Programming Models & Tools

Researching parallel programming models and exploring tools to assist in developing parallel programming languages.
The High Performance Computing Center of Stuttgart (HLRS) of the University of Stuttgart is the first National Supercomputing Center in Germany and is offering services to both academic users and industry. Apart from the operation of supercomputers, HLRS activities include teaching and training in distributed systems, software engineering and programming models, as well as development of new technologies. HLRS is an active player in the European research arena with special focus on Scientific Excellence and Industrial Leadership initiatives.

**Our Network:** HLRS is tightly connected to academia and industry through long term partnerships with global market players such as Porsche and T-Systems, as well as worldwide companies, HPC centres and Universities. Particular attention is given to collaboration with Small and Medium Enterprises (SMEs).

**Our Infrastructure:** HLRS operates a CRAY XC40 supercomputer (peak performance > 7 PetaFlops), as well as a variety of smaller systems, reaching from clusters to cloud resources.
Our Experience: HLRS has been at the forefront of regional, national and European research and innovation over the last 20 years. During this time, HLRS has participated successfully in more than 90 European research and innovation projects.

Our Expertise: HLRS is a leading innovation center, applying software engineering methods to HPC and Cloud for the benefit of multiple application domains such as automotive, engineering, health, mobility, security, and energy. Thanks to the close interaction with industry, the center’s capabilities and expertise support the whole lifecycle of simulation covering research aspects, pre-competitive development and preparation for production. The HLRS innovation group, which actively examines and tests new technologies, can bring into projects expertise on leading edge technologies hardware and scale up data analysis techniques.
Supercomputing serves as the frontline of computational innovation. In terms of scientific discovery, supercomputing is an indispensable tool in enabling research findings too dangerous or risky to be done through other means. However, being at the vanguard of computing technology also requires supercomputing centres to continually innovate ways for research and development teams to take full advantage of these world-class resources. The Programming Models and Tools activities at HLRS address the heavy lifting in the realm of computer science so that users can spend less time programming, and more time running simulations and analyzing data. Thus, HLRS has two primary focus areas—researching parallel programming models and exploring tools to assist in developing parallel programming languages. For the scientific computing community, the contribution to standards is vital, as it drives interoperability and reusability of the developed codes and software. In addition to being user-friendly, this leads to sustainable impact of new technological innovation. The centre is thus highly active in evaluating OpenMP, and regularly gives feedback on the language’s features and newest implementations. As for OpenMPI, HLRS is a regularly contributing member of the Open MPI consortium, one of the main communities for open-source MPI implementation. Furthermore, there is a strong interaction with the MPI forum—the standardization body of MPI.
Project Overview

Smart-DASH - Smart Data Structures and Algorithms with Support for Hierarchical Locality

PHANTOM - Cross-layer and multi-objective Programming approach for next generation heterogeneous parallel computing systems

Open MPI

OpenMP Validation Suite

Mont-Blanc 2/3

EXPERTISE EXperiments and high PERformance computing for Turbine mechanical Integrity and Structural dynamics in Europe
Smart-DASH is a collaborative research project funded for 3 years by the German Research Foundation (DFG) as part of the priority programme „Software for Exascale Computing – SPPEXA“ (2013-2019). Smart-DASH is a follow-up to the project “DASH”. Smart-DASH aims to ease the efficient programming of future supercomputing systems for data-intensive applications. These systems will be characterized by their extreme scale and a multi-level hierarchical organization. Smart-DASH adopts the concept of Partitioned Global Address Space (PGAS) and provides the C++ template library “DASH” for distributed containers such as multidimensional arrays, lists and hash tables. Unlike other PGAS approaches, DASH will furthermore allow a developer either to control and explicitly take advantage of the hierarchical data layout of global data structures, or, to rely on smart handling of data-locality by the runtime system. The runtime and C++ template library will be extended to support a task-based execution model which allows to specify data-dependencies amongst distributed tasks on the global address space. We will develop ‘smart’ data structures that capture frequently encountered application scenarios to enable a productive transition onto new hardware platforms and assist in code modernization efforts. To address fault-tolerance and reliability, we will explore concepts for the redundant storage of data items and with the DASH data dock we will explore the usage of the PGAS approach in general and NVRAM in particular for the coupling of applications. Several case studies will explore the utility of these new features in the context of important scientific problem classes.
Within the project HLRS will lead in the development of the core runtime system, in particular the tasking and communication backend, respectively. Additionally, HLRS will contribute to the user-facing C++ template library, in particular when related to the tasking model.

