Keldysh Institute of Applied Mathematics of RAS
A.M. Prokhorov Institute of General Physics of RAS
University of Montenegro

Thirteenth International Seminar

MATHEMATICAL MODELS & MODELING IN LASER PLASMA PROCESSES & ADVANCED SCIENCE TECHNOLOGIES

PROGRAM and ABSTRACTS

May 30 — June 6, 2015

***Petrovac,* Montenegro**

Supported by:

Ministry of Science of Montenegro

Ministry of Education and Sports of Montenegro

Municipality of Budva

Computer processing of the press Olga Koroleva, Moscow, Russia.
Press: "AP PRINT", Podgorica, Montenegro

SCIENTIFIC COMMITTEE

Prof. Dr. sc. Nat. Vladimir I. Mazhukin (Russia) – Chairman

Prof. Dr. sc. Nat. Serge V. Garnov (Russia) – Vice- Chairman

Prof. Dr. sc. Nat. Pavičević, Zarko (Montenegro) – Vice- Chairman

Academician of the RAS, Prof. Dr. sc. Nat. Boris N. Chetverushkin (Russia)

Corresponding Member of the RAS, Prof. Dr. sc. Nat. Vitaly I. Konov (Russia)

Academician of the RAS Prof. Dr. sc. Nat. Yuri I. Zhuravlev (Russia)

Prof. Dr. sc. Nat. Boris N. Chichkov (Germany)

Prof. Dr. sc. Nat. Vukčević, Labud (Montenegro)

Organizing Committee

Zarko Pavićević (Montenegro) – Chairman
Olga Koroleva (Russia)
Ranko Pavićević (Montenegro)
Zdravko Vukčević (Montenegro)
Alexander Mazhukin (Russia)
Dejana Popović (Montenegro)
Tamara Pavićević (Montenegro)

Technical co-organizer

Forum of University Professors and Researchers of Montenegro

CONTENTS

PROGRAM

Saturday, May 30	
11.00-20.00	**Registration, Check-in at Hotel "Castellastva"**
Sunday, May 31	
10.00-17.00	**Registration, Check-in at Hotel "Castellastva"**
WELCOME PARTY	
Monday, June 1	
10^{00}-10^{40}	**Opening ceremony** **Prof. Dr. sc. Nat. V.I. Mazhukin, Chairman** XIII Seminar. The goals and objectives of the Seminar
10^{40}-10^{55}	Oral Presentation **V.I. Mazhukin**, A.V. Shapranov, M.M. Demin Peculiarities of modern mathematical modeling *Keldysh Institute of Applied Mathematics of RAS, Moscow, Russia*
10^{55}-11^{25}	Plenary Presentation **A.A. Rukhadze** Main development stages of fundamental physics of plasma without collisions. Modeling, analysis. *A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia*
11^{25}-11^{55}	Plenary Presentation **B.N. Chichkov** Laser printing of nanoparticles *Laser Zentrum, Hannover, Germany*
12^{00}-12^{30}	***Coffee break***
12^{30}-13^{00}	Plenary Presentation **A.A. Samokhin[1],** V.I.Mazhukin[2] Continual and molecular-dynamic modeling of phase transitions during laser ablation *[1]A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia* *[2]M.V. Keldysh Institute of Applied Mathematics of RAS, Moscow, Russia*
13^{00}-14^{00}	***Lunch time***

14^{00}-14^{20}	Invited Presentation Mindaugas Gedvilas[1], Bogdan Voisiat[1], Simonas Indrišiūnas[1], Gediminas Račiukaitis[1], **Vadim Veiko[2]**, Roman Zakoldaev[2], Dmitry Sinev[2], Elena Shakhno[2] Thermochemical recording of interference patterns on thin Cr-films by picosecond laser pulse irradiation - experimental realization & theoretical modeling *[1]Center for Physical Science and Technology, Vilnius, Lithuania* *[2]ITMO University, St.Petersburg, Russia*
14^{20}-14^{40}	Invited Presentation **Irina Potapenko[1,2]**, Stanislav Karpov[2] Kinetic simulation of heat transport in collision laser produced plasmas *[1]Keldysh Institute of Applied Mathematics of RAS, Moscow, Russia* *[2]Dukhov All-Russia Research Institute of Automatics, Moscow, Russia*
14^{40}-15^{00}	Invited Presentation **A.G. Kaptilniy[1],** A.A. Karabutov[2], Lead is a perspective heat carrier of the first contour of supercritical nuclear reactor *[1]Joint Institute for High Temperatures of RAS, Moscow, Russia.* *[2]International Laser Center, Moscow State University, Moscow, Russia.*
15^{00}-15^{20}	Invited Presentation **K.V. Khishchenko** Multiphase equations of state for metals at high dynamic pressures *Joint Institute for High Temperatures of RAS, Moscow, Russia*
15^{20}-15^{40}	Invited Presentation **M.E. Povarnitsyn,** V.B. Fokin, P.R. Levashov, K.V. Khishchenko Two approaches for modeling of laser ablation of metals: hydrocode with a model of nucleation and hybrid molecular-dynamic method *Joint Institute for High Temperatures of RAS, Moscow, Russia*
15^{40}-16^{00}	Invited Presentation **M.P. Galanin[1]**, V.V. Lukin[1], A.S. Rodin[1], I.V. Stankevich[2] The modeling of contact interaction of solids by means of Schwartz method *[1]Keldysh Institute of Applied Mathematics of RAS, Moscow, Russia* *[2]Bauman Moscow State Technical University, Moscow, Russia*

16^{00}-16^{30}	***Coffee break***
16^{30}-16^{50}	Invited Presentation Mikhail E. Zhukovskiy, **Sergey V. Podoliako**, Mikhail B. Markov, Roman V. Uskov, Alexandr S. Vorontsov Mathematical maintenance of experiments with penetrating radiatio *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{50}-17^{05}	Oral Presentation Mikhail E. Zhukovskiy, Mikhail B. Markov, Sergey V. Podoliako, **Roman V. Uskov** Supercomputing the cascade processes of radiation transport *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
17^{05}-17^{20}	Oral Presentation **V.O. Podryga**, S.V. Polyakov Molecular dynamic simulation of rarefied gas flow in metallic microchannel *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
17^{20}-17^{35}	Oral Presentation **N.A. Inogamov**[1], V.V. Zhakhovsky[2], V.A. Khokhlov[1] Separation and 3d-expansion of gold film from substrate under action of femtosecond laser pulse *[1]Landau Institute for Theoretical Physics of RAS, Chernogolovka, Russia,* *[2]All-Russia Research Institute of Automatics, ROSATOM, Moscow, Russia.*
17^{35}-17^{50}	Oral Presentation **I.V. Gasilova** Support operators technique for distributed 3d simulation of dissipative processes *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
19^{00}	**POSTER SECTION**

Tuesday, June 2	
RUSSIAN SPACE	
10^{00}-10^{15}	Oral Presentation **G.K. Borovin,** Yu.F. Golubev, A.V. Grushevskiy, V.V. Korianov, A.G. Tuchin, D.A. Tuchin Mission design in systems of outer planets within model restricted two-coupled three-body proble *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{15}-10^{30}	Oral Presentation **I. Molotov,** V. Voropaev, V. Zolotov, T. Fakhrutdinov, G. Borovin Development of the ISON optical network to imrove the conjuction analysis *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{30}-10^{45}	Oral Presentation **M.V. Mikhaylyuk** A realistic model of the Earth in space simulators *Scientific Research Institute for System Analysis of RAS Moscow, Russia*
10^{45}-11^{00}	Oral Presentation **I.E. Molotov** About possibility of application of EOP-1/EOP-2 miniobservatories of Roscosmos for asteroid observations *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
11^{00}-11^{15}	Oral Presentation **L. Elenin**[1], I. Molotov[1], Yu. Krugly[2] ASPIN - ISON asteroid's research program: history, current state and future prospects [1]*Keldysh Institute of Applied Mathematics of RAS,* [2]*Institute of Astronomy of Kharkiv National University*
11^{15}-11^{45}	***Coffee break***
MATHEMATICAL MODELING	
11^{45}-12^{00}	Oral Presentation **V.I. Mazhukin,** M.M. Demin, A.V. Shapranov Mathematical modeling of pulsed laser melting of aluminum *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*

12^{00}-12^{15}	Oral Presentation **A. A. Samokhin**[1], N. N. Il'ichev[1], P.A. Pivovarov[1,2], A.V. Sidorin[1] Acoustical and optical monitoring of absorbing liquid behavior induced by nanosecond laser irradiation under transparent cover. *[1] A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia* *[2] National Research Nuclear University MEPhI, Moscow, Russia*
12^{15}-12^{30}	Oral Presentation **O.N. Koroleva**, AV. Mazhukin, P.V. Breslavskii Analysis of mathematical models of laser heating and melting of silicon *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
13^{00}-14^{00}	***Lunch time***
14^{00}-14^{15}	Oral Presentation **Žarko Pavićević** Local boundary properties of mappings: a general approach *University of Montenegro, Faculty of Science, Pogdorica, Montenegro*
14^{15}-14^{30}	Oral Presentation **T.K. Kozubskaya** Mathematical models and numerical schemes on unstructured meshes for solving aerodynamics+aeroacoustics problems *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
14^{30}-14^{45}	Oral Presentation **M.A. Trapeznikova**, N.G. Churbanova, A.A Lyupa Simulation of three-phase fluid flow in a porous medium with account of thermal effects *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
14^{45}-15^{00}	Oral Presentation **N.G. Churbanova**, A.A. Chechina, M.A. Trapeznikova Two approaches to the vehicular traffic flows simulation using high-performance computer systems *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
15^{00}-15^{30}	***Coffee break***

15^{30}-15^{45}	Oral Presentation **Sviatoslav A. Stumpf**, Alexander A. Korolev, Sergei A. Kozlov Modelling a stimulated amplification of long-wave wing of a multi-harmonic light beam at propagation in dielectric media with induced plasma and static electric field *ITMO University, Saint-Petersburg, Russia*
15^{45}-16^{00}	Oral Presentation **G. Bagdasarov**, A. Boldarev Numerical studies by means of MARPLE: new tools for parallel simulation of continuous media using unstructured meshes *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{00}-16^{15}	Oral Presentation **A.S. Boldarev** Development of the 3D code for numerical modelling MARPLE: generalized programming and creation of really universal codes *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{15}-16^{30}	Oral Presentation Yu.N. Karamzin, T.A. Kudryashova, **V.O. Podryga**, S.V. Polyakov Multiscale modeling in supersonic gasdynamic sputtering problems *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{30} - 16^{45}	Oral Presentation M.B. Markov, **I. A. Tarakanov**, Y.A. Volkov Approximation of continuous breaking for modeling radiation-induced conductivity of crystals *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{45} 17^{00}	Oral Presentation **L.V. Klochkova**, V.F. Tishkin A critical analysis of the mathematical models and simulation results describing the distribution of impurities in the atmosphere *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
19^{00}	**POSTER SECTION**

Wednesday, June 3	
08^{00}-20^{00}	**SOCIAL PROGRAM**
Thursday, June 4	
10^{00}-10^{20}	Invited Presentation **I.N. Zavestovskaya**[1,2] Laser metal nanocrystallization: theoretical modeling *[1]P.N. Lebedev Physical Institute of RAS, Moscow, Russia* *[2]National research Nuclear University MEPhI (Moscow Engineering Physics Institute), Moscow, Russia*
10^{20}-10^{35}	Oral Presentation **I. Tsymbalov**[1], S. Shulyapov[1], A. Brantov[2], K. Ivanov[1], P. Ksenofontov[2], D. Krestovskikh[1], V. Bychenkov[2], V. Nedorezov[3] and A. Savel'ev[1] Parametric wave excitation in relativistic laser-plasma interaction in long under-critical pre-plasma layer *[1]Faculty of Physics and International Laser Center of Lomonosov Moscow State University, Moscow, Russia* *[2]P.N. Lebedev Physical Institute of RAS, Moscow, Russia* *[3]Institute for Nuclear Research of RAS, Moscow, Russia*
10^{35}-10^{50}	Oral Presentation **V.T. Zhukov**, O.B. Feodoritova, N.D. Novikova Multigrid and explicit-iterative solvers for threedimensional parabolic equations *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{50} - 11^{05}	Oral Presentation **O.B. Feodoritova**, Yu.G. Rykov Numerical investigations of variational representation for generalized solutions of quasilinear hyperbolic equations *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
11^{05} – 11^{20}	Oral Presentation Yu.V.Vassilevski[1], I.V.Kapyrin[1,2], **I.N.Konshin**[1,2] INMOST software platform based development of parallel numerical models on general meshes *[1]Institute of Numerical Mathematics of RAS* *[2]Nuclear Safety Institute of RAS*

11^{20}-12^{00}	***Coffee break***
12^{00}-12^{15}	Oral Presentation **N. Mikhalević** Analysis of the direct spectral problem for inverse problem of an operator of Sturm–Liouville *Maritime Faculty,University of Montenegro, Kotor, Montenegro*
12^{15}-12^{30}	Oral Presentation **Romeo Meštrović**[1], Žarko Pavićević[2] Different metrics and topologies on Privalov spaces on the unit disk [1]*Maritime Faculty,University of Montenegro, Kotor, Montenegro* [2]*Faculty of ScienceUniversity of Montenegro, Podgorica, Montenegro*
12^{30}-12^{45}	Oral Presentation **Zirojević Marina**[1], Jokanović Dušan[1], Baralić Đorđe[2] Software 'Cinderella' and its application in visualization of physic and mathematics [1]*Bosnia and Herzegovina University of East Sarajevo, Production and Management Faculty, Trebinje, BiH* [2]*Serbia Mathematical Institute SASA*
12^{45}-13^{00}	Oral Presentation **Dušan Jokanović**[1], Tatjana Mirković, Generalization of a discrete Opial type inequality applied to the eigenvalues of graph [1]*University of East Sarajevo* *Production and Management Faculty Trebinje* *Stepe Stepanovica bb, 89101 Trebinje, Republic of Srpska, BiH*
13^{00}-14^{00}	***Lunch time***
14^{15}-14^{30}	Oral Presentation **Andrej Novak** Continuum model of gene expression *University of Zagreb, Faculty of Electrical Engineering and Computing, University of Zagreb, Croatia*
14^{30} – 14^{45}	Oral Presentation **Biljana Vojvodic**[1], Milenko Pikula[2] The boundary value problem with n delays and asymptotic of eigenvalues [1]*Ministry of Science and Technology Republic of Srpska, Banja Luka, Republic of Srpska, Bosnia and Hercegovina* [2]*University of East Sarajevo, Faculty of Philosophy, Republic of Srpska, Bosnia and Hercegovina*

14^{45}-15^{00}	Oral Presentation **D. Efimov** Click-Through Rate Prediction - TOP-5 solution for the Avazu contest *American University of Sharjah, Sharjah, UAE*
15^{00}-15^{30}	***Coffee break***
15^{30}-15^{45}	Oral Presentation **A.I. Chernov[1,2],** P.V. Fedotov[1], A.V. Osadchy[1,2], V.L. Kuznetsov[3,4], E.A. Obraztsova[1], A.L. Chuvilin[4,5], E.D. Obraztsova[1,2] One-dimensional structures inside single-walled carbon nanotubes *[1]A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia* *[2]National Research Nuclear University MEPhI, Moscow, Russia* *[3]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia* *[4]Novosibirsk State University, Novosibirsk, Russia* *[5]CICnanoGUNEConsolider, San Sebastian, Spain* *[6]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain*
15^{45} – 16^{00}	Oral Presentation **A.E. Bondarev** Parametric studies of Space-Time Structures for CFD Problems *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
16^{00}-18^{00}	**THEMATIC HEADINGS "SCIENCE LIFE"** **ROUND-TABLE DISCUSSION**
	Invited Presentation **A.A. Samokhin** Scientific society in epoch of changes *A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia*
	Invited Presentation **M.M. Gorbunov-Posadov**, T.A. Polilova Multimedia illustrations for scientific publications *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
	Invited Presentation **I.Yu. Novitsky** Modeling of processes of development of large urban agglomerations *Fuel and Energy Department of the city of Moscow, Russia*
POSTER SECTION	

	Friday, June 5
	BRIEF REPORTS
10^{00}-10^{10}	**A.V. Mazhukin**, O. N. Koroleva, P. V. Breslavskii Statement of calculating experiment of molecular dynamics determination of thermophysical properties of silicon *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{10}-10^{20}	**P. V. Breslavskii**, O. N. Koroleva, A.V. Mazhukin Simulation of the dynamics of plasma expansion into the air induced by nanosecond laser irradiation *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{20} – 10^{30}	Mindaugas Gedvilas[1], Bogdan Voisiat[1], Simonas Indrišiūnas[1], Gediminas Račiukaitis[1], Vadim Veiko[2], **Roman Zakoldaev[2]**, Dmitry Sinev[2], Elena Shakhno[2] Direct recording of Multi-Beam Interference Patterns on Titanium Films by Nano- & Picosecond Laser Pulses *[1]Center for Physical Science and Technology, Vilnius, Lithuania* *[2]ITMO University, St.Petersburg, Russia*
10^{30} – 10^{40}	A.V. Berezin, F.N. Voronin, V.A. Gasilov, **K.K. Inozemtseva,** A.E. Lutskiy, M.B. Markov, S.V. Parotkin Mathematical model of fluid dynamic effects in high-energy electrons flux *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
10^{40} - 10^{50}	**Sanja Jancic Rasovic[1]**, Irina Cristea[2] Multiendomorphisms as a tool to construct new hyperri *[1]Faculty of Natural Science and Mathematics, University of Montenegro, Podgorica, Montenegro* *[2]Centre for Systems and Information Technologies, University of Nova Gorica, Nova Gorica, Slovenia*
10^{50} – 11^{00}	**L. I. Galanina**, L. S. Novikov Mechanisms of nuclear reactions at interaction of cosmic rays with materials of microelectronic elements *Skobeltsyn Institute of Nuclear Physics, Moscow State University*

11^{00}-11^{10}	**B.I.Denker**[1], B.I.Galagan[1], S.E.Sverchkov[1], E.M.Dianov[2] Spectral-luminescence propertiesof Bi-doped oxide glasses *[1]A.M.Prokhorov General Physics Institute of RAS, Moscow, Russia* *[2]Fiber Optics Research Center of RAS Moscow, Russia*
11^{10}-11^{20}	**A.V. Osadchy**[1,2], D.V. Rybkovskiy[1], E.D. Obraztsova[1,2] Usage of the semi-empirical pseudopotention method for the gallium selenide nanomaterials band structure calculation *[1]A. M. Prokhorov General Physics Institute of RAS, Moscow, Russia* *[2]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Moscow, Russia*
11^{20}-12^{00}	***Coffee break***
12^{00}-12^{10}	**S.N. Bokova-Sirosh**[1,2], M. A. Shuvaeva[3,4], A. V. Ishchenko[3,4], D.V. Krasnikov[3,4], V.L. Kuznetsov[3,4,6], A.I. Romanenko[5], E.N. Tkachev[5] and E.D. Obraztsova[1,2] Optical and electrical studies of defect multi-wall carbon nanotubes synthesized with Fe-Co catalysts of variable structure *[1]A.M. Prokhorov General Physics Institute RAS, Moscow, Russia* *[2]National Research Nuclear University «MEPhI», Moscow, Russia* *[3]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia* *[4]Novosibirsk State University, Novosibirsk, Russia* *[5]Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia* *[6]National Tomsk State University, Tomsk, Russia*
12^{10}-12^{20}	**Snežana Jovanović** The concept of college library *Library of natural and technical sciences, University of Montenegro*
12^{20}-12^{30}	**N.D. Novikova**, O.B. Feodoritova, K.V. Manukovskii, Yu.G. Rykov, V.T. Zhukov On high speed flow simulation in model ramjet engine *Keldysh Institute of Applied Mathematics of RAS; Moscow, Russia*
12^{30}-12^{40}	**D. S. Polyakov**, E. B. Yakovlev Limits of applicability of the two temperature model for nonuniform heating of condensed matter by ultrashort laser pulses *ITMO University, Saint-Petersburg, Russia*

12^{40}-12^{50}	**Д. С. Поляков,** В. П. Вейко, А. М. Скворцов, К. Т. Хуинь, Е. С. Чопенко, А. А. Самохвалов Исследование продуктов лазерной абляции кремния в различных средах при облучении наносекундными импульсами иттербиевого волоконного лазера *Университет ИТМО, Санкт-Петербург, Россия*
12^{50}-13^{00}	**Vanja Vukoslavčević** Spline difference scheme on a uniform and piecewise uniform grid *Faculty of Sciences, University of Montenegro*
13.00-14.00	***Lunch time***
SUMMING. CLOSING OF SEMINAR.	
BANQUET, CLOSING SPEECH	
Saturday, June 6	
10.00-13.00	Departure

ABSTRACTS

ОСОБЕННОСТИ СОВРЕМЕННОГО МАТЕМАТИЧЕСКОГО МОДЕЛИРОВАНИЯ

В.И.Мажукин, А.В.Шапранов, М.М.Демин

Институт прикладной математики им. М.В. Келдыша РАН, Москва, РФ
e-mail: vim@modhef.ru

Чрезвычайно широкое распространение методов Математического Моделирования (ММ) и Вычислительного Эксперимента (ВЭ) [1], рис.1 связано не только с несомненными успехами и преимуществами, но и с определенными затруднениями и недостатками. Высокая востребованность в исследованиях методов ММ зачастую приводит к тому, что отдельные элементы ВЭ (см. рис.1) занимают доминирующее положение () в ущерб остальным. Так массовый характер приобрело применение, как правило, в режиме «черного ящика» вычислительных кодов (SOFTWARE) известных разработчиков, зачастую за пределами их применимости. В качестве примера, можно указать применение энтальпийного подхода к численному решению классической задачи Стефана в задачах импульсного лазерного воздействия. Использование вычислительных кодов за рамками их применимости приводит к появлению результатов не вызывающих доверия, но формально совпадающих с данными натурных экспериментов. Вторая проблема современного ММ связана с поспешным и поверхностным использованием математических постановок без должного понимания сути явлений. Примером может служить, так называемая, проблема “blast force”, при численном решении, которой авторы [2] вычислительным путем получили труднообъяснимые неравновесные эффекты. Указанные проблемы требуют внимательного и критического анализа.

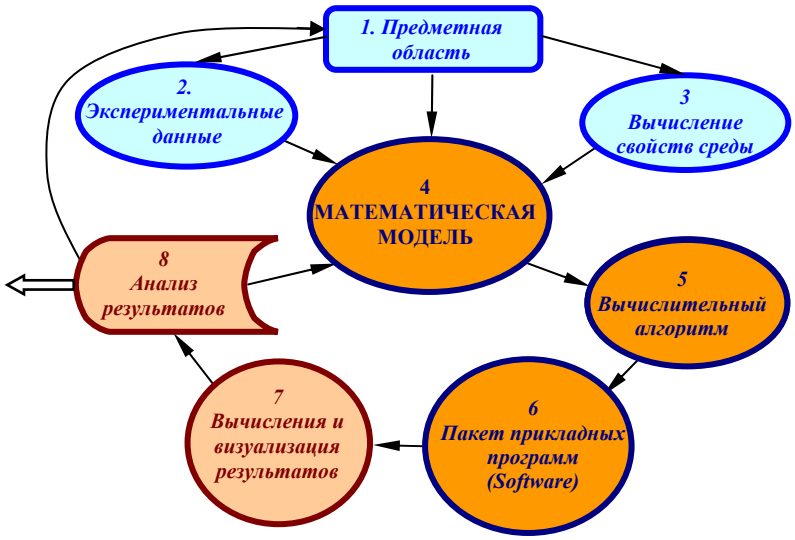


Рис.1 Схема вычислительного эксперимента.

Благодарности: Работа выполнена при финансовой поддержке РНФ № 15-11-00032

Литература:

1. A.A. Samarskii. “Mathematical modeling and computational experiment”. Herald of USSR Academy of science, No. 5, 38-49 (1979)
2. Yonggang Shen, Yong Gan, Wanjun Qi, Yaogen Shen, and Zhen Chen "Effect of the hot electron blast force on ultrafast laser ablation of nickel thin film", Appl. Opt., **54**, 1737-1742 (2015)

PECULIARITIES OF OF MODERN MATHEMATICAL MODELING

V.I. Mazhukin, A.V. Shapranov, M.M. Demin

M.V. Keldysh Institute of Applied Mathematics of RAS
e-mail: vim@modhef.ru

Extremely wide proliferation of the methods of mathematical modeling (MM) and computer experiment (CE) [1] (Figure 1) is connected not only with the undoubted successes and benefits, but also with certain difficulties and disadvantages. High demand for the research methods of MM often leads to the fact that some elements of CE (see. Figure 1) occupy a dominant position () to the detriment of others. For example, massive use of purchased computer codes (SOFTWARE) from the known developers, as a rule, in the "black box" mode, and often outside of their applicability. As an example, one can specify the use of enthalpy approach to the numerical solution of the classical Stefan problem in the problems of pulsed laser action. Using the computational codes beyond their applicability leads to not credible results, but in the formal agreement with the data of field experiments. The second problem in the modern MM is related to the hasty and superficial use of mathematical statements without proper understanding of the phenomena. An example is the so-called problem of "blast force" during the numerical solution of which the authors [2] obtained non-equilibrium effects, which are difficult to explain. These problems require careful and critical analysis.

