Grid as the Country Progress Locomotive

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Ukrainian National Grid Initiative(UNGI) is presented as a powerful computing resource for fundamental and applied scientific research which are carried out at Ukraine. Information on activity and possibilities of UNGI is presented and contribution of UNGI to the European Grid Initiative (EGI) through cooperation with WLCG, EGEE is emphasized. Examples of UNGI activities in developing various Grid applications within various scientific areas are shown.

I. Grid Computing

The popularity of the Internet and the availability of powerful computers and high-speed network technologies as low-cost commodity components is changing the way we use computers today. These technology opportunities have led to the possibility of using distributed computers as a single, unified computing resource, leading to what is popularly known as **Grid computing** .Its principles have been logically and adequately formulated by I. Foster and C. Kesselman [1]. It is the authors's opinion that "*A computational grid is a hardware and software infrastructure that provides dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities*".
The Grid infrastructure provides networking, computing, and data resources in such a way that they are readily available to users regardless of their geographical location and in this way improves the efficiency of scientific and industrial research. It additionally promotes networked collaboration of specialists in joint projects, allowing them to use the same infrastructure for solving different problems. Therefore, today the Grid plays the role of a universal infrastructure for data processing with a great number of services, allowing not only solving the concrete applied tasks but also helping to search for necessary resources to collect information about their state, and to save and to deliver data.

The users interact with the Grid resource broker to solve problems, which in turn performs resource discovery, scheduling, and the processing of application jobs on the distributed Grid heterogeneous resources, which are geographically distributed across multiple administrative domains and owned by different organizations. Grid allows users to solve larger or new problems by pooling together resources that could not be easily coupled before. Hence, the Grid is not only a computing infrastructure for large applications, it is **a technology** that can bond and unify remote and diverse distributed resources ranging from meteorological sensors to data vaults, and from parallel supercomputers to personal digital organizers. For example the Large Hadron Collider (LHC), based in Geneva, generates volumes of data well beyond the capability of conventional computers, meaning clearly necessity for researchers to gain access to greater computing power.

A special Grid *middleware* (Globus, Unicode,NorduGrid, gLite etc.) offers core **services** such as users' authentication and authorization, remote process management, co-allocation of resources, storage access, information registration and discovery, security. It turns a radically heterogeneous environment into a virtual homogeneous one with the Open Grid Services Architecture (OGSA) framework [2]. Grid environment interoperates also the Web services to help interaction of users with the Grid.The evolution of the Grid is a continuous process and the emphasis shifts now to the Semantic Grid as the extension of the current Grid, in which information and services are given well-defined meaning, better enabling computers and people to work in cooperation [3], and to Cload Computing as the more powerful resources environment.

At the beginning, Grid technologies were targeted to solving intricate scientific, production, and engineering problems that cannot be solved in clever terms by separate computing options. Now, however, the application domain of Grid is not limited to these types of tasks. As far as the Grid technologies are disseminated, they penetrate industry and business, and major concerns have begun to create their own Grid for solving their production tasks.

Grid technologies already are actively used in the world by both state organizations (defense and public utility spheres) and private companies, for example, financial and power utilities. Applications of the Grid domain now include nuclear physics, ecological monitoring and environment defense, weather forecasting and design of climatic changes, design in MEMS and aircraft building, biophysics, chemistry, biology, scientific instrumentation, drug design, tomography, high-energy physics, data mining, financial analysis, nuclear simulations, material science, chemical engineering, weather prediction, molecular biology, neuroscience/brain activity analysis, structural analysis, mechanical CAD/CAM, and astrophysics [4].

