

Icelandic HPC National Competence Center for HPC & AI & EuroHPC JU

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24TH SEPTEMBER, RANNIS WORKSHOP, UNIVERSITY OF ICELAND, GROSKA, ROOM ADA



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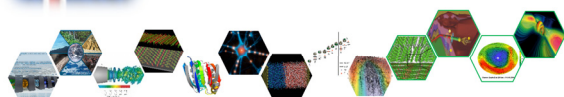
@MorrisRiedel



<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

HELMHOLTZAI | ARTIFICIAL INTELLIGENCE
COOPERATION UNIT

DEEP
Projects



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



JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

RANNIS Workshop & Agenda Items

- EuroHPC JU Administration
 - New Regulation & Governing Board Membership
 - Multi-annual workplan
 - Future Calls (Drafts, no Digital Europe work programme yet)
- EuroCC Phase II (maybe from ~September 2022)
 - Simulation and Data Lab Strategy & IHPC.IS
 - Possibility of co-funding according to 50/50 model of JU
- Future of Centre of Excellences (CoEs)
 - CHEESE (Vedurstofan), RAISE (HI)
- Invitation EuroCC Review
 - Public Event (see Invitation letter for funding authorities)
- Joint Procurements with Industry
 - Exploring possibilities to join with Industry (e.g., Kaiser Global) to host EuroHPC machine?

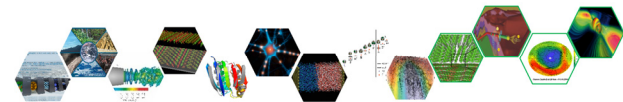
Executive Summary – Major Icelandic HPC Activities

rannís 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

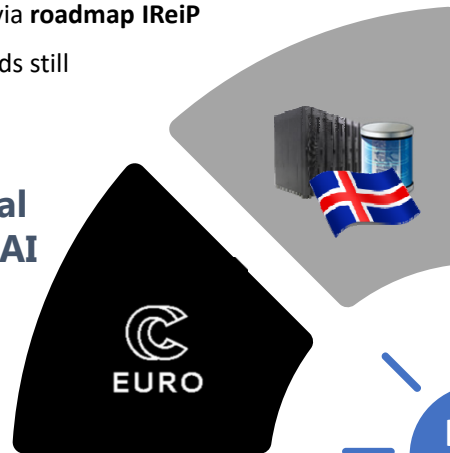
EuroHPC EuroCC National Competence Center for HPC & AI

- ❖ 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**



ISOR **matis** **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)**

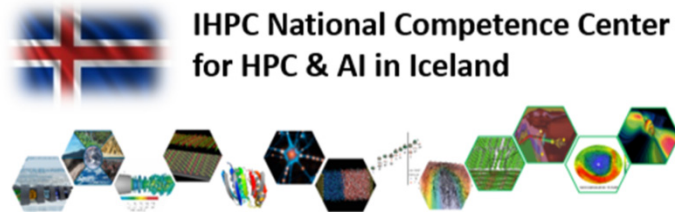


International Cooperations

- ❖ 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



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.

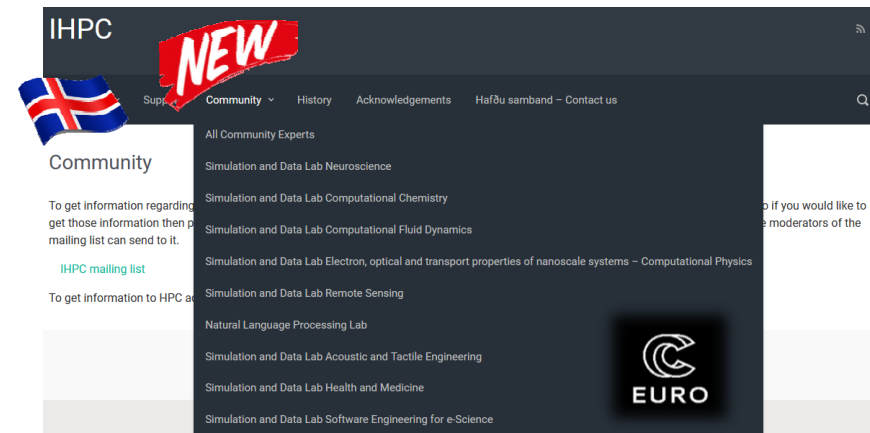
Dr. Pavel Bessarab

Icelandic HPC National Competence Center for HPC & AI

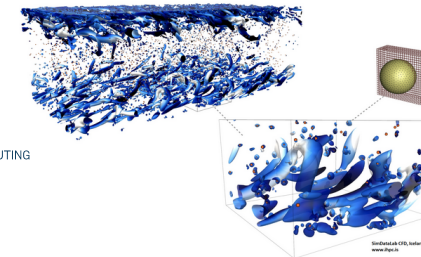


[4] Juelich Supercomputing Centre, Simlabs

[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



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



Perform International & Icelandic HPC Community Workshops

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.



