Introduction

ReiDok-13 is an abbreviation from the Icelandic Reiknifræðileg doktorsverkefni or Computational doctoral projects. The purpose of the symposium is to provide a forum for PhD students and post-docs at the University of Iceland and Uppsala University whose projects are of a computational nature to give a talk on their project, learn from each other, and get to know one another. These projects come from a variety of disciplines, including statistics, computer science, engineering, chemistry and physics. Some involve considerable computer programming and others less, and the computational devices range from laptops to computer clusters. The mini-symposium is jointly organized by the Faculty of industrial and mechanical engineering and computer science and the Faculty of science at the University of Iceland and the Department of Information Technology at Uppsala University.

There has been a substantial increase in the number of computing PhD students and postdocs at the Universities in recent years, and it is interesting to learn more about this flourishing activity. There are many aspects of computational projects that are common across different disciplines, and such a multidisciplinary meeting gives the participants an opportunity to get new ideas and see their own projects in a new light.

Organizing Committee

Kristján Jónasson, Professor, Department of Computer Science, University of Iceland
Sverker Holmgren, Professor, Department of Information Technology, Uppsala University
Sven Þ. Sigurðsson, former Professor, Department of Computer Science, University of Iceland
Ebba Þóra Hvannberg, Professor, Department of Computer Science, University of Iceland
Sæmundur Óskar Haraldsson, PhD student, Department of Computing Science, University of Stirling
Programme

08:15–08:25  Registration, coffee, conference opening.

08:25–08:40  e-Science at Uppsala by Professor Sverker Holmgren

08:40–09:10  Implementation of orbital density dependent functionals for electronic structure and calculations of Rydberg excited states of molecules by Hildur Guðmundsdóttir

09:10–09:35  Scalable Computational and Data Management Solutions for Scientific Applications by Salman Toor

09:35–10:00  Global optimisation applied to metal nanoclusters by Anna Garden

10:00–10:25  Magnetic field and spin influences on the electron transport through a quantum ring in a photon cavity by Thorsten Ludwig Arnold

10:25–10:45  Break

10:45–11:10  Combining efficiency and good software design by Malin Källén

11:10–11:35  Adaptive mesh refinement for high-dimensional PDEs by Magnus Grandin

11:35–12:00  Supervising Learning Linear Composite Dispatch Rules for Scheduling by Helga Ingimundardóttir

12:00–12:25  Diagrammatic perturbation theory for non-equilibrium spin transport by Christoph Hübner

12:25–13:25  Lunch

13:25–13:50  Improved minimum mode following method for finding first order saddle points by Manuel Plasencia Gutierrez

13:50–14:15  Smooth and Sparse Hyperspectral Unmixing using an l0 penalty by Jakob Sigurðsson

14:15–14:40  Computational search for catalysts that enable fuel production from CO2 by Javed Hussain

14:40–15:05  Detection of Multiple QTL in Known Crossings by Behrang Mahjani

15:05–15:20  Break

15:20–15:45  Numerical simulation of the higher harmonic generation process by Emil Kieri

15:45–16:10  A computational approach to catalyst design - Searching for a new way to make fertilizer by Younes Abghoui

