International Young Scientists Conference

High Performance Computing and Simulation

Science Park 123, Amsterdam, Netherlands
2-6 April, 2012

http://promo.escience.ifmo.ru/

Recent Challenges for Computational Science – to Young Generation

Recent advances in experimental techniques such as detectors, sensors, and scanners have opened up new vistas into physical and socio-economic processes on many levels of detail. The complete cascade from the individual components to the fully integrated multi-science systems crosses many orders of magnitude in temporal and spatial scales. This is changing the way we do science into data intensive scientific discovery. The ultimate challenge is to study not only the fundamental processes on the various scales, but also their mutual coupling across scales in the overall system. The sheer complexity and range of spatial and temporal scales on which natural and anthropogenic systems seem to operate defies any existing numerical model or computational capacity. The only way out is by combining data on all levels of detail. This is an open research area. The challenges include understanding how one can reconstruct multi-level systems and their dynamics that connect models to massive sets of heterogeneous and often incomplete data. Conceptual, theoretical and methodological foundations are necessary for understanding these multi-scale processes and associated predictability limits of such large scale computer simulations.

In 2011 we announced a competition for young scientists in the Russian Federation working in the field of computational science and supercomputing to present us their most interesting research results. From the many submission received we selected 20 winners whom all received a ticket and stipend to Amsterdam to present their work at the University of Amsterdam during the International Young Scientists Conference «High Performance Computing and Simulation» 2-6 April, 2012: YSC-2012.

The Conference aims to develop a dialogue on the present and future of computational science, research and applications. The key conference themes are: mathematical modeling of multidisciplinary systems, supercomputer technologies to solve complex computing problems, problem solving computational systems, numerical studies in social sciences and life sciences, etc.

The YSC-2012 presents, in addition to the 20 Russian price winners, PhD students and Postdocs from the computational science research group at the University of Amsterdam (http://uva.computationalscience.nl/) and from the Leading Scientist research group on Advanced Computing at the research institute ITMO in St. Petersburg

Especially we are proud to have the following keynote speakers and invited speakers:

Keynote Speakers:

- Prof. Dr. Jack Dongarra (USA)
- Prof. Dr. Bastien Chopard (Switzerland)
- Dr. Mike Lees (Singapore)
- Dr. Anwar Osseyran(SARA, Amsterdam)

Invited Speakers:

- Prof. Dr. Guz Eiben (VU, Netherlands)
- Prof. Dr. Han La Poutre (CWI and Uni Eindhoven)
- Prof. Dr. Maarten van Steen (VU, Netherlands)
- Prof. Dr. Marian Bubak (AGH Poland and UvA Netherlands)
- Prof. Dr. Cees de Laat (UvA, Netherlands)
- Dr. Jaap Kaandorp (UvA, Netherlands)
- Dr. Alfons Hoekstra (UvA, Netherlands)
- Dr. Robert Belleman (UvA, Netherlands)
- Dr. Valeria Krzhizhanovskaya (StPb Polytech and UvA)

This booklet presents abstracts of invited speakers' presentations and abstracts of young computational scientists from Russian Federation and the University of Amsterdam, The Netherlands.

This international conference is the first of its kind. We hope that it will serve as a regular basis for the internationalization of Russian research and will help to build strong ties within the international community in the field of Computational Science.

Professor Peter Sloot

Professor Alexander Boukhanovsky

Conference Program

Day 1: Monday, 2 April 2012

Time	Sessions	Topic	Chair
9:00-9:30	Registration and welcome coffee		
9:30-10:00	Prof Peter Sloot, Prof Alexander Boukhanovsky	Introduction	
10:00-10:45	Prof. Dr. Han La Poutré (CWI and Uni Eindhoven)	Agents and Intelligence in Logistics and Energy Problems	Prof Peter Sloot
10:45-11:30	Science Speed Date		
11:30-12:00	Coffee break		
12:00-13:00	Young Scientists Presentations		
13:00-14:00	Lunch		
14:00-14:45	Prof. Dr. Cees de Laat (UvA, Netherlands)	Mastering Complex Networked Cyber Infrastructure	Prof Alexander Boukhanovsky
14:45-15:45	Young Scientists Presentations		
15:45-16:00	Networking Tea Break		
16:00-16:45	Dr. Mike Harold Lees (Nanyang Technological University (NTU) Singapore)	Agent-based models by example	Prof Alexander Boukhanovsky
16:45-17:30	Young Scientists Presentations		
17:30-19:00	Welcome reception	http://www.usc.uva.nl/algemeen/cafe_en.php	

Day 2: Tuesday, 3 April 2012

Time	Sessions	Topic	Chair
9:00-9:30	Registration and welcome coffee		
9:30-10:15	Prof. Dr. Marian Bubak (AGH University of Science and Technology, Kraków, Poland & UvA, Netherlands)	Collaborative applications on distributed e-infrastructures	Prof Peter Sloot
10:15-11:00	Young Scientists Presentations		
11:00-11:30	Coffee break		
11:30-12:15	Young Scientists Presentations		
12:15-13:00	Young Scientists Presentations		
13:00-14:00	Lunch		
14:00-14:45	Dr. Jaap Kaandorp (UvA, Netherlands)	Modelling gene regulation of morphogenesis	Prof Alexander Boukhanovsky
14:45-15:45	Prof. Dr. Maarten van Steen (VU, Netherlands)	Challenges in measuring geospatial social networks	Prof Peter Sloot
15:45-16:00	Networking Tea Break		
16:00-16:45	Young Scientists Presentations		
16:45-18:00	Young Scientists Presentations		
18:00-19:00	Transfer to Central Station (by train), address: Prins Hendrikkade 25		
19:00-20:00	Amsterdam canal boat trip		

Day 3: Wednesday, 4 April 2012

Time	Sessions	Topic	Chair
9:00-9:30	Registration and welcome coffee		
9:30-10:15	Prof. Dr. Bastien Chopard (University of Geneva, Switzerland)	The lattice Boltzmann method and its applications to science and engineering	Prof Peter Sloot
10:15-11:00	Dr. Paul Duijn (Computational Criminology, The Netherlands)	Computational criminology and criminal network research	Prof Peter Sloot
11:00-11:30	Coffee break		
11:30-12:15	Prof. Dr. Gusz Eiben (Vrije University, Amsterdam, Netherlands)	Embodied Artificial Evolution: the Next Big Thing?	Prof Peter Sloot
12:15-13:00	Prof. Dr. George Kampis (Eötvös Loránd University, Hungary)	Information Propagation in Dynamic Sexual Contact Networks	Prof Peter Sloot
13:00-14:00	Lunch		
14:00-14:45	Prof. Dr. Jack Dongarra (University of Tennessee, USA)	On the Future of High Performance Computing: How to Think for Peta and Exascale Computing	Prof Peter Sloot
14:45-16:00	Young Scientists Presentations		
16:00-16:15	Networking Tea Break		
16:15-17:00	Dr. Valeria V. Krzhizhanovskaya (St. Petersburg State Polytechnical University, UvA)	Modelling Dikes and Floods on HPC Clouds	Prof Alexander Boukhanovsky
17:00-18:00	Young Scientists Presentations		
18:00-18:15	Prof Peter Sloot, Prof Alexander Boukhanovsky	Closing discussion	

Day 4: Thursday, 5 April 2012

Time	Sessions	Topic	Chair
9:00-9:30	Registration and welcome coffee		
9:30-10:15	Young Scientists Presentations		
10:15-11:00	Dr. Anwar Osseyran (SARA)	About SARA	Prof Peter Sloot
11:00-11:30	Coffee break		
11:30-12:15	Dr. Robert Belleman	Life saving visualization	Prof Peter Sloot
12:15-13:00	Young Scientists Presentations		
13:00-14:00	Lunch		
14:00-14:45	Dr. Alfons Hoekstra (UvA, Netherlands)	Distributed Multiscale Computing	Prof Alexander Boukhanovsky
14:45-15:15	Young Scientists Presentations		
15:15-15:30	Prof Peter Sloot, Prof Alexander Boukhanovsky	Closing session	
15:30-15:45	Networking Tea Break		
15:45-17:00	SARA Tour	http://www.sara.nl/	
17:00-18:00	Drinks and snacks provided by SARA		

Summaries of keynote and invited speakers presentations

LIFE SAVING VISUALIZATION

Dr. Robert Belleman
Section Computational Science, Faculty of Science, University of Amsterdam

A common denominator in the visualization projects of our research group is the use of interactive visualization environments that help the end-user in taking informed decisions in an effort to save human lives. In all these projects the end-user goes into a dialogue with a graphical system to answer "what if?" questions. In this presentation I will provide an overview of some of these projects and explain the methodologies and choices that underlie the designs of our solutions.

ON THE FUTURE OF HIGH PERFORMANCE COMPUTING: HOW TO THINK FOR PETA AND

Prof. Dr. Jack Dongarra
University of Tennessee, Oak Ridge National Laboratory, University of Manchester

In this talk we examine how high performance computing has changed over the last 10-year and look toward the future in terms of trends. These changes have had and will continue to have a major impact on our software. Some of the software and algorithm challenges have already been encountered, such as management of communication and memory hierarchies through a combination of compile--time and run--time techniques, but the increased scale of computation, depth of memory hierarchies, range of latencies, and increased run-time environment variability will make these problems much harder.

CHALLENGES IN MEASURING GEOSPATIAL SOCIAL NETWORKS

Prof. Dr. Maarten van Steen
Professor of Computer Science, VU University Amsterdam

We are moving into an age in which the so-called fourth wave of science is spreading across many different disciplines, requiring a strong interaction between very different groups to extract information from vast amounts of data. In this talk I will discuss the development of an instrument for extracting social interactions in potentially very large groups of people, leading to a geospatial social network. This network, in turn, can be used to intervene in a social group, thus creating a closed loop of measurement and control. The reported research is ambitious, highly speculative, and raises many questions, which should place the audience in an excellent position to also challenge the sanity of the speaker.

AGENTS AND INTELLIGENCE IN LOGISTICS AND ENERGY PROBLEMS

Prof. Dr. Han La Poutre
Utrecht University

Multi-agent systems and computational intelligence techniques are important branches of AI. Important application areas include logistics as well as future energy systems. These areas are increasingly prominent in the modern society, where efficiency and sustainability are key. In the presentation, the techniques are described with respect to the research in these application areas.

COMPUTATIONAL CRIMINOLOGY AND CRIMINAL NETWORK RESEARCH

Paul Duijn MSc.
Strategic analyst, Dutch Police

Criminology is the scientific study of the nature, extent, causes, and control of criminal behavior in both the individual and in society. One important cause and indicator for criminal behavior is found in the social environment in which potential criminals learn and act. Therefore a main part of criminological theory and research focuses on the structure, appearance and behavior of criminal networks. Traditional criminological research methods are limited to the role of group individuals or organized crime groups. This presentation is about the opportunities and insights that methods of computational science can bring to criminal network research on a macro-level.

EMBODIED ARTIFICIAL EVOLUTION: THE NEXT BIG THING?

Prof. Dr. Gusz Eiben
Vrije University, Amsterdam, Netherlands

Evolution is one of the major omnipresent powers in the universe that has been studied for about two centuries. Recent scientific and technical developments make it possible to make the transition from passively understanding to actively using evolutionary processes. Today this is possible in digital spaces, in Evolutionary Computing, where human experimenters can design and manipulate all components of evolutionary processes. We argue that in the near future it will be possible to implement artificial evolutionary processes outside such imaginary spaces and make them physically embodied. In other words, we envision the ``Evolution of Things", rather than just the evolution of digital objects, leading to a new field of Embodied Artificial Evolution. The main objective of this talk is to present a unifying vision in order to aid the development of this high potential research area. To this end, we introduce the notion of Embodied Artificial Evolution, discuss a few examples and applications, and elaborate on the expected benefits as well as the grand challenges this developing field will have to address.

MODELLING GENE REGULATION OF MORPHOGENESIS

Jaap Kaandorp
Section Computational Science, Faculty of Science, University of Amsterdam

In this presentation we would like to give two examples of coupling a model of a gene regulatory network and a biomechanical representation of morphogenesis. In the first example we use the embryogenesis of the sea anemone Nematostella vectensis as a case study. In this example we couple the model of gene regulation to a cell-based model of embryogenesis. In this case study we are collecting recently published spatio-temporal and quantitative gene expression patterns from various developmental stages in Nematostella in a spatial data base («the virtual embryo»). We use this three-dimensional data for constructing a mathematical model of the regulatory network and for inferring regulatory network parameters. The regulatory network is modelled using a set of coupled reaction-diffusion equations, while the model parameters are inferred from the data base using optimization techniques. Finally the aim is to couple the regulatory network model to a biomechanical model of cell movement and cell division.

In the second case study a computational model of the skeletogenesis and the influence of the physical environment on the morphogenesis of a branching sponge is presented. In the model we assume that the radiate accretive growth process is nutrient limited. Recently much information became available about the gene regulation of morphogenesis in sponges. We demonstrate that the computational model of growth and form of the sponge can be combined with a (preliminary) model of spatio-temporal gene regulation. With this model we can generate in a simulated accretive growth process branching objects with a similarity to the branching sponge.

INFORMATION PROPAGATION IN DYNAMIC SEXUAL CONTACT NETWORKS

Prof. Dr. George Kampis
Eötvös Loránd University, Hungary

Contact networks, among them human sexual networks have been intensively studied recently, in particular in the context of contagious diseases an example for which is HIV. Network epidemiology is a new field that uses the science of complex networks to understand the spreading of infections (or, in general, the propagation of information) in human social systems.

Many earlier information propagation studies were based on aggregate networks, i.e. where all contacts present in an extended time frame have been considered. This is also a natural approach as it is typically more difficult to obtain time stamps for a human interaction than just testing whether it took place at all. Hence human networks are typically «envelope networks»– a friendship network a list of all friends, past and present, a sexual contact network an aggregate of all partners.

Initial results on network epidemiology led to arresting insights, such as the lack of an epidemic threshold for scale-free networks. The epidemic threshold is the proportion of the population that has to be infected (or informed) in order to infect (inform) a significant part of the whole population. Envelope sexual networks are scale-free (or close) so it was expected that the same results apply. But dynamic networks are different. When looking for the spreading of an infection (or a bit of information), past links do not matter. Hence the notion of a causal network is relevant, which corresponds to a shifting time aggregate of the snapshot networks of individual time instances. An egocentric causal network for HIV is the network where are all nodes reachable during the infectious state of the individual are listed.

I will present a simulation study for causal networks in dynamic sexual contact systems, where connections are formed and broken by various algorithms. Of special interest are random, preferential attachment, and various assortative mixing procedures for the formation of contacts, and random as well as uniform terminations of linkages. We will see how the various combinations of these lead to different, changing degree distributions and other interesting network characteristics. We'll find that real data best match up with the assortative models, which puts this property in the focus. (Assortativity is a bias in favor of connections between network nodes with similar characteristics – in this case cumulative degree, or, number of past partners.)

Introducing infections in these systems, we observe that, contrary to expectations, most of the infections either die out or infect the entire population and then stop. No epidemic threshold and no conditions capable of sustaining an ongoing epidemic (or a steady information propagation) were found. By contrast, assortative mating systems do not produce the same "all or none" switching behavior and show a wide variety of intermediate stages in a broad range of parameters. Even more importantly, they can sustain epidemics at various levels of prevalence. Based on this recognition, it is suggested that the observed persistence of the HIV and similar epidemics can be traced back to simple network properties such as the assortativity of human relations.

AGENT-BASED MODELS BY EXAMPLE

Michael Harold Lees (Asst Prof)
Assistant Professor, Nanyang Technological University (NTU) Singapore

In a world of ever increasing complexity agent-based modeling (ABM) is one technique applied by both natural scientist and social scientists to try and gain insight into many of the world's complex systems, from the economy to human crowds. These complex systems often consist of many interacting entities that together exhibit emergent macro level dynamics.

Such phenomena are ideally captured by agent-based models, which consist of many, perhaps thousands, of autonomous, social agents. Agents are described at varying levels of detail and complexity, from simple rule-based reactive components to sophisticated systems that can learn, adapt and plan. These agent-based models commonly try to capture aspects of human behavior, with individual agents often mirroring individual humans and their rational or irrational behavior.

In the first half of this talk I will cover a brief introduction to agent-based modeling, including its historical beginnings from the fields of mathematics, economics, artificial intelligence and computer science. Through illustrative examples the talk will showcase typical forms of agent-based models and how they are constructed. The talk will go on to present some of the software tools available to the ABM community and how young scientists might use these tools to develop their own models.

