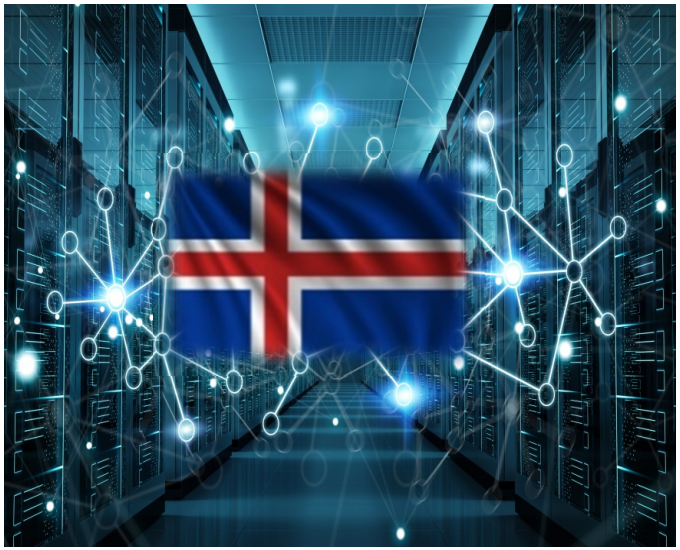


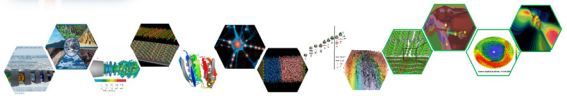
Icelandic HPC National Competence Center for HPC & AI – Welcome Address & HPC @ Iceland

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

19TH MAY 2022, RESPONSIBLE HPC WORKSHOP, REYKJAVIK DOWNTOWN

@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 · EUPEX European Pilot for Exascale · 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

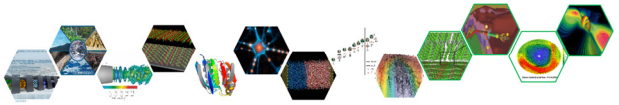
Executive Summary – Major Icelandic HPC Activities

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

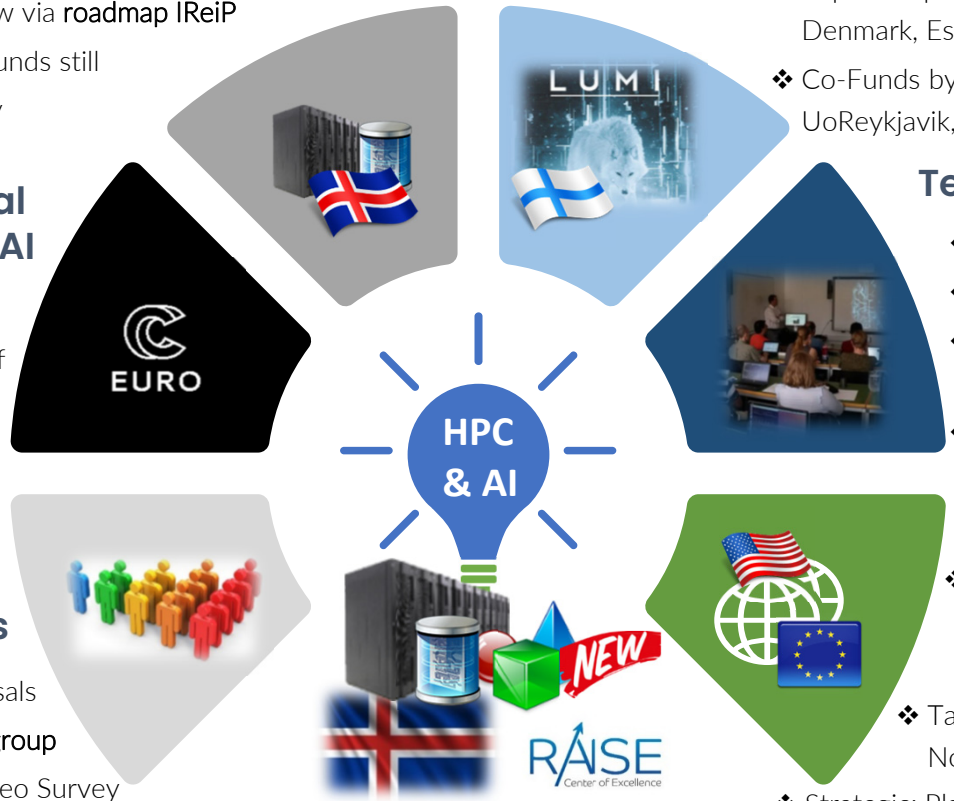
EuroHPC EuroCC National Competence Center for HPC & AI