16:10–16:35  Fourier-based quantum optimal control by Katharina Kormann

16:35–17:00  Electrons and holes in a quantum dot by Pei-yi Lin

17:00–19:00  Social event in Hôtel Holt

20:00-  Symposium dinner at Restaurant Caruso
## List of presenting participants

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<tr>
<td>Anna Garden</td>
<td>Egill Skúlason</td>
<td><a href="mailto:annagarden@gmail.com">annagarden@gmail.com</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Behrang Mahjani</td>
<td>Sverker Holmgren</td>
<td><a href="mailto:behrang.mahjani@it.uu.se">behrang.mahjani@it.uu.se</a></td>
<td>Uppsala University</td>
</tr>
<tr>
<td>Christoph Hübner</td>
<td>Viðar Guðmundsson</td>
<td><a href="mailto:chuebner@physnet.uni-hamburg.de">chuebner@physnet.uni-hamburg.de</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Emil Kieri</td>
<td>Sverker Holmgren</td>
<td><a href="mailto:emil.kieri@it.uu.se">emil.kieri@it.uu.se</a></td>
<td>Uppsala University</td>
</tr>
<tr>
<td>Helga Ingimundardóttir</td>
<td>Tómas Philip Rúnarsson</td>
<td><a href="mailto:hel2@hi.is">hel2@hi.is</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Hildur Guðmundsdóttir</td>
<td>Hannes Jónsson</td>
<td><a href="mailto:hildur.gud@gmail.com">hildur.gud@gmail.com</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Jakob Sigurðsson</td>
<td>Magnús Orn Ulfarsson, Jóhannes R. Sveinsson</td>
<td><a href="mailto:jakob.sigurdsson@gmail.com">jakob.sigurdsson@gmail.com</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Javed Hussain</td>
<td>Hannes Jónsson</td>
<td><a href="mailto:jah1@hi.is">jah1@hi.is</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Katharina Kormann</td>
<td>Sverker Holmgren, Eric Sonnendrücker</td>
<td><a href="mailto:katharina.kormann@tum.de">katharina.kormann@tum.de</a></td>
<td>Uppsala University</td>
</tr>
<tr>
<td>Magnus Grandin</td>
<td>Sverker Holmgren</td>
<td><a href="mailto:magnus.grandin@it.uu.se">magnus.grandin@it.uu.se</a></td>
<td>Uppsala University</td>
</tr>
<tr>
<td>Malin Källén</td>
<td>Sverker Holmgren</td>
<td><a href="mailto:malin.kallen@it.uu.se">malin.kallen@it.uu.se</a></td>
<td>Uppsala University</td>
</tr>
<tr>
<td>Manuel Plasencia Gutierrez</td>
<td>Hannes Jónsson</td>
<td><a href="mailto:mpg2@hi.is">mpg2@hi.is</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Pei-yi Lin</td>
<td>Viðar Guðmundsson</td>
<td>wagamama@<a href="mailto:jan@gmail.com">jan@gmail.com</a></td>
<td>University of Iceland</td>
</tr>
<tr>
<td>Salman Toor</td>
<td>Sverker Holmgren</td>
<td><a href="mailto:salman.toor@helsinki.fi">salman.toor@helsinki.fi</a></td>
<td>Uppsala University</td>
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<td>Thorsten Ludwig Arnold</td>
<td>Viðar Guðmundsson</td>
<td><a href="mailto:tla1@hi.is">tla1@hi.is</a></td>
<td>University of Iceland</td>
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<td>Younes Abghoui</td>
<td>Egill Skúlason, Hannes Jónsson</td>
<td><a href="mailto:yoa2@hi.is">yoa2@hi.is</a></td>
<td>University of Iceland</td>
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Global optimisation applied to metal nanoclusters.

Anna L. Garden, Andreas Pedersen, Egill Skúlason and Hannes Jónsson
Science Institute, University of Iceland

The task of determining the lowest energy arrangement of atoms in nanoclusters is a serious global optimisation challenge already for a cluster containing a hundred atoms. As the size of the system grows, the number of minima on the potential energy surface increases exponentially and a thorough sampling becomes difficult. In the current study an optimisation algorithm based on the adaptive kinetic Monte Carlo (AKMC) algorithm is employed to determine the lowest energy configurations of metal nanoclusters.

Nanoclusters with up to a few thousand atoms are known to exhibit interesting and novel properties, which differ drastically from those of the bulk crystal. The catalytic activity of such clusters is often very high and strongly dependent on the cluster size. In addition to size effects, it is known that catalytic activity on metal surfaces can be dominated by steps and defects in the surface. Thus it follows that, to accurately predict the catalytic activity of a cluster, it is necessary to determine the global minimum energy structure of the cluster, including a full description of the edges and any defects.

