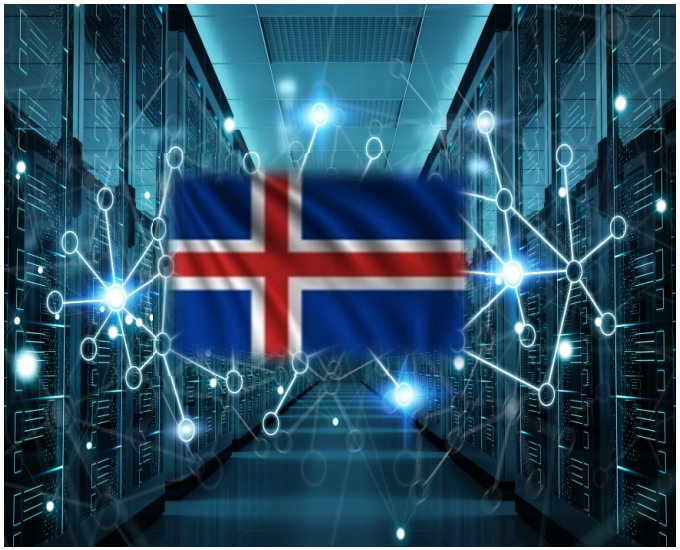


Icelandic HPC National Competence Center for HPC & AI – Welcome & Workshop Objectives

PROF. DR. – ING. MORRIS RIEDEL, UNIVERSITY OF ICELAND & JUELICH SUPERCOMPUTING CENTRE (GERMANY), EVENT CHAIR

28TH OCTOBER, 2ND ICELANDIC HPC COMMUNITY WORKSHOP, UNIVERSITY OF ICELAND, GRÓSKA, ROOM ADA

@ProfDrMorrisRiedel @Morris Riedel @MorrisRiedel @MorrisRiedel https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg

IHPC National Competence Center for HPC & AI in Iceland

EuroHPC Joint Undertaking

EOSC NORDIC

RAISE Center of Excellence

ADMIRE

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

EURO

HELMHOLTZAI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

DEEP Projects

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Setting the Scene:
IHPC National Competence Center for HPC & AI in Iceland

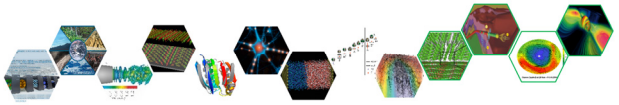
Executive Summary – Major Icelandic HPC Activities

Icelandic National Infrastructure for HPC

- **HPC hardware funds** by RANNIS; now via **roadmap IReiP**
- Proposals yearly required to obtain funds still
- Joint proposal from IHPC community

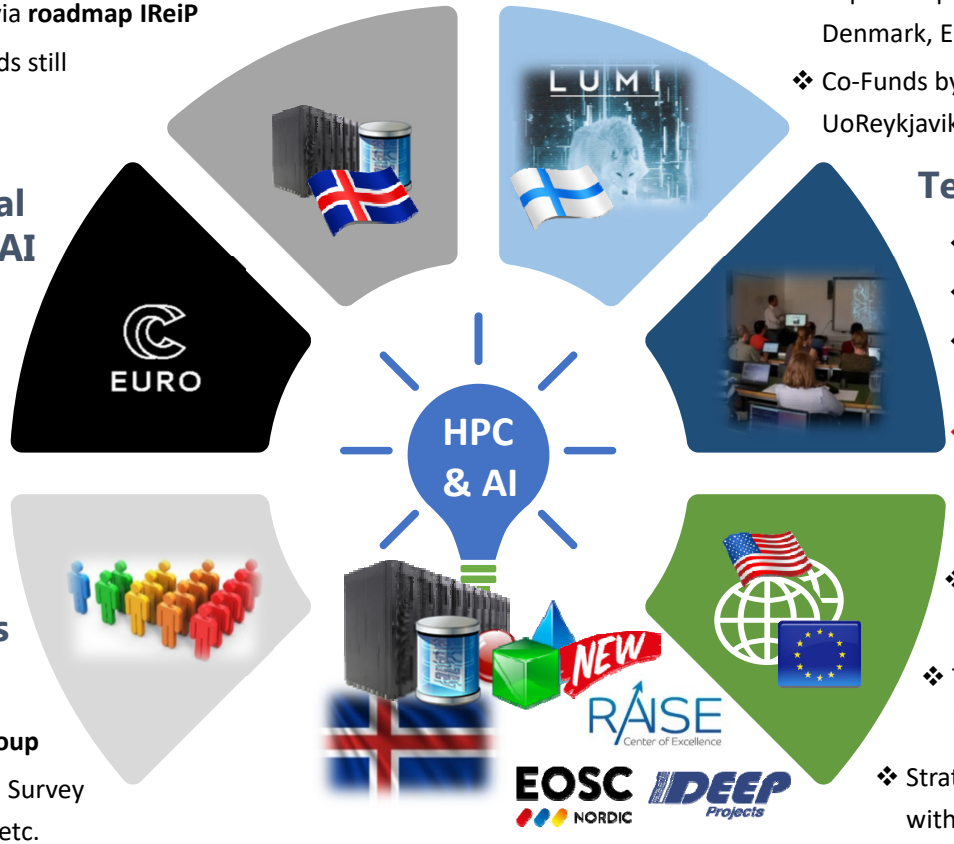
EuroHPC EuroCC National Competence Center for HPC & AI

