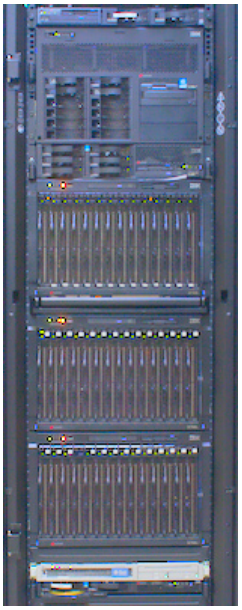

Nordic High Performance Computing & Applications Workshop

23-25 August 2017, University of Iceland, Reykjavík

The University of Iceland is offering a free cross-national training workshop on high-performance computing and applications at the University of Iceland in Reykjavík, Iceland, 23-25 August 2017 (noon-to-noon).

The University of Iceland (HÍ) has resident expertise in software engineering, distributed computing, and closely collaborates with the Jülich Supercomputing Centre (JSC) in High-Performance Computing (HPC) research and teaching. The university's computing centre (RHÍ) has expertise in cross-national Nordic scientific computing through having hosted the Nordic High Performance Computing (NHPC) cluster Garðar and now on the national level with the Icelandic HPC cluster (IHPC) Garpur. Iceland, in particular the University of Iceland, furthermore has a strong user community, e.g. in computational physics and chemistry, systems biology, and glaciology.

The workshop is organized in cooperation with the Jülich Supercomputing Centre (JSC), associated with the NordForsk e-science NCoE eSTICC (e-Science Tools for Investigating Climate Change), and funded via NordForsk's Nordic e-Infrastructure Collaboration (NeIC) Pooling Competencies focus area.

Topics and Trainers

The three-day training workshop will be run by distinguished experts with over a decade of experience in their fields, and cover the following topics, both via lecture and partly hands-on experience (so bring you own laptop to connect via SSH to the provided HPC clusters):

High Performance Computing (Morris Riedel, HÍ/JSC)

The availability of High-Performance Computing (HPC), powered by large-scale supercomputers and scalable cloud computing resources, has changed the way how science and engineering is done today. Innovative HPC technologies enable us to create "bridges" between the traditional scientific pillars "experiment" and "theory" by performing simulations of the real world or technology. Covered topics are parallel programming using MPI and OpenMP as well as more recent approaches using GPGPUs. General elements and challenges of parallel programming like concurrency, domain decomposition, load imbalancing, stencil methods, ghost/halo regions, and related topics will be covered using examples in the programming language C.

The Icelandic HPC Cluster (Hjörleifur Sveinbjörnsson & Máni Marius Viðarsson, RHÍ)

Short presentation on the High Performance Computing facilities and services available at the University of Iceland aimed at new users: how to log in, how to submit jobs, how to use the module system used to set up the appropriate tool environment. Finally, we will have a short walk to the premises of RHÍ to see the HPC hardware and infrastructure (such as cooling) face to face.

Simulations of atomic scale systems using HPC (Hannes Jónsson, HÍ)

Computer simulations of atomic systems based on fundamental equations of physics can in many cases be used to help interpret experimental measurements and even predict properties of new

materials and chemicals. The more fundamental the description is, the more challenging the computations become. Progress in this field is driven by development of better computational algorithms and faster implementations, as well as progress in the theoretical description of the systems. An overview of some ongoing projects in the theoretical chemistry group at University of Iceland will be given with main emphasis on computational methods that can be applied in a wide range of applications, some well outside the realm of atomic scale systems.

A physicist's guide to parallelization at the IHPC (Viðar Guðmundsson, HÍ)

Experience from computational physics on parallel processing at the IHPC.

HPC Requirements Engineering in the Interaction Room (Matthias Book, HÍ)

The Interaction Room (IR) is a collaboration technique that uses large interactive displays to facilitate the elicitation, joint understanding and prioritization of requirements in teams composed of stakeholders from different backgrounds, such as software engineers and scientific domain experts. By encouraging pragmatic modeling, the IR helps to deal with the complexity of scientific computing applications and map them to HPC solution techniques.

Refactoring and Testing (Helmut Neukirchen, HÍ/eSTICC)

Scientific software evolves over time and as part of this, the source code quality decays, making the code hard to understand, hard to modify, and hard to extend. Refactoring is a systematic approach of re-structuring source code to improve its readability and maintainability. Software tests are used as a safety net to make sure that behaviour is not changed as part of refactoring. In addition, software testing is an important means of software quality management. By designing test cases in a systematic way and executing them in an automated way, the quality of scientific software can be assured. Foundations and practical applications are covered.

Performance Analysis (Brian Wylie, JSC)

Parallel and scalable scientific software used in the simulation sciences and data mining often has performance problems that are specified in terms of execution patterns representing situations of inefficient behaviour. Such patterns are the input for an analysis process that recognizes and quantifies the inefficient behaviour in event traces that are created after instrumenting scientific code with a modern toolset such as that offered by Scalasca.

Scientific Workflows (Shahbaz Memon, JSC/HÍ/eSTICC)

This lecture offers a more abstract use of HPC resources through the use of scientific workflow tools. This contribution offers insights to the available tools and the key idea of combining several HPC runs to a greater whole modelled as scientific workflows. The lecture will include practical examples from the eSTICC project of how scientific workflows can be modelled and executed on resources available in the Nordic region.

Agenda

The tentative schedule is as follows:

Day 1: *Morning: Arrival of international participants*
Introduction of High Performance Computing (Morris Riedel)

Introduction to IHPC, the Icelandic HPC Cluster (Hjörleifur Sveinbjörnsson, Máni Maríus Viðarsson)

Day 2: A Physicist's Guide to Parallelization at the IHPC (Viðar Guðmundsson)
Simulations of atomic scale systems using HPC (Hannes Jónsson)
HPC Systems Engineering in the Interaction Room (Matthias Book)
Performance Analysis (Brian Wylie)
Scientific Workflow Implementation (Shahbaz Memon)

Day 3: Testing and Refactoring of Scientific Applications (Helmut Neukirchen)
Hands-on Performance Analysis Tools (Brian Wylie)
Scientific Workflow Applications (Shahbaz Memon)
Afternoon: Departure of international participants

Location and Travel Information

The workshop will take place in the Tæknigarður building (Dunhagi 5, but entrance is rather from Suðurgata) on the campus of the University of Iceland in Reykjavík.

The campus is in walking distance of Reykjavík's city centre, which offers a wide variety of accommodation options (the closest being the Radisson Blu Saga Hotel, right next to the workshop venue -- contact workshop organizers to get 15 percent special workshop reduction on the rates shown in their booking system; but in general, guesthouses are much cheaper).

Iceland can be reached from many European and American cities within a few hours through its international airport at Keflavík (KEF). The Flybus service provides frequent transfers (no schedule for arrivals, the schedule is rather: each arrival has a matching bus trip) to Reykjavík city center. The Flybus terminal in Reykjavík (BSÍ) is in walking distance to the university campus.

If you would like to extend your stay, there is plenty to see and do around Reykjavík. Have a great time!

Registration

To participate in the workshop, **please register until 15 August**.

Participation in the workshop is free of charge and includes lunch and coffee breaks through funding from Nordforsk NeIC. Participants are responsible for their own travel and accommodation.

We are looking forward to welcoming you at the University of Iceland!

Workshop Organization

- Helmut Neukirchen, University of Iceland
- Morris Riedel, Jülich Supercomputing Centre
- Matthias Book, University of Iceland