ABSTRACTS

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The German-Russian conference "Supercomputing in Scientific and Industrial Problems" aims to bring together researchers from universities and research labs of Russia and Germany to discuss the state of the art for supercomputing in solving scientific and industrial problems. It will focus on relevant numerical methods and supercomputing technologies, on the analysis of such methods and technologies, and on supercomputer modeling of complex problems related to continuum mechanics and industrial applications.

Суперкомпьютерные вычисления в науке и промышленности, Германо- российская конференция, тезисы докладов, Вычислительный центр Штутгарта, 2017. 26 с.

Германо-российская конференция "Суперкомпьютерные вычисления в науке и промышленности" ставит своей целью объединить исследователей из университетов и исследовательских лабораторий России и Германии, чтобы обсудить использование суперкомпьютеров для решения научных и производственных задач. Тематика конференции — соответствующие численные методы и суперкомпьютерные технологии, анализ таких методов и технологий, а также суперкомпьютерное моделирование сложных задач, связанных с механикой сплошных сред и промышленным применением.

TABLE OF CONTENTS

FLOW PAST BODIES IN MUTUAL MOTION

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KEY WORDS: computational fluid dynamics, free boundary method, Cartesian grids, mesh refinement, flow past moving bodies.

The features of the flow past a pair of coaxially placed bodies in mutual motion were considered.

During the separation of the successively arranged bodies of rotation, two regimes of flow can be observed [1-3] depending on the distance between bodies. The first regime can be observed at the initial stage of separation, when the distance between bodies is less than critical. The external flow is formed in the space between the bodies with closed current as a solid continuation of the front body. With the distance increasing to critical closed separated flow between bodies collapses. Restructure of the flow occurs. After the front body a bottom current and in front of the rear body a head shockwave form. A second flow regime forms. Similar regimes emerge in the flow past a group the motionless bodies.

In the flow during separation, one can distinguish several specific stages. When the front part of retracting body is in the subsonic flow behind the front bow shock wave it has little effect on the outside flow. Then body interacts with the bow shock wave and reverse flow region is formed. For some time the two bodies with the region of the reverse flow between them are flown around by external flow as one.

Numerical simulation of moving bodies was made using free boundary method (variation on immersed boundary method) [4,5]. A Cartesian grid is used, which covers both the region of the flow and the area occupied by the solid bodies. To fulfill the boundary condition on the body surface compensatory fluxes of mass, momentum and energy are introduced. One of the major advantages of this approach is the simplicity of grid construction which does not depend on the complexity of the body geometry. Results were obtained on multilevel Cartesian grids with local adaptation. For local evaluation of the smoothness of the grid function a criteria based on wavelet decomposition on local templates is applied [6], which allows us to clearly see the location of the discontinuities and large gradients, which in turn helps in the understanding of flow physics.

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DIRECT NUMERICAL SIMULATION OF MICROFLOWS IN CORE SAMPLES WITH QUASI-HYDRODYNAMIC EQUATIONS

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KEY WORDS: digital rock physics; pore scale flow; rarefied gas; Klinkenberg effect; multicomponent flow; diffuse interface method; quasi-hydrodynamic equations.

Quasi-hydrodynamic (QHD) equations are the specific modification of the Navier-Stokes equations for viscous compressible fluid flows with additional physically based dissipative terms [1,2]. On the one hand, these terms have regularization properties and allow to construct logically simple explicit finite-difference schemes which offer advantageous opportunities for parallelization and, on the other hand, simulation results obtained with the QHD equations agree with experimental data for gas flows in microchannels and near sphere for the Knudsen numbers ~0.1 [1,2]. In the present work, the QHD approach is used as the basis for construction of numerical simulation techniques for direct description of microflows in pore space of core samples to determine their macroscopic properties.

Simulation results for one-phase isothermal fluid flow and corresponding values of absolute permeability coefficients for several core samples are presented. Results obtained with regard to slippage effect are presented as well. In the latter case, the classical Maxwell slippage boundary conditions are used. The qualitatively correct Klinkenberg slippage coefficient dependence on the coefficient of absolute permeability is noted. Simulation of displacement of one fluid by

another is illustrated for two-dimensional artificial pore space. To this end, multicomponent QHD equations which take into account surface effects are applied [3,4].

The obtained results demonstrate that numerical techniques based on the QHD approach are promising for direct numerical simulation of microflows in core samples for determination their macroscopic properties by reason of its physically motivated basis and opportunity of usage simply implementable finite-difference approximations.