- EU Project (09/2020-12/2022), ~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, Borealis Data Centers, 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

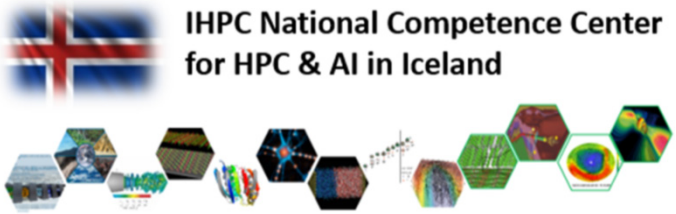
Teaching & Education in HPC & AI

- University of Reykjavik
- University of Iceland
- Arctic Webinar Series (with US partners)
- YouTube Online HPC Lectures

International Cooperations

- Tactical: ~5 Joint PhDs with Juelich Supercomputing Centre in Germany (#1 HPC System in Europe, Quantum computing)
- 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) 'Reykjavik Institute'

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.

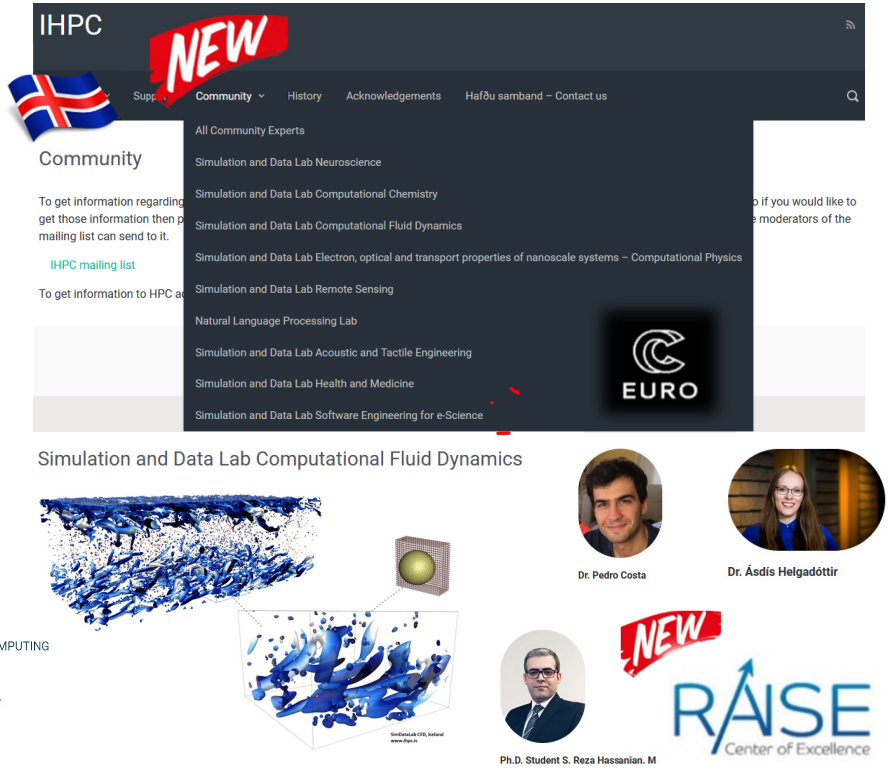
Prof. Hannes Jonsson

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



[2] IHPC SimDataLab CFD Web Page

Supercomputing 2021 Conference St. Louis – „Data Centers by Iceland“

Morris Riedel (He/Him)
Professor & Head of Research Group High Produc...
3w •

Day one at #Supercomputing #SC21 #SC2021 conference at our Data Centers by #Iceland booth & meeting our US partners
National Center for Supercomputing Applications
.
Green by Iceland
Business Iceland
Háskóli Íslands
Borealis Data Center
Verne Global
atNorth
CoE RAISE
EuroCC
EuroHPC Joint Undertaking
Forschungszentrum Jülich ...see more

Chadi Barakat and 38 others 2 comments

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Ministry Report on HPC & Reykjavik Institute

IHPC National Competence Center for HPC & AI in Iceland

UNIVERSITY OF ICELAND

HÁSKÓLINN Í REYKJAVÍK
REYKJAVIK UNIVERSITY

Reykjavík Institute & High Performance Computing – Benefits for the Icelandic Science Community

Executive Summary

Computing in general and scientific computing, in particular, have outstanding track records of providing breakthrough research results, advancing society and providing a strong basis for commercialization and growth.[1] As a result, Icelandic researchers from various academic and industry organizations have formed the Icelandic High-Performance Computing (IHPC) National Competence Center[2]. The conceptual idea of the Reykjavík Institute was co-designed by this IHPC community in close collaboration with Kaiser Global and William (Bill) Patrowicz. IHPC community members have formulated this report on the benefits of the Reykavík Institute for the Icelandic science community:

Benefit #1 Enable Access to Advanced Computing: The planned shared infrastructure usage with the Reykjavík Institute will provide an enormous improvement of Iceland's access to computational HPC resources and consequently increase the competitiveness of Iceland significantly. Hence, access to such a computing infrastructure is needed to reach Iceland's science, technology, and innovation goals.