The second part of the talk will provide an overview of two examples of on-going work in Singapore. The first of these is an agent-based egress simulation, called Dynamic Egress Planning Through Symbiotic Simulation (DEPATHSS). This is an advanced evacuation system that intends to use intelligent buildings coupled with real-time simulation to provide active dynamic evacuation routing. The second will describe work of the TUM-Create programme in Singapore and the early development of the Scalable Electro-Mobility Simulator (SEMSim), designed to help analyze the impact of electric vehicles on the Singaporean road system. In particular, this example will help illustrate the benefits of a true agent-based simulation in answering important design questions for the future transportation infrastructure of Singapore. Finally, through the two real-world examples I will conclude by outlining two of the main challenges faced by agent-based modeling as a paradigm.

SARA NATIONAL HIGH PERFORMANCE COMPUTING & ESCIENCE SUPPORT SERVICES

Dr. Anwar Osseyran
SARA, Amsterdam

How can we improve the quality of life in the Netherlands when it comes to the dispersion of pollutants? How can we deduce macroscopic material properties from quantum mechanical phenomena? How can we reduce noise from aircraft engines? How doe algae spread and clump together in lakes and coastal seas? How do the rapid changes in Atlantic ocean circulation influence the climate in Western Europe? Which impact have atmospheric turbulence on our weather? How do we develop materials for the post-silicon electronics era? How to predict the aerodynamic properties of wind farms?

All those kind of questions evolve with time and capabilities and mark the need for high performance computing (HPC) to solve complex scientific, social or industrial challenges. Most challenges are nowadays large scale and multidisciplinary, and “Computational science” is now recognized as absolutely necessary in each sector, from traditional scientific and industrial domains, to financial, social and community areas like economy, energy, logistics, healthcare, national heritage and security. HPC infrastructure offers researchers, developers and engineers in academia and businesses huge processing power, high bandwidth, large storage facilities and software eco-systems, for rapid simulation, modeling and large scale data-processing. Use of HPC provides a better insight in complex scientific and engineering problems leading to scientific discoveries, patents and competitive products.

SARA was founded in 1971 and is an independent (hybrid) organization with ~170 fte’s in 2 locations (Amsterdam and Almere). As the national HPC en eScience Support Center, the mission of SARA is two-fold:

1. Support research in the Netherlands by providing high-end not-for-profit ICT services to Dutch education and research communities (SARA BV for Science & Innovation);
2. Offer commercial high-end on-demand cloud services based on the expertise built in the high-end activities (Vancis BV for adVANCed Ict Services).

SARA offers a variety of HPC facilities to enable each application to run on the system architecture that is most efficient for it. SARA runs its services on four classes of HPC architectures, which are complementing each other:

1. Low-latency, high-bandwidth architectures, running capability computing services. This type of architecture is typically suited for large parallel computational problems, which in general also demand large memory and I/O capabilities (supercomputer services).

2. Capacity compute cluster architectures, running capacity computing services. A fairly wide range of applications can be run on those clusters, which typically feature a combination of commodity processors, moderate amounts of memory per processor core, moderate I/O facilities and a moderate interconnect architecture between the nodes (capacity computing services).

3. Loosely coupled compute farm architectures, running large-scale data processing services. This is the type of architecture that is very well suited to embarrassingly parallel applications.

4. Special-purpose architectures (accelerators), running hybrid computing services. This is the type of architecture which is mostly connected to innovative projects.

The presentation will give an overview of the national e-infrastructure services at SARA, the projects supported and the innovation program in 2012.

Abstracts of young scientists

PROGRAMMING GRAPHICS PROCESSORS WITH EXTENSIBLE LANGUAGES

A.V. Adinetz
Research Computing Center, Lomonosov Moscow State University, Joint Institute for Nuclear Research

GPUs are widely used to solve computationally intensive problems, which makes important the creation of higher-level system for GPU programming. In this paper, we propose creating such a system using extensible languages, i.e. languages whose syntax and semantics can be easily extended to simplify development. We present NUDA, a set of GPU programming extensions for Nemerle, an extensible programming languages. NUDA macros simplify moving data and code to GPU, while annotations enable easy loop optimizations. Internally, OpenCL is used for GPU program generation. The system has been tested on a number of problems and GPU architectures. Using macros and annotations enabled acceleration several times compared to naive GPU variant, while retaining clarity and small code size.

TOWARDS A WORKOW ORIENTED PROGRAMMING LANGUAGE

Mikolaj Baranowski[1], Adam Belloum[2], and Marian Bubak[1;2]
[1] University of Amsterdam, Amsterdam, Netherlands
[2] AGH University of Scie
01nce and Technology, Krakow, Poland

This paper discusses the objectives of developing the new work oriented programming language. Research is based on the experience of translating Ruby[1] script applications that use the Grid Object abstraction[2] to access a heterogeneous Grid infrastructure into workows - as it is described in [3]. Theories of the CCS[4] (Calculus of Comminicating Systems), CSP[5] (Communicating Sequential Processes) and the pi process algebras[6], the actor model approach[7] and the previous attempts of creating workflow oriented programming languages - the SMAWL[8] (Small Workflow Langauge Based on CCS) and a Prologbased langage for workow programming[9]. The notable XML based workflow description languages including the YAWL[10] (Yet Another Workflow Languages) ware taken into consideration. It also evaluates the opportunities of translating existing workflow models into the developing programming language basing on the set of 20 control Workflow Patterns[11] as well as the advantages of using programming language instead of XML based workflow models including human readable format, formal denition and portability. The motivation for creating the new language are taken from the already mentioned Ruby-based Grid solution which provides programming environment where complex applications are easy to understand and extend. This is a real value of general purpose dynamic programming languages. The other motivation was taken from the Ptolemy II[12] workflow system where the facilities of general purpose programming languages are substituted by the Ptolemy expression language - the internal interpreter with complex types like arrays and records, based on Matlab syntax.The initial idea is to design S-expression based programming languageto achieve syntax exibility and keep similarities with previous work described in [3].

1. Yukihiro Matsumoto. Ruby programming language home page. http://www.ruby-lang.org.
2. Tomasz Bartyski, Maciej Malawski, and Marian Bubak. Invocation of grid operations in the virolab virtual laboratory. In Cracow Grid Workshop 2007 Workshop Proceedings, pages 59{64. ACC CYFRONET AGH, 2008.
3. Mikolaj Baranowski, Marian Bubak, and Maciej Malawski. Constructing workflows from script applications. 2012.
4. R. Milner. A Calculus of Communicating Systems. Springer-Verlag New York, Inc., Secaucus, NJ, USA, 1982.
5. C. A. R. Hoare. Communicating sequential processes. Commun. ACM, 21(8):666{677, August 1978.
6. Robin Milner. Communicating and mobile systems - the Pi-calculus. Cambridge University Press, 1999.
7. Carl Hewitt, Peter Bishop, and Richard Steiger. A universal modular actor formalism for articial intelligence. In Proceedings of the 3rd international joint conference on Articial intelligence, pages 235{245, San Francisco, CA, USA, 1973. Morganaufmann Publishers Inc.

8. Christian Stefansen. SMAWL: A small workflow language based on CCS, volume 161, page 132. 2005.
9. Steve Gregory and Martha Paschali. A prolog-based language for workflow programming. In Proceedings of the 9th international conference on Coordination models and languages, COORDINATION'07, pages 56{75, Berlin, Heidelberg, 2007. Springer-Verlag.
10. A. H. M. Ter Hofstede. Yawl: yet another workflow language. Information Systems, 30:245-275, 2005.
11. Nick Russell, Arthur T. Hofstede, Wil M. P. van der Aalst, and Nataliya Mulyar. Workflow control-flow patterns: A revised view. Technical Report BPM-06-22, BPMcenter.org, 2006.
12. J. Eker, J.W. Janneck, E.A. Lee, Jie Liu, Xiaojun Liu, J. Ludvig, S. Neuendorffer, S. Sachs, and Yuhong Xiong. Taming heterogeneity - the ptolemy approach. Proceedings of the IEEE, 91(1):127 { 144, jan 2003.

MATHEMATICAL MODEL OF THE POSITION OF HIGH-LATITUDE BOUNDARY OF THE OUTER RADIATION BELT DURING QUIET CONDITIONS IN THE EARTH'S MAGNETOSPHERE IN DEPENDENCE ON UT AND MLT TAKING INTO ACCOUNT THE EFFECT OF MAGNETOSPHERIC CURRENT SYSTEMS

Wera Barinova, Vladimir Kalegaev, Maria Riazantseva, David Parunakian, Irina Myagkova and Lev Starostin
Skobeltsyn Institute of Nuclear Physics of the Moscow State University

The global magnetospheric structure and its dynamics in the 2009 epoch was studied using satellite measurements during extremely quiet geomagnetic conditions. It allowed us to determine the mean position of the outer radiation belt (ORB) boundary and inspect its daily dynamics near the Earth surface separating the effects induced by internal and external factors and build a model of the ORB boundary dynamics in dependence on UT (Universal Time) and MLT (Magnetic local time).
The model is based on the statistical processing and analysis of the energetic electron fluxes data measurements of E > 200 keV electron fluxes onboard Coronas-Photon since March till November 2009. It was obtained that the high-latitude ORB boundary is controlled by both geomagnetic (internal) and magnetospheric magnetic fields.

It has been found that at the ionospheric level the high-latitude boundary of ORB rotates with the Earth but slightly shifts to the night side due to large-scale magnetospheric currents

.

PARTICLE-IN-CELL PLASMA SIMULATION ON HETEROGENEOUS CLUSTER SYSTEMS*

Sergey Bastrakov[1], Arkady Gonoskov[2], Roman Donchenko[1], Evgeny Efimenko[2], Alexander Malyshev[1], Iosif Meyerov[1]

[1]Lobachevsky State University of Nizhni Novgorod, [2]Institute of Applied Physics, Russian Academy of Sciences, Nizhni Novgorod

One of the currently high-demand areas of computational physics is simulation of plasma dynamics with Particle-In-Cell (PIC) approach, which nowadays is widely used as an efficient tool for research in astrophysics, high intensity laser-matter interactions, and inertial and magnetic confinement fusion. Many of the applications require simulation of order of 10^9 and more particles in an area represented by order of 10^8 grid cells, thus use of supercomputer technologies is of primary importance. During the last years except traditional supercomputer codes development (OSIRIS, QUICK-PIC, VPIC, VLPL, UPIC) there is a growing interest in GPUs as a source of immense computational power. There are lots of PIC codes for GPU under research and development, some provide very promising results. While both CPU and GPU codes are being developed simultaneously, new supercomputers more and more often are designed to share performance among both CPUs and GPUs thus raising a problem of heterogeneous codes development. We present Picador — a tool for three-dimensional electromagnetic relativistic plasma simulation using the Particle-in-Cell method for heterogeneous cluster systems with several CPUs and GPUs on each node. The eventual goal is to fully utilize computational resources of heterogeneous clusters for research of high intensity laser applications including generation of radiation with tailored properties and laser-driven particle acceleration. The simulation area is statically decomposed into subareas, which are handled in parallel by separate MPI processes, each process uses either one or several CPU cores or a GPU. In the implementation for CPUs we use the widespread technique of ordering particles in memory to enable a cache-friendly memory access pattern on the most time-consuming stages of current deposit and particle push. OpenMP-parallelization is mostly straightforward, guard cells are used for parallel current deposit. GPUs are utilized with OpenCL, we use a modification of supercell approach used in some PIC codes for GPU. Nearby cells are grouped into supercells, all particles of a supercell are handled by a single workgroup with intensive usage of local memory as a user-managed cache for both particle push and currents deposit. This allows to achieve high device occupancy and an effective GPU global memory access pattern, so-called coalescing. The computational experiments demonstrate the efficient scalability on CPU cluster systems for up to at least 2048 cores. The efficiency of strong scalability on 2048 cores relative to 512 cores is 71% and 85% on MVS-100K and Akka clusters. When increasing computational complexity proportionately to the number of used cores (weak scalability) execution time increases 11-12% for 1280 cores relative to 512 cores and stabilizes on that level for up to at least 2048 cores. On NVIDIA Tesla X2070 the GPU version demonstrates speedup of 3-4 times relative to 8 CPU cores. It achieves performance of 71.4 and 141 GFLOPS in double and single precision, respectively, which in both cases is about 14% of peak performance. The weak scalability on GPU-enabled cluster Lomonosov

is as follows: execution time for 128 GPUs increases by 50% related to 16 GPUs and stays around this level up to 512 GPUs (229376 CUDA-cores). The goals for further research are increasing performance and scalability on CPUs and GPUs, enabling simultaneous usage of all computational devices, as well as implementing improved numerical methods and adding new features.

*This work was prepared in the Information Technology laboratory of the CMC department of the UNN and was supported by the Federal Targeted Program “Science and science education personnel of the innovative Russia”, government contract No. 02.740.11.0839.

PARALLEL ALGORITHMS FOR SOLVING LINEAR SYSTEMS WITH BLOCK-TRIDIAGONAL MATRICES ON MULTI-CORE CPU WITH GPU*

Dmitry Belousov, Elena Akimova
Institute of Mathematics and Mechanics, Ural Branch of RAS, Ekaterinburg, Russia
Ural Federal University named the first President of Russia

Systems of linear algebraic equations (SLAE) with block-tridiagonal matrices arise in many applied problems, in particular, geoelectrics problems. The geoelectrics prob-lems are very important for investigating the crust heterogeneity. The well known method for their solving is the method of vertical electrical sounding (VES). After using a finite-difference approximation, the problem is reduced to solving a SLAE with block-tridiagonal matrix [1]. Another important problem is one of lateral logging (LL). As a re-sult, of interpretation of the logging data, we get the formation resistivity, which is close to the real one. It is shown [2] that after using a finite-difference approximation, the LL problem is reduced to solving a SLAE with block-tridiagonal matrix of large dimension.

In the work these problems are considered and efficiency and optimization of pa-rallel algorithms are investigated. The problems with quasi-model data are solved.

The parallel algorithms are incorporated into the elaborated system of remote computations "Specialized Web-Portal for solving geophysical problems on multi-processor computers". The Web-Portal is installed at the Department of Ill-posed Prob-lems of Analysis and Applications of the Institute of Mathematics and Mechanics of the Ural Branch of RAS (Ekaterinburg).

The parallel algorithms were implemented on NVIDIA GPU using the technology of CUDA [6], on multi-core Intel processor using the technology of OpenMP [7], and the Windows API development tools [8].

With the help of the parallel matrix sweep algorithm, preconditioned conjugate gradient method, and square root method, we solved the problem of finding a poten-tial distribution in a conducting medium with known quasi-model solution.
The basic data and quasi-model solution of the problem were provided by the De-part-ment of Borehole Geophysics of the Institute of Petroleum Geology and Geophysics of the Siberian Branch of RAS (Novosibirsk).

After discretization, the problem is reduced to solving a SLAE with an ill-condi-tioned symmetric positive definite block-tridiagonal matrix of dimension with 248 square blocks.

The numerical solution of the problem is compared with the quasi-model solution by means of calculating the relative error. This problem was solved by the parallel con-jugate gradient method (PCGM) with preconditioner, parallel matrix sweep algo-rithm (PMSA), and parallel square root method (PSRM). The numerical solution
of the problem coincides with the quasi-model solution with accuracy

$$\sigma_{PCGM} \approx 10^{-7}, \sigma_{PMSA} \approx 2 \cdot 10^{-7}, \sigma_{PSRM} \approx 6 \cdot 10^{-7}.$$

The computation times of solving the SLAE in the potential distribution problem on the hybrid computing system are presented in Table 1. This system is installed in the Department of Ill-posed Problems of Analysis and Applications of the Institute of Mathematics and Mechanics UB RAS. The computing system consists of 4-core processor Intel Core I5-750 with graphics accelerator NVIDIA GeForce GTX 285. Note that the time for solving the problem by PCGM without preconditioner on one core Intel Core I5-750 for

$$\sigma_{CGM} = 10^{-3}$$

was 55 min. Table 1 shows that the pre-conditioner decreases essentially the time of solving the problem.

Table 1. Computation times of solving SLAE

Method	Computing system	T_m, sec.(Windows API)	T_m, sec. (OpenMP)
PCGM	Intel Core I5 (1 core)	57	21
	Intel Core I5 (2 core)	46	16
	Intel Core I5 (4 core)	36	14
	NVIDIA GeForce GTX	—	14
PMSA	Intel Core I5 (1 core)	52	21
	Intel Core I5 (2 core)	28	18
	Intel Core I5 (4 core)	16	14
	NVIDIA GeForce GTX	—	10
PSRM	Intel Core I5 (1 core)	12	7.4
	Intel Core I5 (2 core)	9	4.6
	Intel Core I5 (3 core)	10	3.8
	Intel Core I5 (4 core)	12	4.2
	NVIDIA GeForce GTX	—	3

At the beginning, for a multi-core processor with shared memory, the PCGM, PMSA, and PSRM parallelization was implemented by means of the operating system (OS) threads by the development tools Windows API [8].

At the beginning, for a multi-core processor with shared memory, the PCGM, PMSA, and PSRM parallelization was implemented by means of the operating system (OS) threads by the development tools Windows API [8].