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RECALCULATION TECHNIQUE FOR EXASCALE COMPUTING SYSTEMS

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KEY WORDS: High performance computing (HPC), fault tolerance, checkpointing, exascale computing, recalculation

On the way to exascale computing there are some crucial challenges [1]. An exascale resilience is probably the most challenging of them. In order to increase performance HPC systems dramatically scale up in all components and become significantly unstable. The mean time between failures may be an hour or less on exascale platforms [2]. So we have to find the way to continue computations in spite of hardware and/or software faults which might happen during calculations. The most popular solution to this problem is a rollback recovery approach using a global checkpoint restart on the system-level or the application-level. The system-level checkpoint approach is unusable for exascale computing systems [2]. As for application-level, the approach of multilevel checkpointing presented in [3] seems to be the best rollback recovery approach. It can significantly reduce the overheads caused by restoration. But its usability on

exascale computer systems is unclear yet as the overheads grow proportionally to the size of the system.

In this paper we introduce an alternative local recalculation approach for the applications based on hyperbolic systems of partial differential equations or those ones which may be hyperbolized. The approach does not generally require recovery from a global checkpoint neither use such technique as message logging, but it needs a small amount of additional processors which do not take part in calculations unless a fault occurs. This approach relies on the properties of hyperbolic systems, for which the domain of influence on the solution is localized in space. As a result, the necessary part of the solution can be rapidly recalculated on additional processors without restarting or suspending the whole calculation process. Though generally the hydrodynamic equations are not hyperbolic, in some cases parabolic systems can be transformed to a hyperbolic form by adding appropriate small terms for the second partial time derivatives in each equation. Thus we obtain a hyperbolic system with almost identical solution which allows us to use explicit numerical schemes for its calculation. Then due to the solution locality the lost part of the solution can be rapidly recalculated by adding some spare processors in calculations. We estimated the number of additional processors required for recalculation instead of one failed processor [4]. This number is rather small, it is determined by the parameters of the simulated problem and does not depend on the number of processors used for the program execution, contrary to the multilevel checkpointing approach and others.

So what are the advantages of the suggested technique? First, it ensures that the runtime of the program remains the same regardless of the faults occurred. But of course we have to monitor system failures during calculations, restore MPI after them and these activities take some additional time. And second, this technique ensures that the program execution is provided with great certainty even if repeated faults occur during the time of recalculation of lost data, if only the newly added processors are not involved in these faults until they catch up with the others.

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USING MODERN SUPERCOMPUTERS FOR SCALE-RESOLVING SIMULATION OF COMPLEX TURBULENT FLOWS ON UNSTRUCTURED MESHES

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Currently, the scale-resolving LES and hybrid RANS-LES approaches for turbulent-flow simulation are mainly used on structured meshes and, correspondingly, exploit "structured" algorithms. Using this way, it is easier to satisfy the requirements for scale-resolving approaches which are high accuracy and minimization of numerical dissipation while maintaining the stability of the numerical scheme for the approximation of convective fluxes. At the same time, the applicable scope of LES and especially hybrid RANS-LES approaches for industrial problems while using structured meshes is limited. The use of unstructured meshes can improve the workability of these scale-resolving approaches and promote their implementation in massive industrial computations.

The numerical algorithm implemented in research code NOISEtte [1] for unstructured meshes is briefly considered. It is based on the edge-based reconstruction (EBR) higher-accuracy numerical scheme [2]. Thanks to the quasi-1D property, it possesses moderate computational cost. We use the new enhanced version of hybrid RANS-LES non-zonal approach DDES [3] which accelerates RANS-to-LES transition in shear layers.

The present work is focused at the improvements recently developed to increase the algorithm's robustness for the simulation of complex compressible turbulent flows using scale-resolving approaches. They mostly consist in adjusting the numerical scheme with the varying characteristics (stencil size, amount of numerical dissipation, shock-capturing capacities) to the solution and mesh peculiarities.

Some recent supercomputer computations of industry-oriented problems are considered to demonstrate a performance of the algorithm and its improvements. In particular, the simulations of single round jets and the near-wall turbulent flow over axial-symmetric cylindrical body are considered. The comparison with the experimental data is given both for the aerodynamic and far and near field acoustic characteristics. Special aspects of effective usage of computational resources towards robust scale-resolving simulation of turbulent flows are discussed.

Supercomputers Lomonosov of MSU, MVS-10P of JSCC, K100 of KIAM, HPC4 of Kurchatov institute have been used for our calculations and performance tests. The authors thankfully acknowledge these institutions.