Participation in epistasis (PAS)

Behrang Mahjani and Sverker Holmgren
Uppsala University

Most important traits in humans, animals and plants can be seen as quantitative traits and affected both by the genetic composition and the environment. Quantitative traits are traits that exhibit a continuous phenotype distribution. The underlying genetic architecture of a quantitative trait can be described by identifying a set of quantitative trait loci (QTL) in the genome for a population and attributing effect values to these loci using a suitable statistical model. In a QTL search, the evaluation of the statistical model is repeated for a large set of candidate positions in the genome to determine the QTL locations that results in the best model fit. Mathematically, this corresponds to solving a global optimization problem using some optimization scheme.

We present an efficient and reliable multiple QTL scans algorithm for experimental populations. Other optimization approaches, e.g. the DIRECT optimization algorithm, have earlier been adopted to QTL search problems. Speedups of several orders of magnitudes in DIRECT permits high dimensional QTL scans to be performed. However, since a heuristic termination criterion must be used in these types of algorithms the accuracy of the optimization process cannot be guaranteed. Indeed, previous results also show that a small bias in the significance thresholds is sometimes introduced. Our new optimization scheme, PruneDIRECT, has a well-defined error bound and can in practice be guaranteed to be equivalent to a corresponding exhaustive search. We present simulation results that show that for simultaneous mapping of three QTL using permutation testing, PruneDIRECT is typically more than 50 times faster than exhaustive search.
Diagrammatic perturbation theory for non-equilibrium spin transport

Christoph Hübner and Viðar Guðmundsson
Science Institute, University of Iceland

The real time diagrammatic transport theory from König et al., based on the Keldysh formalism, is used to determine the diagonal elements of the reduced density matrix in the stationary limit. As a specific case, spin transport between two non-polarized electron reservoirs via an idealized single level quantum dot with an incorporated magnetic impurity is investigated. A mathematica script was used for the calculations. It is capable of switching between analytic transformations, diagrammatic conversions and numerical computations. The build in functions allow to display intermediate results in any desired form. In particular for the investigated system this allowed to point out critical points in the formalism. The transparency of the computation steps leads to a deep insight into the physical mechanism leading to the computed results for sequential and cotunneling. The advantages and disadvantages of such a mathematica script compared to an intermediate-level programming language like C++ are going to be presented.

Numerical simulation of the higher harmonic generation process

Emil Kieri
Division of Scientific Computing, Department of Information Technology,
Uppsala University

In higher harmonic generation (HHG) from atomic gases, atoms are ionised by a laser beam. The detached electrons are accelerated in the oscillatory electric field of the laser, and may return and recombine with the nucleus. A high energy photon, a higher harmonic, is then emitted. The HHG process has extensive applications in experimental physics as the generator of short pulses in the extreme ultraviolet regime. Such pulses can be used e.g. for time-resolved spectroscopy of electron dynamics. We consider simulation of the process using the time-dependent Schrödinger equation. In this talk we will discuss two of the main challenges which emerge when this equation is to be solved numerically. First, the Coulomb potential, which describes the interaction between charged particles, is singular. This limits the regularity of the solution, high order methods are therefore not performing to their full potential. Second, the computational domain must be truncated to finite size. It must then also be equipped with absorbing boundary conditions such that escaping electrons are not reflected back into the domain, polluting the solution.
The study introduces a framework in which dispatching rules for job-shop and permutation flow-shop scheduling problems are discovered by analysing the characteristics of optimal and sub-optimal solutions. Training data is created via randomly generated problem instances and their corresponding optimal solution by inspecting optimal versus suboptimal dispatches. Linear classification is applied in order to identify good choices from worse ones, at each dispatch iteration, in a supervised learning fashion. The method is purely data-driven, thus less problem specific insights are needed from the human heuristic algorithm designer. Experimental studies show that the learned linear composite dispatching rules outperforms common single priority dispatching rules, with respect to minimum makespan. Moreover, models created by training data from problem sizes of low dimension are reasonably robust for higher dimensions.