So, the PSRM is the fastest method. The computation time for solving the SLAE on 4-core CPU Intel and graphics processors is reduced to several seconds (compare with 55 min by CGM without preconditioner).

References

1. Tikhonov, A.N., Samarskii, A.A.: Equations of Mathematical Physics. M.: Nauka (1966).
2. Dashevsky, J.A, Surodina, I.V., Epov, M.I.: Quasi-three-dimensional mathematical model-ling of diagrams of axisymmetric direct current probes in anisotropic profiles. Siberian J. of Industrial Mathematics. Vol. 5, № 3 (11), pp. 76–91 (2002).
3. Samarskii, A.A., Nikolaev, E.S.: Methods for solving the grid equations. M.: Nauka. (1978).
4. Akimova, E.N.: Parallelization of the matrix sweep algorithm. Mathematical Modelling. Vol. 6, № 9, pp. 61–67 (1994).
5. Faddeev, V.K., Faddeeva, V.N.: Computational methods of linear algebra. M.: Gos. Isdat. Fizmat. Lit. (1963).
6. Berillo, A. NVIDIA CUDA – ungraphics computing on graphics processors. URL: http://www.ixbt.com/video3/cuda-1.shtml.
7. Voevodin, Vl.V.: Parallel programming technologies. URL: http://parallel.ru.
Methods of multithreaded applications development: principles and practical implementation.URL: http://www.rsdn.ru/article/baseserv/RUThreadingMethodology.xml

* The work was supported by the Ural Branch of RAS (Presidium RAS Program No. 15, project No. 12-P-1-1023) and by the RFBR (project No. 12-01-00106-a).

PRINCIPLES OF DISTRIBUTED MULTISCALE COMPUTING, FROM FORMALIZATION TO EXECUTION

Joris Borgdorff, Jean-Luc Falcone, Eric Lorenz, Bastien Chopard, and Alfons G. Hoekstra*
J. Borgdorff, E. Lorenz, and A.G. Hoekstra are with the Section Computational Science of the University of Amsterdam, Amsterdam, the Netherlands.
J.-L. Falcone and B. Chopard are with CUI of the University of Geneva, Carouge, Switzerland.

In several disciplines, a multiscale approach is being used to model complex natural processes yet a principled background to multiscale modeling is not clear [1,2]. Additionally, some multiscale models requiring distributed resources to be computed in an acceptable timeframe, while no standard framework for distributed multiscale computing is place [3]. In this contribution a principled approach to distributed multiscale computing is taken, formalizing multiscale modeling based on natural processes. Based on these foundations, the Multiscale Modeling Language (MML) [4,5] is extended as a clear, general, formal, and high-level means to specify scales and interactions in, and as a guide to a uniform approach to crystalize, communicate, develop and execute a multiscale model. With an MML specification, a multiscale model can be analyzed for scheduling or deadlock detection using a task graph [6]. The potential of this method is shown by applying it to a multiscale model of in-stent restenosis [7,8].

References:

[1] P.M.A. Sloot, A.G. Hoekstra, Multi-scale modelling in computational biomedicine, Briefings in Bioinformatics. 11 (2010) 142–152.

[2] G.D. Ingram, I.T. Cameron, Challenges in Multiscale Modelling and its Application to Granulation Systems, Dev. Chem. Eng. Mineral Process. 12 (2004) 293–308.

[3] B. Chopard, J.-L. Falcone, A.G. Hoekstra, J. Borgdorff, A Framework for Multiscale and Multiscience Modeling and Numerical Simulations, in: C. Calude, J. Kari, I. Petre, G. Rozenberg (Eds.), Lncs 6714, Springer Berlin / Heidelberg, Berlin, Heidelberg, 2011: pp. 2–8.

[4] J.-L. Falcone, B. Chopard, A.G. Hoekstra, {MML}: towards a Multiscale Modeling Language, Procedia Computer Science. 1 (2010) 819–826.

[5] J. Borgdorff, J.-L. Falcone, E. Lorenz, B. Chopard, A.G. Hoekstra, A principled approach to distributed multiscale computing, from formalization to execution, in: Proceedings of the 7th IEEE International Conference on E-Science, IEEE Computer Society Press, Stockholm, Sweden, 2011.

[6] J. Borgdorff, J.-L. Falcone, E. Lorenz, C. Bona-Casas, B. Chopard, A.G. Hoekstra, Foundations of Distributed Multiscale Computing: Formalization, Specification, Analysis and Execution, Journal of Parallel and Distributed Computing, Submitted. (2011) 1–31.

[7] H. Tahir, A.G. Hoekstra, E. Lorenz, P.V. Lawford, D.R. Hose, J. Gunn, et al., Multiscale simulations of the dynamics of in-stent restenosis: impact of stent deployment and design, Interface Focus. 1 (2011) 365–373.

[8] D.J.W. Evans, P.V. Lawford, J. Gunn, D. Walker, D.R. Hose, R.H. Smallwood, et al., The application of multiscale modelling to the process of development and prevention of stenosis in a stented coronary artery, Phil. Trans. R. Soc. A. 366 (2008) 3343–3360.

GENE EXPRESSION QUANTIFICATION IN NEMATOSTELLA: CAN WE EXTEND COMPUTATIONAL ANALYSIS FROM DROSOPHILA TO OTHER ANIMALS?

Daniel Botman
PhD student, Informatics Institute,
University of Amsterdam

For many years, topological and dynamical properties of the gene regulation network in Drosophila are analyzed. From parameter estimation to confirming and explaining moving expression domains, these powerful techniques are based on accurate quantifications of gene expression patterns. Drosophila is extremely suitable gene expression quantification due to its constant and radially symmetric shape during early development, as well as spreading of the gap and pair rule genes along the anterior-posterior axis. Unfortunately, these unique properties are not observed in other model animals.

In our approach, complex expression patterns in the Nematostella embryo are mapped to its curved and changing morphology. This provides a convenient framework for gene expression quantification and subsequent analysis. Comparing and clustering gene expression profiles may indicate modules in the regulatory network and in which regions the majority of cell division occurs. Eventually, we want to explore to what extent computational and analytical techniques successfully applied on Drosophila can be generalized for other model species in genetics.

EFFICIENT ITERATIVE SOLVERS FOR TIME-HARMONIC MAXWELL EQUATIONS USING DOMAIN DECOMPOSITION AND ALGEBRAIC MULTIGRID

Dmitry Butyugin
Novosibirsk State University, Novosibirsk, Russia,
Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Novosibirsk, Russia

Paper presents a set of parallel iterative solvers and preconditioners for the efficient solution of systems of linear equations arising in the high order finite-element approximations of boundary value problems for 3-D time-harmonic Maxwell equations on unstructured tetrahedral grids. Balancing geometric domain decomposition techniques combined with algebraic multigrid approach and coarse-grid correction using hierarchic basis functions are exploited to achieve high performance of the solvers and small memory load on the supercomputers with shared and distributed memory. Testing results for model and real-life problems show the efficiency and scalability of the presented algorithms.

IN STENT RESTENOSIS: A 3-DIMENSIONAL MODEL

Carles Bona-Casas, Hannan Tahir, Joris Borgdorff, Eric Lorenz, Alfons G. Hoekstra.
Universiteit van Amsterdam (UvA)

One of the most common surgical interventions used to treat coronary heart disease consists in inserting an artificial tube inside a blocked artery in order to act as a scaffold, that is, to sustain the artery wide open so that blood supply is not constricted anymore. This artificial tube is called a stent. But the long term outcome of stent implantation can be affected by a process called in stent restenosis (ISR)[1][2], which causes the blood supply to be constricted again. Multiple contributory factors have been identified [2], but clear understanding of the overall underlying mechanism remains an enigma. By developing a computational model of ISR [3] we are able to obtain a test bench in which we can check the outcome of our hypothesis, identify the main processes involved and, in the long run, become a source for patient-specific predictions which can assess medical intervention. However, the multi-science and multi-scale nature of ISR poses a series of challenges that we have to overcome [4].

[1] Restenosis after PCI. Part 1: pathophysiology and risk factors. J. Wouter Jukema, Jeffrey J. W. Verschuren, Tarek A. N. Ahmed and Paul H. A. Quax. et al. Nat. Rev. Cardiol. 9, 53-62 (2012)
[2] Restenosis after PCI. Part 2: prevention and therapy. J. Wouter Jukema, Jeffrey J. W. Verschuren, Tarek A. N. Ahmed and Paul H. A. Quax. et al. Nat. Rev. Cardiol. 9, 79-90 (2012)
[3] Multi-scale simulations of the dynamics of in-stent restenosis: impact of stent deployment and design. Hannan Tahir, Alfons G. Hoekstra, Eric Lorenz, Patricia V. Lawford, D. Rodney Hose, Julian Gunn and David J.W. Evans. Interface Focus 6 June 2011 vol. 1 no. 3 365-373
[4] A Principled Approach to Distributed Multiscale Computing, from Formalization to Execution. Joris Borgdorff, Eric Lorenz, Alfons G. Hoekstra, Jean-Luc Falcone, Bastien Chopard. esciencew, pp.97-104, 2011 IEEE Seventh International Conference on e-Science Workshops, 2011.

MODELLING GROWTH AND FORM OF THE SCLERACTINIAN CORAL POCILLOPORA VERRUCOSA AND THE INFLUENCE OF HYDRODYNAMICS

Nol Chindapol [1], Jaap A. Kaandorp [1], Carolina Cronemberger[1], Tali Mass[2] and A. Genin[2]

[1] Section Computational Science, University of Amsterdam, [2] The Interuniversity Institute For Marine Sciences, The Hebrew University, Israel

Scleractinian corals are known to have a high degree of morphological plasticity along different environmental gradients (Hennige 2010; Todd 2008; Muko et al. 2000). Two important factors related to the morphological variation are light and water motion (Todd 2008). When the gradient of water movement increases, it is observed that different morphologies emerge in response to the change of hydrodynamics energy (Veron and Pichon 1976; Kaandorp 1999). In order to investigate the observed morphological plasticity in the flow, we present a computational approach which use accretive growth model (Merks et al. 2004) and couple with advection-diffusion equations. We have simulated coral growth under no-flow and uni-directional flow conditions and compared our results with a series of Computed Tomography (CT) scans of real corals Pocillopora verrucosa exposed to various in-situ flow conditions in a controlled flume setup (Mass T & Genin A (2008). Our results qualitatively agree with the experiments and demonstrate the effect of flow on the growth of branching corals. Under uni-directional flow conditions asymmetrical growth forms develop in the upstream direction. Our finding emphasize the impact of external environmental trait contribute to the colony level morphology.

Hennige SJ, Smith DJ, Walsh SJ, McGinley MP, Warner ME, et al. (2010). Acclimation and adaptation of scleractinian coral communities along environmental gradients within an Indonesian reef system. J. Exp. Mar. Biol. Ecol. 391, 143–152.

Kaandorp JA (1999) Morphological analysis of growth forms of branching marine sessile organisms along environmental gradients. Mar Biol 134:295-306

Mass T, Genin A (2008) Environmental versus intrinsic determination of colony symmetry in the coral Pocillopora verrucosa. Mar Ecol Prog Ser 369:131-137

Merks, R.M.H., Hoekstra, A.G., Kaandorp, J.K. & Sloot, P.M.A. (2004). Polyp oriented modelling of coral growth. J. Theor. Biol. 228, 559-576.

Muko, S., Kawasaki, K., Sakai, K., Takasu, F. & Shigesada, N. (2000) Morphological Plasticity in the coral Porites sillimaniani and its adaptive significance. Bull. Mar. Sci., 66: 225-239

Todd, P.A. (2008). Morphological plasticity in scleractinian corals. Biol. Rev. 83, 315-337.

Veron J, Pichon V (1976) Scleractinian of eastern Australia Monograph 1. Families Thamnasteriidae, Astrocoeniidae, Pocilloporidae. Aust Inst Mar Sci Monogr Ser, Townsville, Australia

SPECIFIC PROBLEMS OF BILLING IN DISTRIBUTED COMPUTATIONAL ENVIRONMENT

Timofey Churov

e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia

Technologies of distributed computing has been actively developed nowadays in the direction of the integration various resources and tools. The investigation of methods and platforms for trouble-less interacting between different technologies is one of the main features of this process. But there are some others features necessary for supporting of progress of these technologies, for example, security and reliability of systems and theirs parts, and a billing –accounting of consumption of computing and network resources and managing of cash operations between services consumers and suppliers. Complicated billing system is the implicit parts for commercial instances of distributed computational environment, and main theirs challenge is to arrange accounting for different resources' suppliers.

This work is related with specific problems that compose topicality of investigation of new billing models and methods that will be decrypted below.

First feature is the big number of resources' suppliers and local accounting services. Arranging communications and cash flows between different suppliers can be a problem as on organizational as on technical layer. This problem can be solved by using payment systems, however, distributed environment suppose to raise a lot of transactions and generate many exceptions.

Another problem is a variety of measurement units. There are a lot of types of services that could need payment and they all can have own measurement unit. They are simple units like seconds of processor's time and Mb of hard drive's usage and more specific like number of I/O operations and volume of RAM memory per time unit. So solution for this problem needs a special synthetic measurement unit that should be simply related with money and can be gotten by applying rates for different resources.

Some organization problem is uncertainty of users groups. The resources can be used by different participants of distributed computational environment like common consumers and owners of software or hardware and have special rights. And also resources can be used by their owners without methods of distributed platform.

Last problem observed in this work is an inaccuracy of prediction of workflow's execution features. The total price of WF includes prices of atomic tasks and depends on such execution parameters as calculation time and volume of transferred data. All these features can be unpredictable in common case because of dependencies by data between different tasks, transfer delays, hardware problems and etc. For example, estimated execution time of single task can't be accurately calculated before data

for its execution is gotten.

Billing module prototype of CLAVIRE (CLoud Applications VIRtual Environment) distributed computational environment uses some principles observed in this work. Billing module is now developing using Microsoft .Net technology and consists of three sub modules: accounting service for interaction between users and platform, billing service for platform and resources and rating service for defining rates for resources' usages.

PROVENANCE FEEDBACK LOOP FOR AUTO WORKFLOW COMPOSITION ABSTRACT

Cushing Reginald Steven

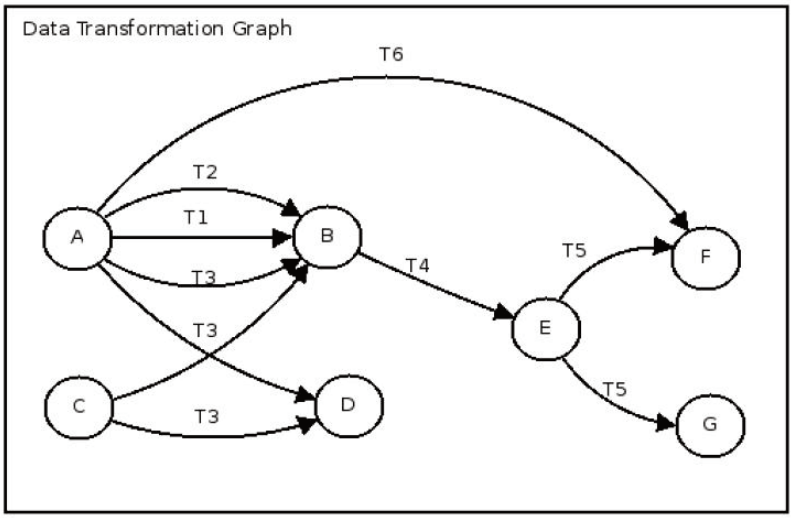
Considering future scientific community task libraries containing hundreds of atomic modules how can we auto compose a workflows and deal with ambiguities that rise from tasks implementing the same transformation? With many modules available for a scientific community it may be a daunting task constructing a workflow for the required experiment that ultimately transforms the input dataset into the requested output dataset. Having the available modules in the library semantically annotated on what input data is required and what output data it produces a system can easily construct a data transformation network as shown in the figure below. Thus a scientist merely specifies the input data and chooses the output result that can be produced through the transformation network. Inevitably with many tasks being contributed to the community some tasks will provide the same semantic transformation with different implementation (e.g. different versions of implementations). This will lead to and ambiguity in finding a path between the input dataset and the result dataset. Using provenance feedback we can annotate tasks with weights which describes the performance of a task.

