

PRACE Course: Intermediate MPI

9-11 November 2022

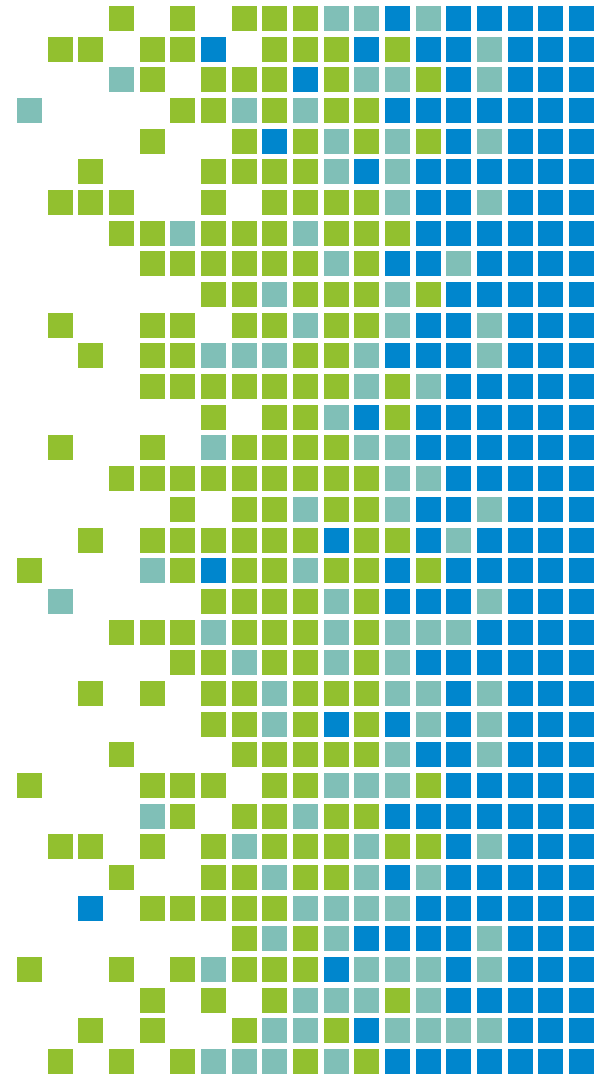
Dr. Adam Ralph and Dr. Buket Benek Gursoy

ICHEC



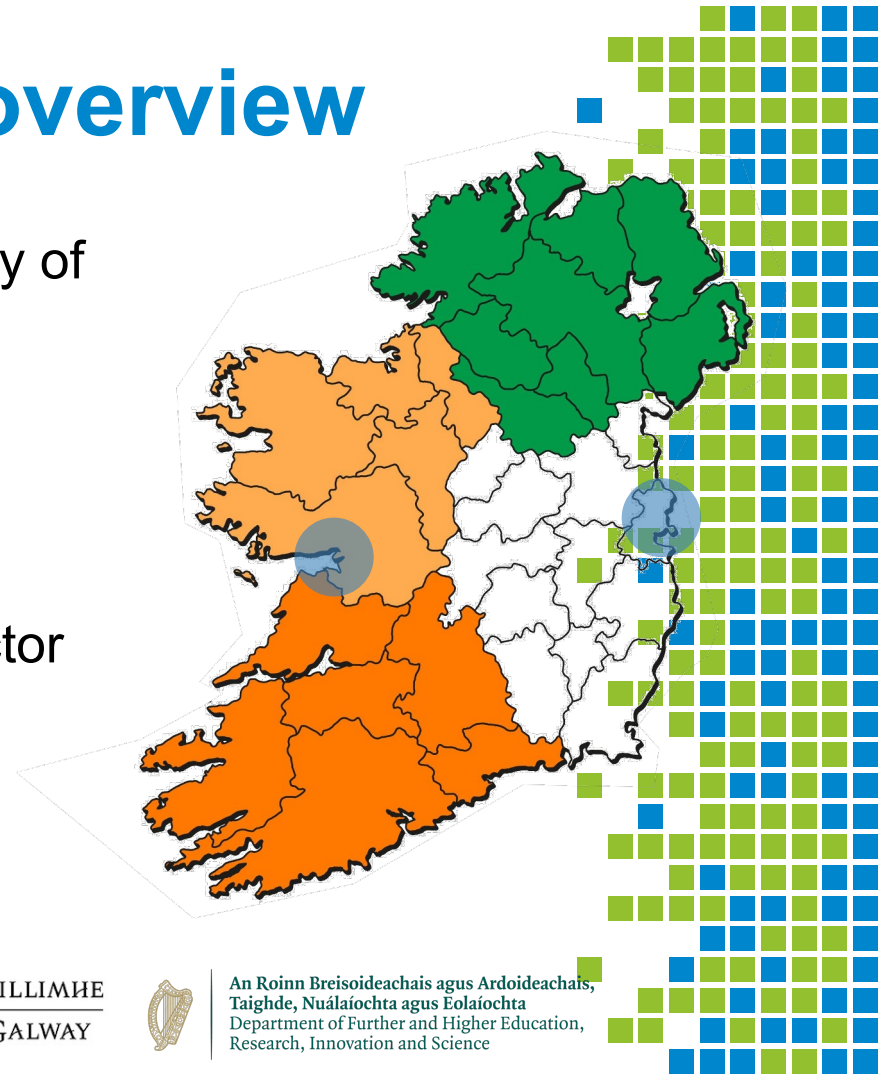
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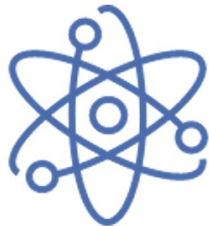


ICHEC: an overview

- **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.



ICHEC activities



National service &
user support



Training & outreach



Performance
engineering



Novel technologies: AI and
Quantum Computing



Earth observation &
climate research



Industry & public sector



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

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)



Univerza v Ljubljani






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
15:30 - 16:00	
16:00 - 17:00	Practical

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**, Morgan 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.

* *Special Thanks to Rolf for the **Train the Trainer** programme.* H L R I S