HP-SEE

High-Performance Computing Infrastructure
for South East Europe's Research Communities

INSTITUTE OF PHYSICS
BELGRADE

HP-SEE User Forum 2012

October 17-19, 2012, Belgrade, Serbia

Book of Abstracts

Edited by: Danica Stojiljkovic, Institute of Physics Belgrade

e-infrastructure

CAPACITES

Government of the Republic of Serbia
Ministry of Education, Science
and Technological Development

HP-SEE User Forum 2012 took place on October 17-19, in Belgrade, Serbia. It gathered scientists from the SEE Region and beyond whose work strongly relies on HPC resources, with the main focus on the fields of Computational Physics, Computational Chemistry, Life Science, Scientific Computing and HPC Systems and Network Operations.

HP-SEE project (http://www.hp-see.eu) works across several strategic lines to link the existing and upcoming HPC facilities in the region into an integrated South-East European HPC Infrastructure, implement solutions for it, and open it to the wide range of research communities with specific needs for massively parallel execution on powerful computing resources. It brings together research communities, HPC users and operators from 14 countries in the SEE region, enduing them to share of HPC facilities, software, tools, data and results of their work, thus fostering collaboration and strengthening the regional and national human network.

Conference topics:

- Computational Physics
- Computational Chemistry
- Life Science
- Scientific Computing
- HPC Systems and Network Operation

Invited Lectures:

Regional eInfrastructure Development for South East Europe's Research Communities
Ioannis Liabotis, GRNET, Greece

International HPC - Building bigger pyramid
Richard Kenway, NeSC, UK

LinkSCEEM2: Development of an HPC ecoSystem in the Eastern Mediterranean
Jens Wiegand, CaSToRC, Cyprus

Monte Carlo methods for Electron Transport: Scalability Study using HP-SEE infrastructure
Aneta Karaivanova, IICT-BAS, Bulgaria

Numerical Study of Ultracold Quantum Gases: Formation of Faraday Patterns, Geometric Resonances, and Fragmentation
Antun Balaz, IPB, Serbia

Use of High Performance Computing in (Bio)Chemistry
Ivan Juranic, FCUB, Serbia

The impact of GISELA Science Gateway (GSG) on the supported Latin America VRC's
Jesus Cruz Guzman, UNAM, Mexico

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Acknowledgement: HP-SEE User Forum 2012 is organised with the support of the European Commission through the project High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE), co-funded by EC (under Contract Number 261499) through the Seventh Framework Programme.
The organizers of the HP-SEE User Forum 2012 would like to thank the National Library of Serbia for the permission to use their premises and for organizational support.

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Book of Abstracts

Computational Physics

Numerical Study of Ultracold Quantum Gases: Formation of Faraday Patterns, Geometric Resonances, and Fragmentation

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Dusan Vudragovic, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*
Axel Pelster, *Technical University of Kaiserslautern*

Presenter:
Antun Balaz, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*

Contribution type: Invited Lecture

Abstract

In this talk we will present our recent results of the study of ultracold quantum gases, obtained using the NUQG high-performance computing application developed in the framework of HP-SEE project. First, by extensive numerical simulations of the underlying Gross-Pitaevskii equation [1], we will show how parametric excitation of Bose-Einstein condensed systems can lead to formation of Faraday patterns [2]. For two-component systems we will show that the excited Faraday waves far from resonances are of similar periods, emerge simultaneously, and do not impact the dynamics of the bulk of the condensate. We will also show that for a modulation frequency close to twice that of the radial trapping, the emergent surface waves fade out in favor of a forceful collective mode that turns the two condensate components miscible. Second, we will investigate effects of the geometry of the trap to the behavior of Bose-Einstein condensates [3,4]. By changing the anisotropy of the confining potential, we numerically observe strong nonlinear effects: shifts in the frequencies and mode coupling of collective modes [5], as well as geometric resonances. Finally, motivated by recent experimental results on the dynamics of a cigar-shaped Bose-Einstein condensate subject to periodic modulation of the scattering length, we investigate the dynamics of the condensate and show that for resonant drives of large amplitude the condensate reaches a fragmented state. The fragmented state is a mixture of a quadrupole collective oscillation mode on top of which a longitudinal resonant density wave is grafted.

[1] D. Vudragović, I. Vidanović, A. Balaz□, P. Muruganandam, and S. K. Adhikari, Comp. Phys. Commun. 183, 2021 (2012).
[2] A. Balaz□ and A. I. Nicolin, Phys. Rev. A 85, 023613 (2012).
[3] I. Vidanović, H. Al-Jibbouri, A. Balaz□, and A. Pelster, Phys. Scr. T149, 014003 (2012).

[4] H. Al-Jibbouri, I. Vidanović, A. Balaz□, and A. Pelster, arXiv:1208.0991 (2012).
[5] I. Vidanović, A. Balaz□, H. Al-Jibbouri, and A. Pelster, Phys. Rev. A 84, 013618 (2011).

Monte Carlo methods for Electron Transport: Scalability Study using HP-SEE infrastructure

Author(s):
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Emanouil Atanassov, *IICT-BAS*
Todor Gurov, *IICT-BAS*

Presenter:
Aneta Karaivanova, *IICT-BAS*

Contribution type: Invited Lecture

Abstract

In this work we consider Monte Carlo methods for solving quantum-kinetic integral equations which describe the electron transport in semiconductors. The corresponding algorithms are included in SET (Simulation of Electron Transport) application. Here we study the scalability of the presented algorithms using HPC resources in South-Eastern Europe. Numerical results for parallel efficiency and computational cost are also presented. In addition we discuss the coordinated use of heterogeneous HPC resources from one and same application in order to achieve a good performance.

Reflections on Parallelization of Gravity Inversion

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Betim Cico, *Polytechnic University of Tirana*

Presenter:
Neki Frasheri, *Polytechnic University of Tirana, Faculty of Information Technology*

Contribution type: Oral presentation

Abstract

In the paper there is presented a summary of results obtained for the parallelization of 3D gravity inversion using the principle of algorithm CLEAN [Hogborn 1974], undertaken in framework o f FP7 project HP-SEE. The problem is “ill posed” with the definition of [Hadamard 1902].
The core of our algorithm consists in cross-calculation of the effect of 3D array of underground nodes to each of 2D array ground surface points. The process is iterative, updating at each iteration the mass density of one node with a predefined step in order to decrease of the least squares error. The volume of calculations for each iteration was

calculated of the order O (N^5). The number of iterations to obtain the same anomalous body resulted of the order O (N^3), leading to an order of calculations O (N^8).
Experiments were carried out in two HPC systems – the HPCG system of IICT-BAS in Sofia, Bulgaria, and in the SGE system of NIIFI at University of Pécs, Hungary, using both OpenMP and MPI. Obtained results confirmed the order of calculations of O (N^8). The absolute user-time and wall-time was obtained. For moderate sized models with geosection 4000m*4000m*2000m using 3D arrays of 101*101*51 nodes, using up to 1,000 parallel cores, the run-time reached the level of 100,000 seconds (27 hours).
Tests with models and field data resulted with clear mass density contrasts between the anomalous bodies and the medium where they were situated, in the same way as in real geological structures. Tests with multi-bodies geosections indicated the tendency of the algorithm to converge towards single body solutions.
MPI tests carried out in HPCG system of IICT-BAS showed a systematic time overhead when the number of parallel processes increased from 8 to 32. Hypothesizing that this was caused because of inter-process communication between computer nodes, a prediction of potential run-time in multi-cluster MPI grid platforms was undertaken, taking into consideration the relative low bandwidth of campus and metropolitan links (compared with the bandwidth of the BUS connecting cores of a computer node). The extrapolation of data led to the hypothesis that the increase in cores using multi-cluster grids may not result in reduction of the run-time.