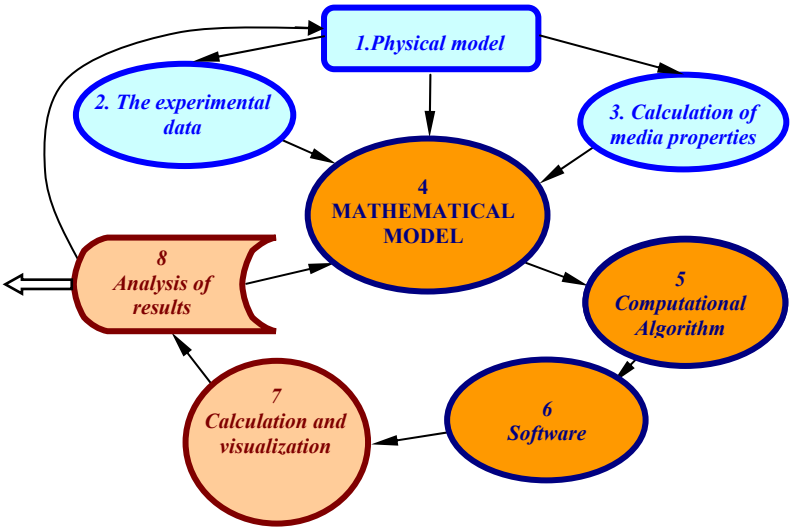


Fig.1. Computational experiment scheme.

Acknowledgements: This work was supported by RSCF grant № 15-11-00032.

References:

1. A.A. Samarskii. “Mathematical modeling and computational experiment”. Herald of USSR Academy of science, No. 5, 38-49 (1979).
2. Yonggang Shen, Yong Gan, Wanjun Qi, Yaogen Shen, and Zhen Chen “Effect of the hot electron blast force on ultrafast laser ablation of nickel thin film”, Appl. Opt., **54**, 1737-1742 (2015).

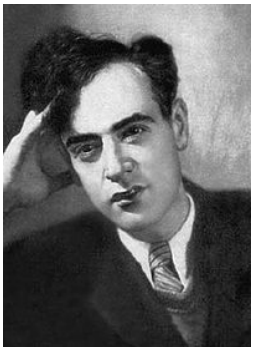
ОСНОВНЫЕ ЭТАПЫ РАЗВИТИЯ ФУНДАМЕНТАЛЬНОЙ ФИЗИКИ ПЛАЗМЫ БЕЗ СТОЛКНОВЕНИЙ. МОДЕЛИРОВАНИЕ, АНАЛИЗ

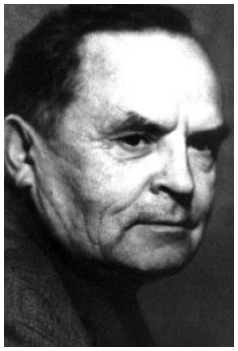
А.А. Рухадзе

Институт общей физики им. А.М Прохорова РАН, М. ул. Вавилова 38.

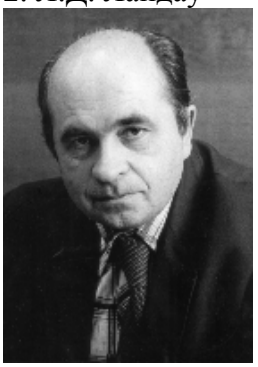
Дается краткий исторический обзор развития фундаментальной физики плазмы, в котором основные этапы были определены следующими физиками.


1. И. Ленгмюр


2. Л.Д. Ландау


3. А.А. Власов


4. Н.Н. Боголюбов


5. Б.Б. Кадомцев


6. В.П. Силин

И. Ленгмюр впервые экспериментально исследовал свойства плазмы, нашел основные характеристики плазмы и определил условия реализации плазменного состояния; Л.Д. Ландау первым понял причину неприменимости газового приближения для описания плазмы, но пренебрег самосогласованным полем и не достиг цели; А.А. Власов показал важную роль самосогласованного поля, и первый получил правильное уравнение, описывающее плазму, а также теоретический обосновал эксперименты И. Ленгмюра по наблюдению плазменных волн и их дисперсию; Н.Н. Боголюбов развил общий метод вывода динамических уравнений для плазмы и показал, что в первом приближении по параметру Ландау справедливо уравнение Власова, а втрое приближение приводит к поправке Ландау к уравнению Власова; Г.В. Гордеев впервые показал, что звуковая ветвь колебаний отличается от звука в газах, звук в плазме изотермический и существует только в неизотермической плазме; Б.Б. Кадомцев и В.П. Силин показали, что в плазме существуют незатухающие моды ионно-звуковых колебаний и впервые построили теорию турбулентности плазмы на незатухающих модах Власова.

LASER PRINTING OF NANOPARTICLES

B. Chichkov

Laser Zentrum Hannover e.V., Hollerithallee , 30419 Hannover, Germany

I will report on our recent progress in the development of laser printing technologies for fabrication of complex nanoparticle structures [1,2]. Fabrication, characterization, and applications of the generated nanoparticle arrays in nanophotonics, plasmonics, and optical sensing will be demonstrated and discussed.

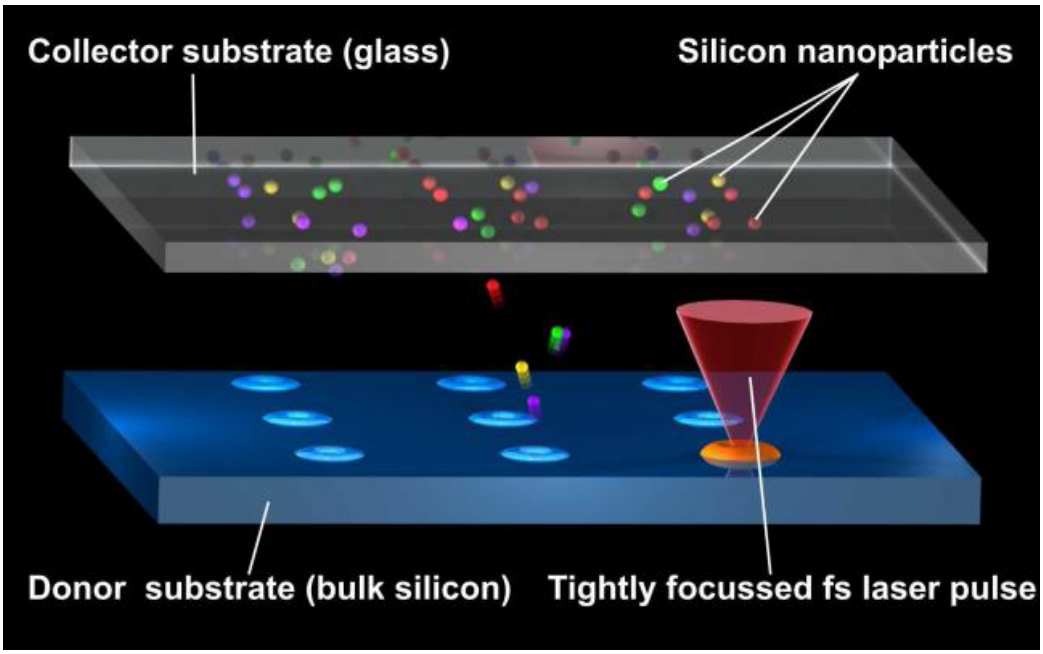


Fig. 1 Experimental setup applied for laser printing of nanoparticles.

References

[1] U. Zywietz et. al. Appl Phys A, **114**, 45 (2014).
[2] U. Zywietz et. al. Nature Commun. 5, 3402 (2014) .

CONTINUAL AND MOLECULAR-DYNAMIC MODELING OF PHASE TRANSITIONS DURING LASER ABLATION

A.A. Samokhin[1], V.I.Mazhukin[2]
[1]*Prokhorov General Physics Institute,Russian Academy of Sciences, Vavilov Str., 38, 119991 Moscow, Russia*
[2]*M.V. Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Myusskaia sq. 4, 125047 Moscow, Russia*
E-mail address: asam40@mail.ru

In this report a comparative description of various theoretical methods in modeling of phase transition induced by intense laser pulses in condensed matter is presented.

The methods include, in particular, continual (fluid dynamics), kinetic and molecular-dynamic modeling. Non-equilibrium features of laser initiated phase transitions such as explosive boiling or spinodal decomposition and their description in different approaches are discussed in details. The discussion is necessary because of some important points of the problem are not yet completely clarified.

For example, appearance of explosive boiling in metals irradiated with intense laser pulses is not evident beforehand because of high values of thermal conductivity and small radiation penetration length. For this reason in some theoretical descriptions of the explosive boiling process in irradiated metals (see [1] and cited there earlier papers) it is declared that in such a case subsurface superheating is impossible. However, our recent results [2,3] obtained with the help of molecular-dynamic modeling show that it is the subsurface superheating which gives rise to metal explosive boiling during nanosecond laser pulse irradiation. At shorter laser pulses which generate negative pressure values in the subsurface region one observes spallation effect that takes place (in the terms of equation of state) near spinodal line in its negative pressure part (see, e,g,, [4,5] and references therein).

According to Van der Waals equation of state constant pressure heat capacity diverges and changes its sign at spinodal line. In real physical systems no such well defined line exists because of growing unstable thermodynamical fluctuations. Spinodal and critical point manifestations in strongly non-equilibrium conditions of laser ablation need more experimental and theoretical investigations [6].

Acknowledgements: This work was supported by RFBR projects Nos 13-02-01129, 15-07-05025, 13-07-00597.

References

1. M. Q. Jiang, Y. P. Wei, G. Wilde, L. H. Dai. Appl. Phys. Let. **106**, 021904 (1-6), (2015).
2. V.I.Mazhukin, A.A. Samokhin, M.M. Demin,A.V.Shapranov. Quantum Electronics. **44**, No. 4, 283–285, (2014).
3. V.I.Mazhukin, A.A.Samokhin, M.M.Demin, A.V.Shapranov. Math. Montisn. **29**, (2014).
4. C. Wu, L.V. Zhigilei, Appl. Phys. A, 114, 11-32, (2014).
5. A. K. Upadhyay, N.A. Inogamov, B. Rethfeld, H.M. Urbassek. Phys. Rev.B, 78, 045437, ┌ (2008).
6. I. A. Artyukov, D. A. Zayarniy, A. A. Ionin, S. I. Kudryashov, S.V. Makarov, P.N. Saltuganov, PZhETF, **99**, 1, 54-58, (2014).

THERMOCHEMICAL RECORDING OF INTERFERENCE PATTERNS ON THIN CR-FILMS BY PICOSECOND LASER PULSE IRRADIATION - EXPERIMENTAL REALIZATION & THEORETICAL MODELLING

Mindaugas Gedvilas[1], Bogdan Voisiat[1], Simonas Indrišiūnas[1], Gediminas Račiukaitis[1], Vadim Veiko[2], Roman Zakoldaev[2], Dmitry Sinev[2], Elena Shakhno[2]

[1]Center for Physical Science and Technology, Savanoriu Ave. 231, LT- 02300, Vilnius, Lithuania
[2]ITMO University, Kronverksky Ave. 49, St.Petersburg, 197101, Russia

Interference of laser beams with the high pulse power density opens an opportunity of direct structuring over large areas. We report results of the thermo-chemical treatment of thin metal films irradiated by multi-beam interference picosecond pulses combined with the following chemical etching.

The essence of laser-induced thermo-chemical recording consists in a local heating of a metallic film for a temperature about a melting point at the normal atmosphere where a surface oxidation takes place [1]. Pulsed laser irradiation initiate formation of thin layer of the chromium oxide Cr2O3 at irradiated zones of the surface, and the oxide preserve metallic film from etching in a proper chemical solvent (some alkali or acids). In this way, the image written by a laser can be developed and registered on a metallic film [2]. The spatial resolution of this method can be quite high due to so-called thermo-chemical sharpening [3] and can even be close to the diffraction limit.

The laser beam was split into two, tree, four or six beams by using the diffractive optical elements. The confocal imaging system was used to produce interference pattern on the chromium films. As a result, 1D and 2D planar structures with a period varying from 1.5 μm to 3.5 μm were produced on the glass surface after chemical treatment (Fig. 1).

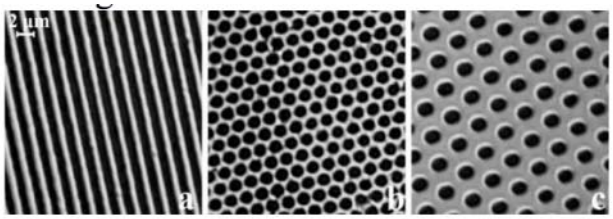


Fig. 1 The micro image of chromium planar structures formed on the glass surface after chemical etching followed the nanosecond laser irradiation.

Acknowledgements:

This work was supported by the Russian Scientific Fond Grant No. 14-12-00351 (on 50%), RFBR grant No. 14-29-07227 ofi_m, the President of the Russian Federation Grant No. NSH 1364.2014.2., and the Government of the Russian Federation Grant No. 074-U01).

References:

1. V.P. Veiko, G.A. Kotov, M.N. Libenson, M.N. Nikitin. “Thermochemical action of laser radiation”. Sov Phys Doklady, 18, 83-85 (1973)

2. V. Veiko, E. Shakhno, A. Poleshchuk, V. Korolkov et al. “Local laser oxidation of thin metal films: ultra-resolution in theory and in practice”. Journal of Laser Micro/Nanoengineering, **3**, 3, 201-205 (2008).

3. V.P. Veiko, V.L. Korol'kov, A.G. Poleshchuk, et al. “Study of the spatial resolution of laser thermochemical technology for recording diffraction microstructures”. Quantum Electronics, **41**, 7, 631-636 (2011).

KINETIC SIMULATION OF HEAT TRANSPORT IN COLLISION LASER PRODUCED PLASMAS

Irina Potapenko[1,2], Stanislav Karpov [2]
[1] *Keldysh Institute of Applied Mathematics RAS, 125047 Moscow, Russian Federation*
[2] *Dukhov All-Russia Research Institute of Automatics, 127055 Moscow, Russian Federation*
firena@yandex.ru

Sincethe early 1970s, in connection with the development of laser technology and the performance of the first ICF experiments, interest in the problem of interaction of intense laser radiation with plasma increased substantially. Such interaction results in the appearance of high temperature and density gradients, which casts doubts on the possibility of describing actual laser experiments in the framework of the classical transport theory. To date, there are a lot of experimental data [1] confirming the idea about the nonlocal character of heat transport in laser produced plasmas. This concerns, first of all, the description of the heat flux, because the electron heat transport plays a crucial role in the energy balance in laser produced plasmas. The problem of the heat flux intensity is one of the key problems to be solved for successful implementation of inertial confinement fusion (ICF), because most energy of the incident laser radiation is absorbed near the critical density (i.e., far from the ignition region) and is then carried deep into the plasma by the electron heat flux, which determines the heating rate, temperature, and compression ratio of the target.

The analytical theory of nonlocal transport is designed only for the small temperature perturbations [2]. So the only way to calculate the parameters of the heat transport in plasma with the temperature inhomogeneity scale length less or equal to one hundred electron mean free path lengths is the numerical simulation of the kinetic equation with Landau-Fokker-Planck collision operator.

We suggest an effective approach to the numerical solution of the plasma kinetic equation that is based on a new DSMC method [3, 4] for the nonlinear collision operator. For wide range of parameters the relaxation of the initial temperature perturbation in a collisional plasma is investigated in 1D3V geometry. The obtained numerical results are compared with many various transport models which describe the process with some differences. A good agreement with nonlocal heat transport model [5] is found. Also the heat wave propagation from the heating region deep into the plasma is considered. The temperature profile and flux dependence on time is examined. The structure of the temperature wave front, particularly, the difference from the hydrodynamic description is investigated.

Acknowledgements: Support of Program n 18 of Presidium RAS and Grant RFFI № 14-02-31407 is acknowledged.

References :

[1] R.E. Harrington, Journal of Appl. Phys. **37**, 2028 (1966).
[2] S. Brunner, E. Valeo, Phys. Plasmas **9**, 923 (2002).
[3]A.V. Bobylev, I.F. Potapenko, S.A. Karpov, AIP Conference Proceeding 1501, 541, (2013).
[4] A.V. Bobylev, I.F. Potapenko, J. Comp. Phys. **246**, 123 (2013).
[5] A. Marocchino et al., Phys. Plasmas **20**, 022702 (2013).

СВИНЕЦ - ПЕРСПЕКТИВНЫЙ ТЕПЛОНОСИТЕЛЬ 1 – ГО КОНТУРА СВЕРХКРИТИЧЕСКОГО РЕАКТОРА АТОМНОЙ ЭЛ. ГЕНЕРИРУЮЩЕЙ УСТАНОВКИ

А.Г. Каптильный[1], А.А. Карабутов[2]
[1]*Объединенный институт высоких температур РАН, 125412, Москва, ул. Ижорская, д. 13, стр. 2*
E-mail: Kalexandr48@gmail.com
[2]*Международный учебно-научный лазерный центр МГУ имени М.В. Ломоносова, 119991, Москва, Ленинские горы, д. 1, стр. 62*
E-mail: aak@ilc.edu.ru

Технологические процессы, основанные на использовании Сверхкритических Флюидов (СКФ), являются процессами следующего поколения новых экологически чистых технологий 6-го технологического уклада.

Но при этом в СКФ-средах имеется ряд фундаментальных проблем: недостаточно исследованы физико-химические свойства СКФ высокие скорости процессов переноса, настраиваемая плотность, низкая вязкость, и др.

В современной энергетике переход на теплоносители сверхкритических параметров позволяет резко увеличить КПД «тепловой» части оборудования с 24% до ~40% атомной эл. генерирующей установки (докритический свинец – теплоноситель 1 контура нагрева, вода (СКФ) теплоноситель - 2 контура нагрева). В данном случае сверхкритическим теплоносителем является вода во втором контуре нагрева. Свинец непосредственно омывает тепловыделяющие сборки ТВЭЛ в энергетическом реакторе. Исследование теплофизических свойств свинца, вплоть до критической точки необходимо для проведения комплексных работ по математическому моделированию безопасной работы реактора в широко диапазоне режимных параметров. В первом приближении необходимо знать о наличии или отсутствии особенностей поведения свинца в высокоэнергетической области параметров состояния.

В настоящей работе было проведено исследование лазерно-индуцированных состояний свинца «**Pb**» и графита «**C**» в до и сверхкритической области при квазиизохорном нагреве механически нагруженной облучаемой поверхности вещества.

Получены данные по динамике изменения термодинамических параметров состояния: давление **P** и температура **T** в процессе лазерного нагрева. Представлены результаты измерения отражательной способности в этих условиях. При экспериментальном исследования установлено, что отражательная способность свинца «**Pb**» падает более чем в 5 раз относительно первоначального значения, что указывает на существенные изменения в электронном спектре металла в этой области.

В случае графита показано, что при температурах **T** ~ 5700 K и давлениях **P** ~ 0.77Gpa (7700 бар) отражательная способность снижается практически на порядок.

Литература:

1. Ivochkin A.Yu., Kaptilniy A.G., Karabutov A.A., Ksenofontov D.M. “Laser opto-acoustic study of phase transitions in metals confined by transparent dielectric”, Laser Physics (ISSN 1054-660), **22**, N. 7, 1220-1228 (2012).
2. Ivochkin A.Yu., Kaptilniy A.G., Karabutov A.A., Ksenofontov D.M “Pulsed laser heating of metal surface confined by thin layer of transparent dielectric: an experimental approach for creation of supercritical chemical reactor”, Mendeleev Communications. **23**, 4, ISSN 0959-943, (2013).

LEAD IS A PERSPECTIVE HEAT CARRIER OF THE FIRST CONTOUR OF SUPERCRITICAL NUCLEAR REACTOR

A.G. Kaptilniy[1], A.A. Karabutov[2],
[1]*Joint Institute for High Temperatures, Russian Academy of Science, Moscow, Russia.*
E-mail: Kalexandr48@gmail.com
[2]*International Laser Center, Moscow State University, Moscow, Russia.*
E-mail: aak@ilc.edu.ru

Technological processes based on supercritical fluids (SCF) are the processes of future generation of new ecologically clear technologies of 6th technological style. But some important fundamental problems appear here: SCF physical-chemical properties has not been studied sufficiently (high speed of transfer processes, low surface tension, adjustable density, dissolving capacity, low viscosity, etc.).

In modern energetics, using of supercritical heat transfer agents allows to increase considerably the efficiency of "heat" part of the equipment from 24% to 40% of nuclear electro generated plant (subcritical lead is the heat transfer agent of the first contour, supercritical water is the heat transfer agent of the second contour). The lead directly flows past heat generating unit assembly of nuclear reactor.

Investigation of heat-transfer properties of lead up to critical point is required for extensive mathematical modelling for the safe operation of nuclear reactor in wide range conditions. At first, it is required to learn the specifics of lead behavior in near critical region of state parameters.

In present investigation we studied laser induced SCF of lead and carbon by quasi-isochoric heating of metal surface covered by transparent dielectric.

We received data on dynamic of changes of thermodynamic parameters of lead states: pressure P and temperature T during laser heating process. We represent the results of reflectivity measuring in these conditions.

It shows that lead reflectivity decreases in these conditions more than 5 times as compared with initial state. For carbon with temperature $\boldsymbol{T} \sim 5700$ K and pressure $\boldsymbol{P} \sim 7700$ bar, reflection possibility decreases by 10 times

Literature:

1. Ivochkin A.Yu., Kaptilniy A.G., Karabutov A.A., Ksenofontov D.M. "Laser opto-acoustic study of phase transitions in metals confined by transparent dielectric". Laser Physics, **22**, N. 7, 1220-1228 (2012), (ISSN 1054-660)
2. Ivochkin A.Yu., Kaptilniy A.G., Karabutov A.A., Ksenofontov D.M. "Pulsed laser heating of metal surface confined by thin layer of transparent dielectric: an experimental approach for creation of supercritical chemical reactor". Mendeleev Communications. **23**, N. 4, (2013), (ISSN 0959-943)

MULTIPHASE EQUATIONS OF STATE FOR METALS AT HIGH DYNAMIC PRESSURES

K.V. Khishchenko

Joint Institute for High Temperatures RAS, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
konst@ihed.ras.ru

Multiphase equations of state (EOSs) of materials over a broad region of pressures and temperatures are necessary for numerical simulationsof processes with intense pulsed influences on media where phase transformations are possible. Accuracy of numerical modeling results is determined mainly by adequacy of thermodynamic description of materials under consideration. In this work, some EOSs for specific metals are presented.

A thermodynamically full EOS model is proposed describing the Helmholtz free-energy function F(V, T) with taking into account polymorphic transitions, melting and evaporation. Basing on the model, multiphase EOS calculations are carried out for aluminum, tin, titanium, beryllium, iron, tantalum, tungsten and bismuth over a wide range of pressures and temperatures.

Obtained EOSs are in a good agreement with data available from experiments at high energy densities, such as measurements at static high-pressure conditionsas well as in shock and release waves. The EOSs can be used efficiently in hydrodynamic simulations of processes in materials and plasmas under intense laser influences.

Acknowledgements
The work is supported by the Russian Science Foundation grant 14-50-00124.

TWO APPROACHES FOR MODELING OF LASER ABLATION OF METALS: HYDROCODE WITH A MODEL OF NUCLEATION AND HYBRID MOLECULAR-DYNAMIC METHOD

Povarnitsyn M.E., Fokin V.B., Levashov P.R., Khishchenko K.V.
JIHT RAS, Izhorskaya 13 bldg 2, Moscow 125420 Russia
povar@ihed.ras.ru

Simulation of femtosecond laser ablation of a bulk aluminum target is performed using two approaches. The first method is a single-fluid two-temperature hydrodynamics completed with a two-temperature equation of state. The second approach is a combination of classical molecular dynamics and continuum model of a free electron subsystem. In both methods an identical and accurate description of optical and transport properties of electron subsystem is based on wide-range models, that gives opportunity to reproduce electron heat wave propagation, electron-phonon/ion coupling and laserenergy absorption on a time-dependent profile of complex dielectric function. Besides, phase diagram of equation of state and molecular dynamic potential are in a good agreementthat gives opportunity to compare the dynamics of laser ablation obtained by both methods directly. Results of simulation are presented in the range of fluences 0.1-20 J/cm^2 and match well with experimental findings for the ablation crater depth. Hydrodynamic approach demonstrates good qualitative agreement in dynamics of phase explosion and spallation. Molecular dynamics accurately reproduces nonequilibrium phase transitions and takes into account surface effects for nanoobjects. Other advantages and disadvantages of both approaches areinvestigated and discussed.

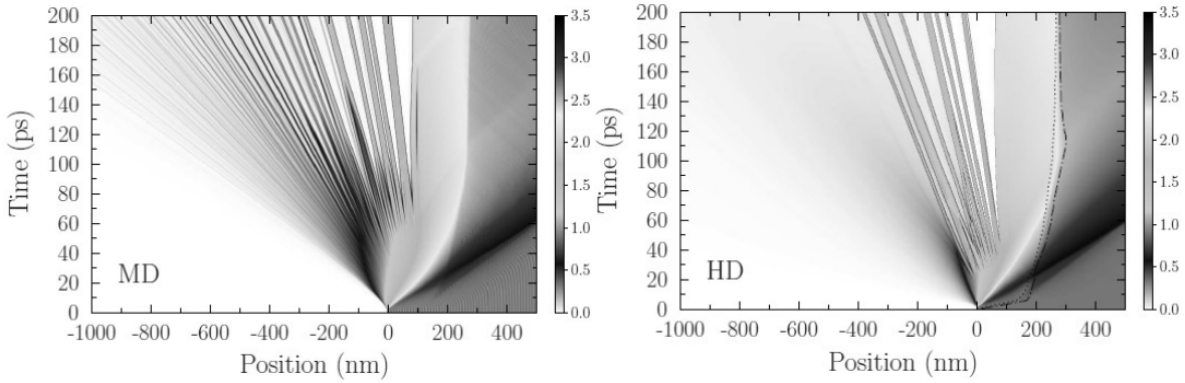


Figure 1. Density contour plots for ablation of Al target by 100 fs laser pulse with the fluence F= 2 J/cm^2 for MD (left) and HD (right) simulation. Zone of melting is bounded by the dashand-dot line in HD panel.

Acknowledgements:

The research was sponsored the Russian Foundation for Basic Research (Project Nos. 13-08-01179 and 13-02-91057-CNRS).