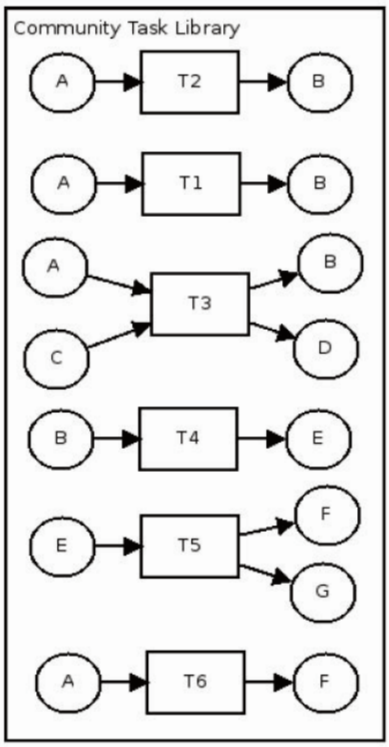
The weighting system will help the auto workflow construction deal with ambiguities. In the example below a scientist defines that he has input dataset A and needs resulting dataset F. From the network

A.F translates:

A.F = ((T2|T1|T3).T4.T5)|T6

The shortest path is obviously using T6 transition but that does not say anything about the performance thus provenance feedback can be instrumental in deciding which path to take for best performance, precision, etc.




Community Task Library
A
T2
B
A
T1
B
A
C
T3
B
D
B
T4
E
E
T5
F
G
A
T6
F

MODIFICATION OF ALGEBRAIC MULTIGRID FOR EFFECTIVE GPGPU-BASED SOLUTION OF NONSTATIONARY HYDRODYNAMICS PROBLEMSD

E. Demidov[1], D. V. Shevchenko[2]

[1]Russian Academy of Sciences, Kazan Branch of Joint Supercomputer Center, Kazan, Russian Federation

[2]Kazan Federal University, Institute of Mathematics and Mechanics, Kazan, Russian Federation

Algebraic multigrid (AMG) is one the most effective methods for solution of large sparse unstructured systems of equations, arising, for example, from discretizations of elliptic differential equations. AMG applies ideas of geometric multigrid (smoothing and correction on coarse grid) to solution of certain classes of algebraic systems of equations. The main advantage of AMG (besides robustness and efficiency) is its ability to solve elliptic partial differential equations discretized on unstructured grids. AMG can be used as a black-box solver for various computational problems, since it does not require any information about underlying geometry.

The algorithm of AMG has two major stages: setup phase and solution phase. The setup phase in classic formulation of AMG is very hard to parallelize because of its intrinsic serial nature. To the contrary, the solution phase allows straightforward parallelization. When GPGPU technique is applied to the solution phase, tenfold acceleration rate is easily achieved. However, according to Amdalh's law, we cannot exceed acceleration rate of 3x for solution of single system of equations, since about 30% of computational work belongs to setup phase. It is shown in this work that this restriction may be loosened when solving nonstationary problems with constant or slowly changing coefficients.

In practice, AMG is more often used not as a standalone solver, but as a preconditioner for one of Krylov subspace methods, such as conjugate gradients. This increases robustness of AMG and reduces number of V-cycles required to achieve convergence. Such usage of AMG also allows us to cut down number of times when setup phase is necessary. When solving nonstationary problems, there is a strong chance that AMG which was built for matrix Ai at time step i will still be a reasonably good preconditioner for matrix A_{i+1} at next time step. We base our technique for solution of nonstationary problems on this assumption. (1) At the first time step both setup and accelerated solution stages of AMG are performed. (2) On each subsequent step: (2.1) in case the solution step on previous time step took more V-cycles than some predefined threshold N_{cr}, AMG is rebuilt for the new matrix. Otherwise, we leave AMG intact. (2.2) The current system of equations is solved with a Krylov subspace method. AMG (either new or old) is used as a preconditioner. The value of Ncr should depend on the convergence rate of the problem at hand. We found that N_{cr}=20 works reasonably well for our needs. In the worst-case scenario of this algorithm we will perform as

many setups of AMG as in classic algorithm. However, it is more probable that AMG built for a previous time step will work reasonably well as preconditioner on the current time step. Since setup phase takes up to 90% of computation time when using CUDA based GPGPU acceleration for solution phase, we may hope for substantial decrease of total computation time.

The suggested modification of AMG for GPGPU-based solution of nonstationary hydrodynamics problems allowed us to save substantial amount of computation time by means of less frequent AMG setups. This modification is easy to implement and should work well enough for problems with slowly changing coefficients.

MODELLING FLOW-INDUCED VIBRATIONS OF FLOOD BARRIER GATES

C.D. Erdbrink

University of Information Technologies, Optics and Mechanics, Russia

University of Amsterdam, The Netherlands Deltares, The Netherlands

Movable barriers form essential parts of many flood defence systems. Large sector gates are built to close off waterways during storm surge events. Coastal sluice structures use hydraulic gates to provide protection from high sea levels and to regulate the discharge of river flow to sea. These gated engineering structures are for instance found in The Netherlands and in Saint Petersburg, Russia, where a large dam with multiple gates protects the city from floods. Optimal control of hydraulic gates and prevention of gate failure are crucial for reliability of flood defences.

Interaction of hydraulic gates with water flow is known to involve dynamic loads on the structure caused by flow-induced vibrations. This topic is part of the research field of fluid-structure interaction, which involves both hydrodynamics and structural mechanics. The traditional way of investigating vibrations of large gates of hydraulic structures is to perform measurements on a physical scale model in the laboratory or on the real-life structure itself. However, the development of automated control and decision systems of barriers –which is done in the UrbanFlood project– requires quick and accurate prediction of gate stability for unanticipated conditions. This is the motivation to conduct numerical modelling of gate vibrations.

My PhD study started in July 2011 and focuses on computational modelling of flow-induced vibrations. The point of departure is a data set of physical scale model tests of underflow gates that were done at Deltares (Delft, The Netherlands) in April 2011. Results from the experimental data analysis will be used for validation of the computational efforts.

Work so far has resulted in a proposal for a hybrid data-driven system to control dynamic gate behaviour. Submitted for FLOODrisk 2012, a conference on water management, the main idea of this system is as follows. Sensors on the gate collect response data (acceleration signals) from which the most important features (frequencies, amplitudes) are extracted and fed into a database. A combination of machine learning and finite-element modelling is applied to this database to make decisions about when and how to open the barrier gates.

Machine learning techniques are employed to classify the vibration data. Firstly, a force thres¬hold separates the regular vibrations from low-level noise. Secondly, a classi¬fication into safe and unsafe regions is made using the gate opening and the 'reduced flow velocity' parameter as attri¬butes. The decision boundaries resulting from the classification thus indicate the contours of the vibration regions.

Finite-element modelling is performed using Comsol Multiphysics software. A

two-dimensional vertical model is set up consisting of a flow domain and a structural domain containing a flat-bottom underflow gate. These computational fluid-structure interaction simulations are presently under development.

Apart from simulation of the gate behaviour and comparison of the results with experimental data, future work will look at various computational methods to judge the nature of vibrations. For instance, when the damping coefficient in the motion equation becomes negative, non-linear self-excited vibrations occur.

SIMULATION OF PARAXIAL ULTRA-SHORT LASER PULSE PROPAGATION ON GPU

Daniil Fadeev
Institute of Applied Physics of Russian Academy of Sciences
Nizhny Novgorod, Russian Federation

In this work the problem of numerical simulation of ultra-short laser pulses propagation is discussed. In most cases using Maxwell equations turns to be redundant since reflected waves could be neglected and propagation has paraxial character. Such a situation is typical for filamentation, gas and solid optical breakdown, interaction of strong relativistic laser pulses with plasma etc. As a reduced model we use Cauchy problem with scalar wave equation for dominant component of laser pulse electric field in the following form (for circular polarization equation supposed to be complex where real and imaginary part of represents transverse electric field components):

$$\frac{\partial^2 E}{\partial z \partial \tau} + \Delta E + N(E) = 0$$

where z is the evolutionary variable,

$$\tau = t - z / c$$

is local laser pulse time, $\triangle$ is a Laplacian unidimentional operator corresponding to cylindrical symmetry or planar geometry, N (E) is a nonlinear term which is a problem specific. We restrict our approach with nonlinearities, which are local along spatial coordinates. We allow responses delayed along T though.

In order to solve the stated problem we use split-step fourier approach. Decomposing wave equation onto linear part (first two terms) and nonlinear part (first and last terms) we obtain two equations, which could be integrated numerically with most suitable method. Applying evolution operators for each problem step by step we get the solution of initial problem. Since nonlinear part is local along transverse coordinates the most interesting part from numerical point of view is linear one. In order to solve it we apply fast fourier transformation (FFT) along T obtaining independent partial differential equations for each frequency. Each equation is solved with Crank-Nicholson method, which requires inversion of tridiagonal matrix. Proposed technique utilizes advantages of fourier approximation of data along T which is usually more convenient for wave packet description and unitarity of Crank-Nicholson propagation operator which provides stability of proposed scheme.

The proposed scheme is principally parallel as it is described above. It requires spatial coordinate independent FFT and frequency independent sweep procedure in order to invert tridiagonal matrix. When all arrays are of cache size this approach works quite well. But for parameters of interest none of CPU cache or GPU shared memory

is enough. Here we propose a efficient scheme of tridiagonalization on GPU. The scheme utilizes both the advantages of simple parallel approach based on independence of different frequencies and methods of parallel sweep for unidimentional tridiagonal systems in order to increase the load of GPU.
Whole two-dimensional data is decomposed on small blocks, which fits the shared memory of GPU. Each thread of each GPU's SM sequentially process one data corresponding to one frequency of each block. This results in partial diagonalization of matrix. For final diagonalization last simple processing is performed. Advantages of proposed algorithm are based on typical relation between grid sizes along spatial and temporal variables. Usually we need high precise grid along spatial coordinates. Performed tests shows speed up ratio from 0.8 to about 4 for different ratios between amount of points in grid along spatial and temporal coordinates.

Proposed algorithm of tridiagonalization allows efficient calculation of light matter interaction problems. It shows good performance in tests with typical parameters of numerical grid. It could be used in large systems with several nodes (multi GPU systems or CPU clusters).

A PARALLEL APPROACH TO IMPROVEMENT AND ESTIMATION OF THE APPROXIMATE OPTIMAL CONTROL

Oles V. Fesko

Program Systems Institute of Russian Academy of Sciences,

Pereslavl-Zalesskii, Russian Federation

We consider the following optimal control problem:

$$\dot{x}(t) = f(t, x(t), u(t)), x(t_I) = x_I, t \in [t_I, t_F], u(t) \in D_u: \quad \{u(t) \mid \underline{u}(t) \le u(t) \le \overline{u}(t)\}, \quad F(x(t_F)) \to \min$$

where the state

$$x = (x_1, \ldots, x_n)^T \in R^n, \quad x_i(t), i = \overline{1, n}$$

is piecewise smooth and the control

$$u = (u_1, \ldots, u_p)^T \in R^p$$

belongs to the set of piecewise linear functions or piecewise constant functions

$$u = (u_1, \ldots, u_p)^T \in R^p$$

The interval $[t_1, t_F]$ is divided by the points

$$t_I = \tau_0 < \tau_1 < \tau_2 < \ldots < \tau_{m+1} = t_F$$

where m is the number of «switching points». The vector of control parameters w is restricted by the condition

$$w^i \in W = \{w^i \mid \underline{u} \le w^i \le \overline{u}\}$$

The dynamic optimization problem can be transformed into the conditional finite-dimensional problem of multidimensional function minimization

$$F(x(t_F)) = G(w)$$

The approach to solving the given problem consists of using alternate numerical algorithms: the Runge-Kutta method for solving a Cauchy problem and the modified gradient descent with the Newton method to minimize a multiextremal function G(w). It is required to estimate a found approximate control numerically. The continuous problem can be transformed into a discrete optimal control problem. The Krotov estimate function for discrete problem can be written in a form:

$$\Delta(\tilde{z}, \tilde{w}, \varphi) = F(\tilde{z}(m+1)) + \varphi(0, z_0)$$

where

$$(\tilde{z}, \tilde{w})$$

is an admissible solution of the discrete problem. The parallel algorithm for computing an initial approximation to the optimal control problem and calculating the estimate of

the solution on the basis of sufficient conditions of optimality consists of the following modules: «Initial approximation» (parallel module), «Improvement of control» and «Estimation» (parallel module). The estimate provides us with information about the quality of the approximate optimal solution obtained by applying the improvement control procedure. The steps of solving the recursive Bellman-type relations with respect to the Krotov function ϕ(k,z) in modules «Initial approximation» and «Estimation» can be fulfilled independently for different sets of the controls that have been obtained by constructing the grid. Taking into account this fact, the algorithm can be executed in parallel. To parallelize the computations a model of a processor farm is used. The main processor reads input parameters, constructs the control grid and thereafter distributes the vectors of control parameters to the worker processors; each processor solves its own recursive relations. At the end, the main processor captures the results and chooses the best solution. The program for solution of the optimal control problem is written in C++ and the parallel version is implemented in T++ programming language in the OpenTS parallel programming system. The benefit of this approach is that the T-system provides «automatic dynamic parallelization'», the scheduling and load balancing and so on without a programmer's participation. All numerical experiments have been carried out on the «BLADE» computational cluster at the Program Systems Institute of RAS. The cluster consists of 8 compute nodes; each with 2 Intel Xeon E5472 CPUs – 4 cores each, 8 cores total, running at 3.0 GHz. Each node has 16 GB RAM. The results of running parallel algorithm for solving the bifunctional catalyst blend optimization problem demonstrate that the algorithm is quite efficient for up to 7 compute nodes. The described algorithm is the part of a set of parallel programs «SControl» intended for optimization of controllable dynamical systems. The package of programs is located on the problem-oriented Web-server which is intended to run problems on the «BLADE» cluster through the web interface.

CONCURRENT SIMULATION OF MULTIBODY SYSTEMS COUPLED WITH STRESS STRAIN AND HEAT TRANSFER SOLVERS

Victor V. Getmanskiy, Efim S. Sergeev, Alexander S. Gorobtsov, Timur D. Ismailov, and Oleg V. Shapovalov

Volgograd State Technical University, Faculty of Electronics and Computer Science

Lenin Av. 28, 400131,Volgograd, Russian Federation

Multiphysics models have high computing complexity because they include several physical domains coupled with each other. For multiphysics simulation high-performance computing is required. In case of weak coupling [1] efficient strategy of concurrent simulation is cluster computing. Considered simulation technique based on constrained multibody dynamics solver coupled with additional subsolvers for several bodies. As a result it is possible to view the non-stationary processes in bodies. In case of coupled solvers simultaneous solution is the only way to obtain correct physical picture. Full vehicle simulation is required to design certain construction parts of the vehicle. During the vehicle running on random road profile parts with the same geometry shape has different responses from adjacent parts so it is important to observe all instances if the parts for correct design decisions. There are two physical processes considered. Heat transfer in hydropneumatic spring and deformations of suspension arms. The first kind of simulation is required to prevent poor spring-damping characteristic of suspension at high temperatures. The second kind of simulation is performed for fatigue and durability analysis. Constrained multibody dynamics simulation is performed using augmented Lagrangian formulation [2]. Numerical integration using 4-th order explicit Runge-Kutta method gives stable solution at time-stepping of 10^{-4} second. For heat transfer simulation heat conduction equation in discrete form is used. Deformable body represented as a set of discrete solid elements with flexible links for stress-strain solver implementation. Newton-Euler's formulation is used for simulation of unconstrained multibody representation of deformable body. Solvers interaction is based on dependencies of right-hand side parameters and boundary subdomains parameters. For considered concurrent multiphysics simulation software system is developed. As an example simulation of truck model is performed. Truck multibody model consists of 45 bodies. It has 6 independent suspension subsystems with the same parts. Suspension subsystem includes lower arm submodel and hydropneumatic spring submodel. Stress-strain solver assigned to the lower arm and heat transfer solver assigned to cylinder and piston parts of hydropneumatic spring. Thus there are 18 subsolvers in total. In practical simulation cases subsolvers are more computing intensive than multibody solver. They have a large dimension and 10 times less time-stepping as a rule so using computing cluster is efficient in considered case. Concurrent simulation is performed with two synchronization points. There are

data exchanges between coupled solvers at the end of multibody solver iteration and before new iteration of multibody solver. For reducing amount of transferring data efficient scatter and gather collective exchange operation are used. They are implemented in MPI [3]. Data to exchange is the dependent parameters in coupled solvers. It is stored in single buffer at the main solver which is sorted according to subsolvers order to perform exchange with single synchronous collective operation. Data amount for each solver depends on number of dependent parameters which are counted before simulation and there are no extra data. This technique sufficiently reduces latency during synchronization. Unified subsolvers interface allow to develop different implementation of solvers for one physical phenomena and use them in developed simulation software. For example we have heat transfer solver implemented for CPU and GPU. In considered truck vehicle model all subsolvers are computing balanced so theoretical estimation of speedup reduced to simple expressions. The experimental results testify that concurrent simulation efficiency remains high with increasing number of cluster nodes only in case of large mesh dimensions of 300000 nodes. In case of 20000 nodes efficiency reduces from 0.85 for 2 nodes to 0.45 for 6 nodes. This results are agreed with a theoretical estimation. Further development of simulation software is directed to general implementation of decomposition of large-scale domains [4] and task mapping algorithms for load balancing.

