PRACE Course: Intermediate MPI

9-11 November 2022

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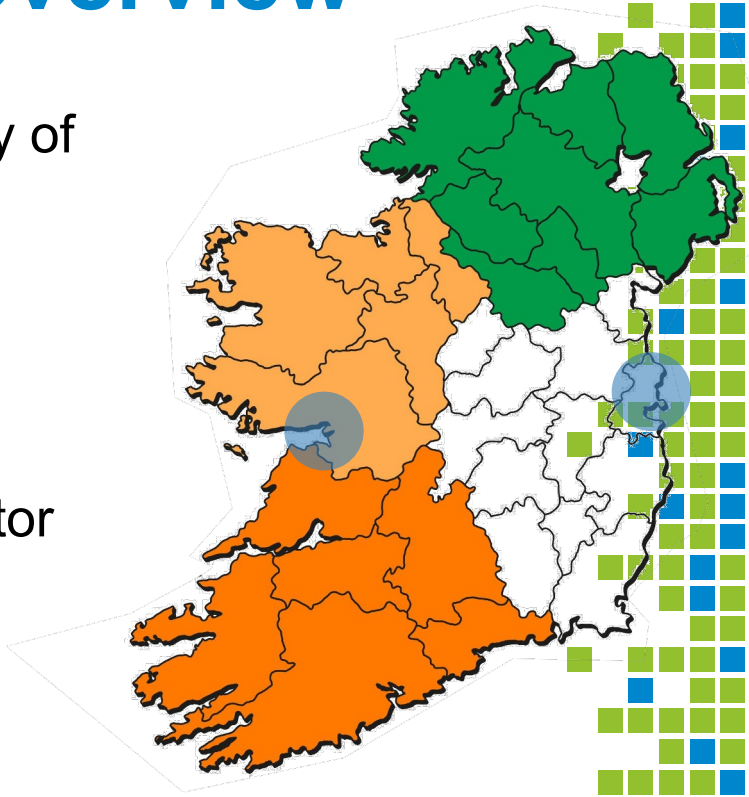
ICHEC

ICHEC: an overview

- **National HPC** hosted by University of Galway and funder by DFHERIS
- Provides e-infrastructure, services and expertise
- Academia, industry and public sector
- Staff: sysadmins, computational scientists, researchers, etc.



Ollscoil na Gaillimhe
University of Galway

An Roinn Breisoideachais agus Ardoideachais, Taighde, Nuálaíochta agus Eolaíochta
Department of Further and Higher Education, Research, Innovation and Science

ICHEC activities

National service & user support

Training & outreach

Performance engineering

Novel technologies: AI and Quantum Computing

Earth observation & climate research

Industry & public sector

ICHEC
Irish Centre for High-End Computing

KAY

Kay Antonelli

- **Thin**: 336 nodes (2x20 cores) Intel Xeon Gold 6148, 2.4Ghz, 192 GiB RAM 400 GiB SSD
- **Shmem**: 6 nodes (2x20 cores) Intel Xeon Gold 6148, 2.4Ghz 1.5 TiB RAM, 1 TiB SSD
- **GPU**: 16 nodes 2x NVIDIA Tesla V100 16GB
- **Phi**: 16 nodes Intel Xeon Phi KNL 64 cores @ 1.3 GHz, 192 GiB RAM 400 GiB SSD
- **Storage**: 1PiB DDN Storage

www.ichec.ie/academic/national-hpc

PRACE Training

14 **PRACE Training Centres** that started in 2012-2017-2020:

- Barcelona Supercomputing Center (Spain)
- CINECA Consorzio Interuniversitario (Italy)
- CSC – IT Center for Science Ltd (Finland)
- EPCC at the University of Edinburgh (UK)
- Gauss Centre for Supercomputing (Germany)
- Maison de la Simulation (France)
- GRNET – Greek Research and Technology Network (Greece)
- ICHEC – Irish Centre for High-End Computing (Ireland)
- IT4I – National Supercomputing Center VSB Technical University of Ostrava (Czech Republic)
- SURFsara (The Netherlands)
- TU Wien – VSC Research Center (Austria)
- University ANTWERPEN – VSC & CÉCI (Belgium)
- University of Ljubljana – HPC Center Slovenia (Slovenia)
- Swedish National Infrastructure for Computing (SNIC) (Sweden)

Mission: Serve as **European hubs and key drivers of advanced high-quality training** for researchers working in the computational sciences.

http://www.training.prace-ri.eu/

About the Course

- Objectives:
  - summarises basic concepts and describes them in more detail
  - more advanced concepts will be described

- The main topics covered:
  - datatypes, communicator management and one-sided communication

- Topics not covered:
  - Remote Memory Operations, MPI Shared Memory, Parallel I/O, Dynamic Process Management

- Prerequisites:
  - Knowledge of C/Fortran, basic knowledge of Unix/Linux commands and exposure to MPI

- Learning Outcome:
  - write parallel programs using the MPI library
  - define custom data types, groups and communicators
  - set up and use different communication modes

- Course Webpage: https://github.com/ICHEC-learn/intermediate-mpi

Agenda – Day 1

09:30 - 10:00	Introduction to Course and ICHEC Cluster
10:00 - 10:30	Introduction to MPI
10:30 - 11:00	MPI Point-to-Point Communication - Blocking
11:00 - 11:30	
11:30 - 12:30	Practical (Ping pong benchmark)
12:30 - 13:00	MPI Point-to-Point Communication - Nonblocking
13:00 - 14:00	
14:00 - 14:30	Practical (Communication in a ring)
14:30 - 15:30	MPI Collective Communication
15:30 - 16:00	
16:00 - 17:00	Practical (array increment)

Agenda – Day 2

10:00 - 10:30	MPI Error Handling
10:30 - 11:00	MPI Groups and Communicators
11:00 - 11:30	
11:30 - 12:30	MPI Virtual Topologies
12:30 - 13:30	Practical (2d Cartesian)
13:00 - 14:00	
14:00 - 14:30	MPI Derived Datatypes
14:30 - 15:00	Practical (Matrix row/column/submatrix)
15:00 - 15:30	Practical (game of life serial)
15:30 - 16:00	
16:00 - 17:00	Practical (game of life parallel)

Agenda – Day 3

10:00 – 11:00	Intercommunicators
11:00 - 11:30	
11:30 - 12:30	Persistent communications, Packing
12:30 - 13:00	Practical (persistent comms in ring)
13:00 - 14:00	
14:00 - 15:30	One-sided Communications
15:30 - 16:00	
16:00 - 16:30	Practical (ring one sided)
16:30 - 17:00	Discussion and Close

References

1. All MPI standard documents: www.mpi-forum.org
2. William Gropp et al.: **MPI: The Complete Reference**, Vol. 2, 1998.
3. William Gropp et al.: **Using MPI: Portable Parallel Programming With the Message-Passing Interface,** MIT Press, 3rd edition, Nov. 2014.
4. William Gropp et al.: **Using Advanced MPI: Modern Features of the Message-Passing Interface,** MIT Press, Nov. 2014.
5. Peter S. Pacheco: **Parallel Programming with MPI,** Morgen Kaufmann Publishers, 1997.
6. **https://hpc-tutorials.llnl.gov/mpi/**
7. Neil MacDonald, Elspeth Minty, Joel Malard, Tim Harding, Simon Brown, Mario Antonioletti: **Parallel Programming with MPI,** PRACE Training @ EPCC.
8. Rolf Rabenseifner, **Parallel Programming Workshop (Train the Trainer),** PRACE Training @ HLRS, October 2021.

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