Using Structured Adaptive Computational Grid for Solving Multidimensional Computational Physics Tasks

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Presenter:
Peter Bogatencov, *RENAM Association*

Contribution type: Oral presentation

Abstract

In the work described the algorithm and program for solving multidimensional problems represented by differential equations with partial derivatives adopted for using SEE regional HPC resources. The algorithm based on the AMR method - adaptive mesh refinement of the computational grid. Utilization of AMR method can significantly improve the resolution of the difference grid in areas of high interest and accelerate the processes of the multi-dimensional problems calculating.
One of the methods that allow developing optimized applications and speeding up the process of complicated models execution is the method based on adaptive refinement of computational mesh – AMR (Adaptive Mesh Refinement) method. Many complex problems of continuum mechanics are numerically solved on structured or unstructured grids. To improve the accuracy of the calculations is necessary to choose a sufficiently small grid (with a small cell size). This leads to the drawback of a substantial increase of computation time. Therefore, for the calculations of complex problems it is reasonable to use AMR method. That is, the grid refinement is performed only in the areas of interest of the structure, where

e.g. the shock waves are generated, or a complex geometry or other such features exist. Applying AMR the computing time is greatly reducing and the execution of the application on the resulting sequence of nested, decreasing nets can be parallelized. We are considering solution of two- and three- dimensional tasks of gas dynamics that have obvious practical interest. These solutions can be applied to many nowadays problems. However, the making of three-dimensional calculations for high definition grids requires large computational resources.
In all cases, at the beginning of solving the problem we define a way to highlight areas in which we need to construct the grid, and then the program builds a sequence of grids and makes a decision on them. During calculations in the computational area there are domains with large gradients of the parameters - such as temperature, pressure, density and others. These areas are contiguous with areas with a smooth behavior of the investigated functions. Therefore, to reduce the requirements for computing resources a detailed grid with small mesh sizes can be created only in areas of high gradients. Approach to creation of such area - adaptive mesh refinement will significantly clarify the definition of the multi-dimensional flows features. The proposed AMR method is the most suitable method of grid generation for solving three-dimensional problem of the collapsing star.
Calculations using of AMR method based on the hierarchical grid cells, which can significantly improve the quality of the calculations in the various fields of science and engineering. Program based on AMR technology uses object-oriented approach, which is available in the current version of Fortran 90.

Numerical Simulations of the Structure and Transport Properties of the Complex Networks

Author(s):
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Milan Zezelj, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*
Jelena Smiljanic, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*

Presenter:
Igor Stankovic, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*

Contribution type: Oral presentation

Abstract

In this talk we review our recent numerical study of various complex networks. First, we will introduce results of Monte Carlo simulations of the percolation and conductivity of two-dimensional random stick systems. Based on the renormalisation group considerations, generalized scaling function is introduced to describe the scaling behaviour of the percolation distribution moments, i.e., average percolation density and percolation density variance [1]. We show that the prefactors in the generalized scaling function depend on the system aspect ratio. The definite parity of the prefactors in the generalized scaling function for the first two moments is a generic feature of whole class of percolating systems. The conductivity of the random stick systems is investigated from the percolation up to ten times percolation density. An analytic model is proposed describing transition from the conductivity

determined by the structure of a percolating cluster to the conductivity of the dense random stick networks. The derived model for conductivity should be broadly applicable to the random networks of the rodlike particles [2].
In the second part of the talk, we will present paths for optimization of the transport capacity of the complex networks without changing average connectivity or total network capacity. The focus is on efficient routing [3]. The routing strategies are compared using two generic models, i.e., Barabási-Albert scale-free network and scale-free network on lattice, and academic router networks of the Netherlands and France. The nodes without buffers are considered, so, if congestion occurs, packets will be dropped. We propose a dynamic routing algorithm which automatically extends path of the packet before it arrives at congested node. Simulation results indicate that proposed routing strategy can further reduce number of dropped packets in a combination with the efficient path routing proposed by Yan et al. [4].

[1] M. Zezelj, I. Stankovic and A. Belic, "Finite-size Scaling in Asymmetric Systems of Percolating Sticks", Phys. Rev. E 85, 021101 (2012).
[2] M. Zezelj, I. Stankovic, “From percolating to dense random stick networks: conductivity model investigation”, submitted.
[3] Jelena Smiljanic, Milan Zezelj, and Igor Stankovic, “Study of routing strategies in the small complex networks”, Telekomunikacije 9, to appear.
[4] G. Yan, T. Zhou, B. Hu, Z.-Q. Fu, and B.-H. Wang, “Efficient Routing on Complex Networks”, Phys. Rev. E 73, 046108 (2006).

Determination of zone of flow instability in a gas flow past a square particle in a narrow microchannel

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Stefan Stefanov, *Institute of Mechanics - BAS*

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Contribution type: Oral presentation

Abstract

Rapidly emerging micro-electro-mechanical devices create new potential microfluidic applications. Fluid flow regime is important for their design. For a gas flow the transition between steady and unsteady regimes occurs at small Knudsen number Kn < 0.1 (Kn = l0 / L, where l0 is the mean free path of the gas molecules and L is the characteristic length). A continuum approach based on the Navier-Stokes-Fourier equations is applicable for this investigation. On the other the microfluidic application requires the problem to be investigated starting at very low Mach numbers (M=0.1), close to incompressible regime. This makes pressure based methods very suitable for this investigation. The system of Navier-Stokes-Fourier equations is calculated numerically using pressure based algorithm SIMPLE-TS 2D. The results are validated by comparison to data obtained by using molecular approach (direct simulation Monte Carlo (DSMC) method).

