LITHUANIAN GRID PROJECTS
(problems and applications needing grids)

Feliksas Ivanauskas
Vilnius University

Problems and applications in PHYSICS

Institute of Physics

Stellar systems physics department

- Space observatory Gaia: data modeling and analysis.
- Project Astrovirtel (Astronomical Archives as Virtual Telescopes): data reduction and analysis.
- Modeling star formation history in nearby resolved galaxies.
- Modeling of galaxy chemical and spectrophotometrical evolution.
- Solution of the 3-D radiative transfer problem in dusty galaxies.

Nonlinear optics and spectroscopy laboratory

- 3D modeling of variation of the spatio-temporal structure of short high power laser pulses in the homogeneous and nonhomogeneous (periodical) media with second and third optical nonlinearities in the strong energy exchange regime taking into account the diffraction, dispertion, temporal delay and other parameters of the pulses and media.

Problems and applications in PHYSICS

Institute of Physics

Department of Molecular Compound Physics

- Modeling of the spectral density function of the phonon and bath modes in optical lines of spectrally disordered molecular aggregates. Systems under consideration: light-harvesting pigment – protein complexes.

- Recognition of the dispersion of the molecular site excitation energies in newly resolved structures of the light harvesting pigment – protein complexes by using genetic algorithm.

- Molecular aggregate structure development from the comparative analysis of the transient absorption measurements and Monte Carlo simulations of nonlinear dynamics of multiple exciton excitations. Real time hydrodinamic simulations of the pollutant dispersion in Lithuanian lake and Baltic sea waters.

Problems and applications in PHYSICS

Institute of Physics

Nuclear and environmental radioactivity research laboratory

- Microscopic nuclear structure calculations.
- The analysis of experimental nuclear decay data with heuristic algorithms.
- Evaluation of delayed neutrons production in accelerator driven systems.
- Simulation of transmutation of transuranium elements in innovative nuclear reactors.
- Migration of radionuclides in biosphere.
- Analysis of ionizing radiation induced damage in biomolecular systems.

Problems and applications in PHYSICS

Institute of Theoretical Physics and Astronomy

Prof. Pavel Bogdanovich group

The problems investigated in atomic physics involve the solution of complex second order integro-differential equations and determination and diagonalization of matrices of extra-high order. To obtain reliable results of high quality and accuracy, one must solve the above mentioned systems of several ten to several hundred equations self-consistently. The order of matrices formed and diagonalized in a calculation on a single (super)computer now is of the order of 20000. The nearest future development of theory will certainly demand the order of matrices to be several hundred thousand. It is likely that solving such problems would be impossible without a Baltic Grid system.

Problems and applications in PHYSICS

Institute of Theoretical Physics and Astronomy

Dr. habil. Gediminas Gaigalas group

The large-scale theoretical calculations of the energy spectra and hyperfine structure of atoms and ions using multiconfiguration Hartree-Fock, multiconfiguration Dirac-Fock and configuration interaction methods.

Dr. habil. Gražina Tautvaišienė group

Investigation of chemical composition of the star atmospheres and modeling of their synthetic spectra are the tasks currently routinely performed by the Nordic grid and other grids. The solid theoretical developments of Lithuanian astronomers in this field remain ineffective without the analogous Baltic grid here and without its connection to other grids.

Problems and applications in PHYSICS

Institute of Theoretical Physics and Astronomy

Dr. Andrius Bernotas group

Simulation of biologically plausible even medium-size neural networks must involve thousands and tens of thousands model neurons, each simulated in a separate thread or even on a separate computer node in parallel.

Future and emerging technologies aiming at the use of "best performers" in various model environments that are selected by genetic algorithms are better developed through grid technology.

A number of new hypotheses regarding the self-organization and emerging phenomena in various natural and social environments have been proposed recently. Parallel computing and grid technologies may aim at supporting or declining them.