МОДЕЛИРОВАНИЕ КОНТАКТНОГО ВЗАИМОДЕЙСТВИЯ СИСТЕМЫ ТЕЛ МЕТОДОМ ШВАРЦА

М.П. Галанин[1], В.В. Лукин[1], А.С. Родин[1],И.В. Станкевич[2]

[1]*ИПМ им. М.В. Келдыша РАН, Москва*
e-mail: galan@keldysh.ru;
[2]*МГТУ им. Н.Э. Баумана*
e-mail: aplmex@yandex.ru

Доклад посвящен разработке алгоритма численного решения поликонтактной задачи термомеханического взаимодействия системы многих тел. Представлен краткий обзор распространенных методов. Использованных алгоритм основан на итерационном методе Шварца, специальным образом модифицированном для решения рассматриваемого класса задач. Дискретизация решаемой нелинейной дифференциальной задачи выполнена методом конечных элементов. Представлены результаты расчетов, в том числе расчета термомеханического взаимодействия 350 тел.

Работа выполнена при частичной финансовой поддержке Программы поддержки ведущих научных школ (грант № НШ-1432.2014.8) и при поддержке РФФИ (проекты № 15-01-03073, № 14-01-31496).

THE MODELING OF CONTACT INTERACTION OF SOLIDS BY MEANS OF SCHWARTZ METHOD

M.P. Galanin[1], V.V. Lukin[1], A.S. Rodin[1], I.V. Stankevich[2]

[1]*Keldysh Institute of Applied Mathematics of Russian Academy of Sciences, Moscow*
e-mail: galan@keldysh.ru;
[2]*Bauman Moscow State Technical University, Moscow*
e-mail: aplmex@yandex.ru

The algorithm of numerical solution of polycontact problem for thermomechanical interaction of big amount of solids is discussed. The brief overview of methods of numerical solution of such problems is given. The used algorithm is based on Schwartz iteration method which is specially modified for the solution of considered class of problems. The discretisation of nonlinear differential problem is performed by the finite element method. The calculation results are demonstrated including the results of calculation for thermomechanical interaction of 350 bodies.

This work was partially funded by leading scientific schools support Program (grant # NS-1432.2014.8) and RFBR (projects 15-01-03073, 14-01-31496).

MATHEMATICAL MAINTENANCE OF EXPERIMENTS WITH PENETRATING RADIATION

Mikhail E. Zhukovskiy, Sergey V. Podoliako,
Mikhail B. Markov, Roman V. Uskov, Alexandr S. Vorontsov

Keldysh Institute for Applied Mathematics of RAS; Moscow, Russia
posev66@yandex.ru

Base of technology of mathematical maintenance of experiments with penetrating radiation is worked out. Main idea is to construct operators of transforming the initial radiation to the transmitted one as well as operators of transforming the transmitted radiation to the measured values [1]. Simulating the radiation transport is based on the Monte Carlo modeling of interaction of X-radiation and electrons with matter. The proposed method permits to construct, for instance, the operator connecting the initial radiation spectrum with the energy distribution of photons penetrating an object of inquiry. The developed method provides the possibility of effective mathematical modeling of radiography testing the complex multi-component objects. Moreover, the method can be used to construct operator equation for solving inverse problems, e.g. the reconstruction of the radiation spectrum by use of simple experimental measurements. Comparison with some experimental measurements is presented.

Acknowlegments:

This work is supported by Russian Fund for Basic Researches, grants N 14-01-00350 and N 15-01-03027

References:

1. Zhukovskiy, M.E., Jaenisch, G.-R., Deresch, A., Uskov, R.V. "Monte Carlo modeling of electron transport using CUDA technology Beitrag zu einem Tagungsband". 18th WCNDT - World conference on nondestructive testing (Proceedings), Paper 89, 1-8 ISBN 978-0-620-52872-6 (2012).

СУПЕРКОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ КАСКАДНЫХ ПРОЦЕССОВ ПЕРЕНОСА ИЗЛУЧЕНИЯ

Жуковский М.Е, Марков М.Б., Подоляко С.В., Усков Р.В.
ИПМ им. М.В.Келдыша РАН, Москва, Россия
roman.uskov@gmail.com

Рассматривается моделирование развития фотонно-электронного каскада внутри многокомпонентных объектов сложной геометрической структуры на гибридной вычислительной технике. Разработан подход к моделированию каскадных процессов, который имеет три ключевые особенности, позволяющие эффективно использовать гетерогенную структуру вычислительной техники для расчета переноса излучения в сложных разномасштабных структурах. Во-первых, применяется два различных геометрических описания объекта при моделировании распространения фотонов в веществе (поверхностно ориентированная модель, дискретизация которой проводится с помощью триангуляции) и переноса электронов (объемно ориентированная или «воксельная» модель объекта, рис. 1).

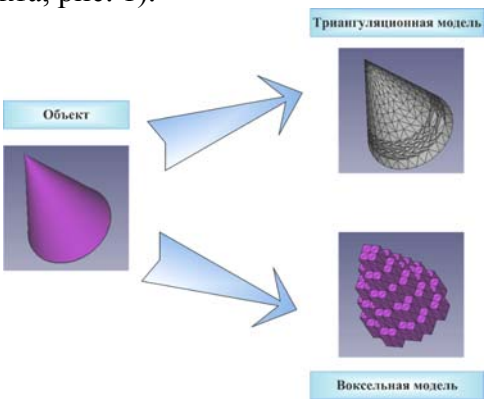


Рис. 1.

Во-вторых, для моделирования поверхностных эффектов (таких, например, как радиационная электронная эмиссия [1]) явным образом учитывается малый параметр задачи – отношение длины тормозного пути электрона к длине среднего свободного пробега фотона. Это позволяет на порядки сократить объем вычислений для моделирования указанных эффектов. В третьих, разработанная эффективная декомпозиция вычислений между центральным и графическим процессорами позволяет значительно повысить скорость моделирования рассматриваемых процессов. С помощью разработанного метода проведено моделирование эксперимента по исследованию характеристик тормозного излучения, генерируемого пучком электронов ускорителя. Сравнение результатов расчетов и экспериментальных данных показало удовлетворительное согласие.

Работа выполнена при поддержке грантов РФФИ № 15-01-03027 и № 14-01-00350.

Литература:

1. M. E. Zhukovskiy, M. B. Markov, S. V. Podoliako and R. V. Uskov. “Hybrid Parallelization of Computing the Electron Fluxes produced by Photon Radiation”. Mathematica Montisnigri. **XXXI**, 43 -53 (2014).

MOLECULAR DYNAMIC SIMULATION OF RAREFIED GAS FLOW IN METALLIC MICROCHANNEL

V.O. Podryga, S.V. Polyakov
Keldysh Institute of Applied Mathematics, Russian Academy of Science,
4 Miusskaya square, 125047, Moscow, Russia
E-mail: pvictoria@list.ru

The simulation problem of rarefied gas flows in microchannels of technical systems in a multiscale computational domain is considered. Problem of the gas flow in microchannel of installations for supersonic cold gasdynamic sputtering is chosen as an example [1]. This problem is one of the basic parts of a general list of sputtering problems, which includes: 1) the features of the gas and nanoparticles motion through microchannels; 2) targeted delivery of nanoclusters to sputtering places; 3) guaranteed attachment of the nanocluster to the substrate surface; 4) providing a specified time and a desired quality of sputtering single act; 5) ensuring a repeatability and mass character of deposition process; etc.

For solution of selected problem the multiscale approach is used, combining the solving of a quasigasdynamic (QGD) [2] equations and the correcting of the solution by molecular dynamics method (MD) [3]. At interaction of the gas mixture with metallic walls of sputtering system (nozzles and microchannels), and also with the nanoparticles, phenomena occur, which are well described only at the molecular level. This applies primarily to determining the equation of state of gas mixture in the flow, as well as component values of the velocity, pressure and temperature on the walls. Therefore, the main attention of this work is devoted to the calculation of macroparameters of the gaseous medium as far away from the walls of microchannels, as well as in the boundary layer. The calculations of medium macroparameters by MD methods are used as in specific calculations, as well as for database accumulation that is used in subsequent QGD computations.

In this work the investigated object (molecules of gas mixture and atoms of metallic surface) is represented by a set of particles that move according to the laws of Newton. The system of equations is solved by the Verlet difference scheme [4]. The interaction of particles is described by potentials determining the basic properties of system components under selected conditions. The system of nitrogen molecules is considered as a gas, at this stage, the system of nickel atoms is regarded as the walls of microchannel. By now the equilibrium states of microsystems gas-gas, metal-metal and metal-gas are already well researched by us. These data already allow calculations for quasi-equilibrium states, and thus determine the necessary macroparameters of the medium.

Acknowledgements: This work is supported by Russian Fund for Basic Researches. Work partially supported by grants RFBR №№ 13-01-12073-ofi-m, 15-07-06082.

References:

1. A. Papyrin, V. Kosarev, S. Klinkov, A. Alkhimov, V. Fomin, "Cold Spray Technology", Amsterdam: Elsevier Science (2007)
2. T.G. Elizarova, "Quasi-gasdynamic equations", Springer (2009)
3. J.M. Haile, "Molecular Dynamics Simulations. Elementary Methods", NY: John Wiley & Sons Inc. (1992)
4. L. Verlet, "Computer «experiments» on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules", Phys. Rev., **159**, 98–103 (1967)

МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ТЕЧЕНИЯ РАЗРЕЖЕННОГО ГАЗА В МЕТАЛЛИЧЕСКОМ МИКРОКАНАЛЕ

В.О. Подрыга, С.В. Поляков
ИПМ им. М.В. Келдыша РАН,
125047, Москва, Россия, Миусская пл., д. 4,
E-mail: pvictoria@list.ru

Рассматривается проблема моделирования течений разреженных газов в микроканалах технических систем в условиях многих масштабов расчётной области. В качестве примера выбрана задача о течении газа в микроканале установки сверхзвукового холодного газодинамического напыления [1]. Эта задача является одной из базовых частей общего списка проблем напыления, в который входят: 1) особенности движения газа и наночастиц по микроканалам; 2) адресная доставка нанокластеров к местам напыления; 3) гарантированное прикрепление нанокластера к поверхности подложки; 4) обеспечение заданного времени и заданного качества единичного акта напыления; 5) обеспечение повторяемости и массовости процесса напыления; и т.д.

Для решения выбранной задачи используется мультимасштабный подход, сочетающий решение уравнений квазигазодинамики (КГД) [2] и корректировку решения методом молекулярной динамики (МД) [3]. При взаимодействии газовой смеси с металлическими стенками системы напыления (сопел и микроканалов), а также с наночастицами, происходят явления, которые хорошо описываются только на молекулярном уровне. Это относится, в первую очередь, к определению уравнения состояния газовой смеси в потоке, а также значениям компонент скорости, давления и температуры на стенках. Поэтому основное внимание в данной работе уделяется расчету макропараметров газовой среды как вдали от стенок микроканалов, так и в пограничном слое. При этом вычисления макропараметров среды методами МД используются как в конкретном расчете, так и для накопления базы данных для последующих КГД-вычислений.

В представленной работе исследуемый объект (газовая смесь и атомы металлической поверхности) представляется совокупностью частиц, которые двигаются по законам Ньютона. Система уравнений решается с помощью разностной схемы Верле [4] в скоростной форме. Взаимодействие частиц описывается с помощью потенциалов, определяющих основные свойства компонент системы в выбранных условиях. В качестве газа рассмотрена система молекул азота, в качестве стенок микроканала на данном этапе рассматривается система атомов никеля. К настоящему моменту нами уже хорошо изучены равновесные состояния микросистем газ-газ, металл-металл и газ-металл. Эти данные уже позволяют проводить расчеты для квази-равновесных состояний и, тем самым, определять необходимые макропараметры среды.

Благодарности: Работа выполнена при поддержке Российского фонда фундаментальных исследований, проекты №№ 13-01-12073-офи-м, 15-07-06082.

Литература:

1. А.П. Алхимов, С.В. Клинков, В.Ф. Косарев, В.М. Фомин. *Холодное газодинамическое напыление. Теория и практика*, М.: Физматлит (2010)
2. T.G. Elizarova, “Quasi-gasdynamic equations”, Springer (2009)
3. J.M. Haile, “Molecular Dynamics Simulations. Elementary Methods”, NY: John Wiley & Sons Inc. (1992)
4. L. Verlet, “Computer «experiments» on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules”, Phys. Rev., **159**, 98–103 (1967)

SEPARATION AND 3D-EXPANSION OF GOLD FILM FROM SUBSTRATE UNDER ACTION OF FEMTOSECOND LASER PULSE

N.A. Inogamov[1], V.V. Zhakhovsky[2], V.A. Khokhlov[1]
[1]*Landau Institute for Theoretical Physics, Russian Academy of Sciences, Russia, 142432 Chernogolovka, Moscow region, prospect Akademika Semenova, 1A*
[2]*All-Russia Research Institute of Automatics, ROSATOM, Russia, 127055 Moscow, ulitsa Sushchevskaya, 22*
e-mail nailinogamov@gmail.com

Many laser applications use "film on substrate" targets with a thin metal film and a dielectric substrate. This situation is interesting and is weakly investigated. Indeed, a system with a thin film between a substrate from the one side and vacuum from the other side is very different from a case of bulk targets and from a case of a freestanding film, where both boundaries of a film are boundaries with vacuum. In the report the action of an ultrashort pulse onto the "film on substrate" target is considered. Modern model of two-temperature (2T) physics is used [1]. We show that for 40-100 nm thick thin films the conductive leveling of electron temperature across film thickness takes 1-2 ps in gold, copper, and silver (heat conduction in dielectric is neglected). This duration is small in comparison with the electron-ion temperature equalization time (2-3 ps for copper, 5-7 ps for silver, and 5-9 ps for gold [2]) and is small in comparison with acoustic time defined by thickness of film and speed of sound in metal. At the same time the equalization time and the acoustic time are comparable. Thus electron-ion coupling coefficient (taken from [3]) and 2T equation of state [1] are important ingredients of 2T physics since they define a rate of electron cooling and electron pressure dynamic significance. Interplay of rarefaction waves in a film and dynamic interaction between the film and the substrate control a process of film separation from substrate. Finite size of a heated spot on a film surface is included into consideration. Velocity of a film after its separation from substrate has a maximum at the axis of a beam in case of Gaussian distribution of pulse intensity across a cross-section of a laser beam [2]. That's why the film (separated from the substrate) expands having a shape of cupola with an apex of cupola at the axis of a laser beam. An area of surface of a target under the cupola is defined by a radius of a laser beam. Absorbed fluence is above a melting threshold in our applications. Therefore a shell of cupola is made from molten metal. Surface tension plays the decisive role in a stopping of expansion of cupola [2]. Tension focuses mass flow inside a shell in direction to the axial region forming a jet and droplets. Mutual action of capillary effects and cooling/freezing process define a final shape of a cupola. Microbumping phenomena are important for laser bio-printing and LIFT applications (Chichkov, Ivanov et al.), for formation of arrays of nanoholes (Nakata et al.), and for nanophotonics (creation of nanoantennas, Ionin, Kudryashov et al.).

Acknowledgements: Authors acknowledge Russian Science Foundation, grant 14-19-01599.

References:

1. Yu. Petrov et al., "Two-temperature equation of state for aluminum and gold with electrons excited by a ultrashort laser pulse", Appl. Phys. B, (2015). DOI: 10.1007/s00340-015-6048-6
2. N. Inogamov et al., "Jet Formation in Spallation of Metal Film from Substrate under Action of Femtosecond Laser Pulse", JETP, **120**(1), 15-48 (2015).
3. Yu. Petrov et al., "Thermal Conductivity and the Electron–Ion Heat Transfer Coefficient in Cond. Media with a Strongly Excited Electron Subsystem", JETP Lett., **97**, 20-27 (2013).

SUPPORT OPERATORS TECHNIQUE FOR DISTRIBUTED 3D SIMULATION OF DISSIPATIVE PROCESSES

Irina Gasilova
Keldysh Institute of Applied Mathematics, Miusskayasq., 4, Moscow, 125047, Russia
igasilova@gmail.com

Problems related to transient high-temperature gas/plasma flows often reveal an essential dependence of a solution on various dissipative effects. A predictive simulation in that area of CFD is supported by finite difference or finite volume methods which satisfy common conditions like conservativity, monotonicity, stability in a wide range of flow parameters, high resolution etc. An important property of any CFD technique is a possibility of its implementing using general computational meshes (block-structured, unstructured, mortar etc.) while general properties of original differential operators persists in their difference analogues [1]. The support operators method is remarkable as it allows building approximations to differential operators using general meshes while the resulting difference operators preserve not only basic properties mentioned above, but, additionally, they provide rotationally-invariant difference schemes [2]. It's important to pay special to the rotational invariance while working with systems describing deformations and dissipations in gas or liquid media, e.g. Navier-Stokes equations.

Differencing via support operator method guarantees preserving of this property provided it is inherent to original differential operator. The method allows building robust numerical procedures suitable for multiscale simulations requiring very finely discretized computational domains – and it is just a case that requires the use of high performance computing. The support operator technique is developed for meshes formed with hexahedral, tetrahedral, prismatic cells and their various combinations. 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]

Acknowledgements: All the work was done in KIAM RAS under the guidance of my supervisor Professor Yu.A. Poveshchenko.

References:

1. A.A. Samarskii et Al. “Difference Schemes on Irregular Meshes”, Minsk (1999).
2. A.V. Koldoba et Al. “Numerical Schemes of the Support Operators Method for Elasticity Theory Equations”, Matem. Mod, **24**, No. 12, 86-96 (2012).
3. V.A. Gasilov et Al. “Towards an Application of High-performance Computer Systems to 3D Simulations of High Energy Density Plasmas in Z-Pinches”. Applications, Tools and Techniques on the Road to Exascale Computing. K. de Bosschere et Al (Eds). IOS Press, Series “Advances in parallel Computing”, **22**, 235-242 (2012). Doi: 10.3233/978-1-61499-041-3-235.

РАЗРАБОТКА СТРАТЕГИЙ ИССЛЕДОВАНИЯ СИСТЕМ ВНЕШНИХ ПЛАНЕТ ПРИ ИСПОЛЬЗОВАНИИ МОДЕЛИ СДВОЕННЫХ ОГРАНИЧЕННЫХ ЗАДАЧ ТРЁХ ТЕЛ

Г.К. Боровин, Ю.Ф. Голубев, А.В. Грушевский, В.В. Корянов, А.Г. Тучин, Д.А. Тучин

Институт прикладной математики им. М.В. Келдыша РАН, Москва, Россия
e-mail: borovin@keldysh.ru

С использованием реальных эфемерид внешних планет и их естественных спутников осуществлена модельная реализация алгоритма преодоления «пар адокса сольных пертурбаций» [1-2] с целью сближения с одним из этих спутников путём совершения обхода зоны повышенной радиации по «верхней секции» диаграммы Тиссерана-Пуанкаре [3]. Одновременно проводится почти беззатратная редукция асимптотической скорости космического аппарата (КА), необходимая для сближения со спутником, которая становится возможной при переходе от поиска в модели ограниченной задачи трёх тел к условиям сдвоенных ограниченных задач трёх тел.

Для параметрического попадания в вышеуказанную зону диаграммы в баллистический сценарий миссии вводятся Bi-Тиссерановы координаты и используются сопряжённые «косые» гравитационные манёвры ещё до завершения фазы редукции периода обращения КА. Таким образом, разумное увеличение длительности миссии удаётся разменять на резкое снижение суммарной дозы полученной радиации (TID). В результате демонстрируется открывающаяся возможность как «комфортабельных» по накопленной дозе радиации полётов в системе КА с TID, не превышающими значений 70 Krad для защиты “Galileo” 8-10 mm Al, так и для «легких» КА с толщиной защитного корпуса 4-5 mm Al при стандартных ограничениях на TID 300 Krad. Указанное обстоятельство может обеспечить как значительный выигрыш в полезной нагрузке КА миссий к Юпитеру и Сатурну и другим внешним планетам, так и повышение степени надёжности работы его научной аппаратуры

Благодарности:
Авторы благодарны С.М. Лавренову за полезные обсуждения и рекомендации.

Ссылки:

1. G. K. Borovin, Yu. F. Golubev, A. V. Grushevskii, V. V. Koryanov, A. G. Tuchin, "Flights in Jupiter system using gravity assist maneuvers near Galilean moons", Preprint No. 72, IPM RAN (Keldysh Institute of Applied Mathematics, Russian Academy of Sciences) (2013). http://library.keldysh.ru/preprint.asp?id=2013-72.
2. Yu.F. Golubev., A.V. Grushevskii, V.V. Koryanov V, A.G. Tuchin. Gravity Assist Maneuvers of a Spacecraft in Jupiter System, Journal of Computer and Systems Sciences International, Pleiades Publishing, Ltd. 2014. **53**, № 3. 445–463 (2014).
3. S. Campagnola, R. P. Russell, "Endgame problem. Part 2: Multi-body technique and TP Graph," J. Guidance, Control, Dynamics, **33**, 476-486 (2010).

DEVELOPMENT OF THE ISON OPTICAL NETWORK TO IMPROVE THE CONJUNCTION ANALYSIS

I. Molotov, V. Voropaev, V. Zolotov, T. Fakhrutdinov, G. Borovin

Keldysh Institute of Applied Mathematics, RAS
im62@mail.ru

ISON optical network represents one of the largest ground-based systems specialized in observation of space debris and other objects in high geocentric orbits. In 2015 quantity of telescopes of 40 observatories that collaborate with ISON project in 17 coun tries will be exceeding 100 units. These telescopes are combined in 4 subsystems – for GEO survey, bright and faint objects follow up, and for asteroids (ASPIN). KIAM collected 10.866 million astrometry measurements during 2014.

Since 2010, ISON is involving in operations of the Roscosmos Automated system of warning on dangerous situations in space (ASPOS OKP). In this system KIAM is responsible for the conjunction analysis at high orbits and developed special software for ASPOS c enter. In 2013-2014 KIAM is created other software complex ADAPS to provide commercial service for industry entities.

To improve the quality of these activities ISON is deploying additional subnetwork for extended GEO surveys from 7 small (18-19.2 cm aperture) automated telescopes with field of view 7x7 degree with centralized scheduling at KIAM. Each telescope is surveying visible part of GEO and provides up to 12 thousands measurements for 600 objects (with brightness down to 14-14.5 magnitude) per night with duration of object tracks up to a few hours. While 22-25 cm telescope of existing ISON global GEO survey subsystem has limiting magnitude down to 15 - 15.5 and provides the duration of tracks between 15 and 40 minutes. Extended surveys of new ISON subnetwork allows to KIAM to determine more precise GEO orbits for conjunction analysis, to detect maneuvers of active satellites and to help maintain the orbits of GEO objects in clusters.

VT-78a 19.2-cm telescopes are working in Tiraspol (Moldova), Kislovodsk (North Caucasus), Khuraltogot (Mongolia) and Ussuriysk (Far East). VT-52c 18-cm telescope – in Nauchniy-1 (Crimea). In addition, VT-78a will be installed in Multa (Altay region) and 2xVT-52c – in Macon (Argentina) to cover almost all GEO. During 2014, VT-78a in Khuraltogot can obtain 1.2 million measurements in 174.5 thousands tracks, VT-52c in Nauchniy-1 – 1 million measurements in 138 thousands tracks. Many HEO objects were detecting as background.

The analysis of results obtained with this new subsystem will be presented and discussed.

РЕАЛИСТИЧНАЯ МОДЕЛЬ ЗЕМЛИ В КОСМИЧЕСКИХ ТРЕНАЖЕРАХ

М.В. Михайлюк, П.Ю. Тимохин
Научно-исследовательский институт системных исследований РАН, Москва, Россия
Email: mix@niisi.ras.ru

В настоящее время в космических тренажерах часто возникает задача моделирования и визуализации в реальном масштабе времени поверхности Земли. Это важно для проведения обучения космонавта ориентированию по поверхности Земли, мониторингу стихийных бедствий, ручному фотографированию отдельных участков Земли, представляющих специальный интерес и т.д. В тренажерах для моделирования вида Земли из космоса используются текстуры большого объема и высокого разрешения, полученные на основе космических снимков. Для работы с ними необходимы эффективные по скорости алгоритмы, использующие разбиение текстуры на куски (тайлы), кэширование, динамическую подкачку тайлов, а также расчет освещенности модели поверхности Земли.

Предлагаемая технология включает комплекс шейдерных программ по определению тайлов, участвующих в закраске текущего кадра, подкачке этих тайлов в текстурный кэш, нахождению нужного тайла в кэше и закраске соответствующих пикселов.

Стандартные средства графической библиотеки OpenGL не обеспечивают необходимый уровень реалистичности освещения с учетом атмосферы. В то же время моделирование освещенности на основе общего уравнения переноса излучения не позволяет обеспечить реальный масштаб времени визуализации. Поэтому необходимо использовать более простую модель переноса, позволяющую обеспечить необходимую скорость синтеза изображений. В нашей модели поверхность Земли является сферой с постоянным коэффициентом отражения света, а атмосфера моделируется как тонкий сферический слой, состоящий из молекул воздуха и аэрозольных частиц, плотность которых уменьшается по мере отдаления от поверхности Земли. Рассеяние лучей, прошедших только через атмосферу или один раз отраженных от Земли, вычисляется по точному уравнению освещения с использованием предрассчитанной таблицы коэффициентов прозрачности атмосферы. Рассеяние переотраженных от Земли лучей вычисляется по приближенному уравнению освещения. Все вычисления в этой модели выполняются в расширенном диапазоне яркостей, а затем переводятся в формат с глубиной цвета 24 бита с помощью тонального отображения. Для обеспечения реального масштаба времени визуализации в качестве такого отображения предложен модифицированный глобальный оператор Рейнхарда и алгоритм его эффективного вычисления.

Описанные алгоритмы расчета освещенности в модели поверхности Земли разработаны и реализованы при поддержке РФФИ (грант № 14-07-31332) в рамках системы визуализации GLVIEW для тренажерных комплексов, созданной в НИИСИ РАН. Апробация системы показала соответствие предложенных алгоритмов требованиям к системе визуализации для космических тренажеров.