1. Arnold, M.: Numerical methods for simulation in applied dynamics. In: Arnold M., Schiehlen W. (eds.) Simulation Techniques for Applied Dynamics. CISM Courses and Lectures, 191-246. Springer, Wien/New York, (2008)

2. Bayo, E., De Jalon, J.G., Serna, M.A: A modified Lagrangian formulation for the dynamic analysis of constrained mechanical systems. Computer Methods in Applied Mechanics and Engineering 71, 2, 183-195, (1988)

3. Pjesivac-Grbovic, J., Angskun, T., Bosilca, G., et al.: Performance Analysis of MPI Collective Operations, luster Computing 10, 127-143, (2007)

4. Gorobtsov A.S., Getmanski V.V., Sergeev E.S., et al.: Concurrent Simulation of Large-Scale Multibody Systems Using MPI, Proceedings of IMSD2010, Lappeenranta, Finland, May 25-27, (2010)

MATHEMATICAL MODELING OF THE FOREIGN EXCHANGE MARKET WITH THE HELP OF A FRACTAL BROWNIAN MOTION

Alexander Goncharenko
Magnitogorsk State Technical University named after G.I. Nosov,
Magnitogorsk, Russian Federation

Traditional models of the financial market assessment (Mean-Variance Model, Capital Asset Pricing Model, the model of Black-Scholes and other numerical models) don't always show the real process. They have some limitations: the market is rational and returns are normally distributed but the yields are different from the normal distribution, diagrams of the distribution density have a "sharp top" and "heavy tails". Fractal analysis has more complex mathematics, but the results are much closer to practical experience. However, the tools of the fractal analysis are not fully developed, models are few and their economic interpretation is complicated. This approach is not a replacement of "normal" models; it generalizes them all rather than contradicts them. Fractal structure of the foreign exchange market generates cycles, trends, and the set of possible "fair price". It depends on human decisions and can be measured quantitatively. Fractal statistics indicates randomness and complexity of the market. This paper is dedicated to fractal analysis of the foreign exchange market on the example of the following pairs: EUR/USD, RUB/USD and CHF/USD. The data exchange rates simulate using a Fractal Brownian Motion and Monte Carlo method for modeling Gaussian noise. The first two courses have an unstable structure which is subject to changes. CHF/USD rise reverts to summer values after the fall in September. Due to their novelty and lack of research these methods have prospect in the development of the subject. Application of mathematical apparatus and fractal statistics to the study of the market is possible because of its fractal nature. It would mean modernization of the traditional model, taking into account the fractal properties of multi-fractal analysis.

MONTE CARLO SIMULATION OF BRAIN SENSING BY OPTICAL DIFFUSE SPECTROSCOPY

Anton V. Gorshkov[1], Mikhail Yu. Kirillin[2], Victor P. Gergel[1]

[1] Lobachevsky State University, Nizhny Novgorod, Russian Federation

[2] Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russian Federation

Modern advances in neurosciences require novel diagnostic techniques for non-invasive brain sensing. Traditional techniques such as magneto-resonant imaging (MRI) or electroencephalography (EEG) are expensive and their application is limited by high requirements to infrastructure. Recent studies propose application of optical diagnostics for non-invasive brain sensing. Optical diagnostics techniques are based on illumination of the studied object by probing radiation beam and further analysis of scattered energy distribution. The wavelengths of probing radiation are chosen in visible or near IR (NIR) ranges and usually belong to so-called optical transparency window for which absorption of the radiation in biotissues is extremely low. This ensures deep penetration of radiation into studied biological tissues. Employment of several wavelength allows to obtain spectroscopic information about the studied object and in particular cases extract its chemical composition. Optical brain sensing is based on the significant difference in absorption spectra of oxy- and deoxyhemoglobin in NIR range. Brain activity is accompanied by blood oxygenation variation in the corresponding area of cortex and, consequently, affects its local optical properties. By illumination of certain cortex area with radiation at wavelengths where absorption spectra of oxy- and deoxyhemoglobin differ most one can effectively monitor oxygenation status dynamics in target area. This technique is called optical diffuse spectroscopy. Choice of the probing wavelengths from optical transparency window usually ensures penetration of the probing radiation to the target area. However, targeting of the probing radiation is complicated by its multiple scattering in human head tissues. A suitable solution for the problem of prediction of probing light propagation and determination of measurement volume is offered by numerical methods for calculation of light propagation in media with complex geometry. Existing numerical methods which are currently applied to study light propagation in turbid media can be separated into two classes: finite elements methods and statistical Monte Carlo (MC) approaches with ray tracing techniques. It has been generally considered, that the MC method is a gold standard of modeling of light transport in multilayered heterogeneous tissues, but it has the significant limitation: the great computational load. We report on development of novel Monte Carlo code for simulation of light propagation in turbid media with complex geometry aimed for simulation of optical diffuse spectroscopy technique for noninvasive brain sensing. There are some distinctive features of the algorithm. A boundary

of areas with different optical properties is determined by a surface (or surfaces) consisting of a number of triangles which allows to simulated light transport in media with complex geometry. For numerical simulation of brain sensing we introduce a class of detectors, and during the simulation we store information about the weight of photons that have been caught by each detector, and accumulate trajectories of photons. After launching a large number of photons (10^7-10^9) for each detector we know the total weight and trajectory density distribution of photons that passed through it. Simulation will allow to determine optimal characteristics for construction of device prototype for optical diffuse brain sensing. The developed Monte Carlo code can be efficiently parallelized both for SMP and distributed memory systems. We show that the speed-up of the developed algorithm almost linearly depends on the number of nodes/threads in utilized system.

The study is partly supported by FTP "Scientific and scientific-pedagogical personnel of innovative Russia" (project # 02.740.11.0839), grant of the President of Russian Federation МК-1652.2012.2, RFBR projects 11-02-97062 and 11-02-01129 and grant of the Government of Russian Federation № 11.G34.31.0066.

TRANSPORT PHENOMENA IN SPONGES (PORIFERA): A MODELING APPROACH TO UNDERSTAND FLOW AND RELATED PHYSIOLOGICAL PROCESSES

Hammel, J.U.1,2, Jahn, H.1, Wilde, F.3, Beckmann, F.3, Kaandorp, J.1, Nickel, M.2

Research fellow

1 Section Computational Science, Faculty of Science, University of Amsterdam, PO Box 94248, 1090 GE Amsterdam, The Netherlands.

2 Institut für Spezielle Zoologie und Evolutionsbiologie mit Phyletischem Museum, Friedrich-Schiller-Universität Jena, Ebertstr. 1, D-07743 Jena, Germany.

3 Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Str. 1, 21502 Gesthacht, Germany.

Sponges (Porifera) are an evolutionary ancient group of animals which are sessile organisms living on dissolved and particulate organic matter like suspended detritus, bacteria and plankton. Sponges acquire their food source by filtration of enormous amounts of water. Filtration is achieved by an efficient filtration system in the form of a highly structured 3-dimensional network of canals which are supposed to be hierarchically organized.

This so called aquiferous system of the Porifera represents the interface between the sponge and its environment. It is involved in ingestion, excretion, gas exchange, etc. Until the discovery of bypass elements in the complex 3D network of incurrent and excurrent canals the sponge aquiferous system has been understood as a unidirectional fluid transport system powered by the high number of choanocyte chambers (flow generating units) distributed within the entire mesohyl. So far the biological function of bypass elements and their impact on flow in sponges is not understood. Our knowledge about configuration, architecture and function of aquiferous systems is mainly based on scanning electron microscopic studies and investigations of serial sections. But it is almost impossible to understand a three-dimensional network structure of such high complexity based on these data.

In order to overcome these limitations we are using corrosion casting techniques and high density and spatial resolution synchrotron radiation based micro computed tomography (SRμCT) imaging to generate replicates of sponge aquiferous systems. By applying 3D morphometric analysis we studied general architectural patterns of canal systems. This studies revealed a much higher complexity (e.g. highly asymmetric bifurcations, none strictly hierarchical organization) of the canal systems. This calls for a refinement of the presently accepted standard model of flow in sponges in order to understand flow and transport phenomena related to physiological processes.

In combining morphological data, experimentally determined flow velocity data, computational fluid dynamics and advection diffusion modeling results, the present

theoretical standard model of flow in sponges will be refined and expanded to fit our deeper knowledge on the higher complexity of canal system architectures. Following a modeling approach we will bring forth information on fluid dynamics inside sponges and specific canal system elements, like bypass structures, based on high resolution morphological data. Modeling diffusion processes of oxygen and nutrients will provide insight into general physiological processes in sponges. The overall resulting expanded knowledge on sponge canal system functional morphology will lead to a deeper understanding of sponge physiology in general and thus support still ongoing efforts to establish sponge cultivation methods which are an important prerequisite for marine biotechnology and applied natural product research on sponges.

DYNAMICS OF IN-STENT RESTENOSIS: FROM TWO DIMENSIONAL COMPUTATIONAL RESULTS TO IN-VIVO DATA COMPARISON

Hannan Tahir, Carles Bona-Casas, Alfons G. Hoekstra
Computational Science, Informatics Institute,
University of Amsterdam
The Netherlands

Neointimal hyperplasia, a process of smooth muscle cell re-growth, is the result of a natural wound healing response of the injured artery after stent deployment. Excessive neointimal hyperplasia following coronary artery stenting results in instent restenosis (ISR). The influence of stent design parameters such as strut thickness, shape, and the depth of strut deployment within the vessel wall on the severity of restenosis have already been highlighted but the details of the underlying mechanisms remain unclear. These factors impact on local haemodynamics and vessel structure and affect the rate of neointima formation. This study presents first results of a mathematical multi scale model of in-stent restenosis. The development of the simulated restenosis as a function of strut deployment depth is quantitatively compared to an in vivo porcine data set. Moreover, the influence of strut size and shape is investigated and the effect of drug released at the site of injury, by means of a drug-eluting stent, is also examined. The effects of re-endothelialization and a subsequent release of nitric oxide from endothelial cells on the progression of ISR are also studied, showing a direct relationship between the amount of neointima and the availability of a functional endothelium.

WHOLE TRANSCRIPTOME ANALYSIS OF THE CORAL ACROPORA MILLEPORA REVEALS COMPLEX RESPONSES TO OCEAN ACIDIFICATION DURING THE INITIATION OF CALCIFICATION

A. Moya†‡1, L. Huisman*§1, E.E. Ball–, D.C. Hayward–, L.C. Grasso*–, C.M. Chua*, H.N. Woo**, J.P. Gattuso†‡, S. Foret* And D.J. Miller*††*

**ARC Centre of Excellence for Coral Reef Studies, James Cook University, Townsville, Queensland 4811, Australia*

†INSU-CNRS, Laboratoire d'Oce´anographie de Villefranche, B.P. 28, 06234 Villefranche-sur-mer Cedex, France

‡UPMC University of Paris 06, Observatoire Oce´anologique de Villefranche, 06230 Villefranche-sur-mer, France

§Section of Computational Science, Universiteit van Amsterdam, Science Park 904, 1098 XH, Amsterdam, The Netherlands

–Evolution, Ecology and Genetics, Research School of Biology, Bldg. 46 Australian National University, Canberra, A.C.T. 0200, Australia,

*** Macrogen Inc., 10F World Meridian Center, 60-24 Gasan-dong, Gumchun-gu, Seoul 153-781, South Korea, ††School of Pharmacy and Molecular Sciences, James Cook University, Townsville, Queensland 4811, Australia*

1 These authors contributed equally to this work

The impact of ocean acidification (OA) on coral calcification, a subject of intense current interest, is poorly understood in part because of the presence of symbionts in adult corals. Early life history stages of Acropora spp. provide an opportunity to study the effects of elevated CO2 on coral calcification without the complication of symbiont metabolism. Therefore, we used the Illumina RNAseq approach to study the effects of acute exposure to elevated CO2 on gene expression in primary polyps of Acropora millepora, using as reference a novel comprehensive transcriptome assembly developed for this study. Gene ontology analysis of this whole transcriptome data set indicates that CO2-driven acidification strongly suppressed metabolism but enhanced extracellular organic matrix synthesis, whereas targeted analyses revealed complex effects on genes implicated in calcification. Unexpectedly, expression of most ion transport proteins was unaffected, while many membrane-associated or secreted carbonic anhydrases were expressed at lower levels. The most dramatic effect of CO2-driven acidification, however, was on genes encoding candidate and known components of the skeletal organic matrix that controls CaCO3 deposition. The skeletal organic matrix effects included elevated expression of adult-type galaxins and some secreted acidic proteins, but down-regulation of other galaxins, secreted acidic proteins, SCRiPs and other coral-specific genes, suggesting specialized roles for the members of these pro-

tein families and complex impacts of OA on mineral deposition. This study is the first exhaustive exploration of the transcriptomic response of a scleractinian coral to acidification and provides an unbiased perspective on its effects during the early stages of calcification.

CRAWLER FOR MINING COMMUNITIES IN SOCIAL NETWORKS

Andrei V. Iakushev
PhD student
e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia

My researches in Saint-Petersburg University ITMO cover social networks, that reflect structure and processes that take place in real society, and searching hidden communities of people with deviant behavior. For example people that are interested in drugs or suicide. Research of these communities can help to better understand laws of information propagation in them and can help to better influence on them.

Creating instruments and algorithms for community searching in big social networks with limited computational resources is the first part of work. To search communities we need special program - crawler – that downloads information about users and relationships between them. Also we need special algorithms and approaches for searching relatively small community in big network, because we simply don't enough resource to crawl full network.

In the core of community searching algorithms lays algorithms of text mining that classify user's document to given theme (drugs or suicide). To create text classification algorithm for the given theme we need human made knowledge base that contains words and phrases which describes given theme. But even at this step different challenges arise, like allowing different word forms and creating words weight function. Because of word's cases, plural forms and a lot of suffixes in Russian language nouns can have multiple word forms and adding each word form to knowledge base can't be performed so we need automatic way of word forms consideration. Another task is creating word weight function for words and phrases from knowledge base. We need weights for words because different words have different relationship to the given theme, and differently characterize text. In addition creating scalable crawler that can traverse networks of big sizes in small time and resources is also very interesting task. Second part of my work is concentrated on data analysis that was gathered by crawler. We try to research not only individual properties of nodes in the network but also relationships between them and different communities of nodes that can be explicit and hidden. Hidden communities consist not only from nodes that directly specified some property (for example nodes that are interested in drugs) but also from nodes that have many connections with these nodes.

We search for people interested in drugs in social network Livejournal.com which is very popular in Russia. For that purpose we created knowledge base of 375 words and 1392 phrases that describes different drugs, ways of their preparation and using. Using this base we created text classifier and crawled network of 136022 users. Using text mining algorithms we classify these users on four groups depending on the fre-

quency of using words from knowledge base and we found that sizes of these groups approximately the same as sizes of groups of people involved in drug culture that were estimated by experts using real life data. This shows that research of social network can be used in order to study and model processed that take place in real life.

METHOD AND ALGORITHMS OF THE ADAPTIVE ORGANIZATION OF THE DISTRIBUTED COMPUTATIONS IN A DECENTRALIZED GRID

Anatoly I. Kalyaev

Scientific Research Institute of Multiprocessor Computing Systems of Southern Federal Uni-versity, Taganrog, Russia

The new method of the organization of the distributed computations in a GRID-system is offered in the presented paper. The method allows using resources of private computers united by a network for solving coherent tasks. The main feature of the given method is adaptive correcting of process of com-putation if parameters of com-puting nodes are varying. This ability is achieved because of system decentralization. Also paper presents algorithms based on the developed method and program model of decentralized GRID.

Keywords: distributed computations, GRID, adaptability, decentralization, communities, agents.

THE DATA ASSIMILATION IN THE FLOOD FORECASTING MODEL FOR SAINT-PETERSBURG

Anna V. Kalyuzhnaya

e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russian Federation

For several centuries, floods were a threat for many European centers such as London, Amsterdam, Saint-Petersburg. Nowadays, special complexes are developed and continuously improved to protect high population cities from economic and cultural damage, which could cause by flood. To protect Saint-Petersburg from destruction a dike, which separates Neva Bay from the Gulf of Finland, was built.

High water level are almost always meteorologically induced water level disturbances that originate in the western and central Baltic Sea, which then propagate and intensify going eastward, leading to increased level in Saint-Petersburg.

To predict extremely level rising a mathematical model based on shallow water equations is taken. This model performs only synoptic component of oscillation (long-term oscillations are not produced at all). To account for so-called background level additional procedure is need to be applied in a couple with hydrodynamic model. For this aim and for enhance the forecasting accuracy applied the assimilation of measured water level in the model. The difference between the modeled and observed water level at a station in the model is used to adjust model results in the neighborhood of that station. Optimal interpolation and Kalman filtering are the relevant approaches to data assimilation and used before operating the barrier's gates. But data assimilation block requires to be upgraded, because of constantly increasing amount of new data and systematically improving quality of forecast model.

