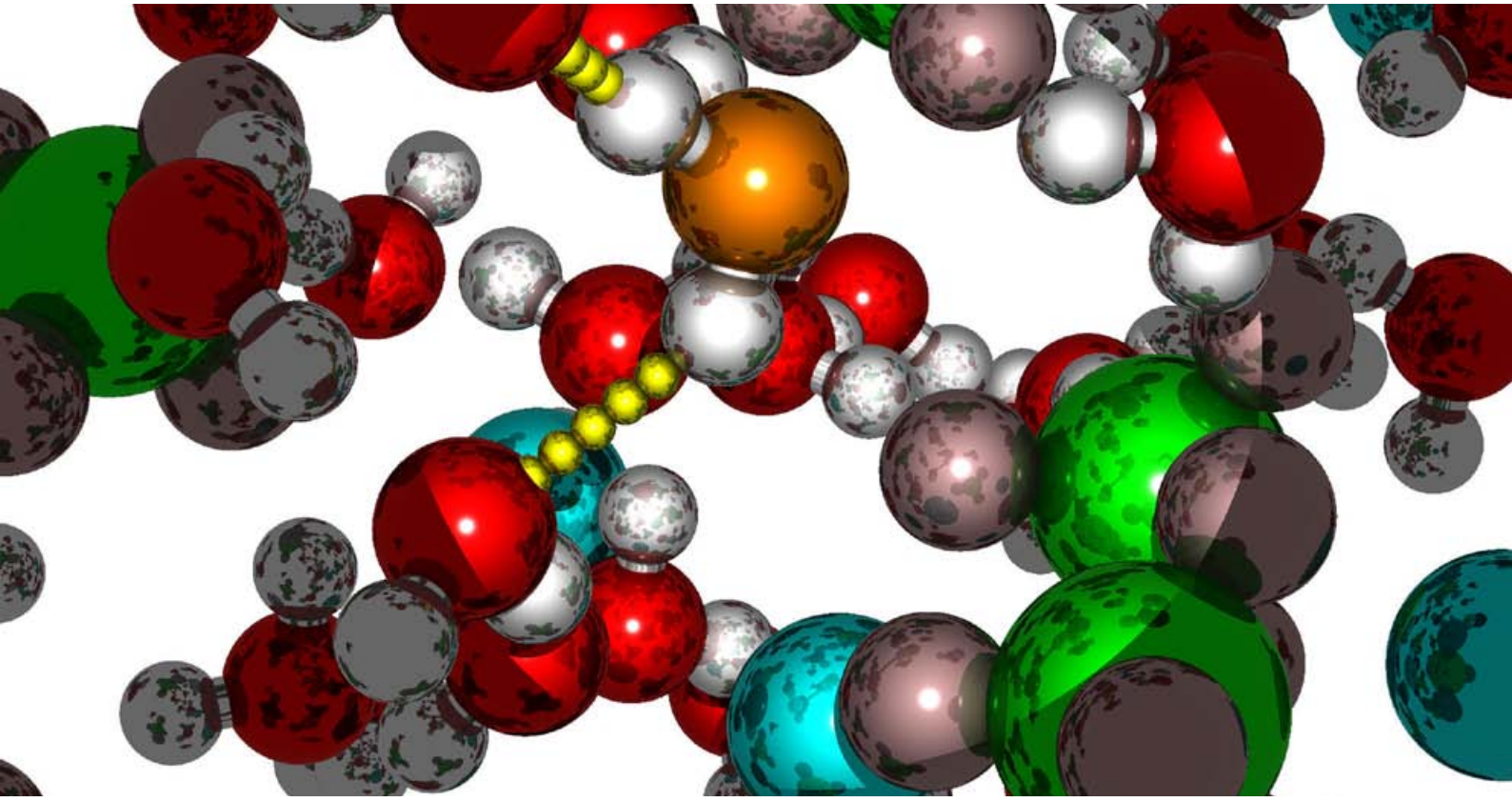
NSC News
National Supercomputer Centre at Linköpings universitet
2010:2

Aqueous solution



Hydrogen bond exchange in aqueous solution

Liquid water is held together in an ever fluctuating network of hydrogen (H) bonds, which determines its peculiar properties. In a combination of ab initio molecular dynamics simulations and infrared spectroscopy, Michael Odelius and collaborators have resolved the basic step for H-bond rearrangement.