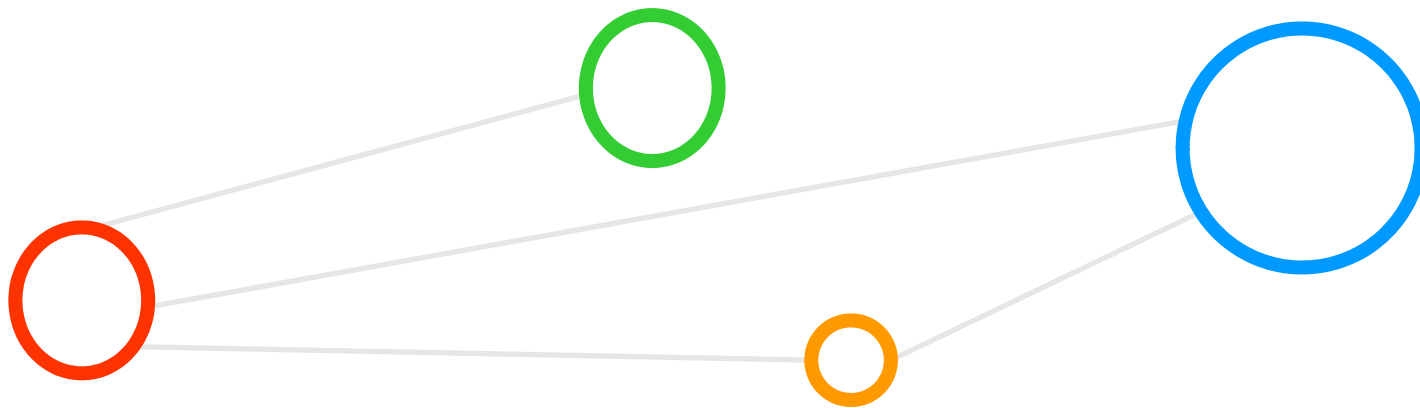
DOCUMENT COMPETENCIES

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.

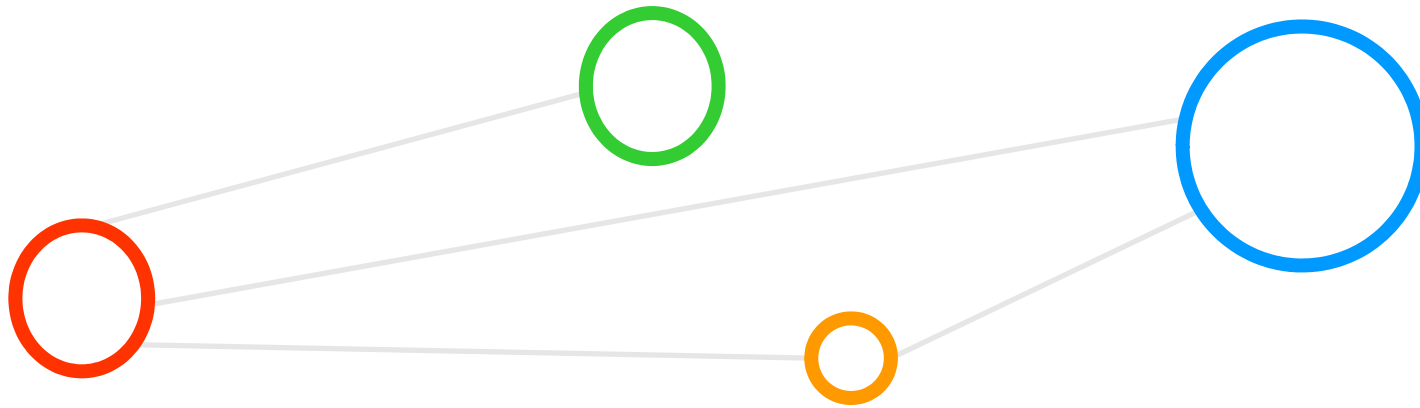
Selected References



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:
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ACKNOWLEDGEMENTS



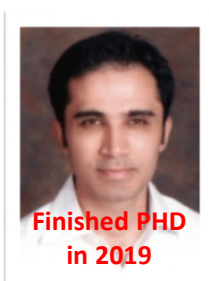
Acknowledgements – High Productivity Data Processing Research Group



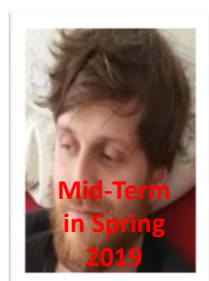
PD Dr.
G. Cavallaro



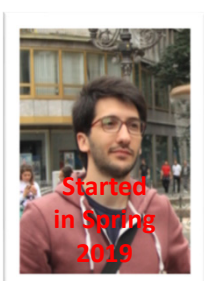
Senior PhD
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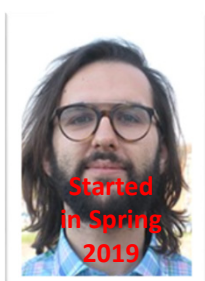
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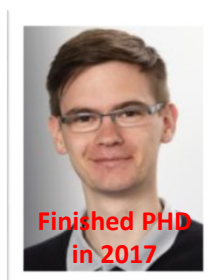
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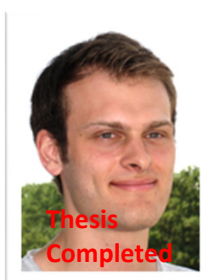
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P. H. Einarsson



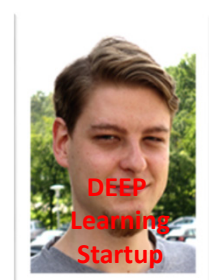
Dr. M. Goetz
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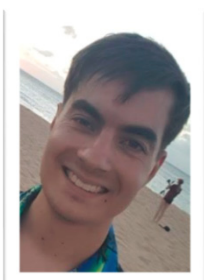
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Richerzhagen
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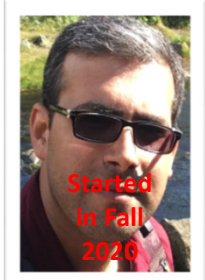
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