Project Partners
- LMU Munich, MNM Team
- IHR, University of Stuttgart
- TU-Dresden, ZIH
- HLRS (Germany)

Project Information
- Runtime: 08.2016 – 07.2019
- Funding Organisation: DFG

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Further Information
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www.sppexa.de
Modern software applications have to cope with a great variety of hardware platforms, ranging from the commodity Intel’s and low-power ARM’s CPUs to the accelerators like NVIDIA’s GPU, reconfigurable-logic systems like Xilinx’s FPGA or dedicated systems like Movidius’ Myriad2. Consequently, the selection of the best possible platform for the specific application, which has to fulfill the user-imposed functional and non-functional requirements, is a very challenging task, even without considering the required development efforts. Furthermore, the challenge is getting even more complex when taking the assumption that all this hardware is working in a collaborative way within the common infrastructure (which might range from the “server-on-chip” to the cluster-like distributed systems). So the term “Cloud” has become common for such restrictive hardware domains like embedded systems as well.
PHANTOM is a EU-H2020 project (under grant agreement No. 688146) that has the ambition to provide a platform, which allows the components constituting the application (within the specified control- and data-flow) to be executed in heterogeneous, parallel, and distributed hardware environments (see the figure on the left) without any hardware-specific adaptation of the source code.

Role of HLRS
- Use case provider: Dynamic simulation of aero- and gas-dynamic processes in real-time
- Technology provider: Monitoring and Resource Management Framework, Parallelisation Toolkit

Project Partners
- The Open Group (UK)
- Easy Global Market (France)
- GMV (Portugal)
- Intecs (Italy)
- HLRS (Germany)
- University of York (UK)
- Unparallel Innovation (Portugal)
- WINGS ICT Solutions (Greece)

Project Information
- Funding Organisation: EU-H2020
- Runtime: 10.2015 - 03.2018

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Further Information
www.phantom-project.org
Open MPI

The Message Passing Interface (MPI) is the most important standard for inter-node communication on any kind of HPC system today. Since the first version MPI-1 from 1994 it has evolved a lot and many implementations of the standard have been developed. Open MPI is one of the most used implementations today. It started 2005 as the merger between the three well-known MPI implementations FT-MPI, LA-MPI and LAM/MPI.

The success of Open MPI is based on its goals...

- to deliver a production quality implementation of the latest MPI standard
- to provide extremely high performance
- to provide an extensible platform for 3rd-party research and commercial development
- to be a community driven project involving feedback from researchers, vendors and users
- to support a wide variety of HPC-platforms

Concept of OPEN MPI

- Modular design with component architecture
- Support of many network protocols such as openib, libfabric, usnic, udapl, ugni and tcp
- Support for accelerators such as Intel MIC and CUDA

HLRS contribution to OPEN MPI

- Nightly test on HPC Systems
- MPI standard conformance tests
- Add support for RDMA Bit Transfer Layer using Network Direct
- Work on advanced internal concurrent-threading features
- Memory debugging features supporting Intel pin and valgrind
- I/O optimization for GPFS
Members of OPEN MPI

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The OpenMP validation suite is a collection of C and Fortran programs with OpenMP directives that were designed to validate the correctness of an OpenMP implementation according to the OpenMP standard specification. It is a joint effort of the High Performance Computing Center Stuttgart, the Center for Information Services and High Performance Computing (Dresden) and the University of Houston.

The suite is designed to cover the 3.1 version of the OpenMP specification. It is currently extended to cover the new 4.0 standard with special focus on the task dependency model.

The OpenMP specification for the C/C++ language binding consists of more than twenty different constructs, and up to a dozen clauses that can be applied to these constructs. Although not all clauses can be used together with all constructs, this results in a sufficient complexity to make the implementation of an OpenMP compiler a difficult task.

