

Icelandic HPC National Competence Center for HPC & AI – Supporting the Reykjavik Institute Plans

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

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@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



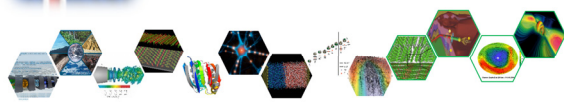
@MorrisRiedel



<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

HELMHOLTZAI | ARTIFICIAL INTELLIGENCE
COOPERATION UNIT

DEEP
Projects

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE



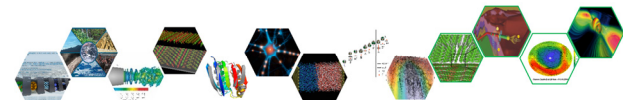
Executive Summary – Major Icelandic HPC Activities

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

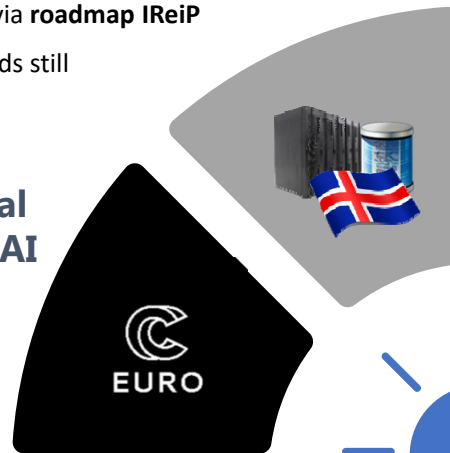
EuroHPC EuroCC National Competence Center for HPC & AI

- ❖ 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)

International Collaboration – Juelich Supercomputing Centre – Europe #1 HPC



JÜLICH
SUPERCOMPUTING
CENTRE



[2] YouTube, 'flexible and energy-efficient supercomputer: JUWELS is faster than 300 000 modern PCs'

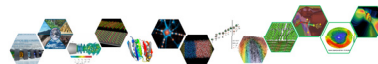


2018
12 PF



Europe #1 HPC
System in Top500

Application Co-Design



[6] S. Kesselheim et al., 'JUWELS Booster - A Supercomputer for Large-Scale AI Research', ICS 2021, to appear



2023

1 EF

Potentially first
Exascale system
in Europe



[3] DEEP Series of Projects Web Page

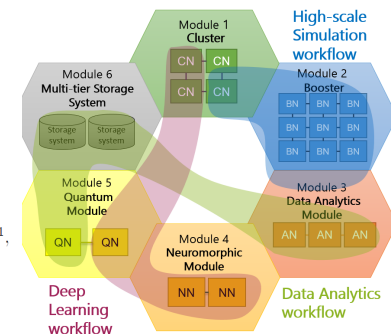
JUWELS Booster – A Supercomputer for
Large-Scale AI Research

Stefan Kesselheim^{1*}, Andreas Herten^{1*}, Kai Krajsek^{1*}, Jan Ebert^{1*},
Jenia Jitsev^{1*}, Mehdi Cherti^{1*}, Michael Langguth^{1*}, Bing Gong^{1*},
Scarlet Stadler^{1*}, Amirpasha Mozaffari^{1*}, Gabriele Cavallaro^{1*},
Rocco Sedona^{1,2*}, Alexander Schug^{1,3*}, Alexandre Strube¹, Roshni Kamath¹,
Martin G. Schultz¹, Morris Riedel^{1,2}, Thomas Lippert¹

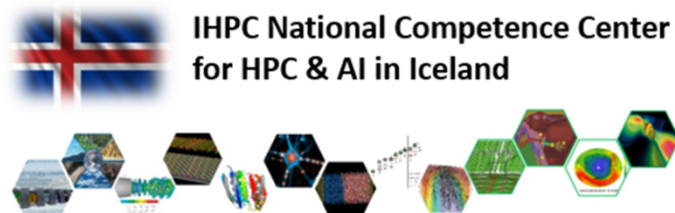
¹ Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, Germany,
contact <n>.<surname>@fz-juelich.de

² School of Engineering and Natural Sciences,
University of Iceland, Reykjavik, Iceland

