ANALYSIS OF EXECUTION TIME AND ITS COMPONENTS IN PARALLEL ESTIMATION OF ADDITIVE RELATIONSHIP COEFFICIENTS

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Computing relationship matrix (or its inverse) for a large population uses a lot of computer time and memory, so the scientists' efforts concentrated on reducing both of them. The tabular method has been proposed by Cockerham [1954] and further developed by Henderson [1975, 1976]. The existing tools (packages) like PEDIG [Boichard, 2002] or PyPedal [Cole and Franke, 2002] focus on speed, memory, disk space, flexibility, user-friendliness etc. Parallel computing already speeded up calculations eg. in animal breeding value estimation [see eg. Lidauer et al., 1998, Lidauer and Strandén, 1999, Strandén and Lidauer, 2001]. So the aim of the work was to design and test a fast parallel computer program to calculate relationship matrix, applying directly the formula used in tabular method, using recursion instead of creating auxilliary tables in computer memory.

The solution was to design the algorithm which would create a hierarchical structure of recursive function calls for each pair of animals.

The data were 63264 one-generation cattle pedigrees. The recursive function defined in the FORTRAN program used directly the formula "$a_{ij} = 0{,}5\,(a_{ip} + a_{iq})$"; the relationship coefficient between animals i and j (i is older than j) is the average relationship of animal i with the parents (p, q) of animal j. The FORTRAN program was parallelized via "DOACROSS" directive with "DYNAMIC" scheduling: the lower triangular part of (symmetric!) relationship table was divided into "slices" 4000 rows each (except the last one). The Fortran 77 compiler and SpeedShop package were used on SGI 2800 computer ("grizzly") with Irix 6.5 operating system. The crucial calculations were divided into 1, 2, 4, 8 (, 16*) processes.

Real execution time changed from ca. 13500s to ca. 2500s (2800s*), total CPU time - from ca. 13400s to ca. 18400s (20500s*), Real process' execution time - from ca. 13500s to ca. 13900s (28600s*), and the sum of process' times - from ca. 13400s to ca. 14500s (19500s*). The sum of relationship calculation times (13100-13200s) did not depend on the number of processes. The SpeedShop analysis revealed that defining 1000-row slices and analyzing the upper triangular part of the matrix would reduce idle time used by processes.

Paralellizing calculations of relationship coefficients reduced computing time by the factor of over 60% of the number of processors, and this can be still improved by defining smaller parts of work for processes and by analyzing upper triangular matrix.

Keywords: animal breeding, relationship matrix, parallel computing

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Application of Waterloo MAPLE 9.5 and Wolfram MATHEMATICA 5.1 software for analytic solving of certain nonlinear partial differential equations of physics

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1. Introduction

Nonlinear partial differential equations (NPDE's) are very important tool for description of many phenomena in the nature. In recent years some new analytic methods of solving of such equations were developed, for example: a concept of strong necessary conditions [1], [2], homogeneous balance method [3] an auxiliary equation method [4]. However, it is possible, that they will not give all solutions of nonlinear partial differential equation or their usage can be hard. I would like to present an application of some alternative method [5] of analytic solving of certain NPDE's.
These NPDE's are among others: Navier-Stokes equation, [6], [7] and Monge-Ampere equation [6].

2. Description of a problem solution

I have inserted some ansatzes in the investigated equations. Thus the form of the investigated equation has been changed and now (if it is possible) I have transformed it into some convenient form, which gives a possibility of finding the answer on the question, whether such solutions, described by these ansatzes, exist. The solutions are arbitrary functions of some arguments.

3. Applied algorithms and methods; software and hardware used

After inserting each of these ansatzes, I have transformed these equations (using MAPLE 9.5 software) into some convenient form. Both: the answer on the question, whether the mentioned solutions of the equation exist and the conditions of their existence, have been found with the help of: MAPLE 9.5 and MATHEMATICA 5.1. The figures have been plotted using also these two packages. The computations and plotting the figures were executed on the machine Sun Fire 6800 (saturn) in ACK CYFRONET AGH (grant No. MNiI/Sun6800/WSP/008/2005).

4. Results

As the results, some wide classes of analytic solutions of the investigated equations and figures has been obtained.

5. Conclusions and future work

I expect that the mentioned method of decomposition can be extended towards application of it for solving of the equations describing certain models of nonlinear field theory with some classes of potentials.

Keywords: analytic solutions, exact solutions, nonlinear partial differential equations, Euler equation, Navier-Stokes equation, Monge-Ampere equation, isentropic flow equation

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CRITICAL LOADS CALCULATIONS OF ANNULAR THREE-LAYERED PLATES WITH SOFT ELASTIC OR VISCOELASTIC CORE

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Introduction

The three-layered, annular plates under lateral loads are subjected to investigation. Compressive load acting in the plane of outer plate layers causes the loss of the plate stability. It could be the static or for the loads variable in time the dynamic one. The transverse structure of examined plate is symmetric composed of the elastic, steel facings with the equal thickness and the thicker, foam core with the viscoelastic properties. This undertaken problem is the complement of the analyses of the widely applied sandwich structures. It shows the possible behaviours of examined elements in the range of their critical and overcritical loads. The formulated problem is the multi-parameter task requiring the evaluation of the influence of both material, geometrical and load plates parameters on their behaviours. Also, the way of building of the proper computational model of analysed plate in the finite element method is the essential problem.

Calculations and some observations

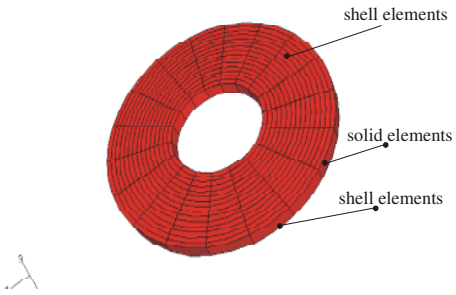

Fig.1.

In model building the participation of the plate layers in carrying the basic stresses: normal by the facings and shear by the core has been used. The shell and solid elements in creating facings and core plate mesh were applied. The proposal of such selection of elements in sandwich mesh structure has been presented in work [1]. Using he surface contact interaction the surfaces of facings mesh elements have been tied with the surfaces of the core elements. The model of full plate annulus is presented in Fig.1.

The viscoelastic properties of the core material have been described by the single term of Prony series for the shear relaxation modules [2]:

$$G_R(t) = G_o\left(1 - q_1^p\left(1 - e^{-t/\tau_1^G}\right)\right) \qquad (1)$$

where: q_1^p, τ_1^G – material constants, G_o – instantaneous shear.

In the description of the rheological properties of core material the formulation of the standard model of the linear viscoelastic medium has been adopted.

The calculations were carried out at the Academic Computer Center CYFRONET-CRACOW using the ABAQUS system (KBN/SGI_ORIGIN_2000/PŁódzka/030/1999).

As the criterion of loss of plate stability, the criterion presented by Volmir [3] was adopted. According to this criterion the loss of plate stability occurs in the moment of time when the speed of the point of maximum deflection reaches the first maximum value. The form of the plate deformation corresponding to the minimal value of the critical plate load has the importance in the plate stability problem. The calculations show that the plate with both slidably clamped edges compressed on the inner edge (Fig. 2a) loses it stability in the form of axially-symmetrical, regular form (Fig. 2b) but the plate compressed on outer perimeter (Fig. 3a) loses it stability in the wavy form (Fig. 3b).

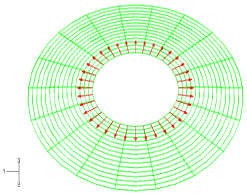

Fig.2a.

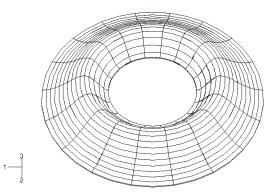

Fig.2b.

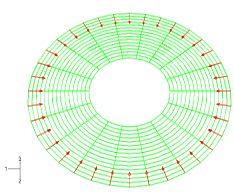

Fig.3a.

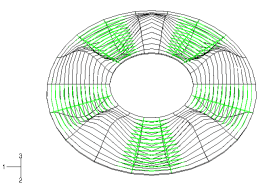

Fig.3b.

The number (described by *m*) of the circumferential waves strongly depends on the plate material and geometrical parameters.

The example table 1 shows the results of static, critical loads p_{cr} and the forms of buckling.

Table 1.

p_{cr} [MPa]	**35.04**	35.46	35.57	36.94	37.19	38.98	40.87	42.48	47.01
m	6	5	7	8	4	9	3	10	2

In the evaluation of the dynamic plate stability the critical time, load and deflections are analysed. The calculations were carried out for plates subjected by the quickly increasing, linear load expressed by:

$$p=st \qquad (2)$$

where: p – compressive stress, s - rate of plate loading growth, t – time.

The rates of plate imperfection and the loading growth are importance in dynamic analysis. Table 2 shows the example results of critical dynamic p_{crdyn} and static p_{cr} loads and maximum deflection w_{dcr} of plates compressed on inner edge, which lose their stability in axially-symmetrical form.

Table 2.

h_2/G_2 [m /MPa]	p_{crdyn} [MPa]	w_{dcr} [m]	p_{cr} [MPa]
0.005/5.0	62.72	$1.78 \cdot 10^{-3}$	64.0
0.005/15.82	118.72	$2.13 \cdot 10^{-3}$	119.92
0.02/5.0	141.77	$3.11 \cdot 10^{-3}$	143.20
0.02/15.82	333.7	$4.33 \cdot 10^{-3}$	324.01

The parameters h_2 and G_2 are the core thickness and Kirchhoff's modulus of core material, respectively.

Figure 4 shows the example diagrams of the time histories of plate maximum deflection (Fig. 4a) and velocity of deflection (Fig. 4b). The first maximum value of plate velocity of deflection describes the critical parameters of examined plate.

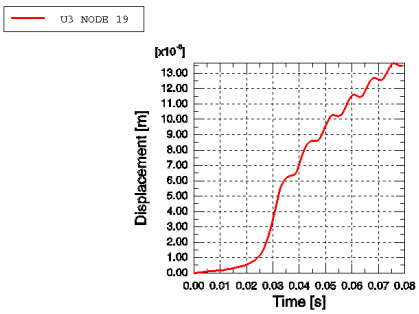

Fig. 4a.