Problems and applications in PHYSICS

Institute of Theoretical Physics and Astronomy

Dr. Arvydas Tamulis group

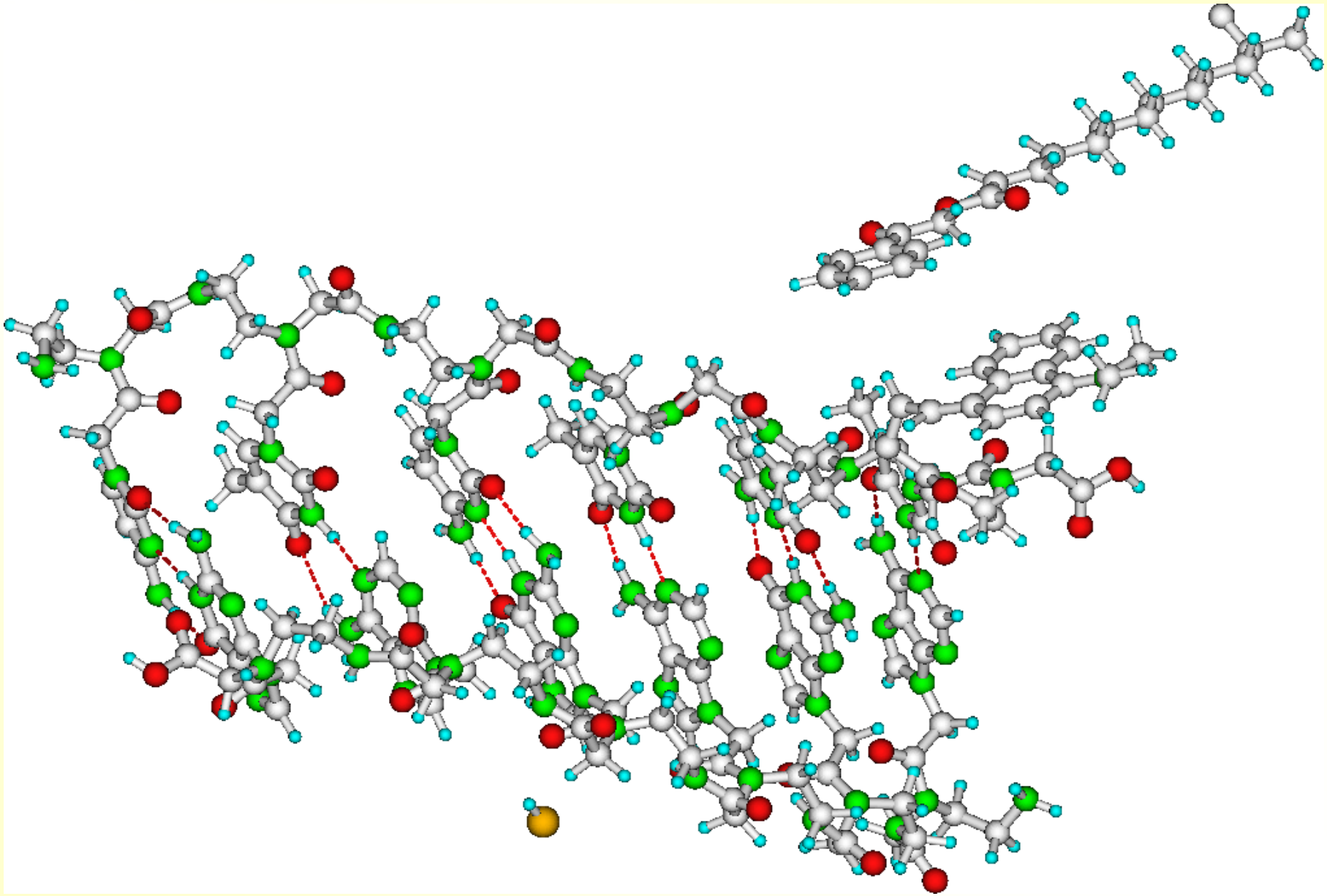
Quantum Modelling of Processes in Artificial Living Organisms and Elements of Molecular Computers

I. Quantum Modelling of Artificial Photosynthetic Systems Based on Assemblies of Modified Peptide Nucleic Acids (PNA) and Lipid Molecules

This research is performed in the framework of EU FP6 granted consortium: 'Programmable Artificial Cell Evolution (PACE)'

We need Baltic Grid sources because we are doing now exact quantum mechanical simulations of self-assembly and electron migration processes in peptide nucleic acids surrounded by lipid molecules in the excited states using Time Dependent Density Functional Theory

The main components of artificial living organism



Problems and applications in PHYSICS

Institute of Theoretical Physics and Astronomy

Dr. Arvydas Tamulis group:

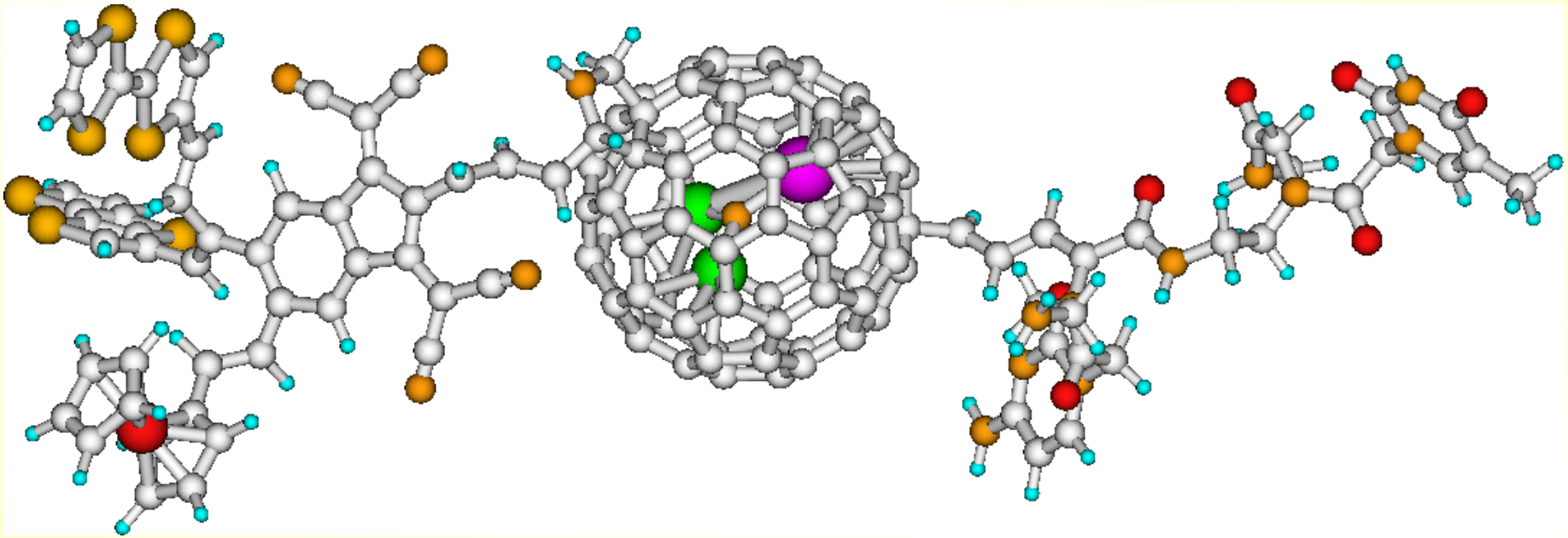
Quantum Modelling of Processes in Artificial Living Organisms and Elements of Molecular Computers

II. Quantum Modelling of Elements of Molecular Computers

This research is performing in the framework of NorFA granted consortium: 'Quantum Modelling of Molecular Materials'

Quantum mechanical modelling using parallel programmes running on Baltic Grid PC clusters should allow to predict the geometry, electronic and spintronic structure in ground state of biological supermolecules and supramolecules consisting from arround 10,000 atoms, and spectra, electron charge and spin transfer in excited states for biological molecules consisting from arround 1,000 atoms.

Quantum mechanical modelling of electron and spin transfer in logically controlled artificial photosynthetic systems (see figure bellow) needs Baltic Grid sources



Problems and applications in PHYSICS

Vilnius University, Faculty of Physics

Main tasks requiring powerful (parallel) computations:

- Quantum mechanical computations for determination of stable molecular geometries and vibrational spectra of main and excited molecular states.
- Accurate non empirical determination of excited potential surfaces of biological molecules for further investigation of quantum molecular dynamics, determination of lifetimes of excited electronic states.
- Molecular dynamics computations of large biological structures by means of semiempirical methods.

These investigations are carried out mainly in Theoretical physics department and Common physics department

Problems and applications in PHYSICS

Vilnius University, Faculty of Physics

Mentioned methods may be used for modeling of solid state surfaces and its interactions with other molecules. The only answer why there are no such investigations in our faculty – computers power is too small.

