, workshops and other teaching events often benefit from immediate and on-demand access to preconfigured, interactive environments.

For low resource requirements these interactive environments can be run on workstations. However, as user count and resource demand increase, these setups become more complex. While these frameworks typically provide good support for cloud based deployments in container orchestrations, it is often preferable to deploy them on existing compute infrastructure that provides access to both software packages and the data to be analysed. The deployment on HPC batch systems specifically brings challenges on how to handle authentication, user identities, and job submissions.

The architecture of these applications can be considered as following the master – minion paradigm in most cases. One central component manages user access and acts as a gateway. It launches one or multiple per-user instances of a compute component, that provides the actual user environment.

We want to demonstrate how we provide applications like Galaxy [1], Jupyterhub [2], RStudio [3] and XPRA [4] to scientists of the Vienna Biocenter. The presentation will focus on the similarities and pitfalls of these deployments. We run the web application gateway based on our standardized container environment. The compute components run as SLURM jobs on the CLIP batch environment (CBE). Specific focus will be placed on the integration of web-based Single-Sign-On, and how we address the management of user identities for starting jobs on the batch system. Source and configuration examples on the specific setup will be provided.

After the operator's perspective, we will pan to the end-users view. Beginners and workshop situations typically prefer a static, pre-configured setup of the user session. Contrary to that, advanced users will want to customize their execution environment as much as possible. We will explore how scientists can tailor the setup to their individual needs.

Finally, we will summarize the different setups of the applications in a high-level comparison from both the operators and the end-users perspective. We wish to start a discussion and exchange experiences of other system operators with regards to both, deploying the applications and acceptance of users.

References

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Open OnDemand – A web-based client portal for the VSC

David Fischak, Elias Wimmer

VSC Research Center, TU Wien

Overview So far, the only way of accessing the VSC systems has been via the good old command line, which requires quite some effort to learn. As of late, Open OnDemand [1], developed mainly at the Ohio Supercomputer Center, offers our users access to all VSC systems via a modern web-based portal. The portal's basic functionality includes a graphical file browser with up- and download capabilities, a job composer app for the creation of batch jobs, a searchable list view of job queues and a web-based command line terminal with the same functionalities as the native shell. Additionally, Open OnDemand is easily extensible especially by users with custom apps.

OPEN OnDemand
https://openondemand.org/

Benefits Besides the default system apps, such as the job composer, users are furthermore enabled to develop their own Open OnDemand apps and to install various 3rd party apps that allow the integration of commonly used scientific software, such as MATLAB or ParaView. A prime example for this is Jupyter, where our users only need a few clicks to start the development of programs in Julia, Python and R in interactive notebooks that run on our clusters. Another promising user-developed app is the Git Manager [2], which allows for a graphical Git versioning workflow. Due to the fact that all these apps run in the user's home directory with no more than user privileges, further security considerations, except for authentication, need not be taken into account. If a user prefers to work with a graphical shell instead of the web-based command line, several desktop environments, such as Gnome or Xfce, can also be launched within the browser. Open OnDemand is developed with a multi-cluster and multi-scheduler environment in mind, whereby users can easily switch between our clusters. Moreover, installable themes allow the customization to include the HPC Center's brand.

VIENNA SCIENTIFIC CLUSTER

TU WIEN

Our very own installation can be found at: `https://ood.vsc.ac.at/`

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IT4Innovations in the EuroHPC era

Branislav Jansik

IT4Innovations, Ostrava, Czech Republic

The talk will introduce the Czech national supercomputing center IT4Innovations, its current technology and scope. Further, the future outlooks will be presented, including the EuroHPC EURO_IT4I petascale machine, its architecture, intended use as well as challenges we are likely to face using future HPC technologies.

Biography: Branislav Jansik has obtained his PhD in computational chemistry at Royal Institute of Technology, Sweden in 2004. He took postdoctoral position at IPCF, CNR, Italy, developing high performance computational methods for molecular optical properties. Since 2006 he worked on development of highly parallel optimization methods in the domain of electronic structure theory at Aarhus University, Denmark. In 2012 he joined IT4Innovations, the Czech national supercomputing center as a head of supercomputing services. At IT4Innovations, he leads the supercomputer procurement, deployment and service operations. He published over 35 papers and co-authored the DALTON electronic structure theory code.

Taking VSC to the next level – Open discussion on VSC-5

Dieter Kvasnicka and Irene Reichl

VSC Research Center, TU Wien

VSC-5 should be a continuation of the successful VSC path providing appropriate resources for researchers from the partner universities. Keeping the application procedure as convenient as possible, researchers across many faculties and research areas enjoy easy access to the hardware, support, HPC consulting, and training. Furthermore, the good mix of small, medium and large projects leads to very high utilization of the cluster.

