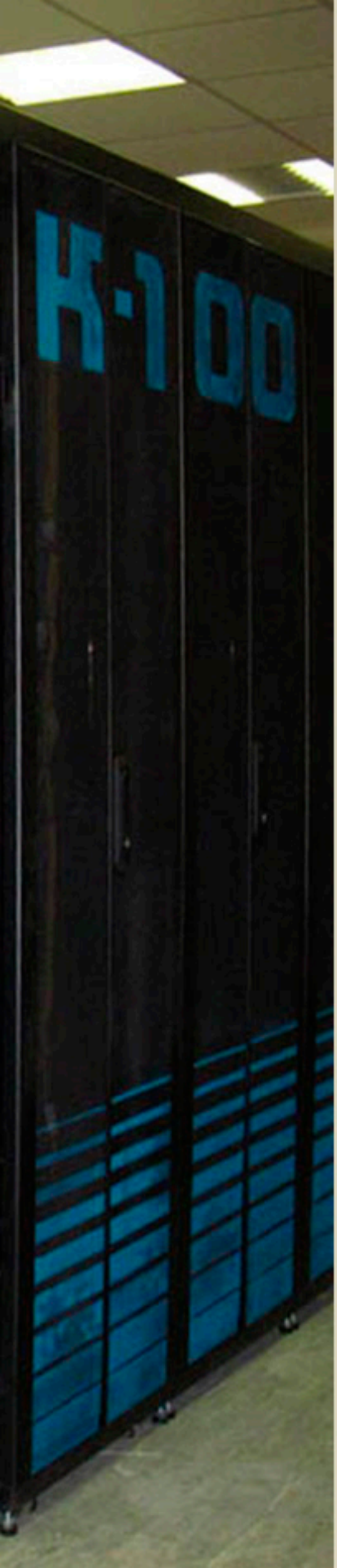

SUPERCOMPUTING IN SCIENTIFIC AND INDUSTRIAL PROBLEMS

9-11.03.2016, Moscow

Abstracts

ABSTRACTS

GERMAN-RUSSIAN CONFERENCE "SUPERCOMPUTING IN SCIENTIFIC AND INDUSTRIAL PROBLEMS"

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Supercomputing in Scientific and Industrial Problems. German-Russian Conference: Abstracts. — M.: ИПМ им. М.В. Келдыша. 2016. 32 p.

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. — М.: ИПМ им. М.В. Келдыша. 2016. 32 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.

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SUPERCOMPUTING TECHNOLOGIES FOR CFD AND CAA SIMULATIONS ON UNSTRUCTURED MESHES

I. Abalakin, P. Bakhvalov, V. Bobkov, A. Duben, A. Gorobets, T. Kozubskaya, N. Zhdanova
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The work is devoted to the development of supercomputing technologies based on the original higher-accuracy schemes [1] based on quasi-1D reconstruction of variables on unstructured hybrid meshes for computational fluid dynamics and aeroacoustics problems. The schemes have been developed both in vertex-centered and cell-centered formulations. On arbitrary meshes they provide higher accuracy in terms of error values in comparison with most 2^{nd}-order schemes and are significantly cheaper than most very high-order schemes. On grid-like (translationally-symmetric) meshes their accuracy grows up to the 5^{th}-6^{th} order.

The corresponding parallel computing algorithms and implementations in the in-house code NOISEtte [2] for large-scale simulations of turbulent compressible flows are presented in detail. Two-level MPI+OpenMP parallelization capable of running thousands of MPI processes with hundreds of OpenMP threads each allows engaging tens of thousands of CPU cores and using hybrid supercomputers with Intel Xeon Phi accelerators.

On a base of the quasi-1D approach various numerical techniques have been developed and implemented, including higher-accuracy sliding mesh interfaces, immersed boundary methods, turbulence modeling approaches RANS (SA, KE, KO, SST), LES (Smagorinsky, S3PQ, S3QR, S3PR [3], WALE, Sigma, Vreman, Verstappen), and hybrid approaches DES, DDES, IDDES, PANS and a new subgrid-scale calculation approach [4] variant for vertex-centered schemes.

Finally, a set of recent supercomputer simulations performed with the developed numerical methods and software is presented. It includes turbulent flows around various backward-facing step and cavity configurations, turbulent jets, simulations of helicopter main and tail rotors, flow deflectors.

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Multilevel Wavelet Based Non-uniform Cartesian Grids Adaptation in CFD

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Algorithm for the wavelet based multilevel non-uniform mesh refinement will be discussed. For solution smoothness evaluation we use sliding window method with the patterns of different size and shape. To capture areas where the high resolution is required we use wavelet decomposition of grid functions on these local patterns. Calculations of several test (2D) and supersonic flows about cavity and blunted body (3D) will be given presented.

Acknowledgements
The work is supported by the Russian Science Foundation grant No 14-11-00872.

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3. *Афендиков А.Л., Луцкий А.Е., Меньшов И.С., Меркулов К.Д., Пленкин А.В., Ханхасаева Я.В. Алгоритм динамической локальной адаптации сеток на основе вейвлет-анализа с использованием метода свободной границы Препринт ИПМ им.М.В.Келдыша № 94, 20 с., ISSN 2071-2898, 2015 http://library.keldysh.ru/preprint.asp?id=2015-94*

MONOTONE BICOMPACT HIGH RESOLUTION SCHEMES FOR SOLVING LINEAR MULTIDIMENSIONAL TRANSPORT EQUATION

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Processes of radiation and particle propagation are described by a linear transport equation. This equation is integral-differential one with respect to

distribution function in phase space, so condition of positivity of numerical solution is important for robust calculation of integral at the right hand side of the equation.