CRIMINAL NETWORKS ANALYSIS

Victor V. Kashirin
PhD student
e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia

Criminal Networks is the topic, which requires usage of wide range of analysis technics available. Considering its both social and business nature, networks of criminals are great objects for studying not only scientific, but also practical and strategic interests too. The bitter part of work in this field is the troubles with obtaining data about the networks. The data has to be gathered from different sources with various levels of validity, informativeness and, sometimes questionable completeness. Therefore the methods and approaches of analysis depend upon it.

The present work investigations are based on two datasets of different kinds about criminal offenders. First is presented by police criminal records about suspects. Its advantages are bulkiness, accessibility, different types of crime involved and personal criminal details are available. Another dataset is brought via criminal intelligence and collected directly from criminal networks by informants. This dataset reveals blind spots in network structure, uncovers hierarchical properties of value network and spots on social aspects of the structure.

This work is aimed to answer two conditionally defined groups of questions. First group of questions could be described as «scientific»: What are the general properties of criminal networks structure? Are there any preferences in terms of role and criminal activity in co-offending network formation? What are the differences in organization of criminal networks for specific crime types? These questions are answered mostly by statistical calculations. They show that criminal networks demonstrate distinctive characteristics of social networks, preferences in terms of role and activity. These calculations also prove that criminal network structure depends on role of an individual in the network of a definite type.

Second group of questions is specified from law enforcement point of view: What are the key actors/edges that can be eliminated from the criminal network to disrupt the criminal network and process? Which actors/edges are important for durability of criminal network after elimination of key elements from network? How effective are law enforcement interventions on the criminal network and production process? These questions require more in-depth research due to inhomogeneous properties of network elements. Importance of actors is determined not only by their function in structure connectivity or by certain centrality characteristic, but also by their place and role in value network and amount of actors with the same role as neighbors or just within the network. For listed purposes we introduce replaceability property of an actor within network as mixture of described characteristics. The lesser replaceability the actor

has, the better candidate he is to cause large disruption of value network while being isolated from it. With the help of that property we can answer the questions about key actors in criminal processes.

SCIENTIFIC WORKFLOW DESIGN TECHNOLOGY USING DOMAIN-SPECIFIC LANGUAGES

Konstantin V. Knyazkov
PhD student
e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia

Scientific workflow is a widespread formalism for computational experiment description. There is a plenty of existing workflow management systems (WMS) devoted to solving of scientific problems (e.g. Kepler, Pegasus, Askalon). These systems vary by used models of workflow (e.g. DAG, Petri-nets, Pi-calculus), workflow representation facilities (textual, graphical), supported workflow block types. This work deals with three aspects of WMS design: a method of software package embedding, textual WF representation and framework implementing interactive WF model. The research results presented below were used in the CLAVIRE (CLoud Applications VIRtual Environment) project which is being developed in the e-Science Research Institute. CLAVIRE is a WMS for distributed computing based on Intelligent Problem Solving Environment (iPSE) concept. CLAVIRE acts as a platform which can be extended with computational resources (clouds, Grids and clusters) and adjusted for using in a specific domain by embedding domain software. The platform is based on an idea of utilization of existing legacy software packages. And the general WF block in CLAVIRE is a single software package run.

One of the main issues is simplification of software package installing. Here package is considered as a piece of software working in batch mode. Usually package is a black box and it's not possible to edit its source code. During execution package processes input data extracted from files and environment and then generates output data which are usually represented by files. Automatic package embedding is complicated by heterogeneity of computational environment, diversity of data representational formats, differences in ways of configuration and running. For this purpose the domain-specific language for package describing is proposed. The language allows to represent declarative and imperative information about package. The description of package in this language consists of several sections: general package info, input parameters, output parameters, execution parameters. Imperative part of description allows to describe data file formats and map them to parameters. Package description is like a container for domain-expert knowledge about the particular package. In the platform the description is used by many WMS components for different purposes: assisting user, checking formed jobs, workflow execution scheduling, package execution. The approach of using a package description as a base for package handling gives an advantage of ability to generate dynamic and interactive domain-specific user interface for packages.

Next issue concerns the workflow representation method. Graphical representation in a majority of reviewed WMS is considered as a basic means for workflow designing. Textual representation is often used as a backend. There is a plenty of existing workflow languages but most of them are not intended to be used as a main workflow design facility (and usually are based on XML). In this work we made an attempt to design a textual language which is clear and easy to use for scientists and has enough flexibility and expressiveness to represent workflows. It is based on DAG model and represent in declarative manner nodes of workflow and dependencies between nodes. For package execution nodes it uses package programming interface derived from package descriptions.

Batch mode of execution of workflows and its nodes is not enough for effective representation of computational experiments in some domains, e.g. urgent computing using computational steering, real time control systems, data mining tasks where large amount of data is processed. As an extension to basic workflow model we propose the model of interactive workflows. The three aspects of such workflows are investigated in this work: support of infinitely working nodes, support of communication between nodes at runtime, the ability of changing workflow graph at runtime. Implemented framework allows to develop interactive packages which can be embedded to the platform.

ACCESS TO LARGE BINARY DATA ON THE CLOUD

S. Koulouzis
University of Amsterdam, Informatics Institute,
Science Park 904, 1098 XH Amsterdam, The Netherlands

Just like cloud computing, cloud storage has also been increasing in popularity for many of the same reasons as cloud computing. Cloud storage delivers virtualized storage on demand, over a network.There is no need to purchase storage or in some cases even provision it before storing data. However, in the scope of some domains such as collaborative medical applications it cannot be assumed that data are located in a single cloud storage infrastructure. Moreover, for security reasons, institutes and hospitals may opt for private cloud storage, or prefer to use their existing storage infrastructure. When considering public cloud storage, there is also a risk of a vendor lock-in. In the case of data-intensive applications and HPC, although computational and storage resources may be abundant, access to large data sets often proves a signi_cant drawback. Thus, to transport, access and process large data in the cloud, e_cient solutions must be put forward. Cloud federation is a concept for addressing issues such as vendor lockin, scalability and fault tolerance. Cloud federation combines services from di_erent providers aggregated in a single pool in order to support resource migration, resource redundancy and combination of complementary resources.

The Large OBject Cloud Data storagE fedeRation (LOBCDER) adopts the federation concept in order to provide reliable, managed access to large binary objects stored in various storage frameworks and providers. LOBCDER transparently integrates multiple autonomous storage resources, and exposes all available storage as a single name-space. This approach attempts to address issues such as vendor lock-in and scalable access of large data sets in a collaborative environment.

Keywords: cloud federation, large data, collaborative environments

HIGH-LEVEL GRAPHICAL WORKFLOW COMPOSITION FOR COMPLEX SYSTEM SIMULATION

Sergey V. Kovalchuk
Senior researcher
e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia

Nowadays scientific experiment often requires complex computation procedures to be performed during simulation process. Moreover today we can speak about a new paradigm for scientific research often called e-Science. This paradigm introduces many issues that have to be solved by collaboration of IT-specialists and domain scientists. These issues become more urgent as appropriate hardware and software turn into large complex systems. In this case solution composition become one of the most complex issues because currently there is a lot of software developed for solving particular domain problem. Today's common approach for solving integration problem is typically based on service-oriented architecture (SOA) which allows developing of composite application using sets of services that give access to diverse resources in unified way. But in case of composite application construction using diverse existing software and hardware resources, implementing complex domain-specific simulation algorithms we are faced with the following issue: user (which is usually domain-expert with week technological background) needs special tools for domain-specific services composition within one complex application aimed to solve particular domain-specific task.

This work (currently performed within e-Science Research Institute) is aimed to develop high-level conceptual graphical user interfaces (GUI) implemented within software tool. This tool should allow the user to develop composite application for complex system simulation without deep technical knowledge on software pieces remote running and integration. Such an interface should have ability to interact with user using general simulation and domain-specific (for particular problem domain) concepts allowing describing task need to be solved. After the task describing information, presented by the user, should be translated into sequence of service calls which can be processed as a workflow which can be run within distributed computational environment.

Presenting approach is based on iPSE concept (Intelligent Problem Solving Environment), which extends well-known PSE (Problem Solving Environment) approach with strong knowledge support. This concept uses formal knowledge acquired from domain experts and IT-specialists to build and run composite software. Within iPSE concept workflow is processed on three layers: meta-workflow (MWF) which forms general task description; abstract workflow (AWF) which defines sequence of procedures to be performed for task solving; concrete workflow (CWF) which is sequence of appointed services to be executed. Concerning this three-layered procedure, pre-

sented project is aimed to form conceptual and technological basis for MWF construction.

During MWF formalization this approach offers to the user a set of palettes containing general graphical elements (representing modeling objects, used models, simulated values etc.) which can be used to describe complex system to be simulated and task to be solved during this simulation (e.g. computing any unknown characteristic of the system in a distant moment of time). This structure is constructed using knowledge of domain-experts mapped onto general simulation conceptual structure. Such approach allows converting automatically or semi-automatically constructed MWF structure into AWF.

Software prototype based on presented approach is now developing using Microsoft Silverlight technology and can act as an extension to CLAVIRE (CLoud Applications VIRtual Environment) distributes computational environment. The CLAVIRE platform developed using iPSE approach allows building composite applications using set of domain specific software available within service-oriented distributed computational environment. This platform gives ability to run AWFs, which can be constructed with the developed software prototype.

PLATELET TRANSPORT BEHAVIOR IN INTRACRANIAL ANEURYSMS

Lampros Mountrakis, Eric Lorenz and Alfons G Hoekstra
Computational Science, Informatics Institute, University of Amsterdam, Netherlands
Correspondence

Intracranial aneurysms are local abnormal deformations of brain vessels and their possible rupture can be lethal to patients. The natural self-repair mechanism is the formation of a thrombus inside the cavity, which significantly lowers the risk of rupture and can also be induced by positioning a stent in the orifice of the aneurysm. Platelets are essential to the initiation and the formation of a thrombus and special attention has to be given to their transport properties. The excess of platelet concentration near the vessel walls is considered to be due to the complex motion of red blood cells. This proximity of platelets to the vessel wall ensures a more effective response to tissue damages.

Several methods have been proposed and used to describe platelet transport in blood flow, from advection diffusion models to fully resolved red blood cells and platelets suspensions. To date, research has mainly focused on the transport of platelets in straight channels providing adequate results, but little has been done for more complex geometries where most of them may lack in confidence. This contribution focuses on the transport behavior of platelets in aneurysm geometries by explicitly simulating platelet-sized and deformable membraneous RBC-shaped particles in realistic dimensions.

The aim of the fully resolved simulation is to obtain a better level of detail on the platelet transport by explicitly considering the enhancing effect of the presence of RBCs. The rich behavior of platelets in complex geometries can give insights on the thrombus formation inside intracranial aneurysms. This way the accuracy of coarser methods can be assessed and in case these simpler models are sufficient, coefficients for the less computationally expensive advection-diffusion models can be provided.

PARALLEL COMPUTATIONS IN DRILLING PROCESS

Lind Yuliya B.
Bashkir State University, «BashNIPIneft» LTD
Ufa, Russian Federation

Construction of oil and gas wells is a basic process in the chain of actions for hydrocarbons extraction. Drilling of each well is carried out on the base of design documentation for its construction; both technical and economic parameters of drilling, as well as its environmental safety and trouble-free construction, depend on correctness of data contained in the project. Most precise results can be obtained by use of science-based algorithms and development of software for automation of calculations in designing of wells construction. The main purpose of this work is development of software for accurate and fast calculation of drilling parameters during designing of well construction; necessity of processing of high data level from database and use of complicated algorithms such as neural networks causes significant computational complexity of the problem, which calls for expediency of parallel computations use. To achieve this object it is necessary to solve the following practical problems:
1) to create a uniform relational database of field data on wells drilled in all fields and management system of the database;
2) to develop and implement a science-based methodology for designing of optimal horizontal wells profiles;
3) to construct maps of intensity for troubles in the drilling process and to develop software for prediction of possible troubles occurring during the wells construction;
4) to construct adequate mathematical models for technological parameters of drilling fluids and to develop software for optimization of their composition and management of their properties based on constructed models;
5) to implement parallel algorithms and to develop uniform software with intuitively clear user interface, which will issue on the basis of suggested algorithms valid recommendations for design of each well depending on its geological and mining conditions.

Uniform software which combines capabilities of all considered programs has been developed. It allows issuing of science-based recommendations for design of each concrete well according to its geological and mining conditions, and provides for use of a PC as well as a multiprocessor system. This allows working with this program for both engineers in research and design institutes, and drillers in the field conditions. Recommendations having been issued by this software allow to reduce time and material costs on troubles elimination, drilling fluid treatment and drilling equipment rent, and this in its turn can lead to rise of technical and economic indices of wells construction.

SKIPPING REDUNDANT SCALES - HETEROGENEOUS MULTISCALE SIMULATIONS OF SUSPENSION FLOW

Eric Lorenz
Section Computational Science
University of Amsterdam

The macroscopically emergent rheology and transport properties of suspensions are very sensitive to the details of fluid-particle, and particle-particle interactions. For systems where the typical spatio-temporal scale of the particle dynamics is much smaller than that of macroscopic properties the scales can be split (see [1] for a classification of multiscale problems). We present a heterogeneous multiscale method (HMM) approach to modeling suspension flow [2] in which, at the macroscale, the suspension is treated as a continous non-Newtonian fluid. Using local shear rate and volume fraction as boundary conditions, in a simulation of the fully resolved suspension microdynamics the apparent viscosity and shear-induced diffusivities are computed. These are then used to complete the macroscopic constitutional relations. On both levels the lattice-Boltzmann method (LBM) is applied to model the fluid phase, coupled to an advection-diffusion solver at the macroscale, and a fully resolved particle dynamics at the microscale, respectively.

Temporal scale splitting between viscous and diffusive dynamics has also been exploited to accelerate the macroscopic equilibration dynamics. Additionally, Galileian and rotational symmetries allow to make very efficient use of a database from which the results of previous simulations can be retrieved, again reducing the computational effort by several orders of magnitude.

The proposed HMM suspension model is applied to the simulation of a 2-dimensional flow through a straight channel of macroscopic width where we can reproduce experimental findings for low Reynolds numbers. We are also able to predict macroscopic properties in the shear-thickening regime not accessible through existing theoretical suspension flow models.

At the end of the presentation an outlook towards HMM simulations of blood flow will be given.

[1] Complex Automata: Multi-scale Modeling with Coupled Cellular Automata. A.G. Hoekstra, A. Caiazzo, E. Lorenz, J.-L. Falcone, and B. Chopard, In A.G. Hoekstra, J. Kroc, and P.M.A. Sloot (Eds.), Simulating Complex Systems by Cellular Automata (Understanding Complex Systems), Springer, 2010.
[2] Heterogeneous Multiscale Simulations of Suspension Flow, E. Lorenz, A.G. Hoekstra; Multiscale Model. Simul. 9, pp. 1301-1326, 2011.

IDENTIFICATION OF THE REGIONAL STRATIFICATION MODEL USING HPC ON THE EXAMPLE OF THE KIROV REGION

Dolmatova A. I., Maltsev K. A.
Vyatka State University

The economic situation in the Kirov region in recent years is quite unfavorable. The economic crisis has had a profound impact on the regional economy. Anti-crisis measures have not shown themselves as effectively as they were expected to be. Why did this happened and how it is necessary to carry out anti-crisis policy? What factors influence the success or failure of any economic program? The answers to such questions are not easy to obtain.

People that have approximately the same position in society, equal levels of income and education, usually have equal views at any problem. The division of society into strata based on major factors of the quality of life is called stratification. Strata - a united group of people - can be described by only a few parameters. Thus, studying the society and dividing it by the strata, one can make predictions about the reactions and, consequently, the effectiveness of any methods of economic development.

The upper stratum consists of a real ruling class, which includes the elite groups that occupy the most important positions in government, in economic and security structures. The middle stratum consists of small entrepreneurs, managers of medium and small businesses, mid-level bureaucrats, senior military officers, the most qualified and capable professionals and workers. In the future, a full-fledged middle class in Russia will be formed on the basis that stratum. Basic social class covers more than two thirds of Russian society. Its members have an average professional qualifications and limited employment potential. The bottom layer closes the main, socialized part of society. The distinctive features of its members are the low activity-potential and the inability to adapt to the tough socio-economic conditions of the transition period.

Model of the regional economy is based on the allocation of social strata associated with certain sectors of the regional economy. It is assumed that each stratum produces value-added in the sector of the economy, and the interaction of strata and sectors of the economy in the model is reduced to a redistribution of value added.