Benefit #2 Empower Researchers via Joint Labs: The IHPC Simulation and Data Labs (SDLs) with experts in various science and engineering areas can increase and enlarge their international visibility and obtain additional grants. Dual affiliations of researchers enable very close cooperation.

Benefit #3 Expand Computing Skills & Capabilities: HPC is a research and engineering capability that delivers a clear impact. Joint university courses, hands-on training, and internships with the Reykjavík Institute increase Icelandic researchers' and students HPC skills and scientific computing capabilities.

While this report primarily focuses on the scientific community benefits, we would like to use this opportunity to emphasize the enormous impact on the local industry and Icelandic economy shortly:

Establish a new knowledge-based industry built on local know-how, resources, and location: Unlike some existing resource-based industries, a compute based knowledge industry creates high-value modern jobs, both direct and derived. The Reykjavík Institute plans to build 150 expert-level jobs in Iceland over the next five years, with an equal number of derived jobs, including digital-tech spin-offs.

Attract computing-based value-added industries, including space exploration and energy transition: A successful establishment of the Reykjavík Institute will attract enterprises and development groups benefitting from proximity to experts and computing resources. It constitutes a unique opportunity for Iceland to contribute meaningfully to the energy transition and decarbonization beyond our borders.

[1] PRACE – The Scientific Case for Computing in Europe 2018 – 2026, Online: https://prace-ri.eu/wp-content/uploads/2019/08/PRACEScientificCase.pdf
[2] Icelandic HPC (IHPC) National Competence Center & Community, Online: https://ihpc.is/community/

Benefit #1 Enable Access to Advanced Computing

'[...] the competitiveness of European science & industry will be jeopardized if sufficiently capable computers are not made available, together with the associated infrastructure and skilled people necessary to maximize their exploitation.'[3]

Scientific and engineering applications of HPC underpin all aspects of our lives. For example, HPC can quickly process scientific data and perform complex calculations at extremely high speeds. As a result, it has become an integral part of the scientific method for the physical sciences (e.g., see Figure 1 for avalanche simulations based on known physical laws).

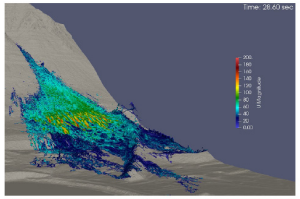

Figure 1: Avalanche simulation at Flateyri, Iceland that is only possible to compute using HPC; *Image: Tómas Jóhannesson, Icelandic MetOffice, 3rd IHPC Workshop*

The past decade showed a vast increase in HPC use across different scientific communities in Iceland. For example, the Principle Investigators (PIs) in Iceland that are part of RANNIS HPC proposals grew from roughly 17 to over 52 today. Many of those PIs are part of IHPC Simulation and Data Labs, and the number of PIs is expected to grow in the following years. That demonstrates the need for HPC resources in Iceland and benefits to cooperate closely with the Reykjavík Institute to co-design a computational infrastructure for energy, space, and the environment in Iceland.

The benefit includes usage access to that shared infrastructure in exchange for skills provided by Icelandic researchers to use and maintain scientific application codes on the Reykjavík Institute infrastructure used by a broader set of infrastructure users in the Icelandic private & public sector.

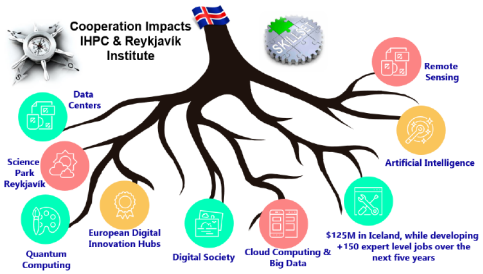

Figure 2: Selected impacts of the close cooperation between the Icelandic HPC (IHPC) community and the Reykjavík Institute, including building 150 expert-level jobs in Iceland over the next five years.