A new class of difference schemes for a transport equation solving has been suggested. These schemes have fourth order of approximation in space variables and arbitrary order in time. A space stencil is minimal and consists of two nodes in each space direction, so the schemes are called *bicompact*. This approximation is possible due to the expansion of the list of the required quantities and the inclusion of integral averages of desired function on edges, faces and volume for the each space cell along with the nodal values. Semi discrete equations of bicompact scheme for basic and additional unknowns are derived by the method of lines. For this purpose, the original transport equation and some its differential consequences are integrated over spatial cell. To calculate some integrals which occur in this procedure the Euler–Maclaurin formula is applied. The third or fifth order approximation single diagonally implicit Runge–Kutta method is applied for solving the evolutionary ODEs derived by the method of lines. At every time step, the difference equations of the bicompact scheme might be resolved by a marching method with respect to any space variable. A hybrid monotone scheme on the basis of the high resolution bicompact scheme and a scheme of first order approximation in time with minimal dissipation has been suggested.

The radiation and particle propagation processes can be considered as stationary ones in a lot of applications. Numerical solving of this problem by means of unsteady difference schemes leads to unreasonable waste of calculation resources. The steady bicompact scheme of fourth order of approximation for solving the steady multidimensional problems has been constructed. In accordance with Godunov's theorem it is not monotonic. At present paper a hybrid monotone scheme is proposed on the basis of the first order short characteristic method and the bicompact scheme. Under condition of absorption absence the first order short characteristic method is reduced to analogue of well known upwind first order schemes for steady problems. It is shown that these schemes have the minimal dissipation among all monotone schemes constructed at minimal space stencil. Offered variant of a hybrid scheme preserves high order of convergence of the numerical solution in regions where it is smooth and its positivity at all calculation region including zones with high gradient of the solution.

Effective parallel algorithm had been implemented to solve the transport equation by using the high accuracy bicompact schemes.

FAULT TOLERANT ALGORITHM FOR HPC

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Fault-tolerance is one of the problems which appear on the road to exascale computing. We consider ULFM (User Level Failure Mitigation) a perspective tool for solving fault-tolerant challenge. ULFM is a set of Message Passing interface extensions enabling Message Passing programs to restore MPI and handle faults on user level. We develop a fault-tolerant algorithm for simulation of interaction between gas mixture and metal surface based on molecular dynamics techniques. For this algorithm we propose a resiliency scheme which is based on checkpointing in the memory of computing nodes and implements hybrid method of checkpointing both in operative memory and in the distributed file system. For fault simulations we developed special library which realize some of the ULFM functions (designed for upcoming MPI 4.0) in current MPI standard 3.1. This library allows us to simulate faults on computer system which works without faults.

We tested different checkpointing methods on a model problem of simulation of 1D steady-state heat-equation. The experiments show that checkpointing in operative memory can reduce overhead to 40% compared to hybrid checkpointing.

Also we consider multilevel checkpointing by using two types of faults for our resiliency scheme: light faults and heavy faults. Light faults require only local data for application recovery. Heavy faults assume that some MPI process will need for the recovery some part of consistent global checkpoint that is not saved in the memory of corresponding local storage device. We estimate that if the average time between faults is less than an hour then the computation time can be reduced by more than 10% by using multilevel checkpointing tools which can handle light and heavy faults.

Acknowledgements
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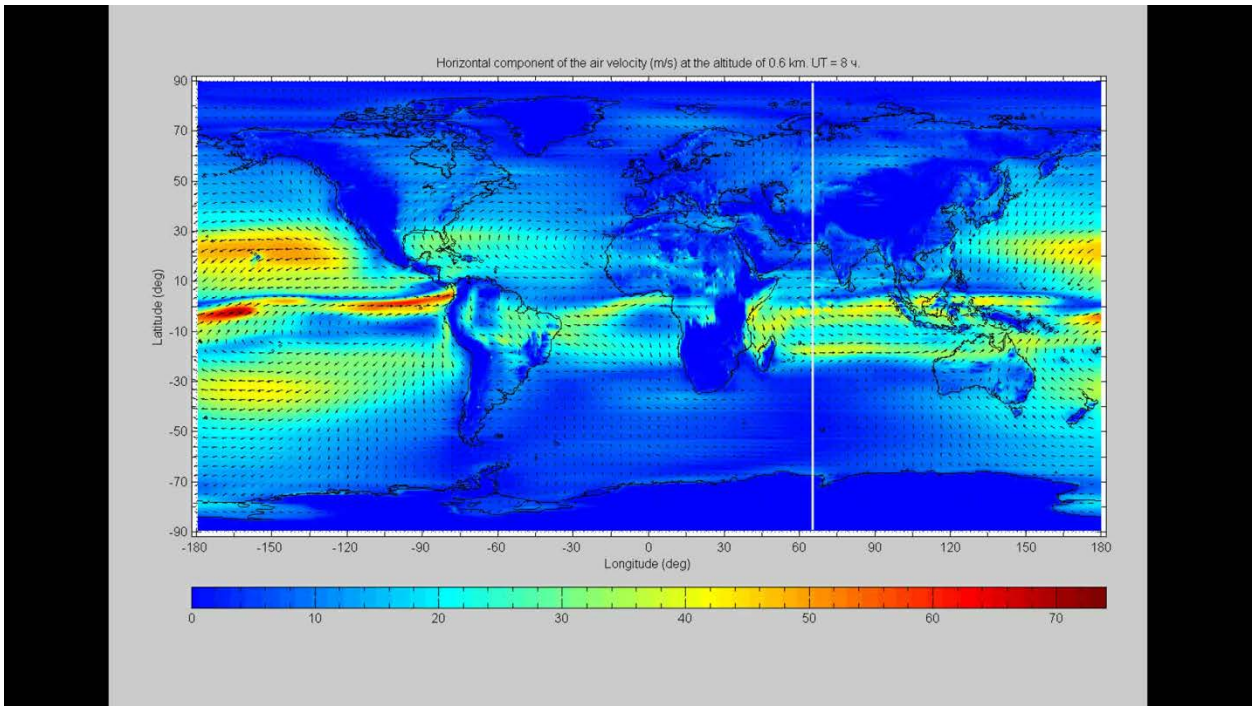
A simulation study of the formation of polar lows and tropical cyclones

V.M. Chechetkin, I.V. Mingalev

The model takes into account heating/cooling of the air due to absorption/emission of infrared radiation, as well as due to micro drops of water and ice particles, which play an important role.