Computational approaches for electronic properties of semiconducting materials and nanostructures

Author(s):
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Presenter:
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Contribution type: Oral presentation

Abstract

Density functional theory (DFT) provides a reliable theoretical framework for studying the electronic properties of atoms, molecules, bulk materials, surfaces, interfaces, etc. However, due to its computational effort, the calculations based on DFT are typically performed only for relatively small molecules or for crystalline materials where periodicity of the structure can be exploited. There is a wealth of highly relevant systems which are currently beyond the reach of standard DFT calculations, such as, for example, disordered conjugated polymers, inorganic nanocrystals, and polycrystalline materials. To study these systems, one typically needs to do the calculation for a supercell containing thousands of atoms to get reliable information about the properties of the system.
The methods that can be used to study even such systems will be presented and computational aspects of the applications of these methods will be discussed.
Charge patching method (CPM) [1] is the method for the construction of electronic charge density of the system that avoids demanding self-consistent DFT calculations. It is based on the idea that electronic charge density in the neighborhood of an atom depends mainly on its local environment. Such an assumption is typically valid in semiconducting and insulating materials without any long-range charge transfer. The contribution of each atom to electronic charge density of the system is therefore extracted from the calculation of some small prototype system where atoms have the same environment as in the large system under study. Electronic charge density of the large system is then simply obtained by adding the contributions of each atom. With electronic charge density at hand, one gets the single-particle Hamiltonian by solving the Poisson equation for the Hartree potential and using the local density approximation formula for the exchange-correlation potential.
To study the electrical properties of the material, one does not need to calculate all the electronic states of the Hamiltonian but only these in the region near the band gap. Overlapping fragments method (OFM) [2] was developed to efficiently find these states. The method is in particular suited to study disordered conjugated polymers [3]. It is based on the divison of the system into fragments and the representation of the Hamiltonian in the basis of molecular orbitals of these fragments. It is typically sufficient to use only a few molecular orbitals of each fragment. This approach strongly reduces the size of the Hamiltonian matrix that needs to be diagonalized down to the size of several hundreds.
Finally, several applications of these methods in the studies of organic solar cell materials will be briefly presented.

[1] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 128, 121102 (2008).
[2] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 134, 094119 (2011).
[3] N. Vukmirovic and L.-W. Wang, J. Phys. Chem. B 115, 1792 (2011).

Emergence of resonant waves in cigar-shaped Bose-Einstein condensates

Author(s):
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Presenter:
Alexandru Nicolin, *Horia Hulubei National Institute for Physics and Nuclear Engineering*

Contribution type: Oral presentation

Abstract

Motivated by the continuous interest shown to the nonlinear dynamics of quantum gases we present in this talk the emergence of resonant waves in cigar-shaped Bose-Einstein condensates using which has been reported in Ref. [1].
We introduce the analytic treatment of the dynamics of a trapped, quasi-one-dimensional Bose-Einstein condensate subject to resonant and nonresonant periodic modulation of the transverse confinement. The dynamics of the condensate is described variationally through a set of coupled ordinary differential equations, and the period of the excited waves is determined analytically using a Mathieu-type analysis. For a modulation frequency equal to that of the radial confinement we show that the predicted period of the resonant wave is in agreement with the existing experimental results. Finally, we present a detailed comparison between the resonant waves and the Faraday waves that emerge outside of resonance.
[1] A.I. Nicolin, Phys. Rev. E 84, 056202 (2011).

Iterative Perturbative Method for a Study of Disordered Strongly Correlated Systems

Author(s):
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Milos Radonjic, *Scientfic Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*
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Presenter:
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Contribution type: Oral presentation

Abstract

Twenty years after the introduction of the Dynamical Mean Field Theory as a means of solving the Hubbard model, the focus has moved towards computationally very intensive

multi-site and multi-orbital calculations, which are aimed at including spatial correlations, disorder and detailed atomic structure to the otherwise fairly simple model. However, limited computational resources create a need for faster and more optimized codes and even approximative solutions. We present here a highly optimized parallel implementation of the approximative second order perturbative approach especially suitable for a study of strongly disordered correlated systems. On this example, we give an overview of numerical challenges that arise in dealing with large systems of non-linear equations, ill-behaved discretized functions and self-consistent calculations in general. In the end, we discuss results of performance tests, outline possible improvements and make a comparison to the exact, but computationally very demanding Quantum Monte Carlo method.

Electronic Structure and Lattice Dynamics Calculations of FeSb2 and CoSb2

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Zoran Popovic, *Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade*

Presenter:
Milos M. Radonjic, *Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade*

Contribution type: Oral presentation

Abstract

First principles calculations of the electronic structure and lattice
dynamics of FeSb2 and CoSb2 are performed using the Quantum Espresso package. Calculated vibrational modes and frequencies are used for proper assignation of the normal modes in the corresponding Raman scattering experiments.

Using Parallel Computing to Calculate Quark-Antiquark Potential from Lattice QCD

Author(s):
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Artan BORIÇI, *Physics Department, Faculty of Natural Sciences, University of Tirana Bvd. Zog I, Tirana, Albania*

Presenter:
Dafina Xhako, *Department of Engineering Science, Professional Studies Faculty "Alexander Moisiu" University, Durres, Albania*

Contribution type: Poster

Abstract

Lattice Quantum Chromo-dynamics (LQCD) is an algorithmic formulation of QCD, the mathematical model that describes quarks and their interactions. Computations in LQCD are typically very expensive and run on dedicated supercomputers and large computer clusters for many months. In this paper the calculations are performed in one of the clusters for supercomputing of HP-SEE (High-Performance Computing Infrastructure for South East Europe's Research Communities) project, that is located in Bulgaria (BG HPC). We use parallel computing with Fermiqcd software, to determine the static quark-antiquark potential. In LQCD the static quark-antiquark potential can be derive from the Wilson loops. The standard method use rectangular Wilson loops, while we test 3-D Wilson loops, using simulation with SU(3) gauge field configuration for different values of coupling constant and for different lattice sizes. The calculations are made for 100 configurations, statistically independent, of gauge fields of the lattice. We extrapolate in continuum limit for different lattice constant to take string tension parameter and to compare with the experimental value.

Quenched Hadron Spectroscopy Using FermiQCD

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Contribution type: Poster

Abstract

FermiQCD is a C++ library for fast development of parallel Lattice Quantum Field Theory computations. It has been developed following a top-down fully Object Oriented design approach with focus on simplicity of use. We present simulations for the hadron spectrum with the Wilson action in quenched QCD carried out on the BG HPC cluster, using this tool kit. Testing Fermiqcd as a tool kit for parallel lattice QCD applications and see how parallel calculations are implemented in this package are some aims of this work. Simulations are made with the plaquette gauge action on 8^4, 12^4 and 16^4 lattices at three lattice spacings, for a total number of 300 SU(3) gauge configurations. The masses of pi and rho –meson, nucleon and delta baryons are computed for these conditions. For a constant physical volume we study the dependence of the hadron masses on the lattice spacing. After chiral and continuum extrapolations, the agreement of the calculated mass spectrum for this kind of fermions with experiment is reasonable.

EagleEye: Feature Extraction from Satellite Images Using a Hybrid Computing Architecture

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Contribution type: Poster

Abstract

Feature extraction from satellite images has become a wide area of interest in the last two decades with the increase in the number of commercial earth observation satellites. This work focuses on extracting roads and cities from true color multi-spectral images that suffer from different quality problems like blurriness, increased amount of noise or abnormal color variations. To assist in the feature extraction process we extract city location information from almost 200 military maps. We present an approach for automatic and independent road detection in satellite images, an automatic city detection process in military maps and a semi-automatic (assisted) method of detecting street layout inside cities in satellite images. We also evaluate the accuracy and performance of our implementation by tests that are done using a parallel infrastructure running over different types of blades inside an HPC computing cluster.