II. Ukrainian National Grid Initiative

For a long time Ukraine in the framework of the former USSR had strong traditions in the fields of cybernetics, mathematics, and computer sciences. For example, in 1952 Ukraine was the third country after the USA and Great Britain capable of building a computer. In spite of social and economic problems, Ukraine has made progress, especially after Geneva’s WSIS-2003, in the direction of creating the information society. This aim was recognized as one of the priorities of the state. First of all, a several related laws were adopted. Among them – the Decree of Cabinet of Ministers of Ukraine from September ‘23’, 2009 № 1020, which is dedicated to building the high-quality national Grid infrastructure with corresponding services for giving possibility to native scientists to collaborate fruitfully in European Research Area (ERA).

Nowadays there is none of highly developed countries which rejects an idea to build up a proper Grid network. We can state with assurance a country that has not Grid infrastructure and is not drawn into the world Grid community could not even pretend to be a developed one. Thus, a development and application of Grid technologies for the daily social life becomes a strategic trend for each state which is anxious about scientific, economic and social progress.

Ukrainian National Grid Initiative (UNGI) is a Grid infrastructure to share the computer resources of the National Academy of Science institutes and universities as well. The principal tasks of the UNGI are to develop the distributed computings and Grid technologies to advance computationally intensive fundamental and applied studies. Besides, UNGI has to ensure a participation of the Ukrainian scientists in various topical international Grid projects. At present the UNGI shares resources (29 clusters, more than 3300 CPU and 320 TB of disk memory) of the next organizations (Fig. 1):

Fig. 1. Fiber optic channels for UNG

The main goals of national Ukrainian Grid are [5]:
1) creating the powerful information computing environment for solving scientific and practical computer tasks of any complexity;
2) providing the wide access to computational resources for specialists who need extraordinary computational capacities for research and solving scientific, scientific-technical and the other tasks;
4) implementation of new methods of population medical service (creation of distributed diagnostic data bases, consultation with the use of telecommunication means, including large scale computer data analysis);
5) providing efficient, real-time processing the results of geophysical, meteorological, and space observations;
6) creating conditions for grid technologies implementation in economics, industry, financial activity, and social sphere;
7) supporting servicing of Ukrainian World Data Centre (WDC "Sustainable development and Geoinformatics"), providing its clients with remote access to world scientific data repositories, possibility of efficient common share of computers, unique experimental sets, and devices:
8) integrating the Ukrainian institutes, establishments and separate specialists into the world Grid community, their participation in the international research and technical projects.

Among a number of key factors that promote Grid installation are not only a rise in the efficiency of the use of resources and economy of charges but also the possibility of a flexible change of infrastructure according to new requirements. Most organizations presently have opened small Grid installations with a limited set of equipment and applications. An important task is the effective use not only of computing but also of human resources because the Grid promotes networked collaboration of specialists in joint projects, allowing them to use the same infrastructure for solving different problems. Below it is an appropriate list of the scientific areas where new UNGI facilities have been already used [6]:

High energy physics:
- LHC (CERN) experimental data processing, their analysis and comparison to the theoretical results and phenomenological models aiming the full scale participation of the Ukrainian institutes in the ALICE experiments *(Bogolyubov Institute for Theoretical Physics, Kiev National University, Kharkov Institute of Physics and Technology, Institute of Scintillation Materials , National Technical University "Kiev Polytechnic Institute", Institute of Cybernetics*) and CMS ones (*Kharkov Institute of Physics and Technology*).

Astrophysics and astronomy:
- Dynamical computing of an evolution of the star concentration in the Galaxy external field. The hydrodynamic modeling of collision and fragmentation of the molecular clouds. Analysis of N-body algorithm and parallel computing on the GRAPE clusters. Cooperation with AstroGrid-D (*Main Astronomy Observatory*).
- Theoretical analysis and the observation processing of primary, roentgen and gamma radiation data which are obtained from the satellite telescopes INTEGRAL, SWIFT and others (*Bogolyubov Institute for Theoretical Physics, Kiev National University, Main Astronomy Observatory*).
- Creation and formation of VIRGO – VIRtual Gamma and Roentgen Observatory (*Bogolyubov Institute for Theoretical Physics, Kiev National University, Main Astronomy Observatory*).
- Development of nuclei activity models of Galaxy and star concentrations. Testing the dark matter and dark energy models. Collaboration with Lausanne and Geneva universities (*Bogolyubov Institute for Theoretical Physics, Main Astronomy Observatory*).