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HIGH PERFORMANCE SIMULATION OF SHORT-RANGE MOLECULAR DYNAMICS

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Molecular modelling and simulation has become a well established method, being applied in a wide range of areas, such as thermodynamic properties of fluids, phase equilibria, phase transitions and transport coefficients. When only short-ranged potentials are used, linear complexity algorithms can be deployed, making it feasible to investigate very large systems on high performance computers and thereby opening the range to more complex phenomena like phase transitions, adsorption, and protein folding. However, to leverage this powerful method, reliable software tools are necessary. In this presentation, two state of the art simulation codes ms2 and ls1 mardyn will be presented, focussing on their respective unique value propositions.

ANALYZING SCALABILITY OF PARALLEL ALGORITHMS BASED ON SIMULATION MODELING

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The problem of studying the properties of scalability of parallel algorithms for their implementation in future exaflops-class supercomputers reached the level of technological challenges and requires a research. Computational algorithms are generally more conservative compared with the development of computer technology. Evaluating behavior of an algorithm developed by the computational scheme can be done by their implementation in the simulation model. Such model can represent thousands or millions of CPU cores. Simulation model allows

finding bottlenecks in algorithms for understanding how to modify them to achieving efficient scaling on a large number of cores. In this work, we propose simulation modeling results for astrophysics [1], physics of plasma[2], geophysics [3] algorithms and codes that were developed by authors. All applications for simulation is launched many times on different supercomputer's (NKS-30T [4], MVS-10P[5], Lomonosov[6], Polytechnic[7]) hardware. All network delays time functions execution time and scheme of simulating application is used as initial data for simulation modeling. The output data from simulation modeling system consists of scalability prediction data. This data helped to improve our astrophysics, physics of plasma, geophysics codes. Finally, we achieved predicted scalability for our codes for up to 1 mln of CPU cores. This prediction is in a good accordance with real runs on 50K+ cores supercomputers.

Acknowledgements

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TOWARDS EXASCALE CFD WITH HIGH-ORDER METHODS AND UNSTRUCTURED MESHES

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The worldwide exascale race imposes many challenging problems related with the variety and complexity of hybrid massively-parallel computing architectures and the required extreme levels of parallelism. The present work is focused on development of highly scalable and portable parallel CFD algorithms and software implementations for time-accurate simulations of compressible turbulent flows using unstructured hybrid meshes.

The multilevel MIMD-based MPI+OpenMP parallelization of our in-house CFD/CAA research code NOISEtte is outlined, performance details are provided for up to 24K CPU cores and particular problems are discussed including the use of Intel Xeon Phi accelerators.

Then, our research work on heterogeneous computing on whatever hybrid architectures is presented. A finite-volume cell-centered parallel algorithm and its portable stream processing-based MPI+OpenMP+OpenCL implementation are described. Performance study is reported for a wide range of computing devices including various multi-core CPUs, NVIDIA and AMD GPUs, Intel Xeon Phi accelerators. Scalability is tested on different hybrid systems including a fat-node with 8 GPUs and a supercomputer with up to several hundreds of GPUs engaged.

Finally, our cooperative research on large-scale heterogeneous computing with the Heat and Mass Transfer Technological Center of UPC, Barcelona, Spain, is briefly outlined. It is focused on development of a highly-portable CFD solution for modeling of incompressible turbulent flows on unstructured hybrid meshes.

This work has been financially supported by the Russian Science Foundation, project 15-11-30039 (heterogeneous implementations) and the Russian Foundation for Basic Research, grant 15-07-04213-a (parallel mesh processing). Supercomputers Lomonosov of MSU, MVS-10P of JSCC, K100 of KIAM, HPC4 of Kurchatov institute have been used for our calculations and performance tests. The authors thankfully acknowledge these institutions.

PARALLEL METHODS AND TECHNOLOGIES IN THE LIBRARY KRYLOV FOR SOLVING SLAES

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We consider the parallel methods and technologies for solving the systems of linear algebraic equations (SLAEs) with large sparse matrices, symmetric or non-symmetric, which arise in finite difference, finite volume and finite element approximations of the multi-dimension boundary value problems on the non-structured grids. The scalable parallelism is provided by two level iterative domain decomposition approaches in the Krylov subspaces. The convergence rate is accelerated by using the parametrized overlapping of the computational grid subdomains and various interface Steklov–Poincare type conditions at the internal boundaries, as well as coarse grid correction, deflation, augmentation and low rank approximation of the original matrix. The auxiliary subsystems in subdomains are solved simultaneously by direct or preconditioned iterative algorithms. The set of the advanced approaches are implemented in the library Krylov – multi-preconditioned semi-conjugate residual methods, FGMRES, ADI algorithms in rational Krylov subspaces, as well as least square techniques including. The matrices of SLAEs can be presented in the different formats, Compressed Sparse Row, in particular. Hybrid programming techniques are applied for implementation of the algorithms on the different languages, by means

of MPI tools, Open MP, and CUDA for GPGPU. In conceptual sense, Krylov presents the integrated environment for wide class of the computational algebra problems, adapted to extension of the new tasks, algorithms and to evolution of computer platforms. The library is open for the reusing of the external codes, as well as for coordinating participation of the various development groups.