Self-avoiding Hamiltonian Walks Counting in Parallel processing mode

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Contribution type: Poster

Abstract

We have developed a program for counting self-avoiding Hamiltonian walks to run on multiple processors in a parallel mode. We study Hamiltonian walks (HWs) on the family of two-dimensional modified Sierpinski gasket fractals, as a simple model for compact polymers in nonhomogeneous media in two dimensions. We apply an exact recursive method which allows for explicit enumeration of extremely long Hamiltonian walks of different types: closed and open, with end-points anywhere in the lattice, or with one or both

ends fixed at the corner sites. The leading term ωn is characterized by the value of the connectivity constant $\omega 1$, which depends on fractal type, but not on the type of HW.

Data analysis in high energy physics using CUDA and OpenCL

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Contribution type: Poster

Abstract

We developed an aplication that allows both the analysis of data and also the real-time visualisation on the same time. This is possible with the help of the GPU. To use the power of GPU is need of an specific framework (we use CUDA and OpenCL).
The application use data generated by UrQMD (Ultra relativistic Quantum Molecular Dynamics) to run a variety of algorithms and 3D visualization. How it works: As a front-end to the user, the application uses Qt libraries to create the GUI (graphical user interface library) and user interaction. The input data, obtained from a SQLite3 database file, is fetched and loaded on the graphic device. After this, the data is processed on GPU using CUDA (Compute Unified Device Architecture) or OpenCL (Open Computing Language), depends on the GPU use. The processed data is output in a OpenGL(Open Graphics Library) viewport and in ROOT's graphs or histograms. Using widgets, one can select/filter events, frames or particles that are going to be processed. Also, render all frames in an event continually, such that one sees the evolution of particles as a fluid animation. Just like movie player, with buttons to play/pause or go forward, backward.
When one wants fast analysis and real-time animation, one chooses parallel processing. Having this in mind, we put move all processing on the best and cheapest parallel unit one can afford: GPU parallel processing. The framework developed by NVIDIA named CUDA and the framework developed by Khronos Group named OpenCL allows one to harness the power of the GPU device using parallel processing. The programming execution model on GPU in CUDA is SIMT (Single Instruction Multiple Thread) and in OpenCL is SIMD(Simple Instruction Multiple Data). This means, only one function (running in multiple threads or instances) can run on the GPU at one time processing the data. In CUDA and OpenCL terminology, this function is named a kernel.
After querying database for the interested data, and loading it in GPU, depending on the one's action, a CUDA or OpenCL kernel (depends on the GPU used) is launched accordingly. The kernel above, takes in particles information (x,y,z,px,py,pz,E,...) and outputs the computed values of: transverse momentum, direct and elliptic flow parameters, pseudo-rapidity and OpenGL's necessary data to render the particles. The representation of the processed data can be seen in OpenGL viewport (particles as spheres) and parameters in ROOTs graphs and histograms.

Evolution of an gravitotional bound n-body system with DLA (Diffusion Limited Aggregation) initial mass distribution using GPU parralel computing

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Contribution type: Poster

Abstract

In this paper we present a collection of algorithms to generate power law mass distribution as initial conditions for gravitational N-body simulations. This type of algorithms are highly parallizable and can analyze large data customary on clusters. The input data will be high resolution images in the most used format in astrophysics, FITS and diffusion limited aggregation generated clusters. The application will algorithm running on GPU (with CUDA and OpenCL), for the generation of initial mass distribution and fort the evolution of the n-body sysytem. Data analysis and plotting is done in ROOT Framework.
General scientific image on the formation and evolution of the galaxies is that they formed by gravitational collapse of matter. The study of the mass distribution of spiral galaxies will shade new light on the formation and evolution of galaxies. The application will provide new data of spiral arms and their morphology.
The method is name all-pairs that is a brute-force technique that evaluates all pair-wire interactions among the n bodies. The all-pairs method is combined with a faster method based on a far-field approximation of longer-range forces, which is valid only between parts of the system that are well separated. Fast N-body algorithms of this form include the Barnes-Hut method (BH) (Barnes and Hut 1986), the fast multipole method (FMM) (Greengard 1987), and the particle-mesh methods (Hockney and Eastwood 1981, Darden et al. 1993).
The benchmarks was done on an server with 4 GPU (Nvidia Tesla) with 480 cores each.
The tests was been maid on 480, 960, 1440, 1920 cores on CUDA and OpenCL and the difference was 5-10% in CUDA favor.

Formation of Faraday And Resonant Waves in Driven High-Density Bose-Einstein Condensates

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Contribution type: Poster

Abstract

Extended parametric resonances are one of the recurrent themes in the dynamics of quantum gases. Following some inceptive theoretical works Faraday waves have been observed in parametrically driven 87Rb BECs and 4He cells subject to vertical vibrations. These experimental observations have catalyzed the research activities and many theoretical investigations followed shortly. Among them we mention the emergence of density waves in dipolar and binary condensates, the transition to miscibility observed in non-miscible condensates and the suppression of Faraday waves in condensates loaded into optical lattices.
In this work we present the variational method introduced in Ref. [1] to describe the dynamics of cigar-shaped Bose-Einstein condensates of high density subject to periodic modulations of the radial component of the confining potential. The key ingredient of the variational treatment is the q-Gaussian radial envelope which describes the Thomas-Fermi regime of the condensate. A longitudinal density wave is grafted to the ansatz to account for Faraday and resonant waves. Using the variational equations, we investigate the dynamics of a realistic condensate for frequencies close to the radial frequency of the trap and show the emergence of the Faraday waves excited outside of resonance and that of the resonant wave that appears straight on resonance.

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Computational Chemistry

Use of High Performance Computing in (Bio)Chemistry

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Contribution type: Invited lecture

Abstract

A short overview of computational modeling is presented. The major features of molecular geometry optimization are given, and the computational demands are analyzed. Short outlines of strategies that are in use for speeding-up of computation are presented, too.
In the second part of presentation, the specific examples, and accompanying results of computational applications in chemistry are given. The aim is to make a rational design of efficient drugs, and, on other hand, to explain the mechanisms of complex chemical reactions. In last two centuries of Chemistry, the models are in heart of amazing progress made in it. Many models deal with non-observables, and validity of model can be tested only by simulations. These simulations could be done on various levels of complexity, and some illustrative examples are presented.
A study of molecular potential energy surface (PES) is done on QM level in order to explain the mechanism of the reaction of carbonyl compounds with bromoform. A successful application of non-observable molecular descriptor – partial atomic charges - is presented, too.
The application of MM and MD simulations for the description of interaction of small molecules with proteins was successfully done on several examples. The computationally derived molecular descriptors were used for statistical modeling of the correlation between molecular structure and biological activity of compounds. These correlations give the leverage for the design of more potent drugs.