Due to preliminary information from our key partners concerning funding we expect a system size similar to the predecessor systems, 5-10 M€, including private nodes.

The objective of this session is to identify the requirements of the various groups and to create an understanding for the respective problems and methods. The knowledge gained in this discussion will serve as a valuable basis for the tender. However, there should be enough room to adapt the tender to technological developments over the next few years.

Users' needs may include -among others- maximizing the number of multiply-add operations, easy access to resources, fast availability without long waiting times, a productive development and debugging environment, multiple compatibility requirements, availability of software, huge memory, network connectivity, largest possible space for files, and fast file systems for irregular access patterns. From an administrative point of view, further requirements such as component reliability, homogeneity of the nodes, and continuity with previous systems come into play.

Important components of an HPC system are CPU, network, memory, GPU (or other accelerators), file systems, and infrastructure (electricity, cooling, emergency power, space, reliability, ...). The discussion will focus on the main optimizable costs, primarily determined by the CPU, and secondarily by the network and main memory. Further questions will address the CPU architecture (Intel, AMD, ARM, Power, ...) and type and amount of accelerators.

The discussion approaches active and future users of the VSC systems and aims for finding a balance between large and small projects, as well as between groups that have already expressed their needs in the past and those that have not been sufficiently heard.

Moderation:

Dieter Kvasnicka
Irene Reichl
VSC Research Center, TU Wien

List of participants

Name	Affiliation
Amman, Fabian	IST Austria
Ban, Nikolina	University of Innsbruck
Bartel, Michael	University of Vienna
Beatriz, Vicoso	IST Austria
Bergner, Andreas	Boehringer Ingelheim
Birngruber, Erich	Vienna Biocenter (VBC)
Birringer, Gerald	Boehringer Ingelheim
Blaas-Schenner, Claudia	VSC, TU Wien
Bodruzic, David	Karl-Franzens-Universität Graz
Boresch, Stefan	University of Vienna
Bourgouin, Pierre	CTBTO
Buchner, Bianca Allegra	acib GmbH
Dellago, Christoph	University of Vienna
Elefante, Stefano	IST Austria
Ernstbrunner, Robert	University of Vienna
Fahringer, Thomas	University of Innsbruck
Fäßler, Florian	IST Austria
Fink, Michael	University of Innsbruck
Fischak, David	VSC Research Center
Fischer , Michael H.	University of Vienna
Flicker, Karl	Montanuniversität Leoben
Fonseca Faraj, Marcelo	University of Vienna
Forai, Petar	IMP
Franchetti, Franz	Carnegie Mellon University, PA, USA
Gesek, Georg	Novarion
Ghodrati, Mojgan	Medical University of Vienna
Goldenberg, Florian	University of Vienna
Großöhme , Peter	Megware, Germany
Gschwandtner, Philipp	University of Innsbruck
Haase, Gundolf	University of Graz
Hajek, Andreas	Rittal GmbH
Hashem, Elham	Montanuniversität Leoben
Haunschmid, Ernst	VSC, Tu Wien
Heydemueller, Joerg	Data Direct Networks, Germany
Hickel, Markus	VSC Research Center
Hinsche, Ralph	Nvidia, Germany
Hoefinger, Siegfried	VSC, TU Wien
Höller, Harald	IMS Nanofabrication GmbH
Hunner, Markus	IMS Nanofabrication GmbH
Husinsky, Wolfgang	TU Wien
Hüther, Patrick	IMP
Imbert, David	IMS Nanofabrication GmbH
Jansik, Branislav	IT4Innovation national computing center, Czech Republic
Jodlbauer, Daniel	RICAM, ÖAW
Kashansky, Vladislav	University of Klagenfurt
Kauch, Anna	TU Wien
Kemetmüller, Josef	IMS Nanofabrication GmbH