HETEROGENEOUS PARALLEL COMPUTATIONS FOR SOLVING PHYSICS PROBLEMS

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Manycore processors play an important role in modern supercomputers. The most of the supercomputers in the world are based on manycore processors such as Intel Xeon Phi, NVIDIA GPUs. Some of them did not use classical CPUs. The distinct advantages of this approach are energy efficiency and high density of computing performance, but this approach requires careful attention to many programming details. We propose the co-design technique for development of algorithms and parallel codes for massively parallel supercomputers. By the example of this technique, we present the modification of PPML method for solving astrophysical problems on Intel Xeon Phi (KNL) based supercomputers [1], a parallel direct algorithm to solve boundary value problems for 3D Helmholtz equation discretized with help of finite differences for solving geophysics problems [2]. It should be noted that we use a different kind of supercomputer nodes for the geophysical code at the same time. We use SMP node with 1TB of RAM and 80 CPU cores as well as MPP nodes of NKS-30T [3] cluster in Siberian Supercomputer Center at the same time. The geophysical code detecting SMP node and using it for data processing as one of the MPI processes with internal OpenMP parallelization, MPP nodes are used for arithmetic-intensive part of the algorithm. In astrophysical code, we use memory access reconfiguration on some Intel Xeon Phi (KNL) nodes for optimization and load balancing of arithmetic intensively part of the algorithm.

Acknowledgements

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DEPENDENCIES BETWEEN POWER CONSUMPTION AND PERFORMANCE ON HPC PLATFORMS

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A modern Petascale System consists of millions of different components, which consume a huge amount of energy. The power rating of each component depends on the type of the current instructions executed on cores, memory controllers, network units and other various components. On the other hand, the modern processors are able to switch the core frequencies during the operating, which has a great influence on the energy consumption of the processors and memory.
This talk presents a way to identify and understand the dependencies between power dissipation and performance by consideration of kernel operations. In particular, the underlying approximation approach will be presented.

HIGH-FIDELITY SIMULATION OF ROTORCRAFT AEROMECHANICS

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Over the last decades, Numerical Simulation has established as a key technology in Aeronautics. In research as well as in the development of new products, Numerical Simulation is nowadays an essential tool in engineering for the improvement of the products' safety, performance, and environmental impact, and also for the reduction of development time and costs. Moreover, for exploring new grounds, simulations are indispensable. This holds true also and in particular for the helicopter industry.

The development and deployment of simulation methods ready for industrial use is one important task of academia and research establishments. The presentation will focus on current research work performed at the University of Stuttgart that aims on the application and further development of state-of-the-art Computational Fluid Dynamics (CFD) methods for solving challenging aerodynamic problems on today's and future rotorcraft. The actual capabilities of the

CFD methods in use will be demonstrated on various exemplary topics, as e.g.: flight in ground effect, tail-shake, dynamic stall, and noise emission.

The investigation into physically complex problems like these requires the capability to simulate the complete helicopter including main and tail rotor, fuselage, empennage, and even excrescencies like e.g. skids. It also requires the consideration of the blade dynamics, i.e. the pitching, flapping and lagging motion of the blades as well as their aero-elastic deformation during their revolution, by coupling the flow solver to a structural dynamics code. Finally yet importantly,

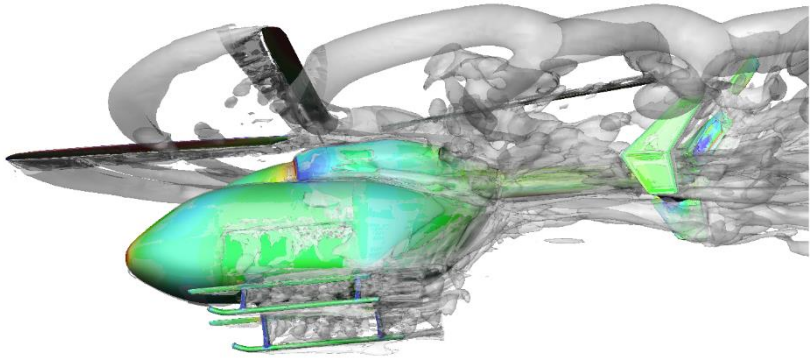

Fig.1: Flow simulation of a full helicopter

for validation of the numerical results by wind tunnel measurements and for a reliable transfer of the results to full size free flight conditions, a 3- or 6-degrees-of-freedom trim, respectively, has to be performed in order to guarantee accordant forces and moments.