ABOUT POSSIBILITY OF APPLICATION OF EOP-1/EOP-2 MINIOBSERVATORIES OF ROSCOSMOS FOR ASTEROID OBSERVATIONS

I. Molotov

Keldysh Institute of Applied Mathematics, RAS
im62@mail.ru

KIAM proposed and elaborated the conception of six dedicated mini-observatories of two series (four EOP-1 and two EOP-2) sponsored by Roscosmos grants. It was planned that these mini-observatories created using the best ISON project experience would allow to quickly doubling the performances of ISON network to improve the conjunction analysis in the Automated System for Prediction and Warning on the dangerous situations in the ne arEarth space. The main target of the project is a signicant improvement of the situation with detecting and tracking of HEO objects and increasing the regularity of the GEO surveys in

Western Hemisphere. EOP-1 includes twin 19.2 cm telescope VT-78a with FOV of 7x9 degree, one 25-cm telescope ORI-25 with FOV 3.3 degree and one 40 cm telescope ORI-40 with FOV 2.3 degree in pavilions with moving roof. Observatories EOP-1 are installed in Kislovodsk (North Caucasus), Byurakan (Armenia) and two in Naucnniy (Crimea). EOP-2 includes quadruple VT-78a with FOV of 14x9 degree, one 40 cm telescope ORI-40 with FOV 2.3 degree and one 65 cm telescope SANTEL-650 with FOV of 2.2 degree in rotating domes. First observatory EOP-2 is installed in Kislovodsk (North Caucasus), second will be installed in Blagoveschensk (close to Far East).

There is good chance that four EOP-1 will be added with 65 cm telescopes SANTEL-650, and two more EOP-2 will be ordered in next two years. In common nine 65-cm telescopes (including one in Ussuriysk observatory) and eight 40-cm telescope will be operating in nearest future. It will be a biggest opportunity to provide Russian share to solving the asteroid-comet hazard problem. Up to now, 95% potentially hazard asteroids (PHA) is discovered by dedicated USA survey programs. The investment of Russia in this research is very small.

In the case of using of EOP-1/EOP-2 telescopes for the asteroid survey during part of observing time we can realize the conception of second boundary of PHA detection – USA surveys use large aperture telescopes and can detect faint objects but are not able to survey all sky in reasonable time, Russia can use middle aperture telescope and can detect bright objects but can provide the survey of all sky for each three-four days.

Test asteroid surveys that were arranged by KIAM/ISON team with 40-cm and 65-cm telescopes of Roscomos allowed discovering one NEA, ISON comet, and few tens main belt asteroids that confirm the reliability of proposed idea.

In addition, 24 telescopes VT-78 may be used for comet searching. Such quantity of telescopes allowed covering all sky twice per night. Test surveys with VT-78 allowed discovering 3 comets and 1 PHA.

ASPIN - ISON ASTEROID'S RESEARCH PROGRAM: HISTORY, CURRENT STATE AND FUTURE PROSPECTS

L. Elenin[1], I. Molotov[1], Yu. Krugly[2]
1Keldysh Institute of Applied Mathematics RAS,
2Institute of Astronomy of Kharkiv National University
l.elenin@gmail.com

This presentation will be briefly describe history, current state and future prospects of Asteroid Research Project of the ISON Optical Network (ASPIN)[1]-ISON asteroid's researchprogram, working by support of Keldysh Institute of Applied Mathematics RAS. First observations started in September 2003 at Andrushivka astronomical observatory (Andrushivka, Ukraine) with Zeiss-600 telescope with small CCD camera. In 2009, telescope upgraded with new full-format CCD camera and lens corrector. During first 7 years observatory discovered more than 350 asteroids, include two NEAs. At current time, observations of small bodies of Solar System (SBSS) at Andrushivka observatory had stopped.

Below we will describe observatories, which works until current date. Survey work atISON-NM observatory (Mayhill, USA) started in July 2010 and continues until this day. First telescope of this observatory was Centurion-18, 0.45-m f/2.8 with full-frame CCD camera. In September 2013 with telescope replaced by our new telescope Santel-400AN (0.4-m f/3) with 105'x105' FOV. Both telescopes was controlling remotely from KIAM. At ISON-NM observatory discovered more than 1,500 asteroids, include five NEO and three comets – wellknown C/2010 X1 (Elenin), P/2011 NO1 (Elenin) and P/2014 X1 (Elenin). Obtained more than 580,000 observations of small bodies. Except survey work, ISON-NM carry out photometric observations of NEAs, obtained dozens lightcurves, determined rotational period for more than 30 NEAs, include extremely close and fast rotators, such a 2012 KP24, 2012 KT42, 2012 LZ1 and Duende (2012 DA14)[2]. Since April 2012, another observatory joined to ASPIN – ISON-Kislovodsk. At observatory installed Santel-400AN telescopes with fullframe CCD camera, provided 105'x105' FOV. At present time, ISON-Kislovodsk - second of all APSIN observatories by number of measurements and discoveries. For 3 years observatory discovered about 100 new asteroids, include one NEA and famous comet C/2012 S1 (ISON). More than 110,000 measurements obtained. In 2013, ISON started using very wide-field telescope VT-73e (0.19-m f/1.5) with FOV 7°x4.5°, for chasing comets and bright NEAs. As first result – discovering new comet C/2013 V3 (Nevski). Next step of ASPIN program was installation of our biggest wide-field telescope Santel-650A (0.65-m f/2) in September 2013 at ISON-Ussuriysk observatory. For now, this telescope obtained more than 13,000 measurements and discovered three new asteroids. In 2014 three new observatories obtained his MPC codes and join to ASPIN program (ISON-Khureltogot, ISON-Uzhgorod, ISON-Byurakan).

In April-May 2015, ISON will install new dedicated telescope for SBSS observation at Siding Spring observatory (Australia). This will allow us to control South hemisphere, where not presented big, professional surveys. After realization of this object, next telescope will be installed at Macon mount (Argentina).

References:

1. I. Molotov, V. Agapov, Yu. Krugly, L. Elenin, "ASPIN - Asteroid Research Project of the ISON Optical Network". ACM 2012, LPI Contribution No. 1667, id. 6408.

2. L. Elenin, I. Molotov, "Lightcurve Analysis of Extremely Close Near-Earth Asteroid - 2012 DA14." MPB, **40**, No. 4, 187-188 (2013).

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ИМПУЛЬСНОГО ЛАЗЕРНОГО ПЛАВЛЕНИЯ АЛЮМИНИЯ

В.И. Мажукин, М.М. Демин, А.В. Шапранов
Институт Прикладной Математики им. М.В. Келдыша.

Исследуется механизм плавления тонких и толстых пленок Al ультракороткими лазерными импульсами с $\tau = 10^{-11}$-10^{10}с и F=0.2-0.4Дж/см^2. Моделирование осуществлялось с использованием континуальных (неравновесная 2-х температурная гидродинамическая модель) [1] и молекулярно-динамических [2] моделей. Результаты моделирования сравниваются между собой (рис. 1). Установлено, что интегральные характеристики процесса плавления, такие как толщина расплава, показывают хорошее согласие, погрешность не превышает 5-7%. Вблизи пороговых значений флюенса фазовый переход формируется в перегретом приповерхностном слое в виде гомогенных зародышей, которые, сливаясь, образуют межфазный фронт. Рост жидкой зоны обеспечивается гетерогенным распространением фронта от облучаемой поверхности вглубь перегретой твердой фазы. Роль гомогенного плавления незначительна. С ростом F роль гомогенного плавления усиливается. В приповерхностном перегретом слое образуется несколько жидких зон, и гетерогенное распространение межфазных фронтов происходит не только от поверхности, но и от образовавшихся жидких областей. При очень больших значениях F фазовый переход характеризуется сверхбыстрым гомогенным механизмом.

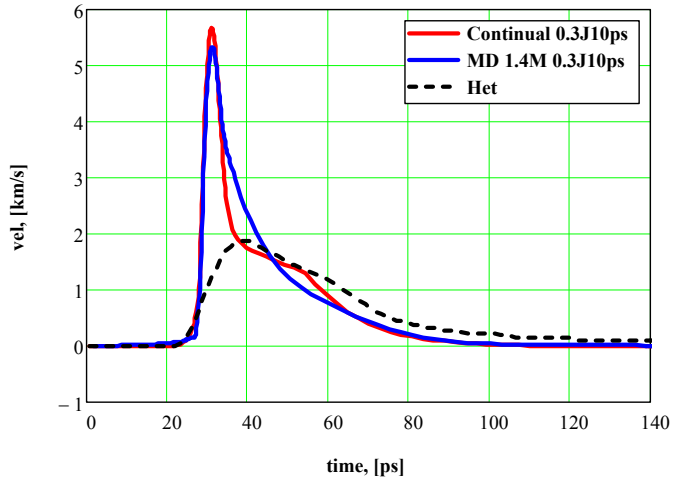


Рис. 1. Скорости фронта плавления, полученные при континуальном и МД моделировании.

Благодарности: Работа выполнена при финансовой поддержке РНФ № 15-11-00032.

Литература:

1. VI Mazhukin, MM Demin, AV Shapranov, “High-speed laser ablation of metal with pico-and subpicosecond pulses”, *Appl. Surf. Sci*., **302**, 6-10 (2014)
2. C. Wu and L. V. Zhigilei, “Microscopic mechanisms of laser spallation and ablation of metal targets from large-scale molecular dynamics simulations”, *Appl. Phys. A,* **114**, 11-32, (2014).

MATHEMATICAL MODELING OF PULSED LASER MELTING OF ALUMINUM

V.I. Mazhukin, M.M. Demin, A.V. Shapranov
M.V. Keldysh Institute of Applied Mathematics
email: vim@modhef.ru

Mechanism of melting of thin and thick Al films using ultrashort laser pulses with $\tau = 10^{-11}$ -10^{10}c and F=0.2-0.4J/cm^2 is investigated. Modeling was performed using continual (non-equilibrium 2-temperature hydrodynamic model) [1] and molecular-dynamic [2] models. The simulation results are compared with each other (Fig.1). It is found that the integral characteristics of the melting process, such as the thickness of melt show good agreement, the difference does not exceed 5-7%. Near the threshold fluence, the phase transition is formed in the superheated surface layer in the form of homogeneous nucleation, which merge to form a interphase front. The growth of the liquid zone is provided by a heterogeneous liquid front propagation from the irradiated surface into the superheated solid. The role of homogeneous melting is insignificant. As F increases, the role of homogeneous melting increases as well. Several liquid zones are formed in the surface superheated layer, and heterogeneous propagation of the fronts takes place not only from the surface but also from the formed liquid regions. For very large values of F, phase transition is characterized by ultra-fast homogeneous mechanism.

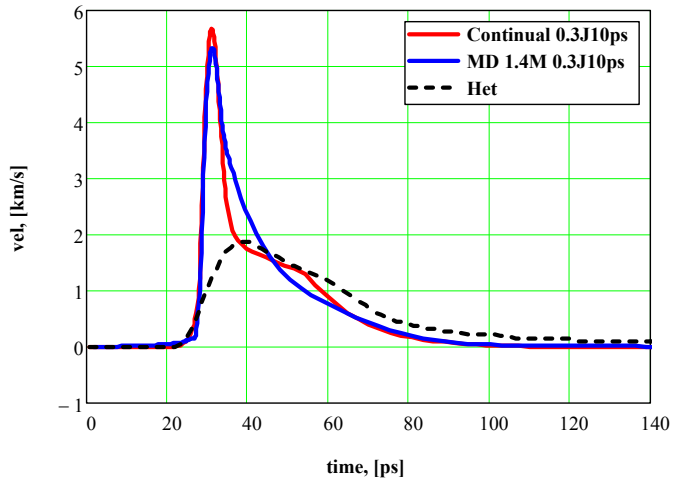


Fig.1. Velocities of melting front obtained by the continuous and MD simulation.

Acknowledgements: This work was supported by RSCF grant № 15-11-00032.

References:

1. VI Mazhukin, MM Demin, AV Shapranov, "High-speed laser ablation of metal with pico-and subpicosecond pulses", *Appl. Surf. Sci.*, **302**, 6-10 (2014)
2. C. Wu and L. V. Zhigilei, "Microscopic mechanisms of laser spallation and ablation of metal targets from large-scale molecular dynamics simulations", *Appl. Phys. A* **114**, 11-32, (2014).

ACOUSTICAL AND OPTICAL MONITORING OF ABSORBING LIQUID BEHAVIOR INDUCED BY NANOSECOND LASER IRRADIATION UNDER TRANSPARENT COVER

A. A. Samokhin[1], N. N. Il'ichev[1], P.A. Pivovarov[1,2], A.V. Sidorin[1]
[1] *A.M. Prokhorov General Physics Institute of RAS,*
Vavilov str. 38, 119991 Moscow, Russia
[2] *National Research Nuclear University MEPhI,*
Kashirskoye sh. 31, Moscow, 115409, Russia
asam40@mail.ru

Laser vaporization process of absorbing liquids under transparent cover differ significantly from the free surface case ablation. In the last case photoacoustic (PA) signal at low laser intensity has a bipolar form which at high intensities transforms to monopolar signal due to vaporization process development (see e.g. [1,2] and references therein). In the covered case PA signal at low intensity has a monopolar form which at increasing intensity becomes bipolar. This somewhat counterintuitive behavior may be due to cavity formation under the transparent cover and this suggestion is on accordance with the acoustical monitoring of irradiated zone displacement [3]. At higher intensity PA signal transforms again to monopolar form because of vaporization pressure contribution [2].

In the present paper absorbing liquid behavior (water and ethanol at λ=2,9 μm pulsed laser irradiation) under the transparent (sapphire) cover is investigated using acoustic monitoring [3] combined with optical diagnostic (λ=0,53μm, CW) of irradiation zone. Two optical diagnostic scheme are used which are based on total internal reflection effect and thin films reflectometry.

Optical diagnostic results suggest that the cavity formation occurs somewhat lower then boundary between liquid and transparent solid cover due to cooling effect of the cover. The cavity lifetime determined from the optical signals durations amounts to about several hundreds microseconds at the laser fluency ~1J/cm^2 and the pulse duration 150ns. In the case of ethanol covered with sapphire plate it is observed up to ten reflexes during 200 μs which are probable due to condensation process. During the laser pulse no distinctive oscillations of optical signals are visible. At low fluencies the signal demonstrates threshold behavior (E_{th}~0,1J/cm^2) with subsequent saturation. Cavity collapse is accompanied with additional pressure perturbations due to cavitations effect which takes place after some delay with respect to the end of optical signal.

Acknowledgements: This work was partially supported by Russian Fund of Basic Research grant № 13-02-01129.

References:

1. A.A.Samokhin, Proceedings of the A.M. Prokhorov General Physics Institute, **13**, (1990)
2. A. A. Samokhin, and N. N. Il'ichev, P.A. Pivovarov, A.V. Sidorin, Mathematica Montisnigri, **30**, 46-55 (2014)
3. A. A. Samokhin, N. N. Il'ichev, Quantum Electronics, **40,** № 8, 659-660 (2010)

АНАЛИЗ МАТЕМАТИЧЕСКИХ МОДЕЛЕЙ ЛАЗЕРНОГО НАГРЕВА И ПЛАВЛЕНИЯ КРЕМНИЯ

О.Н. Королева, А.В. Мажукин, П.В. Бреславский
Институт Прикладной Математики им. М.В.Келдыша РАН,
125047, Москва, Миусская пл. 4, Россия
vim@modhef.ru

В сообщении анализируются математические модели нагрева, гетерогенного и гомогенного плавления кремния. Сложность математического описания фундаментальных механизмов, лежащих в основе быстрых фазовых переходов в полупроводниках, вызванных короткими и мощными лазерными импульсами, связана как с большим разнообразием и необычностью физических процессов протекающих в зоне лазерного воздействия, так и с необычайно высокими скоростями движения границ раздела расплава и твердой фазы. Быстрые фазовые переходы сопровождаются сильными перегревами твердой фазы при плавлении и сильными переохлаждениями жидкой фазы при затвердевании расплава. Для качественного и количественного описания подобных ситуаций разрабатывается в настоящее время особый класс локально-неравновесных моделей. Разрабатываемые модели охватывают процессы макро и микро уровня. Для характеристики макропроцессов используются локально-неравновесные модели, базирующиеся на уравнениях механики сплошной среды [1] с резкой границей, представляющие собой различные варианты задачи Стефана [2]. Для процессов атомарного уровня – молекулярно динамический подход, суть которого состоит в прямом нахождении траекторий молекул в соответствии с заданными свойствами межатомарного взаимодействия [3,4]. Кроме этого используются комбинированные модели, включающие оба: континуальное и молекулярно-динамическое описание [5]. Решение континуальных локально-неравновесных моделей позволяет определять тепловые и гидродинамические поля, температурные градиенты, скорости перемещения фазовых фронтов, степени перегревов твёрдой фазы при плавлении и переохлаждения жидкой при кристаллизации. Знание скорости движения фазовых фронтов позволяет также определить размеры области фазовых превращений в твёрдом теле и жидкости. Модели молекулярной динамики используются для определения структурных, динамических, термодинамических и кинетических свойств молекулярных или атомарных систем.

Благодарности: Работа выполнена при финансовой поддержке РФФИ №№ 13-07-00597, 15- 07- 05025.

Литература:

1. Henry M. van Driel. Kinetics of high-density plasmas generated in Si by 1.06- and 0.53-μm picosecond laser pulses. J. Phys. Rev. B, **35**, № 15, 8166-8176, (1987).
2. В.И. Мажукин, В.В. Носов, Математическое моделирование неравновесных нагрева и плавления кремния лазерным излучением Nd-YAG лазера на длине волны излучения 1,06 μm. SPIE, Proceedings 5th International Conference on Industrial Lasers and Laser Applications 95, **2713**, 236-247, (1995).
3. V.I. Mazhukin, A. V. Shapranov, O.N.Koroleva, A.V. Rudenko. Molecular dynamics simulation of critical point parameters for silicon, Mathematica Montisnigri, **XXX**, 56-76, (2014).
4. Dorel Buta, Mark Asta, Jeffrey J. Hoyt. Kinetic coefficient of steps at the Si (111) crystal-melt interface from molecular dynamics simulations. J. Chem. Phys., **127**, 074703 (2007).
5. V.P. Lipp, B. Rethfeld, M.E. Garcia, D.S. Ivanov. Atomistic-continuum modeling of short laser pulse melting of Si targets. Phys. Rev. B, **90**, 245306, (2014).

ANALYSIS OF MATHEMATICAL MODELS OF LASER HEATING AND MELTING OF SILICON

O.N. Koroleva, AV. Mazhukin, P.V. Breslavskii
Keldysh Institute of Applied Mathematics Russian Academy of Sciences
Miusskaya sq., 4, Moscow, 125047, Russia
vim@modhef.ru

Mathematical models of heating, heterogeneous and homogeneous melting of silicon in the report are analyzed. The complexity of the mathematical description of the fundamental mechanisms underlying the rapid phase transitions in semiconductors, caused by short and intense laser pulses, are associated with both the great variety and uniqueness of the physical processes occurring in the area of laser exposure, and with an extremely high speeds of the interfaces melt and the solid phase. The rapid phase transitions are accompanied by severe overheating during melting of the solid phase and liquid phase and by strong supercooling during solidification of the melt. For qualitative and quantitative description of these situations a special class of locally-equilibrium models is currently being developed. The developed models include the processes of macro and micro level. To characterize the macro processes, locally non-equilibrium models are used based on the equations of continuum mechanics [1] with a sharp boundary, representing the different types of the Stefan problem [2]. For the processes at the atomic level, molecular dynamic approach is used, the essence of which is in direct finding trajectories of molecules in accordance with the desired properties of the interatomic interaction [3,4]. Besides, the combined models are used, which include a continuum and molecular dynamic description [5]. The solution of the continual locally nonequilibrium models allows to determine the thermal and hydrodynamic fields, temperature gradients, the phase velocity of the fronts, the superheating of the solid phase during melting and supercooling of the liquid phase during crystallization. Knowing the speed of the phase fronts can also determine the size of the field of phase transformations in solids and liquids. Molecular dynamics models are used to determine the structural, dynamic, thermodynamic and kinetic properties of molecular and atomic systems.

Acknowledgements: This work was supported by RFBR grants №№ 13-07-00597, 15- 07-05025.

References:

1. Henry M. van Driel. Kinetics of high-density plasmas generated in Si by 1.06- and 0.53-μm picosecond laser pulses. J. Phys. Rev. B, **35**, № 15, 8166-8176, (1987).
2. V.I. Mazhukin, V.V. Nosov. Matematicheskoe modelirovanie neravnovesnykh nagreva i plavleniia kremniia lazernym izlucheniem Nd-YAG lazera na dline volny izlucheniia 1,06 μm. SPIE, Proceedings 5th International Conference on Industrial Lasers and Laser Applications 95, **2713**, 236-247, (1995).
3. V.I. Mazhukin, A. V. Shapranov, O.N.Koroleva, A.V. Rudenko. Molecular dynamics simulation of critical point parameters for silicon, Mathematica Montisnigri, **XXX**, 56-76, (2014).
4. Dorel Buta, Mark Asta, Jeffrey J. Hoyt. Kinetic coefficient of steps at the Si (111) crystal-melt interface from molecular dynamics simulations. J. Chem. Phys., **127**, 074703 (2007).
5. V.P. Lipp, B. Rethfeld, M.E. Garcia, D.S. Ivanov. Atomistic-continuum modeling of short laser pulse melting of Si targets. Phys. Rev. B, **90**, 245306, (2014).

LOCAL BOUNDARY PROPERTIES OF MAPPINGS: A GENERAL APPROACH

Žarko Pavićević

University of Montenegro, Faculty of Science, Pogdorica, Montenegro

E-mail address: zarkop@ac.me

To successfully solving local boundary properties of functions $f: D \to \mathbb{R}^n,\ D \subset \mathbb{R}^n,\ n \in \mathbb{N},$ it is necessary the following „infrastructure" of a domain D:

- it is possible to define the hyperbolc metric on D (distance);
- the existence of a group $\Im$ of automorphisms of D;
- the hyperbolc metric (distance) is invariant with respect to a group $\Im$.

***Example* 1.** Let $B^n, n \in \mathbb{N},$ be the *n*-dimensional ball on $\mathbb{R}^n$. For this domain, the previously mentioned three properties are satisfied for study local boundary properties.
Let $f: B^n \to \mathbb{R}^n$ be an arbitrary function, $\zeta \in \partial B^n$ and let (w_n) be a sequence in B^n such that $\lim_{n\to\infty} w_n = \zeta$. Let $C(f, \mathrm{A})$ denote a cluster set of a function f along a set *A*. Then for arbitrary compact subset K of B^n there holds $C\left(f, \bigcup_{n=1}^{\infty} g_{w_n}(K)\right) = \{\alpha\},\ \alpha \in \overline{\mathbb{R}^n}$, if and only if a sequence $\left(f \circ g_{w_n}\right)$ converges uniformly on K to a constant α.

The second important moment that gives a necessary condition for the existence of local boundary properties of mappings $f: D \to \mathbb{R}^n$ is the normality of of the family $\{f \circ g \mid g \in \Im\}$. This is indicated by Example 1.

The third important moment for the study of local boundary properties of mappings $f: D \to \mathbb{R}^n,\ D \subset \mathbb{R}^n,\ n \in \mathbb{N},$ is in relation to the question of the validity of „some" uniqueness theorem for a mapping f.

***Example* 2.** Let $f: B^n \to \mathbb{R}^n$ be a normal quasiconformal mapping, $\zeta \in \partial B^n$, and let (w_n) be a sequence such that $\lim_{n\to\infty} w_n = \zeta$. If there exists a „small" ball $L,\ L \subset B^n$ such that $C\left(f, \bigcup_{n=1}^{\infty} g_{w_n}(L)\right) = \{\alpha\}$ with $\alpha \in \overline{\mathbb{R}^n}$, then $C\left(f, \bigcup_{n=1}^{\infty} g_{w_n}(L)\right) = \{\alpha\}$ for every ball $L,\ L \subset B^n$.

MATHEMATICAL MODELS AND NUMERICAL SCHEMES ON UNSTRUCTURED MESHES FOR SOLVING AERODYNAMICS+AEROACOUSTICS PROBLEMS

Tatiana Kozubskaya
Keldysh Institute of Applied Mathematics RAS, Miusskaya Sq., 4, Moscow 125047, Russia
tatiana.kozubskaya@gmail.com

The talk begins from a brief overview on mathematical models used for solving complex aerodynamics and aeroacoustics problems. Generally, the modeling is built basing on the Navier-Stokes equations (including the averaged and spatially filtered formulations if necessary) in the region of nonlinear distributed acoustic source, the linearized equations systems in the near-field propagation region and the wave equation in the far field.

The aeroacoustics in aviation applications is mostly determined by unsteady turbulent flows. It is very sensitive both to the correctness of turbulence modeling and the accuracy of numerical methods used for the simulation of these flows. The situation is additionally complicated by a possible presence of shocks. All these points are to be carefully considered at the numerical implementation.

We develop the higher-accuracy lower-cost EBR (Edge Based Reconstruction) schemes for solving aerodynamics+aeroacoustics problems on unstructured meshes which are suitable for applications of complex geometry. The schemes are based on quasi-1D reconstruction of variables and provide accuracy of the 2^{nd}-6^{th} order depending on the mesh quality.

Finally, the examples of aerodynamics and aeroacoustics problems simulated recently are presented.

Acknowledgements:
The work is supported by the Russian Foundation for Basic Research (RFBR Project 15-01-07911).

