Impact and Legacy of PRACE Implementation Phase Projects

Back in 2010, the first PRACE Implementation Phase (PRACE-1IP) project was launched. Recently, in December 2022, the 6th and final PRACE-IP project was completed. These EU-funded projects invested substantial amounts of money (€ 282 million from EU and national funds) and personnel (about 500 active persons from 58 HPC centres and organizations around Europe) to undertake activities such as peer review, organizational, and legal support, dissemination and event organization, training, technology assessments, joint operations, application support, and software solutions for exascale computing. These activities supported and complemented the core offering of the PRACE Research Infrastructure (RI): to offer access to the Tier-0 supercomputers provided by the five hosting members to the benefit of the European HPC ecosystem.

The highlights of the PRACE-IP projects – to mention just a few – include: the first Pre-Commercial Procurement in HPC in Europe; support for the industrial use of HPC through the SME HPC Adoption Programme in Europe (SHAPE); the pioneering collaboration with CERN, SKAO, and GEANT to overcome challenges related to the use of high-performance computing (HPC) and to support large, data-intensive science projects; and the 10 pioneering software solution projects that provided the building blocks for community software for the European pre-exascale and exascale landscape.

In the last decade, PRACE also established a trusting relationship with the HPC user communities. The Scientific Steering Committee (SSC) and the Industrial Advisory Committee (IAC) were founded in order to steer and guide the PRACE RI. The PRACE-IP projects strongly supported the user-driven development of the RI by involving the SSC and IAC in the events (e.g. PRACEdays), publications (e.g. Scientific Case) and software, and user support. With the EuroHPC Joint Undertaking now delivering HPC resources in Europe, PRACE has decided in future to focus on HPC users and HPC centre representation. It will also aim to foster the creation of a European HPC user association for academics, industrial users, and HPC centres. In this new role, PRACE will be an important part in the European HPC ecosystem, giving a voice to users.

Further details can be found on the PRACE website. A historical overview has been published as a timeline.

Contact: Veronica Teodor

JSC@ISC2023

The ISC High Performance 2023 conference will take place from 21 to 25 May in Hamburg, Germany. JSC, together with its partners within the Gauss Centre for Supercomputing (GCS) – HLRS in Stuttgart and LRZ in Garching – will present its wide-ranging supercomputing activities at the GCS booth. The focus will be on topics including the path to exascale with JSC's modular supercomputing architecture (MSA) concept; the steadily increasing importance of AI in HPC, which is reflected by developments such as the Helmholtz AI Cooperation Unit; and quantum computing technologies, with the expanding Jülich UNified Infrastructure for Quantum computing (JUNIQ) being presented.

JSC employees will also contribute to the event with numerous talks, tutorials, and workshops. For example, Estela Suarez will give a keynote presentation entitled "HPC Achievement and Impact – Past and Future". Kristel Michielsen will be part of the ISC Invited Program committee as Track Chair for Quantum Computing. Andreas Herten and Lena Oden will be co-organizing the tutorial "Efficient Distributed GPU Programming for Exascale" together with NVIDIA. In conjunction with the Barcelona Supercomputing Center, Jedrzej Rybicki will present the tutorial entitled "Introduction to the eFlows4HPC Software Stack and HPC Workflows as a Service Methodology". Bernd Mohr and Morris Riedel are organizing the tutorial "Introduction to HPC Applications, Systems, Programming Models and Machine Learning and Data Analytics". Claire Wyatt will be hosting the BoF session "Scientific Software and the People Who Make It Happen: Building Communities of Practice". Estela Suarez will be co-organizing two workshops: the "International Workshop on Smart Networks, Data Processing and Infrastructure Units" and the "2nd

International Workshop on Malleability Techniques Applications in High-Performance Computing". The Jülich "Women in HPC" Chapter JuWinHPC is also involved in the planning of the "ISC 2023 – Diversity Day", which will feature an early career poster session and networking reception.

Detailed information on JSC's participation and activities can be found at https://go.fzj.de/isc23.