Although for the time being most of the presented simulations can yet be handled only on high performance supercomputers due to grid sizes of more than 100 Mio. cells, the rapid progress in computer performance will render the tackling of these kinds of problems possible not only in academia but also in daily industry work within the next years to come.

PARTNERSHIP INITIATIVE COMPUTATIONAL SCIENCE - USING HPC EFFICIENTLY

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High performance computing is going through constant changes, from the times of the early single processor supercomputers to massively parallel machines with accelerators. One observation sticks out: The complexity is steadily increasing and despite many ideas in simplifying the programming model, using the fastest computers on the planet becomes even more challenging. As a consequence, improved models of support mechanisms need to be applied. Using the observations from the LRZ extreme scaling workshops, we present the

challenges in using HPC efficiently and provide a series of observations and ideas for improving the current situation.

NUMERICAL SIMULATION OF THREE-DIMENSIONAL PROBLEMS OF GAS DYNAMICS BY DISCONTINUOUS GALERKIN METHOD ON DIFFERENT PARALLEL ARCHITECTURES

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Design and creation of parallel software modules that implement the numerical solution of complex gas-dynamic problems and effectively work on different parallel architectures is not a trivial task, especially when used in the calculations on unstructured grids. Furthermore, this problem becomes more complicated when using high accurate numerical methods. As an example of such method the Galerkin method with discontinuous basis functions or Discontinuous Galerkin Method (DGM) [1] can be proposed, which works well for solving the problems of gas dynamics. This method for all its virtues, has a significant computational complexity, so the question of the most effective use of all the possibilities of modern computer technology is very serious. In this paper, during the creation of a computational module that implements the discontinuous Galerkin method for solving the three-dimensional Navier-Stokes equations, in order to accelerate calculations the grid-operator approach to programming is used [2-4]. This approach allows to write mathematical formulas in compact form in code and facilitates the porting of programs on parallel architectures, such as NVidia CUDA and Intel Xeon Phi. The usage of this approach allows, for example, to transfer the program to NVidia CUDA simply recompiling the source code by corresponding compiler and obtain acceleration from 4 to 9 times (for different programs) compared to the consistent version of program. In addition, the methods of template meta-programming of language C ++ are used actively to speed up the calculations [5]. The paper presents the characteristics of the effectiveness of the programs for numerical simulation of three-dimensional problems of gas dynamics using discontinuous Galerkin method on different parallel architectures.

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NUMERICAL TREATMENT OF INTERFACES

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The treatment of interfaces is still a challenge for the numerical simulation. In this talk we will consider the “volume of fluid” technique for the treatment of interfaces for arising bubbles including curvature effects and the phasefield model for the treatment of interfaces for two phase flows with phase transition. Finally we will show some recent results concerning transport on moving interfaces.

These results have been obtained together with S. Burbulla, D. Diehl, J. Gerstenberger, M. Kränkel, T. Malkmus, T. Müller, M. Nolte, C. Rohde.

EIGENMODES OF NONLINEAR SYSTEMS

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Even if eigenvalue and eigenvector decomposition seems to be restricted to linear operators at first glance, it turns out that it is also applicable to nonlinear operators by embedding these in a much larger space and analyzing the Koopman operator which let the nonlinear operator appear linear. Spectral analysis will be enabled for very general settings. We show a numerical approach, which allows to separate different parts of instationary data in a time vanishing part and a remaining part in coincidence with mathematical theory.

INVESTIGATION OF POSSIBILITY TO APPLY OPENMP FOR SPEEDING UP DYNAMICS SIMULATION FOR A MODEL OF LOW DIMENSION

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The modeling of dynamics of continuously variable car transmission is considered.

This problem is extraordinary because it requires the development of a specific physical model describing the behavior of nonlinear system composed of 3D elastic bodies interconnected with many contact interactions; it also requires the development of problem-oriented software.

Due to the specific features of the transmission structure (nonlinear system of elastic 3D bodies, many contact interactions) and its model, the authors have reasonably refused to formally use the finite element method, due to the impossibility to obtain a convergent and adequate result even on a fine finite element mesh with a large number of degrees of freedom. Therefore, a different approach to the modeling has been chosen, which has allowed to adequately describe transmission behavior using quite few degrees of freedom while taking into account all major effects under various regimes of loading. Model validation has been carried out against experiments with real transmission on a test stand.

The process of a dynamics simulation boils down to the time integration of the ordinary differential equation (ODE) system describing model behavior.