References:

1. Ilya V.Abalakin, Alain Dervieux, Tatiana K.Kozubskaya, “On the accuracy of direct noise calculations based on the Euler model”, in “Computational Aeroacoustics”, Multi-Science Publishing, Essex SS5 4AD, UK, 141-166 (2008)
2. P.A.Bakhvalov, T.K.Kozubskaya, E.D.Kornilina, A.V.Morozov, M.V.Jakobovskii, “Technology of predicting acoustic disturbances in flow far field”, Mathematical Models and Computer Simulations, **4,** 3, 363–373 (2012)
3. Ilya Abalakin, Pavel Bakhvalov, Tatiana Kozubskaya, “Edge-based reconstruction schemes for prediction of near field flow region in complex aeroacoustic problems”, Int. J. of Aeroac., **13** (3&4), 207-234 (2014).

МОДЕЛИРОВАНИЕ ТЕЧЕНИЯ ТРЕХФАЗНОЙ ЖИДКОСТИ В ПОРИСТОЙ СРЕДЕ С УЧЕТОМ ТЕРМИЧЕСКИХ ЭФФЕКТОВ

Трапезникова М.А., Чурбанова Н.Г., Люпа А.А.
Институт прикладной математики им. М.В. Келдыша РАН, Москва, Россия
e-mail: mtrapez@yandex.ru

Математическое моделирование течений в пористых средах находит широкое применение при конструировании гидросооружений, при решении экологических задач о загрязнении почвы и грунтовых вод, при разработке технологий добычи углеводородов. В наши дни перспективными являются термические методы нефтедобычи: внутрипластовое горение, закачка теплоносителя в пласт и др. Поэтому возникает необходимость адекватного моделирования термических эффектов.

Работа посвящена дальнейшему развитию оригинальной математической модели многофазных течений в пористых средах, построенной по аналогии с квазигазодинамической системой уравнений [1]. Моделирование крупномасштабных процессов в подземных горизонтах является весьма трудоемким, и его практически невозможно проводить без использования высокопроизводительных вычислительных систем. Поэтому предпочтение отдается алгоритмам явного типа, так как они могут быть эффективно адаптированы к суперкомпьютерам с гибридной архитектурой.

Модель обобщена на случай трехфазного течения (вода-нефть-газ) и учитывает возможные источники тепловыделения. Жидкости слабосжимаемые, присутствуют гравитация и капиллярные силы. Уравнения неразрывности фаз модифицированы: они содержат регуляризаторы и производные второго порядка по времени с малыми параметрами. Эти гиперболические уравнения могут быть аппроксимированы трехслойной явной схемой с достаточно мягким условием устойчивости, конвективные члены аппроксимируем центральными разностями. Так как температура всех фаз и породы считается одинаковой, система включает единое уравнение сохранения энергии, которое аппроксимируем также явной схемой.

С целью верификации решен ряд тестовых задач просачивания и нефтедобычи в изотермическом и неизотермическом случаях. Созданный ранее комплекс параллельных программ [2] дополнен новыми модулями. Достигнута высокая эффективность распараллеливания при расчетах как на классическом кластере, так и на кластере с графическими ускорителями вычислений.

В ближайшем будущем модель будет преобразована в композиционную для учета многокомпонентного состава жидкостей.

Работа поддержана РФФИ (гранты 13-01-12073-офи, 15-01-03654, 15-01-03445).

Список литературы:

1. D. Morozov, M. Trapeznikova, B. Chetverushkin, N. Churbanova, "Application of explicit schemes for the simulation of the two phase filtration process" Math. Mod. & Comp. Sim., **4**, No.1, 62-67 (2012)
2. D. Morozov, M. Trapeznikova, B. Chetverushkin, N. Churbanova, "Simulation of filtration problems on hybrid computer systems" Math. Mod. & Comp. Sim., **5**, No.3, 208-212 (2013)

SIMULATION OF THREE-PHASE FLUID FLOW IN A POROUS MEDIUM WITHACCOUNT OF THERMAL EFFECTS

Trapeznikova M.A., Churbanova N.G., Lyupa A.A.
Keldysh Institute of Applied Mathematics RAS, Moscow, Russia
e-mail: mtrapez@yandex.ru

Mathematical modeling of fluid flows in porous media is widely used in practice, in particular, at the construction of hydraulic facilities, at the solution of ecological problems concerning the soil and groundwater contamination and, of course, at the development of hydrocarbon recovery technologies. Nowadays the oil-and-gas industry faces global problems connected with the drop in production by traditional methods. Among perspective methods of oil recovery there are thermal methods such as in-situ combustion, heat carrier pumping into the stratum etc. Thus appropriate numerical predictions of thermal effects are necessary.

The present work deals with further development of an original mathematical model of multiphase porous media flows constructed by the analogy with the quasi-gas dynamic system of equations [1]. Simulation of large-scale processes in the subsurface is time-consuming and impossible without the use of HPC systems. Therefore algorithms of the explicit type are preferable, as they can be efficiently adapted to supercomputers with hybrid architectures. The proposed model is generalized to the case of three-phase flow (water-oil-gas) and takes into account possible heat sources. Fluids are slightly compressible and immiscible; the gravitational and capillary forces are present. The distinguishing feature of the model is modification of phase continuity equations: they get regularizing terms and second order time derivatives with small parameters. These hyperbolic equations can be approximated by the three-level explicit scheme with rather a mild stability condition; convective terms are approximated by central differences. As the temperature of all phases and the rock is identicalthe system involves a single equation of the total energy conservation approximated also by an explicit scheme.

The approach is verified by solving a number of test problems of infiltration and oil recovery in isothermal and non- isothermal cases. The parallel software created by the authors earlier [2] is supplemented with new computational modules. High parallelization efficiency is achieved on a classical cluster as well as on a GPU-based cluster.

In the nearest future the model will be transformed to the compositional one to take into account a multi-component structure of fluids.

Acknowledgements:
The work is supported by RFBR (grants No. 13-01-12073-ofi, 15-01-03654, 15-01-03445).

References:

1. D. Morozov, M. Trapeznikova, B. Chetverushkin, N. Churbanova, “Application of explicit schemes for the simulation of the two phase filtration process” Math. Mod. & Comp. Sim., **4**, No.1, 62-67 (2012)
2. D. Morozov, M. Trapeznikova, B. Chetverushkin, N. Churbanova, “Simulation of filtration problems on hybrid computer systems” Math. Mod. & Comp. Sim., **5**, No.3, 208-212 (2013).

ДВА ПОДХОДА К МОДЕЛИРОВАНИЮ ПОТОКОВ АВТОМОБИЛЬНОГО ТРАНСПОРТА С ИСПОЛЬЗОВАНИЕМ ВЫСОКОПРОИЗВОДИТЕЛЬНЫХ ВЫЧИСЛИТЕЛЬНЫХ СИСТЕМ

Чурбанова Н.Г., Чечина А.А., Трапезникова М.А.

Институт прикладной математики им. М.В. Келдыша РАН,
Москва, Миусская пл., 4
e-mail: nataimamod@mail.ru

Работа посвящена моделированию автотранспортных потоков на городских улицах и автомагистралях. Представлены оригинальные макро- и микроскопические модели многополосного движения для описания потоков с учётом реальной геометрии дороги. Макроскопическая, или гидродинамическая, модель синхронизованного транспортного потока использует приближение сплошной среды и построена по аналогии с квази-газо-динамической (КГД) системой уравнений [1]. В отличие от существовавших ранее моделей автотранспорта, здесь вводится переменная поперечная скорость, а именно, скорость смены полос. В рамках этой модели можно описывать многофазные потоки, когда каждая фаза имеет свои собственные плотность и скорость. Микроскопическая модель основана на теории клеточных автоматов [2] и обобщена на многополосный случай.

Описанные выше модели сравнивались на большом числе тестовых расчётов в ситуациях, когда они обе применимы. Полученные результаты показали хорошее согласование моделей, как по качественным, так и по количественным параметрам.

Численный алгоритм макроскопической модели был адаптирован для расчётов на многопроцессорной вычислительной системе. Распараллеливание основано на технике декомпозиции области (разделение данных) и обмене данными между узлами кластера. Расчеты были выполнены на гибридной системе К 100, сконструированной в Институте прикладной математики им. М.В. Келдыша с пиковой производительностью 100 TFLOPS. Было получено достаточно высокое ускорение.

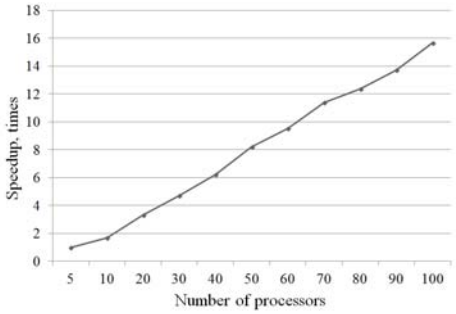


Рис. 1. Ускорение в зависимости от числа процессоров

Рисунок 1 демонстрирует ускорение более чем в 15 раз на 100 процессорах по сравнению с 5 процессорами на сетке 3 миллиона расчетных точек.

Работа была поддержана грантами РФФИ № 13-01-00781, 13-01-12008-офи.

Литература:

1. A.B. Sukhinova, M.A. Trapeznikova, B.N. Chetverushkin and N.G. Churbanova. "Two-Dimensional Macroscopic Model of Traffic Flows". Mathematical Models and Computer Simulations, **1**, No. 6, 669–676 (2009).
2. K. Nagel, M. Schreckenberg, A Cellular Automation Model for Freeway Traffic. J. Phys. I France, **2,** 2221 (1992).

TWO APPROACHES TO THE VEHICULAR TRAFFIC FLOWS SIMULATION USING HIGH-PERFORMANCE COMPUTER SYSTEMS

Churbanova N.G., Chechina A.A., Trapeznikova M.A.
Keldysh Institute of Applied Mathematics RAS, 4 Miusskaya Square, Moscow
e-mail: nataimamod@mail.ru

The paper deals with the simulation of vehicular traffic flows in urban streets and at motorway. Original 2D macro- and microscopic models of multilane traffic to predict flows for the real road geometry are presented. The macroscopic or hydrodynamical model of synchronized traffic flow uses the continuum approach and is constructed by analogy with the quasi-gas-dynamic (QGD) system of equations [1]. Contrary to the earlier traffic flow models, a variable transverse velocity (namely the velocity of lane changing) is introduced. In the frame of this model the multiphase flow can be described where each phase has its own density and velocity. The microscopic model is based on the cellular automata theory [2] and is generalized to the multilane case.

The models described above are compared by a large number of test predictions for situations when both models are applicable. The results obtained demonstrated good agreement of the models in both qualitative and quantitative sense.

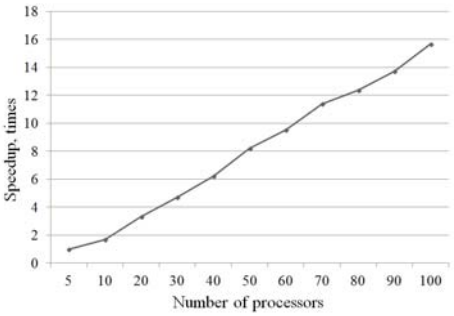


Fig. 1. Speedup depending on the number of processors

The numerical algorithm of macroscopic model was adapted to multiprocessor computer system. Parallelization is based on the domain decomposition (data partitioning) technique and message passing between nodes of the cluster. Computations were performed on hybrid system K100 built in Keldysh Institute of Applied Mathematics. with the peak performance 100 TFLOPS. The high enough speedup was obtained: Figure 1 demonstrates more than 15 times speedup using 100 processors versus 5 processors on the 3 million cells mesh.

Acknowledgements: The work was supported by RFBR projects № 13-01-00781, 13-01-12008-ofi

References:

1. A.B. Sukhinova, M.A. Trapeznikova, B.N. Chetverushkin and N.G. Churbanova. “TwoDimensional Macroscopic Model of Traffic Flows”. Mathematical Models and Computer Simulations, **1**, No. 6, 669–676 (2009).
2. K. Nagel, M. Schreckenberg, A Cellular Automation Model for Freeway Traffic. J. Phys. I France, **2,** 2221 (1992).

MODELLING A STIMULATED AMPLIFICATION OF LONG-WAVE WING OF A MULTI-HARMONIC LIGHT BEAM AT PROPAGATION IN DIELECTRIC MEDIA WITH INDUCED PLASMA AND STATIC ELECTRIC FIELD.

Sviatoslav A. Stumpf, Alexander A. Korolev, Sergei A. Kozlov
ITMO UNIVERSITY, 49 Kronverksky pr., Saint-Petersburg, Russia 197101
stumpf@rain.ifmo.ru

A generation of spectral supercontinuum by a pair of synchronized few-cycle pulses, including a generation of radiation in terahertz range (THz), is an object of complex and thorough studies this decade [1-2]. Fine tuning of generation procedure, opening a way to cost-effective and efficient generation of long-wave radiation (up to 1 mm) [3-4], is being developed in parallel with a theory combining optical processes in dielectric media with highenergetic processes such as plasma induction. We derived the theory several years ago [5] and applied it to numerical simulation and mathematical modelling of mentioned processes. The computed data shown an excellent correlation with experimental quazi-periodic dependence of generated THz radiation energy on interacting pulses spatial shift.

Noticing a fast progress of experimental set-ups, allowing generation and combination of multiple synchronized optic pulses, we found out that theoretically it is possible to increase an efficiency of THz generation by adding pulses of tripled basic wavelength to an interaction scene. So the present paper shows some results of modelling and simulating such multiwave high-intense femtosecond pulse propagation through dielectric media with plasma excitation. The additional feature of this study is an simulation of high-intense few-cycle pulse interaction with media at presence of quasi-static electric field, causing a separate ponderomotive dynamics of free electrons induced by input pulse. We report several scenes modelling such dynamics and predicting notable generation of THz radiation stimulated by static field. Also the dependence of optical energy redistributed to THz range on 'filament length' is presented and examined by a correlation with known experimental results.

Acknowledgements:
The authors would like to thank the Russian Fund of Fundamental Researches for supportingthe research program; professor Yuri A. Shpolyansky for contributing into the numerical modelling; professor Victor G. Bespalov for discussing experimental studies.

References:

1. Karpowicz N, Lu X, Zhang X-C "Terahertz gas photonics" J. Modern Opt., **56**, 1137–1150 (2009).
2. Dai J, Karpowicz N, Zhang X-C "Coherent polarization control of terahertz waves generated from two-color laser-induced plasma" Phys. Rev. Lett., **103,** 023001 (2009).
3. Kosareva O G, Kandidov V P, Chin S L et al "Optimization of a femtosecond pulse self-compression region along a filament in air" Appl. Phys. B., **91**, 35–43 (2008).
4. S. Tsortakis , B. Prade, M. Franco et al, "Femtosecond laser-guided electric dischage in air" Phys. Rev., **64**, 057401 (2001).
5. Stumpf S A, Korolev A A, Kozlov S A Izv. RAN, Ser. Phys. **71**, 158-161 (2007).

NUMERICAL STUDIES BY MEANS OF MARPLE: NEW TOOLSFOR PARALLEL SIMULATION OF CONTINUOUS MEDIAUSING UNSTRUCTURED MESHES

Bagdasarov G., Boldarev A .
Keldysh Institute of Applied Mathematics RAS, Moscow, Russia
gennadiy3.14@gmail.com

Code MARPLE [1] is an Eulerian numerical tool designed for 3D simulations of radiative magnetohydrodynamic problems related to experiments with magnetically driven high energy density plasmas. In recent years new features and optimizations were implemented in the code with the view of preparing it for comprehensively scaled multiphysics and upcoming exascale computations.

Data structures based on binary relations are used in the code to operate with unstructured meshes. New storage scheme was implemented in order to improve performance, add support for oct-tree type of meshes and adaptive mesh refinement technique.

Initial support for scripting languages was embedded in the code. Python wrappers for equation-of-states module were implemented which allow storing only indispensable minimum amount of computed values for post-processing.

The renovated code demonstrates good scalability and ability to handle large data volumes needed for HPC multi-parameter numerical studies.

The work was supported by RFBR grant No.14-01-31154.

References:

1. Boldarev A., Gasilov V., Olkhovskaya O., Dyachenko S., Bagdasarov G., Boldyrev S., Gasilova I., Dorofeeva E. “Object-oriented code MARPLE3D: simulations of radiative hydrodynamic/MHD effects at high-performance computer systems.” In: 6th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012), Vienna, Austria, 10–14 September 2012.

РАЗВИТИЕ КОДА ТРЕХМЕРНОГО ЧИСЛЕННОГО МОДЕЛИРОВАНИЯ MARPLE: ОБОБЩЕННОЕ ПРОГРАММИРОВАНИЕ И СОЗДАНИЕ ДЕЙСТВИТЕЛЬНО УНИВЕРСАЛЬНЫХ КОДОВ

А. С. Болдарев
Институт Прикладной Математики им. М. В. Келдыша РАН, Москва
boldar@imamod.ru

В течение ряда лет в нашем отделе ИПМ РАН разрабатывается и используется трехмерный код MARPLE для моделирования процессов в высокотемпературной плазме. Исследовательский характер этого кода налагает требование максимальной гибкости и универсальности, чтобы можно было легко добавлять учитываемые физические процессы, менять термодинамическую модель среды, аппроксимации, способы учета тех или иных явлений и т. д. Кроме того, разнообразие типов решаемых нами задач и естественное желание использовать при их решении имеющуюся в MARPLE инфраструктуру (распределенная работа с неструктурированными сетками, общая организация вычислений, аппроксимации, визуализация результатов и т. д.) привело к тому, что с помощью кода MARPLE проводятся расчеты в различных предметных областях, помимо физики плазмы.

Код MARPLE изначально создавался как универсальный легко достраиваемый код, это достигалось благодаря его структуре и широкому использованию объектно-ориентированных возможностей языка C++. В результате, в настоящее время к коду легко могут быть добавлены новые солверы, уравнения состояния, граничные условия и т. д. Однако в коде остались некоторые"жестко зашитые" элементы, такие как набор величин в ячейках сетки, и это приводит к определенным проблемам при переходе к другой предметной области. Например, газодинамические задачи приходится трактовать как частный случай двухтемпературной МГД, в результате хранятся и обрабатываются нерелевантные для данной предметной области величины, такие как вторая энергия, компоненты магнитного поля...

Грамотное использование обобщенного программирования (с помощью шаблонов в C++) позволяет решить проблему создания большого количества однотипных солверов – например, одно- и двухтемпературной МГД, газодинамики, моделей турбулентности и др. Солвер становится шаблоном, в котором содержатся все общие черты перечисленных частных солверов– организация вычисления потоков и их учета, вычисление"наветренных" величин с той или иной коррекцией и т. д., в то время как конкретные алгоритмы вычисления и сложения потоков и т. п. для выбранной конкретной системы уравнений передаются в шаблон в виде параметров.

Обобщенное программирование позволяет также оптимизировать работу с различными типами сеток. Как и в предыдущем случае, сведение всех возможных частных случаев к одному наиболее общему приводит к неэффективной реализации.

Например, хранение индексно прямоугольной сетки в виде неструктурированной приводит к необходимости хранения отношений инцидентности элементов, в данном частном случае имеющих очевидную структуру и потому в хранении не нуждающихся.

В рамках обобщенного программирования солвер должен работать с сеткой как с абстрактным объектом, способным отвечать на запросы определенного вида.

MULTISCALE MODELING IN SUPERSONIC GASDYNAMIC SPUTTERING PROBLEMS

Yu.N. Karamzin, T.A. Kudryashova, V.O. Podryga, S.V. Polyakov
Keldysh Institute of Applied Mathematics, Russian Academy of Science, Moscow, Russia
E-mail: pvictoria@list.ru

The simulation problem of technological processes in installations for supersonic cold gasdynamic sputtering (SCGS) of micro- and nanoparticles on the substrates is considered [1]. This theme is relevant in connection with the transfer of sputtering technology on a nanometer range. In the electronics industry SCGS technology is proposed to use for creating of the polysilicic nanofilms with the inclusion of carbon nanostructures and / or nanoclusters made of rare-earth metals [2]. However, there are difficulties related to management of a sputtering process and providing the required quality of the films. To overcome these difficulties detailed investigations of processes occurring in the installations are needed. In this paper focus is on a transport part of the sputtering problem. Its decision is connected with a technical device of SCGS installation. In simplified form, the installation consists of Dewar flask with rarefied gas, which has a table with a substrate for deposition. Sputtering subsystem is located above the table. It consists of cylinders channels with pure gas mixture and the gas mixture with nanoparticles, the matrix of micronozzles and microchannels in which the nanoparticles are supplied into the near zone of the substrate. Pure gas mixture is used for process control. Gas mixture with the inclusion of nanoparticles is used to give them a starting pulse. The mathematical problem is to calculate the motion of the gas and nanoparticles in all parts of the installation, and determining the optimum mode of nanoparticles moving to the individual sputtering places. It is necessary to take into account that the simulated environment near solid surfaces is not continuous, and the equation of state of gas mixture with the inclusion of nanoparticles is unknown. For decision of this problem multiscale approach is proposed, combining the solution of a quasi gasdynamic (QGD) [3] equations and correction of gasdynamic parameters by molecular dynamics method (MD) [4]. QGD system is considered in relaxational approximation and is written for a case of gas mixtures. It is solved by method of finite volumes on a suitable grid. The system of equations of the Newtonian dynamics is used as the sub-grid algorithm, which is applied in each control volume. The proposed method has been parallelized, passed a partial validation and confirmed its operability and efficiency.

Acknowledgements: This work is supported by Russian Fund for Basic Researches. Work partially supported by grants RFBR №№ 13-01-12073-ofi-m, 15-07-06082.

References:

1. A. Papyrin, V. Kosarev, S. Klinkov, A. Alkhimov, V. Fomin, “Cold Spray Technology”, Amsterdam: Elsevier Science (2007).
2. D. Resnick, “Nanoimprint lithography”. In “Nanolithography. The art of fabricating nanoelectronic and nanophotonic devices and systems” (Edited by Martin Feldman), Woodhead Publishing Limited (2014).
3. T.G. Elizarova, “Quasi-gasdynamic equations”, Springer (2009).
4. J.M. Haile, “Molecular Dynamics Simulations. Elementary Methods”, NY: John Wiley & Sons Inc. (1992).

МУЛЬТИМАСШТАБНОЕ МОДЕЛИРОВАНИЕ В ЗАДАЧАХ СВЕРХЗВУКОВОГО ГАЗОДИНАМИЧЕСКОГО НАПЫЛЕНИЯ

Ю.Н. Карамзин, Т.А. Кудряшова, В.О. Подрыга, С.В. Поляков
ИПМ им. М.В. Келдыша РАН, Москва, Россия
E-mail: pvictoria@list.ru

Рассматривается проблема моделирования технологических процессов в установках сверхзвукового холодного газодинамического напыления (СХГН) микро- и наночастиц на подложки [1]. Данная тематика актуальна в связи с переходом технологии напыления в нанометровый диапазон. В электронной промышленности технологию СХГН предлагается использовать для создания поликремниевых нанопленок с включением углеродных наноструктур и/или нанокластеров, изготовленных из редкоземельных металлов [2]. Однако при этом возникают трудности, связанные с управлением процессом напыления и обеспечением нужного качества пленок. Для преодоления этих трудностей необходимы детальные исследования протекающих в установках процессов. В данной работе основное внимание уделяется транспортной части проблемы напыления. Ее решение связано с техническим устройством установки СХГН. В упрощенном виде установка состоит из дюаровского сосуда с разреженным газом, в котором имеется стол с подложкой для напыления. Над столом расположена подсистема напыления. Она состоит из каналов от баллонов с чистой газовой смесью и газовой смесью с наночастицами, матрицы микросопел и микроканалов, по которым наночастицы подаются в ближнюю зону подложки. Чистая газовая смесь используется для управления процессом. Газовая смесь с включением наночастиц используется для придания последним стартового импульса. Математическая задача состоит в расчете движения газа и наночастиц во всех частях установки и определении оптимального режима подачи наночастиц к индивидуальным местам напыления. При этом необходимо учесть, что моделируемая среда вблизи твердых поверхностей не является сплошной, а уравнение состояния газовой смеси с включением наночастиц неизвестно. Для решения задачи предлагается мультимасштабный подход, сочетающий решение уравнений квазигазодинамики (КГД) [3] и коррекцию газодинамических параметров методом молекулярной динамики (МД) [4]. КГД система рассматривается в релаксационном приближении, записана для случая смеси газов и решается методом конечных объёмов на подходящей сетке. Система уравнений ньютоновской динамики используется в качестве подсеточного алгоритма, применяющегося внутри каждого контрольного объёма. Предложенная методика была распараллелена, прошла частичную валидацию и подтвердила свою работоспособность и эффективность.

Благодарности: Работа выполнена при поддержке Российского фонда фундаментальных исследований, проекты №№ 13-01-12073-офи-м, 15-07-06082.

Литература:

1. А.П. Алхимов, С.В. Клинков, В.Ф. Косарев, В.М. Фомин, "Холодное газодинамическое напыление. Теория и практика", М.: Физматлит (2010).
2. D. Resnick, "Nanoimprint lithography". In "Nanolithography. The art of fabricating nanoelectronic and nanophotonic devices and systems" (Edited by Martin Feldman), Woodhead Publishing Limited (2014).
3. T.G. Elizarova, "Quasi-gasdynamic equations", Springer (2009).
4. J.M. Haile, "Molecular Dynamics Simulations. Elementary Methods", NY: John Wiley & Sons Inc. (1992).

APPROXIMATION OF CONTINUOUS BREAKING FOR MODELING RADIATION-INDUCED CONDUCTIVITY OF CRYSTALS

M.B. Markov, I. A. Tarakanov, Y.A. Volkov
Keldysh Institute of Applied Mathematics of Russian Academy of Sciences,
Miusskaya sq.4, Moscow, 125047, Russia
e-mail:liu_roach@mail.ru

The mathematical model of radiation-induced conductivity in non-degenerate semiconductors and dielectrics is submitted. The most common materials of semiconductor devices are considered: silicon and silicon dioxide.

