ROOTS OF RUSSIAN-GERMAN COOPERATION IN COMPUTATIONAL SCIENCE

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Комментируются первые шаги сотрудничества ученых России и Германии в области вычислительных наук, установленные между Институтом вычислительных технологий и Компьютерным центром высокой производительности университета Штутгарта. После достаточно долгого начального периода контактов между отдельными учеными с 30 сентября по 2 октября 2003 года было организовано первое Российско-Германское рабочее совещание по вычислительным наукам и высокопроизводительному программированию. В данной статье представлен краткий обзор докладов, затрагивающих широкий круг вопросов, представленных на этом рабочем совещании.

1. Introductory remarks — the early contacts

One of the first contacts between Russian and German scientists in the field of computational science was established by Academician Yurii I. Shokin when he visited the author at the Aerodynamisches Institut of the Rheinisch-Westfälische Technische Hochschule Aachen in 1974. It so happened that Dr. Paul Kutler, one of the leading scientists of NASA Ames Research Center, California, USA, was also visiting the Aerodynamisches Institut at the same time, and it did not take long to reach the unanimous decision to organize an international workshop on the spot together with some German scientists, among them Prof. Karl Foerster of the University of Stuttgart, Prof. Ernst Heinrich Hirschel and Prof. Dietrich Rues of the Deutsche Forschungs- und Versuchsanstalt fuer Luft- und Raumfahrt, and Prof. Karl Roesner, at that time at the Max Planck-Institut fuer Stroemungsforschung in Goettingen. In passing it is mentioned, that the lectures could not be held in the seminar room of the Aerodynamisches Institut, since it was carnival, and the carnival fools would not let anybody in, who did not want to celebrate carnival with them. So the lectures had to be held in the library of the institute.

Scientific meetings on computational technologies were rare in those days. On the occasion of the 70^{th} birthday of Prof. Maurice Holt of the University of California at Berkeley the author recalled in his tribute to Prof. Holt in 1989 [1]:

“When the author first heard about the Second International Conference on Numerical Methods in Fluid Dynamics, to be organized by Professor Holt at the University of California at Berkeley in September 1970, he was surprised for several reasons. Until 1970 there was no conference dealing with the subject in question. The idea to initiate a series of conferences for this field on a worldwide basis was greeted with great enthusiasm. Finally, the “numerical community” as Gino Moretti once called the scientists working with numerical methods, was given the chance to meet and discuss their problems in the frame of international conferences. To be admired was also the courage the organizers must have had in order to overcome the difficulties, typical for such ventures. The associated problems were already signalized by the fact, that little or nothing was known about the first conference of the series proposed. Rumors had it, that it had taken place in Novosibirsk in 1969, at that time almost unbelievable in view of the relatively sparse scientific contacts between East and West.

Nevertheless, the second conference was a great success. Altogether 65 papers were presented by scientists from the USA, USSR, France, Germany, England, the Netherlands, Canada, and Australia. That then the third conference would follow two years later in Paris was no surprise to anybody anymore. The Berkeley conference was a sound scientific affair. The participants had the impression, that it was just one of a well-established series, but not one which was just initiated. It opened new dimensions, mainly due to Professor Holt and his colleagues who worked with him on the conference committee."

After Yurii I. Shokin's visit to Aachen in 1974 scientific contacts to Russian scientists could be increased — although slowly — on a personal and individual basis. Yurii Shokin visited Aachen several times and others followed. Among them was Prof. Victor V. Russanov of the Keldysh Institute of Applied Mathematics in Moscow.

Contacts were substantially widened in the following years, when the author joined the Committee for the International Conferences on Numerical Methods in Fluid Dynamics. In the meetings of the committee he met academician N. N. Yanenko, the man who — as the author had learned in the mean time — in 1969 had initiated the first International Conference on Numerical Methods in Fluid Dynamics in Akademgorodok. In 1980 the eighth conference of this series was held at the Rheinisch-Westfaelische Technische Hochschule in Aachen, organized by the staff of the Aerodynamisches Institut. Substantial scientific contributions to the conference were made by the Russian delegation, and it seemed that a sound basis for increasing and broadening contacts was eventually established. In 1983 the author visited the Institute of Theoretical and Applied Mechanics of the Russian Academy of Sciences in Akademgorodok, which at that time was headed by Prof. Yanenko. During this visit, an agreement was signed, in which the exchange of Russian and German scientists and an extensive cooperation between the Institute of Theoretical and Applied Mechanics and the Aerodynamisches Institute was proposed.