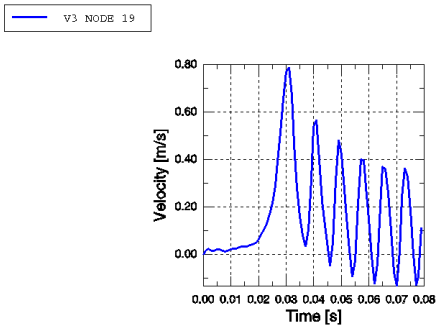

Fig. 4b.

For the plate compressed on the outer edge essentially the form of dynamic, critical deformation does not correspond to the static one. The problem is more complicated.

Conclusion

The work contains the general evaluation of the critical loads of annular plates with sandwich structure with the taking notice of the way of FEM model building and the evaluation of the influence of the some plate parameters on it critical behaviour.

Keywords: sandwich annular plate, static, dynamic stability, finite element method

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Design of a Load Balancing Algorithm for Computational Chemistry Applications

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Abstract:

Significantly growing demand for higher quality computational chemistry results for big molecular systems can be recently observed. As a result, the theoretical chemistry community needs for computational power are constantly growing. While this trend is accompanied by quick development of high performance hardware solutions, the typical architecture of modern supercomputers requires also algorithmic changes in software to efficiently use the accessible resources.

The key issue is that virtually all modern supercomputers are designed as highly parallel. This necessitates the switch from traditional sequential algorithms to the ones that are able to exploit the parallelism of the hardware architecture. Fortunately, most of the typical quantum chemistry problems are relatively easy to reformulate in such a way. As a result, basically all the existing quantum chemical programs are parallelized, at least to some extent. The most prominent examples of highly parallel ones are MOPAC2007, MPQC and NWChem. Nevertheless, some basic issues regarding the construction of efficient highly parallel algorithms are not fully explored. One of them are the techniques of optimal partitioning of the workload between the computational nodes.

Majority of the existing procedures used for commonly executed quantum-chemical calculations are parallelized within the Single Program Multiple Data (SPMD) model. This approach is in general case not optimal from the efficiency point of view. It is however justified by its conceptual simplicity and near optimal performance for typical applications. The SPMD model requires a scheduler to partition the problem between computational nodes. In this work we analyze the crucial factors determining scheduling quality and propose an efficient and flexible scheduling algorithm. Its key design feature is near optimal run-time adaptivity of the scheduling process achieved with negligible computational overhead.

The algorithm was implemented in Niedoida[1], a general-purpose computational chemistry package built as a set of libraries implementing quantum-chemical and microelectrostatic calculations. Niedoida is a parallel program designed according to the SPMD model. Message Passing Interface (MPI) is used as the low-level parallelization framework. The main reasons for using Niedoida in this work is that it provides a plug-in scheduler interface and a wide range of production quality quantum-chemical procedures, allowing for benchmarking different schedulers in a realistic and consistent environment.

Performed tests confirmed key design decisions. Additionally, obtained results allow to fine-tune the load-balancing parameters for a given range of constraints imposed by both hardware environment and application specific requirements. Future plans include introducing cache affinity to the scheduling process.

Keywords:

computational chemistry, parallel programming, high-performance computing

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Development and Optimization of Computational Chemistry Algorithms

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Significantly growing demand for higher quality computational results for big molecular systems can be recently observed. This trend is accompanied by advances in theoretical chemistry resulting in proliferation of quantum-chemical models. As a result, the needs of computational chemistry community are constantly rising. Efficient algorithms and tools facilitating software development are necessary to fulfill them.

Niedoida[1] is a general-purpose computational chemistry package, built as a set of libraries implementing quantum-chemical and microelectrostatic calculations. Main Niedoida's design objectives are clear modular structure and extensibility to facilitate its usage as a development platform for new software and hardware solutions in the field of computational chemistry.

The object-oriented design is used to achieve loose coupling among components. Generic programming techniques are applied to increase efficiency. Advanced memory management simplifies the implementation of modern algorithms and methods of computational chemistry. These features are rather untypical for existing quantum-chemistry packages.

Niedoida is implemented in C++. The choice of the implementation language allows one to obtain both clear expression of the artifacts from the problem domain and efficient implementation of the computationally demanding kernels. The key algorithms are parallelized along the lines of Single Program Multiple Data (SPMD) model. Message Passing Interface (MPI) is used as the implementation framework.

The basic infrastructure provided by Niedoida includes the Self Consistent Field (SCF) algorithm, the Fock matrix and the Kohn-Sham matrix generators, selected post-Hartree-Fock methods and the Time-Dependent Density Functional Theory implementation. Basing on them, some new algorithms were designed, implemented and tested. The most significant ones are an efficient formulation of two-electron integrals engine[2] and an improved scheme of microelectrostatic polarization calculations[3]. Niedoida was also used as a testbed for implementing other quantum-chemical models, like the Nalewajski-Mrozek bond indices[4].

A promising modification of Time Dependent Density Functional Theory (TDDFT) effectively describing excited states having significant contribution from double-excited configurations[5] is worked on. A project in collaboration with ACK Cyfronet aimed at creating a hybrid solution in which some of the computational kernels are implemented using hardware acceleration (Field Programmable Gate Array, FPGA)[6] is currently under way.

Keywords:
computational chemistry, software framework, hardware acceleration

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Effect of wave propagation velocity on the dynamic response of multiple-support structures: FEM analysis and *in situ* investigation

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ABSTRACT

In the paper results of calculations of the dynamic response of mulitiple-support structures to kinematic excitation of seismic and paraseismic origin are presented. In the case of multiple-support structures consideration of non-uniformity of excitation is necessary [1, 2, 3]. In the case of structures of small foundation dimensions identical kinematic excitation in every point of structure base may be assumed. In the case when the length of the structure base is comparable with the length of the wave propagating in the ground, occurrence of various values of amplitudes and phases characterizing kinematic excitation in particular points must be taken into account [4, 5, 8, 9 , 10, 11] . The conducted investigations included two types of structures subjected to non-uniform kinematic excitation: bridges and large-dimensional earth dams. Theoretical calculations of the earth dam dynamic response to seismic shock as well as calculations of bridge response to paraseismic tremor of mining origin were performed [6, 7]. Different shock wave velocities in the ground were assumed: 400 – 3000 m/s. The dynamic response in case of uniform kinematic excitation was also calculated. The relation of the dynamic response of the structure and velocity of the wave propagation in the ground was also shown. On the basis of the carried out calculations it was demonstrated that the effect of wave propagation in the ground and decrease in the velocity may cause occurrence of significant quasi-static effects resulting from changes of geometry of the structure during non-uniform movement of its supports.

For proper determination of the dynamic response of large-dimensional bridges and earth dams velocity of shock wave propagation in the ground under structure was determined in experimental way. Methods of *in situ* investigations and results interpretation were proposed. For calculations of the dynamic response of dams and bridges to non-uniform kinematic excitation the program ABAQUS– a general-purpose system for static and dynamic calculations of engineering structures based on finite element method – was used. Analysis of the measured signals, constituting the basis of determination of wave velocity in the ground, was performed by using MATLAB – a general-purpose system for spectral analysis. These programs are available at Academic Computer Centre CYFRONET AGH on computers SGI ALTIX 3700 and SUN FIRE 6800.

In consequence necessity of a proper recognition of physico-mechanical properties and, consequently, recognition of wave propagation velocity in the ground was proved when performing such a type of calculations. A proper adoption of wave propagation velocity is specially important in analysis of massive bridges in which increasing of dynamic response occurs at the assumption of a non-uniform excitation in relation to the dynamic response obtained at application of uniform excitation. In case of these structures incorrect adoption of wave propagation velocity may cause underestimation of values of inner forces in the structure.

Key words: *dynamics of earth dam, dynamics of bridges, non-uniform kinematic excitation, wave propagation*

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Elastic properties of doped tetragonal yttrium stabilized zirconium dioxide

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Abstract

Superplastic properties of doped zirconium dioxide have been an active field of research during the last decade (see e.g. review [1]). Many experiments show that doping of ZrO_2 with different metal oxides such as GeO_2, TiO_2, SiO_2, MgO and Al_2O_3 strongly increase the plasticity of the material [1-5]. Such phenomenon is usually explained by the grain boundary sliding. Another theoretical explanation has been proposed recently by A. Kuwabara et alter [2] using GeO_2 and TiO_2 dopants. They have calculated the changes in net ionic charges of Zr, dopant atom and oxygen, and found the correlation between the experimental critical stress and average product of net charges. This phenomenon is explained by stronger covalent interactions between dopant atoms and oxygens than in the primary matrix.

In the present work we study elastic properties of the doped tetragonal Y-stabilized zirconia, in particular calculate bulk modulus and shear elastic constants as function of dopant concentration. Our purpose of present studies is to find out whether there is a correlation between changes in superplasticity and changes of elastic properties. Also we observe changes in net charges of cations and anions in order to check Kuwabara's results and study more properly how local changes in covalency influence the elastic properties.

Atomistic calculations of elastic properties require advanced quantum methods to describe efficiently systems consisting of hundred or more atoms. Calculations were performed within density-functional theory (DFT) [6] with generalized-gradient approximation (GGA) [7] for exchange-correlation functional using LCAO (linear combination of atomic orbitals) basis set as implemented in SIESTA program [8]. The calculations were performed at ACK CYFRONET AGH using SGI Altix 3700 (*baribal*). As this computer is equipped with Intel Itanium processors, for better performance we have compiled SIESTA with MPI, using Intel Fortran Compiler and Intel MKL libraries. According to the results of several performance tests, the calculations on “baribal” with a use of 4 processors run approximately twice faster than a serial computation on Intel Core 2 Duo workstation (for the system of 40-160 atoms.) The same performance is achieved by other researchers using SIESTA reported in private communications and on SIESTA mail list. Starting atomic coordinates of pure ZrO_2 were prepared using Accelrys Cerius on SGI Onyx 300 computer (*cezar*).