- EU Project (09/2020-08/2022), 2 years
- Building **Simulation and Data Labs (SDLs)** of the IHPC Community of Users
- **Supports industry engagement in HPC**



IHPC Community of Users

- Organized around RANNIS proposals
- **~53 scientific experts & research group**
- UoIceland/UoReykjavik, Iceland Geo Survey ÍSOR, Met Office & **industry: Matis**, etc.



EuroHPC LUMI Supercomputer in Finland

- Supercomputer funded by Finland, Belgium, Czech Republic, Denmark, Estonia, Iceland, Norway, Poland, Sweden, Switzerland
- Co-Funds by EC and Iceland participation funds from: UoIceland, UoReykjavik, and Hannes Jonsson & Egill Skulason

Teaching & Education in HPC & AI

- University of Reykjavik
- University of Iceland
- Arctic Webinar Series (with US partners)
- **H2020 MSc in HPC Pilot (EduHPC proposal)**

International Cooperations

- Tactical: ~4 Joint PhDs with **Juelich Supercomputing Centre** in Germany (#1 HPC System in Europe)
- Tactical**: EC Projects** like DEEP-EST, EOSC-Nordic, RAISE Center of Excellence (CoE), etc.
- Strategic: Plans of building an **Icelandic National Lab** with international cooperation together with Industry (e.g. Kaiser Global, other investors)

EuroCC Activities – Selected Benefits towards Bottom-Up Community Building

[1] Icelandic HPC Community Web page

- Simulation & Data Lab Communities
  - Experts w.r.t. **HPC in domain-specific topics**
- Based on extensive community experience
  - Juelich Supercomputing Centre in Germany works with the model for ~16 years

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

[4] Juelich Supercomputing Centre, Simlabs

Simulation and Data Lab Computational Chemistry

General Information

Advancement of theory and methodology for atomic scale simulations, with broad ranging applications for chemistry and physical chemistry, reaction rate theory, adsorption spectroscopy, and magnetism, to name a few.