Unfortunately the activation of the cooperation conceived was delayed for several reasons, and years passed by without any progress. It was long after Prof. Yanenko had passed away, that the agreement could be filled with life. Eventually substantial joint experimental scientific campaigns could be planned and executed in the nineties of the last century by scientists of both institutes, vigorously pushed forward by Profs. V.M. Fomin and A.M. Kharitonov. This cooperation was so successful, that the Siberian Branch of the Russian Academy of Sciences and the Deutsche Forschungsgemeinschaft decided to show results of the cooperation among other results in a public exhibition in Akademgorodok in 2004.

2. The first joint workshop

Almost at the same time, in 2003, exactly twenty years after the agreement of cooperation was signed, a far-reaching and extensive cooperative venture was initiated in the field of computational science. An advanced research workshop on computational science and high performance computing was proposed to be organized by the Institute of Computational Technologies in Akademgorodok under the auspices of Academician Yurii I. Shokin, together with Prof. Michael

Resch, the head of the High Performance Computing Center of the University of Stuttgart in Germany.

The aim of the workshop was to discuss recent results in various branches of the computational sciences, as for example computational fluid dynamics, to present new mathematical methods for the development of new materials, to construct new prediction methods for the solution of environmental problems, and, above all, to initiate cooperation between Russian and German scientists in the development of algorithms, soft- and hardware support for high-performance computation, and of visualization techniques for numerical simulations.

Participation to the workshop was by invitation only. Scientists of 15 universities and research centers readily followed the invitation extended by the Institute of Computational Technologies in Akademgorodok and the High Performance Computing Center of the University of Stuttgart and contributed scientific papers to the program. The names of the institutions invited are listed below in alphabetical order:

The All-Russia Research Institute of Experimental Physics in Sarov, the Center for High Performance Computing (ZHR) of Dresden University of Technology, Dresden, the Institute of Applied Mathematics of the University of Freiburg i. Br., the Institute of Aerodynamics and Gasdynamics, the Institute for Fluid Mechanics and Hydraulic Machinery, and the High Performance Computing Center Stuttgart (HLRS), all three of the University of Stuttgart, the Institute of Computational Mathematics and Mathematical Geophysics (SB, RAS), Akademgorodok, the Institute of Computational Modelling (SB, RAS), Krasnoyarsk, the Institute of Computational Technologies (SB, RAS), Akademgorodok, the Institute of Fluid Mechanics and the Institute of Informatics, both of the University of Erlangen-Nuremberg, Erlangen, the Institute of Theoretical Astrophysics of the University of Tuebingen, the Regional Computing Center Erlangen of the University of Erlangen-Nuremberg, Erlangen, and the Kemerovo State University, Krasnaya, the Russian Federal Nuclear Center, Snezhinsk.

Previous experience with international cooperative ventures has shown that the long-term success is best guaranteed by tying in young scientists. It was therefore decided to enable young postgraduates of Novosibirsk University, of Novosibirsk Technical University and young researchers of the Institute of Computational Technologies to participate in the scientific sessions of the workshop.

In order to document the scientific content of the workshop, the Springer Verlag was asked to publish the contributions in the series "Notes on Numerical Fluid Mechanics and Multidisciplinary Design". Volume 88 of this series, edited by M. Resch, Y.I. Shokin, N. Shokina, and the author, contains the contributions to the workshop, which will briefly be reviewed in the following. The contributions can roughly be grouped under the two headings "General Computational Technology" and "Physics of Fluids".