The finite-difference method and explicit scheme are applied for solving the system of governing equations. The calculated parameters are determined on a uniform grid. The latitude step and longitude step are equal to 0.04 and height is equal to 200 m. For detail description of Earth atmosphere we need to use the grid, which contains about 10^8 cells.

We are obtained the picture of kinetically atmosphere of Earth



The distribution of horizontal wind (m/s) at the altitude of 600 m after the beginning of calculations.

Dynamic Approach to Scheduling Scientific Workflows in Heterogeneous HPC Environments

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High Performance Computing infrastructures are getting increasingly heterogeneous, which offers opportunities to the applications in terms of performance improvement. However, the “hardware-concise” heterogeneous resource allocation requires a deep knowledge of the scheduled applications’ characteristics. The challenge is getting more difficult if the scheduler has to balance the optimization policies between the application- and the infrastructure-specific properties, e.g. the overall energy consumption, resource utilization, etc. We introduce a heuristic-based approach to adaptive scheduling, enabled by in-depths monitoring technologies. Our solution has been applied on top of the native schedulers like Torque or Maui but is open per design and thus can be seamlessly integrated into the core scheduling algorithms.

Simulation of magnetogasdynamics problems on exascale computer systems

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MHD model is very important for simulation of many interesting problems such as: astrophysics, physics of high energy density matter, controlled thermonuclear synthesis, etc.

For their numerical realization they need massive HPC systems up to exascale performance.

Let us consider one important MHD problem which arise while using systems with performance more than 100 TFLOPS.

Problem has fundamental character. We need logically simple but effective algorithms. However logical simplicity of an algorithm is not equivalent to its efficiency.

For MHD model this problem can be solved by means of introducing complex local maxwellian distribution function

$$f_m = \frac{\rho}{(2\pi RT)^{3/2}} exp \frac{-\left(\xi_k - u_k - i\frac{B_k}{\sqrt{4\pi\rho}}\right)^2}{2RT}$$

here ρ is density, T is temperature, u is mean velocity, ξ is velocity variable, B is stress of magnetic field.

Using the Boltzman equation and the distribution function in the form of f_m one can obtain an ideal MHD system as well as MHD system including dissipative effects.

This gives the opportunity for construction of algorithm which can be easily adapted to HPC architectures with extramassive parallelism.

Here we demonstrate the result of numerical simulation related to 3D MHD problems solved with use of computational meshes including more than 10^9 vertices.

Acknowledgements

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SOME APPLICATIONS OF THE LOCAL ADAPTIVE MESHES.

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Implementation of algorithms for solving problems of gas dynamics for parallel computing systems has some difficulties. In order to improve the accuracy of calculation a detailed grid is required and, as a result, calculations can proceed for a very long time. Cartesian grids are ideal for algorithms that are adapted for use with the GPU but in order to obtain a good result often require the use of meshes of such a large size that the computational experiments can take a very long time. Therefore it is expedient to use local adaptive meshes. Indicator for the cell to be divided is based on wavelet analysis.

An approach for storage and processing of three-dimensional local adaptive meshes will be considered. Grid data is proposed to be retained in the form of associative arrays. Separate arrays for cells and faces in three directions are used. Thus at any given time mesh is an unstructured face-based grid with cube elements.

Some ways of parallelization of algorithms for local adaptive meshes, based on slicing of base mesh will be discussed. Namely, let us consider the basic grid as a set of cross sections (slices) for one, two or three directions. Since the base mesh topology is a cube, it is quite easy to do. Each processor handles several such slices, sharing boundary information via MPI. Some examples of 3D calculations

will be presented. For example, the flow around cylinder with a square cross section and in a rectangular cavity.

Also some 2D examples will be presented. The influence of a narrow wake with the reduced Mach number and total pressure values on the flow about blunt body has been investigated with the use of local adaptive mesh based on wavelet analysis. Two variants of the wake formation have been considered: after the energy source and small moving body ahead of the cone. The free boundary method was used for the flow simulation about moving bodies. The dynamics of the bow shock interaction with the small body and the reverse flow region formation have been studied. For the regimes considered it has been shown that the wake before the body results in a significant reduction of wave resistance.

Acknowledgements

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Supercomputer modeling of space radiation effect on satellites

Berezin A.V., Volkov Yu.A., Gasilov V.A., Zhukovsky M.E., Markov M.B., Tarakanov I.A.

The investigation of space radiation effect on satellites is an actual technical problem. Electrons, heavy charged particles and photons of cosmic space can destroy satellite protective coats, cause electrical pickups in radio equipment and failures of microelectronic devices. Experimental research of these effects is a very complex, expensive and frequently unsolvable problem.

Let us consider the satellite in operation as a complex media, which scatters space radiation. Satellite is made up of complex composite materials and is surrounded by ionized atmosphere. Thrusters operation and skin evaporation create

this atmosphere. Communication and control equipment generates electromagnetic field in the satellite and in its vicinity.

Specialists of Keldysh Institute of Applied Mathematics design software package for modeling the interaction of charged particles and photons with complex technical objects in real operating conditions. Package includes computation modules with unified data exchange protocol and user interface.

Classic transport equations model the scattering of free particles in materials of satel-lite. Corresponding module uses Monte-Carlo method for this equation numerical solving. Direct modeling of charged particle scattering is used. It allows considering low scale effects, when charge particle free path is comparable with material heterogeneity. Classic kinetic equations with scattering and field effects describe the radiation propagation in gas and vacuum. Maxwell equations model the field. Computation modules are united in program script with KIAM's program code MARPLE-3D. It models effects of radiation gas dynamics. Script allows taking into account materials dynamics under radiation influence.

Recently we designed new computational module for calculating radiation conductivity in active areas of microelectronic devices. External free particles create excess charge carriers – electrons of conductivity and holes of valence band. They cause radiation conductivity, modeling by quantum kinetic equations. The energy loss of free particles in active area determine source of electrons and holes. Collision's integral in quantum equations describes charge carriers scattering on phonons and impurities. The statistic particle method is carried out for quantum and classic kinetic equations numerical solving. This method combines stochastic modeling of carrier scattering and particles motion in electromagnetic field equations solving between collisions.