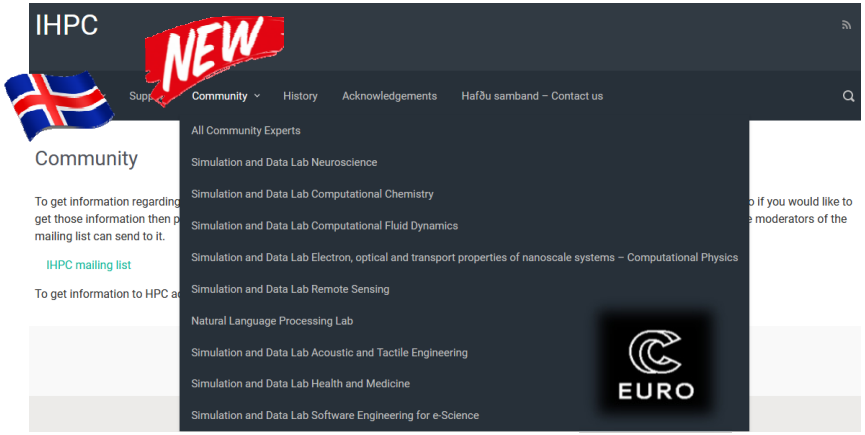
Prof. Hannes Jonsson

Dr. Elvar Örn Jónsson

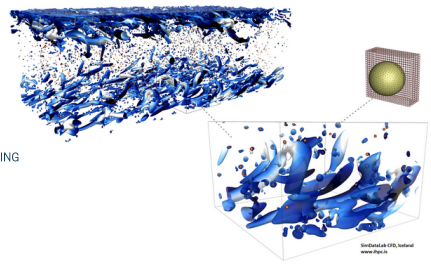
Development of explicit polarizable classical solvent models and methodology for hybrid simulations coupling classical and quantum mechanics for the simulation of solvated molecules and the solid / liquid interface.

Dr. Pavel Bessarab

[3] IHPC SimDataLab Computational Chemistry Web Page



Simulation and Data Lab Computational Fluid Dynamics



Dr. Pedro Costa

Dr. Ásdís Helgadóttir

Ph.D. Student S. Reza Hassanian. M

NEW

RAISE Center of Excellence

Prologue

The Simulation and Data Lab computational fluid dynamics (SimDataLab CFD) is leading parallel computing in Computational fluid dynamics in Iceland at the University of Iceland. The SimDataLab is Iceland's representative in the international projects in CFD and parallel computing. SimDataLab CFD aims to develop parallel code applications in CFD and support users who have already developed parallel application codes. SimDataLab CFD participates in the European project network in parallel computing and has an infrastructure and access to powerful parallel systems in-memory optimization, processing system architecture, high scalability, and have performance optimization computer nodes.

[2] IHPC SimDataLab CFD Web Page

1st Icelandic HPC Community Workshop

Workshop Objectives

F2F WORKSHOP

Bring together a diverse group of Icelandic and international stakeholders to discuss the role of HPC and related areas within Iceland without losing sight of its international links.

PERFORM COMMUNITY BUILDING

Perform community building in developing new successful joint activities between academia and industry, potentially creating new joint Simulation and Data Labs or collaborations.

DOCUMENT COMPETENCIES

Document competencies, achievements, activities, and lessons learnt from participating stakeholders of Icelandic HPC efforts and associated international activities.

RECOMMENDATIONS

Identify best practices and core principles with a set of recommendations for developing the future Icelandic HPC ecosystem, including necessary skills, funding opportunities, applications, Centre of Excellences, community events, and sustainable infrastructure developments.

Selected Results – 1st Workshop

- Facts
  - Active on Social Media
  - Visibility in EuroCC Project Review
  - ~25 participants
- Report per Workshop
  - Will be available soon
  - Updates also on IHPC Web page

5:00 – 5:15	Informal Welcome – Participant Introduction & Discussions *(Coffee/Tea/Refreshments, Snacks, and Sandwiches available)*	All
5:15 – 5:25	Opening remarks & Workshop objectives & Introduction EuroCC IHPC National Competence Center for HPC & AI	Prof. Dr. – Ing. Morris Riedel (University of Iceland)
5:25 – 5:30	Q & A	All
5:30 – 5:40	Infrastructure, Services, and HPCFlow from atNorth	Rui Gomes (atNorth)
5:40 – 5:45	Q & A	All
5:45 – 5:55	Simulation and Data Lab Computational Fluid Dynamics	Seyedreza Hassanianmoaref (University of Iceland)
5:55 – 6:00	Q & A	All
6:00 – 6:10	An Overview of the Reykjavik Institute and its Strategic Planning for Icelandic Stakeholders	Bill Patrowicz (Kaiser Global)
6:10 – 6:15	Q & A	All
6:15 – 6:25	From Management Games to the idea of „Dig In" and its future	Baldvin Albertsson & Björn H. Helgason (Vitargames)
6:25 – 6:30	Q & A	All
6:30 – 6:40	Accurate Virtual Acoustics Enabled by High-Performance Computing	Finnur Pind (Treble)
6:40 – 6:45	Q & A	All
6:45 – 7:00	Workshop Closing – Concluding remarks with next steps *(Coffee/Tea/Refreshments, Snacks, and Sandwiches available)*	All