3. The contributions to the first joint workshop on computational science

3.1. General Computational Technology

The first paper presented at the workshop is concerned with the development and secure handling of information and telecommunication systems for emergency management. The authors Y.I. Shokin and L.B. Chubarov of the Institute of Computational Technologies in Akademgorodok in [2] discuss problems associated with collecting and sharing timely, reliable and accurate information in catastrophic situations in order to improve humanitarian response, maximize the availability of resources, and to minimize human suffering. The paper explains in detail the principles of humanitarian information management and exchange, comments on its best practices, describes new communication and information technologies, explains existing projects of emergency telecommunications, as for example the EPIX-Project, the emergency preparedness information exchange on the world wide web, and others. This is a relatively new field in computational science, which is bound to gain more importance in the future.

In the second article [3], M. Resch of the High Performance Computing Center (HLRS) of the University of Stuttgart describes the latest developments in the field. He shows, how simulation techniques of high performance computing have become indispensable research tools in science and engineering. As an example he comments on the Accelerated Strategic Computing Initiative, the ASCI Project in the USA, which aims at replacing atomic bomb tests by advanced simulation on supercomputers, a topic closely related in a certain way to the first contribution. Resch also describes the dominant role high performance computing plays in industry, summarizes the basic problems, and describes the state of the art. The paper is supplemented by an extensive list of references.

In reference [4] the distributed software environment, developed at the High Performance Computing Center of the University of Stuttgart, for visualization is described by U. Lang. The environment enables the visualization of results either on a desktop computer or on stereo projection environments. The software architecture can make efficient use of distributed computing resources as well as of high speed networking infrastructures. The paper gives details of the software and shows impressive results of projects in which it was used. It is made clear that scientific visualization has become a support technology that enables scientists and engineers to understand complex relationships typically represented by large sets of data. In the analysis of complex problems in science and engineering the visualization process has become part of the overall simulation-process. Several examples demonstrate the application of the visualization technique developed at the HLRS.

V.V. Moskvichev of the Institute of Computational Modeling in Akademgorodok in [5] reviews research activities in reliability and safety of technical systems of the period 1990–2002. Results are presented for failure causes of complex technical systems in industry, test calculations regarding fracture toughness, life-cycle design of welded structures, and residual lifetime-, reliability-, and risk-assessment. The calculations rest on data obtained from numerous tests on fracture toughness and analyses of technological and operational defects of complex technical systems. The applications described include buildings, crane and ship structures, welded joints of reactors and excavators, propeller blades of airplanes, frame structures of spaceships, pressure vessels, pipeline systems, and others. Future research is focussed on determining safe residual lifetimes of machines and structures, which have exceeded their normative lifetime.

In [6] I.D. Sofronov describes the structure of the institutional complex of computer simulations of the All-Russia Research Institute of Experimental Physics in Sarov. Expertise in numerical simulation was gained there in a period of over fifty years. The fields of basic research presently being worked on, developments in simulation techniques for solid mechanics, energy transfer and radiative transport, numerical studies of hydrodynamic instabilities, and other problems are briefly described. The paper also mentions research programs in which computational methods for the description and solution of problems posed by the development of nuclear and thermonuclear weapons are designed. For security reasons the corresponding scientific activities are not open to the scientific community.

In reference [7] an overview is given by M.P. Fedoruk of the Institute of Computational Technologies in Akademgorodok on the joint efforts in the field of mathematical modeling of dispersion-managed solitons in optical communication fiber lines, carried out by his own Institute, together with scientists of the Aston University in Birmingham in the United Kingdom, and the Institute of Automation and Electrometry in Akademgorodok. Three of the most widely used mathematical models of dispersion-managed solitons and the corresponding numerical techniques are discussed. Some results of numerical simulations for important practical dispersion maps are presented. It is shown, how the results of the fundamental soliton theory can be successfully exploited for the solution of practical problems.

Problems of mechanics of composite plates and shells are discussed by S.K. Golushko of the Institute of Computational Technologies in Akademgorodok with direct and indirect methods of solution in [8]. Several models of fibrous composites are considered, as for example a filament model, a model with one-dimensional fibres, a special model with one-dimensional fibres, and a model with two-dimensional fibres. In the paper it is shown, how the models influence the stress-deformed state of constructions of composite materials. In addition the formulation of the problem of rationally designing composite plates and shells is discussed. Several analytical solutions are obtained for problems of rational designing of nodoid shells.