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Materials simulations for technology-oriented energy research

The newest compute resource at NSC will serve the Network of Excellence "MATerials simulations for Technology-oriented Energy Research", MATTER.

Read further on page 5

More application experts and computational scientists at NSC

After a warm and nice summer in Sweden, I wish you all welcome back to a new academic year with new fresh ideas to solve your important scientific problems. Thanks to governmental financial support to the e-science consortia via SNIC, several additional application experts will be employed at the SNIC centres in the near future. At NSC, we will now have application expertise in chemistry, materials sciences and bioinformatics. These application experts will help our users in installing software, testing new programs and selecting the proper parameters for the most efficient execution of the programs.

In addition, we also have computational scientists' expertise at NSC that can help our users with code optimisation. This is becoming increasingly important when using massively parallel systems both within Sweden and at the European level with the new PRACE resources. NSC is therefore now launching a call for code optimisation projects and I would kindly invite all of you that have codes which need to be optimised to run more efficiently on parallel systems to this call. The proposals will be prioritised depending on scientific value and technical feasibility, and a number of projects will have the opportunity to get assistance from NSC. During autumn, we will also expand our software developer staff in order to meet the increased requirements from SNIC national storage development, needs for secure and user-friendly data access, international collaborations in climate data storage, and additional projects.

NSC has during summer started the preparations for a new, larger computer hall, which is necessary to host future NSC systems. In order to meet the exponentially increasing user requirements, the next generation of computers will not fit in the current hall. Even though new systems are more energy efficient when looking at computational capacity per kW, the total energy consumption for the complete cluster still grows, since the demands increase more than energy efficiency gains. The new hall is expected to be ready during autumn 2011.

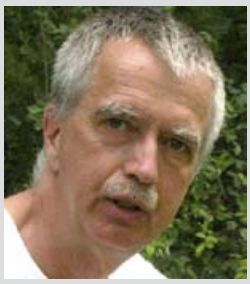
Finally, on behalf of NSC, I would like to cordially congratulate our sister centre PDC in Stockholm on their 20th anniversary which will be celebrated on August 30 and 31. We are looking forward to continued good collaborations within the high performance computing field.

BENGT PERSSON, NSC DIRECTOR

Increased number of application experts at the SNIC centres

The increased governmental resources to the e-science consortia SERC and ESSENCE that are channelled via SNIC have now resulted in that a number of new application experts will be employed at several SNIC centres. The additional experts at NSC will be in the subjects material sciences, electron structures, and bioinformatics. At PDC in Stockholm, there will be new experts in flow mechanics/turbulence and biomolecular simulations. UPPMAX in Uppsala will get expertise in material modelling and C3SE in Gothenburg in material sciences. Furthermore, increased grid computing competence will be set up also in Uppsala, Lund, and Umeå. All these experts give important addition to the SNIC centres and they are expected to provide appreciated support for users in the different scientific fields to more efficiently utilise the SNIC resources in the future. Since the governmental e-science commitment is gradually increasing over the next years, there will be additional application experts appointed during 2011 and 2012. The topics for these will be decided upon towards the end of 2010.

BENGT PERSSON



Staff highlight

Time flies when you are having fun so I suddenly find myself going on my 14:th year here at NSC. I joined just after the Cray T3E was purchased and have been involved in just about everything since then. Currently my primary task at NSC is managing our relations with our partners Saab and SMHI, involved in long as well as short term planning of projects and resources ar tions continue to be carried out in an efficient w of the management group at NSC I participate ir planning process but I also find time to work on related issues and problem solving for parallel c