Software package is oriented toward supercomputer with heterogeneous architecture. This package can be used on supercomputer K-100 as united program and as separate modules. In the first case imbalance of computing resources is observed. Module with Monte-Carlo method is the slowest part of package. Graphic accelerators effectively eliminate this imbalance.

SUPPORT OPERATORS METHOD FOR FLUID DYNAMICS 3D SIMULATIONS

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A predictive simulation in CFD area is supported mainly by finite difference or finite volume methods, which satisfy common conditions: conservativity, monotonicity, numerical stability, high resolution. The theory of difference approximations explains how to construct difference approximations possessing such properties of original differential operators as positivness/nonpositiveness, self-adjointness, etc. The support operators method (SOM) is a versatile tool for

building difference schemes which retain listed above properties when using general irregular meshes [1]. A remarkable property of SOM is that the resulted schemes are rotationally invariant if this invariance is inherent to the governing system of differential equations [2]. Rotational invariance is very important in modeling of deformation and dissipation processes in gas or liquid media.

Presented work deals with implementation of SOM via 3D irregular meshes for the 3D simulations of thermo-hydrodynamics processes. The appropriate numerical algorithms are incorporated into the scientific object-oriented, parallel CFD code MARPLE3D (Keldysh Institute of Applied Mathematics - KIAM), designed for scientific simulations at systems performing distributed computations [3]. The correspondent mathematical model, that describes the system of mass-energy balances of fluid dynamics in the porous media, containing gas-hydrates, is presented. The basic dissipative “hydrate” equation, that defines thermodynamics evolution of the parameters of the system, is obtained. Numerical examples show a high quality of SOM-based simulations related to recovery processes in underground collectors with gas-hydrate depositions.

Acknowledgements
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DNS of the incompressible fluid flows

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Many phenomena in the nature may be considered in the frame of the incompressible fluid flows. Such flows are described by the Navier-Stokes equations. As usually we have deal with the flows with large gradients of hydrodynamic parameters (flows with free surface, stratified fluid flows, separated flows, etc.). For direct numerical simulation of such flows finite difference schemes should possess by the following properties: high order of accuracy, minimum scheme viscosity and dispersion and monotonisity. The Splitting on the physical factors Method for Incompressible Fluid flows (SMIF) with hybrid explicit finite difference scheme (second-order accuracy in space, minimum scheme viscosity and dispersion, ca

pable for work in wide range of Reynolds and Froude numbers and monotonous) based on Modified Central Difference Scheme (MCDS) and Modified Upwind Dif ference Scheme (MUDS) with special switch condition depending on the velocit y sign and the signs of the first and second differences of transferred functions ha s been developed and successfully applied [1]. The Poisson equation for the press ure has been solved by the Preconditioned Conjugate Gradients Method. The parall elization of the algorithm has been made and successfully applied on the massive parallel computers with a distributed memory.

The numerical method SMIF has been successfully applied for solving of the differ ent problems: 3D separated homogeneous and stratified fluid flows around a sphe re and a circular cylinder including transitional regimes [2-4]; the flows with free surface including regimes with broken surface wave [1]; the air, heat and mass t ransfer in the clean rooms. Some examples will be demonstrated.

This work has been partly supported by Russian Foundation for Basic Research (grants No. 14-01-00428, 15-51-50023), by the programs of the Presidium of RAS No.1.5П, 1.32П and by the program of the Department of Mathematical Sciences of RAS.

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SIMULATION ON HPC-CLOUDS

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This presentation will show approaches which make best use of the complementarity of High Performance Computing and Clouds both, in terms of a paradigm exchange and interaction of technologies. HPC access mechanisms for simulations will be presented together with examples of successful provisioning of Simulation as a Service over a dedicated marketplace. This is work of the ongoing EC FORTISSIMO project.

In addition to that, technological work in progress will be presented, which aims to overcome the performance losses for I/O when virtualizing systems by working on improved

Energy Efficient Environmental Computing on SuperMUC

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Among the many applications of the world-class high-performance computing system SuperMUC hosted at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich, environmental computing has some special interest. This talks describes the environmental computing initiative at LRZ, which intends to support users in the field of environmental research with high performance computing power. In total, SuperMUC phase 1 and 2 provide more than 230.000 compute cores and a theoretical peak performance of more than 6 Petaflop/s. Developing applications for SuperMUC is a non-trivial task for users, as both, scalability as well as energy efficiency need to be taken into consideration. Results from a series of extreme scaling workshops at LRZ show how users utilize large numbers of cores for their applications while operating in the innovative cooling environment of LRZ.

ANISOTROPIC SOLUTION ADAPTIVE GRIDS FOR SUPERSONIC FLOW CALCULATIONS

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The framework of high resolution gridding technology for automatic unstructured grid generation and viscous flow adaptation presented in [1] is applied to supersonic flow calculations. The goal is to iteratively resolve strongly anisotropic solution features adjusting grid cell aspect ratio and the stretching direction to follow the numerical solution anisotropy at every point in space including boundary layers and shocks. The use of adaptive grid for supersonic viscous flows calculations with a complex system of shocks enhances the solution accuracy and reduces the needed mesh size. Hessian based metric is employed to describe optimal grid cell size and stretching direction distribution in space based on numerical solution and some regularization is needed.

In the proposed approach a combination of the regularization of the Hessian metric and the grid elements in real space is used. The concept of macro-grid introduced in [2] is a practical implementation of such an approach at the expense of deviation from the strict grid optimality but with a possibility to directly control the grid quality and optimize boundary conforming grid. An initial grid is needed to begin the adaptation procedure. Usually a coarse isotropic grid is enough for

that. The combination of stretched and isotropic grid cells in the course of the adaptive grid generation is then obtained by subsequent refinement/de-refinement operations on the macro-grid.

Parallel CFD solvers from the open source OpenFoam toolbox are employed for calculations of steady-state 2D supersonic flows in a channel with a wedge. The results of the computations on the Keldysh Institute cluster K-100 are compared to the experimental data with Mach number M=2.7 at the channel entrance. Different turbulence models and wall functions in the boundary layers are explored. Preliminary results on adaptive grids are cross checked versus the calculations on large regular grids. The adaptive grid quality deterioration leads to slower solver convergence but does not result in significant solution accuracy deterioration. The solver/grid generator compatibility and 3D extensions as well as possibility of multiple steady-state solutions are discussed.