The problem has the following features:

- Problem dimension is not high (about 2000 generalized coordinates in total), so the memory requirements are low.
- Many contact interactions between model parts.
- ODE system with high frequencies about 10^8 rad/s, which is caused by the presence of low flexibility in model parts. However, the interpretation of the ODE system as a “stiff” one is doubtful.
- As a consequence, long simulation time due to the necessity to use small time step.

Simulation process consists of a sequence of steps of an explicit Runge-Kutta method. At each step, most of the time is spent on the evaluation of ODE right hand side, which in turn boils down to the calculation of generalized forces and also computation and decomposition of the inertia matrix (in some cases, the inertia matrix is non-constant due to a constraint between moving pulley and deformable shaft). Those two operations consume about 90% of total time spent for each step.

Therefore, to speed up dynamics simulation, it is desirable to parallelize the evaluation of generalized forces and the inertia matrix. Since memory requirements are low, but there are frequently alternating parallel (generalized forces) and sequential (state vector) sections, the

natural choice for the parallelization technology is one considering the parallelization within a single process, e.g., OpenMP.

The results of sequential code profiling indicate that about 60% of ODE right hand side calculation time is spent on the internal forces in the transmission chain, and about 12% — on the forces of contact interaction between the chain and the pulleys. Therefore, the code computing these forces should be parallelized first. Currently the code computing transmission chain internal forces is parallelized using OpenMP. The structure of the chain gives the clue to the choice of structural unit passed to an OpenMP thread: such a unit is either a pin or a link of the chain. The choice between the two options is dictated by the force component being computed, so both of them are actually used in our implementation.

Simulations with a chain consisting of 84 links have shown satisfactory scalability when the number of OpenMP processes does not exceed 6, which can be seen from the table below (in each column, the first row is the number of OpenMP threads, the second row is the value of acceleration relative to the sequential version). Further growth of the number of OpenMP threads leads to saturation, and the acceleration remains close to 6.

Thread count	1	2	3	4	5	6	7	8	9	10	11	12
Acceleration	1	1.91	2.85	3.72	4.50	5.28	5.81	6.05	6.32	6.66	6.86	6.78

Notice that the simulations were run on a node containing two Intel Xeon CPUs, each having 6 cores and supported the Hyperthreading technology.

Further directions of our work are as follows: the improvement of scalability of parallel calculation of transmission chain forces and overcoming the saturation effect, as well as the parallelization of pin-pulley contact force evaluation.

Apart from that is the problem of parallel evaluation and decomposition of the inertia matrix. This procedure takes about 16% of total step time, which is second after chain forces. First thing to do here is to take the block-diagonal structure of the inertia into account, as well as the fact that only a small number of blocks actually vary in time.

MULTISCALE MULTILEVEL APPROACH TO SIMULATION OF GASDYNAMIC PROCESSES IN MICROSYSTEMS

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The present work is devoted to multiscale multilevel modeling of nonlinear gasdynamic processes in technical systems of micron sizes. This problem is relevant for many applications related to the implementation and the use of nanotechnology in various industries [1]. As an

example the calculation of a binary gas mixture flow in channel with metal walls is considered. The multiscale multilevel approach is based on combining the calculations of gasdynamic processes at the macrolevel and at the micro- and the nanolevels. Macrolevel is determined by the quasigasdynamic equations [2], micro- and nanolevels – by molecular dynamics [3]. Such mathematical model allows describing the gas flow accurately. It works on the rules of splitting on physical processes. The presented approach can be used in two ways [4]: 1) to apply calculations at macro- and microlevels alternately at each time step; 2) to create a database of necessary system properties by means of MD calculations and further make all calculations using this base or completely, or partially instead of molecular computing. The both ways are applied in this work. The results confirm the efficiency of the developed algorithms and the possibility of its use to optimize the parameters of gas flows in technical microsystems. Also they show that the numerical algorithm is suitable for the analysis of physical processes in microinstallations and its parallel implementation is productive in the calculations on clusters and supercomputers with hybrid architecture. Calculations of the flow are in agreement with the results of experiments.

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EDUCATION AND TRAINING IN HPC

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HPC poses ever new challenges and it is hard to keep up with them. At the same time simulation becomes part of many disciplines and is based on a variety of technologies that include among others HPC. In this talk we will discuss the needs for training and education in HPC and propose a concept for such training and education.