IHPC National Competence Center for HPC & AI in Iceland

EuroHPC Joint Undertaking

EURO

1st Icelandic HPC Community Workshop
Endurmenntun HI, Dunhaga 7, 107 Reykjavik – Room Náma
11th August 2021 – 5:00 – 7:00 p.m. GMT

Background
The Icelandic High-Performance Computing (IHPC) activities are increasing in academia and industry that also includes related areas such as Artificial Intelligence (AI), Machine Learning (ML), Data Analytics, and Data Sciences. As a result, the IHPC community members created Icelandic Simulation and Data Labs (SDLs)[1], including academic and industrial partners. They form together in a bottom-up fashion the IHPC National Competence Center for HPC & AI in Iceland partly funded by the EuroHPC Joint Undertaking EuroCC project. The IHPC community seeks more collaborations and new members.

Objectives
This workshop aims to bring together a diverse group of Icelandic and international stakeholders to discuss the role of HPC and related areas within Iceland without losing sight of its international links. The specific objectives of the workshop are to:
- **Document competencies, achievements, activities, and lessons learnt** from participating stakeholders of Icelandic HPC efforts and associated international activities.
- **Perform community building** in developing new successful joint activities between academia and industry, potentially creating new joint Simulation and Data Labs or collaborations.
- **Identify best practices and core principles with a set of recommendations** for developing the future Icelandic HPC ecosystem, including necessary skills, funding opportunities, applications, Centre of Excellences, community events, and sustainable infrastructure developments.

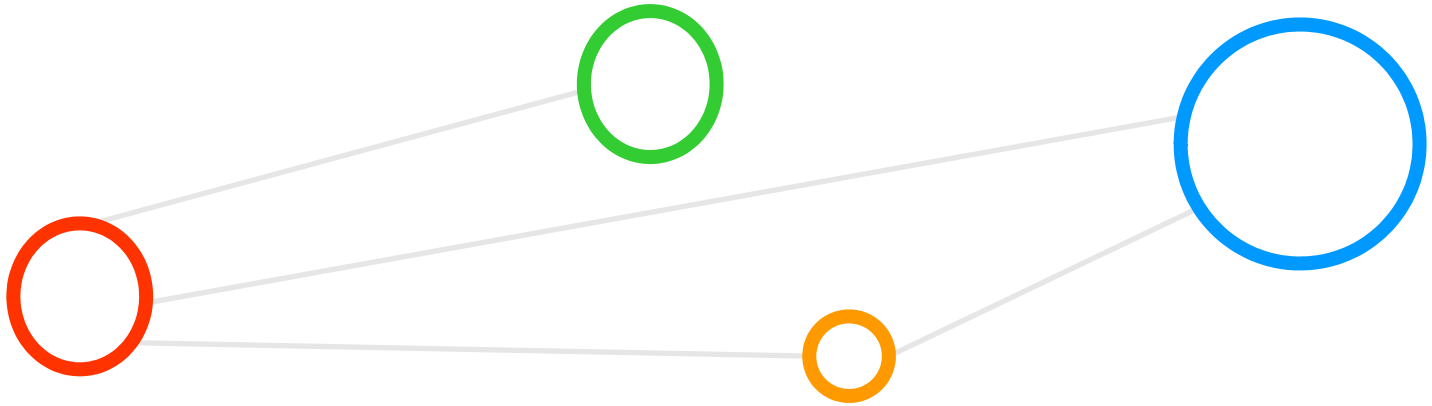
Participants
Approximately 20-25 participants from Iceland, Germany, and the USA. Participants will include:
- Selected Icelandic companies and SMEs from different sectors with interest in HPC & AI
- Academic representatives from the University of Iceland and Simulation and Data Labs
- The Icelandic Centre for Research (Rannís), Startup Iceland, and Icelandic Technology Clusters
- US company that forms government, industry, and academic cooperative research coalitions