Bulk modulus and shear elastic constants as function of Y/dopant concentration (it was the same for Y and dopant) are shown on **Fig. 1** and **Fig. 2**, respectively. We can see that addition of dopants do not affect “bulk” elastic properties of the material, but obvious decrease of shear elastic constant is observed, especially in the direction 66. Having calculated net ionic charges of all the cations and anions we have confirmed that dopant atoms attract electron density and stronger dopant-oxygen bonds are created (because dopant atom has larger electronegativity then Zr). As a result, regions with weaker Zr-O bonds surrounds dopant atom, and the overall elasticity increases in selected directions.

To conclude, our calculations have shown that addition of dopant atom into Y-stabilized tetragonal zirconium dioxide reduces its selected elastic properties, which is driven by the attraction of electron density by dopant atom and creation of stronger dopant-oxygen bonds. This can be an additional factor which influences the increase of superplasticity of doped material.

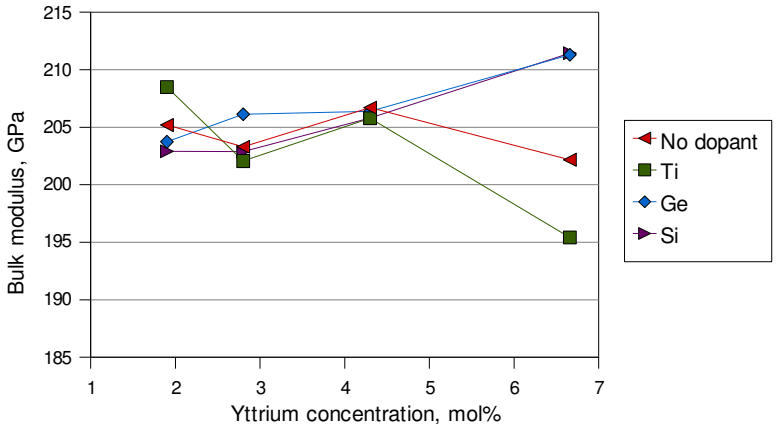

Fig. 1. Bulk modulus as a function of yttrium concentration

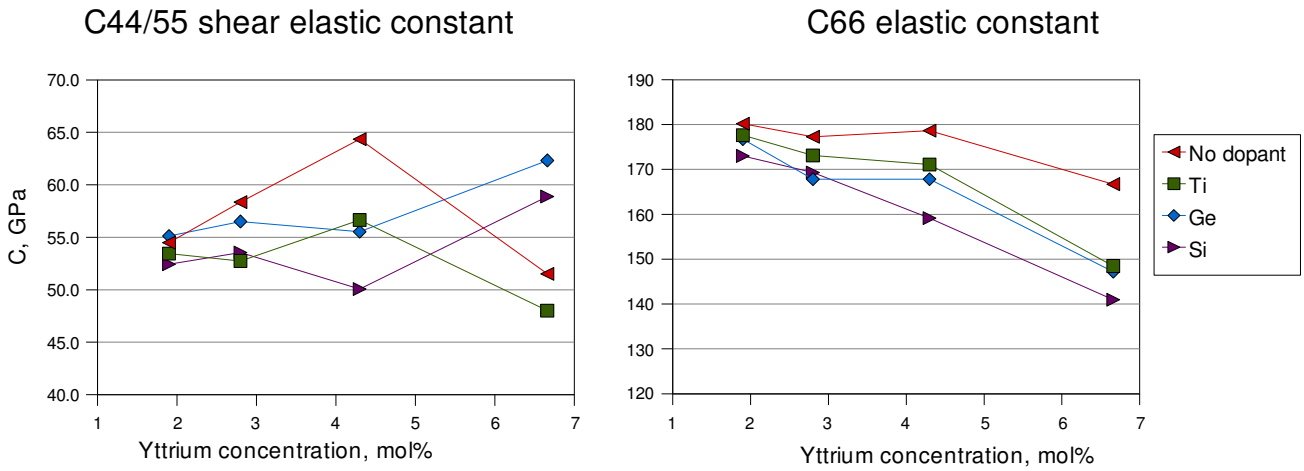

Fig. 2. Shear elastic constants versus yttrium concentration for different dopant atoms

Keywords: Y-stabilized zirconia, superplasticity, net charge, ab initio calculations, SIESTA

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Electronic structure and conformation of cobalt(II) acetylacetonate: CASPT2 and DFT study

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Bis(acetylacetonate) cobalt(II) [$Co(acac)_2$] and its derivatives have been proposed as mediators in controlled free-radical polymerization of olefines [1]. In theoretical studies on such reactions the issue of great importance is to identify the spin symmetry and the lowest-energy conformation of the cobalt moiety. Two alternative spin states (doublet or quartet) as well as two conformations (planar-square or tetrahedral) were proposed for [$Co(acac)_2$]. To the best of the authors' knowledge, no definite conclusions can be made solely on the basis of the available experimental results [1-4]. The correct assignment of the ground state is also a great challenge for quantum-chemical modeling. In this context the considered cobalt(II) compound is a valuable benchmark case (apart from being an interesting problem itself).

We carefully studied all the candidates for the ground state (low-lying states of various spin and spatial symmetry) for the alternative conformations, employing various quantum chemical methods. The widely used Density-Functional Theory (DFT) methods were applied, but as this methodology cannot unambiguously identify the ground state in our case (see below), we focus on the *ab initio* multi-reference perturbation theory (CASPT2): computationally more demanding, but also more reliable (i. e., providing more balanced description of the electronic exchange and correlation e. g., for some iron(II) compounds [5]).

The DFT calculations were performed with the `Turbomole` quantum-chemical package. Both hybrid and non-hybrid functionals were used. Solvent effects were estimated using the COSMO model. The CASPT2 energy calculations (for DFT geometries) were performed with the `Molcas` suite. The active space was composed of the 3d and 4d orbitals of the cobalt atom with additional ligand orbital(s) for the covalent metal-ligand bond(s). The Atomic Natural Orbitals basis sets employed in these calculations were verified to accurately reproduce the ^4F–^2G splitting in free cobalt(II) ion. Cobalt 3s3p semi-core electrons were correlated and the scalar relativistic effects were included by means of the Douglas-Kroll transformation.

The vibrational analysis at the DFT level identified the stable minima: the doublet one for the square-planar conformation and the quartet one for both conformations. The DFT results are not conclusive with respect to their relative energies. The hybrid functionals (B3LYP, PBE0) predict the high-spin tetrahedral quartet ground state, whereas the low-spin state lies significantly higher (10–20 kcal/mol above). In contrast, the non-hybrid functionals (BP86, PBE) predict the high- and the low-spin states to lie close in energy (within 5 kcal/mol range); in some calculations the doublet even becomes the ground state. In CASPT2 the ground state is the tetrahedral quartet; the lowest doublet is lying 13–16 kcal/mol above.

Therefore, by applying the CASPT2 we have solved the doubts regarding the ground state (it is high-spin and tetrahedral). Since the hybrid functionals follow the CASPT2 results rather close they can be advised for studying the similar problems. The CASPT2 appears to be a very promising alternative for the DFT in the organometallic chemistry. It is presently applicable only to small- or medium-size systems, but the scope of this method is still growing due to the hardware and software progress, and the better understanding of the method itself.

Keywords: cobalt(II) acetylacetonate; quantum chemistry; conformational analysis; spin-splitting; DFT; CASPT2

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Elongation cutoff technique for linear SCF scaling

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Application of electronic structure calculations to large molecular systems is limited due to unfavorable scaling properties of a given computational method with the system size. For bio- and nanostructures, molecular orbital calculations deal with a huge number of basis functions and any decrease in the computational cost is of great importance. For these reasons, the efforts of quantum chemists over the last two decades have been directed towards development of order-*N* methods. There are two main approaches leading to linear scaling [O(*N*)] in quantum chemical calculations. On one side, new algorithms and formalisms are developed which linearize every step in Hartree-Fock (HF) and Kohn-Sham (KS) schemes, or diminish the scaling properties in the post-HF methods. Here, the best example is the continuous fast multipole method.[1] On the other side are the fragmentation techniques. These techniques are based on nearsightedness approximation; the electronic structure of a given part of a molecule is mainly determined by its nearest neighborhood and the very distant parts of the molecule have practically no effect on it. Two types of fragmentation techniques can be distinguished: the electron density based schemes and energy based schemes. The former schemes build the electron density of the whole system from subsystem densities while the latter compute the total energy or other quantities using the matching rules. The best example of density based approaches is divide-and-conquer of Yang,[2] while the example of energy based methods is the fragment molecular orbital method of Kitaura.[3] The elongation cutoff method that is the subject of this presentation belongs to density based approaches.[4]

The elongation method[5] uses the concept of locality and works in localized molecular-orbital (MO) basis set. The whole molecular system during the elongation procedure is partitioned into several frozen fragments and an active one. If the coupling between a given frozen part and the active part is small enough one can discard it in further calculations. In this presentation we investigate such a "cut-off" variant of elongation method. This exact construction in the limit of perfect localization reduces the computational time in comparison to Hartree-Fock (HF) reference calculations since substantially limits the number of computed two-electron integrals (TEI).

The cutoff elongation scheme has been implemented and linked to the GAMESS program package. The test calculations are performed for two model systems, i.e. weekly bound water chains and polyglycine conformers. Two variants of cutoff scheme are considered: 'conventional' with TEI stored on a disc and 'direct' with TEI computed in every SCF iteration. The effect of basis set and the assumed type of partitioning on CPU (central processing unit) time and accuracy is discussed. It is demonstrated that the number of TEI in the elongation cutoff calculations increases linearly with the system size thus, allowing to extend the 'conventional' type of calculations to larger systems.[6] The step CPU time in the elongation cutoff calculations is much lower than in the HF reference calculations. Such behavior reduces significantly the prefactor in the quadratic scaling relation. The total CPU time in the elongation calculation is about 40% lower than in the conventional HF calculations or comparable to 'direct' type of calculations with the quantum fast multipoles method employed. It is shown that by introducing the interaction radius the linear scaling in the SCF calculations is obtained. In contrast to 'conventional' type of calculations, the 'direct' cutoff technique is linear when the continuous fast multiple method is employed.