The main task of the study - is to create scenarios of economic development of the Kirov region. Determination of the parameters directly from the statistics is not possible because of the unreliability or lack thereof. The number of parameters that do not have statistical counterparts, in this model is very high that causes the need for high performance computing. Therefore, it is useful to find parameters which will describe the regional economy more adequately by the parallel calculations. The model parameter estimation can be realized by maximization of the proximity criteria convolution of the calculated and statistical data. The parallel program of modeling identifi-

cation was written on C++ language using the massage passing interface MPI and it was executed on Vyatka State University supercomputer. The parameters identification of the Kirov Region data helps to use the model at analytical calculations. The first approximate calculations based on scenarios of economic development of the Kirov region with respect to interacting strata were made.

HIV RESERVOIRS AND IMMUNE SURVEILLANCE EVASION CAUSE THE FAILURE OF STRUCTURED TREATMENT INTERRUPTIONS: A COMPUTATIONAL STUDY

E. Mancini1,, F. Castiglione2, M.Bernaschi2, Andrea de Luca5,6, P.M.A. Sloot1,3,4*

1 University of Amsterdam, Computational Science, Amsterdam, Netherlands

2 Institute for Computing Applications "Mauro Picone", National Research Council, Roma, Italy

3 National Research University, ITMO, St. Petersburg, Russia

4 Nanyang Technological University, Singapore

5 Institute of Clinical Infectious Diseases, Catholic University, Roma, Italy

6 Infectious Diseases Unit, Siena University Hospital, Siena, Italy

** Corresponding author*

Continuous antiretroviral therapy is currently the most effective way to treat HIV infection. Unstructured interruptions are quite common due to side effects and toxicity, among others, and cannot be prevented. Several attempts to structure these interruptions failed due to an increased morbidity compared to continuous treatment. The cause of this failure is poorly understood and often attributed to drug resistance.

Here we show that structured treatment interruptions would fail regardless of the emergence of drug resistance. Our computational model of the HIV infection dynamics in lymphoid tissue inside lymph nodes, demonstrates that HIV reservoirs and evasion from immune surveillance themselves are sufficient to cause the failure of structured interruptions. We validate our model with data from a clinical trial and show that it is possible to optimize the schedule of interruptions to perform as well as the continuous treatment in the absence of drug resistance.

Our methodology enables studying the problem of treatment optimization without having impact on human beings. We anticipate that it is feasible to steer new clinical trials using computational models.

A PARALLEL ITERATIVE SOLVER FOR POSITIVE-DEFINITE SYSTEMS WITH HYBRID MPI/OPENMP PARALLELIZATION FOR MULTI-CORE CLUSTERS

Igor Mitin, Alexander Kalinkin, Yuri Laevsky

Institute of Computational Mathematics and Mathematical Geophysics SB RAS

This article is devoted to the development and study of a software package for solving large systems of linear al-gebraic equations with sparse stiffness matrix on super-computer by using the preconditioned conjugate gradi-ent method (PCG). An efficient preconditioner is con-structed on the basis of domain decomposition method (the additive Schwarz method) which makes it possible to implement the algorithm on several computing nodes. We describe the parallel algorithm for computing the ac-tion of the stiffness matrix and the preconditioner on a vector. In addition, to increase the computational effi-ciency we use the routines from Intel@MKL: the direct solver (PARDISO) and the matrix-vector multiplication for sparse matrices (Sparse BLAS). We also use OpenMP di-rectives on each computational node and exploit paral-lelism of the Intel@MKL routines. Our analysis of the testing results shows the efficiency of the proposed algo-rithm in the sense of a good scalability of the developed parallel code on distributed memory parallel computers.

MODELING BIOSILICIFICATION IN DIATOMS

Narges Javaheri a, Jaap A. Kaandorp a, Werner E.G. Müller b, Heinz C. Schröder

a) Section Computational Science, University of Amsterdam, Science park 904, 1098 XH Amsterdam, The Netherlands

b) Institute for Physiological Chemistry, University Medical Center of the Johannes Gutenberg University Mainz, Duesbergweg 6, D-55128 Mainz, Germany

Diatoms are unicellular algae which are one of the largest silicifying organisms. They have walls made of amorphous silica deposited in a delicately nanopatterned form, which is why they attract increasing interest from a material science point of view. The wall architecture is a species-specific characteristic of diatoms and this shows that the synthesis of silica is highly genetically controlled, in addition to chemical and physical controls. Since the entire genome of some species of diatoms has been sequenced, there have recently been more insights into genetic control; it is believed that such control takes place mainly through two processes. First, via special biomolecules that regulate uptake and transport of Silicon and, second, via an organic matrix (mainly proteins and polyamins) which plays the role of a scaffold in structure formation. In our model, we focus on the uptake and transport of silicic acid through the cell membrane and cytoplasm -- the step that is vital in providing the material for the special silica depositing compartment and, consequently, vital for the cell division.

The diffusion-reaction model used here consists of several compartments and includes polymerization reactions and nutrient transport by Silicon transporters. In this way we can compare the kinetics of silica condensation in a cell with in vitro chemical experiments and achieve an insight into the biocontrol of silicification. Moreover in a compartmental model, we model mass transport equations to estimate the temporal silicon content in each compartments with an optimization method.

There are a large group of sponges which have siliceous skeletons. Since diatoms are single-cellular and their silicification process is better understood (still a lot to be studied) and they have a lot in common in terms of silica-related life, we use diatoms as a simpler case-study for biosilicification in order to also attain a better understanding of sponges skeleton growth.

PARALLEL ALGORITHM OF 3D WAVE-PACKET DECOMPOSITION OF SEISMIC DATA: IMPLEMENTATION AND OPTIMIZATION FOR GPU

Viktor Nikitin

Trofimuk institute of petroleum geology and geophysics SB RAS

Seismic data sets are characterized by multidimensionality, large volume and irregular sampling. Here we address optimal representation of 3D seismic data volumes using wave-packet basis (curvelet-type redundant representation). It can be further used for seismic data compression, de-noising, and interpolation. The wave-packet decomposition appears to be a computationally-intensive operation. We have implemented a forward and inverse 3D wave-packet transform on GPUs using NVIDIA CUDA technology. The code was tested on different types of graphical processors achieving the average speedup up to 46 times on Tesla M2050 compared to the sequential code on CPU. Also we analyzed its scalability for several GPUs. The code was tested for processing synthetic seismic data set.

USING NVIDIA CUDA TECHNOLOGY FOR NEURAL NETWORKS OPTIMIZATION

V. Parubets[1], D.Devjatyh[1], O. Berestneva[1]

[1]National Research Tomsk Polytechnic University, Institute of Cybernetics, Tomsk, Russia

The application of artificial neural networks in medical diagnosis problems. Describes the opportunity to network optimization technology for the NVIDIA CUDA parallel processing in learning and pattern recognition network. The increase productivity and establish the most optimal network structure.

MULTI PARTICLE STATES CALCULATIONS AND PARTICLES STORAGE IN PERTURBED NANOLAYERS

S.I.Popov, M.I.Gavrilov, I.Yu.Popov

St. Petersburg National Research University of Information Technologies, Mechanics and Optics

Problem of particles storage in nanolayered structure is considered. Local perturbations of the nanolayers can lead to appearance of eigenvalues of the corresponding one-particle Hamiltonian. To study the particles storage it is necessary to deal with multi particle problem. It faces with essential computational difficulties due to great increasing of space dimension. Composition of natural physical models, analytical methods and computational approaches allows one to simplify the problem and to obtain results useful for applications. Particularly, Hartree method and FEM are used. The discrete spectrum of the Hamiltonian of two interacting particles is considered. Two different types of the perturbation is considered: deformation of the layer boundary, small window in a wall between two layers. Relation between the system parameters (interaction intensity - waveguide deformation) ensuring the existence of non-empty discrete spectrum is studied. Comparison of particles storage efficiencies in these two casesis made.

PACS 02.30.Tb - Operator theory
PACS 73.21.Ac - Multilayers
PACS 03.65.Ge - Solutions of wave equations: bound states

SOME ASPECTS OF PERCOLATION MODELS APPLYING TO SIMULATION OF SIGNAL PROPAGATION IN A SYSTEM OF MOVING OBJECTS

Valery Prokoshev, Vasily Sklyarenko
Vladimir State University named after Alexander and Nikolay Stoletovs,
Vladimir, Russian Federation

Taking into account a role which is played by cyclic periodic and almost periodic processes, we consider a problem of signal transmission in the system consisting of objects, moving cyclically (on a circle). We show that existing percolation models require significant corrections to model processes in dynamic systems. The possible approach for reduction of dynamic system models to earlier researched models [1] is proposed.

Suppose that in nodes of a flat rectangular lattice with step d the centers of circles are located. All circles has the same radius r (d>2r) and objects rotate on these circles with incommensurable speeds. The signal is sent to all objects on first layer, and it is considered the transmitted through system if it will reach the last layer. The signal can be transmitted instantly and without a delay from object only to the neighbors if the following condition is met: the distance between objects of communication is less than k. Unlike a classical percolation case (see a review in [2]), signal transmission possibility between two objects depends on time.

Simulation was performed on parallel network simulator that was developed earlier and installed on high performance cluster system[4]. For a simulation the extension modules were developed.

Results of simulation allow to estimate the existence of the percolation threshold with sufficient accuracy. The signal transmits through the system with p = 0.6. The resulting value differs on 20% from the value 0.5, which is the percolation threshold for the case of percolation on a square lattice described in [3]. The reason for this effect is the dependencies between links. That leads to a significant change in the threshold value.

It is suggested that if the signal transmission to the next object is not instantaneous, but for some “time to live” interval T, then with increasing T conditional probability of a signal transmission from i-th to i+1-th dependence on the number of the object i will decrease. This dependence can be estimated through the ratio of the probability of signal transmission to the i+1-th object to the probability of signal transmission to the i-th. Also, it is suggested that the sequence of ratios generate a sample of random variables which distributed normally.

From the results obtained in the simulation, we can conclude that the adding the “time to live” parameter on the node is planned to stabilize the sequence of probabilities ratios. Hypothesis of normal distribution random variables sample formed by the se-

quence is rejected and nature of this sequence needs to be clarified further.

References

1. Minlos R.A., Hrapov P.V. O protekanii v konechnoj polose dlja nepreryvnyh sistem // Vestn. MGU. Ser. mat. meh. – 1985. – T. 1. – № 1. – C. 56–59. О протекании в конечной полосе для непрерывных систем.

2. Men'shikov M. V., Molchanov S. A., A. F. Sidorenko A. F. Teorija perkoljacii i nekotorye prilozhenija. V kn.: Itogi nauki i tehniki. Ser. Teorija verojatnostej. Matematicheskaja statistika. Teoreticheskaja kibernetika. — T. 24. — M. 1986. — S. 53–110. Теория перколяции и некоторые приложения.

3. Kesten H. The critical probability of bond percolation on the square lattice equal 1/2 // Commun. Math Phys. – 1980. – T. 74. – № 1. – S. 41 – 54.

4. Shamin, P.U. Parallel'nyj setevoj simuljator: koncepcija i perspektivy razvitija / P.U. Shamin, A.S. Aleksanjan, V.V. Prokoshev // Nauchno-tehnicheskie vedomosti Sankt-Peterburgskogo gosudarstvennogo politehnicheskogo universiteta. — SPb. 2009. — № 3. — S. 18–24. Параллельный сетевой симулятор: концепция и перспективы развития.

NATURE PROCESSES INFORMATION

Rick Quax [1], Andrea Apolloni [2], Peter M.A. Sloot [1,3,4]
PhD student, Computational Science, Informatics Institute,
University of Amsterdam
The Netherlands

Nature processes information. We observe this from physical systems, which register information in the system state and its associated components, transfer information through interactions, and lose information due to thermal noise. Being able to quantify this information processing could lead to a unifying framework for a better understanding of complex systems. In this talk I describe how to use information processing to describe to what extent a macroscopic system is affected by the microstates of its constituents. We study this numerically for a scale-free network of Ising-spins, a prototypical complex system, and shed light on the unexplained phenomenon that real systems with a heterogeneous topology are mainly controlled by nodes with fewer connections. Counter to intuition we find that due to selective information dissipation, not the hubs but rather the intermediately connected nodes are remembered best by the system. Our study reveals that the framework of information processing provides a better understanding of complex systems at large.

Preprint:
http://arxiv.org/abs/1111.5483

Affiliations:
1. Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam,
The Netherlands
2. Institut des Systèmes Complexes Rhone-Alpes (IXXI) and Laboratoire de Physique, École
Normale Supérieure de Lyon, 46 Allée d'Italie, 69007 Lyon, France
3. National Research University of Information Technologies, Mechanics and Optics (ITMO),
Kronverkskiy 49, 197101 Saint Petersburg, Russia
4. Nanyang Technological University, 50 Nanyang Avenue, 639798 Singapore

ACROPORA SKELETAL PROTEOME REVEALS CORAL SPECIFIC PROTEINS AND COMMON PATTERNS IN BIOMINERALIZATION

Paula Ramos-Silva[1,2], Isabelle Zanella-Cleon[3], Lotte Huisman[1], Laurent Plasseraud[2], Jaap Kaandorp[1] and Frédéric Marin[2]

1. Section Computational Science, Faculty of Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

2. UMR CNRS 6282 (ex 5561) CNRS Biogéosciences, Université de Bourgogne 6 Bd. Gabriel, 21000 Dijon, France

3. Service de Spectrométrie de Masse, FR3302, UMS3444/US8 Institut de Biologie et Chimie des Protéines (IBCP), Université Lyon 1, 7 Passage du Vercors, 69367 Lyon, France

4. ICMUB, UMR CNRS 5260, Faculté des Sciences Mirande, Université de Bourgogne, 21000 Dijon, France

Acropora species are one of the best-studied Scleractinian corals taking part in the construction of coral reefs. The genus Acropora has been used to study evolutionary and developmental processes in corals. It also has been the subject of several ecological studies to elucidate coral responses to environmental changes such as ocean acidification. In these contexts, biological sequence data has been made available as EST and nucleotide libraries from general (NCBI) and coral specific (SymBioSys) databases. Moreover the first coral genome from Acropora digitifera was released publicly in 2011. Despite the available sequence data little is known about the genes and proteins that control biomineralization - the process by which corals form their large calcified skeletons. Biomineralization proteins are secreted by the calcifying epithelium and sealed within the skeleton during its growth, constituting the skeletal organic matrix (SOM). So far, in the field of calcium carbonate biomineralization, the composition of the organic-matrix has only been revealed for some structures in vertebrates (ex: eggshell), mollusks (shell) and sea urchins (test, spine, tooth and spicules). To fill this gap and identify new candidate biomineralization proteins in corals we extracted the extracellular matrix from an adult skeleton of Acropora millepora by an improved method. A first characterization of the SOM was performed by SDS-PAGE, FTIR and in vitro interaction with CaCO3. Subsequently we analyzed the OM digested fractions by nanoLC ESI MS/MS and interrogated the transcriptomic sources of Acropora spp. using the MASCOT algorithm. Combining proteomics with transcriptomics enabled the identification of 35 proteins directly involved in biomineralization. These proteins were further analyzed by uptdate sequence analysis methods in a functional and evolutionary perspective. This data analysis revealed simultaneously common patterns to other biomineralizing organisms and a coral specific repertoire.

Keywords: Biomineralization, corals, Acropora millepora, skeleton, extracellular matrix, proteins, sequence analysis.

USING MODELING AND AUTOMATIC DIFFERENTIATION TOOLS IN A FRAMEWORK FOR PARALLEL LARGE-SCALE GLOBAL OPTIMIZATION

Vladimir Voloshinov[1] and Sergey Smirnov[2]

[1] Institute for System Analysis RAS, [2] Moscow Institute of Physics and Technology

The article concerns a number of ways to increase usability of the BNB-Solver global optimization framework by the use of algebraic modeling languages, optimization frameworks and automatic differentiation tools. Several methods of describing optimization problems are discussed and compared in terms of computational performance. Then an approach based on an algebraic modelling language is implemented and benchmarked.

MODELING OF MOLECULAR DOCKING ON A RECONFIGURABLE COMPUTER SYSTEM

Alexey I. Dordopulo, Ilya I. Levin, Dmitry A. Sorokin,
Academician A.V. Kalyaev Scientific Research Institute of Multiprocessor Computer Systems at Federal State University, Taganrog, Russia

The paper contains the description of molecular docking modeling. In contrast to well-known solutions the authors suggest an all-in-one solution that is implemented on a reconfigurable computer system and that provides coordinated functioning of all fragments of the task within a single computational structure. The authors analyse application of methods of optimization of the task's fragments. Adaptation of architecture of a reconfigurable computer system to the structure of the solving task is also viewed.

PROGRAMMING TEMPLATES FOR ACTIVE STORAGES

Ekaterina Tyutlyaeva[1] and Alexander Moskovsky[2]

[1]Program Systems Institute of Russian Academy of Sciences,

Pereslavl-Zalessky, Russian Federation

Storing and processing data in a most efficient way is a major concern in every aspect of human activity. In this paper, we consider the Active Storage concept, implemented using the TSim template parallel programming library and the Lustre parallel file system.