Biophysics and biology:
- Computing of thermodynamic characteristics, infrared and electron spectra of sputter DNA fragments. Study of bionanohybrid system structures composed by DNA and RNA of different sequence (*Institute of Low Temperatures Physics and Engineering, Institute of Cybernetics*).
- Molecular dynamic computing of Fts-Z-protein systems with the low-molecular associations (*Institute of Cell Biology and Genetic Engineering*).

- Computer simulation of the spatial structure and molecular dynamics of cytokine-tyrosine-RNA synthetase (*Institute of Molecular Biology and Genetics*).

Nanotechnologies:

- Computing of nanostructure oxides which seem to be perspective high-temperature superconductors, as well as physical characteristics of the DNA fragment with transition metal ions which could be good nano-conductors.
- Computing of structures and interaction energy of bio-nano-hybrids on basis of the single-shell carbon nano-tubes with the various bio-objects (*Institute of Low Temperatures Physics and Engineering, Institute of Cybernetics, Institute of Metal Physics*).

Environment monitoring:

- Weather forecast parameters on the Ukrainian terrain based on the computer simulation and satellite data. Estimate of biodiversity as ecologic parameter on Ukrainian terrain (*Institute of Space Researches , Institute of Cybernetics*).
- Development of GEO-UA information infrastructure (*Institute of Space Researches*).

Grid may be considered as a new reinforced instrument for scientific and technological international cooperation. Grid becomes one of the principal factors and locomotives of the globalization process. Science has always an international nature but at the end of previous century because of the fight with the background of economic globalization the proper attention to developing the cooperation principles in the science management was not given in necessary extent. Nevertheless, due to Internet and new scientific projects (for example, Space exploration, the largest colliders in CERN and USA, European project of thermonuclear reactor ITER etc.) the tasks of world science integration have been brought to the forefront. New international project called the World Grid could be realized by creating the national and big international Grid projects (WLCG, EGEE, GLORIAD, TERAGRID and others). Realizing a stable character of unification tendency and availability of this process in the country the organizers of UNGI pay the special efforts to the integration and consolidation of the Ukrainian Grid into the international Grid community.

III. Networked MEMS Designer for Grid

Let us consider remote design tool NetALLTED as an example of integrated multidisciplinary application of distributed simulation and methodology, which allows to design remotely different Nonlinear Dynamic Complex Technical systems (first of all, for Microelectronics) using Web-based CAD framework . Such tools support the co-operation of several groups of designers working on the common tasks at project different stages in Grid environment.

The proposed interdisciplinary Networked Computer-Aided Design System NetALLTED with invariant computational procedures was developed for design, verification and optimization of micro- electro-mechanical systems (MEMS) and large-scale integrated circuits (fig.2).

The developed methodology and modeling toolkit allow collective designing of various MEMS, being adapted for the newest submicron technologies, on the system and circuit levels using available or creating new parameterized model of MEMS subsystems. This toolkit is named by NetALLTED (Network ALL Technology Designer) and it is devoted for schematic design of complicated technical systems (including Nonlinear Dynamic Systems) composed of either/and electronic, hydraulic, pneumatic, mechanical, electromagnetic, and other subsystems.
NetALLTED is based on **the original numerical algorithms** for all the stages of design [7]: starting from steady state, frequency and transient analyses till parametrical optimization of a designed device output characteristics, optimal component tolerances assignment, centering of solution, and Yield maximization. NetALLTED can be used in distributed Grid environment or it can be embedded in every Intranet domain with client-server base configuration.