Keywords: linear scaling methods, elongation method, cutoff elongation method, continuous fast multipole method, fragmentation techniques

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Evaluation of dynamic characteristics of masonry arch bridges: linking full-scale experiment and FEM modeling

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ABSTRACT

The paper presents the results of theoretical calculations and measurement-interpretation methods of *in situ* investigation of dynamic characteristics of masonry arch bridges. Elaborated of this topic was connected with the program of adapting these objects to increased loads and to the required gabarite of the road at preservation of their monumental character.

Old masonry arch bridges are structures used up till now in the road system all over the world. The basic condition of further functioning of these objects in the road network is adaptation of the roadway and foot pavements to the increased road traffic. Another problem is appearance of new dynamic loads induced by heavy vehicle passages on road surface or paraseismic loads transmitted by the ground such as high-speed train-induced vibrations, mining shocks and firing of explosives in quarries.

Determination of frequency and free vibration modes is a starting point for calculations of the dynamic response of the structure to all types of dynamic loads. Proper recognition of dynamic characteristics of the structure permits for proper interpretation of the investigation results of the structure response to dynamic influences. This requires elaboration of a proper physical and numerical models of the structure. The adopted models become more valuable at the moment of their positive experimental verification. Experimental verification of dynamic characteristics is necessary especially in the case of monumental objects [1, 2, 3]. Lack of documentation makes it impossible to recognize properly the physic-mechanical data of structure, way and depth of founding and parameters of the ground. In this situation experimental verification of dynamic characteristics of the object is of special value.

The paper presents the results of the theoretical calculations of frequency and free vibration modes of two masonry arch bridges used in the Malopolska road network [6]: the road viaduct at Zaborów-Czudec and the bridge at Kamienica Dolna. Physical and numerical models of the bridges were applied considering all componential parts of the structure: bearing arch, spandrel walls, sand-gravel fill, asphalt, soil-structure interaction.

For verification of computational models of chosen bridges a program of *in situ* investigations of dynamic characteristics of these objects was elaborated and realized. Applied methods used in full-scale experiment and in calculation are in a good agreement with methods adopted by other authors [4, 5, 7, 8, , 10]. As a basic ways of realization of dynamic loads serving for determination of frequency, modes of vibrations and damping, impulse excitation was applied: drop of a lorry wheels from a threshold located on the bridge span and kinematic forcing – train passage under the viaduct. For theoretical determination of free vibration frequencies Fourier's transform, power spectral density function as well as transmittance function of measured signals was applied. Basing upon the records of damped free vibrations the value of logarithmic decrement of structure damping was evaluated.

For calculations of dynamic characteristics the ABAQUS program was used – a general-purpose system for static and dynamic calculations of engineering structures based on finite element method. Spectral analysis of the signals was carried out by use of the MATLAB system. These programs are available at Academic Computer Centre CYFRONET AGH on computers SGI ALTIX 3700 and SUN FIRE 6800.

Finally the results of measured and calculated frequencies of free vibrations of bridges were compared and these results were in good agreement. With regard to the degree of complexity of physical and numerical models the existing differences (reaching 12%) between experimental and computational results can be accepted. The frequencies of natural vibrations of bridges obtained are respectively high and the frequency spectrum is dense. This fact made identification of the obtained experimental frequencies difficult, since bending and torsional shapes of vibrations occurred together in dynamic response. In the light of comparison of results obtained experimentally and numerically it may be stated that adopted physical and computational models of masonry arch bridges are correct.

Key words: *dynamic characteristics, masonry arch bridges, in situ dynamic investigation*

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Highly efficient twin module structure of 64 bit exponential function implemented on SGI RASC platform

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It was examined (based on code profiling) that exp() function is employed by plenty of calculation routines. Therefore exp() was chosen as promising software section to be accelerated with FPGA technology. It is worth mentioning that the exp() function by itself has a lot of features making it good candidate for hardware acceleration.

This paper presents a FPGAs implementation of the exponential function in the double precision floating point format. Most presented exponent implementations confine to the single precision format, and increasing data precision requires a novel implementation approach. Employing of massive parallelism results in high performance of the module. Table-based architecture together with short Taylor expansion provide low latency (30 clock cycles) which is comparable to 32 bit implementations. As this work shows, FPGA-based double precision elementary functions implementation achieve huge performance with a satisfactory accuracy and latency.

Low area consumption of a single exp() module (roughtly 4% of XC4LX200) allows implementation of several parallel modules on a single FPGAs. The exp() function was implemented on the SGI RASC platform, thus external memory interface limitation allowed only a twin module parallelism. This implementation aims primarily to meet quantum chemistry's huge and strict requirements of precision and speed. Each module is capable of processing at speed of 200 MHz with max. error of 1 ulp, RMSE equals 0,62.

HLA Component Model for Multiscale Simulations

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Introduction

Building a simulation system from modules of different scale is an interesting, but non-trivial issue. There are many approaches to combine different models and scales in one problem solution is difficult and depends on actual models being combined. When designing a problem solving environment [PSE] for simulation of multiphysics multiscale systems, one can identify issues related to actual connection of two or more models together (this includes support for joining models of different internal time management [PPAM07], efficient data exchange between two modules of different scale etc.). Apart from that, there are also issues related to reusing of existing models and their composability. For scientists working on multiscale systems it would be useful to find already existing models needed and connect them either together or include into their own models.
To facilitate that, there is a need to wrap simulations into recombinant components that can be selected and assembled in various combinations to satisfy specific requirements. There is also a need for an infrastructure that allows to exchange these components between scientists in a relatively easy way across administrative domains. To summarize, there is a need for a component model with support specific for multiscale simulations (complex time interactions, efficient data transfer between modules of different scale etc) and for the environment that would allow to build and reuse such components across administrative domains [ICCS08].
An important approach to using services and component technology to distributed simulations is described in [TURNER] and is addressed in general to distributed simulations, without special focus on multiscale simulations systems. Another worth to be mentioned component framework for simulations [PARKER] is specifically designed for partial differential equations.

Description of a problem solution.

As a solution, we propose to integrate solutions from the High Level Architecture [HLA] (such as advanced time and data management) with possibilities given by component technologies [CCA] (such as reusability and composability) and the Grid [GRID] (such as joining geographically distributed communities of scientists). This approach will allow users working on multiscale applications to more easily exchange and join the simulations already created. The particular focus of this paper is on design of HLA component. We show how to insert a simulation logic into a component and to make possible to steer from outside its connections with other components. Its functionality is shown on the example of a multiscale simulation of a dense stellar system.

Applied algorithms and methods, software and hardware used

As any of the existing component models does not explicitly address requirements of multiscale simulations, we have presented the idea of model based on HLA. The difference between the component view proposed in this paper and the original HLA approach is that the particular behavior of a component and it's connections are defined and set by an external module on the user request. The main advantage of this approach over original HLA is that it enables the user to create simulation systems (federations) from simulation modules (federates)

developed by others without ingerating into their implementation. The particular federation, in which federate is going to take part, does not need to be defined by a federate developer, but can be created later -- from outside -- in the process of setting up the distributed simulation system. Therefore, the presented approach increases the reusability and composability of simulations. As a a Grid framework we have chosen H2O [H2O] platform as it is lightweight and enables dynamic remote deployment. The HLA component is implemented as a H2O pluglet. The component developer has to provide a simulation logic code which is connected with the pluglet by interfacing the compoHLA library. The use of the compoHLA library does not free the developer from understanding HLA mechanisms, but simplifies use of them and allows the HLA component to be steered from outside.

It is worth noticing that components of multiscale simulation systems are often computationally intensive and need a high performance hardware like dedicated clusters (e.g. nbody simulation of star dynamics used in as the example in this paper needs clusters of GRAPE architecture [GRAPE]).
The experiments described in this paper were performed on DAS-3 (The Distributed ASCI Supercomputer 3) [DAS3] which is a five-cluster wide-area distributed system in the Netherlands. We also plan to use CYFRONET Grid node Zeus.

Results

For this research we have used simulation modules of different time scale taken from the Multiscale Multiphysics Scientific Environment (MUSE) [MUSE] for simulation of dense stellar systems like globular clusters and galactic nuclei. Components were built with two MUSE modules: evolution (macro scale) and dynamics (meso scale) that run concurrently. We have created two prototype HLA components for dynamics and evolution simulations, then, we measured execution time of requests to them. The experiments show that the overhead of designed component layer is rather small -- for all requests of order of a few milliseconds.

Conclusions and Future Work

The purpose of the solution presented in this paper is to offer scientists working on multiscale simulations a component model that facilitates joining elements of different scale and the environment supporting applications in that model running on the Grid. We have also build the preliminary prototype of the HLA component that stores the simulation logic and makes possible to steer from outside its connections with other components. This approach differs from that in original HLA, where all decisions about actual connections are made by federates themselves. The functionality of the prototype is shown on the example of multiscale simulation of dense stellar system -- MUSE environment. The results of the experiment show that the execution time of requests are promising and that the component layer does not introduce much overhead.
In the future we plan to fully design and implement the environment supporting applications build from HLA Components. We also plan to extend the prototype of HLA Component.