Contact: Jens Henrik Göbbert, Michael Bresser

Official Handover of SDL Neuroscience Lead at Joint Lab SMHB General Assembly 2023

After ten successful years, Abigail Morrison officially passed on the role of scientific lead of JSC's Simulation and Data Lab (SDL) Neuroscience to her successor, Sandra Diaz Pier, to the applause of the General Assembly of the Helmholtz Joint Lab Supercomputing and Modeling for the Human Brain (SMHB), which was held from 4 to 5 April 2023 at Forschungszentrum Jülich. Prof. Morrison, who is also a research group leader at the Institute of Neuroscience and Medicine – Computational and Systems Neuroscience (INM-6), had led the SDL Neuroscience since it was founded in 2013 as a core element of the Helmholtz Joint Lab SMHB, which at the time was launched as a Helmholtz Portfolio Theme. Under her scientific guidance, the SDL Neuroscience – a high-level support team for neuroscientists and part of the Bernstein Network Computational Neuroscience – grew continuously in size and scope, and played key roles in strategic projects such as the European Human Brain Project. Innovative in-house developments such as the Arbor simulator and the NESTML modelling language for the NEST simulator were started during Morrison's reign. An area she was particularly committed to was the development of neuromorphic computing technology within the Jülich Advanced Computing Architectures (ACA) project and beyond. Morrison also acted as a supervisor for several PhD, master's, and bachelor's students working in the SDL Neuroscience.

In Dr. Diaz Pier, an experienced member and recognized leader of the SDL Neuroscience team – with a research focus on the meta-optimization of bio-inspired networks – has now taken over the scientific lead of the SDL Neuroscience. JSC would like to sincerely thank Abigail Morrison for her excellent work and commitment over the past decade and wishes her successor Sandra all the best for the future in her new role.

Contact: Dr. Boris Orth

NFDIxCS Project Started

On 1 March 2023, the new National Research Data Infrastructure for and with Computer Science (NFDIxCS) was started. The project is coordinated by the University of Duisburg-Essen (UDE) and funds 17 project members for a period of five years. The main goal of the consortium is to identify, define, and, ultimately, deploy services to store complex domain-specific data objects from the particular variety of sub-domains from computer science (CS) and to comprehensively implement the FAIR principles. This includes producing reusable data objects specific to the various types of CS data, which not only contain these data along with the related metadata, but also the corresponding software, context, and execution information in a standardized format. These data objects can be of any size, structure, or quality.

The key aim of NFDIxCS is to assemble an organizational, technical, cooperative, and inter-operable infrastructure to bring together the relevant services and actors regarding CS. The services developed will be designed for sustainable operation. Among its objectives, NFDIxCS will promote the implementation of the FAIR data principles for CS research data and software artifacts, simplify the citation of software and CS data, and support the application of CS methods such as big data, artificial intelligence, and machine learning in other scientific disciplines. In addition, it will work towards generally accepted standards, in particular for the sustainable storage, retrieval, and availability of CS research data. JSC is contributing to the task areas HPC performance management and data for benchmarking.

Contact: Dr. Bernd Mohr

Destination Earth Use Case to Improve Air Quality Forecasts During Extreme Weather Events

The European Centre for Medium-Range Weather Forecasts (ECMWF) has tasked a team of scientists from IEK-8 and JSC at Forschungszentrum Jülich with developing an interactive air quality forecasting system and an assessment tool for their DestinE digital twin model of the Earth. The scientists are working on a web-based user interface that will provide high-resolution air quality analyses and forecasts based on machine learning methods as well as on the chemistry transport model EURAD-IM, which was developed in collaboration with Forschungszentrum Jülich. The EURAD-IM model has the significant advantage of providing daily forecasts and analyses of air quality in Europe with a horizontal resolution of one kilometre. The machine learning applications and data analysis tools for air quality issues will be integrated into the various components of the digital twin that ECMWF is building on behalf of the European Union. The overall system will be developed with a degree of flexibility, making it possible to test and implement the system's transferability to other European EuroHPC super-computers.

The project – called DE370C – is being developed in cooperation with the German Environment Agency (UBA) and the North Rhine-Westphalia Office of Nature, Environment, and Consumer Protection (LANUV) as core users. It is set to run for 16 months. Destination Earth is an EU-funded initiative and is

being implemented by ECMWF, ESA, and EUMETSAT (see https://www.ecmwf.int/destine for details).