Keywords: Scheduling & Composite dispatching rules & JSP & PFSP & Generating training data & Sampling & Scalability & Ordinal Regression

Orbital density dependent functionals and Rydberg states of molecules

Hildur Guðmundsdóttir
Science Institute, University of Iceland

We have implemented a recently developed method for optimizing functionals of orthonormal functions that are not invariant under unitary transformation [1]. The method is implemented in the electronic structure software package GPAW [2], and has enabled us to carry out self-interaction corrected density functional theory (DFT) calculations of electronically excited molecules. The calculations are carried out for the valence electrons, represented on a real space grid, and the core region is treated with the projector-augmented wave method [3].

First a Rydberg state orbital is estimated using DFT with Perdew-Zunger self-interaction correction [4] by means of an optimized effective potential. In the subsequent step, the binding energy of the excited electron is obtained by placing it in the Rydberg state orbital, while a self-consistent DFT calculation is carried out for the rest of the electrons [5].

Results are presented for the first few Rydberg states of Ne, H₂O, NH₃ and trimethylamine. The accuracy in the energy of the molecular Rydberg states is typically on the order of 0.1 eV. The computational effort scales as $NM^2$ where $N$ is the number of orbitals and $M$ is the number of grid points included in the calculation. Due to the slow scaling of the computational effort with system size and the high level of parallelism in the grid approach, the method makes it possible to estimate Rydberg states of large molecules.

References

Smooth and Sparse Hyperspectral Unmixing using an l0 penalty

Jakob Sigurðsson
School of Engineering and Natural Sciences, University of Iceland

Hyperspectral unmixing is an important technique for analyzing hyperspectral remote sensing images. We propose an estimation algorithm that, simultaneously, encourages smoothness in the endmembers and sparseness in the abundances by using first order roughness and l0 penalties. The method is evaluated both on simulated data and real hyperspectral imagery.

Computational search for catalysts that enable fuel production from CO₂

Javed Hussain, Egill Skúlason and Hannes Jónsson
Science Institute and Faculty of Physical Sciences, University of Iceland

Density functional theory (DFT) for describing approximately systems of even up to a thousand electrons and transition state theory methods for finding the mechanism and rate of atomic scale transitions have made it possible to simulate, for example, elementary steps in catalyzed chemical reactions. This methodology has become an efficient tool for the design of new and improved heterogeneous catalysts. We are using this approach to identify catalysts that can be used for electrochemical reduction of CO₂ to form hydrocarbons such as methanol and methane. In combination with renewable electricity sources such as hydro, solar, wind and geothermal, such a process could potentially enable CO₂ neutral and sustainable fuel production. The electrochemical reduction of CO₂ on stepped surfaces and edges of nanoparticles have, in particular, been studied. The calculations provide an explanation for why copper is a uniquely efficient catalyst for electrochemical reduction of CO₂ to hydrocarbons, while nickel and palladium show only moderate efficiency and other commonly used catalysts such as platinum have negligible catalytic efficiency.
Fourier-based quantum optimal control

Katharina Kormann
Zentrum Mathematik, Technische Universität München

The dynamics of quantum systems can be steered by the interaction with a tuned electric field. The problem of designing an optimal field can be posed as an optimal control problem. We reformulate the optimization problem by using a Fourier transform of the electric field, and narrow the frequency band. The resulting problem is less memory intense and can be solved with a superlinearly convergent quasi-Newton method. Moreover, this formulation allows the inclusion of additional physical constraints such as phase-only optimization. We show computational results for a Raman-transition example and give numerical evidence that our method can outperform the standard monotonically convergent algorithm. Also, potential application to higher harmonic generation (cf. talk by E. Kieri) will be discussed.

Acknowledgements. Different parts of the presented work where done in collaboration with Sverker Holmgren, Hans O. Karlsson, Markus Kowalewski, and Emil Kieri.