Design of novel nano-photonic materials

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Presenter:
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Contribution type: Oral presentation

Abstract

We have designed or selected a series of derivatives, which have very high linear and nonlinear optical L&(NLO) properties and which are likely to be useful for photonic applications. The compounds belong to three families:
(a) Noble gas derivatives. These involve one or more noble gas (Ng) atoms inserted in the chemical bond A-B [1-2]. We have considered a number of such derivatives, for example HArF, HXeC2H. It has been found that, in general, the inserted noble gas atom increases remarkably the NLO properties. Two novel Xe derivatives have also been proposed: HXeOXeF and FXeOXeF. Their electronic ground state, the stability and their L&NLO properties have been studied [2].
(b) Ni-dithiolene derivatives. We discuss how the diradicaloid character (DC) of Ni(SCH)4, which is used as model derivative, affects the L&NLO properties. It has been found that the quasidegeneracy of the two lowest-energy singlet states, 1 1Ag and 1 1B1u, the clear DC nature of the former and the very large number of low-lying states increase the NLO properties. The very large effect of Ni on the properties of interest is demonstrated. A series of Ni-dithiolene derivatives with very large NLO properties are proposed [3].
(c) Fullerenes. Using a wide variety of quantum-chemical methods we have analyzed in detail the L&NLO properties of [60]fullerene-chromophore dyads of different electron-donor character [4]. The dyads are composed of [60]fullerene covalently linked with 2,1,3-benzothiadiazole and carbazole derivatives. Substitution of 2,1,3-benzothiadiazole by the triphenylamine group significantly increases the electronic first and second hyperpolarizabilities.
These studies have been performed by employing a series of methods: HF, DFT, MP2, MS-CASPT2, CCSD and CCSD(T).
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Development of a Hybrid Statistical Physics – Quantum Mechanical Methodology for Computer Simulations of Condensed Phases and its Implementation on High-Performance Computing Systems

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Contribution type: Oral presentation

Abstract

A hybrid, complex statistical mechanics – quantum mechanical approach which enables exact computational modeling of condensed phases at finite temperatures has been developed and implemented on high-performance computing systems. The computational approach is robust and inherently sequential. First, the studied physico-chemical system is modeled by a statistical physics approach, either Monte Carlo (MC) or molecular dynamics (MD). Though in the first phase it is often sufficient to carry out a classical MC or MD simulation, in particular cases, when it is necessary, one can also perform a quantum molecular dynamics simulation (e.g. ADMP, BOMD or CPMD). Even the classical MC/MD simulations carried out in the first phase can be based on interaction potentials which have been derived by quantum chemical calculations. Sequentially to the first phase of the computation, which actually generates either a MD trajectory or an appropriate sample of the system's configurational space, the generated trajectories are analyzed employing time-series analytic methods. In the case of e.g. MC simulations, this is done most frequently by computation and subsequent integration of the energy autocorrelation function, which leads to the so-called correlation step. The last quantity is then used to choose a representative number of configurations representing the state of the physico-chemical system at finite temperature which will be further analyzed by a quantum mechanical approach. These, appropriately chosen configurations for the system of interest, are further modeled by exact quantum mechanical (QM) approach. The particular approach that needs to be implemented depends on the quantity that needs to be computed. For example, in the case of X-H stretching vibrations, the anharmonic X-H vibrational frequency is computed in a quantum mechanical manner with respect to both electronic and nuclear subsystem. In this case, first a 1D cut through the vibrational potential energy surface is computed at series of suitably generated points, and subsequently, the vibrational Schrodinger equation is solved either by diagonalization approach or using a variant of the discrete variable representation (DVR) methodology. As the statistical mechanics simulations are often done implementing periodic boundary condition, the exact QM calculations in the final simulation phase are often done implementing some sort of embedding of the relevant part of the system. All these aspects of our developed methodology are illustrated through a particular example – the fluoroform solvated in liquid Kr and the noncovalently bonded complexes which are formed between fluoroform and dimethylether in liquid Kr. A vast variety of condensed phase systems can be treated by the developed approach. Achieving good parallel efficiency for calculations of such type is far from a trivial task without the use of high-performance low-latency MPI interconnect (such as, e.g. a supercomputer or HPC cluster).

Dynamics of uninhibited and covalently inhibited cysteine protease on non-physiological pH

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Contribution type: Oral presentation

Abstract

Cysteine proteases involved in degradation of proteins, widespread in plants, parasites and vertebrates, are an important medicinal chemistry target implicated in the diseases ranging from immunological processes to cancer. Due to conserved cysteine residue in their active site, unsaturated ketones and their analogs represent one of the major chemotypes used for inhibitors design [1]. In this communication the dynamics of the papain-like cysteine protease isolated from the fruit, uninhibited and inhibited with covalent inhibitor E-64, on non-physiological pH, were reported merging results and experiences from our biochemical and medicinal chemistry laboratories.The aim of our study is to explain some experimental findings. Proteins are modeled using similar ones with the known 3D structure, taken from Protein Data Bank [2]. After sequence alignment residues that differentiate templates from the experimental proteins were manually changed. Afterward the eventual existence of close contacts, bumps or similar was carefully checked. The protonation states of the aminoacid residues and the inhibitor ionizable groups were adjusted to pH 1.5, using empirical function [3]. Systems were neutralized with explicit counterions, than embed in explicit water, obtaining the sphere having ~ 100 Å radius. Systems under simulations were minimized during 30000 steps, than heated to 300 K during 10000 steps. After equilibration, the 5 ns unconstrained and unbiased molecular dynamics simulation, on 300 ± 10 K, were performed on the each system. CHARMm22 force field and Geisteiger charges were used. Electrostatics was treated by Particle Mesh Ewald method. The periodic boundary conditions were applied, and 12 Å cut-off (8 Å switching), with pair list distances set to 13.5 Å. Each simulation was performed in duplicate, using different random seeds and giving comparable results. The root-mean-square deviation of the backbone atoms and the energy profiles of the systems under the study proved stable, converged simulation. The movement of the loops and the (flexible) inhibitor, as well as radius of gyration of the selected amino-acid side chains was analyzed and conclusion derived on the influence of the covalently bound inhibitors on the dynamics of the enzyme on pH 1.5. All calculations were performed by NAMD 2.8 [4] on the multimode Linux cluster. For the preparation of the systems, and analysis of the results VegaZZ 2.4.0 were used [5].

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Free-energy surfaces of 2-[(carboxymethyl)sulfanyl]-4-oxo-4-arylbutanoic acids. Molecular dynamics study in explicit solvents.