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A CARTESIAN GRID METHOD FOR COMPRESSIBLE AERODYNAMICS

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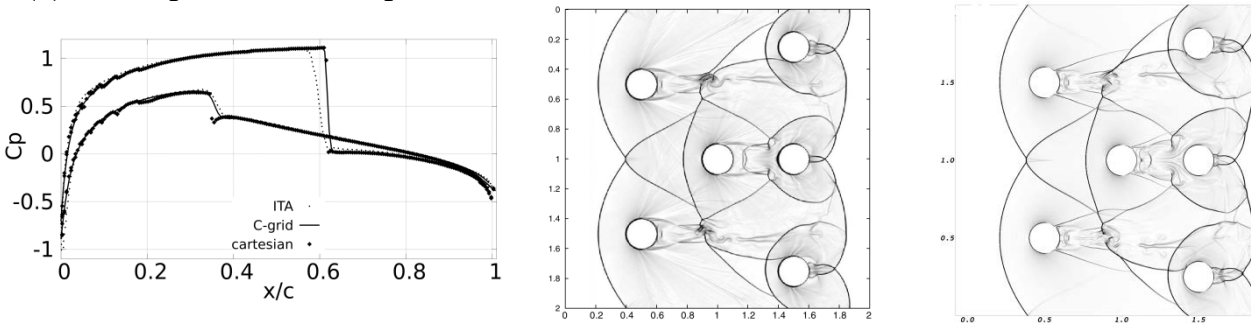
We propose a Cartesian-grid numerical method that allows one to perform calculations of gas dynamics equations in complex geometry domains by using simple geometry non-fitted Cartesian grids. This approach possesses an important feature of algorithm homogeneity (computational primitivism) which makes it quite suitable for massive parallel architectures (e.g., multi-GPU computer systems). The method steams from an alternative mathematical formulation of the boundary value problem where boundary conditions are modeled by a so-called compensation flux – a surface-defined function introduced in the right-hand side of the governing equations. It is shown that the compensation flux can be chosen in such a way so that the solution to the modified equations in the whole space projected onto the problem domain coincides with the solution to the initial boundary value problem [1]. The numerical method for solving the modified equations is hybrid explicit-implicit [2] based on the Godunov approach. The system of discrete equations is solved with the LU-SGS approximate factorization method. We also describe an effective multi-GPU two-levels parallel realization

based on executing staggered (chess-type) counting loops. Fig. 1(a) illustrates comparison between numerical solutions for the NACA0012 airfoil flow obtained with a body fitted structured grid and a Cartesian grid, respectively; figs. 1(b) and 1(c) - comparison of the presented method with an alternative one [3].



(a) (b) (c)

Fig.1. (a) Cp distribution, NACA0012, M=0.8, α=1.25°; solid line- body fitted grid , markers —Cartesian grid. Flow around a set of cylinders, M=3: present (b) и alternative [3] (c).

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HPC and Big Data: Is there any change?

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Parallelism and scalability have become the major issues in all areas of Computing. Nowadays, pretty much everybody – even beyond the field of classical HPC – uses parallel codes. Nevertheless, the number of cores on a single chip – homogeneous as well as heterogeneous cores – is significantly increasing in future. Soon, we will have millions of cores in one HPC system. The ratios between flops and memory size, as well as the bandwidth for memory, communication, and I/O, will worsen. At the same time, the need for energy might be extraordinary, and the best programming paradigm is still unclear.

Furthermore, we have reached the point where data becomes the primary challenge, let it be complexity, size, or rate of the data acquisition. While Cloud services at least announce to solve many problems, it is clear that our backbone networks have to deal with the new situation where data generation, data analysis, and data storage might not be localized at a single site.

This talk will describe technology developments, software requirements, and other related issues to identify challenges for the community, which have to be carefully addressed.

HIGH-PERFORMANCE SIMULATIONS OF CONTINUOUSLY VARIABLE TRANSMISSION DYNAMICS

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The present paper describes a parallel computational model simulating continuously variable transmission (CVT) dynamics. A specific feature of the CVT model is the combination of relatively small problem sizes (about 1000 unknowns) and high computational costs (up to several weeks of sequential code computations for a thirty seconds simulation period). The main source of computational complexity here is the calculation of non-linear contact forces acting between transmission parts at each step of the explicit time integration procedure. Below we analyze simulation workflow and runtime load distribution among the application modules. Based on the profiling data, we present a task parallel multithreaded implementation of the model over shared memory and discuss steps towards further parallelization.

COMPUTER MODELING OF INFLUENCE OF ICE STRUCTURES ON SEISMIC REPLIES IN THE ARCTIC

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Abstract. The aim of this work is simulation of wave propagation in the Arctic with the presence of different ice structures, using high-performance computing. In the given report grid-characteristic method is applied, which provides correctly describing the contact and boundary conditions.
Key words: numerical modeling, Arctic, seismic prospecting, grid-characteristic method, ice ridges, ice field.

Introduction

The question of developing the Arctic in Russia is of current importance as there are eight hydrocarbon fields, and their supplies are estimated approximately 2,7 trillion $м^3$. The considerable barrier on way of oil extraction in north seas is presence of different ice formations, particularly, ice ridges, icebergs. One of the main stages of planning geological survey works is mathematical modeling, that allows significantly bring down the cost of carrying

out seismic exploration. In this very work numerical experiments on solving problems of seismic exploration in the conditions of the Arctic shelf were carried out.d then applied to calculate the fluxes in the finite volume discretization of the governing equations.