Yu.M. Laevsky of the Institute of Computational Mathematics and Mathematical Geophysics in Akademgorodok offers a review-like commentary on the key areas of numerical methods for the solution of partial differential equations, based on the analysis of recent reviews. The paper summarizes the state-of-the-art of new tools of modern computational technology: New generations of numerical methods of solution and algorithms for large-size problems of mathematical physics, approximation techniques, iteration procedures of linear systems, design of efficient preconditioners, and solution techniques for non-stationary problems [9].

In [10] the behavior of multilayered conic shells is analyzed by V.V. Gorshkov of the Institute of Computational Technologies in Akademgorodok with non-classical models. The stress-deformed state is investigated in a parametric study, in which the influence of the structure of the reinforcement of a composite material, the cross shift of binding and the order of arrangement of the reinforced layers on the behavior of the shell are analyzed with vectorially linear and non-linear variants of classical and non-classical theories. Numerical results obtained with the methods of spline collocation and discrete orthogonalization are compared with those obtained with the method of invariant immersing. The high efficiency of the numerical methods used is demonstrated for the solution of a boundary-value problem described by a system of stiff differential equations.

H. Mix and W.E. Nagel of the Center for High Performance Computing (ZHR) of Dresden University of Technology in Dresden discuss the problem of how to effectively utilize the large performance potential of the microprocessors on parallel computers in addition to the problem of parallel programming. With the ever growing demands in computer-modeling and simulation, the programming conversion techniques for efficient algorithms and procedures have to keep up with the rapid development progress on the instrumental platforms in computer architectures. In many cases the sustained single PE performance of a large HPC application is in the order of a few percent of the peak speed announced for the microprocessor. This still limits the success of such machines especially in large scale environments. The paper discusses aspects of programming and optimization in HPC applications on parallel computers [11].

3.2. Physics of Fluids

The problem of discretizing the Navier-Stokes equations is discussed in a paper by I.V. Kireev, V.V. Shaidurov of the Institute of Computational Modelling in Krasnoyarsk, and U. Rüde of the

Institute of Informatics of the University of Erlangen-Nuremberg, Erlangen. The authors explain their joint work on a finite-element solution of the Navier-Stokes equations for two-dimensional time-dependent flows in a rectangular domain in [12]. They divide the problem on the physical level into a convection-diffusion and action of pressure process. Advantages and disadvantages of the method proposed are discussed in detail. The development of the discretization by fractional steps is supplemented by a numerical experiment, allowing estimates of the numerical errors. The paper closes with remarks on future work.

Another detailed problem of fluid flow simulation by numerical techniques, namely the computation of the flow passing a shock wave in supersonic flow, is reviewed in [13] by V.F. Kuropatenko of the Russian Federal Nuclear Center in Snezhinsk. The author compares the specific characteristics of the Neumann — Richtmyer-scheme, the Lax-scheme, and the Godunov-scheme with his own non-divergent and divergent schemes. The distraction, i. e. the width of the layer, in which the shock is smeared, the monotoniscity and stability properties, and empirical constants, needed in the computation, are used for the comparison. The results, obtained in a comprehensive derivation, are summarized in a table at the end of the paper, giving the numerical stability limits of the schemes, the distractions, and the monotoniscity properties. It is shown that the Lax-, Godunov- and the Kuropatenko-schemes do not have to rely on empirical constants.

The next contribution under the heading of physics of fluids is concerned with a theoretical problem of high-speed aerodynamics. At the Institute of Aerodynamics and Gasdynamics of the University of Stuttgart, A. Pagella and U. Rist in [14] study the interaction of a shock wave impinging on the hypersonic boundary layer of a flat plate with numerical techniques. The analysis shows the influence of wall cooling on transition and on the flow in the separated region. It was found that the cooled wall yields a separated region of shorter length. It could also be shown with linear stability calculations, that the first instability mode can completely be suppressed by wall cooling, while the higher acoustic modes are destabilized. The paper discusses the details of the transition process, including the formation of longitudinal vortices, which are not observed in undisturbed hypersonic boundary layers.