Another field of applications for powerful computing in Faculty of Physics are:

- Electromagnetic waves scattering by set of bodies of arbitrary shape
- Nonlinear optics

Parallel computation facilities able to reduce calculation time by several orders could be very suitable in these cases

Problems and applications in PHYSICS

Vilnius University, Faculty of Physics

Equations of nonlinear optics

$$\frac{\partial A_1}{\partial z}+\frac{1}{u_1}\frac{\partial A_1}{\partial t}-\frac{i}{2}g_1\frac{\partial^2 A_1}{\partial t^2}+\beta_1\frac{\partial A_1}{\partial x}+\frac{i}{2k_{01}}\left(\frac{\partial^2 A_1}{\partial x^2}+\frac{\partial^2 A_1}{\partial y^2}\right)=-i\sigma_1 A_2^* A_3\exp(-i\Delta kz),$$

$$\frac{\partial A_2}{\partial z}+\frac{1}{u_2}\frac{\partial A_2}{\partial t}-\frac{i}{2}g_2\frac{\partial^2 A_2}{\partial t^2}+\beta_2\frac{\partial A_2}{\partial x}+\frac{i}{2k_{02}}\left(\frac{\partial^2 A_2}{\partial x^2}+\frac{\partial^2 A_2}{\partial y^2}\right)=-i\sigma_2 A_1^* A_3\exp(-i\Delta kz),$$

$$\frac{\partial A_3}{\partial z}+\frac{1}{u_3}\frac{\partial A_3}{\partial t}-\frac{i}{2}g_3\frac{\partial^2 A_3}{\partial t^2}+\beta_3\frac{\partial A_3}{\partial x}+\frac{i}{2k_{03}}\left(\frac{\partial^2 A_3}{\partial x^2}+\frac{\partial^2 A_3}{\partial y^2}\right)=-i\sigma_3 A_1 A_2\exp(i\Delta kz),$$

Numerical solution of such kind equations requires a lot of computer facilities and is time consuming. Even when the radiation possesses radial symmetry and number of dimensions can be reduced from 3 to 2 it can take a long time of the numerical processing, especially when the narrow patterns are accompanied with the large backgrounds (or even with some randomization) what means extremely wide spatial-temporal spectrum and thus requires large number of the numerical grid points.

Problems and applications in CHEMISTRY

Institute of Chemistry

Computational chemistry methods are applied for:

- Modeling of organic and bioorganic molecules and metal clusters
- Simulation of organic reactions
- Modeling of the SAM (self-assembled mono layers) on metal surfaces

For calculation GAUSSIAN, GAMESS and MOPAC programs are used. The structures of molecules and their both vibrational and NMR spectra, obtained owing to the modeling help to interpret the experimental data.

All calculations are carried out on personal computers, therefore even simple calculations take a good deal of time. The "Baltic grid" project will considerably increase our possibilities in modeling of more complex molecules and will reduce the calculation time.

Problems and applications in CHEMISTRY and BIOCHEMISTRY

Vilnius University, Faculty of Chemistry

Application areas:

- chemo-informatics
- bioinformatics
- pharmaceutical sciences

Namely – protein folding, virtual screening, QSAR, etc.

However, the lack of specialists in chemo-informatics and bioinformatics and special programming problems may retard the effective explorations of GRID

Biochemistry Institute

Molecular dynamics of proteins; protein-protein and protein-substrate interaction; protein mutation in silico; de nova protein design

Problems and applications in EDUCATION

Kaunas University of Technology

Since 2002 Kaunas University of Technology (KTU) is a partner in two EU IST Grid Projects.

KTU as a partner aims to integrate into EU Grid Learning space and to achieve two main goals:

- Using Grid technologies to establish Virtual Learning Organizations including science and academic institutions.
- E-Science Grid resources have to be used for advanced studies (especially by MSc and PhD students) at higher education institutions.

FP5 Thematic network project IST-2001-38763, 2002 - 2004

Learning Grid of Excellence Working Group (LeGE-WG) LITHUANIAN NODE

http://www.lege.ktu.lt

KTU partner in the EU IST Grid Project

The *Learning Grid of Excellence Working Group (LeGE-WG)* aims to facilitate the establishment of a European Learning Grid Infrastructure by supporting the systematic exchange of information and by creating opportunities for close collaboration between the different actors.