Hydrogen bond exchange in aqueou

Very early on it was recognised that computers are ideal tools to obtain numerical solutions to complex problems which would require crude approximations in analytical theory. In the field of statistical thermodynamics, computer simulations have over the years grown into a third branch of science on equal footing with experiments and analytical theory. Computer simulations can, by the ability to explore and lift approximations, bridge the gap between theory and experiments. Ever since the molecular dynamics(MD) simulation study by Rahman and Stillinger in 1971 [1] liquid water has remained the prime target for new techniques. Monte Carlo and MD simulations have played a key role in acquiring fundamental knowledge about molecular liquids in general and liquid water in particular, along with the appearance of new experimental probes. With the rapid increase of computational power, it has been possible to investigate increasingly complex and realistic models and to derive observables for direct comparison to novel experiments. Thereby, concepts derived from molecular dynamics simulations give strong stimuli to the refinement of liquid theory.

Ab initio molecular dynamics

In ab initio MD simulations, the forces are calculated on-the-fly from the electronic structure in contrast to classical MD simulations, which rely on pre-parametrised force-fields. There are strong limitations in terms of size, simulation time and available methods, but they give a balanced description of many-body effects and allow us to directly access electronic properties. For example, electric dipole fluctuations can be used to calculate infra-red spectra and the influence of electronic polarisation can be studied. We performed a series of ab initio MD simulations of 6 M $NaClO_4$(aq) solution in various isotope mixtures (180 atoms / 20 picoseconds) using 9 nodes (72 cores) and over 100.000 core-hours. Periodic DFT calculations in the CPMD program [2] employs pseudopotentials to describe the core-electrons in combination with a plane-wave expansion of the wave-function. It uses MPI, FFT and the high-band width in the Neolith architecture.

Insight into molecular details

Ab initio and classical MD simulations of 6 M $NaClO_4$(aq) gave a detailed molecular understanding of the structure and dynamics. The local structures around the water molecules and ions were analysed in terms of radial and spatial distribution functions, which showed the ion solvation and different classes of H-bond environment. From the MD simulations, we could also follow the H-bond exchange and reorientational dynamics for direct comparison to measured correlation functions. The O-H_p groups, H-bonded to an anion, exhibit fast initial reorientation. At longer time-scales they reorient slower than the O-H_w groups H-bonded to water. Free O-H groups only occur as transient species, and in particular the O-H_p groups undergo frequent H-bond breakage and reformation evens. Based on an analysis proposed by Laage and Hynes [3], the H-bond exchange mechanism between O-H_p and O-H_w was shown for involve ultra-fast reorientations. The H-bond dynamics is best described by a reorientational jump model, which was used to analyse the experimental data.

Infrared vibrational spectroscopy

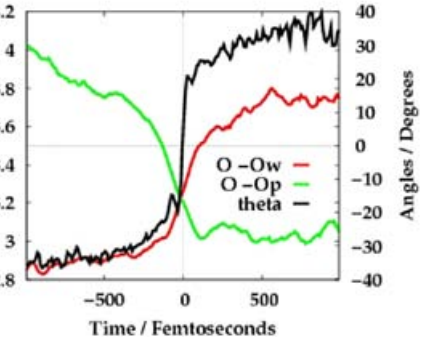
Infrared spectroscopy is a well established probe of H-bonding. In time-resolved spectroscopy, dilute isotope substitution (H/D) is necessary to avoid rapid energy relaxation. Sodium perchlorate, 6 M $NaClO_4$(aq) is a suitable model system with a double peak in the O-D stretching region. The high-frequency peak increases with ion concentration and in the MD simulations we can assign the peaks to O-D groups H-bonded to water or anions. Reorientation in water has been investigated with nuclear spin relaxation since the 1970s, but with time-resolved IR spectroscopy we can study the full correlation function and even single out the actual H-bond switching event. The purpose of investigating sodium perchlorate solution was to utilise the split peak to follow the H-bond exchange, which unfortunately is difficult in pure water. With carefully controlled ultra-short IR pulses, we can measure how the frequency of a molecule changes in time due to changes in environment. Thereby in photon-echo 2DIR spectroscopy, we acquire a map of the correlation of frequencies at varying time delays and can study the H-bond exchange [4]. Reorientation during the exchange from O-H_p to O-H_w, was obtained by controlling the polarisation of the light [5]. Through molecular dynamics simulations a detailed molecular mechanism for the H-bond exchange was identified. The emerging picture is that H-bond rearrangement involves intermolecular motion on the picosecond time-scale that triggers an