Furthermore there is a rich API including library calls and environment variables that have to be checked as well. Currently the suite consists of 122 different tests. Each of these tests comes with a cross test, which verifies its capability of finding issues within a given runtime, identifying possible false positive.
Project Partners

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Mont-Blanc 2
The limiting factor in the development of an Exascale High Performance Computer System is power consumption. The Mont-Blanc2 project focused on the task to develop a next generation HPC system using embedded technologies to reach this difficult task. After the development of the hardware architecture in the first phase of the Mont-Blanc project, Mont-Blanc2 focused more on the developed of the necessary system software stack and evolution of the system design. It examined a new programming model allowing to write efficient code for the new computer architecture. It emphasized tools for the programmer like debugger and performance analysis tools, which increase the usability of such a system for the users. The main contribution of HLRS is the development of scalable debugging tools. In particular, HLRS extended the task-based graphical debugger Temanejo with support for the OmpSs programming model, and support for multi-node debugging. In addition, HLRS also contributed to evaluation of the programming model and prototype system by porting and benchmarking an application from the engineering domain.

**Funding Organisation:** EC FP7  
**Runtime:** 10.2013 – 01.2017

Mont-Blanc 3
The Mont-Blanc project aims to design a new type of computer architecture capable of setting future HPC standards, built from energy efficient solutions used in embedded and mobile devices. The project has been running since 2011 and was extended in 2013 (Mont Blanc 2) and 2015 (Mont Blanc 3), respectively. In particular, Mont Blanc 3 will enable further development of the OmpSs programming model to automatically exploit multiple cluster nodes, transparent application checkpointing for fault-tolerance, support for ARMv8 64-bit...
processors, and the initial design of the Mont-Blanc Exascale architecture. HLRS contribution to the project is twofold. Firstly, we will participate in the development of the programming model, in particular combining MPI and OmpSs into a hybrid, task-aware MPI/OmpSs. This will allow to overlap MPI communication with computation with minimal effort for the application programmer. Secondly, HLRS will contribute to the evaluation of the programming model and the architecture by porting a representative scientific application.

**Funding Organisation:** EC H2020  
**Runtime:** 10.2015 – 09.2018

**Project Partners**

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**Further Information**  
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EXPERTISE
EXperiments and high PERformance computing for Turbine mechanical Integrity and Structural dynamics in Europe

EXPERTISE is a European Training Network (ETN) that will contribute to train the next generation of mechanical and computer science engineers. Within the network 15 Early Stage Researchers (ESRs) will work on the big challenges on the way to a fully validated nonlinear dynamic model of turbo-machinery components. Along their way they are supervised by experts at world leading institutions from across Europe in this multidisciplinary project. The ultimate research objective of EXPERTISE is to develop advanced tools for the dynamics analysis of large-scale models of turbine components to pave the way towards the virtual testing of the entire machine. Key aspects addressed thereby will be the understanding and accurate modeling of physics of frictional contact interfaces, new, highly efficient and accurate nonlinear dynamic analysis tools as well as the integration of all this into high performance computing (HPC) techniques, enabling for the first time the accurate dynamic analysis of a large scale turbomachinery model.

The research program of EXPERTISE is based on the following Work Packages (WPs):
- WP1 – Advanced modeling of friction contacts
- WP2 – Identification of contact interfaces
- WP3 – Structural dynamics of turbine and its components
- WP4 – High Performance Computing for structural dynamics
HLRS as expert in the field of high performance computing (HPC) will lead the HPC activities in EXPERTISE. Also, HLRS will have a key role in the network by training all the researchers in modern HPC techniques and furthermore add its own research project, addressing the tremendous problem of handling the huge amounts of data that are produced during these full model simulations and bring HPC systems to their limits.

Beneficiaries
Imperial College of Science Technology and Medicine London | Universität Stuttgart | University of Oxford | CRAY UK Limited | École Centrale de Lyon | Middle East Technical University | Vysoka Skola Banska – Technicka Univerzita Ostrava | Barcelona Supercomputing Center – Centro Nacional de Supercomputacion | Mavel AS | Technische Universität München

Project Information
- **Runtime:** 03.2017 – 02.2021
- **Funding Organisation:** Horizon 2020, Marie Sklodowska-Curie Actions, Innovative Training Network (H2020-MSCA-ITN)

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