Numerical modelling of flows of reacting gases is addressed in [15] by A.D. Rychkov of the Institute of Computational Technologies in Akademgorodok and by N.Yu. Shokina of the High Performance Computing Center of the University of Stuttgart. The paper describes the numerical solution of three problems: The filtration combustion of a gas mixture in an inert porous medium, the combustion of fuel granules in a hard fuel gas generator, and the non-stationary combustion of hard fuel in an automotive safety device (airbag). The main emphasis is placed on the numerical aspects of the problems mentioned. These include the description of the physical and fluid-mechanical models, the discussion of the associated boundary and initial conditions, and their numerical implementation. The general considerations are supplemented by a discussion of numerical results obtained so far.

Another problem of fluid mechanics is discussed by A.M. Frank of the Institute of Computational Modelling in Krasnoyarsk in [16]. The so-called particle-method is described together with its application to the simulation of incompressible flows with free surfaces. The method used is a free-Lagrangian method, a special kind of the Galerkin method, in which convective transport is calculated by means of material particle motion. The material derivatives are calculated in Lagrange variables, while the mass forces, inner and surface stresses are obtained in Eulerian formulation. The main advantages of the method are a good accuracy, a high efficiency for smooth flows combined with the possibility of simulating complex flows in arbitrarily shaped regions with moving and free boundaries, as for example surface waves, ball suspension by a thin liquid jet, and thin-film flows on locally heated substrates.

Interest in processes taking place in plasma-chemically etching reactors is motivated by their wide-spread use in industrial production of semiconductor devices. Yu.N. Grigoryev and A.G. Gorobchuk of the Institute of Computational Technologies in Akademgorodok discuss the problem of optimization of plasma-chemical etching reactors in [17]. Since the experimental optimization is markedly limited by the large number and complicated interconnection of factors that determine the quality and etching rate of wafers the authors suggest optimization with the aid of mathematical modelling of the relevant processes as an alternative. In the paper a numerical model for plasma-chemical reactors is proposed. The model is based on a numerical solution of the Navier — Stokes equations and the Boussinesq approximation. The capability of the model proposed is illustrated with applications.

The method of smoothed particle hydrodynamics (SPH), used by S. Holtwick and H. Ruder of the Institute of Theoretical Astrophysics of the University of Tübingen mainly to simulate astrophysical phenomena, is extended to simulate flows with free surfaces and flows in technical applications, as e. g. the injection of diesel fuel in automotive engines. The method, a grid-free numerical particle method, applicable to incompressible and compressible flows, provides a numerical algorithm for solving a system of coupled partial differential equations by transforming them to a system of coupled ordinary differential equations for magnitudes at discrete sampling points, the locations of the SPH-particles. The paper gives details of the parallalisation of the method [18].

A similar topic is addressed by T. Zeiser of the Regional Computing Center Erlangen and F. Durst of the Institute of Fluid Mechanics, both of the University of Erlangen-Nuremberg in Erlangen. These authors explain recent developments in the area of lattice Boltzmann methods for simulating incompressible fluid flows [19]. The application of a particular method is shown for the simulation of the flow in a complex geometry of a randomly packed fixed bed reactor. The paper also addresses general aspects of high performance computing, as for example, efficient handling of large amounts of data produced in time-dependent simulations, performance of recent commodity off-the-shelf (COTS) high performance computers, and optimization strategies for them.

Solutions of hydrodynamic problems of an ideal incompressible fluid with a free surface are discussed by K.E. Afanasiev and S.V. Stukolov of Kemerovo State University in Kemerovo. The authors use a boundary element method, based on the Cauchy integral formula and the third of Green's formulas, and describe solutions for flow over obstructions, for unsteady two-dimensional problems, as the horizontal movement of a semi-infinite body in a fluid and of a semi-circular cylinder along a plane bottom, for the collapse of a cavity of a given form in a pool of finite depth, and others. The main numerical developments are explained, along with a discussion of the algorithms developed, including the parallelization of the algorithms [20].