VIRTUALISATION AND HPC

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HPC in the framework of the Baden-Württemberg state initiative bwHPC is meeting new challenges. User groups have successfully set up their own computing environments which they want to move onto HPC systems. Modern research data management requires archiving of run time environment, as operating system updates or new versions of mathematical libraries may influence the computation of research data. At Freiburg University we currently evaluate how HPC systems can provide virtual environments to address these needs and whether the inevitable performance loss is acceptable. Our first experiences are presented in talk.

TOWARDS A SYSTEM TO ASSESS BIOMECHANICAL DEVICES IN VIRTUAL CLINICAL TRIALS

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The development as well as the application of biomechanical implants like total hip endoprostheses in orthopaedic surgery or stent grafts in vascular surgery is down to the present day based on empirical procedures. Even though this leads to durable implants, complications arise in a non-negligible number of cases c.f. e.g. [1].

During the past years there has been significant effort from various groups all around the world to develop numerical simulation methods towards a stage where it can be beneficial as a clinical decision support method as well as in biomechanical device development to improve device performance and reduce complication rates. Even though biomechanical simulation methods have been lifted to a quite mature state, a problem that persists in their application is the deterministic character of numerical results, which foils the natural variance of biological systems.To overcome this problem, in this talk we propose the implementation of a system that will allow the assessment of biomechanical devices in virtual clinical trials. The system will use numerical tools to combine patient-specific information measured before the operation and during rehabilitation with information from a central, dynamically growing case database. The feedback of information from many patients at different stages of treatment into the central database will lead to a ‘self-learning’ system that will enhance over time and will be able to account for future developments and problems by the application of recent methods from the field of data-analytics. Further on we will focus on the detailed discussion of our estimated HPC resource requirements necessary for the implementation and efficient execution of the system.

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FORTISSIMO: BRINGING INDUSTRY AND HPC INFRASTRUCTURE PROVIDERS TOGETHER

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With the advent of computer aided engineering and the constantly growing demand for accurate and cost-effective simulations, the access to high performance computing resources and technology consulting for academia, small and medium sized companies as well as industries is mandatory and represents the key to success in the evolving market. Within the FORTISSIMO project, advanced simulation for small and medium sized companies has been targeted, realizing a “one-stop-shop” in order to enable state-o-the-art hardware access, expertise, applications, visualization and tools in an efficient fashion.

FORTISSIMO 2 takes the key findings of its predecessor and enhances it with Big Data Analytics and coupled high performance computing simulations by having a clear focus on the adoption of next generation information and communications technology for the manufacturing domain. As a result, an enhanced one-stop-shop will be developed and operated, following the business requirements of the manufacturing industries to drive the uptake of advanced modelling, simulation and data analytics for improved design processes, better products as well as services and improved competitiveness.

As its predecessor, FORTISSIMO 2 is be driven by clear and sound end-user requirements, which are being brought into the project by Open Calls in order to solve real-world customer problems. Thus, FORTISSIMO 2 not only strengthens the market shares and opportunities of the participating parties, but also contributes to the competitiveness of the European manufacturing industry through its innovative infrastructure built around the FORTISSIMO 2 Marketplace, the “one-stop-shop” for the European manufacturing domain.

FORECASTING MODELLING STORM ELEVATION IN THE AZOV SEA BY MEANS OF EXPLICIT REGUARIZED SCHEMES ON MULTIPROCESSOR SYSTEM

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The main subject of this work is to present the experience of modelling extreme storm elevation in Taganrog bay of the Azov Sea, September 24-25, 2014, when the velocity of wind was more than 40 m/s during 30 hours on multiprocessor system. Under this huge wind the elevation of free surface water was more than 420cm. It is important to predict such natural accidences in accelerated time scale – in several decades of minutes or less. This important problem leads to the solution of two tasks. One of them is constructing conservative and numerically stable discrete model for extreme values of wind tension; the second one is the task of building highly effective algorithms for parallel computing. First task has been decided on the basis of three dimensional hydrodynamics models, using three momentum equations and special splitting method in physical processes (variant of pressure correction method), which has been developed authors for coastal sea systems. The problem of parallel realization of discrete models has been decided in two manners. First of all we have used implicit difference schemes and parallel variant of improved SSOR method for grid equations with non-selfadjoint operator, which has been constructed earlier author team. The acceleration on HPC of Southern Federal University in Taganrog was in comparison of sequential algorithm near the 50 times (on Hewlett multiprocessor system with 2048 processor units -PU), when the total number of used PU was 128. Further increasing of this number was non-effective for implicit schemes. Total modelling time was more than 10 hours. The second approach to construct effective parallel algorithm has been based on explicit difference schemes, which have been built by involving of second order time difference member with small multiplier (method of B. Chetverushkin) in momentum equations. It allowed to accelerate total time decision in comparison of firs approach more than 10 times and to obtain total modelling results for grid of 501x501x101 nodes; total modelling time was near the 1 hour.