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Contribution type: Oral presentation

Abstract

The 2-[(carboxymethyl)sulfanyl]-4-oxo-4-arylbutanoic acids (Scheme 1) exert antiproliferative potency and significant selectivity toward human tumor cells in vitro in low micromolar to submicromolar concentrations [1]. In the congeneric set of compounds we observed the regularity between the selectivity and the properties derived from the conformational assemblies of compounds [2]. As the part of ongoing studies, in this communication we repot the free-energy surfaces of the representative congeners, as obtained by molecular dynamics simulations, using adaptive biasing force (ABF) procedure [3] to speed-up sampling of the systems. All simulations were performed involving simulation of explicit solvents having different polarity and hydrogen bond donor/acceptor abilities (water, chloroform, dimethyl-sulfoxide, ethanol, n-octanol/water mixture), lasting from 20 to 50 ns. For comparison, the molecular dynamics simulations on the representative system without applied biasing forces was also reported. The differences in the free-energy surfaces of the same, representative, congener in different solvents reflect the fact that flexible molecules change conformations in a way to mimic surroundings (i.e. solvent in which are dissolved) [4]. Ranges of property spaces [5] of compounds under the study were analyzed and compared. In all simulations molecules were treated in their neutral form. The effect of using different types of atomic charges on the final results is also commented. All systems under the study were minimized during 20000 steps, than heated to 310 K for 10000 steps. Molecular dynamics simulation, on 310 ± 10 K, with applied ABF procedure was performed on the each system. CHARMm22 force field and Geisteiger charges, or charges derived from the semiempirical calculations, were used. Electrostatics was treated by Particle Mesh Ewald method. The periodic boundary conditions were applied, and 12 Å cut-off (8 Å switching), with pair list distances set to 13.5 Å. All calculations were performed by NAMD 2.8 [6] on the multimode Linux cluster. For the preparation of the systems and analysis of the results VegaZZ 2.4.0 was used [7].

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In the search of the HDAC-1 inhibitors. The preliminary results of ligand based virtual screening.

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Contribution type: Oral presentation

Abstract

Acetylation and deacetylation of histone is an important mechanism to regulate the DNA expression. Two main classes of enzymes catalyze this regulatory mechanism: histone acetyltransferase (HAT) and histone deacetylase (HDAC). HDACs are involved in signal transduction, cell growth and cancer [1]. We report the results of the preliminary ligand-based virtual screening in the search of the novel HDAC-1 inhibitors. By this virtual screening study, we aimed to test the performances of the OpenEye applications installed on our home cluster PARADOX. As the template, we used the ligand from 3MAX PDB entry [2]. The ChemBank set of 2346 molecules was taken from the ligand.info [3]. After the filtering (exclusion of the metal containing compounds, and limiting of the number of HBA (10) and HBD (5)) we obtained 1990 molecules, which are submitted to OMEGA [4] to generate conformational assemblies of the molecules studied. The OMEGA options were set to default, yielding ~ 142000 conformers in total. We searched the shape and the pharmacophoric similarity of the multiconformer ligand set against the template molecule by ROCS program [5]. The best-ranked solution of the 100 hits by TanimotoCombo score (1.305) was Nifenazone, that has been used as the analgesic drug and was withdrawn due to heavy side effects. The subset of ligand conformers prepared with ROCS is further submitted to EON [6], to search for the electrostatic similarity to the template molecule. The compound labeled as the itdac-7 in ChemBank appears as the best-ranked solution by the ET-combo score (1.403) maid. There is no literature data on this compound, but ChemBank results from the high-throughput screening campaigns indicates itdac-7 as active toward enzymes involved in deacetylation. Our preliminary screen, as reported in this communication, involves the MMFF94s charges ascribed by default. Further work will be directed to assignation of the semiempirical charges for the electrostatic similarity screen, using the larger database of the compounds. All calculations by OpenEye applications were performed in BJD work group on PARADOX cluster, Institute of Physics, Belgrade.

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Investigations of biomolecular systems within the ISyMAB simulation framework

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Contribution type: Oral presentation

Abstract

ISyMAB is an integrated framework that provides secured access to a distributed set of molecular dynamics tools for modeling and simulation of large bio-systems using high-performance computing. It relies upon open-source software (such as NAMD, MMTSB tool set, VMD) and in-house developed analysis scripts, which are made available through a user-friendly graphical interface.
ISyMAB brings a significant contribution to the optimization of the creation of the files needed by the job management system and the simulation description files. Also, it minimizes the time between successive runs, making the nodes within the HPC clusters run with maximum efficiency.
The use and the performances of the framework is illustrated through the molecular dynamics study of an acid-sensing ion channel in a 200x200 Angstrom lipid bilayer simulated within a 800 000 atoms system.

Efficient Parallel Simulations of Large-Ring Cyclodextrins on HPC cluster

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Contribution type: Oral presentation

Abstract

A new class of compounds, the large-ring cyclodextrins (LR-CDs), attracted attention in recent years, and advances were marked in the study of their physicochemical properties in spite of existing difficulties in their synthesis, isolation and purification. Practical applications were also reported of this new class of compounds. Understanding the mechanism of their action requires knowledge of the macroring conformational dynamics. In view of the

difficulties with the experimental examination of the conformations of LR-CDs, computational modeling and simulation methods provide useful tool to gain information about their conformational dynamics, the energetics, and the complex-forming ability.
Using molecular dynamics simulations as a conformational search protocol, post-processing of the simulation trajectories is carried out by: (i) the MM/GBSA (Generalized Born/Surface Area (LCPO)) methodology in order to estimate energy data, and (ii) principal component analysis (PCA), also called quasiharmonic analysis or essential dynamics method. With the methodology used we can monitor the concerted motions of the atoms of the molecule in a few dimensions, making it easier to visualize and investigate these motions. After examining the conformational interconversions in some lower-size LR-CDs (CDn, n=10, 11, …, 30),1-3 our efforts are focused now on treating problems with much higher dimensionality, e.g. CD100, as well as on inclusion complexes of LR-CDs. Due to the access to more powerful computational resources and parallelized software it became practically feasible to execute molecular dynamics conformational searches with longer duration for large cyclodextrins examined by us earlier with very short simulations, 5.0 ns (CDn, n=40, 55, 70, 85, 100; Giant cyclodextrins).4
Such studies require enormous computational resources and it is of crucial importance to make the proper choice of optimal hardware, as well as software configurations in order to execute the computations efficiently. We present in this report results produced at the HPC cluster at IICT-BAS with Infiniband interconnection, which is part of the HP-SEE infrastructure. All tests are in support for optimal execution of the specifically parallelized module PMEMD of AMBER v.11 with 64 cores on eight nodes.

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Some aspects of the comparative study of semi-empirical combustion models on FLUENT and OpenFOAM codes

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Contribution type: Poster

Abstract

Development of an optimal medium power gas burner started under the FP6 project and was continued in HP-SEE project. CFD simulations were initially performed using FLUENT and partly StarCD Adapco sotware, but due to limited computing resources were limited to simulations of small segments with assumptions of absolute radial symmetry. In HP-SEE project we used OpenFOAM for full scale model simulations using solver for combustion with chemical reactions using density based thermodynamics package (rhoReactingFoam). An

analysis of the differences in the results obtained was performed. The advantages of the new approach to CFD modeling of combustion are demonstrated.