EC Framework 6 Integrated Project, 2004 - 2008

European Learning Grid Infrastructure (ELEGI) LITHUANIAN NODE

http://www.elegi.ktu.lt

KTU partner in the EU IST Grid Project

The *European Learning Grid Infrastructure (ELeGI)* project has the ambitious goal to develop Grid technologies for effective human learning, focused on knowledge construction.

It will be done by using experiential based and collaborative learning approaches to replace the current information transfer paradigm focused on content.

ELEGI identified the following learning Service Scenarios:

- **Learning services for Large Community**
- **Organic Chemistry (17 millions formulae)**
- **e-Qualification**
- **Masters in ICT**
- **Physics Course (4 semesters)**

KTU partner in the EU IST Grid Project

In parallel to the EU project activities, KTU is going to create Service Oriented Grid Infrastructure (within university) on the basis of LITNET network as well as to create Grid aware applications for studies at MSc and PhD levels.

Problems and applications in EDUCATION

Kaunas University of Technology

Educational tools of Finite Elements Analysis implemented into computational GRIDs:

- **education-through-distance techniques** (course materials, examples, problems and solutions bases, reference materials to accompanying courses);
- **“numerical laboratory” base enabling to implement computational schemes and strategies**
- **access to commercial FE software and license management**

Sample Grid services

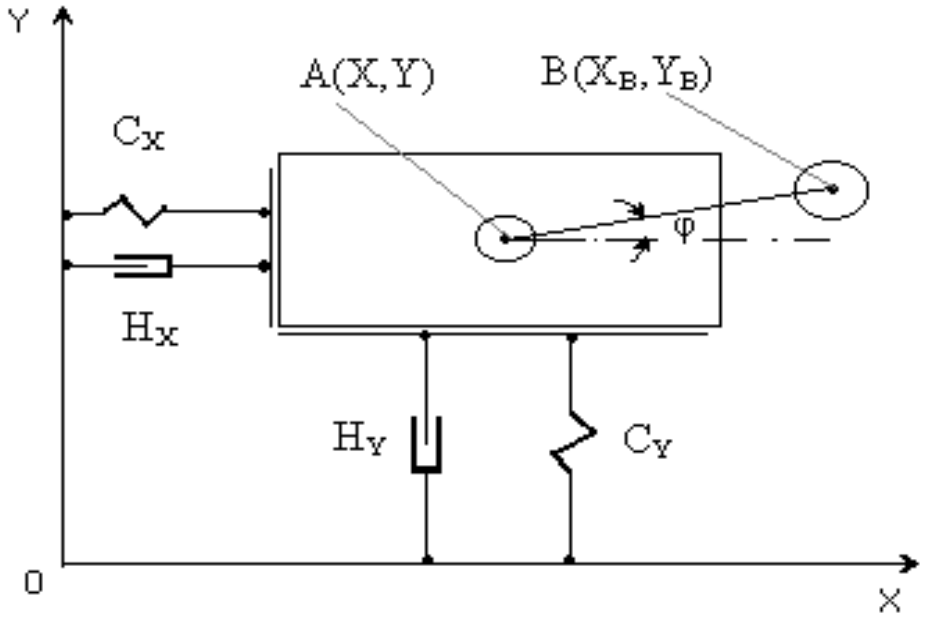
Grid architecture levels

	FEA using licensed software	FEA by implementing computational processes in mathematically oriented environments (MATLAB+FEMLAB), High-level programming languages (C++, FORTRAN)	Using numerical and graphical libraries (IMSL, OpenGL)	Learning through distance
	VO1	VO2	VO3	VO4
Collective (application-specific)	Input language service, source data and results transport	Function library organization and retrieval, multi-language compilation, access to visualization tools		-
Collective (generic)	Resource discovery, resource brokering, system monitoring, community authorization, certificate revocation, help and content information			
Resource	Access to computation; access to data; access to information about system's structure, state, performance			
Connectivity	Communication (IP), service discovery (DNS), authentication, authorization, delegation			
Fabric	Storage systems, computers, networks, code repositories, catalogs			

Expected advantages:

- ✓legal, easy and standardized access to up-to-date Finite Elements software systems and libraries;
- ✓building a flexible and creative environment for a researcher;
- ✓providing the educational course materials and tutorials with “numerical laboratory” examples and software tools

The real model and specifying system



Alternative receiving of energy

The wave (flowing liquid) energy straight dynamically, without any kinematics forced relationships, stimulates rotational motion of the output term.