Acknowledgments

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Keywords

Components, Grid computing, HLA, distributed multiscale simulation, problem solving environments

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Modelowanie procesu krystalizacji wybranych stopów metali nieżelaznych przy pomocy programu FLUENT

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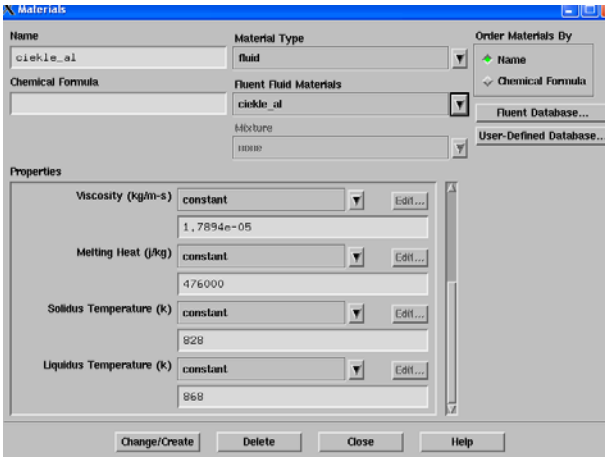
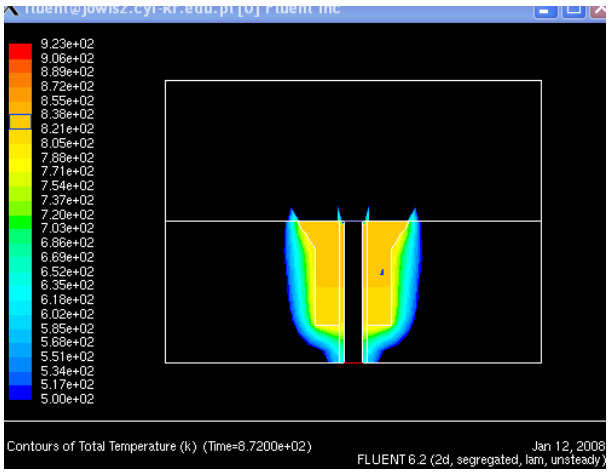
W pracy przedstawiono rezultaty badań symulacyjnych procesu krystalizacji stopów metali nieżelaznych ze szczególnym uwzględnieniem wybranego stopu aluminium. Symulacje realizowano wykorzystując zainstalowany w ACK – CYFRONET program FLUENT.
Opisano podstawowe procedury i funkcje FLUENTA wykorzystywane podczas symulacji procesu krystalizacji. Wyniki badań symulacyjnych porównano z eksperymentami fizycznymi prowadzonymi w ramach projektu badawczego realizowanego w Katedrze Automatyki Akademii Górniczo-Hutniczej. Rozpatrywany jest odlew ze stopu aluminium w kształcie tulei cylindrycznej z rura stalową w środku. Badany jest wpływ chłodzenia wodą przepływającą przez rurę chłodząca na rozkład temperatury w czasie krzepnięcia odlewu oraz na mikrostrukturę odlewu.

Przyjmuje się określone właściwości materiałów takich jak przewodność cieplna formy, odlewu i rury chodzącej - zapisanych zgodnie z wymaganiami programu. Przykład danych charakteryzujących badany stop aluminium podano na rys.3.3.1a (Określenie właściwości ciekłego metalu - stopu aluminium)





Rys. 3.3.1a

Rys. 3.3.1f

Wyniki symulacji są przedstawione między innymi w postaci umożliwiającej ocenę procesu krzepnięcia w czasie. Na rys. 3.3.1f przedstawiono przykładowy rozkład temperatury [K] po 872sek.
Prezentowana praca jest związana z eksperymentem fizycznym w którym zmieniano czas przepływu wody chłodzącej i mierzono rozkłady temperatur termoparami w krzepnącym odlewie oraz termowizją na powierzchni nadlewu.

Monte Carlo fitting of data from Muon Catalyzed Fusion experiments in solid hydrogen

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For a wide range of physical problems the only applicable way to compare experiment with theory is via the Monte-Carlo (MC) method. However, the MC method has several limitations, mostly related to calculation time and the nature of random sampling. Modelling of events which are fairly rare and hidden inside many other processes often requires long calculation time to establish sufficient statistics for comparison.
As is fairly well known, finding the best fit parameters describing a multitude of data requires repeated calculation of some statistical estimator (e.g. χ^2). When the χ^2 minimum depends on two or more variables, the error determination on the parameters as well as the study of the possible occurrence from several minima requires calculations of several thousands theoretical functions, and hence, the calculations becomes extremely time-consuming. Even if the calculation time were acceptable, the intrinsic nature of MC simulations makes such an approach impossible since instabilities will arise resulting from the statistical nature of the results. Clearly, the statistical fluctuations of the MC method can cause entirely false gradients (calculated numerically from difference quotients), and thus such a minimization procedure is not suitable.

We proposed a modification in the calculation of the theoretical functions $M(\vec{p})$ which describe the data for a given parameter vector $\vec{p}(p_1, p_2, \ldots, p_n)$. Before fitting, one generates a set (a "grid") of theoretical functions $\{M\} = \{M_{\gamma,\delta,\ldots,\varphi}, M_{\gamma',\delta',\ldots,\varphi'}, \ldots\}$ for all permutations of a *chosen* discrete set of parameter values $(p_1^{\gamma}, p_2^{\delta}, \ldots, p_n^{\varphi})$, where $\gamma, \delta, \ldots, \varphi$ are the function indexes in the set. Once the $\{M\}$ set is known, the interpolation procedure (relatively fast), is used to find $M(\vec{a})$ (theoretical function for any set of parameters $\vec{a}$ required by fitting procedure), which is used to calculate the χ^2. It means that the time-consuming calculations are only executed for a select and limited parameter set.

The Monte-Carlo simulation was performed using developed in Fortran 77 the FOW code [1]. Simulation of the diffusion processes and interaction of muonic atoms with a solid hydrogen and the experimental hardware were the main task of the code. The output of the simulation are the γ-ray and converted muons time spectra which can be, after normalisation, directly compared with the experimentally measured ones. The computational time necessary for realization of a single simulation was equal to ca. 2h of the CPU on SGI 2800 computer, for the programme in scalar version. For the "grid" with dimensions 11x11 the real time of generation was ca. two weeks of the CPU time.

The procedures were used for the data analysis of experiments devoted to study behaviour of muonic atoms inside structure of solid hydrogen. The existence of the minimum in the cross-section dependence of elastic scattering of muonic atoms was confirmed [2] and the rate of a $pd\mu$ muonic molecule formation was determined [3].

Keywords: *data fitting, Monte Carlo simulation ,chi-square estimator, gradient calculation, diffusion simulation, muonic atoms and molecules,*

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Multivariate tools for tau identification in the ATLAS experiment

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Introduction. The new particle accelerator LHC (Large Hadron Collider) is being commissioned at CERN, Geneva, Switzerland. The LHC represents a significant step on the energy and luminosity frontier, thus allowing searching for new physics phenomena. Elementary particle physics experiments, searching for very rare processes, require the efficient analysis and selection algorithms able to separate signal from the overwhelming background. Three of such algorithms have been applied to identify tau leptons in the ATLAS (A Toroidal LHC ApparatuS) experiment at LHC: Probability Density Estimator with Range Searches (PDE-RS), Neural Network (NN) and Support Vector Machine (SVM). Tau leptons play an important role in the physics to be observed at LHC; they enter electroweak measurements, studies of the top quark and searches for new phenomena such as Higgs boson, Supersymmetry and Extra Dimensions.

Description of a problem solution. For the track-based tau reconstruction algorithm several discriminating variables are defined to separate real tau jets from background jets. The variables are not independent and no single variable provides good signal and background separation, which emphasizes a need for efficient selection algorithms and multivariate techniques.

Applied algorithms and methods; software and hardware used. Beside the standard cut analysis three multivariate algorithms were applied to select tau candidates. The PDE_RS discriminant is determined by taking a number of signal and background events in a small volume around point being analyzed. Neural Network is an another statistical non-linear data modeling tool. For the NN emulation the *Stuttgart Neural Network Simulator* was used and the resulting network was included into the official reconstruction software. We have also implemented the SVM algorithm, in which the separation is performed by building a hyperplane separating signal from background. The position of the hyperplane is defined by the subset of all training vectors called support vectors. The extension into non-linear SVM is performed by mapping input vectors into a high dimensional feature space, in which data can be separated by a linear procedure.

The ACK Cyfronet "Zeus Cluster" was used to run the simulation and reconstruction jobs in the grid environment, which were needed to prepare training data samples and later to validate the methods.

Results. Identification of tau candidates by the track-based tau identification algorithm is significantly improved by using multivariate analysis tools, as compared to the standard cuts. All three multivariate methods applied give similar results, which suggest that the performance of these algorithms is close to the Bayesian limit.

Conclusions and future work. The use of multivariate tools greatly enhances the performance of the tau selecting procedure. The Support Vector Machine wasn't, up to now, commonly used in HEP. We have shown that SVM can be successfully used to analyze high energy physics data. In view of real ATLAS data we are searching for better discriminating variables and improving selection algorithms.

Keywords: multivariate methods, High Energy Physics, ATLAS, tau lepton physics

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Numerical simulation of the laser welding

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Laser based welding of alloys is one of the most applied techniques of welding process for the sake of connection of high speed, precision and small deformation in comparison with conventional welding process. The process using high power density beam is more and more often used in industrial manufacturing. During laser welding in a very short time occur such complicated phenomena such as temperature dependency of material properties, phase transformations, formation and convection of the liquid phase caused, among other things, by Marangoni effect.

Experiment based traditional optimization of the process requires great expenses and is time-consuming. The use of computer simulation allows replace a part of experimental research with modeling of physical processes. Following computer applications have been used in this work: the Gambit for the shape modeling and to build of finite elements and the Fluent with the help of which calculations have been carried out. Calculations have been carried out using the calculation cluster of the IBM Blade Center HS21 at the Academic Computer Center Cyfronet AGH.

The model takes into consideration thermophysical and metallurgical properties of the remelting steel, laser beam parameters and boundary conditions of the process. As a result of heating the material, in the area of laser beam operation the weld pool is being created, which shape and size depends on convection caused by the Marangoni force. The direction of the liquid stream depends on the temperature gradient on the surface and on the chemical composition as well. Created model allows to predict the weld pool shape depending on material properties, beam parameters and boundary conditions of the sample.

The model takes into consideration the stage of heating. Taking into consideration the CCT diagram of the material, it is possible to calculate the shape of zones for individual metallurgical transformations during the cooling of the material.

Key words: laser treatment, computational fluid dynamics (CFD), Marangoni effect, metallurgical transformation, geometry of the melted zone

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On optimal acceleration of iterative solution methods of Simultaneous Algebraic Equations

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Keywords: *simultaneous algebraic equations, Gauss-Seidel iterative method, relaxation approach, solution increment approach, non-linear algebraic equations*

Solution of the simultaneous linear algebraic equations SLAE is usually obtained by means of either the elimination methods or iterative ones. The iterative solution methods are convenient in practical calculations due to their simplicity and minimised storage requirements. On the other hand they may be not efficient enough, especially for large systems of equations. Several techniques were already proposed in order to speed up the iteration process. Some new concepts are discussed here using an example of the well-known Gauss-Seidel method.