[3] PRACE – The Scientific Case for HPC in Europe 2012 – 2020, Online: https://exdci.eu/sites/all/themes/exdci_theme/images/prace_-_the_scientific_case_-_full_text_-.pdf

Áslaug Arna Sigurbjörnsdóttir

Embætti:	Háskóla-, iðnaðar- og nýsköpunarráðherra
Ráðuneyti:	Háskóla-, iðnaðar- og nýsköpunarráðuneytið
Kjördæmi:	Reykjavíkurkjördæmi suður
Þingflokkur:	Sjálfstæðisflokkur

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Benefit #2 Empower Researchers via Joint Labs

'[...] the European industry needs increased support in application development: to develop effective HPC applications is intrinsically difficult – and the adoption of such codes to new hardware (for example, to accelerators such as GPUs) requires detailed expertise.'[4]

Icelandic researchers already have excellent skills in a wide variety of HPC application areas (e.g., members of IHPC Simulation and Data Labs) and forming joint laboratories with the Reykjavík Institute will enable an amplification factor for their research.

Compared to many other data centre strategies, the Reykjavík Institute plans to create 150 expert-level jobs in Iceland over the next five years. Those job areas are in computer science and the realm of science and engineering applications that take advantage of HPC. Therefore, it makes sense to enable from the start close cooperation between the IHPC community and the Reykjavík Institute and its computational infrastructure activities. Furthermore, the dual affiliations of Icelandic researchers with the Reykjavík Institute make it possible not to lose identities with their Icelandic home organization (e.g., HI, HR, HA, MetOffice, etc.). Figure 2 shows expected initial cooperation impacts, to list a few.

The benefit for Icelandic researchers in engaging in joint laboratories with the Reykjavík Institute is to strengthen the IHPC Simulation and Data Labs by gaining more international visibility, career path options for its younger scientists, and being in a better position to win additional research grants. Apart from having a more substantial footprint in Digital/Horizon Europe EU programs, researchers can also engage in US grants (e.g., National Science Foundation, Department of Energy, etc.).

Benefit #3 Expand Computing Skills & Capabilities

HPC is a research and engineering capability built using technology, people, and processes to deliver clear business value and scientific impact. It is not just supercomputing, AI, and Quantum, and therefore it is instrumental for Iceland to enlarge its number of experts having those capabilities in the future. They enable a deeper scientific understanding and breakthroughs in nearly every scientific field.

The benefit of cooperation between the Reykjavík Institute and the IHPC community will enable a broader range of education options through new joint university courses, student education, internships, and hands-on training to massively increase the HPC research and engineering capability of Icelandic researchers.

Figure 3: William (Bill) Patrowicz (CEO, Kaiser Global) discusses the Reykjavík Institute with members of the IHPC community at the first IHPC workshop in 2021.

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University of Iceland (Prof. Morris Riedel, Prof. Jón Atli Benediktsson, Prof. Sigurður Magnús Garðarsson)
University of Reykjavík (Prof. Gísli Hjálmtýsson)

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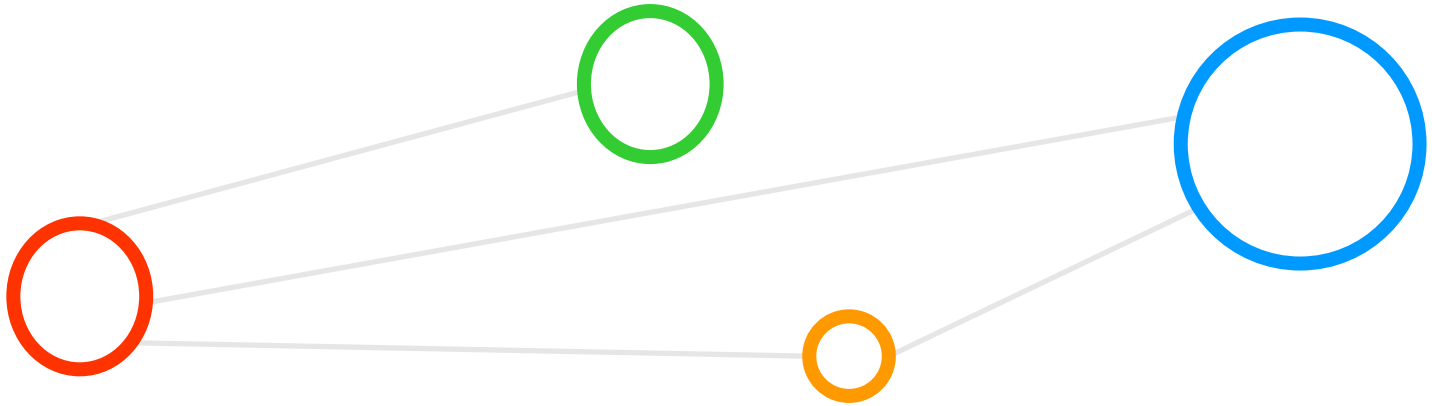
The Icelandic HPC Competence Center has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 763558 (DEEP-EST EU Project) and grants agreement No 951740 (EuroCC EU Project) & 951733 (RAISE EU Project).