The main idea of active storages is, in the context of parallel file systems, to use computational power of the storage node to process data located on this node. Processing data directly on the storage units can give a dramatic performance increase, by avoiding redundant transfers of data.

The TSim base scheduler provides support for different load balancing strategies and scheduling policies.

For our Active Storage system we developed the Active Storage policy class. User just needs to change the template parameter for the TSim scheduler's registration to change the strategy of the scheduler for the Active Storage policy and back.

```
//MyScheduler::Registrar<RoundRobin<TaskBase> >(NAME);
MyScheduler::Registrar<ActiveSched<TaskBase> >(NAME);
TSimRuntime rt(new MyScheduler);
```

For fault tolerance support we have implemented the modified scheduler and derived type T-variables (also known as futures) with timeout. This technique allows to complete the execution in a determined period of time even if a number of tasks has been uncompleted. Example of usage the T-variable with timeout:

```
TValT<int, N> fin;
 t = new ActiveTask(i, fin);
TSubmit(t);
```

Besides, we study testing results for our Active Storage system using reprojection remote sensing data task and compare it with the standard round robin scheduling policy. Study shows that the Active Storage system is effective even for a small grain of parallelism.

Finally, we suggest a cost model for estimate storing and processing costs for N duplicates in Active Storage environment. We analyzed a large amount of works on characterizing failures in computer systems to choose a statistical distribution that can provide the best fit.

DISTRIBUTED DICTIONARY–BASED MORPHOLOGICAL ANALYSIS FRAMEWORK FOR RUSSIAN LANGUAGE PROCESSING

Dmitry Ustalov
Institute of Mathematics and Mechanics UrB RAS,
Yekaterinburg, Russian Federation

Every natural language processing task depends on morphological analyzer, which is able to annotate the text and perform various transformations on the annotated text (e.g., word inflection: pony → ponies).

The problem of morphological parsing of the text means performing the morphological interpretation of every word of the input text. Usually, this interpretation contains word's POS (part of speech), a set of grammatical descriptors, detected stem and affixes, etc.

Nowadays, one of the most popular scientific fields is procession of big documents collections called the text corpora. For example, this is confirmed by existence of the RAS Presidium Program of the fundamental research "Corpus linguistics". Morphological annotation is one of the important stages of this program, but amounts of text to be analyzed can be measured by decades and hundreds of megabytes of data. So, annotation of these collections at one computing node may take unacceptable time.

In view of wide popularity of the cloud computing technology and large development of the cloud–based natural language processing systems (i.e., GATE Cloud), the problem of creating the distributed morphological analyzer becomes more actual because of high requirements to text processing frameworks that works in cloud.

Myaso (the word is composed as acronym of phrase "my analysis system is open") is a general purpose morphological parser that is developed with the aim of evaluation of the novel morphological analysis methods for Russian and English languages.

The Myaso analyzer is available as an embeddable solution and as a scalable RESTful Web–service with following structure:

1. HTTP request with source data is accepted from a client by a frontend server, i.e., by one of the load balancers (LB);
2. Every load balancer contains the workload table of the backend servers, i.e., application servers (AS), and passes the request to the less–loaded application server that is suitable to process the initial data;
3. The application server (AS) checks existence of the analysis results of the requested word in the cache, and if cache contains necessary data, application server sends a response to the client and terminates the HTTP–connection;
4. If the cache does not contain analysis information of the requested word, the AS

performs morphological analysis using morphological dictionary, saves results into the cache, returns computed results to the client, and terminates the HTTP–connection.
A prototype of distributed morphological analysis system of Russian language is presented. The following advantages of the presented Myaso analyzer can be noticed:

1. In contrast to the closest analogue, the Myaso analyzer is a free software that is licensed under terms and conditions of MIT License and is fully available to anybody;
2. The Myaso analyzer can be used as a typical Ruby library (Ruby Gem), but it includes embedded mechanisms to construct the linear–scalable Web–services of morphological analysis;
3. This analyzer is built on algorithms that were proven at such fields as information retrieval, corpus linguistics, etc.

A source code repository of Myaso is available by URL: https://github.com/eveel/myaso.

COMBINING SOCIAL AND GENETIC DATA TO RECONSTRUCT HIV TRANSMISSION NETWORKS

Narges Zarrabi[1], Mattia Prosperi[2], Robert Belleman1, Andrea De Luca[3], Peter Sloot[1]*

[1] University of Amsterdam, Computational Science, Science park 904, 1098 XH Amsterdam, The Netherlands.

[2] University of Florida, College of Medicine, Department of Pathology, Emerging Pathogens Institute, P.O. Box 103633, 1376 Mowry Road, Gainesville, FL, 32610-3633, USA.

[3] Catholic University of Sacred Heart, Infectious Diseases Clinic, Largo F. Vito,100168, Rome, Italy.

**Corresponding author*

Inferring disease transmission networks is important in epidemiology in order to understand and prevent the spread of infectious diseases. Reconstruction of the infection transmission networks requires insight into viral genome data as well as social interactions. For HIV-1 epidemic, the current research either uses genetic information of patients virus to infer the past infection events or uses statistics of sexual interactions to model the network structure of viral spreading. Methods for a reliable reconstruction of HIV-1 transmission dynamics, taking into account both molecular and societal data are still lacking. The aim of this study was to combine information from both genetic and epidemiological scales to characterize and analyse a transmission network of the HIV-1 epidemic in central Italy. We introduce a novel filter-reduction method to build a social network of HIV infected patients. The social network is combined with a genetic network of patients, to reconstruct the infection transmission network. We apply this method to a cohort study of HIV-1 infected patients in central Italy and find that patients who are highly connected in the network have longer untreated infection periods. We also find that the structure of the transmission network for homosexual males is heterogeneous, consisting of a majority of 'peripheral nodes' that have only a few sexual interactions and a minority of 'hub nodes' that have many sexual interactions. Inferring HIV-1 transmission networks using combined epidemiological and genetic networks reveals novel correlations between high out-degree individuals and having longer untreated infection periods. These findings signify the importance of early treatment and support the potential benefit of wide population screening, management of early diagnoses and anticipated antiretroviral treatment to prevent viral transmission and spread. The approach presented here for reconstructing HIV-1 transmission networks can have important repercussions in the design of intervention strategies for disease control.

References

1. Ferguson N, Capturing human behavior, Nature, vol. 446, no. 7137, p. 733 (2007).
2. Smith RJ, Okano JT, Kahn JS, Bodine EN, Blower S, Evolutionary dynamics of complex networks of HIV drug-resistant strains: the case of San Francisco. Science, vol. 327, no. 5966, pp. 697-701 (2010).

3. Lewis F, Hughes GJ, Rambaut A, Pozniak A, Leigh Brown AJ (2008) Episodic Sexual Transmission of HIV Revealed by Molecular Phylodynamics. PLoS Med 5(3): e50. doi:10.1371/journal.pmed.0050050
4. Prosperi, M.C.F., et al. A novel methodology for large-scale phylogeny partition. Nat. Commun. 2:321 doi: 10.1038/ncomms1325 (2011).
5. Mei S, Quax R, Van de Vijver D, Zhu Y, Sloot PMA, Increasing risk behaviour can outweigh the benefits of antiretroviral drug treatment on the HIV incidence among men-having-sex-with-men in Amsterdam. BMC Infectious Diseases, vol. 11, no. 1, p. 118, (2011).
6. Metzger VT, Lloyd-Smith JO, Weinberger LS (2011) Autonomous Targeting of Infectious Superspreaders Using Engineered Transmissible Therapies. PLoS Computational Biology, vol. 7, no. 3, p. 12.
7. Pilcher CD, Wong JK, Pillai SK (2008) Inferring HIV Transmission Dynamics from Phylogenetic Sequence Relationships. PLoS Med 5(3): e69. doi:10.1371/journal.pmed.0050069
8. DeGruttola V, Schooley RT, Antiretroviral therapy as prevention: linking the mainframe to Main Street. Clinical Infectious Diseases, vol. 52, no. 8. pp. 1050-1052 (2011).

About participants

LIST OF KEYNOTE AND INVITED SPEAKERS

#	name	position	email
1	Belleman Robert	Dr., Informatics Institute, Universiteit van Amsterdam, The Netherlands	R.G.Belleman@uva.nl
2	Bubak Marian	Prof. Dr. , Informatics Institute, Universiteit van Amsterdam, The Netherlands & AGH University of Science and Technology, Krakow, Poland	bubak@agh.edu.pl
3	Boukhanovsky Alexander	Prof. Dr., e-Science Research Institute, National Research University ITMO, Saint-Petersburg, Russia	avb_mail@mail.ru
4	Chopard Bastien	Prof. Dr., University of Geneva, Switzerland	Bastien.Chopard@unige.ch
5	de Laat Cees	Prof. Dr., Informatics Institute, Universiteit van Amsterdam, The Netherlands	delaat@uva.nl
6	Dongarra Jack	Prof. Dr., University of Tennessee, USA	dongarra@eecs.utk.edu
7	Duijn Paul	Strategic analyst in Computational Criminology, Dutch Police,The Netherlands	Paul.Duijn@haaglanden.politie.nl
8	Eiben Guz	Prof. Dr. , VU, Netherlands	gusz.eiben@gmail.com
9	Hoekstra Alfons	Dr., Informatics Institute, Universiteit van Amsterdam, The Netherlands	a.g.hoekstra@uva.nl
10	Kaandorp Jaap	Dr., Informatics Institute, Universiteit van Amsterdam, The Netherlands	J.A.Kaandorp@uva.nl
11	Kampis George	Prof. Dr., Eötvös Loránd University, Hungary	kampis.george@gmail.com
12	Krzhizhanovskaya Valeria	Dr., St. Petersburg State Polytechnical University, UvA	V.Krzhizhanovskaya@uva.nl
13	La Poutre Han	Prof. Dr., CWI and Uni Eindhoven	Han.La.Poutre@cwi.nl

#	name	position	email
14	Lees Michael Harold	Assistant Professor, Nanyang Technological University (NTU) Singapore	MHLEES@ntu.edu.sg
15	Lopatukhin Leonid	Prof. Dr., e-Science Research Institute, National Research University ITMO, Saint-Peters-burg, Russia	leonid-lop@yandex.ru
16	Osseyran Anwar	Dr., SARA, Amsterdam	Anwar.Osseyran@sara.nl
17	van Steen Maarten	Prof. Dr., VU, Netherlands	steen@cs.vu.nl
18	Sloot Peter	Prof. Dr., Informatics Institute, Universiteit van Amsterdam, The Netherlands	p.m.a.sloot@uva.nl

LIST OF YOUNG SCIENTISTS

#	name	position	email
1	Adinetz Andrey	Research assistant, Lomonosov Moscow State University, Research Computing Center	adinetz@gmail.com
2	Baranowski Mikolaj	Informatics Institute, Universiteit van Amsterdam, The Netherlands & AGH University of Science and Technology, Krakow, Poland	baranowski@uva.nl
3	Barinova Vera	Institute of Nuclear Physics of the Moscow State University,Leninskie Gory 1, Moscow, Russia	http://smdc.sinp.msu.ru/
4	Bastrakov Sergey	Student, N.I. Lobachevsky State University of Nizhni Novgorod (UNN)	sergey.bastrakov@gmail.com
5	Belousov Dmitry	Programmer, Institute of Mathematics and Mechanics (IMM), Ural Branch of the Russian Academy of Sciences	rtfdeamon@mail.ru
6	Borgdorff Joris	Section Computational Science of the University of Amsterdam, Amsterdam, the Netherlands	j.borgdorff@uva.nl
7	Botman Daniel	PhD student, Informatics Institute, Universiteit van Amsterdam, The Netherlands	d.botman@uva.nl
8	Butyugin Dmitry	PhD student, Researcher, Institute of Computational Mathematics and Mathematical Geophysics SB RAS	dm.butyugin@gmail.com
9	Bona-Casas Carles	PhD student, Informatics Institute, Universiteit van Amsterdam, The Netherlands	carlesbona@gmail.com
10	Chindapol Nol	PhD student, Section Computational Science Faculty of Science, Universiteit van Amsterdam, The Netherlands	nol.chindapol@gmail.com
11	Churov Timofey	PhD student, University of Information Technologies, Optics and Mechanics, Russia	tchurovtim@gmail.com
12	Cushing Reginald Steven	PhD student, Computational Science, Informatics Institute, University of Amsterdam The Netherlands	r.s.cushing@uva.nl

#	name	position	email
13	Demidov Denis	Researcher, Joint Super Computer Center, Kazan Branch	ddemidov@ksu.ru
14	Erdbrink C.D.	PhD student, University of Information Technologies, Optics and Mechanics, RussiaUniversity of Amsterdam, The Netherlands-Deltares, The Netherlands	chriserdbrink@gmail.com
15	Fadeev Daniil	Researcher, The Institute of Applied Physics of the Russian Academy of Sciences (IAP RAS)	fadey.d.a@gmail.com
16	Fesko Oles	Engineer, programmer, The Program Systems Institute of RAS	fov@pereslavl.ru
17	Getmanskiy Victor	PhD student, Volgograd State Technical University	getman_w@rambler.ru
18	Goncharenko Alexander	Student, Magnitogorsk State Technical University named after G.I. Nosov	alex.gonzao@hotmail.ru
19	Gorshkov Anton	PhD sudent, N.I. Lobachevsky State University of Nizhni Novgorod (UNN)	anton.v.gorshkov@gmail.com
20	Hammel Jörg U.	Research fellowUniversity of AmsterdamFaculty of ScienceSection Computational Science	j.u.hammel@uva.nl
21	Hannan Tahir	Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	h.tahir@uva.nl
22	Huisman Lotte	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	
23	Javaheri Narges	PhD student, Computational Science, Informatics Institute, University of Amsterdam The Netherlands	
24	Iakushev Andrei	PhD student, University of Information Technologies, Optics and Mechanics, Russia	yaja30@gmail.com
25	Kalyaev Anatoly	Programmer, Taganrog Institute of Technology, Southern Federal University	anatoly.kaliaev@gmail.com
26	Kalyuzhnaya Anna	Researcher, University of Information Technologies, Optics and Mechanics, Russia	kalyuzhnaya.ann@gmail.com

#	name	position	email
27	Kashirin Viktor	PhD student, University of Information Technologies, Optics and Mechanics, Russia	kashirin.victor@gmail.com
28	Knyazkov Konstantin	PhD student, University of Information Technologies, Optics and Mechanics, Russia	constantinvk@gmail.com
29	Koulouzis Spiros	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	S.Koulouzis@uva.nl
30	Kovalchuk Sergei	Senior Researcher, University of Information Technologies, Optics and Mechanics, Russia	sergey.v.kovalchuk@gmail.com
31	Lind Yuliya	Associate Professor, Bashkir State University	LindYuB@yandex.ru
32	Lorenz Eric	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	e.lorenz@uva.nl
33	Maltsev Kirill	Student, Vyatka State University	kir109@yandex.ru
34	Mancini Emiliano	Postdoctorial researcher, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	mancini.emiliano76@gmail.com
35	Mountrakis Lampros	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	L.Mountrakis@uva.nl
36	Mitin Igor	Student, Novosibirsk State University	mitin_igor@ngs.ru
37	Nikitin Viktor	Laboratory assistant, A.A. Trofimuk Institute of Petroleum Geology and Geophysics SB RAS	nikitinVV@ipgg.nsc.ru
38	Parubets Valeriy	Student, National Research Tomsk Polytechnic University	vparubets.mail@gmail.com
39	Popov Sergei	Master student, St. Petersburg National Research University of Information Technologies, Mechanics and Optics	popov1955@gmail.com

#	name	position	email
40	Prokoshev Valery	The Vladimir State University named after Aleksandr Grigorevich and Nikolay Grigorevich Stoletov	valery.prokoshev@gmail.com
41	Quax Rick	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	
42	Ramos-Silva Paula	PhD student, Computational Science, Informatics Institute, University of AmsterdamThe Netherlands	p.sequeirados-ramossilva@uva.nl
43	Smirnov Sergey	PhD student, Moscow Institute of Physics and Technology (MIPT)	sasmir@gmail.com
44	Sorokin Dmitry	Researcher, Southern Federal University	ordi@xgl.pereslavl.ru
45	Tyutlyaeva Ekaterina	Programmer, The Program Systems Institute of RAS	
46	Ustalov Dmitry	Senior programmer, Institute of Mathematics and Mechanics (IMM), Ural Branch of the Russian Academy of Sciences	dau@imm.uran.ru
47	Zarrabi Narges	PhD student, Computational Science, Informatics Institute,University of AmsterdamThe Netherlands	N.Zarrabi@uva.nl

Content