Mathematical model and ways of describing it

The models of continuum, described by linear-elastic statement, were considered in the work [1] given.

$$\rho \frac{\partial}{\partial t}\vec{v} = (\nabla \cdot \boldsymbol{\sigma})^{\mathrm{T}}$$

$$\frac{\partial}{\partial t}\boldsymbol{\sigma} = \lambda(\nabla \cdot \vec{v})\mathbf{I} + \mu(\nabla \otimes \vec{v} + (\nabla \otimes \vec{v})^{\mathrm{T}})$$

Numerical method

In the given work the grid-characteristic method is used [2]. It solves equations of the particular form:

$$\frac{\partial \vec{q}}{\partial t} + \mathbf{A}_1 \frac{\partial \vec{q}}{\partial x_1} + \mathbf{A}_2 \frac{\partial \vec{q}}{\partial x_2} = 0$$

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NUMERICAL MODELLING OF COMPOSITE DESTRUCTION DUE TO LOW-VELOCITY STRIKE

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Low-velocity strikes are considered as one of the most dangerous load types for composites, especially in aviation. They don’t lead to an immediate destruction of a whole detail, but inner damage – delamination between layers or between fiber and matrix – lowers material strength and can lead to destruction during the flight. This inner damage can only be noticed via complex study.

Modern composite destruction theory is an actively developing science field, but none of the existing criteria can give results reliable enough for engineering purposes [1]. The given work is dedicated to the comparison between several destruction criteria, which are mostly used in commercial software packages and use parameters which can be directly obtained in experiments.

A hybrid grid-characteristic method of 1-2 order on irregular tetrahedral grid is used [2, 3, 4]. A carbon fiber and a glass fiber polymer matrix unidirectional composites are modeled as orthotropic media with a single distinguished direction along the fiber [5]. Drucker-Prager, Hashin, Puck, Tsai-Hill and Tsai-Wu destruction criteria are used. Several problem statements are considered and the comparison of examined criteria is given.

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The role of algorithms in modern HPC

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Modern HPC technologies are reaching the end of Moore’s law in the coming ten years. Even though we see an increase in speed for some time to come we have to face the fact the hardware will not be able to satiate the computational needs of research and industry. In this talk we will work out the roadmap for HPC over the coming years and will describe how algorithms can help to further push the speed of modern HPC systems.

USING SUPERCOMPUTING TO SIMULATE DETONATION COMBUSTION

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The present paper deals with the numerical investigation of the detonation combustion with using supercomputing. In the paper we discussed mathematical model, kinetics schemes for different fuels, parallelization technics and structure of the software. Our approach is based on the set of equations for 2D and 3D transient flow of inviscid, compressible, multicomponent, explosive gaseous mixture. The numerical procedure for solving Euler equations is based on the finite volume approach, explicit time integration, interpolation procedure to enhance the spatial accuracy of the scheme. The fluxes through the computational cells faces are calculated with Godunov's method. The numerical investigations were implemented with the use of up to 3000 processor cores of multiprocessor systems MVS-100k (Joint Supercomputer Center RAS) and LOMONOSOV (Research Computing Center of the Moscow State University).

In the paper we presented several examples of numerical investigations detonation propagations in homogeneous and non-homogeneous reactive mixtures with using developing software. Fig.1 illustrates “numerical soot footprints” (gas pressure maximums distributions) in planar channel which fulfilled the hydrogen-air mixture with transverse concentration gradient of hydrogen. The results of numerical investigations are revealed that there is strong periodically arising transverse wave, which burns rich mixture at the upper part of the channel. The results of numerical investigation the detonation initiation and propagation in channels and tubes with special shapes to improve the detonation initiation process are presented. Numerical modelling of detonation processes in heterogeneous mixtures also discussed.

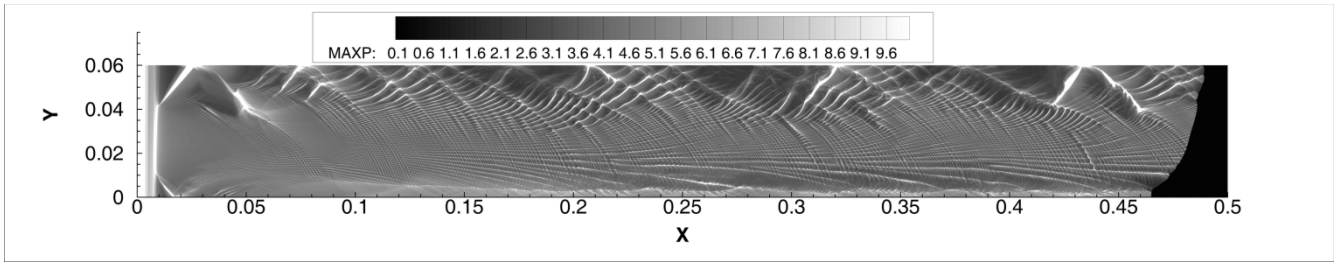

Fig. 1 Cellular structure of DW in channel with transverse concentration gradient of hydrogen for the case of averaged volumetric concentration of hydrogen in channel 40%.

COMPUTING ENVIRONMENTS FOR LONG TERM RESEARCH DATA MANAGEMENT

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Research data can be a valuable asset by itself (example: satellite data) and thus should be preserved for a longer period. Nowadays the interpretation of research data depends on more and more complex environments - the use of mathematical libraries during data generation, of data bases for efficient storage, etc. Despite precise bit preservation there are well known cases where the re-execution of old software in new environments leads to different results. One cause are new algorithms in system libraries and the way they handle round-off errors.

So it is desirable not only to archive data but to provide a computing environment which can be archived "in toto".

The new HPC system in Freiburg will provide such an environment. The talk will cover the necessary details, both design issues and technical realization.

Material statistics in cancellous bone and their influence upon continuum mechanical simulations

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To perform patient specific biomechanical simulations of bone implant systems three prerequisites are necessary. (1) The patient specific geometry of the simulated bone structures and muscle strands, (2) the patient specific boundary conditions determined by means of the bodyweight and the muscle forces acting on the simulated bone structures and (3) the patient specific material distribution within the bones. By implementing these three prerequisites it would be possible to derive a patient specific continuum mechanical model, which would allow predicting the bone remodelling and with this ultimately the healing process of fractured bone structures stabilized by implants along with the possibility of mechanically induced complications.

This talk will focus on the third prerequisite defined above since one very critical aspect for the prediction of bone remodelling is the correct determination of the local strain field with-in the simulated bone structures as it is one of the essential triggers for bone remodelling.