$$x'' + x = f_x \qquad y'' + y = f_y \qquad \mu^* \varphi'' = f_\varphi$$

$$f_x = a_x - h_x x' + \left(q_{1x} - q_{3x} x'^2\right) x' + \mu\left(\varphi'' \sin\varphi + \varphi'^2 \cos\varphi\right)$$

$$f_y = a_y - h_y y' + \left(q_{1y} - q_{3y} y'^2\right) y' - \mu\left(\varphi'' \cos\varphi - \varphi'^2 \sin\varphi\right) + g^*$$

$$f_\varphi = \mu_\varphi^* - h_\varphi \varphi' + g^* \cos\varphi + \mu\left(x'' \sin\varphi - y'' \cos\varphi\right)$$

Peculiarities of the computer realization

The operator method appears to be a successful extension of numerical methods. In applying an operator method, the sought-for solutions are represented as operator series, where from polynomials of various degrees - approximate solutions - are obtained. Desirable accuracy is available. Various characteristics of differential equations (their systems) can be found out and analyzed. The calculation time for operator and Runge-Kutta methods realization makes acceptable using (for parallelization) a particular computer network. The symbolic differentiation (time of calculation about 80%) is realized using Maple tools, the computer network is used applying MPI tools. ·

KTU – Educational tools of Finite Elements Analysis

Distributing actions of algorithm to 3 groups and three computers of personal cluster are used. Then execution of actions sequences and transmissions between processors time is less than 0.5 s. Calculation time of parallel executed sequences is between 550 s. and 600 s. Using 10 computers (10 groups of algorithm) this time is less than 85 s., whereas using 1 computer (1.2 GHz, RAM 516 MB) algorithm execution time is about 0.5 h.

On purpose to solve complicated systems, describing energy transmission, it's in urgent need to use computer network.

Computational strategies and parallelization of the operator and numerical algorithms in use lead to considerable time and computer memory savings.

Kaunas University of Technology

CHIP design online

- *Increased operating frequency, nano technologies place increasing demands on the noise simulation of systems containing large-scale integrated circuits.*
- *Signal nets noise coupling is very hard to analyze using traditional circuit simulation techniques.*
- *The size of the netlist required to simulate a multi-chip system, and the analysis of the complex multiple couplings between power supply and signal nets, have forced to use* ***grid approach****.*

Problems and applications in MATHEMATICAL MODELING

Partners:

- Faculty of Informatics and Mathematics, Vilnius University
- Faculty of Physics, Vilnius University
- Faculty of Chemistry, Vilnius University
- Institute of Materials Science and Applied Research, Vilnius University
- Kaunas University of Technology
- Gediminas Technical University of Vilnius
- Military Academy of Lithuania
- Mathematics and Informatics Institute
- Institute of Biochemistry
- Institute of Physics
- Institute of Theoretical Physics and Astronomy
- Institute of Lithuanian Scientific Society

Problems and applications in MATHEMATICAL MODELING

Problems:

- The development of computational methods and software for simulating the penetration of deformable bodies to textile structures
- Numerical methods and applications to ballistics
- The development of computational methods and software for simulating a slow movement of rigid formations in biological media accompanied by atrophy and proliteration processes
- Numerical algorithms and applications to biomedicine
- Self formation of artificial objects (in micro and nano scale)

Problems and applications in MATHEMATICAL MODELING

Problems:

- Modeling of generation dynamics of microchip lasers with multilayered semiconductor switches and mirrors, mode-locked VCSELs, fiber and other solid-state lasers enabling to obtain high repetition rate (~1010 Hz) sequences of short (~1 ps) pulses and low jitter
- Development of mathematical models, efficient numerical algorithms and convenient software packages for the second- and third-order nonlinear optical effects (generation of harmonics, parametric interactions, transient scattering and other processes) in heterogeneous media, including optical waveguides of small transverse size (close to the optical wavelengths)
- *and many others…*

Problems and applications in MATHEMATICAL MODELING

The main aim of mathematical modeling is the creation of integrated research potential with a modern research basis, which is still absent in Lithuania, for computational modeling the quality of which could be competitive on the international level. The use of the GRID would be a tool for:

- *research which cannot be carried out by experiment or the cost of which is very high*
- *algorithms and software testing and preparations for work in other research centres*

Thank You for Your Attention