nd that the opera-
ay. As a member
n the strategic
performance
omputers, bench-

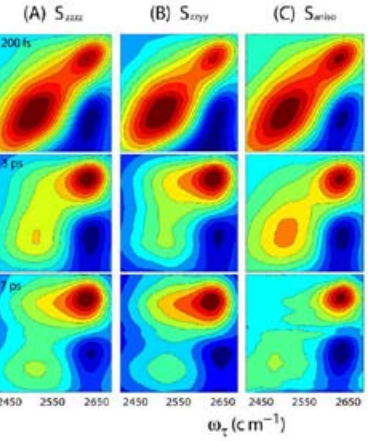
marking for future resources and EU projects in climate, tasks that are close to my heart! My background in meteorology and computer science at Uppsala University coupled with 10 years in the HPC industry both in Sweden and USA, working for Alliant Computer, Kendall Square Research and SGI, has been a very good fit for this job. Finding my way and solving problems is something I enjoy both at work and privately through orienteering in the Linköping Orientering Club (let me know if you are interested in trying it out!).

TORGNY FAXÉN

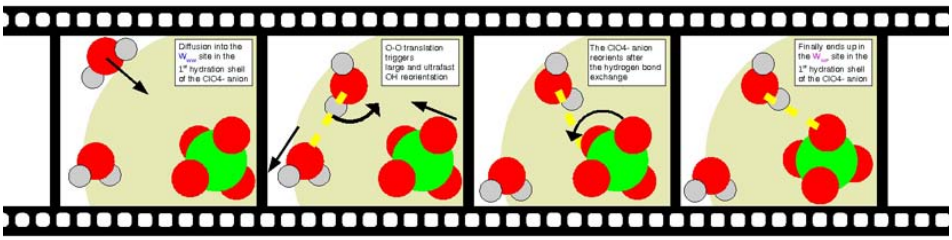
s solution



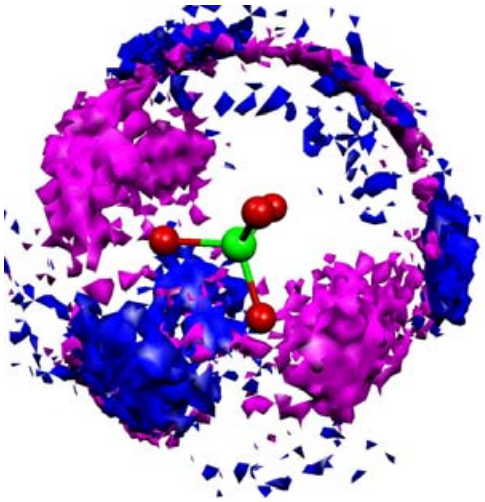
termolecular variables were sampled for different ex-
ange events. The exchange involves gradual changes in
e O-O distances which trigger a large amplitude reorien-
tional jump, as seen in the evolution of the projection of
e O-H vector onto the O-O-O plane, denoted "theta".



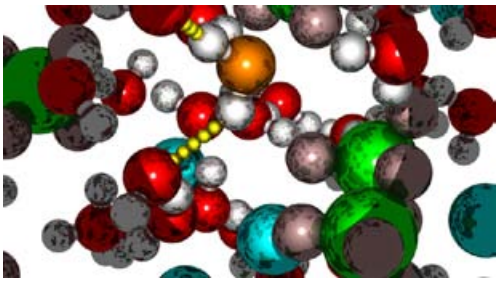
ater molecules in different environment exhibit a varia-
n in vibrational frequency. From 2DIR spectroscopy, the
rrelation in the vibrational frequency for a molecule at
fferent times is obtained. Molecules in similar environ-
ent occur along the diagonal. The upper-left cross peak
the O-D stretching region contains information about
e exchange of H-bonds to water molecules (O-H_w) and
anions (O-H_p). The reverse process should appear in the
wer-right cross peak, but it is obscured by excited-state
sorption.
anisotropy measurements, we can specifically measure
e reorientation of water molecules undergoing H-bond
change. The lack of anisotropy in the cross-peak indi-
tes that the O-H group undergoes an orientational jump
th an amplitude close to the magic angle 54.7°.