The development of a procedure for the determination of high resolution anisotropic material data of cancellous bone based on micro-focus computer tomography (μ-CT) was subject to research carried out during the last years at HLRS [1], [2], [3]. First of all a short overview of the developed procedure and its

current implementation state will be given. After that, based on the aforementioned developments and recent findings [4], the talk will present the statistical evaluation of 21-dimensional data fields, representing the anisotropic distributions of material parameters resulting from the application of the developed procedure across a complete human femoral head. The talk will show results arising from cube shaped, overlapping decompositions of the μ-CT in the range of 0.3mm to 1.2mm which had shown to be the transition area between a linear and non-linear transfer path between the relative density and scalar properties of the calculated anisotropic material data.
Finally it will be shown how the independent parameters of the derived 21-diemensional, anisotropic material fields can be reduced by means of principle component analysis and how this reduction influences stress and strain results calculated on the continuum mechanical scale with the help of the derived material data.

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Cut-Cell Method Based Analysis of Freely Moving Particles in Viscous Flows

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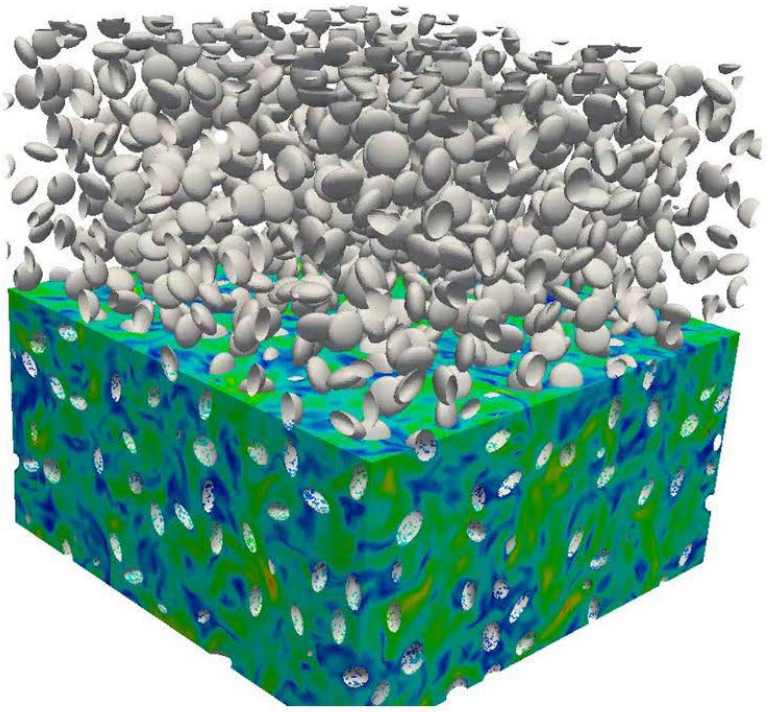
A Cartesian cut-cell method for viscous flows interacting with freely moving boundaries will be presented. The method provides a sharp resolution of the embedded boundaries and strictly conserves mass, momentum, and energy. A new explicit Runge-Kutta scheme is introduced which significantly reduces the computational time for tracking moving boundaries and subsequently reinitializing

the solver without lowering stability or accuracy. The structural motion is computed by an implicit scheme with high stability due to an iterative strong-coupling strategy. A new formulation for the treatment of small cut cells is presented with high accuracy and robustness for arbitrary geometries based on a weighted Taylor-series approach solved via singular-value decomposition. Unphysical oscillations occurring in Cartesian grid methods applied to moving-boundary problems are eliminated. The efficiency and the accuracy of the new method are demonstrated for several three-dimensional cases of laminar and turbulent particulate flow such as a spherical particle settling in a quiescent fluid, rotation of an ellipsoidal particle in simple shear flow, and a cloud of particles in homogeneous turbulence.



1600 disc-like particles in decaying homogeneous isotropic turbulence

COMPUTER-INTENSIVE SIMULATIONS OF COMBUSTION IN FIRES

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Keywords: CFD, fire modeling, buoyant turbulent diffusion flame, thermal radiation, soot

Natural fires are mainly driven by turbulent diffusion combustion in buoyancy dominated flames. The effect of buoyancy, wide range of stoichiometry covering very lean (over-ventilated) and very reach (under-ventilated) flames, large amount of soot and importance of soot radiation makes combustion in natural fires to be rather distinct from that in jet flames occurring in engines and turbines. Most of current research on CFD fire modeling is essentially reliant upon the specially designed open-source software. At the same time, general-purpose commercial CFD codes are intensively used in industry, hence the justification of adapting it to predict fires and fire-related phenomena. It is therefore important, that the models validated for conditions of engines and turbines may not be transferrable to fire conditions.

The purpose of this work is to elaborate methodology of CFD fire modeling by means of ANSYS FLUENT. We use the large eddy simulation approach (LES), which makes the methodology computer-intensive. Buoyant turbulent diffusion flames fueled by methane and heptane are simulated in unconfined atmosphere with no cross-winds. Non-premixed combustion is considered using the subgrid eddy dissipation model. The focus of this study is placed on thermal radiation emission, transfer and absorption. To model the radiative transfer, we use the discrete ordinate method (DOM), and the spectral properties of the combustion products including CO2, H2O and soot are accounted for by means of the weighted sum of the grey gases model (WSGG). In the methane flame, thermal radiation is controlled by the gaseous products, while soot radiation dominates in the heptane flame. As such, soot modeling approaches available in ANSYS FLUENT are thoroughly examined against the existing experimental data, both for methane and heptane. We found that none of the soot models can be used with confidence for modeling buoyant turbulent diffusion flames with the default settings. We demonstrate that the soot oxidation models could be equally important as soot formation ones to predict the soot yield in the overfire region. We also calibrate the Moss-Brooks soot formation model to replicate the experimental radiative fluxes and soot yields.

Current results show that ANSYS FLUENT offers powerful tools to predict dynamics, structure and radiative impact of buoyant turbulent diffusion flames occurring in fires, although it requires lengthy multi-processor simulations.