Conformational Analysis of Kyotorphin Analogues Containing Unnatural Amino Acids

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Contribution type: Poster

Abstract

The dipeptide kyotorphin (Tyr-Arg, Kyo) plays a role in pain modulation in the mammalian central nervous system (CNS), and is one of the most investigated neuropeptides. The Tyr-Arg motif exists widely throughout the brain not only as kyotorphin, but also as the N-terminal part of several endogenous analgesic peptides1,2. Also, this peptide is very rapidly degraded by aminopeptidases3. One of the successful strategies in the design of neuropeptides with enhanced stability and improved delivery to the CNS is that with the use of non-protein amino acids, like canavanive (Cav), a structural analogue and antimetabolite of arginine (Arg). In our previous in vivo experiments we demonstrated that Tyr-Cav exerted a strong-reversible analgesic effect, more pronounced than that of Kyo. Bearing in mind these and the fact that norsulfoarginine (NsArg)4 is a structural analogue of arginine and canavanine, we synthesized a series of new peptides with expected analgesic activity, containing NsArg residues in their molecules: NsArg-Tyr, Tyr-NsArg, Tyr-NsArg-NH2 and Tyr-NsArg-OBzl5,6.
The conformational features of these dipeptides are of particular interest, both from theoretical and pharmacological point of view. Since no single-crystal X-ray diffraction data for the compounds are available until now, we undertook a quantum-chemical modelling of their structure.
We have undertaken a profound conformational study of kyotorphin and its synthetic analogues, containing unnatural amino acid nor-sulfoarginine (NsArg).
Here we present our preliminary computational results for Kyo, NsArg-Tyr and Tyr-NsArg. Molecular mechanics (MM+ force field) conformational search for the two species was performed, and the global minimum-energy conformations thus obtained, were further optimized at HF ab initio (3-21G** basis set) level of theory. In the three cases (Kyo, NsArg-Tyr, and Tyr-NsArg) specific, scorpion-like conformations are realized, with hydrogen bonds involving the guanidino-group and the phenolic hydroxyl. Numerical results are obtained using HPC cluster deployed at the Institute of Information and Communication Technologies. This cluster is part of High-Performance Computing Infrastructure for South East Europe's Research Communities.

Life Science

Quantum-Chemical Calculations for the Quantitative Estimations of the Processes in DNA

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Contribution type: Oral presentation

Abstract

Investigated the DNA tendency to denaturation using Dencity Functional(DFT) Theory method.
Presence of the polaric solvents with small polarity index Et - such as ethanol, in the aquatic ambient causes protons transfer between nucleobases pair, which in turn fires DNA denaturation and mutation proceses. Using Software for analysing chemical compounds the tautomeric equilibrium indexes of the nucleobases were calculated. The software was ported on the HPC (NCIT-Cluster) infrastructure.

Performance and scalability evaluation of short fragment sequence alignment applications

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Contribution type: Oral presentation

Abstract

Mapping short fragments to open access eukaryotic genomes at a very large scale presents a data processing challenge to the scientific world. The large volume of data processing requires an immense amount of computing power for the tools to provide feasible response time, which is essential for the researchers. The main tool used for such an application is BLAST which is the one we use in our portlets developed at Obuda University. There are

ways for the scientists to use the BLAST algorithm either executing it locally or using a web based BLAST tool. Usually the scope of usability of these solutions is limited because of the lack of computing power available. The portlets developed at Obuda University are served by a web server but computation takes place in a massively parallel supercomputing environment. The type of the algorithm and the data it has to process make it an ideal candidate for a highly parallel execution on the HPSEE infrastructure. The portlets are available to the scientist community on the Bioinformatics eScience Gateway hosted at OU and powered by gUSE/WS-PGRADE technology, while the backend is being served by the Hungarian HPSEE Infrastructure by NIIF.
Lately most of our work has been focused on evaluating the performance and scalability of our applications by profiling, analyzing the results of the tests and improving the performance of both the portlets and the server-side massively parallel algorithm by environment optimization using the data collected during the testing phase.
In this paper we will describe the two portlets (Deep Aligner and Disease Gene Mapper), discuss the issues and challenges during the development and the performance analysis and present our results on the performance and scalability of the applications.

Dynamical Features of Complex Systems: A Molecular Simulation Study

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Contribution type: Oral presentation

Abstract

The parallel molecular dynamics simulation of complex micellar system consisting of long hydrocarbon chain surfactant was carried out. The GROMACS software package, which is designed for high-performance simulation of large complex system, was applied. The simulations were paralell on Bulgarian BlueGene/P supermachine. The goal of this paper is the detail analysis of surfactant molecules in complex system. The initially random distributed surfactant molecules in aqueous solute hydration have been simulated using GROMOS united atom force field. The computation was carried out on BlueGene/P supermachine using from 256 to 1024 processors. The estimated benchmarks show about 0.5ns per day optimized by 512 processors. It should be noted that the further increase of processors (for instance, 1024 processors) do not lead to significant increase in benchmarking value and therefore 512 processors were chosen for final run. The received data shows that the long hydrocarbon chain surfactant self-assemble into small oligomers since 50ns of simulation run, meanwhile in our previous study with surfactant rich content shows that 43ns is enough for self-assembling of spherical micelle. It is planning to continue the simulation to see the self-assembling process of huge complex systems.

Parallellizing computational models of memory function for the investigation of sustained activity in the prefrontal cortex

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Presenter:
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Contribution type: Oral presentation

Abstract

Neurons in the prefrontal cortex display sustained activity in response to environmental or internal stimuli, that continues until the behavioral outcome or a reward signal arrives. Large-scale modeling studies have proposed intensive recurrence and slow excitation mediated by NMDA receptors as the mechanisms able to support the sustained excitation in these neurons. In addition, electrophysiological studies suggest that single-cell intrinsic currents also underlie the delayed excitation of prefrontal neurons. In order to study learning and memory processes, we develop detailed biophysical computational models of small neural circuits of the prefrontal cortex (PFC). We use these models in order to study the role of biophysical and anatomical mechanisms in the emergence and maintenance of sustained activity. Additionally, we dissect the contribution of different types of interneurons in this sustained activity. This computational work provides (a) some of the most realistic biophysical models of neurons in the brain which are publicly available and used by numerous labs worldwide and (b) generates interesting predictions which steer the interest of the neuroscience community and open up new avenues for experimental verifications. All of our models are developed within the open source Neuron simulation environment and were parallelized for the HPCG Infrastructure provided by HP-SEE. Benchmarks show a significant speedup when simulations are run on parallel environments.