Many iterative solution methods, including Gauss-Seidel method, may be used together with the successive over-relaxation technique (SOR). In the classical SOR approach [1,2] the optimal relaxation parameter value is to be chosen in order to minimise the spectral radius of an error dumping matrix. However, evaluation of such optimal parameter λ is difficult except in the simplest cases. It is often obtained only approximately, based on trying various values λ, and observing its effect on the solution convergence speed. A new simple and effective way of evaluation of the relaxation factor for solution of SAE by means of iterative methods is considered here [3]. Proposed is either minimisation or annihilation of a modified subsequent value of solution residuum. As opposed to the spectral radius minimisation technique [1,2], the above mentioned concept requires only simple calculations to evaluate a new parameter λ in each iteration step.

The other concept accelerating the iteration process is based on the notion of infinite geometrical progression. Its quotient is built using solution increments in several initial subsequent steps separately for each equation. After several iteration steps each solution component is improved by adding solution increment multiplied by evaluated progression sum of infinite number of those steps. Both acceleration mechanisms were combined in order to obtain the best acceleration of the solution process.

Variety of tests were done implicating the optimal relaxation and increment approach parameters. Approach was examined using many linear, and non-linear benchmark problems, with banded and/or sparse systems. The convergence rates were, for relaxed G-S approach, up to 200 times better when compared with the standard ones. Tested were also non-linear SAE, with relaxed Newton-Raphson method, yielding significant convergence improvement. Future plans include further analysis oriented on large systems of SAE, including distributed calculation techniques for additional reduction of solution time.

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Optimalisation of Simulation Model Parameters for Solidification of Metals with Use of Agent-Based Evolutionary Algorithm

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Abstract
The finite elements method (FEM) is currently widely used for simulation of thermal processes. However, one of still unresolved problems remains proper selection of mathematical model parameters for these processes. As far as modelling of cooling casts in forms is concerned, particular difficulties appear while estimating values of numerous coefficients such as: heat transport coefficient between metal and form, specific heat, metal and form heat conduction coefficient, metal and form density. Coefficients mentioned above depend not only on materials properties but also on temperature. Values of these coefficients that may be found in charts are usually approximated. In the paper the idea of optimalisation of simulation method parameters based on adaptive adjustment of curve representing simulation result and result obtained in physical experiment is presented.
In the presented approach, the complexity of algorithm is crucial, because each iteration requires repetition of the procedure of simulating the course of temperature in casting simulation. Using of evolutionary algorithm in agent-based version may enhance the possibilities of reducing the complexity. Decreasing of simulation cost by the means of parallelization and faster convergence is expected. In the paper, the idea of the method and preliminary results obtained with use of ABAQUS system available in ACK CYFRONET and software developed at AGH-UST are presented. Successful solution of considered problem may be very important for opening new research opportunities in the field of metal cooling and solidification research, especially in casting technologies.

keywords: numerical simulation, evolutionary algorithm, agent systems, solidification casting process, casting,

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Parallel clustering algorithm for noisy data

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Abstract

1. **Introduction.** *Cluster analysis, an important unsupervised learning technique, has been well advanced for noiseless data with well defined, compact clusters. However, various experimental data often harbor substantial background noise, i.e. large number of observations that do not steam from the actual phenomena underlying the analyzed data but rather arise from measurement errors or week criteria for selecting cases into the dataset. Some algorithms for clustering such noisy data has been proposed recently. In our research we focus on methods employing similarity measures and data density measures derived from shared nearest neighbors graphs.*
2. **Description of a problem solution.** *In this article a parallel implementation of an algorithm for clustering noisy data with shared nearest neighbor graphs is presented. The implementation is dedicated for shared memory machines and was done with OpenMP standard. A well balanced data decomposition was achieved with an aid of small hash tables of locks.*
3. **Results:** *The algorithm has been evaluated on SGI Altix 3700 machine, running 128 1.5GHz Intel Itanium 2 processors. Parallelization speedup and efficiency as well as an example result for a data set with almost 100,000 data points are demonstrated.*
4. **Conclusions and future work:** *The algorithm scales well for up to 32 processors, which is a good result for shared memory implementation. Our current work focuses on improvements to the clustering method that would allow for more accurate noise identification and on methods for visualizing the clustering structure. In particular, we investigate methods for density estimation that do not require extensive parameterization and methods for identifying low energy minima in stress function used in MDS visualization.*

Keywords: *Cluster analysis, background noise, shared nearest neighbor graphs, parallel implementation for shared memory machines.*

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Parallel simulation of a fluid flow by means of the SPH method: OpenMP vs MPI comparison.

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- Abstract
  1. **Introduction.** The SPH method for simulating incompressible fluids is presented in this article. The background and principles of the SPH method are explained and its application to incompressible fluids simulations is discussed. The parallel implementation of the SPH simulation with OpenMP and MPI environments are demonstrated. Both models of parallel implementation are fully analyzed, and compared, as well as their results.
  2. **Description of a problem solution.** In the article the simulation of fluid flow in an elongated vessel simulation is presented. The details of the initialization of the particle system are depicted. Also, we present the domain decomposition for the MPI implementation, as well as its optimization for the particular particle distribution. We also present the algorithm decomposition for OpenMP implementation.
  3. **Algorithms.** In executed simulations the SPH method was used. The SPH is a computational model, in which the simulated fluid is modeled by a number of particles. The particles interact mutually by means of hydrodynamic forces and follow the motion according to Newton's dynamics. In the parallel implementation we exploited two approaches: domain decomposition, where simulated box is divided into subdomains, and each of them is computed by proper node (MPI implementation), and algorithm decomposition, where blocks of algorithm are indicated to execute in parallel. This approach is realized on the shared memory machines, and parallel scheduling is done automatically (OpenMP implementation).
  4. **Results.** The comparison between two programming paradigms was performed on the SGI Altix machine, for varying number of processors.
  5. **Conclusions and future work.** In future we plan to focus on the optimization of both implementations and to apply the simulation for greater number of particles.

- Keywords: **computational fluid dynamics, SPH, parallel computing, OpenMP, MPI**

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The absorption and fluorescence study of 1,4,5,8-Naphthalenetetracarboxylic dianhydride (NTCDA).

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NTCDA belongs to a family of large organic molecules of the potential significance as optoelectronic devices or sensors in the molecular electronics. For this reason the title molecule was extensively studied in many experiments[1,2]. Since the fluorescence and absorption spectra of NTCDA species show no mirror-image relationship, the dianhydride studied is also attractive and interesting from theoretical point of view.

For the time being, the electronic structure of the low-energy states of NTCDA is investigated in terms of DFT and TD-DFT methods. At this level the Franck-Condon (FC) parameters were estimated for low-energy dipole-allowed $1B_{1u}$, $1B_{2u}$ and $1B_{3u}$ electronic states and for 12 totally symmetric modes of NTCDA molecule. These FC parameters were then employed to simulate[3] the vibrational structures of absorption and fluorescence spectra [Fig 1].

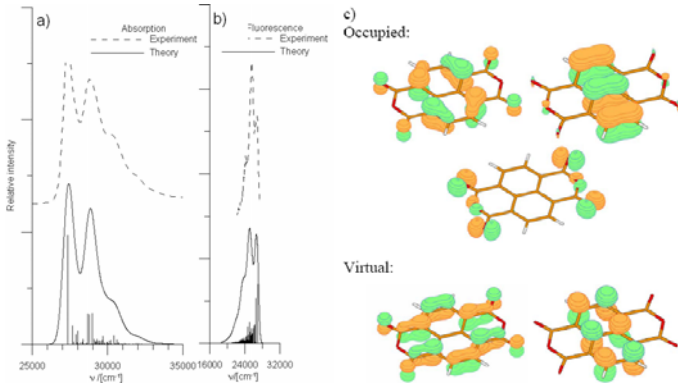

Figure 1. a) Absorption b) fluorescence spectra c) involved molecular orbitals

In series of DFT computations performed with different sets of basis sets and functionals we could found that the absorption spectra is a superposition of two electronic excitations, namely $1A_g \rightarrow 1B_{2u}$ (y-polarized) and $1A_g \rightarrow 1B_{3u}$ (x-polarized), both π-π^* in character. On the other hand, the fluorescence spectrum is very likely due to $1B_{1u} \rightarrow 1A_g$ (z-polarized) transition being n-π in character.

There is still a debate concerning absolute location of out-of-plane $1B_{1u}$ state on the energy scale. While the accurate theoretical location of $1B_{1u}$ state may significantly depend on the methods used in the computations, the experimental data, like these gained from magnetic circular dichroism (MCD) and resonance Raman scattering (RRS), strongly suggest that the out-of-plane $1B_{1u}$ state is in fact emissive one. Works on this topic is now in progress in our scientific group.

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The ATLAS experiment on-line monitoring and filtering as an example of real-time application

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Introduction. The ATLAS detector, recording LHC particles' interactions, produces 1.5 MB events with rate of 40 MHz. The processes with new and interesting physics phenomena are very rare, thus an efficient on-line filtering system (trigger) is necessary. An asynchronous part of that system relays on a few thousands of computing nodes running the filtering software. Applying refined filtering criteria results in increase of processing times what may lead to lack of processing resources installed on CERN site. We propose extension to the system based on submission of the real-time filtering tasks into the Grid.

Description of a problem solution. The ATLAS experiment implemented the filtering and data acquisition system with assumption that all computing power needed (ca. 5000 CPUs) will be available at CERN. In case, some additional CPUs would improve the rate of filtering process, the grid resources could be used. To profit from the grid remote resources with minimal modifications to the existing system we propose to break the processing task (PT) into the proxyPT which fulfills the requirements of the local (CERN) system and the remotePT, running the bulk of computational work, which is to be submitted into the grid. Only sites which confirmed upgrade to the current version of the filtering software and recent updates of the data bases can be taken into consideration. These aspects are taken care of by the dedicated virtual organization (VO). The VO is also responsible for launching pilot jobs to the grid to allocate machines where the remotePT will subsequently be started.