Modeling and Simulation of Energy Storage Technologies

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We provide a review of simulations of electrochemical and thermal energy storage technologies carried out at the University of Stuttgart (Institute of Energy Storage) and at the DLR (Institute of Engineering Thermodynamics).

Application of averaging for solutions smoothing in DG method

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DG is widely used to solve various problems of gas dynamics. This method has discontinuous basic functions and is characterized by high order accuracy of the solution. As is well known, it is necessary to use limiters to guarantee the monotony of the solution, especially if the result has disruptions. However, limiters can negatively affect the accuracy of the solution [1]. Therefore the problem of keeping the high order of the solution and providing it's monotony is of current importance. To solve this problem the usage of smoothing operator is proposed instead of limiting [2, 3]. However, smoothing operator based on WENO reconstruction [3] doesn't provide the high order of the solution for DG method. In this paper the different smoothing operator is proposed. Theoretically it doesn't demote the order of method.

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THREE-DIMENSIONAL CODE FOR LPP EUV SOURSE MODELING

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Laser produced plasma (LPP) is one of the most promising sources of radiation in range 13.5±1% nm (EUV, Extreme Ultraviolet) for needs of lithographic industry [1]. The principal scheme of EUV-machine is following: high-frequency nanosecond laser is evaporating tiny tin droplets throwed into optical focus of collector mirror. Hot dense plasma, produced by laser flux, is emitting EUV radiation, which then is collected and redirected to optical system by the collector mirror. The main problem standing in the way of this technology is source availability, which is bounded by the collector mirror life time. Unevaporated matter, tin vapor and high energy ions are damaging and polluting mirror, causing radical decrease of its reflectivity and, consequently, reduce of output EUV flux.

To understand how tin ions transfers from the target to the mirror we need to find ion flux energy and anisotropy. This often cannot be done in two-dimensional setting due to the circumstances that violate the symmetry (non ideal spatial profile of laser beam, non symmetric target, non-central laser coupling to target...).

Here we present parallel three-dimensional code 3DLINE [2], which includes much of the most important physical processes in tin plasma and liquid droplet, such as laser absorption, radiative and thermoconductive heat transfer, ionization dynamics and wide-range equation of state for target deformation and evaporation, and built on basis of fully conservative arbitrary lagrangian-eulerian numerical scheme.

Also we describe results of simulations of central and non-central laser coupling to tin droplet. Despite of similarity of EUV power dynamics for these two cases, for the shifted pulse ion jet is forming, what causes great differences in ion fluxes.

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EXPERIENCE IN HYBRID RANS/LES SIMULATION OF COMPLICATED INTERNAL FLOWS

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The contribution covers results of numerical simulation of turbulent flows and heat transfer in some model configurations (such as backward-facing step, T-junction of pipes, etc.) that are known to be challenging problems for RANS models. To improve the prediction we used a vortex-resolving method that combines RANS modeling close to walls and LES simulation faraway (with smooth transition from one to another depending on distance to the wall and local grid resolution). Synthetic turbulence was generated at the inlet to provide reasonable turbulent content entering the LES region. The computations were performed by means of an in-house finitevolume parallel code. A semi implicit non-iterative method was used for time advancement and an efficient multigrid solver was elaborated to solve the linear systems at every time step. For T-junction case, the hybrid RANS/LES approach yielded a great improvement of the prediction accuracy. For the backward-facing step flow, the vortex-resolving simulation produced better agreement with experiments for the wall friction, whereas the RANS solutions showed superiority in the heat transfer prediction.

A SINGLE-VELOCITY APPROACH TO DIRECT NUMERICAL SIMULATION OF TWO-PHASE FLOWS*

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A single-velocity numerical model for simulation of two-phase flows of one-component medium is presented. It is supposed that pressure, temperature, viscosity, coefficient of thermal conductivity and other necessary parameters are continuous single-valued functions of density and internal energy. A method for obtaining EOS for multiphase states on the base of EOS for single-phase states is given. The interfacial surfaces are represented by domains of fast but continuous changing of density. The governing equations are the laws of conservation of mass, momentum and energy. Special terms are added in the stress tensor in order to describe effects of surface tension forces. The numerical model is intended for the usage with the supercomputers (with the prospects of achieving of exaflops performance). It is expected that the model is most useful for subcritical and supercritical flows.

The model is implemented as an MPI code for parallel computer K100. On the example of real water it is demonstrated the capacity of proposed methodology

to realistically describe phase transitions, to clearly monitor the boundaries of phases' separation and to follow the processes of the type of bubbles merging. Properties of the parallel code are investigated.

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PARALLEL MULTIGRID METHOD FOR DIFFUSION EQUATIONS

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We consider two approaches for numerical solution of parabolic partial differential equations with anisotropic discontinuous coefficients on ultraparallel computers. These equations are solved by discretizing both in space and time. For 3D space discretization it is used a convenient seven-point stencil on a cartesian grid. We present the results of development of two time-integration schemes.

The first one is the two-layer scheme (the implicit Euler method) which is resolved by the multigrid method [1–4]. We refer to this scheme as the MM scheme. The second one, the LI-M scheme [5], is elaborated to solve a heat equation in high temperature gasdynamics simulation. This scheme is based on explicit iterations with Chebyshev's parameters and here it is studied as a competitor of the MM scheme.

Special attention is paid to development of the parallel multigrid code. The multigrid algorithm represents an efficient parallel implementation of the Fedorenko multigrid method [1–2]. The algorithm is adapted for solving the anisotropic stationary diffusion equations and it is able to solve the general boundary value problems including the semi-definite Neumann problem. Scalability to a large number of processors is achieved by the use of the explicit Chebyshev's iterations to solve the coarsest grid equations and for construction of the smoothing procedures. For discontinuous coefficients it is used so called problem-dependent intergrid transfer operators.

We developed an automatic procedure for adaption of our smoothers to anisotropy and give a few examples, which show that adaptation improves the efficiency of the multigrid method. For both LI-M and MM schemes the results of

comparison are given. Both schemes provide a high performance; they scale efficiently and seem to overcome the difficulty in achieving exaflops performance.

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