³ University of Duisburg-Essen, Germany



Icelandic HPC Community Building – Simulation & Data Labs & Workshops



- Simulation & Data Lab Communities
 - Experts w.r.t. HPC in domain-specific topics
 - UoIceland, UoReykjavik, SMEs, etc.
- 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

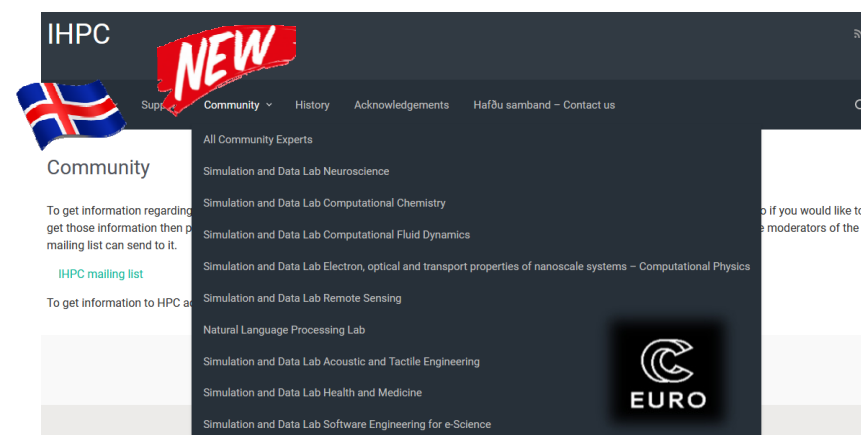


[4] Juelich Supercomputing Centre, Simlabs

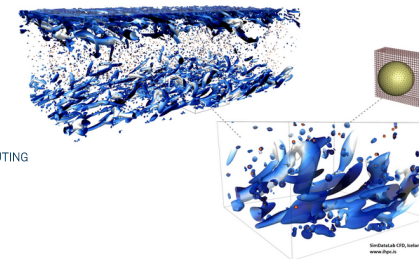
[3] IHPC SimDataLab Computational Chemistry Web Page

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[1] Icelandic HPC Community Web page



