

HPC2N Open House and Kebnekaise Celebration 30 November 2017

High Performance Computing Center North



A national center with first-class resources and expertise

Scalable and parallel high performance computing

High Performance Computing Center North



A national center with first-class resources and expertise

Large-scale storage facilities

High Performance Computing Center North



A national center with first-class resources and expertise

Grid and cloud computing

High Performance Computing Center North



A national center with first-class resources and expertise

Software and advanced support for eScience applications

High Performance Computing Center North



A national center with first-class resources and expertise

International network for research and development

High Performance Computing Center North



A national center with first-class resources and expertise HPC2N is mainly funded by: **SNIC** Our partners:





The Kebnekaise massif – The Beauty!



The Kebnekaise Cluster - The Beast?? No, the Beauty of Computing



































Assembling Hardware – Putting Things in Place















Getting Kebnekaise Ready and Running



Getting Kebnekaise Ready and Running



Getting Kebnekaise Ready and Running














Kebnekaise and Abisko













Lustre Parallel File System



HPC2N Project Portfolio

More than 100 research projects are using Kebnekaise:

- Biosciences and medicine
- Computing science
- Chemistry
- Engineering
- Material science
- Mathematics and statistics
- Physics and astronomy





Three and four-dimensional teraspin systems

Klas Markström Umeå University

Large-Scale Simulations in Stability, Transition, Turbulence and Control

Dan Henningson KTH

Uppsala Computational Biochemistry Initiative

Lynn Kamerlin Uppsala University

Molecular Dynamics Simulations - Theory and Applications

David Van Der Spoel Uppsala University





Molecular level investigations of (organo)clays

Michael Holmboe Umeå University

Computational studies of metalloproteins and ligand binding

Ulf Ryde Lund University

Computational Materials Science: Perovskite solar cell, solar fuel production, sensors, two-dimensional materials, materials for energy storage and solar cell

Rajeev Ahuja Uppsala University

Large Scale Simulations in Biomolecular and Nanomaterial Science

Alexander Lyubartsev Stockholms University





Studies of intense laser-matter interactions

Mattias Marklund Chalmers

Computational condensed-matter chemistry: Ion solvation and metal oxide surfaces

Kersti Hermansson Uppsala University

Atomistic design of functional materials

Levente Vitos Royal Institute of Technology

Theory of simple and complex materials

Sergei Simak Linköping University



Biocompatibility of Biomaterials with Bacterial and Mammalian Membranes

Madeleine Ramstedt Umeå University

Electronic structure and atomistic modelling for materials science

Andreas Larsson Luleå Technical University





Continuous-Space Methods for Natural Language Processing

Joakim Nivre Uppsala University

Physics of the solar atmosphere

Jorrit Leenaarts Stockholm University

NLAFET: Parallel Numerical Linear Algebra for Future Extreme Scale Systems

Bo Kågström Umeå University

Theoretical studies of ultra-fast molecular dynamics and electronic structure in liquids, superconductors and solar cells

Michael Odelius Stockholm University





Targeting the dynamical differences in acetylcholinesterase from mosquito and non-target species for the development of new insecticides to combat malaria and dengue

Anna Linusson Umeå University

Large-scale bio and materials modeling across spatial and temporal scales

Aatto Laaksonen Stockholm University

Deep learning for protein structure prediction

Arne Elofsson Stockholm University

Strongly scalable algorithms for matrix and tensor computations

Lars Karlsson Umeå University





Modeling solar wind interactions

Mats Holmström Swedish Institute of Space Physics

Studies in heterogeneous catalysis and x-ray spectroscopy of water

Lars G.M. Pettersson Stockholm University

Efficient studies of large-scale topological superconductors

Annica Black-Schaffer Uppsala University

Ab-initio Calculations for the Design of Functional Nanoscale Thin Film Materials

Lars Hultman Linköping University





Theoretical studies of complex magnetism

Lars Nordström Uppsala University

Numerical design optimization

Eddie Wadbro Umeå University

Novel Functional Organic Materials and the Organic Materials Database

Alexander Balatsky NORDITA

Membrane heterogeneity and viral binding

Peter Kasson Uppsala University





Computational materials science applied to solid state physics

Olle Eriksson Uppsala University

Wave-particle interactions in the complex environment of a comet

Maria Hamrin Umeå University

Population genomics of conifer trees

Xiao-Ru Wang Umeå University

Large-scale Simulations in Complex Flows

Luca Brandt Royal Institute of Technology





Towards a process-based understanding of speciation and reverse speciation

Åke Brännström Umeå University

Dynamics of complex physical systems

Claude Dion Umeå University

Genome-wide association study and genomic selection to assist forest breeding of eucalyptus

Biyue Tan Umeå University

Computational modelling of discrete metal oxide systems

Andy Ohlin Umeå University





Molecular simulations of biological processes to aid in the understanding of the function of peroxiredoxins and protein tyrosine kinases

Kwangho Nam Umeå University

First Principles Simulations of Nano Electronics and Photonics

Yi Luo Royal Institute of Technology

Investigation of mechanism and structural dynamics in the human MAPEG enzymatic family

Jesper Haeggstrom Karolinska Institutet

Integrated Computational Engineering of High-performance Alloys

Pavel Korzhavyi Royal Institute of Technology



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Thanks and credits!



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