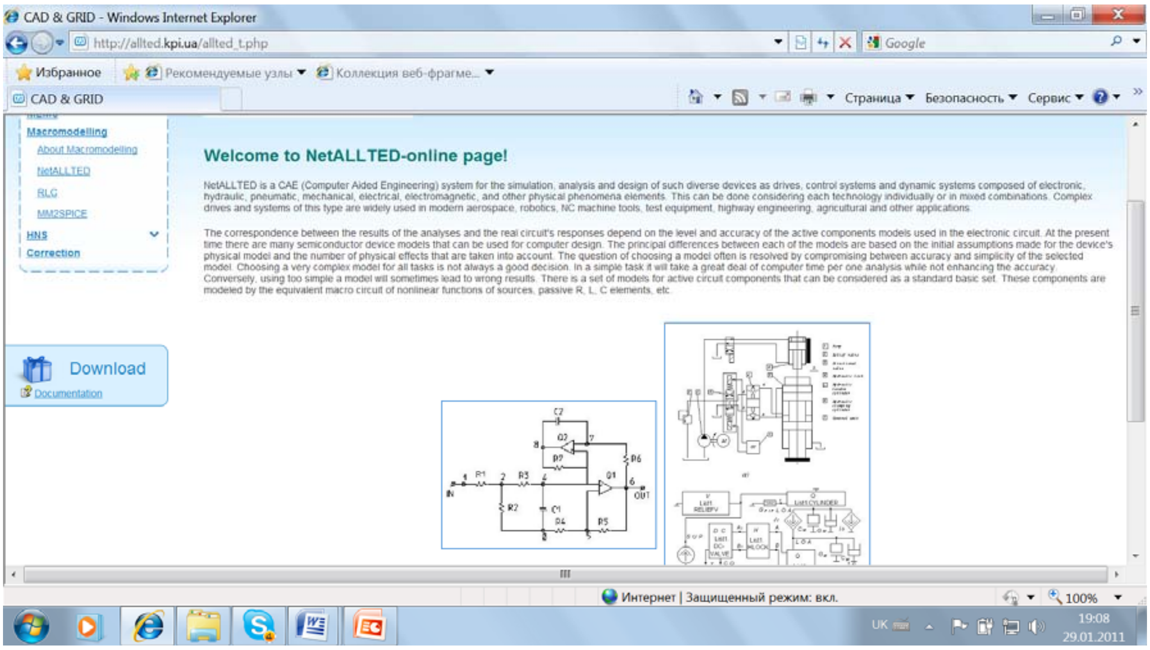


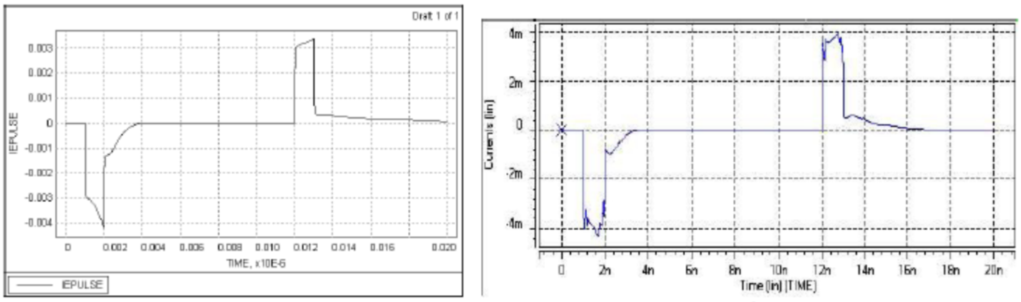
Fig.2. NetALLTED interface window

Area of Application. Advantages of above methods in comparison with numerical methods used in SPICE-like simulators are illustrated by the example of simulation of benchmark circuits set being proposed by North Carolina Microelectronics Centre (table 1).

There are visible false oscillations at the plot (Fig.3).when simulating the circuit *Make2* with default conditions in HSPICE due to used numerical integration methods (2-nd order in HSPICE and variable order (till 6-st) in NetALLTED).