Hydrogen-bond exchange in aqueous sodium perchlorate solution. The exchange mechanism identified in the MD simulations was corroborated by results from 2DIR spectroscopy.



In concentrated electrolyte solution, virtually all water molecules coordinate anions. Hence, both classes (W_{WP} and W_{WW}) of water molecules belong to the 1st hydration shell of the ClO_4^- ion. The simulations show that they form angularly distinct sub-shells, presented in different colours.



Snapshots from the $NaClO_4$(aq) solution show the H-bond network. The water molecules in 6 M $NaClO_4$(aq) can be divided into two classes W_{WP} and W_{WW} which form H-bonds either to an anion and a water molecule and or only to water molecules.

ultra-fast (< 50 femtoseconds) exchange coupled with a dramatic (θ=50°) reorientation of the O-H group. The measurements were carried out at PULSE Institute, SLAC National Accelerator Laboratory, Stanford University. Kelly J. Gaffney, Minbiao Ji and Sungnam Park, who performed all the experiments, are gratefully acknowledged for an exciting collaboration. Magnus Bergvall foundation, Carl Tryggers foundation and the Swedish research council gave financial support.

MICHAEL ODELIUS

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Michael Odelius is a senior lecturer in quantum chemistry at the department of physics, Stockholm university. He is presently working with ultra-fast dynamics, solution chemistry and solar cell applications.

320 million compute hours to ten research projects

In the first application round for access to the Partnership for Advanced Computing in Europe, PRACE, infrastructure ten out of sixty-eight research projects were granted in total 321.4 Million compute hours. Five of the successful projects are from Germany, two from the UK and one each from Italy, the Netherlands and Portugal. But none of the tree Swedish applications were accepted. The projects are in the fields of astrophysics, earth sciences, engineering, and plasma and particle physics. They will have access to the fastest computer in Europe available for public research, the first Petascale HPC system, the IBM BlueGene/P in Jülich, Germany. Read more: http://www.prace-project.eu/news/prace-awards-320-million-compute-hours-to-ten-european-research-projects

PETER MÜNGER

Materials simulations for technology-oriented energy research

Achieving energy sustainability has become the main global concern for the human society in the XXI century. A rapidly growing economy requires new energy resources while conventional technologies face increasing problems with limiting access to sources of energy and negative environmental effects of its production, distribution, and usage. In order to maintain a sustainable development of the modern society these issues have to be resolved. It is recognized that any solution should involve a large variety of actions, ranging from the discovery of qualitatively new energy sources to the changes of our attitudes towards energy consumption. Clearly, science has to be given a leading role in this global challenge. This motivated five leading Swedish groups in materials modeling, together with the National Supercomputer Centre in Linköping, to build the Network of Excellence "MATerials simulations for Technology-oriented Energy Research", MATTER, within the call made jointly by Swedish National Infrastructure for Computing, SNIC, and Knut and Alice Wallenbergs foundation, KAW.

The five groups within the Network are Theoretical Physics (Prof. I. A. Abrikosov) and Computational Physics (Prof. S. Stafström) Groups at the Department of Physics, Chemistry and Biology (IFM), Linköping University, the Division of Materials Theory at the Department of Physics, Uppsala University (Prof. O. Eriksson), Applied Materials Physics Group at the Department of Materials Science and Engineering, Royal Institute of Technology (Prof. B. Johansson), and Inorganic Chemistry Group at the Department of Materials Chemistry, Uppsala University (Prof. K. Hermansson). SNIC and KAW provided the support (14 mln. Sek) for a new computer cluster, and NSC builds and hosts the supercomputer named Matter.