Adaptive mesh refinement for high-dimensional PDEs

Magnus Grandin
Uppsala University

Accurate solution of time-dependent, high-dimensional PDEs requires massive-scale parallel computing and efficient numerical techniques. Spatial decomposition is particularly challenging in higher dimensions, since the memory requirements for uniform grids with fine enough resolution quickly grow prohibitively large and out of reach even for massively parallel computers. We present a framework for adaptive mesh refinement that is tailored for spatial decomposition of localized solutions in domains of high dimensionality. Key features of our framework are: (1) block-structured grids, partitioning the domain into logical hyperrectangles, (2) anisotropic refinement by recursive bisection and (3) an efficient binary tree structure that stores the hierarchy of grid blocks and provides all necessary information on how the blocks relate to each other. We have successfully combined this scheme with high-order finite element and finite difference methods (SBP-SAT) to provide stable and accurate discretizations. Furthermore, we show how to partition and load balance an adaptive grid in a distributed environment, aiming at massive scale parallel computing.
Combining efficiency and good software design

Malin Källén
Uppsala university

HAParaNDA (High dimensional Adaptive Parallel Numerical quantum Dynamics API) is a parallel software framework used for solving the time dependent Schrödinger equation, which arises from problems in quantum dynamics. The time needed for solving the equation increases exponentially with the number of particles. Therefore, an important challenge is to make the computations efficient.

At the moment, we are two PhD students whose main focus is on developing HAParaNDA, and yet another couple of researchers who contribute to the code. The amount of code in HAParaNDA is currently about 20 000 lines, and it will increase in the future. Therefore, another important aspect is the readability.

In order to get the code well structured and readable, I am at the moment working on its design. My goal is to make the design fully object oriented and as flexible as possible. Readability and flexibility are not necessarily contradictory to efficiency, but in some cases compromises have to be done.

In my presentation, I will introduce HAParaNDA and discuss some issues that have to be considered in my work on designing for maintainability while keeping the framework as efficient as possible.

Adaptive mesh refinement for high-dimensional PDEs

Manuel Plasencia Gutiérrez¹, Andreas Pedersen¹ and Hannes Jónsson¹,²
¹Science Institute of University of Iceland, ²Faculty of Physical Sciences

The task of finding first order saddle points on a high dimensional surface arises in many different contexts. One is an estimation of the mechanism and rate of rare events such as thermally driven diffusion or reaction events in atomic systems within harmonic transition state theory. Another is global optimization where one local minimum of an objective function after another is found by traversing through the vicinity first order saddle points [1]. The minimum mode following (MMF) method [2] is an efficient method for finding first order saddle points specially when the evaluation of second derivatives of the objective function and explicit construction of the Hessian is difficult or costly. There, a local minimization of a ‘dimer’, i.e. two replicas of the system variables separated by a fixed, small displacement, is used to determine the direction in which the second derivative is minimal. The gradient is then inverted along this direction and the transformed gradient used in an optimization method such as conjugate gradients to converge on a first order saddle point. The MMF method is often used to find saddle points on surfaces corresponding to more than a thousand variables.

In the present project, various improvements to the method are being developed, in particular by keeping track of moves where the locally minimal second derivative changes sign. Such a move corresponds to crossing the boundary of the basins of attraction of a first order saddle point and special care needs to be taken in the optimization. The revised method is illustrated with 2-dimensional test problems and is being applied to a test system consisting of a 7-atom island on a crystal surface, a system including several hundred degrees of freedom.

References


Electrons and holes in a quantum dot

Pei-yi Lin
Faculty of Physical Sciences

Quantum confinement effect appears when the size of semiconductor is smaller than the Bohr radius of the material that forms potential and traps electrons and holes in the system. Quantum dots are noteworthy for its quantum confinement effects and atom-like energy levels. The atom-like behavior of quantum dots leads outstanding transport properties and are agreed to be one of the fabricated devices. Electron and hole electronic spectrums are demonstrated by combining single band model for electron and four-band Luttinger-Kohn k.p model for the valence holes within the 3D-parabolic potential of a QD.

Scalable Computational and Data Management Solutions for Scientific Applications

Salman Toor¹
¹Helsinki Institute of Physics (HIP), Finland

The need of large-scale computational and storage infrastructures have became an essential part of almost every scientific discipline. Several different architectures have been considered over the time, ranging from batch-oriented cluster computing to elastic solutions based on distributed heterogeneous infrastructures. In this talk I will present two major areas of my research:

- An open-source cloud infrastructure for the Compact Muon Solenoid (CMS) experiment at CERN [a].
- The strength of Chelonia [b] with SciSPARQL [c], a distributed data management solution for scientific applications.