Name	Affiliation
Kero, Stefan	ATOS
Kiss, Janos	IST Austria
Kopecky, Dieter	Boehringer Ingelheim
Kozubek, Tomas	IT4Innovations, VSB, Czech Republic
Kracher, Christian	University of Vienna
Kvasnicka, Dieter	TU Wien
Langer, Matthias	ZAMG
Langer, Ulrich	Johannes Kepler University
Lang, Konrad	Graz University of Technology
Lehr, Markus	TU Wien
Lengyel, Balázs	VSC
Levonyak, Markus	University of Vienna
Libiseller-Egger, Julian	ACIB
Ligon, Becky	Clemson University, SC, USA
Ligon, Walter B.	Clemson University, SC, USA
Linauer, Lukas	TU Wien
Logar, Bernd	TU Wien
Lopez, Jose Manuel	IST Austria
Lovicar, Ludek	IST Austria
Markevich, Alexander	University of Vienna
Markov, Ilia	IST Austria
Marksteiner, Peter	TU Wien
Mayer, Viktoria	University of Vienna
Mitterecker, Daniel	ZAMG
Moghrabi, Issam	Gulf University for Science and Technology, Kuwait
Necker, Tobias	LMU Munich, Germany
Notton, Philippe	Si Pearl, France
Oppel, Markus	University of Vienna
Ostermann, Alexander	University of Innsbruck
Pachajoa, Carlos	University of Vienna
Pacher, Christina	University of Vienna
Panigl, Christian	University of Vienna
Pfennig, Tobias	Megware, Germany
Povh, Janez	University of Ljubljana,Slovenia
Ramos Vieira, Ariane Neale	TU Wien
Reichl, Irene	VSC Research Center, TU Wien
Rembart, Klaus	IMBA,ÖAW
Ren, Zoran	University of Maribor, Slovenia
Riha, Lubomir	VSB-TU Ostrava, IT4Innovations, Czech Republic
Robinson, Matthew	University of Lausanne, Switzerland
Roda, Giovanna	TU Wien
Schafelner, Andreas	Johannes Kepler University Linz
Schlögl, Alois	IST Austria
Schramm, Matthias	TU Wien
Schuller, Lukas	IMS Nanofabrication GmbH
Schwärzler, Hermann	University of Innsbruck
Seibert, Petra	BOKU
Seren, Ümit	Vienna BioCenter
Stadlbauer, Stephan	IST Austria, Klosterneuburg
Stadler, Bernadett	Johannes Kepler University, Linz
Stanzel, Andreas	Lenovo

Name	Affiliation
Stepponat, Manfred	TU Graz
Störi, Herbert	VSC Research Center, TU Wien
Stres, Blaz	University of Ljubljana, Slovenia
Szczech, Oliver	IST Austria
Tan, Kenneth	Sardina Systems, UK
Tomasch, Andreas	Lenovo
Träff, Jesper Larsson	TU Wien
Tron, Uwe	Lenovo
Truhetz, Heimo	Wegener Center for Climate and Global Change, Graz
Ulbin, Miran	University of Maribor, Slovenia
Uncu, Ali	RICAM ÖAW
Vlcsek, Martin	EDV-Design GmbH
von Kirchbach, Konrad	TU Wien
Wallerberger, Markus	TU Wien
Wang, Yin	University of Innsbruck
Wimmer, Elias	VSC Research Center, TU Wien
Winkler, Ursula	University of Graz
Yoshida, Shuhei	TU Wien
Zabloudil, Jan	VSC, BOKU

Three names are not listed, because usage of the name according to the "General Data Protection Regulation" (GDPR) was not confirmed.

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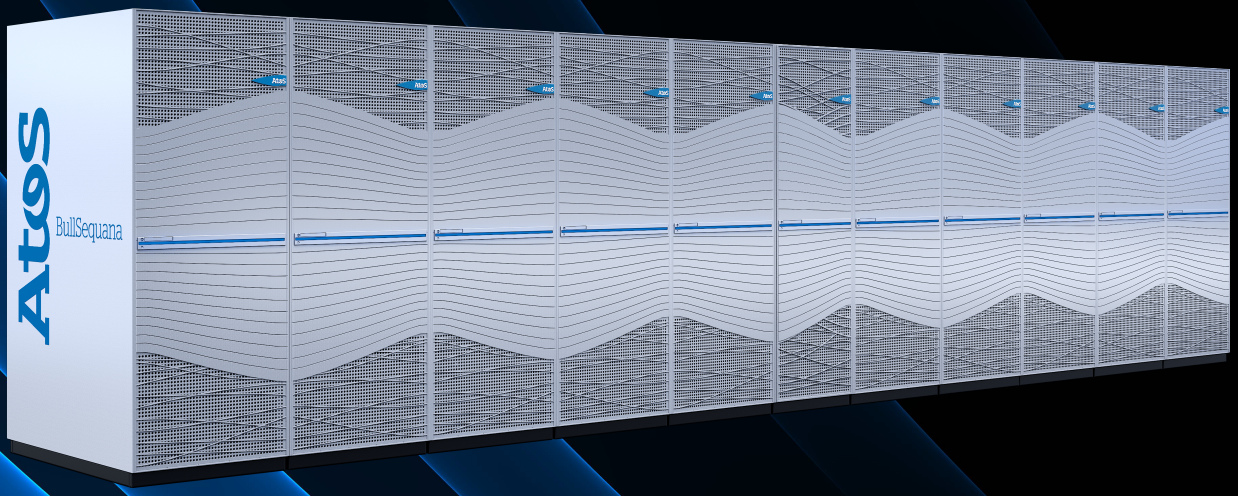

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