The main goal of the Network is to carry out an ambitious research program along the following main directions: new materials for clean energy production, new materials for energy storage, new materials and phenomena for energy saving, materials and phenomena for hydrogen production and emission reduction, as well as materials issues of nuclear waste disposal. The main tool for the research is the so-called first-principles simulations of materials properties, which are based on the atomistic description of condensed matter. A solution to the quantum mechanical problem is provided by the electronic structure theory. The majority of calculations are carried out in the framework of the density functional theory. We use state-of-the-art software developed by us and also available for us via our international collaborations. Moreover, we will continue our methodological developmental work, which will be beneficial for this project, but also for the large community involved in materials simulations. The same basic methodology from the point of view of the computations allows us to use essentially the same hardware for all the groups which enter the network.

Examples of systems and phenomena to be simulated with the new cluster include hydrogen fuel cells based on proton exchange membranes, photovoltaic systems (or "solar cells"), new materials for hydrogen storage, magnetic refrigeration, metal alloys for weight reduction applications, materials and phenomena for hydrogen production and emission reduction, as well as materials issues of nuclear waste disposal. In this way we will participate in and contribute to the truly demanding scientific progress that has to take place in order to solve the global energy problem.

The newly installed Matter system is a cluster with two types of servers. The majority consists of 512 servers with two Intel Xeon E5520 processors and 36 GB of memory, but there are also four servers equipped with two Intel Xeon X5570 processors and 144 GB of memory. In total the cluster has 4128 cores available for computational usage. Network wise all nodes have both 1 GB Ethernet and QDR Infiniband available. Disk storage is shared with the Neolith and Kappa resources already in production at NSC.

I. A. Abrikosov
Department of Physics, Chemistry and Biology, LiU
Andreas Johansson NSC, LiU

UPCOMING EVENTS

Euro-Par 2010; Aspects of Parallel Computing and Distributing Computing
August 31 – September 3, 2010, Ischia, Naples, Italy.
http://www.europar2010.org

PACT; 19th International Conference on Parallel Architectures and Compilation Techniques
September 11 – 15, 2010, Vienna, Austria.
http://www.pactconf.org

ICPP2010; 39th International Conference on Parallel Processing
September 13 – 16, 2010, San Diego, CA, USA.
http://www.cse.ohio-state.edu/~lai/icpp2010

IEEE Cluster 2010
September 20 – 24, 2010. Heraklion, Crete, Greece.
http://www.cluster2010.org

HEPiX Fall 2010 Workshop
November 1 – 5, 2010, Ithaca, NY, USA.
http://indico.cern.ch/conferenceDisplay.py?confId=92498

LISA'10; 24th Large Installation System Admininstration Conference
November 7 – 12, 2010, San Jose, CA, USA.
http://www.usenix.org/event/lisa10

SC10; International Conference for High Performance Computing, Networkng, Storage and Analysis
November 13 – 19, 2010, New Orleans, LA, USA.
http://sc10.supercomputing.org

HiPC 2010; International Conference on High Performance Computing
December 19 – 22, 2010, Goa, India
http://www.hipc.org

PPoPP 2011; 16th ACM SIGPLAN Annual Symposium on Principles and Practice of Parallel Programming
February 12 – 16, 2011, San Antonio, TX, USA.
http://www.ppopp.org

FAST'11; 9th USENIX Conference on File and Storage Technologies
February 15 – 18, 2011. San Jose, CA, USA.
http://www.usenix.org/events/fast11

IPDPS 2011; 25th IEEE International Parallel & Distributed Processing Symposium
May 16 – 20, 2011, Anchorage, Alaska, USA.
http://www.ipdps.org

CCGrid11; 11th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing
May 23 – 26, 2011, Newport Beach, CA, USA.
http://www.ics.uci.edu/~ccgrid11/

The 26th NORDUnet Conference
June 7 – 9, 2011, Reykjavik, Iceland.
http://www.nordu.net/conference/ndn-2011web/welcome.html

ParCo2011; International Conference on Parallel Computing
30 August – 2 September 2011, Ghent, Belgium
http://parco2011.elis.ugent.be/

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National Supercomputer Centre, Linköpings universitet, 581 83 Linköping, Sweden
Tel: +46 (0) 13-28 26 18, fax: +46 (0) 13-28 25 35, e-mail: info@nsc.liu.se
www.nsc.liu.se

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