Mathematical modeling of radiation-induced conductivity is carried out in two stages. At the first stage the scattering of high energy photons and electrons, which excite non-equilibrium distribution of charge carriers in the crystal, is examined. The process is described by Maxwell equations and classic transport equations for photons and free electrons with energies exceeding the ionization potential of the scattering medium [1]. The source of the charge carriers with energies below ionization potential – the conduction electrons and valence band holes – is defined as functional on the space of free electrons transport equation solutions. Next, the carriers dynamics is considered on the basis of quantum kinetic equations for their distribution functions in the phase-space of coordinates and quasimomentum. Scattering of charge carriers is modeled in the approximation of continuous momentum loss.

This model was validated by comparison with experimental data on the electrons average drift velocity in an electric field and the speed of energy transmission from electrons to optical phonons. The effect of drift speed saturation [2,3] – the achievement of a constant value of 10^7 cm/s in increasing electric field strength – is confirmed. The initial distribution of the conduction electrons with average energy of about 2 eV degrades to an equilibrium state during the time of the order of 10^{-13} s, which corresponds to the data of [4]. The condition of simulation and experimental results is limited of energy loss by optical phonon energy. Quantitative agreement with the results of the drift theory is obtained.

The calculation of silicon barrier radiative conductivity, which is uniformly ionized by external source free electrons flux, shows the following. Radiation conductivity exceeds the equilibrium value by five orders of magnitude. Constant conductivity value is stored until the time of conduction electrons and valence band holes recombination.

Acknowledgement :
The reported study was partially supported by RFBR, research project No. 14-01-00350.

References:

1. Markov M. B., Zhukovskiy M. E. “Modeling the radiative electromagnetic field”, International Journal of Computing Science and Mathematics.**2**, No.1/2, 110 –131, (2008).
2. Смирнов Б.М. “Кинетика электронов в газах и конденсированных системах”, УФН, **172**, 1411-1447 (2002).
3. Canali C., Jacobini C., Nava F., Ottavini G., Quaranta A. A. “Electron drift velocity in silicon”, Phys. Rev., B **12**, 2265, (1975).
4. Pop E., Sinha S., Goodson K.E. “Monte Carlo modeling of heat generation in electronic nanostructures”, Proc. of IMECE02/HT-32124, 1-6, (2002).

A CRITICAL ANALYSIS OF THE MATHEMATICAL MODELS AND SIMULATION RESULTS DESCRIBING THE DISTRIBUTION OF IMPURITIES IN THE ATMOSPHERE

Klochkova L.V., Tishkin V.F.
KIAM of RAS, Moscow
klud@imamod.ru

Represented work is directed on the solution of fundamental problems of mathematical forecasting of environment quality at anthropogenous and technogenic influences. In the report results of creation of mathematical models, computing methods and algorithms for the integrated expert systems of forecasting of development of the non-stationary processes described by the differential equations in private derivatives are discussed. The main idea consists in developing systematic approach to mathematical forecasting and formulation of computing experiments at the solution of actual applied problems which researchers face at science and equipment development. It is most the common fundamental problem of computational mathematics.

Methods of the description are a combination of the analytical, asymptotic and numerical decisions received on the basis of mathematical modeling by means of differential schemes and semi-empirical statistical model representations. Also as the known popular expression of the academician A.A. Samarsky that mathematical modeling is based upon three elephants: model – algorithm – the program, and computational mathematics on three foundations: approximation, interpolation, extrapolation. Correctly picked up approximating function allows to carry out correctly regression so that the measured values of sizes experimentally coincided for the set point in coordinate and time space with theoretical model.

For example, in the multiple-factor analysis of influence of development of various social structures for an appreciable length of time on environment of megalopolises it is necessary to solve complex computing problem. The same is required for carrying out researches of concrete characteristics of a condition of atmospheric layers and a ground layer of the hashing defining quality of air in the megalopolis. The problem especially becomes complicated if the task to estimate changing processes of toxic emissions spread from difficult variable sources in a changing environment in canyons of city building is set.

Acknowledgement : The work was supported by RFBR, grant 14-01-00145_a

LASER METAL NANOCRYSTALLIZATION: THEORETICAL MODELING

I. Zavestovskaya[1,2]
[1]*P.N. Lebedev Physical Institute of RAS, Leninsky pr.53, Moscow, 119991, Russia*
[2]*National research Nuclear University MEPhI (Moscow Engineering Physics Institute), Rashirskoe sh.31, Moscow, 115409, Russia*
zavest@sci.lebedev.ru

Laser micro- and nanostructuring of materials is important in many scientific, technological and medical applications. Nanostructures resulting from laser material processing have unique properties and cannot be produced by other, nonlaser techniques.

In optimizing laser nanostructuring conditions, an important point is to optimize the size of the resulting structures. The minimum possible size of the structures (tens of nanometers) produced by direct laser ablation of the surface is possible in two cases: 1) intense laser ablation due to cluster redeposition in and outside the ablation crater and 2) ultrashort laser pulses which ensure very rapid heating, melting and solidification of metal surfaces.

In recent years, controlled direct surface nanostructuring with laser pulses under such conditions has been the subject of intense research. Attempts were made to systematically study laser nanostructuring mechanisms and optimize processing conditions (intensity, duration, number and repetition rate of laser pulses) with consideration for the thermodynamic characteristics, mechanical properties and surface quality of the target material.

This Paper reviews the results of experimental and theoretical studies of micro- and nanomodification processes induced on the surface of metals and other materials by short and ultrashort laser pulses. Particular attention is paid to the possibility of direct laser nanostructuring through melting of the material (with or without ablation), followed by ultrarapid solidification of the molten surface.

The focus of attention have been the results on studying the kinetics of ultra-rapid solidification of the molten surface, and determination of the conditions which ensure forming of surface nano-scale structures.

An analytical solution to the rate equation for the crystallite size distribution after ultrarapid cooling has been found. The average number of atoms per crystallite and the size of crystalline grains resulting from pulsed laser irradiation of metal surfaces have been evaluated.

Determination of the volume fraction of crystallised phase allows one to find the critical cooling rate at which crystallization is impossible and the structure amorphises, i.e. to establish a kinetic amophisation criterion.

The model for laser modification of porous metallic films called as “the instant collapse of the pores” was considered.

The presented data can be used to optimize direct laser micro- and nanostructuring conditions and to ensure process control and reproducibility.

PARAMETRIC WAVE EXCITATION IN RELATIVISTIC LASER-PLASMA INTERACTION IN LONG UNDER-CRITICAL PRE-PLASMA LAYER

I. Tsymbalov[1], S. Shulyapov[1], A. Brantov[2], K. Ivanov[1], P. Ksenofontov[2], D. Krestovskikh[1], V. Bychenkov[2], V. Nedorezov[3] and A. Savel'ev[1]

[1]*Faculty of Physics and International Laser Center of Lomonosov Moscow State University, Moscow, Russia*

[2]*P.N. Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia*

[3]*Institute for Nuclear Research, Russian Academy of Sciences, Moscow, Russia*

E-mail: ivankrupenin2@gmail.com

The electron bunches with high energy and charge may be generated in low dense plasma via different mechanisms of laser acceleration [1]. In this paper we present the experimental research and numerical simulations of the possibility of generation MeV electrons at an intensity around 10^{18} W/cm^2 in an undercritical pre-plasma, formed by additional nanosecond laser pulse with controlled parameters onto the surface of solid targets. The effect may be attributed to the parametric plasma wave excitation.

In our experiments we used Ti:Sapphire laser system (wavelength – 800nm, repetition rate – 10Hz, maximal pulse energy – 30mJ, minimal pulse duration – 45±5fs and maximal intensity on target – $5\cdot10^{18}$ W/cm^2 , level of contrast on ps time scale - 10^{-8}) [2]. The laser radiation was focused by off-axis parabolic mirror (F~5cm) onto the Mo target. To create preplasma layer on the target surface, we use Nd: YAG laser (wavelength –10^{64}nm, repetition rate – 10Hz, maximal pulse energy – 70mJ, pulse duration – about 6 ns and maximal intensity on target – 10^{12} W/cm^2). Varying delay between main pulse and pre-pulse in the range from 10 ns to -50 ns we can change pre-plasma scale in the large range of values. All experiments were performed in a vacuum chamber at a pressure not higher than 10^{-2} Torr. Bremsstrahlung of hot plasma was detected by scintillation detector based on NaI crystal. The fiber spectrometer was used to measure the plasma emission spectra.

Our experimental results are supported by PIC simulation of laser-plasma interaction at the intensity around 10^{18} W/cm^2 (using 3D 3V code Mandor in 2D3V regime). A laser pulse (p-polarized, I – 10^{18} W/cm^2, λ – 1um, τ – 50fs) was focused into 90 um plasma layer with linear density gradient (from 0(0um) to $0.25n_{cr}$ (90um)). The density gradient is corresponding to the results of interferometry and shadowgraphy of the pre-plasma produced by the artificial prepulse. The calculations revealed that the propagation of the laser pulse through corona with rising density is accompanied by the relativistic self -focusing leading to increasing of laser pulse intensity, plasma wave excitation due to Raman scattering at density region around 0.15-0.25 $n_{cr.}$ and generation of an high energy(up to 7 MeV) electron bunch due to wavebreaking and acceleration by the longitudinal electric field of a plasma wave.

Acknowledgements: The work is supported by the Russian Foundation for Basic Research (grants ## 14-02-31871, 13-02-00337, 13-02-00494).

References:

1. D. Umstadter, Phys. D, **36**, 151-165 (2003).
2. Ivanov K A et al. Physics of Plasmas **21**(9) 093110 (2014).

MULTIGRID AND EXPLICIT-ITERATIVE SOLVERS FOR THREEDIMENSIONAL PARABOLIC EQUATIONS

V.T. Zhukov, O.B. Feodoritova, N.D. Novikova
Keldysh Institute of Applied Mathematics, Moscow, Russia.
zhukov@kiam.ru

The problems of numerical solution of time-dependent parabolic partial differential equations are considered. These equations are solved by discretizing both space and time. For space discretization it is used a convenient seven-point stencil on a cartesian grid. We present results of development of two time integration schemes for solving three-dimensional equations with anisotropic discontinuous coefficients on ultraparallel computers.

The first scheme is the implicit Euler method resolved by the multigrid method [1,2]. We refer to this scheme as MM scheme. The second scheme, LI-M [3], is elaborated to solve nonlinear heat conduction equation in high temperature gasdynamics simulation. This scheme is based on explicit iterations with Chebyshev's parameters and represents a rational function of spatial discrete operator. LI-M scheme is studied as a competitor of MM scheme.

Special attention is paid to development of the multigrid algorithm. The proposed algorithm represents an efficient parallel implementation of the Fedorenko multigrid method and is intended for solving the anisotropic stationary diffusion equations. The algorithm is able to solve the first, second and third boundary value problems including semi-definite Neumann problem. Scalability to a large number of processors is based on the use of the Chebyshev's iterations for solution of the coarsest grid equations and for construction of the smoothing procedures. For equations with discontinuous coefficients it is used so called problem-dependent intergrid transfer operators.

We have developed a special procedure for adapting smoothers to anisotropy and present examples, which show that adaptation improves the efficiency of the multigrid method. For LI-M and MM schemes the results of comparison on solving the evolution model problems are demonstrated. Both schemes provide a high performance; they scale efficiently and allow overcoming difficulties in achieving exaflops performance.

Acknowledgements:
This work is supported by the Russian Science Foundation (project № 14-21-00025).

References:

1. V. T. Zhukov, N. D. Novikova, O. B. Feodoritova, "Parallel multigrid method for solving elliptic equations", Math. Models and Computer Simulations, **6**, № 4, 425–434 (2014).
2. V. T. Zhukov, N. D. Novikova, O. B. Feodoritova, "Multigrid method for anisotropic diffusion equations based on adaptive Chebyshev smoothers", Math. Models and Computer Simulations, **7**, № 2, 117–127 (2015).
3. V.T. Zhukov, "Explicit methods of numerical integration for parabolic equations", Math. Models and Computer Simulations, **3**, № 3, 311–332 (2011).

NUMERICAL INVESTIGATIONS OF VARIATIONAL REPRESENTATION FOR GENERALIZED SOLUTIONS OF QUASILINEAR HYPERBOLIC EQUATIONS

O.B. Feodoritova, Yu.G. Rykov
Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Moscow, Russia
e-mail: feodor@kiam.ru

The modern theory of quasilinear conservation laws faces considerable difficulties. The theory is developed well for only one conservation law, see. [1]. In [2] a new approach to investigation of generalized solutions of quasilinear hyperbolic systems is proposed, which is specified for the case of systems of two equations in [3]. This approach is the use of so-called variational principle for generalized solutions. Note that earlier variational principles are built for some particular systems of two equations, see [4].

The proposed approach gives a new view of the nature of generalized solutions of quasi-linear hyperbolic systems. This view is formulated on the basis of general considerations which, in principle, are valid for a wide range of problems in the theory of conservation laws. Generally speaking, for any system of quasilinear hyperbolic equations might be built a number of variational principles. Thus, the problem is to find a form of the variational principle, which would allow a straightforward construction of a generalized solution. This is done in the case of an equation with a convex flow function, namely, the Hopf equation. It is chosen as a typical representative of this class of equations, for which the structural form of the variational principle is known.

The presented numerical scheme is based on the variational principle and characterized by high accuracy of calculation. Here we present the main features of the variational scheme and results of numerical investigations for the particular case of Hopf equation to show the ability of this scheme. This study highlights the way to possible robust algorithm for practical calculations.

Acknowledgements:
This work is supported by the Russian Science Foundation (grant 14-21-00025).

References:

1. S. N. Kruzhkov, "First order quasilinear equations in several independent variables", Mathematics of the USSR-Sbornik, **10**, № 2 , 217–243, (1970).
2.Yu.G. Rykov, "A variational representation of generalized solutions to quasilinear hyperbolic systems and possible algorithms for hybrid supercomputers", Keldysh Institute of Applied Mathematics, preprint № 62, (2011).
3. Yu.G. Rykov, O.B. Feodoritova, "On the methodology of variational representation of generalized solutions to quasi-linear hyperbolic two-equations systems", Keldysh Institute of Applied Mathematics, preprint № 84, (2014).
4. E.Weinan, Yu.G.Rykov, Ya.G. Sinai, "Generalized variational principles, global weak solutions and behavior with random initial data for systems of conservation laws arising in adhesion particle dynamics", Comm. Math. Phys., **177**, 349–380, (1996).

INMOST SOFTWARE PLATFORM BASED DEVELOPMENT OF PARALLEL NUMERICAL MODELS ON GENERAL MESHES

Yu.V. Vassilevski[1], I.V. Kapyrin[1,2], I.N. Konshin[1,2]
[1]*Institute of Numerical Mathematics of RAS*
[2]*Nuclear Safety Institute of RAS*
igor.konshin@gmail.com

A report presents an experience of creation of parallel MPI-platform and graphical environment for developing parallel numerical models on general meshes. Technological platform INMOST (Integrated Numerical Modelling and Object-oriented Supercomputing Technologies) [1,2] is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility and costeffectiveness, cross platform portability, as well as graphical environment for interactive user interface.

INMOST supports basic operations on mesh elements (vertices, edges, faces, and cells), their connectivity, operations on a set of elements, and tag tools to fit the data to a mesh element. The high level distributed mesh operations such as the data exchange for nearest fictitious elements, mesh data redistribution and balancing can also be used. The problem specific discretization module can exploit a special tool to form and solve the constructed linear system by PETSc, Trilinos, or internal linear solvers without taking into account the specificity of the interface for each solver.

The INMOST ideas for developing of the computational code with interactive user interface are demonstrated using the GeRa code, which is oriented on long-term groundwater flow and transport of radionuclides in geological media numerical simulation. GeRa includes modules for geostatistical modelling, grid generation and several types of discretizations for groundwater flow and transport problems. GeRa allows to perform parallel computations directly from the interface. Advanced graphical tools for visualization and verification of computational results are also included. Some results of numerical modelling experiments are presented as well.

References:

1. Yu.Vassilevski, I.Konshin, G.Kopytov, K.Terekhov, INMOST - a software platform and a graphical environment for development of parallel numerical models on general meshes. Moscow State Univ., Moscow (2013).
2. INMOST: a toolkit for distributed mathematical modeling. http://www.inmost.org (2015).

DIFFERENT METRICS AND TOPOLOGIES ON PRIVALOV SPACES ON THE UNIT DISK

Romeo Meštrović[1], Žarko Pavićević[2]

[1] *Maritime Faculty,*
University of Montenegro
Dobrota 36, 85330 Kotor, Montenegro
e-mail: romeo@ac.me
[2] *Faculty of Science*
University of Montenegro
81000 Podgorica, Montenegro
e-mail: zarkop@ac.me

For $p>1$, the class N^p, introduced in 1941 by I.I. Privalov, is defined as the space of holomorphic functions f on the open unit disk $D:|z|<1$ in the complex plane for which the function $(\log^+|f(z)|)^p$ has a harmonic majorant on D. In 1977 M. Stoll introduced the d_p-metric topology on N^p, and showed that the space N^p with the topology given by this metric becomes an $F-$algebra. Another ρ_p- metric topology which is equivalent to the d_p- metric topology on N^p, was considered by R. Meštrović in 2014. In connection with the space N^p, Stoll also studied the space F^p with the locally convex topology given by a certain family of seminorms $(\|\cdot\|_{p,c})_{c>0}$. In 1988 C.M. Eoff proved that F^p with the topology endowed by this family of seminorms is the Frechet envelope of N^p (also see R. Meštrović and Ž. Pavićević [2]). Furthermore, by a result of Eoff (1993), the Privalov space N^p can be expressed as a union of certain weighted H^2 Hardy spaces. This representation was used in [1] to define two topologies on N^p: the usual locally convex inductive limit topology H_p, and a not locally convex topology I_p. As noticed by R. Meštrović and Ž. Pavićević in [1], the topology I_p coincides with the weak topology induced on N^p by the familiy of seminorms $(\|\cdot\|_{p,c})_{c>0}$. Furthermore, it was proved in [1] that the topology H_p coincides with the Stoll's d_p - metric topology. Using the mentioned connections between different topologies on the space N^p and some related results, we establish some applications in Functional and Real Analysis.

References:

1. R. Meštrović, Ž. Pavićević, "Topologies on some subclasses of the Smirnov class", Acta Scientiarum Mathematicarum, **69**, 99-108 (2003).
2. R. Meštrović, Ž. Pavićević, "Weakly dense ideals in Privalov spaces of holomorphic functions", Journal of the Korean Mathematical Society, **48**, 397-420 (2011).

SOFTWARE 'CINDERELLA' AND ITS APPLICATION IN VISUALIZATION OF PHYSIC AND MATHEMATICS

Marina Zirojević[1], Dušan Jokanović[2], Đorđe Baralić[3]

[1]*Production and Management Faculty Trebinje, Stepe Stepanovića bb, 89 101 Trebinje, BiH*
[2]*Production and Management Faculty Trebinje, Stepe Stepanovića bb, 89 101 Trebinje, BiH*
[3]*Mathematical Institute SASA, Kneza Miloša 36, 11 001 Belgrade, Serbia*
marina.zirojevic@live.com

In this paper we present the posibilites to use the 'Cinderella' software in theory of curves and vector fields visualizations as well as in understanding their mechanical and geometric characteristics. These objects are extensively studied in physics, medicine and other sciences. The use of 'Cinderella' is exemplified in animation of cardioid, astroid, cubic curves, quadratic curves and their singularities. We emphasize the educational role of this software and application of its language 'SindyScript' and illustrate the way in which physical processes are modelled by the means of "Cinderella' software.

Acknowledgements:
This research was supported by the Grant 19/6-020/961-120/14 of the Ministry for Science and Technologies of the Republic of Srpska.

References:

1. Đ. Baralić, B. Grbić, Đ. Žikelić, "Theorems about quadrilaterals and conics", International Journal of Computer Mathematics, **91**, No.7, 1407-1421, (2013).
2. Đ. Baralić, I. Spasojević, "Illumination of Pascal's Hexagrammum and Octagrammum Mysticum", Discrete & Computational Geometry, **53**, 2, 414-427, (2015).
3. J. Richter-Gebert, "Perspectives on Projective Geometry", Springer-Verlag Berlin Heidelberg, (2011).
4.Veljko Vranić, Đorđe Baralić, "Cinderella – način da vidimo apstraktnu matematiku", Zbornik radova sa Treće matematičke konferencije Republike Srpske, **2**, 69-77, (2014).
5. Jürgen Richter-Gebert, Ulrich H. Kortenkamp "The Cinderella.2 Manual Working with the Interactive Geometry Software", Springer-Verlag Berlin Heidelberg, (2012).

GENERALIZATION OF A DISCRETE OPIAL TYPE INEQUALITY APPLIED TO THE EIGENVALUES OF GRAPH

Dusan Jokanovic[1], Tatjana Mirkovic

[1]*University of East Sarajevo*
Production and Management Faculty Trebinje
Stepe Stepanovica bb, 89101 Trebinje, Republic of Srpska, BiH
e-mail: dusanjok@yahoo.com

Abstract. In this paper we consider modifications of a discrete Opial type inequality applied to the eigenvalues of the graph G. We obtained a new proof of generalized inequalitiy $-\cos\frac{\pi}{r+1}\sum_{k=1}^{n}x_k^2 \le \sum_{k=1}^{n-m}x_k x_{k+m} \le \cos\frac{\pi}{r+1}\sum_{k=1}^{n}x_k^2$, as well as its special case for $m=1$ and $m=2,$ using the well-known equation for real eigenvalues of the graph $\sum_{k=1}^{n}\lambda_k^2 = 2m,$ where n is number of vertices, and m is number of edges of graph. Those generalizations enables us to derive a number of discrete inequalities related to binomial coefficients.

REFERENCES

[1] R.P. Agarwal, *Difference equations and inequalities: Theory, methods and applications*, Taylor and Francis, (2000).
[2] R.P. Agarwal and P.Y.H. Pang, *Opial inequalities with applications in differential and difference equations*, Kluwer Academi Publ., Dorddrecht, (1995).
[3] G.V. Milovanović and I.Ž. Milovanović, "Some discrete inequalities of Opial's type", Acta Sci. Math. (Szeged), **47**, 413-417 (1984).
[4] G.V. Milovanović and I.Ž. Milovanović and L.Z. Marinković, "Extremal problems for polynomials and their coefficients, Topics in polynomials of one and several variables and their applications", Volume dedicated to memory of P.L. Chebyshev, (Th.M. Rassias, H.M. Srivastava, A. Yanushauskas, eds.), World Scientific Publ., Com. Singapore, (1993).
[5] I.Ž. Milovanović, "An extremal problem for polynomials with a prescribed zero", Proc. Math. Soc., **97**, 1, 105-106 (1986).
[6] Z.-H. Znong, Z.-G. Xiao, "A simple new proof of Fan-Taussky-Todd inequalities", Australian J. Math. Anal. Appl., **2**, 5, 1-5 (2005).

ONE-DIMENSIONAL STRUCTURES INSIDE SINGLE-WALLED CARBON NANOTUBES

A.I. Chernov[1,2], P.V. Fedotov[1], A.V. Osadchy[1,2], V.L. Kuznetsov[3,4], E.A. Obraztsova[1], A.L. Chuvilin[4,5], E.D. Obraztsova[1,2]

[1]*A.M. Prokhorov General Physics Institute, RAS, 38 Vavilov str., Moscow, 119991, Russia*
[2]*National Research Nuclear University MEPhI, Kashirskoe hwy. 31, Moscow, 115409, Russia*
[3]*Boreskov Institute of Catalysis SB RAS, Lavrentieva ave. 5, Novosibirsk, 630090, Russia*
[4]*Novosibirsk State University, Pirogova 2, Novosibirsk, 630090, Russia*
[5]*CICnanoGUNEConsolider, TolosaHiribidea 76, E-20018 San Sebastian, Spain*
[6]*IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain*
al.chernov@nsc.gpi.ru

Single-walled carbon nanotubes can be used as nano-containers for different molecules. Besides the fact that filled aggregates become protected from the environment, nanotubes may serve as a template and support formation of various structures, which may be unfavorable in ambient conditions. We study the formation of hydrogen-terminated graphene nanoribbons inside single-walled carbon nanotubes [1,2]. Coronene molecules are used as filler of nanotubes. Depending on the diameter of nanotubes and synthesis parameters molecules can organize in the form of ordered stacks or graphene nanoribbons. Molecular mechanics modeling allows us to explain the process of transformation from ordered molecular stacks into the nanoribbons. Experimental results, such as optical absorption, photoluminescence and Raman spectroscopy studies, together with transmission electron microscopy are supported by molecular mechanics modeling (Fig. 1). Diameter dependent filling of carbon nanotubes is additionally confirmed by calculations demonstrating that for nanotubes below 1.5 nm in diameter the angle of molecule stacks orientation depends on the nanotube diameter values [3]. Surpassing the coronene stacks formation limit, which is governed by the diameter of nanotubes, results in further conversion of molecules into graphene nanoribbons. Filling of carbon nanotubes also influences on their electronic structure. *Ab-initio* calculations demonstrate that the relaxed cross-section of the nanotube transforms from circular to oval shape after inserting the nanoribbon leading to the changes in the band structure of the system [4].

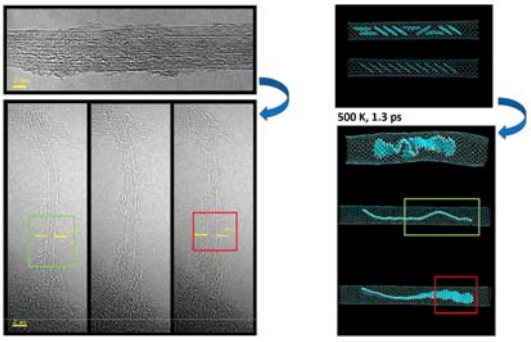


Figure 1. Left – HR TEM images of the 1.4 nm average diameter nanotubes filled with coronene stacks (top) and GNR (bottom). Three bottom images are captured one after another and demonstrate the rotation of the nanoribbon inside the tube. Molecular dynamics calculations are presented on the right and give the schematic view of the structures placed inside the nanotubes.