Contact: Sabine Schröder

Whitepaper on Fenix Service Provisioning and Lessons Learned in ICEI

The Interactive Computing E-Infrastructure for the Human Brain Project (ICEI), a "sister project" of the Human Brain Project (HBP) that is building an initial version of the Fenix Research Infrastructure under the umbrella of the HBP, has published the whitepaper "Fenix e-infrastructure service provisioning – lessons learned". After the ICEI project was started five years ago, the ICEI consortium consisting of the five European supercomputing centres – BSC (Spain), CEA (France), CINECA (Italy), CSCS (Switzerland), and JSC (Germany) – and Fenix partners want to share their experience in providing e-infrastructure services to European researchers from different research areas. The whitepaper, which is addressed to e-infrastructure service providers or similar initiatives, provides a summary of current Fenix services, offers statistics on infrastructure users, and concludes with an overview of lessons learned based on the feedback collected from Fenix users as well as the experiences gained and the know-how obtained. It can be downloaded at https://fenix-ri.eu/news/lessons-learned-hpc-services-provisioning.

Contact: Dr. Anne Nahm

JSC Researcher Wins at QHack 2023

Congratulations to Alejandro Montanez-Barrera from JSC for being one of the winners of QHack 2023 with his project "Enhancing Portfolio Optimization Solutions – Wisely Encoding Constrained Combinatorial Optimization Problems on Quantum Devices". QHack is one of the largest hackathons in quantum computing. At this year's event, there were over 2,800 participants from 105 countries, 31 sponsors, and 90 hackathon projects. For more information on QHack 2023, please visit https://pennylane.ai/blog/2023/04/qhack-2023-highlights/.

Alejandro received awards in two categories: he won the Amazon Braket Challenge category for having one of the best projects using Amazon Web Service (see AWS Blog on the winners) and he received 3rd prize in the "Quantum computing today!" category for implementing a potential research idea in quantum computing.

Alejandro's project uses the recent results from the research project "Unbalanced penalization: A new approach to encode inequality constraints of combinatorial problems for quantum optimization algorithms" that he and colleagues at JSC published under the supervision of Prof. Kristel Michielsen. This method reduces the resources needed for solving constrained combinatorial optimization problems using quantum technology.

Contact: Dr. Alejandro Montanez-Barrera

Events

Introduction to Scalable Deep Learning
Instructors: Dr. Stefan Kesselheim et al., JSC
Date: 8–12 May 2023, 09:00–13:00
Venue: online
https://go.fzj.de/2023-scalable-dl

High-Performance Scientific Computing in C++
Instructor: Dr. Sandipan Mohanty, JSC
Date: 30 May – 2 June 2023, 09:00–16:30
Venue: JSC, building 16.3, room 213a
https://go.fzj.de/2023-hpc-cplusplus

Introduction to Supercomputing at JSC - Theory & Practice
Instructors: JSC employees, representatives of Atos, Intel, and ParTec
Date: 30 May – 2 June 2023, starting on 30 May at 13:00
Venue: online
https://go.fzj.de/2023-sc-1

Data Analysis and Plotting in Python with Pandas
Instructor: Dr. Andreas Herten, JSC
Date: 5 June 2023, 09:00–13:00
Venue: online
https://go.fzj.de/2023-pandas

Unreal Engine for Remote Visualization and Machine Learning
Instructor: Dirk Helmrich, JSC
Date: 5 & 7 June 2023, 09:00–16:00
Venue: hybrid
https://go.fzj.de/2023-unreal-ml

High-Performance Computing with Python
Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC
Date: 12-16 June 2023, 09:00-13:00
Venue: online
https://go.fzj.de/2023-hpc-python

GPU Programming Part 2: Advanced GPU Programming
Instructors: Dr. Jan Meinke et al., JSC
Date: 19-23 June 2023, 09:00-13:00
Venue: online
https://go.fzj.de/2023-gpu-adv

Getting Started with AI on Supercomputers
Instructors: Dr. Alexandre Strube, Sabrina Benassou, JSC
Date: 27-28 June 2023, 09:00-13:00
Venue: online
https://go.fzj.de/2023-ai-2