Table 1. Comparative simulation results of NetALLTED and HSPICE

Circuit	DC Iteration number, *ALLTED*	DC Iteration number, *HSPICE*	TR Iteration number, *ALLTED*	TR Iteration number, *HPSPICE*
Bjtinv	95	96	1340	3239
Gm3	80	185	149	219
Make2	12	10	527 but 256 steps	327 outputs are distorted



a b

Fig.3. The simulation results obtained by ALLTED (a) and by HSPISE (b).

Simulation time depends on using platform (HSPICE was run on *UNIX*-Working Station and ALLTED- on PC under *Windows*) , but ALLTED made at least some time less time steps during simulation what is extremely important for effective realization of such time-consumed procedures as optimization and Monte-Carlo procedures.
The toolkit in hand was used for selection of optimal ratio W/L (width to length) for CMOS in DEC Alpha AXP 64-bit microprocessor resulting in twice increasing its run frequency. The toolkit was used also for General Electric Ultrasonic Transducer simulation (Fig.4).

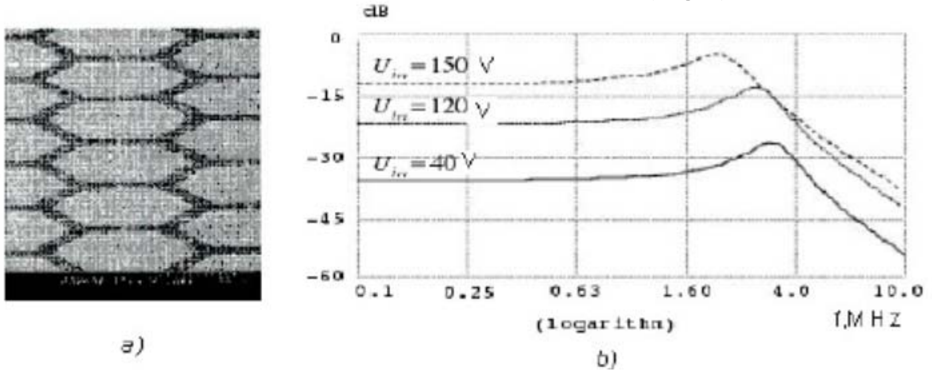


Fig.4. Fragment of ultrasonic transformer (a) and the graph of decreasing a transducer own frequency with applied voltage rise (b).

In comparison with SPICE-like programs Net ALLTED offers:
■ Faster simulation speed and improved numerical convergence;
■ Sensitivity analysis for frequency and transient analyses;
■ Comprehensive optimization procedure and optimal tolerances assignment;
■ Alternative approach to the secondary response parameters determination (delays, rise and fall times, etc.);
■ Powerful user-defined modeling capability,
■ Original way of generating a system-level model of MEMS from FEM component equations which is described below.

MEMS system-level model. A new technology for building of the mathematical model of a MEMS being designed is proposed that includes the following steps:
● the initial equations by finite element method (for example, by means of ANSYS) are constructed for MEMS library components.
● these equations with boundary conditions are transformed into the equivalent equations of a schematic model, which consists of L, C and G components. The boundary conditions for deviation velocities are assigned simply by setting initial values for grounded inductances' current node voltages.
● the MEMS model electrical equivalent circuit assembled from the separate electrical representations of MEMS separate components' finite element models is simplified by means of Y-Δ transformation instead of using Krylov-Arnoldi method or model decomposition, and at that its dimension reduces significantly.
● the reduced MEMS model has a circuit character unlike the existing approaches (for example, in CoventorWare), where it is represented by the reduced system of differential equations, that allows using directly the input interface of NetALLTED domestic circuit simulation package and making use of its unique power optimization and tolerancing procedures.
● taking into account the proposed approach to form MEMS models, the architecture of the MEMS design package that provides for users' servicing remote mode has been developed. Matrices received from ANSYS mor4ansys program [9] are coefficients of equation

$$M\ddot{x} + D\dot{x} + Kx = BF, \qquad y = Cx \,,$$

where *M, D*, and *K* are mass, damping and stiffness matrices correspondingly; *B* is an input matrix; *C* is an output matrix; x is a vector of unknowns, which includes all the degrees of freedom; F is a force vector, and y is a vector of output variables.