Simulation and Data Lab Computational Fluid Dynamics



Dr. Pedro Costa



Dr. Ásdís Helgadóttir



Ph.D. Student S. Reza Hassanian, M

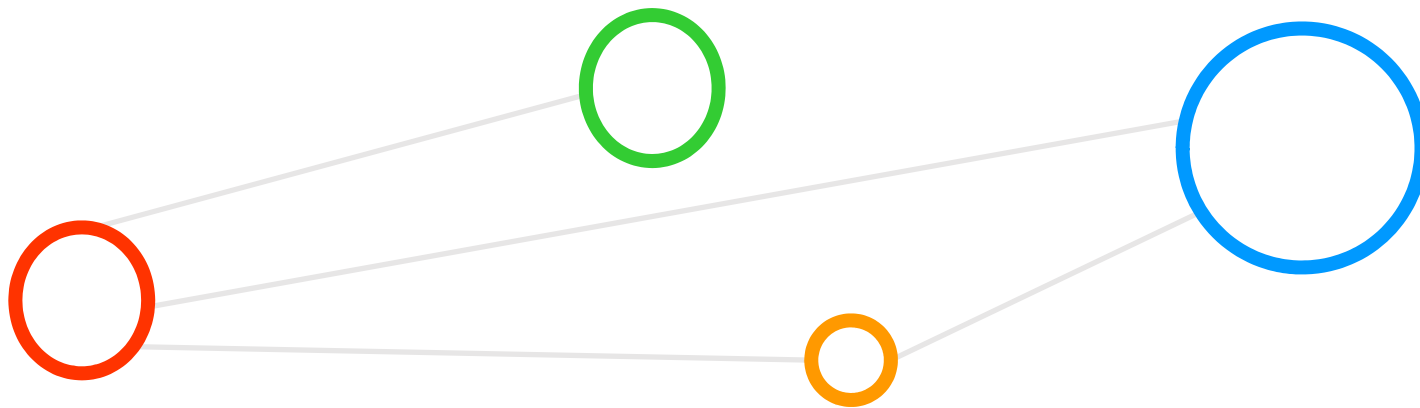


Prologue

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

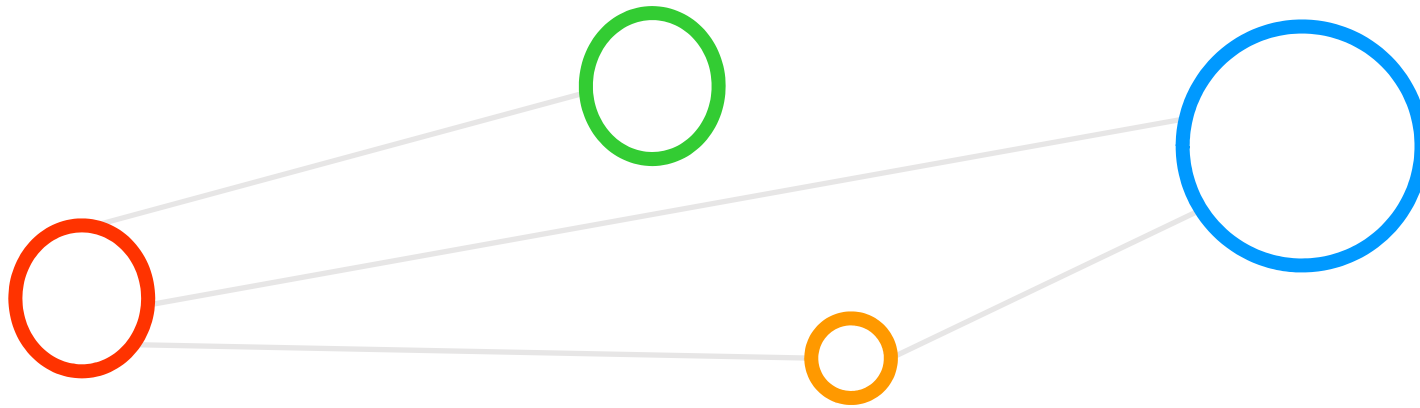
Selected References



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



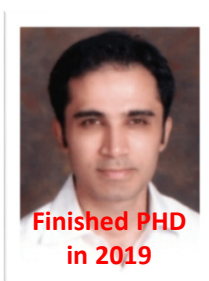
Acknowledgements – High Productivity Data Processing Research Group



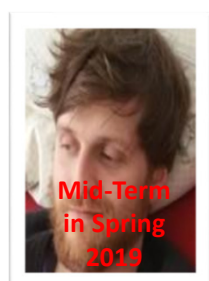
PD Dr.
G. Cavallaro



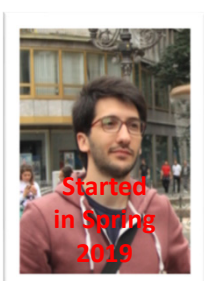
Senior PhD
Student
A.S. Memon



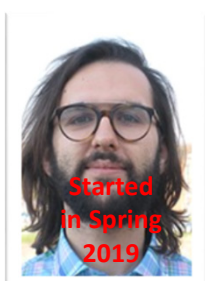
PD Dr.
M.S. Memon



PhD Student
E. Erlingsson



PhD Student
S. Bakarat



PhD Student
R. Sedona



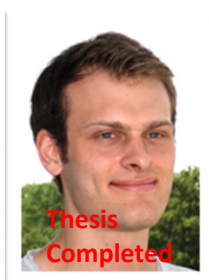
PhD Student
P. H. Einarsson



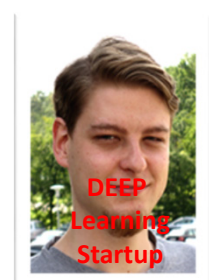
Dr. M. Goetz
(now KIT)



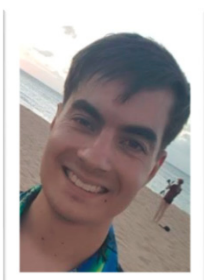
MSc M.
Richerzhagen
(now other division)



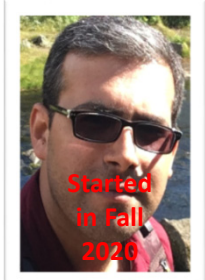
MSc
P. Glock
(now INM-1)



MSc
C. Bodenstein
(now
Soccerwatch.tv)



MSc G.S.
Guðmundsson
(Landsverkjun)



PhD Student
Reza



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