Deploying the filtering task in some distant grid farm increases risk of losing communication with working node, hence losing event, and in addition introduces network delays. The ATLAS filtering software is secured against lost events in case of crashes in filtering software, whereas the latter is to be addressed by the Real Time Dispatcher (RTD). The RTD, designed and implemented within the scope of the Interactive EU Grid project, relays events between the proxy and remotePTs. By using the grid middleware it is able to select sites with available computing resources and nodes with minimal network congestions.

Applied algorithms and methods; software and hardware used. As a part of the EU "CrossGrid" project, IFJ PAN together with Cyfronet participated in network QoS measurements between CERN and Cyfronet using GPS system and network programmable cards. Collected results justified implementation of the system in remote sites and indicated necessary modifications to higher communication protocols aimed on improving usage of installed network capacity.

Results. We designed and implemented system that allows real time applications to be submitted and executed in the grid infrastructure. With the help of the RTD we can perform load balancing and delegate events to nodes optimally positioned from the performance point of view.

Conclusions and future work. We plan to further improve our system and make more consistent studies of performance issues before proposing the solution for the Atlas collaboration. We also plan to investigate other real-time applications which possibly could benefit from our developments. We appreciate the cooperation of ACK Cyfronet director, site administrators and network technicians.

Keywords: High Energy Physics, real-time processing, ATLAS, TDAQ, remote farms
References: https://twiki.cern.ch/twiki/bin/view/Atlas/HltDaqMainPage

The ATLAS experiment simulations as the computing challenge for the ACK Cyfronet AGH

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Introduction. The High Energy Physics (HEP) community is commissioning the Large Hadron Collider (LHC) at CERN, Geneva, Switzerland. The LHC, the particles accelerator, will extend the frontiers of particle physics with its unprecedented high energy and luminosity. One of the four detectors, placed at the beam interaction points is the ATLAS (A Toroidal LHC ApparatuS) detector dedicated to searches for the Higgs boson particle – very important ingredient in understanding the origin of particles masses – and the supersymmetry. The information gathered from the detector is organized in so called physics events. The processes leading to the Higgs boson formation are very rare. The first challenge is to filter on-line interesting events from the bulk of background. The second challenge is to prepare collaboration software for particles reconstruction and identification (e.g. tau leptons) and extensively test them on large statistics Monte-Carlo samples. With use of these algorithms we have prepared analysis tools estimating signal significance (presence of the Higgs boson).

Description of a problem solution. The unprecedented data volumes needed to validate reconstruction and analysis software of the ATLAS collaboration have been produced in so called data challenges, in which the ACK Cyfronet AGH has participated from the beginning. The ATLAS generation, simulation and reconstruction jobs were sent to the Cyfronet cluster as grid jobs and the results were sent back to CERN. The validation of the reconstruction software, particularly algorithm for the tau leptons identification and the analysis software required interactive access to the worker nodes and the batch system, in order to check validation histograms on smaller statistics, for debugging purposes.

Applied algorithms and methods; software and hardware used. As a result of participation in EU "CrossGrid" project, the Cyfronet acquired new computational power – the "zeus" cluster (Racksaver's PCs). It has been used for preparation of large statistics of physics events. The ATLAS production software has evolved very rapidly (several significant release upgrades within few years) leading to re-simulation of events with different versions and validating developed software and comparing overall performance. The support of the ATLAS Virtual Organization has assured availability of the ATLAS collaboration framework (Athena) needed both for developing the reconstruction algorithms and an analysis code.

Results. The infrastructure of the ACK Cyfronet AGH enabled development of analysis code that estimated significance of the Higgs boson discovery region in the Minimal Supersymmetric Standard Model and improvement in low mass around 200 GeV/c (PhD – T. Szymocha, another PhD thesis will be completed next summer). The Cyfronet cluster has been also used in the validation of the tau leptons reconstruction and identification package, developed by IFJ PAN team (A. Kaczmarska, T. Szymocha, P. Malecki, E.Richter-Was). Produced validation Monte-Carlo data were used by the ATLAS Tau Working Group.

Conclusions and future work. The cooperation with the Cyfronet has enabled our participation in world-wide collaboration. In view of arrival of "real" data from the ATLAS detector we plan extensively enlarge the CPU and storage usage, not only by the central production, but mainly by physics analyses performed by local ATLAS HEP community. We appreciate the cooperation of ACK Cyfronet director and site administrators.

Keywords: High Energy Physics, HEP, ATLAS, tau lepton physics

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The simple - $KBrO_3$, H_2SO_4 oscillator

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Na saturnie (Sun Fire 6800, przy użyciu programu MATHEMATICA) wykonano obliczenia dotyczące publikacji, którą załączam. Obliczenia dotyczyły wielokrotnego rozwiązywania dziewięciu równań różniczkowych aż do znalezienia rozwiązań, które odtwarzają wyniki doświadczalne. Wynik doświadczalny jest pierwszym w świecie i dodatkowo upiększony poprzez obliczenia komputerowe, których nie udało się przeprowadzić na zwykłych komputerach za względu na duże potrzeby pamięci. W doświadczeniu, które poprzedziło wykonane obliczenia wykryto oscylacyjne zachowanie się stężeń reagentów w czasie zachodzenia reakcji chemicznych w układzie $KBrO_3$ i H_2SO_4 . Należało napisać równania reakcji chemicznych , a następnie trzeba było napisać tzw. równania kinetyczne i w uproszczonej postaci przez zastąpienie symboli chemicznych prostymi oznaczeniami alfabetu. W ten sposób otrzymano 9 równań różniczkowych, które rozwiązywano przy pomocy Mathematyki na Saturnie. Wprowadzano najpierw doświadczalne stężenia początkowe jako warunki początkowe dla tych równań różniczkowych. Stężenia te modyfikowano tak, by rozwiązania równań różniczkowych przypominały wynik z doświadczenia. Po kilkudziesięciu próbach otrzymano wynik zadawalający. Bez tego wyniku samo doświadczenie byłoby za ubogie do opublikowania w dobrym czasopiśmie jakim jest J.Phys.Chem. Praca ta właśnie tam jest w publikacyjnym cyklu. Wzięto pod uwagę następujące równania reakcji chemicznych, które mogły zachodzić w reaktorku:

(1) $Br^- + BrO_3^- + 2H^+ \rightarrow HOBr + HBrO_2$ $2\ M^{-3}s^{-1}$
(2) $HOBr + HBrO_2 \rightarrow Br^- + BrO_3^- + 2H^+$ $3.3\ M^{-1}s^{-1}$
(3) $Br^- + HBrO_2 + H^+ \rightarrow 2HOBr$ $2.0\ E{+}6\ M^{-2}s^{-1}$
(4) $2HOBr \rightarrow Br^- + HBrO_2 + H^+$ $2.0\ E{-}5\ M^{-1}s^{-1}$
(5) $HOBr + Br^- + H^+ \rightarrow Br_2 + H_2O$ $2.3\ E{+}9\ M^{-2}s^{-1}$
(6) $Br_2 + H_2O \rightarrow HOBr + Br^- + H^+$ $2.0\ s^{-1}$
(7) $2HBrO_2 \rightarrow BrO_3^- + HOBr + H^+$ $3.0E{+}3\ M^{-1}s^{-1}$
(8) $BrO_3^- + HOBr + H^+ \rightarrow 2HBrO_2$ $7.5E{-}9\ M^{-2}s^{-1}$
(9) $BrO_3^- + HBrO_2 + H^+ \rightarrow Br_2O_4 + H_2O$ $33.0\ M^{-2}s^{-1}$
(10) $Br_2O_4 + H_2O \rightarrow BrO_3^- + HBrO_2 + H^+$ $2200\ s^{-1}$
(11) $Br_2O_4 \rightarrow 2BrO_2^{\bullet}$ $7.4\ E{+}4\ s^{-1}$
(12) $2BrO_2^{\bullet} \rightarrow Br_2O_4$ $1.4\ E{+}9\ M^{-1}s^{-1}$

Obok powyższych równań podano stałe kinetyczne, niezbędne czynniki mnożące w równaniach kinetycznych. Zastępując symbole chemiczne prostymi oznaczeniami otrzymano równania różniczkowe, które rozwiązywano właśnie przy pomocy Saturna:$[Br^-] = a$, $[BrO_3^-] = b$, $[HOBr] = c$, $[HBrO_2] = d$, $[BrO_2^{\bullet}] = e$, $[Br] = f$, $[Br_2O_4] = g$, $[H_2O] = w$, $[H^+] = h$

$$\dot{a} = -2abh^2 + 3.3\,cd - 2dah10^6 + 2c^210^{-5} - 2.3cah10^9 + 2f^2w$$

$$\dot{b} = -33bdh + 2200\,gw - 2abh^2 + 3.3cd + 3000d^2 - 7.5bch10^9$$

$$\dot{c} = 2abh^2 + 3.3cd + 4dah10^6 + 4c^210^{-5} - 2.3cah10^9 + 2f^2w + 3000d^2 - 7.5bch10^9$$

$$\dot{d} = -33bdh + 2200gw + 2abh^2 - 3.3cd - 2dah10^6 + 2c^210^{-5} - 2d^23000 + 15bch10^9$$

$$\dot{e} = 14.8g10^{4} - 2.8e^{2}10^{9}$$

$$\dot{f} = 4.6cah10^{9} - 4f^{2}w$$

$$\dot{g} = 33bdh - 2200gw - 7.4g10^{4} + 1.4e^{2}10^{9}$$

$$\dot{h} = 33bdh + 2200gw - 2abh^{2} + 6.6cd - 2dah10^{6} + 2c^{2}10^{-5} - 2.3cah10^{9} + 2f^{2}w - 7.5bch10^{9}$$

$$\dot{w} = 33bdh - 2200gw + 2.3cah10^{9} - 2f^{2}w$$

Theoretical calculation in form of the Monte Carlo for particle collider experiments

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Since early dates of the particle physics accelerator experiments
Monte Carlo programs were used to simulate scattering process.
In recent decades these calculations became more sophisticate,
both as the theoretical physics (quantum field theory) models
and as computational projects, with decades long lifetime cycle.
The corresponding software projects seem to have distict features,
which I would like to review briefly.
For instance: constant change of specifications (long prototyping period)
need of inventing novel numerical methods, the need of ever larger
CPU power, supporting large group of users over long time, etc.
These features can be seen in other branches of computing,
but their mix is here unique and requires special methodology
of the software development.