Moving to electro-mechanical analogies [7], we will receive:

$$\frac{d}{dt}(Mv) + Dv + \int Kvdt = F(t)$$

$$\tilde{C}\dot{v} + \tilde{G}v + \tilde{L}v = F(t),$$

where $\tilde{C} = M, \tilde{G} = D, \tilde{L} = K -$ are equivalent capacitance, conductance and inductance matrices. The elements of *C, G*, and *L* matrices are formed from the elements of *M, D* and *K* matrices by formulas:

$$\tilde{C}_{ij} = m_{ij}, \quad i, j = 1(1)N, \quad i \neq j$$

$$\tilde{C}_{ii} = \sum_{j=1}^{N} m_{ij}, \quad i = 1(1)N,$$

$$\tilde{L}_{ij} = -1/k_{ij}, \quad i, j = 1(1)N, \quad i \neq j$$

$$\tilde{L}_{ii} = 1/\sum_{j=1}^{N} k_{ij}, \quad i = 1(1)N,$$

$$\tilde{G}_{ij} = -d_{ij}, \quad i, j = 1(1)N, \quad i \neq j$$

$$\tilde{G}_{ii} = \sum_{j=1}^{N} d_{ij}, \quad i = 1(1)N,$$

where N is the number of equations for the system given. Using the received C, G, and L matrices, it is possible to move to the equivalent circuit. In particular cases, some of these matrices can be absent. This will mean that the corresponding elements will be absent in the circuit.

The example of such approach is illustrated by fig.5 for the micro-accelerometer which is realized as a square silicone plate (membrane) of the thickness 1 µm and the size 50µm. A square metal plate of size 10µm is fixed at the centre of the plate as an additional load.
The calculation of eigen frequencies and normal modes for the membrane was done using a finite square element SHELL 93 (5x5 µm) by the program ANSYS v10.0 . The calculation of eigen frequencies was done using a standard block Lancoz decomposition method. The first and fours eigen frequencies were defined (n = 1; f = 181.36 kHz; n = 4; f = 3427.8 kHz).

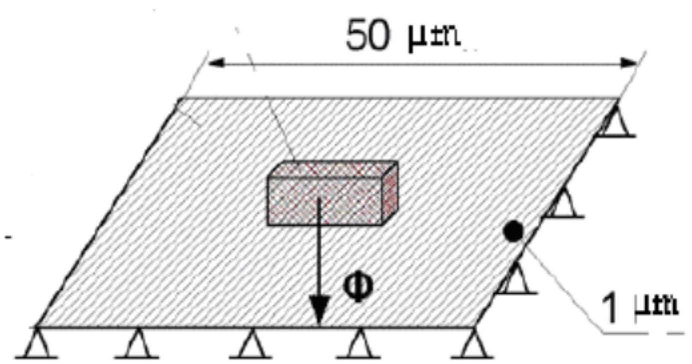


Fig.5. Microaccelerometer membrane

The full-sized matrices, being obtained from ANSYS and mor4ansys program ,have been used to create the source equivalent electrical circuit presented in NetALLTED input language, which after were reduced by means of Y-Δ transformation algorithm with $\tau_{\min} = 10^{-5}$ parameter. Then reduced circuit was simulated for the frequency range of 50 kHz – 3.5 MHz. The number of nodes and elements of the source and reduced circuits as well as the reduced circuit's simulation results are presented in Table 2.
Reduced circuit description in input NetALLTED language (element-node list) is shown in Table 3).