DNA multigene approach on HPC using RAxML software

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Contribution type: Oral presentation

Abstract

Computational phylogeny is a challenging even for the most powerful supercomputers. One of significant application in this area is Randomized Axelerated Maximum Likelihood

(RAxML) which is used for sequential and parallel Maximum Likelihood based inference of large phylogenetic trees.
We choose 5 different genes, two real genes (part of D-loop and Cytochrome b of different European salmond fish species) both from mitochondrial genome and additional three designed genes in order to test reliability of constructed census phylogeny tree. Two of those "fake" genes were designed with phylogeny information similar to phylogeny of real genes while the third one was completely different. Using of multigene option of RAxML software we test contribution of each gene (percentage of base pares in tested genes) in terms of gene contribution in phylogeny tree construction. We additionally test contribution of gene position in analysis in terms of final results of phylogeny reconstruction.
This paper will also cover scalability results of multigene tests on high-performance computers for coarse and fine grained parallelization using MPI, Pthreads and hybrid version.

A new microRNA target prediction tool identifies a novel interaction of a putative miRNA with CCND2

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Contribution type: Oral presentation

Abstract

Computational methods for miRNA target prediction vary in the algorithm used; and while one can state opinions about the strengths or weaknesses of each particular algorithm, the fact of the matter is that they fall substantially short of capturing the full detail of physical, temporal, and spatial requirements of miRNA::target-mRNA interactions. Here, we introduce a novel miRNA target prediction tool called Targetprofiler that utilizes a probabilistic learning algorithm in the form of a hidden Markov model trained on experimentally verified miRNA targets. Using a large scale protein down-regulation dataset we validate our method and compare its performance to existing tools. We find that Targetprofiler exhibits greater correlation between computational predictions and protein down-regulation and predicts experimentally verified miRNA targets more accurately than 3 other tools. Concurrently, we use primer extension to identify the mature sequence of a novel miRNA gene recently identified within a cancer associated genomic region and use Targetprofiler to predict its potential targets. Experimental verification of the ability of this small RNA molecule to regulate the expression of CCND2, a gene with documented oncogenic activity, confirms its functional role as a miRNA. These findings highlight the competitive advantage of our tool and its efficacy in extracting bio-logically significant results.

Scientific Computing

An Analysis of FFTW and FFTE Performance

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Contribution type: Oral presentation

Abstract

One of the most frequently used algorithms in engineering and scientific applications is Fast Fourier Transform (FFT). Its open source implementation (Fastest Fourier Transform of the West, FFTW) is widely used, mainly due to its excellent performance, comparable to the vendor-supplied libraries. On the other hand, even if not yet in a fully production state, FFTE (Fastest Fourier Transform of the East) keeps up with FFTW, and outperforms it for very large transform sizes. Here we present results of the performance and scalability tests of FFTW and FFTE libraries. Comparison is done using different compilers and parallelization approaches on Curie and Jugene supercomputers.

SCL Quantum Espresso Extensions

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Contribution type: Oral presentation

Abstract

Quantum Espresso (QE) software package allows electronic-structure calculations and materials modeling at the nanoscale, based on density-functional theory, plane waves, and pseudopotentials. It extensively uses Fast Fourier Transform (FFT) during all computations. In addition to the built in FFT libraries, QE enables integration of newly developed FFT algorithms. Since Fastest Fourier Transform of the East (FFTE) library has shown performance comparable with the widely used and vendor-supplied libraries, the same behavior is foreseen in QE. In this paper we present FFTE-enabled and thread-enabled FFTW3 extensions of QE, together with benchmarking and performance results.

On HPC for Hyperspectral Image Processing

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Contribution type: Oral presentation

Abstract

Hyperspectral image processing still requires nowadays considerable computational and storage resources, beyond the available ones for a single server. In particular, clustering of images gathered from the current satellites can be done in a reasonable time only using high performance computing facilities.
In this paper we discuss the latest approaches for fuzzy clustering techniques that are adapted to work on hundreds of processors as well as the pre-processing techniques for data splitting and reading. Comparisons between different techniques are based on implementations for BlueGene/P.

The paper exposes part of the concepts presented in [1] and [2],as well as experimental results.

[1] D. Petcu, D. Zaharie, S. Panica, A. S. Hussein, A. Sayed, H. El-Shishiny, “Fuzzy Clustering of Large Satellite Images using High Performance Computing,” In Proceedings of SPIE Volume 8183, SPIE Remote Sensing Conference: High-Performance Computing in Remote Sensing, http://dx.doi.org/10.1117/12.898281, 2011
[2] A.C. Toma, S. Panica, D. Zaharie, D. Petcu, "Computational Challenges in Processing Large Hyperspectral Images", submitted to Grid, Cloud & High Performance Computing Science", RO-LCG 2012, October 2012

Number Theory Algorithms on GPU Cluster

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Contribution type: Oral presentation

Abstract

Many algorithms from Number Theory and their implementation in software are of high practical importance, since they are the building primitives of many protocols for data encryption and authentication of Internet connections. Number theory algorithms are also the basic part of cryptanalytic procedures. Many of these algorithms can be parallelized in a natural way. In this paper we describe our efforts to develop a software package that implements various Number Theory algorithms on GPU clusters and in partial our implementations of integer factorization using NVIDIA CUDA on clusters equipped with NVIDIA GPUs. Also we report results of our experiments regarding the performance of our implementation.

Generalization of the parallel HPC implementation for solving differential equations

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Contribution type: Poster

Abstract

We report our results, obtained so far, in developing a novel, general two step genetic algorithm for finding an analytical solution of systems of ordinary differential equations, ant its generalization for solving more complex systems of ordinary and partial differential equations. We tested extended solution for solving several complex systems of different type of differential equations and achieve excellent results for small number of generations. Due to the computationally intensive calculations the code is implemented and tested in HPC environment with promising results in view of performance and scaling. A possibility for application in more complex research-level models is noted and evaluated.

GPAW optimisations

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Contribution type: Poster

Abstract

GPAW software package implements efficient calculation of electronic structure of materials, based on the density functional theory and projector-augmented wave method. This C/Python code uses real-space formalism that allows flexible boundary conditions and efficient parallelization. Here we present results of the optimization of GPAW hybrid code (OpenMP and MPI). OpenMP performance traps are identified and discussed, as well as general performance gains and tradeoffs between pure message passing and hybrid code.

HPC Systems and Network Operation

Advanced Vulnerability Assessment Tool for Distributed Systems

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Presenter:
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Contribution type: Oral presentation

Abstract

Large-scale high performance systems have significant amount of processing power. HP-SEE's HPC/Supercomputing infrastructure is geologically distributed, and provide 24/7, large scale, high performance computing services primarily for various high-end research communities thus such system can be categorized as critical regional/national infrastructure. System features such as non-stop availability, large scale processing power and community based usage make such infrastructure vulnerable against malicious attacks. In order to decrease the menace, we designed the Advanced Vulnerability Assessment Tool for HPC/supercomputing Systems. We propose the implementation of the tool that are integrated to the HP-SEE infrastructure. Our vulnerability assessment software can submit jobs into the HP-SEE infrastructure and run vulnerability assessment on the components of the infrastructure. The decentralized Security Monitor collects and stores the results from the components and makes them available via a web interface for the local/regional administrators. We tested our solution from reliability and from performance point of view as well.