[4] European Technology Platform for High Peformance Computing (ETP4HPC) Strategic Research Agenda: https://www.etp4hpc.eu/sra.html

WELCOME
RESPONSIBLE HPC WORKSHOP PARTICIPANTS

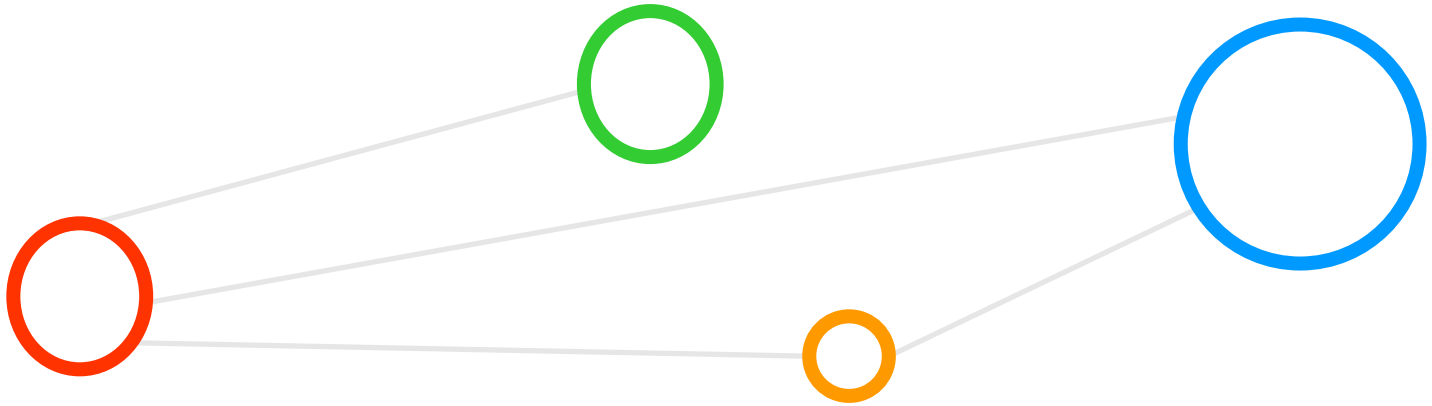
Selected References



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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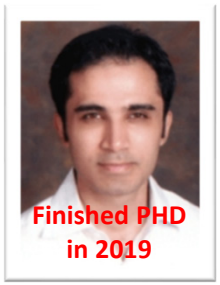
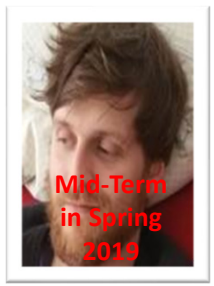


PD Dr.
M.S. Memon



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PhD Student
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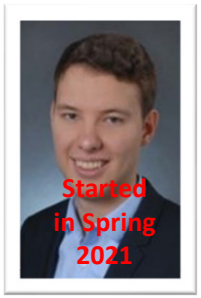
PhD Student
P. H. Einarsson

PhD Student
S. Sharma



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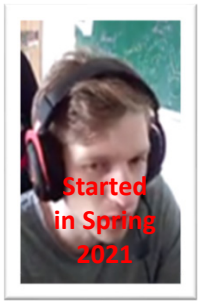

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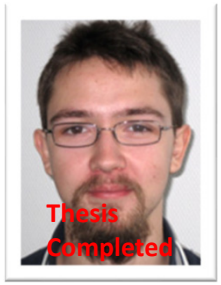

MSc M.
Richerzhagen
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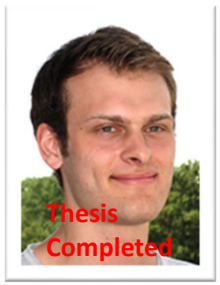

MSc
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(now INM-1)

MSc
C. Bodenstein
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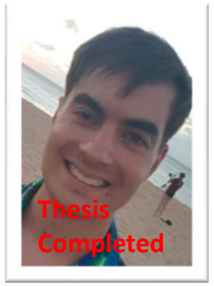
Soccerwatch.tv)



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E. Sumner

This research group has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 763558 (DEEP-EST EU Project) and grant agreement No 951740 (EuroCC EU Project) & 951733 (RAISE EU Project) & 956748 (ADMIRE EU Project)


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Test
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