Theoretical modeling of electrochemical interactions in bimetallic molybdenum nitrosyl complexes incorporating saturated bridges

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Since the preparation of the most renowned example of mixed-valence compound, the Cretuz-Taube ion, $[\{Ru(NH_3)_5\}_2(pz)]^{5+}$, chemists have been interested in the study of molecules with two (or more) redox-active metal centers connected *via* appropriate bridging ligand, showing electronic interactions detectable electrochemically. From the early 1970s many other examples of such mixed-valence compounds, showing a wide range of behavior from fully delocalized to valence-trapped, have been studied because of the possibility of constructing potential elements for molecular electronics, *e.g.* molecule-sized wires, diodes, switches, and the great importance for explaining key processes in biology like the long-range electron transfer in proteins. The electronic interactions may occur either coulombic through-space or through-bond (π – mesomeric effect, σ – inductive effect), dependent on the metal and its environment, the length and the geometry of the bridging ligand and its electronic properties.

Recently a series of bimetallic complexes based on 16-electron $\{Mo(NO)\}^{3+}$ centers were prepared, among them singly bridged $[\{Mo(NO)(Tp^{Me2})X\}_2\{O(CH_2)_2O\}]$ (X = halide) and a doubly bridged $[\{Mo(NO)(Tp^{Me2})(OCH_2CH_2O)\}_2]$ (Tp^{Me2} is tris(3,5-dimethylpyrazol-1-yl)hydroborate) [1]. The electrochemical data, *i.e.* the separation between reduction potentials of 310 mV for the complex with a single C_2 bridge indicating significant metal-metal interactions, prompted us to investigate electronic interactions through saturated alkyl chains in $\{16:17\}^-$ complexes.

In this study hybrid B3LYP DFT formalism has been applied to bimetallic nitrosyl hydrotris(3-methylpyrazol-1-yl)borato complexes of molybdenum with saturated ethane-1,2-diolate bridges and their reduced forms. Direct evidence for localization of an extra electron in mixed-valence monoanions $\{16:17\}^-$ is based on the analysis of electron density, energetic stabilization of asymmetric structures with an electron trapped on one Mo and the splitting of both calculated and experimental ν_{NO} stretching frequencies. Calculated differences in the first and second electron affinities are successfully related to cyclic voltammetry measurements. Electronic interactions through saturated ethane-1,2-diolate bridges are evidenced by the extent of spin density delocalization towards the second Mo centre. These results indicate that the presence of the double bridge causes 10% partial delocalization of unpaired electron.

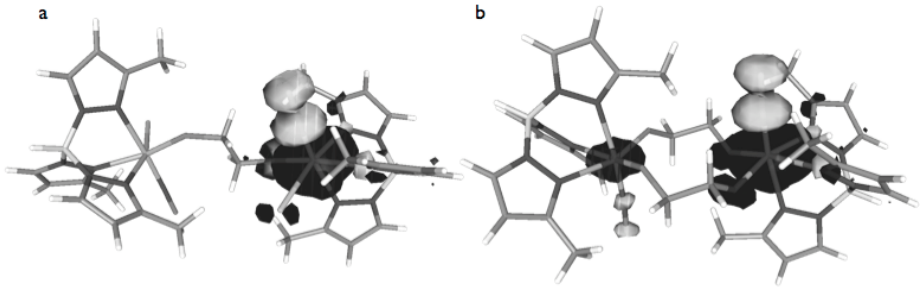

Figure 1. Spin density plots for mixed-valence: (a) singly or (b) doubly bridged complexes (contour value 0.002)

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Theoretical reproduction of vibronic structures for the $A_{1g} \leftarrow B_{1u}$ transition in oligothiophenes containing 2-6 thiophene rings

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Oligothiophenes have been widely studied over the recent years owing to their potential applicability in organic electronics. Vibronic coupling within the molecules and in the corresponding molecular crystals is one of the issues that still remain the subject of vivid discussions. Theoretical modeling of the vibronic spectra requires a way of optimizing geometry of a molecule in its ground state and in some excited state, as well as calculating the normal modes at least for the molecular ground state.

A new implementation of the Turbomole package provides a novel method of calculating the molecular geometries for excited states. Based on the time dependent version of the density functional theory (TDDFT [1]), it is potentially capable of dealing with much larger systems than the highly-correlated *ab initio* methods (CASSCF, CASPT2) available so far. We decided to test the performance of this new approach by using the calculated excited state geometries to simulate the vibronic spectra of a number of oligothiophenes, in the meantime producing sets of Franck-Condon parameters [2] that may be used in further research. Available high-resolution experimental spectra served as the reference.

The procedure entailed the optimization of the molecular geometries both for the ground and for the excited state of the oligothiophene molecules, along with the vibrational analysis for each state. A thorough study of possible conformations and of the ensuing normal coordinates was carried out together with tests concerning the choice of the optimum basis set and of the most suitable exchange-correlation functional. Eventually, the vibronic structures were generated using simple home-made programs based on standard formulas [2]. All the quantum-chemical calculations were carried out on the IBM Blade Centre HS21 (Mars) and the SGI Altix 3700 (Baribal) by means of the Turbomole 5.9 package and, for the ground state, verified by parallel calculations with the Gaussian ’03 package. Also, for bithiophene we were able to compare the DFT-based results with the vibronic structures generated from the CASSCF and CASPT2 calculations.

The simulated vibronic structures obtained by means of the DFT methodology show at least semi-quantitative agreement with the experimental spectra and are clearly superior to the structures generated from *ab initio* results. Although a number of factors still require further investigation, we believe that our results already lend credit to TDDFT as a method of obtaining molecular geometries in their excited states.

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Virtual Laboratory for the Development and Execution of Collaborative Applications

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1. Introduction

The ViroLab project [1] is developing a virtual laboratory [2] for research of infectious diseases to facilitate medical knowledge discovery and provide decision support for HIV drug resistance [3].

Three groups of users have been identified: clinicians using the decision support systems for drug ranking, experiment developers who plan complex biomedical simulations, and experiment users who apply prepared experiments (scripts). The virtual laboratory integrates biomedical information related to viruses (proteins and mutations), patients (viral load) and literature (drug resistance); it enables planning and executing experiments transparently on distributed resources.

This type of research is a good example of a new approach to scientific investigations which, besides analysis of individual phenomena, integrates different, interdisciplinary sources of knowledge about a complex system to obtain an understanding of the system as a whole. This innovative way of research has recently been called system-level science [4]. The virtual laboratory we are developing in the ViroLab project is not limited to biomedical applications -- it may be useful in other areas of system-level science.

Problem-solving environments and virtual laboratories have been the subject of research and development for many years [5]. Most are built on top of workflow systems [6]. Their main drawbacks include limited expressiveness of the programming model and lack of mechanisms for integration of computing resources from grids, clusters and dedicated computers.

2. Description of problem solution

To overcome the limitations of the programming methods, we have defined an experiment plan notation based on a high-level scripting language, namely Ruby, which has a concise and clear syntax combined with a full set of control structures. These features enable the construction of experiments of various degree of complexity. An experiment plan is synonymous with a Ruby script.

For easy interfacing of different technologies, we have introduced a grid object abstraction level hierarchy [7]. Each grid object class is an abstract entity which defines the operations that can be invoked from the script. Each class may have multiple implementations, representing the same functionality. Each implementation may have multiple instances, which may run on different resources [8]. Grid objects may have different properties, such as stateless or stateful interaction mode; moreover, they may be either private or shareable between experiments and users.

The provenance approach [9] in the ViroLab virtual laboratory brings together ontology-based semantic modeling, monitoring of applications and the runtime infrastructure, and database technologies, in order to collect rich information concerning the execution of experiments, represent it in a meaningful way, and store it in a scalable repository [10].

3. Structure of the virtual Laboratory

In this section we shortly describe the main modules of the virtual laboratory [11].

The Experiment Planning Environment is an Eclipse-based development tool supporting rapid experiment plan development. Scientists may use their web browsers to access the web-based Experiment Management Interface where experiments may be loaded and executed.
The Experiment Repository stores experiment plans prepared by developers and published for scientists, and the Laboratory database holds the obtained results.
To enable high-level programming, the virtual laboratory engine, called the GridSpace, includes the Grid Operation Invoker which instantiates grid object representatives (proxies) and handles remote operation invocations.
The GridSpace Application Optimizer is responsible for optimal load balancing on computational servers.
The Data Access Service acquires data from remote databases located in research institutions and hospitals. To meet the specific requirements for exchanging confidential biomedical information within such a virtual environment, the solution introduced in DAS bases on existing Grid technologies: Globus Toolkit, OGSA-DAI, and Shibboleth. The provenance tracking, recording and publishing system enable users to find past experiments, browse archived data and track origins of certain experiment results.

4. Results

The virtual laboratory has already been used to plan and execute important virological experiments, with various types of analysis of HIV virus genotypes such as calculation of drug resistance based on virus genotype, querying historical and provenance information about experiments, a drug resistance system based on the Retrogram set of rules, data mining and classification with Weka [2], and the molecular dynamics NAMD application which has been installed on the CYFRONET EGEE site.

5. Conclusions and Future Work

The virtual laboratory provides an environment to collaboratively plan, develop and use collaborative applications; it is dedicated for multi-expertise task-oriented groups running complex computer simulations.
The most important features of the virtual laboratory are the following: mechanisms for user-friendly experiment creation and execution, possibility of reusing existing libraries, tools etc., gathering and exposing provenance information, integration of geographically-distributed data resources, access to WS, WSRF, MOCCA components and jobs, secure access to data and applications.

The laboratory is under continuous development (see [2]) and it will be extended by a module for management of results produced by experiments, and with a subsystem for handling semantic descriptions of data and computations, so that finding interesting information is made easier and the middleware is able to track the provenance of results in an application-specific way.

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Keywords

System-level science, e-Science, collaborative applications, virtual laboratory, ViroLab

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