In the first project, the infrastructure is based on Openstack [d] components for structuring a private cloud together with the Gluster [e] filesystem. The Openstack cloud platform is one of the fastest growing solutions in the cloud world. The components provide solutions for computational resource (NOVA), instance (GLANCE), network (QUANTUM) and security (Keystone) management all underneath an API layer that supports global applications, web clients and large ecosystems. One important component that is currently not part of the Openstack suite is a network file system. To overcome this limitation we have used GlusterFS, a network-based file system for high availability.

The second project focuses on large scale data management solution. One of the known limiting factor in most of the current solutions is that they only support batch processing in which a complete data file needs to be transferred from the data store to the computational node. This approach is inadequate to meet the requirements of upcoming data-intensive applications. The proposed architecture composed of a database-enabled distributed storage system, Chelonia, and SciSPARQL, a language that extends SPARQL to queries over numeric scientific data. It is developed in Uppsala Database Laboratory (UDBL). The Chelonia storage system is a joint effort of the NorduGirid collaboration. The database extension of Chelonia is locally build for this project, thus not part of the original Chelonia distribution available from NorduGrid. The system is capable of interactive online data analysis by SPARQL queries over simple (numbers and strings) and complex (e.g. matrices or tensors) numeric data.

References

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c http://doi.ieeecomputersociety.org/10.1109/ICDEW.2012.67
d http://www.openstack.org
e http://www.gluster.org
Magnetic field and spin influences on the electron transport through a quantum ring in a photon cavity.

Thorsten Ludwig Arnold
Faculty of Physical Sciences

We investigate time-dependent transport of electrons under non-equilibrium conditions using a time-convolutionless non-Markovian master equation to describe an open system coupled to biased semi-infinite leads. We applied our approach to a two-dimensional broad quantum ring in a photon cavity running numerous calculations for various magnetic field strengths and different photon field polarizations. The calculations required in total about 230,000 CPU hours on the NHPC. We find strong deviations of the lead-system-lead current from Aharonov-Bohm oscillating behavior in the case of photon field polarization perpendicular to the transport direction. The current deviations are associated with the energy difference of the most relevant many-body states. Recently, we implemented the interaction of the electron’s spin with the magnetic field and orbital motion both for the central ring system and the leads. The numerical effort increases by more than a factor of 2 due to complications for the electron-electron, electron-photon and system-leads interaction. Hence, grid and cutoff parameters of the exact numerical calculations have to be selected very carefully. Furthermore, optimization and parallelization is absolutely required. Preliminary results indicate photonic deviations of Aharonov-Casher oscillations.

A computational approach to catalyst design - Searching for a new way to make fertilizer

Younes Abghoui, Hannes Jónsson and Egill Skúlason
Science Institute and Faculty of Physical Sciences, University of Iceland

Density functional theory has made it possible to calculate approximately the properties of electronic systems with up to even a thousand electrons. Together with methods for determining the mechanism and rate of transitions, this has made it possible to simulate elementary steps in chemical reactions in the presence of heterogeneous catalysts. These techniques are being used to help develop a new, electrochemical method for making ammonia, the key step in producing fertilizer. Since the early 20th century, ammonia has been synthesized primarily using the Haber-Bosch process, in which gaseous nitrogen ($N_2$) and hydrogen ($H_2$) are passed over ruthenium or iron-based catalysts at high temperature and pressure. In stark contrast to the industrial process, the enzyme nitrogenase catalyzes the formation of ammonia at ambient temperature and pressure by reacting gaseous $N_2$ with protons ($H^+$) from solution and electrons ($e^-$) from the enzyme. This electrochemical approach avoids the need for harsh industrial conditions. The calculations are used to model electrochemical formation of ammonia on the surface of various transition metal nitrides, in an attempt to find an optimal catalyst that can form ammonia electrochemically at ambient temperature and pressure.