Output
The following outputs are expected:
- A short synthesis paper that documents Icelandic competencies, field experiences and achievements in using and/or offerings HPC & AI solutions and consideration of 'best practices'
- A short strategy paper responding to HPC & AI issues and challenges identified during the workshop, including potential options for jointly engaging in EuroHPC funding opportunities
- Strengthened informal networks and transfer of experiences and lessons learnt

Selected Results – 1st Workshop – Reykjavik Institute Progress

Selected Results – 1st Workshop – Reykjavik Institute Progress

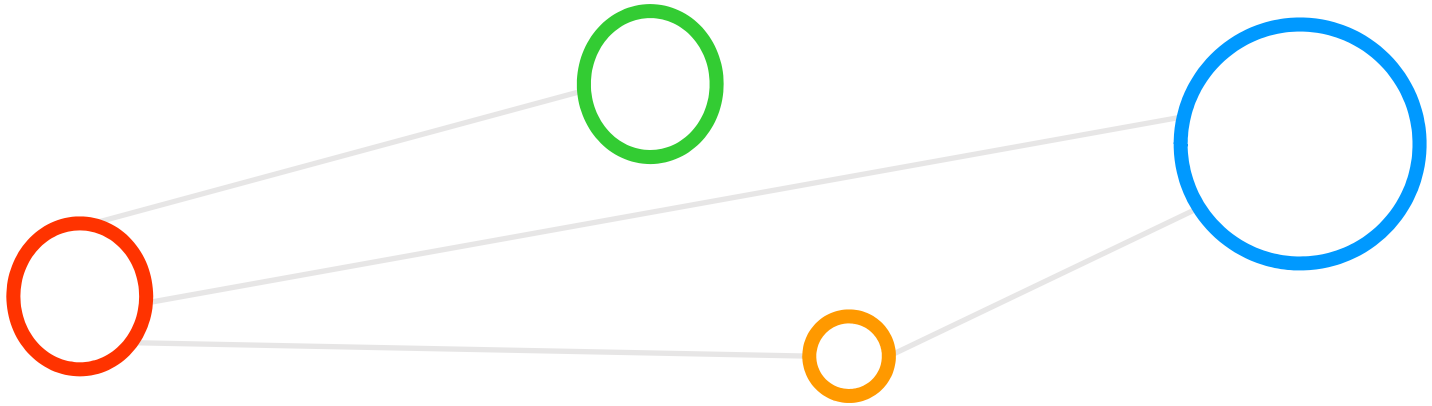
Selected References



Selected References

- [1] Icelandic HPC Community Web Page, Online: ihpc.is/community
- [2] Icelandic HPC Simulation and Data Lab Computational Fluid Dynamics (CFD), Online: https://ihpc.is/simulation-and-data-lab-computational-fluid-dynamics/
- [3] Icelandic HPC Simulation and Data Lab Computational Chemistry, Online: https://ihpc.is/simulation-and-data-lab-computational-chemistry/
- [4] Juelich Supercomputing Centre (JSC) Simulation and Data Labs, Online: https://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/simlab_node.html

ACKNOWLEDGEMENTS



Acknowledgements – High Productivity Data Processing Research Group

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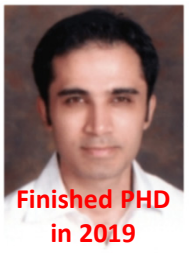
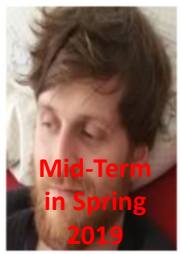
G. Cavallaro

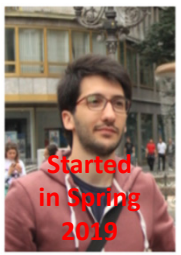
Senior PhD
Student
A.S. Memon



PD Dr.
M.S. Memon



PhD Student
E. Erlingsson



PhD Student
S. Bakarat

PhD Student
R. Sedona

PhD Student
P. H. Einarsson

Dr. M. Goetz
(now KIT)

MSc M.
Richerzhagen
(now other division)

MSc
P. Glock
(now INM-1)

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(Landsverkjun)

PhD Student
Reza

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