In his paper E. Göde of the Institute for Fluid Mechanics and Hydraulic Machinery of the University of Stuttgart discusses results of long-term research on the development of high-performance numerical simulation tools for the design and optimization of hydro power stations. The programs developed so far, in a very impressive way demonstrate, that power output of hydro turbines can accurately be predicted, how the maximum hydraulic efficiency of the turbines can be achieved, how cavitation and vibrations can be avoided or kept to a minimum. The programs proved very useful especially in conjunction with the rehabilitation and upgrading of existing hydro power plants together with the connected plant components. This is of particular interest, since hydro power plants are long-term installations, which can be used for 50 years and more. The new simulation tools very efficiently can help to guarantee smooth and safe operation over the entire life time [21].

The motion and heating of an irregular plasma is simulated numerically by N. A. Huber of the Institute of Computational Technologies in Akademgorodok. The author uses a differential model that rests on the three-fluid approach. It includes the continuity and energy equations of all plasma components, the equations of motion for the heavy particles, and the equations describing the magnetic field. The action of the electric field is simplified by excluding the relatively rapid electron motions, but ionization, heating, heat transfer, and relativistic electron beam action are taken into account. Computational experiments were carried out on heating and motion of a dense ionized gas cloud (plasmoid) in a strong magnetic field. Among other results, the mechanism of the effect of the magnetic field and of the heat source on the plasmoid expansion could be determined [22].

D. Kröner of the Institute of Applied Mathematics of the University of Freiburg i. Br. reports on his numerical work on and simulations of convection dominated flow problems. In his paper he gives a summary of his work on improvements of the performance of existing codes and their validation. Several numerical tools are presented, with which existing codes can be made more efficient: To be mentioned are local grid refinement, based on rigorous a posteriori error estimates; artificial boundary conditions for problems in outer domains; higher-order schemes; and balanced schemes for problems with source terms and relaxation schemes. An application is demonstrated for a problem in magnetohydrodynamics [23].

The problem of oceanic wave propagation is studied by A.V. Styvrin of the Institute of Computational Technologies in Akademgorodok in [24]. The approach is based on the non-linear shallow-water equations, for which a computational scheme for describing the wave propagation is constructed. The time discretization is carried out with the Taylor-Galerkin method, and a mixed modified finite-volume method is employed on an unstructured triangular grid for spatial discretization. Linear base functions are used for the approximation of the wave surface, but quadratic base functions for the approximation of the velocity field in order to avoid non-physical spatial oscillations. The general considerations are supplemented by numerical examples.

4. Subsequent developments and concluding remarks

In order to secure the continuation of the joint work initiated with the first Russian-German Advanced Research Workshop on Computational Science and High Performance Computing, it was agreed on to set up an organizational frame for future cooperations. Y. Shokin and M. Resch proposed to form the German-Russian Center for Computational Technologies and High Performance Computing during the course of the workshop. The initiation of the center was the starting point of further cooperative ventures. As mentioned before, a first measure for future work it was also agreed on to invite postgraduate students of Novosibirsk University and Novosibirsk Technical University and young researchers of the Institute of Computational Technologies to the 2003 workshop, which proved to be very successful.

Other initiatives soon followed. In order to introduce young students to modern programming languages a first Russian-German School on Parallel Programming using High Performance Computation Systems was held in Akademgorodok during the period of July 5 to 10, 2004, and a second school, one year later, from June 27 to July 8, 2005, again in Akademgorodok. Both events were well attended and enjoyed great success.

Also the concept of the advanced workshop was continued. The second Russian-German Advanced Research Workshop on Computational Science and High Performance Computing was held March 14 to 16, 2005 in Stuttgart. While 11 German and 22 Russian scientists attended the first workshop in Akademgorodok, 25 German, 10 Russian, and 2 Kazakh scientist attended the second in Stuttgart. On the initiative of Academician Y.I. Shokin the workshop concept could also be carried over to Kazakhstan: The first Kazakh-German Advanced Research Workshop on Computational Science and High Performance Computing was held in Almaty, Kazakhstan, from September 25 to October 1, 2005.

In 1969 academician N. N. Yanenko dared to take the first steps to lay the fundament for international cooperation in computational science and pave the road for international exchange of scientists. By founding the first International Conference on Numerical Methods in Fluid Mechanics in Akademgorodok he planted a tree which has grown a lot in the meantime and begins to bear fruits in great abundance.

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