PROBLEMS OF PARALLEL SIMULATION TECHNOLOGY

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The parallel simulation technology (ParSimTech) is a research direction of the scientific cooperation between the experts from the area of informatics and simulation technology from the University of Stuttgart, Ulm University and Donetsk National Technical University (Pokrovsk). The main research focus of ParSimTech is investigation and development of new parallel numerical methods, the theoretical analysis of virtual parallel simulation models and their devirtualization. Also development of the powerful and user friendly simulation environments

with an efficient use of the parallel hardware and software resources plays a significant role here. The developed simulation tools allow to solve numerically the complex models of the dynamic systems with concentrated and distributed parameters. As an example processes which are used here are models of mine ventilation systems which are simulated in corresponding problem-oriented distributed parallel simulation environments (DPSE).

NUMERICAL STUDY OF NONLINEAR ABSORPTION OF ALFVEN WAVES BY DISSIPATIVE PLASMA

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In the work, we study numerically the nonlinear absorption of a plane Alfven wave falling on the stationary boundary of dissipative plasma. The factors caused the absorption are the hydrodynamic viscosity, magnetic viscosity and thermal conductivity of electrons and ions, energy exchange between plasma components and bremsstrahlung. The relevance of this investigation is due to some works [1], regarding the heating mechanism of the solar corona and solar wind generation as a result of the absorption of plasma Alfven waves generated in the lower significantly colder layers of the Sun. Numerical analysis shows that the absorption of Alfven waves occurs at wavelengths of the order of skin depth, in which case the classical MHD equations are inapplicable. Therefore, our research is based on equations of two-fluid magnetohydrodynamics that take into account the inertia of the electrons. The implicit difference scheme proposed in the work for calculating plane-parallel flows of two-fluid plasma reveals a number of important patterns of absorption and thus allows us to study the dependence of the absorption on the Alfven wave frequency and the electron thermal conductivity and viscosity, as well as to evaluate the depth and the velocity of plasma heating during the penetration of Alfven waves interacting with dissipative plasma.

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NUMERICAL MODELLING OF RAREFIED GAS FLOWS USING MULTI/MANY-CORE ARCHITECTURES

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Development of numerical methods to solve the Boltzmann kinetic equation with exact or model collision integrals is an important scientific problem. However, the large dimension of the equation requires adaptation of the numerical schemes for massively parallel computers. Over the recent years the author has been developing numerical methods to solve S-model kinetic equation [1] for three-dimensional flows [2,3]. These methods are implemented in the software package “Nesvetay-3D”. Distinguishing features of the methods as compared to other known approaches include the support of both block-structured and hybrid unstructured spatial meshes, use of efficient implicit time evolution method and two-level MPI+OpenMP parallel implementation for modern parallel computers.

The present work is devoted to the discussion of the approaches to solve kinetic equations on computers with large number of cores / hyperthreads per cluster node (up to 244), as implemented in our software. Examples are provided for computing external flows over realistic three-dimensional geometries using up to 61440 hyper threads on the RSK PetaStream computers [4], installed in Joint Supercomputer Center of RAS and Saint-Petersburg Polytechnic University named after Peter the Great.

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INMOST: INTEGRATED NUMERICAL MODELLING AND OBJECT-ORIENTED SUPERCOMPUTING TECHNOLOGIES

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INMOST is a tool for supercomputer simulations characterized by maximum generality of supported computational meshes, distributed data structure flexibility and cost-effectiveness, as well as crossplatform portability. The library is licensed under Modified BSD License (no restrictions of use). The project webpage www.inmost.org provides source archives, installation user's guides, online documentation etc. The principal developer of INMOST is the former PhD student of INM RAS Kirill Terekhov (Stanford University). Igor Konshin, Kirill Nikitin, Alexander Danilov, Ivan Kapyrin, Dmitry Bagaev (INM RAS) took part in the development of INMOST and INMOST-based applications. INMOST was devised to accelerate development of parallel software for supercomputer simulations. One can develop parallel mesh generators, parallel libraries for FD, FEM or FV discretizations, parallel solvers.

-INMOST is the basis of our in-house parallel reservoir simulator and parallel software for modeling geofiltration and geomigration http://proryv2020.ru/kod-gera/.

-INMOST library supports unstructured grids with uniform and mixed topology with arbitrary polyhedral elements

-INMOST library provides internal linear system solvers and supports third party solvers
-INMOST library provides internal mesh partitioners and supports third party partitioners
The lecture gives brief numerical motivation and introduction to the library, reviews its attractive features and presents two applications.