Acknowledgements:
The work was supported by RFBR grants 13-02-01354, 14-02-31829, 14-32-50113, 14-02-00777, RAS research projects, Ministry of Education and Science of Russian Federation grants № 14.513.12.003 and SP-7362.2013.3.

References:

1. A.I. Chernov, P.V. Fedotov, A.V. Talyzin, I. Suarez Lopez, I.V. Anoshkin, A.G. Nasibulin, E.I. Kauppinen, E.D. Obraztsova, "Optical properties of graphene nanoribbons encapsulated in single-walled carbon nanotubes", ACS Nano, 7, 6346-6353 (2013).
2. P.V. Fedotov, A.I. Chernov, A.V. Talyzin, I.V. Anoshkin, A.G. Nasibulin, E.I. Kauppinen, E.D. Obraztsova, "Optical study of nanotube and coronene composites", Journal of Nanoelectronics and Optoelectronics, 8, 16-22 (2013).
3. A.I. Chernov, P.V. Fedotov, A.G. Nasibulin, I.V. Anoshkin, E.I. Kauppinen, V.L. Kuznetsov, E.D. Obraztsova, "Single-walled carbon nanotubes as a template for coronene stack formation", Phys. Stat. Sol. (B), 251, 2372-2377 (2014).
4. A.V. Osadchy, I.V. Vorobyev, D.V. Rybkovskiy, E.D. Obraztsova, "Ab-initio investigation of band structure of graphene nanoribbons encapsulated in single-wall carbon nanotubes", Journal of Nanoelectronics and Optoelectronics, 8, 91-94 (2013).

АНАЛИЗ ПРЯМЫХ СПЕКТРАЛЬНЫХ ЗАДАЧ ДЛЯ ОБРАТНОЙ ЗАДАЧИ ОПЕРАТОРА ТИПА ШТУРМА - ЛИУВИЛЛЯ

Никола Михаљевич

Университет Черногории, Морской факультет
Котор, Черногория
nikolamih@ac.me

Эта статья содержит анализ прямой спектральной задачи и устанавливает связь между спектральными параметрами. Таким образом, открывается возможность для решения обратных задач. Рассчитываются коэффициенты в условии граничного оператора $D^{(2)}$ и значения функции задержки α на правом конце отрезка $[0,\pi]$.

CONTINUUM MODEL OF GENE EXPRESSION

Andrej Novak

University of Zagreb, Faculty of Electrical Engineering and Computing,
University of Zagreb, Croatia
andrej.novak@fer.hr

All living organisms have genes that are differentially activated and repressed to regulate life processes. Gene regulations drives expressions of gene at precise levels, spatial locations and time. We want to describe such process with PDE in order to gain better understanding understanding. One sRNA may regulate several different genes by binding to several mRNA targets creating different effects in the espression of a gene. In our model we have free sRNAs and free mRNAs of different types. It is important to notice that different types of sRNA may have some of the target mRNAs the same. Studies have shown that members of the Argonaute (Ago) protein family are core components of RISC. The RNA-induced silencing complex, or, RISC, is a multiprotein complex that incorporates one strand of a sRNA and uses it as a template for recognizing complementary mRNA. When it finds a complementary strand, it activates argonaute and cleaves the RNA. This is why we are going to include concentrations of Ago and complexes consisting of sRNAs bound to Ago protein in our model. This complex is associated with association rateand it may dissociate to its original components with dissociation rate. Once Ago-sRNA complex is assembled, it may bind to an i^{th} mRNA target and induce mRNA degradation. Of particular importance is the mobility of the RNAs, Argonaute and Ago-sRNA complexes between cells across the tissue. We model it by the system of parabolic PDE.

Joint work with Gabriela C. Racz and Mile Šikic (University of Zagreb).

CLICK-THROUGH RATE PREDICTION - TOP-5 SOLUTION FOR THE AVAZU CONTEST

Dmitry Efimov
Assistant Professor, American University of Sharjah, Sharjah, UAE
defimov@aus.edu

The paper describes the contribution to the Click-Through Rate Prediction contest with the data provided by Avazu. The proposed solution placed in the TOP-5 in this competition on Kaggle platform and involved more than 1600 participants. The described technique includes the robust algorithm for likelihood features engineering and the improvement of the FTRL online learning algorithm proposed by the Google's team. The improvement is obtained by the smart sorting of the provided dataset. The solution also shows the application of the Factorization Machine - the modification of the low rank approximation algorithm with stochastic gradient descent optimization.

References:

1. H. Brendan McMahan, Gary Hold, D. Sculley, Michael Young, Dietmar Ebner, Julian Grady, Lan Nie, Todd Phillips, Eugene Davydov, Daniel Golovin, Sharat Chikkerur, Dan Liu, Martin Wattenberg, Arnar Mar Hrafnkelsson, Tom Boulos, and Jeremy Kubica, "Ad click prediction: a view from the trenches", KDD, Chicago, Illinois, USA, (August 2013)
2. Steffen Rendle, "Social network and click-through prediction with factorization machines", KDD Cup, (2012).

SPLINE DIFFERENCE SCHEME ON A UNIFORM AND PIECEWISE UNIFORM GRID

Vanja Vukoslavčević
Faculty of Sciences, University of Montenegro
e-mail turner@t-com.me

For the problem: $-\varepsilon y''(x)+p(x)y(x)=f(x),\quad x\in D,\ y(0)=\alpha_0,\ y(1)=\alpha_1$, the spline difference scheme on a uniform mesh having the second order of uniform convergence and the fourth order of classical convergence is given. The global approximation is used in the form of spline in tension. Also, some uniformly convergent schemes on a Shishkin mesh are given.

ПАРАМЕТРИЧЕСКИЙ АНАЛИЗ НЕСТАЦИОНАРНЫХ СТРУКТУР В ЗАДАЧАХ ВЫЧИСЛИТЕЛЬНОЙ ГАЗОВОЙ ДИНАМИКИ

А.Е. Бондарев
Институт прикладной математики им. М.В. Келдыша РАН, Москва, Россия
e-mail: bond@keldysh.ru

Ключевые слова: пространственно-временные структуры, многомерные данные, обобщенный вычислительный эксперимент

Работа представляет приближенный комбинированный подход, предназначенный для исследования условий возникновения пространственно-временных структур в нестационарных задачах вычислительной механики жидкости и газа. Рассматриваются различные типы пространственно-временных структур, такие, например, как отрыв пограничного слоя, возникновение циркуляционных зон, возникновение осциллирующих режимов течения, переход от Маховского отражения к регулярному для ударных волн, и т.д. Подход сочетает численные решения обратных задач и параметрический анализ. Для численной реализации подхода используются параллельные вычисления. Предлагаемый в работе подход предназначен для быстрой приближенной оценки зависимости возникновения нестационарных структур в потоке от определяющих параметров задачи [1]. Результаты применения подхода представляются в виде многомерных объемов данных. Для нахождения скрытых взаимозависимостей в этих объемах необходимо применять методы обработки, анализа и визуализации многомерных данных. Предлагаемый подход организован в виде технологической цепочки алгоритмов. В ряде случаев данный подход позволяет получать искомую зависимость в виде квазианалитических соотношений. Предлагаемый подход может рассматриваться как прототип обобщенного вычислительного эксперимента. Схема подобного эксперимента представлена на Рис.1. Приведены примеры применения подхода кряду практических задач.

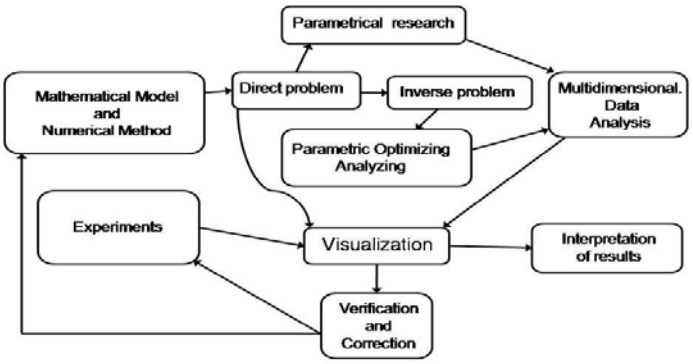


Рис. 1: Схема обобщенного вычислительного эксперимента.

Данная работа выполнена при поддержке Российского фонда фундаментальных исследований (проекты N 13-01-00367a и N 14-01-00769a).

REFERENCES

1. A.E Bondarev and V.A. Galaktionov, “Parametric Optimizing Analysis of Unsteady Structures and Visualization of Multidimensional Data”, *Int. J.l of Modeling, Simulation and Scientific Computing*, **4(supp01)**, 13 p., DOI 10.1142/S1793962313410043, (2013).

PARAMETRIC STUDIES OF SPACE-TIME STRUCTURES FOR CFD PROBLEMS

A.E. Bondarev

Keldysh Institute of Applied Mathematics Russian Academy of Sciences
Moscow, 125047, Russia
e-mail: bond@keldysh.ru

Key words: space-time structures, multidimensional data, generalized numerical experiment

The paper presents a combined approach to finding conditions for space-time structures appearance in non-stationary flows for CFD (computational fluid dynamics) problems. We consider different types of space-time structures, for instance, such as boundary layer separation, vortex zone appearance, appearance of oscillating regimes, transfer from Mach reflection to regular one for shock waves, etc. The approach combines numerical solutions of inverse problems and parametric studies. Parallel numerical solutions are implemented. This approach is intended for fast approximate estimation for dependence of unsteady flow structures on characteristic parameters (or determining parameters) in a certain class of problems [1]. The numerical results are presented in a form of multidimensional data volumes. To find out hidden dependencies in the volumes some multidimensional data processing and visualizing methods should be applied. The approach is organized in a pipeline fashion. For certain classes of problems the approach allows obtaining the sought-for dependence in a quasi-analytical form. The proposed approach can be considered to provide some kind of generalized numerical experiment environment. Proposed scheme for such generalized experiment is presented in Figure 1. Examples of its application to a series of practical problems are given.

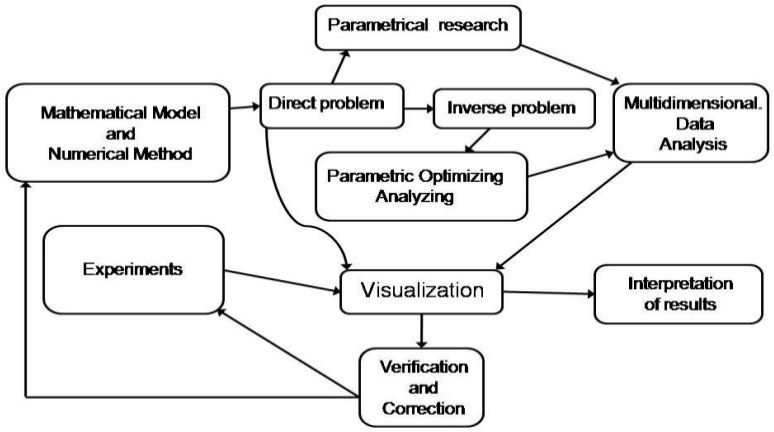


Figure 1: Scheme of generalized experiment

This work is supported by RFBR grant (project 13-01-00367A and project 14-01-00769A).

References:

1. A.E Bondarev and V.A. Galaktionov, "Parametric Optimizing Analysis of Unsteady Structures and Visualization of Multidimensional Data", *Int. J.l of Modeling, Simulation and Scientific Computing*, **4(supp01)**, 13 p., DOI 10.1142/S1793962313410043, (2013).

НАУЧНОЕ СООБЩЕСТВО В ЭПОХУ ПЕРЕМЕН

А.А. Самохин
Институт общей физики им. А.М. Прохорова РАН, Москва, Россия
asam40@mail.ru

Научное сообщество (НС) представляет собой часть российского общества и вместе с ним переживает сходные проблемы и трудности. Реакция НС на внешние и внутренние вызовы может служить достаточно выразительной характеристикой различных аспектов его состояния. В настоящем сообщении рассматриваются и качественно анализируются некоторые примеры такой реакции на общественные события последних лет. Количественная оценка параметров состояния НС затрудняется из-за его неоднородности, которая выражается, в частности, в различной ориентации и степени активности отдельных членов и организаций НС.

Одним из самых непосредственно значимых для академического сообщества событием (и процессом) продолжает оставаться реформирование Российской академии наук, которая в 2013 г. была отрезана от своих бывших институтов. Реакция на этот фактически многолетний процесс оказалась неоперативной и неадекватной как со стороны РАН, так и со стороны Профсоюза работников РАН. Вместо того, чтобы еще в середине прошлого десятилетия четко и принципиально поставить вопрос о решении организационных проблем управления российской наукой посредством, в частности, создания органа, подобного ГКНТ, руководство РАН страстно «бодалось» с руководством МОН с требованиями министерских извинений и прочими подобными претензиями. В то же время руководство РАН оставило без внимания майское 2010 года обращение Общего собрания Отделения физических наук РАН к Общему собранию РАН о необходимости проведения в октябре того же года собрания РАН, специально посвященного накопившимся академическим проблемам. Профсоюз работников РАН также не воспользовался имеющимися у него возможностями для результативного решения этого вопроса. Обстоятельный и содержательный анализ всех основных аспектов истории нынешнего реформирования РАН до сих пор отсутствует.

Вопросы отечественной истории сейчас весьма востребованы обществом, однако роль НС в удовлетворении этой потребности вряд ли соответствует потенциальным возможностям науки. Выступления некоторых представителей научного цеха на главных телевизионных каналах нередко оставляют скорее негативное, чем позитивное впечатление у широкой аудитории. Просветительская и образовательная роль науки и НС значительно возрастает в эпоху перемен, требующих оперативного критического анализа, осмысленных предложений и решительных действий. Эту свою естественную функцию члены и организации НС пока еще реализуют далеко не полностью. (Полный текст размещен на сайте ИОФ РАН http://www.gpi.ru/profcom/gpiras.php)

МУЛЬТИМЕДИЙНЫЕ ИЛЛЮСТРАЦИИ В НАУЧНОЙ ПУБЛИКАЦИИ

М.М.Горбунов-Посадов[1], Т.А.Полилова[2]
[1]*ИПМ им.М.В.Келдыша РАН, Москва, Миусская пл. 4, gorbunov@keldysh.ru*
[2]*ИПМ им.М.В.Келдыша РАН, Москва, Миусская пл. 4, polilova@keldysh.ru*

Интернет уверенно превращается в основной источник научного знания. Научные журналы, монографии, энциклопедии либо получают полнотекстовую интернет-проекцию, на которую с удовольствием переключается подавляющее большинство читателей, либо и вовсе целиком перекочевывают в интернет, постепенно забывая о своих печатных корнях.

Среди многочисленных преимуществ размещения научной публикации в интернете далеко не последнюю роль играет возможность широко использовать звук, видео, анимацию, интерактивную компьютерную графику — богатейший набор средств, о которых не могли и мечтать печатные издания. К сожалению, эти средства мультимедиа включаются в научные публикации недостаточно часто.

А ведь технический арсенал мультимедиа учеными давно освоен. Редкий семинар или защита диссертации проходят сегодня без подготовленной докладчиком динамичной демонстрации сталкивающихся галактик, движущихся циклонов, совершающих головоломные манипуляции роботов и т. д. Почему же эти замечательные иллюстрации до сих пор не украшают собой публикуемые научные работы?

Причин несколько. Прежде всего, инерция представления о публикации как о чем-то абсолютно неподвижном, что обязано в полном объеме отразиться на бумаге. До сих пор чрезвычайно редко встречаются научные журналы, где автору статьи разрешается подготовить мультимедиа иллюстрации для онлайновой версии. Как ни странно, даже если журнал исключительно онлайновый, тем не менее мультимедийные иллюстрации в нем зачастую не допускаются.

Существуют и чисто технические причины, мешающие массовому появлению мультимедиа иллюстраций в научной статье. В то время как у создателя "ненаучного" сайта с появлением HTML5 просто глаза разбегаются от обилия всевозможных доступных приемов работы с мультимедиа, обустройство "научного" интернета вызывает определенные сложности. Дело в том, что для представления текстов научных статей HTML практически не используется, там безраздельно господствует формат PDF. А организация размещения мультимедиа в PDF коренным образом отличается от технологий HTML, причем, увы, не в лучшую сторону.

Анализируется опыт использования видео, анимации и 3D иллюстраций в онлайновом издании "Препринты ИПМ им.М.В.Келдыша".

Работа поддержана грантом РФФИ 13-01-00493-а.

Литература

1. М.М.Горбунов-Посадов, Д.С.Ролдугин, М.И.Слепенков, И.В.Тузов. “Анимация и видео в научной публикации”, Препринты ИПМ им. М.В.Келдыша. 2014. № 104. 32 с. URL: http://library.keldysh.ru/preprint.asp?id=2014-104

ПОСТАНОВКА ВЫЧИСЛИТЕЛЬНОГО ЭКСПЕРИМЕНТА ПО МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОМУ ОПРЕДЕЛЕНИЮ ТЕПЛОФИЗИЧЕСКИХ СВОЙСТВ КРЕМНИЯ

А.В.Мажукин, О.Н.Королева, П.В.Бреславский
Институт прикладной математики им. М.В.Келдыша РАН
Москва, Миусская пл., 4
specimen@modhef.ru

Рассматриваются общие положения математического описания физических процессов в кремнии в молекулярно-динамическом (МД) приближении, в том числе проблема выбора межчастичного потенциала взаимодействия [1]. Представлены результаты вычислительных экспериментов, в которых получены температурные зависимости ряда теплофизических характеристик кремния. Из постановки серии вычислительных экспериментов определены параметры критической точки [2]. Проведено сравнение с экспериментальными данными.

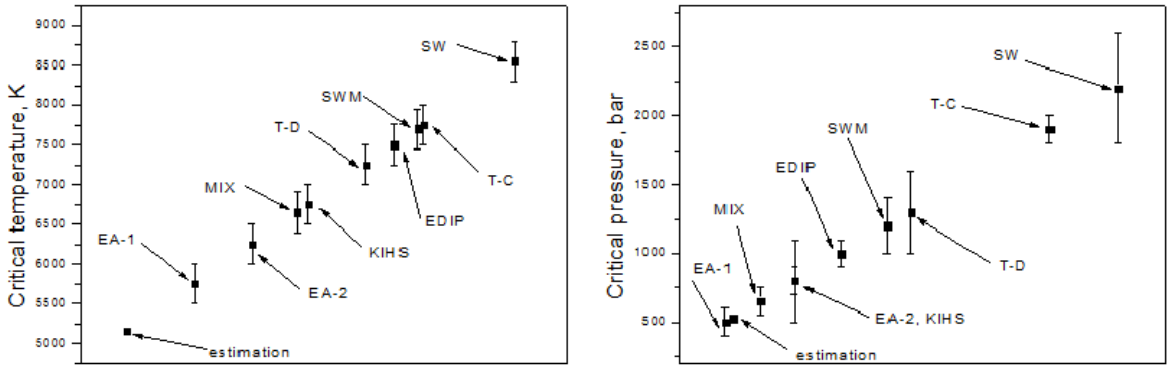


Рис. 1. Критическая температура и давление при различных межчастичных потенциалах взаимодействия.

Благодарность: Работа выполнена при финансовой поддержке РФФИ №№ 13-07-00597, 15- 07- 05025.

Литература:

[1] В.И. Мажукин, А.В. Шапранов, А.В. Руденко. Сравнительный анализ потенциалов межатомного взаимодействия для кристаллического кремния. Mathematica Montisnigri, vol. XXX, 2014.
[2] V.I. Mazhukin, A.V. Shapranov, O.N. Koroleva, A.V. Rudenko. Molecular dynamics simulation of critical point parameters for silicon. Mathematica Montisnigri, vol. XXXI, 2014.

STATEMENT OF CALCULATING EXPERIMENT OF MOLECULAR DYNAMICS DETERMINATION OF THERMOPHYSICAL PROPERTIES OF SILICON

A.V.Mazhukin, O.N.Koroleva, P.V.Breslavsky

Keldysh Institute of Applied Mathematics of RAS
Moscow, Miusskaya sq., 4
specimen@modhef.ru

We consider the general provisions of the mathematical description of physical processes in silicon in the molecular dynamic (MD) approach, including the problem of choosing the interparticle interaction potential [1]. Set the results of computational experiments in which the temperature dependences of a number of thermophysical characteristics of silicon are obtained. From statement of series of numerical experiments were determined the parameters of the critical point. [2] A comparison with experimental data was made.

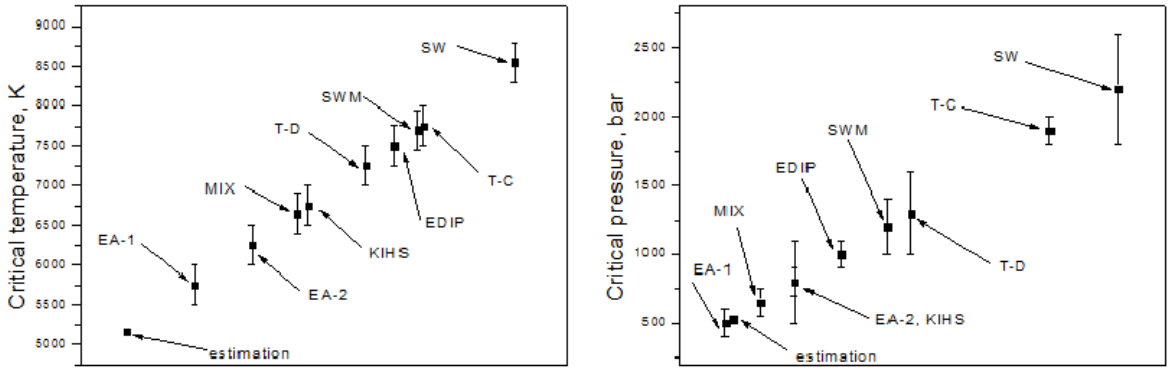


Fig. 1. The critical temperature and pressure at different interparticle interaction potentials.

Acknowledgements: This work was supported by RFBR grants №№ 13-07-00597, 15- 07-05025.

References:

[1] В.И. Мажукин, А.В. Шапранов, А.В. Руденко. Сравнительный анализ потенциалов межатомного взаимодействия для кристаллического кремния. Mathematica Montisnigri, vol. XXX, 2014.
[2] V.I. Mazhukin, A.V. Shapranov, O.N. Koroleva, A.V. Rudenko. Molecular dynamics simulation of critical point parameters for silicon. Mathematica Montisnigri, vol. XXXI, 2014.

МОДЕЛИРОВАНИЕ ДИНАМИКИ РАЗЛЕТА ПЛАЗМЫ В ВОЗДУХЕ ПРИ НАНОСЕКУНДНОМ ЛАЗЕРНОМ ВОЗДЕЙСТВИИ

Бреславский П.В., Королева О.Н., Мажукин А.В.
Институт прикладной математики им. М.В. Келдыша РАН
Миусская пл., 4, Москва, 125047, Россия
vim@modhef.ru

Рассматриваются различные режимы движения фронта плазменного факела в среде с нелинейной теплопроводностью. Показывается, что структура пространственных профилей плотности, скорости и температуры существенным образом связана со степенью нелинейности теплопроводности. Появление изотермических разрывов гидродинамических величин в тепловом потоке обуславливается исключительно взаимодействием тепловых и гидродинамических процессов переноса. Математическая модель реализуется на основе уравнений газовой динамики с учетом теплопроводности. Для численного решения используется метод динамической адаптации с явным выделением возникающих разрывов. Функция адаптации автоматически учитывает изменение плотности, скорости и температуры [1], что позволяет получить решение на расчетной сетке с малым количеством узлов $N = 30$.

Благодарности: Работа выполнена при финансовой поддержке РНФ № 15-11-00032.

Ссылки:
1. P. V. Breslavskii and V. I. Mazhukin, “Dynamic Adaptation Method in Gasdynamic Simulations with Nonlinear Heat Conduction”, *Comp. Math. Math. Phys.* **48**(11), 2102 – 2115, (2008).

SIMULATION OF THE DYNAMICS OF PLASMA EXPANSION INTO THE AIR INDUCED BY NANOSECOND LASER IRRADIATION

P. V. Breslavskii, O. N. Koroleva, A.V. Mazhukin
Keldysh Institute of Applied Mathematics Russian Academy of Sciences
Miusskaya sq., 4, Moscow, 125047, Russia
vim@modhef.ru

Various modes of motion of the front of a plasma torch in a medium with nonlinear thermal conductivity are considered. It is shown that the structure of density, velocity and temperature profiles significantly related to the degree of non-linearity of thermal conductivity. The appearance of isothermal discontinuities for hydrodynamic quantities in heat flow is caused exclusively by interaction of thermal and hydrodynamic transfer processes. The mathematical model is implemented on the basis of the gas dynamics equations with heat conduction. The method of dynamic adaptation with explicitly specified discontinuities is used for the numerical solution. The adaptation function automatically takes into account the change in density, velocity and temperature [1] to provide a solution to the computational grid with a small number of nodes $N = 30$.

Acknowledgements: This work was supported by RSCF grant № 15-11-00032.

References:

1. P. V. Breslavskii and V. I. Mazhukin, "Dynamic Adaptation Method in Gasdynamic Simulations with Nonlinear Heat Conduction", *Comp. Math. Math. Phys.* **48**(11), 2102 – 2115, (2008).

DIRECT RECORDING OF MULTI-BEAM INTERFERENCE PATTERNS ON TITANIUM FILMS BY NANO- & PICOSECOND LASER PULSES

Mindaugas Gedvilas[1], Bogdan Voisiat[1], Simonas Indrišiūnas[1], Gediminas Račiukaitis[1], Vadim Veiko[2], Roman Zakoldaev[2], Dmitry Sinev[2], Elena Shakhno[2]
[1]*Center for Physical Science and Technology, Vilnius, Lithuania*
[2]*ITMO University, Russia*

The laser oxidation of thin metallic films is a promising method to planar metal structures formation on the glass surface. Projecting of such planar structures can be applied to difractive optical element manufacturing. One of the best ways to provide such technique is laser thermochemical recording. Thin films of chromium are traditionally used in this technology, since it make possible to record with high resolution (1-1000 mm^{-1}) [1]. In this case additional chemical treatment after laser exposure is an integral part of this method. That complicates the technological process, makes it less productive and precise.