Table 2. Eigen frequencies calculation

	Source circuit	Reduced circuit
$\tau_{\min}$	-	$5*10^{-5}$
Number of nodes	1883	6
Number of elements	35954	30
Node reduction, %	-	99.68
Element reduction, %	-	99.92
1 peak, kHz (error)	181.36	181.5 (<0.1%)
2 peak, kHz	1018.1	-
3 peak, kHz	1018.1	-
4 peak, kHz (error)	3427.8	3223.3 (6%)

Table 3. Element-node lists for reduced membrane circuit model

$\tau_{\min}$ = 5e-5
C_1(749,681) = 9.81875e-12; C_10(1023,0) = 9.11751e-11; C_11(1023,827) = -1.46106e-11; C_12(1023,1041) = 9.32471e-12; C_13(0,827) = 3.39931e-10; C_14(0,1041) = 9.11359e-11; C_15(827,1041) = -1.32974e-11; L_16(749,681) = 145.945; L_17(749,1023) = 293.424; L_18(749,0) = 1743.16; L_19(749,827) = 81.0146; C_2(749,1023) = -6.76919e-12; L_20(749,1041) = -116.299; L_21(681,1023) = -116.31; L_22(681,0) = 1749.7; L_23(681,827) = 81.0134; L_24(681,1041) = 293.884; L_25(1023,0) = 1748.35; L_26(1023,827) = 81.0241; L_27(1023,1041) = 145.914; L_28(0,827) = -769.548; L_29(0,1041) = 1779.07; C_3(749,0) = 9.11471e-11; L_30(827,1041) = 81.0423; C_4(749,827) = -1.45068e-11; C_5(749,1041) = 9.05184e-12; C_6(681,1023) = 8.85191e-12; C_7(681,0) = 9.11518e-11; C_8(681,827) = -1.25893e-11; C_9(681,1041) = -6.56002e-12;

A reader can run himself this example remotely using the proper code and data on (*http://netallted.cad.kiev.ua*) and also solve there his own tasks.

Parallel NetALLTED version

The purpose of current work is development of the parallel algorithms of numeral integration of the promoted reliability and exactness for dynamic analysis tasks and their implementation into the NetALLTED being run now on the university cluster with 5.83 Tflops productivity[8] . Algorithms were developed which :
- are enable to solve the nonlinear stiff algebra-differential equation systems of 5000 sizes ;
- are suitable for solving wide spectrum of tasks which deal with different hybrid objects (with electronic, mechanical, piezoelectric components, etc.).
- take into account possible heterogeneities of models characteristics (breaks both in functions and derivatives, physical limitations on the area of argument values etc.);
- provide facilities of automatic adaptation to the features of a task being solved.

These algorithms are based on parallel choosing of the best implicit method order from 1 to 6 on an each calculation step comparing a predicted solution exactness for different method order . It is possible due to using implicit methods with high differences instead of usual Gear their presentation. Parallel NetALLTED is preparing for usage in Grid- infrastructure under OS Linux.

CONCLUSIONS

The UNGI project realization allows:
• Ensuring the people’s right of open access to important scientific and educational information,
• Solving the social problems connected with providing equal conditions for access to education and science,
• Creating conditions for continuous life-long education,
• Raising the efficiency of the public administration of education and science,
• Promoting Ukraine’s integration into the global research and educational areas.

Despite all difficulties and problems in developing of grid technologies in NASU the background of the widest application of grid technologies in Ukraine has been provided. There is a good reason to believe that grid exists and operates in Ukraine, the collaboration with international grid community is intensified and Ukrainian National Grid will be built with joint efforts and occupy a fitting place in the world grid infrastructure.

The term eScience is generally used to describe the science that is undertaken over distributed computational infrastructure (involving the use of computational and data Grids). Whereas much of the effort in Grid computing has been devoted to the development of computational infrastructure, eScience has primarily been about empowering the scientist to utilize such infrastructure in a more effective and efficient manner. As much of the science that is undertaken today requires collaboration between distributed scientific research groups/laboratories, eScience includes enabling technologies and applications.

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