That's why we used thin titanium films as a recording medium. Since the titanium oxides becomes optically transparent under direct laser irradiation it is possible to create single-stage process of absolute contrast structures manufacturing [2]. It is important to noticethat during a formation of Ti-oxide the negative feedback takes place due to its transparency for incident laser beam. This is the main feature in comparison with chromium films where positive feedback took place connected with growing of absorbance oxide.

In this work, the high-pulse-energy picosecond and nanosecond lasers were applied to produce interference patterns in thin titanium films by thermo-chemical treatment. The laser beam was split into two, tree, four or six beams by using the diffractive optical elements. The confocal imaging system was used to produce interference pattern on the titanium films. As a result, planar structures with a period varying from 1.5 μm to 3.5 μm were produced on the glass surface.

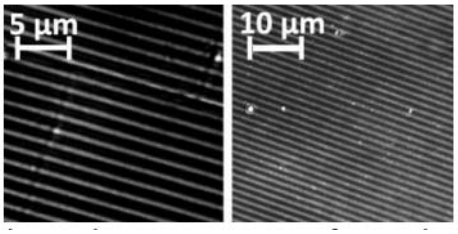


Fig. 1 The micro image of titanium planar structures formed on the glass surface after nanosecond (a) and picosecond (b) laser irradiation.

Acknowledgements: This work was supported by the Russian Scientific Fond Grant No. 14-12-00351 (on 50%), RFBR grant No. 14-29-07227 ofi_m, the President of the Russian Federation Grant No. NSH 1364.2014.2., and the Government of the Russian Federation Grant No. 074-U01).

References:

1. V. Veiko, E. Shakhno, A. Poleshchuk, V. Korolkov, V. Matyzhonok. "Local laser oxidation of thin metal films: ultra-resolution in theory and in practice". Journal of Laser Micro/Nanoengineering, **3**, 3, 201-205 (2008).
2. E.A. Shakhno, D.A. Sinev, A.M. Kulazhkin. "Features of laser oxidation of thin films of titanium". Journal of Optical Technology, **81,** 5, 298-302 (2014).

MATHEMATICAL MODEL OF FLUID DYNAMIC EFFECTS IN HIGH-ENERGY ELECTRONS FLUX

Berezin A. V., Voronin F. N., Gasilov V. A., Inozemtseva K. K., Lutskiy A. E., Markov M. B., Parotkin S. V
Keldysh Institute of Applied Mathematics of Russian Academy of Sciences, Miusskaya sq. 4, Moscow, 125047,
Russia e-mail: inozem.k0@gmail.com

We consider electromagnetic field emerging during particle accelerator experiment [1]. Highenergy electrons flux spreads in a gas medium and interacts with solid-state barrier, generating self-consistent electromagnetic field. Mathematical model of the situation includes description of high-energy electrons transfer, elastic and inelastic scattering, bremsstrahlung and medium excitation [2]. To compute particle propagation we apply modifications of particle-in-cell method to gas medium segment and Monte Carlo method [3,4] to barrier. Electromagnetic field is composed of currents generated by high-energy electrons and by conductance current in ionized medium. It is obtained from finite-difference scheme for Maxwell equations [5]. The key feature is account of influence of fluid dynamic effects caused by energy release during primary electrons propagation on scattering medi um properties. Gas state is described by Euler's equations with particles energy release as energy source [6]. Scattering properties of a solid-state barrier are modeled by equations of magneto fluid dynamics [7]. We consider thermomechanical behavior change insignificant during particle life time. Preliminary results of numerical methods development and testing are represented.

Acknowledgement : The reported study was partially supported by RFBR, research project No. 14-01-00350

References:

1. A. Andrianov A., A. Berezin, A., A. Vorontsov, K. Efimkin, V. Zinchenko, M. Markov, A. Chlenov, "Modeling the electron beam from the accelerator LIA-10 on the multiprocessor computer system", Mahtematical Modeling, **22**, 2, 29-44 (2010).
2. N. Mott, H. S. W. Massey. *The theory of atomic collisions*, IIL, Moscow, (1949).
3. A. Andrianov, A. Berezin, A. Vorontsov, K. Efimkin, V. Zinchenko, M. Markov, "The radiational electromagnetic fields modeling at the multiprocessor computing systems", Mahtematical Modeling, **20**, 3, 98-114 (2008).
4. M. Zhukovskiy, R. Uskov, "Modeling of interaction between gamma rays and matter on hybrid computers", Mahtematical Modeling, **23**, 7, 20-32 (2011).
5. A. Berezin, A. Krukov, B. Plyushchenkov, "The method of electromagnetic field with the given wavefront calculation" Mahtematical Modeling, **23**, 3, 109-126 (2011).
6. L. D. Landau, E. M. Lifshitz, "Fluid Mechanics", 2 nd edition, Nauka, Moscow, (1988)
7. V. Gasilov, S. D'yatchenko , A. Chuvatin, O. Olkhovskaya, A. Boldarev, E. Kartasheva, G. Bagdasarov, "Performance analysis of magnetic flux compression by plasma liner", Mahtematical Modeling, **21**, 11, 57-73 (2009).

MULTIENDOMORPHISMS AS A TOOL TO CONSTRUCT NEW HYPERRINGS

Sanja Jancic Rasovic[1], Irina Cristea[2]
[1]*Faculty of Natural Science and Mathematics, University of Montenegro, Dzorza Vasingtona bb Podgorica, Montenegro*
[2]*Centre for Systems and Information Technologies, University of Nova Gorica,SI-5000,Vipavska 13, Nova Gorica, Slovenia*

Based on the notion of composition ring introduced by Adler, we define the concept of composition hyperring. In this paper we show that the composition structure of a composition hyperring is determined by a class of its strong multiendomorphisms. Then,we deal with a class of Chinese hyperrings. Corsini shows that from every HX-group, hypergroupoid is obtained which is in some case hypergroup (Chinese hypergroup). Similarly, we show that if we start from the ring $(R,+,\cdot)$ then some family of subsets of R, under certain conditions generates a Chinese hyperring.In this paper we deal with a class of Chinese hyperrings associated with a family of subsets of R generated by a class of multiendomorphisms of additive group (R,+).

THE CONCEPT OF COLLEGE LIBRARY

Snežana Jovanović
Library of natural and technical sciences
University of Montenegro
snezaj@ac.me

The true university's collection of books. One as such by the program Stephens College represent "the book as a permanent part of the student's natural environment." College Library is the ultimate culmination of independent learning, learning in the library, not in the classroom. The concept of college libraries and college libraries as a precondition for the birth of the concept of "free art laboratories." The emphasis in the concept of the unbookish materials, primarily on Multimedia and technological advantages, ie images, sound recordings, films. The tendency of this concept is the union of teachers and librarians in a single instruction staff. The concept of "college library" as a result of education at the forefront of discovery, not in the process of filing. In this way encourage the initiative of the students themselves for independent learning, whereby eliminating the lecturers, who have only an indirect role. Their role becomes threefold: as an inspirer, guide and collector. In place of the guide stands library.

References:

1. Sister Helen Sheehan, Library trends, 93-103 (1969).

МЕХАНИЗМЫ ЯДЕРНЫХ РЕАКЦИЙ ПРИ ВЗАИМОДЕЙСТВИИ КОСМИЧЕСКОЙ РАДИАЦИИ С МАТЕРИАЛАМИ МИКРОСХЕМ

Галанина Л.И., Новиков Л.С.
НИИ ядерной физики им. Д.В. Скобельцына
Московского государственного университета им. М.В.Ломоносова
E-mail: galan_lidiya@mail.ru

Проанализирован механизм сбоев бортового электронного оборудования космических аппаратов обусловленный ионизацией ядрами отдачи и вторичными фрагментами, возникающими при ядерных взаимодействиях протонов и легких ионов космической радиации с веществом интегральной микросхемы.

Одиночные сбои возникают, если выделенная в чувствительном объеме элемента интегральной микросхемы энергия превышает пороговую для данного элемента величину E_0. Частота сбоев определяется дифференциальными потоками воздействующих частиц и макроскопическим сечением $\Sigma_i(E, E_0)$ возникновения одиночных сбоев под действием частиц этого вида. Для легких заряженных частиц сечение одиночных сбоев в объеме чувствительного элемента, содержащем N атомов, определяется соотношением

$$\Sigma_i(E, E_0) = N\sigma_i(E, E_0) = N\sum_k \int_{E_0} \frac{d\sigma_i^k(E, E_r)}{dE_r} dE_r .$$

Суммирование проводится по всем каналам взаимодействия $k = (Z, A)$ первичных ионов типа i с энергией E с материалом интегральной микросхемы, в результате которого с вероятностью $\sigma_i^k(E, E_r)$ образуется ядро с массой A, зарядом Z и энергией E_r.

Энергетические спектры всех образующихся в реакции ядер-остатков могут быть найдены экспериментально либо рассчитаны с помощью теоретических подходов. В работе энергетические спектры ядер-остатков рассчитаны в рамках современных моделей ядерных реакций, объединенных в пакете EMPIRE.

Результаты анализа показали, что сечения образования различных ядер отдачи зависят от энергии протонов и типа мишени. Наиболее вероятны каналы реакции с выбиванием одного-трех нуклонов, а в случае ядра ^{28}Si -с выбиванием α-частицы. Частота одиночных сбоев зависит от полного сечения реакции для ядер отдачи с энергией меньшей критической энергии сбоя E_0.

Благодарности: работа поддержана РФФИ (проект № 14-29-09244).

MECHANISMS OF NUCLEAR REACTIONS AT INTERACTION OF COSMIC RAYS WITH MATERIALS OF MICROELECTRONIC ELEMENTS

L.I. Galanina, L.S. Novikov
Skobeltsyn Institute of Nuclear Physics, Moscow State University.
E-mail: galanina@nsrd.sinp.msu.ru

The mechanism of failures in microelectronic elements due to the ionization of atoms by recoil nuclei and secondary fragments, formed at nuclear interactions of cosmic-ray protons and light ions with substance, has been analyzed.

Single failures arise when the energy evolved in a sensitive volume of an integrated circuit element exceeds some threshold (for this element) value E_0. The failure frequency is determined by the differential fluxes of acting particles as well as by the macroscopic single failure cross section $\Sigma_i(E, E_0)$. For light charged particles, the single-failure cross section in a sensitive element volume containing N atoms is

$$\Sigma_i(E, E_0) = N\sigma_i(E, E_0) = N\sum_k \int_{E_0} \frac{d\sigma_i^k(E, E_r)}{dE_r} dE_r$$

The summation is over all interaction channels $k = (Z, A)$ of the primary ions of type i and energy E with the integrated circuit element, as a result of which a nucleus with the mass A, charge Z and energy E_r is formed with the probability $\sigma_i^k(E, E_r)$.

The energy spectra $\sigma_i^k(E, E_r)$ of all recoil nuclei formed in the reaction can be obtained experimentally or calculated within theoretical nuclear models. In this study the macroscopic failure cross section was calculated using the models of nuclear physics combined in the EMPIRE software.

The calculation results show that the production cross sections of different recoil nuclei depend on the acting proton energy and the structure of target nucleus. The most likely channels of nuclear reactions are those with knocking out of one to three nucleons and with knocking out of an α particle (for the 28Si nucleus). The single-failure frequency depends on the total reaction cross section for recoil nuclei with energies below the critical failure energy E_0.

Acknowledgements: the study was supported by the Russian Foundation for Basic Research (project no. 14-29-09244).

SPECTRAL-LUMINESCENCE PROPERTIES OF BI-DOPED OXIDE GLASSES

B.I.Denker[1], B.I.Galagan[1], S.E.Sverchkov[1], E.M.Dianov[2]
[1]*A.M.Prokhorov General Physics Institute of RAS, Vavilov str.38, Moscow, 119991 Russia*
[2]*Fiber Optics Research Center of RAS Vavilov str.38, 119991 Moscow, Russia*
denker@Lst.gpi.ru

The luminescence properties of bismuth-doped glasses are the subject of intense research aimed at both identifying the nature of the emission centers involved and extending the range of lasing wavelengths.[1] It is well known that the luminescence and lasing properties of Bi-doped glasses and fibers strongly depend on the conditions under which they were produced. Note in this context that the development of advanced processes for the fabrication of Bi-containing active materials with reproducible properties is a priority issue. To date, lasing and optical gain have been demonstrated in silica fibers doped with very small amounts of Bi (< 0.01 at %) and containing Al, Ge, and/or P ions or no other dopants. Most of the Bi-doped fibers reported to lase were fabricated by the MCVD process, but recent work has shown that lasing can in principle be achieved in Bi-doped fibers produced by the powder-in-tube method.[2] Note that no lasing of Bi-doped bulk glasses has been reported to date.

This paper compares the absorption and emission properties of bulk glasses prepared by melting in a crucible and optical fibers fabricated by the powder-in-tube method. Both the bulk glasses and fibers were prepared from identical mixtures. The emission properties of the bulk samples and fibers were similar, while the "gray losses" in the fibers were an order of magnitude lower than those in the crucible melted glasses.

References

[1] I.A. Bufetov, E.M. Dianov, "Bi-doped fiber lasers," Laser Phys. Lett., **6**, 7, 487 - 504 (2009).
[2] I. A. Bufetov, M. A. Melkumov, S. V. Firstov, A. V. Shubin, S. L. Semenov, V. V. Velmiskin, A. E. Levchenko, E. G. Firstova, and E. M. Dianov, "Optical gain and laser generation in bismuth-doped silica fibers free of other dopants," Opt. Lett. **36**, 2, 166–168 (2011).

USAGE OF THE SEMI-EMPIRICAL PSEUDOPOTENTION METHOD FOR THE GALLIUM SELENIDE NANOMATERIALS BAND STRUCTURE CALCULATION

A.V. Osadchy[1,2], D.V. Rybkovskiy[1], E.D. Obraztsova[1,2]
[1]*A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia*
[2]*National Research Nuclear University MEPhI (Moscow Engineering Physics Institute, Moscow, Russia*
aosadchy@yandex.ru

The work was carried out computer simulations of the band structure of nanostructures based on layered AIIIBVI semiconductors using the empirical pseudopotential method. The main objects of study were quantum dots, single and few-layered GaSe. A widely used method based on density functional theory significantly underestimates the band gap. This value is the most important characteristic of semiconductors. At the same time, GW approximation, which gives much better results, often not applicable for nanomaterials because of the high computer resource requirements [1,2]. This is especially observed in the simulation of quantum dots based on GaSe and similar materials. This was the main reason for the developing of a computer program to simulate the band structure using the method of empirical pseudopotential. Special computational code allow to perform calculations using cluster of computers, which significantly increases the number of atoms in the system. This approach allows us to obtain results with an accuracy comparable to GW approximation. At the same time, the requirements for computational resources considerably smaller than in the case GW approximation.

Modeling of 1, 2, 3 layered GaSe and GaSe quantum dots using this method showed good agreement with theoretical data obtained by GW approximation and experimental results [3, 4].

Acknowledgements:
This work was supported by the RFBR 15-02-09073

References:

1. Schlüter M, “The Electronic Structure of GaSe”, Nuovo Cimento B., **13**, No. 2, 313-360 (1971).
2. Kshirsagar A., Kumbhojkar N., “Empirical pseudo-potential studies on electronic structure of semiconducting quantum dots”, Bull. Mater. Sci., **31**, No. 3, 297-307 (2008).
3. D. V. Rybkovskiy, A. V. Osadchy, and E. D. Obraztsova, “Transition from parabolic to ringshaped valence band maximum in few-layer GaS, GaSe, and InSe”, Physical Review B, **90**, 235302 (2014).
4. Segura A., Manjón F.J., et. al., “Specific features of the electronic structure of III−VI layered semiconductors: recent results on structural and optical measurements under pressure and electronic structure calculations”, phys. stat. sol. (b), **235**, No 2, 267-276 (2003).

OPTICAL AND ELECTRICAL STUDIES OF DEFECT MULTI-WALL CARBON NANOTUBES SYNTHESIZED WITH FE-CO CATALYSTS OF VARIABLE STRUCTURE

S.N. Bokova-Sirosh[1,2], M.A. Shuvaeva[3,4], A.V. Ishchenko[3,4], D.V. Krasnikov[3,4], V.L. Kuznetsov[3,4,6], A.I. Romanenko[5], E.N. Tkachev[5] and E.D. Obraztsova[1,2]

[1]*A.M. Prokhorov General Physics Institute RAS, Moscow, Russia*

[2]*National Research Nuclear University «MEPhI», Moscow, Russia*

[3]*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

[4] *Novosibirsk State University, Novosibirsk, Russia*

[5]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

[6] *National Tomsk State University, Tomsk, Russia*

sofia@kapella.gpi.ru

Today, carbon nanostructures are one of the most priority materials for use in various fields of science and technology, as components of new structural materials, nanoelectronics, nonlinear optics, etc. The purpose of this work was to study electrical and optical properties of multi-wall carbon nanotubes (MWCNTs) synthesized using catalysts Fe-Co with a variable composition in order to establish the relationship between the physical properties of the structure and its defectiveness.

Raman scattering is widely used for characterization of various types of carbon nanostructures. This method is also sensitive to changing the structure and properties of MWCNTs. For characterization the intensity ratios of D, G and 2D-modes in the Raman spectrum have been used.

It is also planned to carry out a theoretical modeling of the MWCNT Raman spectra by the first principles. The calculation will be made with the method based on density functional theory.

Acknowledgements: This research was partially supported by the RAS research programs and RFBR 14-32-50078 mol_rf_nr

References:

1. S. N. Bokova, E. D. Obraztsova et al. "Raman diagnostics of multi-wall carbon nanotubes with a small wall number", Physica Status Solidi B, 1–4 (2010).
2. V. L. Kuznetsov, S. N. Bokova-Sirosh et al. "Raman spectra for characterization of defective CVD multi-walled carbon nanotubes", Physica Status Solidi B, **251**, No. 12, 2444–2450 (2014).

THE BOUNDARY VALUE PROBLEM WITH N DELAYS AND ASYMPTOTIC OF EIGENVALUES

Biljana Vojvodic[1]

Milenko Pikula[2]

[1]*Ministry of Science and Technology Republic of Srpska*
Banja Luka, Republic of Srpska, Bosnia and Hercegovina

[2]*University of East Sarajevo, Faculty of Philosophy*
East Sarajevo, Republic of Srpska, Bosnia and Hercegovina

e-mail:b.vojvodic@mnk.vladars.net

Abstract. This paper deals with the boundary value problem for the operator Sturm-Liouville type with N constant delays, $L = L(q_1(x), q_2(x), \dots . q_N(x), \tau_1, \tau_2, \dots \tau_N)$:

$$-y''(x) + \sum_{i=1}^{N} q_i(x) y(x - \tau_i) = \lambda y(x), x \in (0, \pi], y(x - \tau_N) \equiv 0, x \in [0, \tau_N]$$

$$y(\pi) = 0, 0 < \tau_1 < \tau_2 < \dots < \tau_N < \pi, q_i \in L_2[0, \pi], i = 1,2, \dots, N$$

The boundary value problems for Sturm-Liouville operators with one constant delay ($N = 1$) are studied in 1-2 and other works. Although the operators with two constant delays ($N = 2$) are least studied, some of the results for this class of operators can be found in 3-4. Construction of the solution for the differential operators with N constant delays is more complex than in the case when $N = 1$, due to complexity of relations between linear combinations of delays $\tau_i, i = 1,2, \dots N$ and also their relations around π. By the method of successive approximation we construct the solution and determine the characteristic function of the boundary value problem. Then we consider the existence and asymptotic behavior of the eigenvalues of the boundary value problem.

References:

1. G. Freiling, V. A. Yurko, "Inverse Sturm-Liouville diferential operators with a constant delay", Appl. Math. Letters, 25 2012, 1999-2004
2. M. Pikula, V. Vladicic, O. Markovic, "A solution to the inverse problem for Sturm-Liouville-type equation with a delay", Filomat, 27:7, 2013, 1237-1245
3. B. Vojvodic, M. Pikula, V. Vladicic, "Determining of the solution of the boundary value problem for the operator Sturm-Liouville type with two constant delays", Symposium Math. and Appl. 2014, Belgrade 2014
4. M. Pikula, N. Pavlovic, B. Vojvodic, "First regularized trace on the limit assigment of Sturm-Liouville type with two constant delays", Conference Analysis, Topology and Applications 2014 (ATA2014), Vrnjačka Banja, 2014

ON HIGH SPEED FLOW SIMULATION IN MODEL RAMJET ENGINE

N.D. Novikova, O.B. Feodoritova, K.V. Manukovskii, Yu.G. Rykov, V.T. Zhukov
Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Moscow, Russia
e-mail: nn@kiam.ru

We present numerical investigations of flows in ramjet engines which will play a key role in the realization of hypersonic flight. Ramjets are the air-breathing engines working at high supersonic speeds. Ramjets are relatively simple in design, and do not have any moving part, such as turbine, but are very susceptible to flow instabilities. Numerical simulation of ramjet components even in isolated mode (as we do, see [1]) is useful for cost and time-savingin process of engine development.

We study high speed flow structures inside the model air intake, the inlet-isolator [2], see sketch on Fig.1. The isolator separates the combustor from the engine inlet. The ramp near exit of the isolator is fully down for the started flow. For this case stable flow structure consists of shock waves interacting with boundary layers. When the configuration starts to destroy various oscillations and unstart event arises. For unstart case, where unsteady flow is registered in the experiment, the ramp is lifted as it is shown on Fig. 1. So it is important to reliably determine the flow parameters when the unstart event occurs.

The flow simulation software OpenFOAM [3] is used. Both started and unstart flows are numerically simulated. Computations are based on the time averaged compressible Navier-Stokes equations with turbulence SST model. Calculations for validation and calibration of the computational model are used the detailed measurements from isolator [2]. The results of 2D and 3D computations are presented.

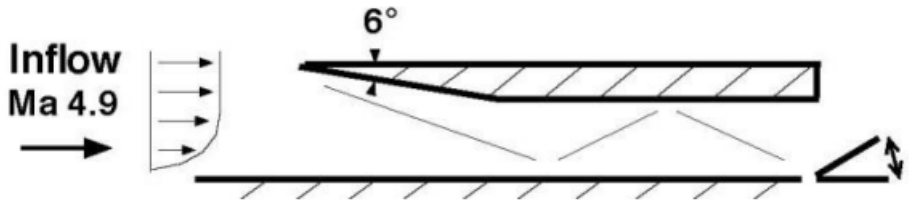


Fig. 1. Sketch of inlet-isolator configuration with the lifted ramp near exit

Acknowledgements:
This work is supported by the Russian Science Foundation (grant 14-21-00025).

References:

1. J.L. Wagner, "Experimental studies of unstart dynamics in inlet/isolator configurations in a Mach 5 flow", PhD Thesis, The University of Texas at Austin, (2009).
2. V.T. Zhukov, K.V. Manukovskii, N.D. Novikova, Yu.G. Rykov, O.B. Feodoritova, "Calculation, analysis and visualization of flow simulation in model ramjet engine on high velocity", Scientific Visualization, **7**, № 1, 78–95 (2015).
3. The OpenFOAM® Foundation, http://www.openfoam.org/index.php.

LIMITS OF APPLICABILITY OF THE TWO TEMPERATURE MODEL FOR NONUNIFORM HEATING OF CONDENSED MATTER BY ULTRASHORT LASER PULSES

D. S. Polyakov, E. B. Yakovlev
ITMO University, Saint-Petersburg, Russia
polyakovdmitry1988@gmail.com

At present time two-temperature model (TTM) is the basic tool for modeling heating of condensed medium by femtosecond laser pulses. This model assumes fast internal thermalization of electron gas. However, it is known that for low-intensity pulses (Qa << 2 mJ/cm^2, where Qa is absorbed fluence) in metals thermalization of electrons proceed after the end of the pulse and stretched for hundreds femtoseconds up to picoseconds. Under these conditions the decrease of the rate of energy transfer from electrons to lattice can be observed [1]. The question of evolution of electron gas distribution function under the action of femtosecond laser pulses with Qa > 2 mJ/cm^2 for metals remains poorly understood. At the same time the form of distribution function directly affects the electron emission, which, according to work [2], may play a decisive role in the oxidation of metals by single femtosecond pulses. Another problem to be solved is the following.
Authors of theoretical works based on kinetic Boltzmann equation consider only uniform situation without energy fluxes. Accordingly, the question of energy redistribution in skin-layer of metal, taking into account nonequilibrium electrons distribution, is not investigated. These problems are also actual for semiconductor and dielectric materials. So, the aim of this work is to study the role of electron's nonequilibrium distribution in general picture of interaction of femtosecond laser pulses with condensed matter and determination of the limits of applicability of TTM. We proposeda model of interaction of femtosecond laser pulses with condensed matter based on kinetic Boltzmann equation for electrons distribution function, which takes into account nonuniformity of the heating of the sample and different types of collisions. The solution was obtained by numerical modeling using the methods of direct statistical simulation. The results of calculations werecompared with predictions of TTM. In case of semiconductor materials the role of the effect of saturation of interband absorption in dynamics of concentration of electron-hole plasma was investigated. It is shown that for typical metals (Al, Ag) in the case of fluences about ablation threshold (Qa ~ 100 mJ/cm^2) TTM gives adequate results, however, for low fluences some deviations from TTM prediction were observed. For semiconductor materials the thermalization of electron gas occurs rapidly in wide range of intensities and role of nonthermal electrons is not significant. Also it is found that effect of saturation of interband absorption has noticeable influence on spatial-temporal distribution of concentration of photo-exited electron-hole plasma.

Acknowledgements: This work is supported by the Russian Scientific Fond № 14-12-00351

References:

1. B. Rethfeld et al. "Utrafast dynamics of nonequilibrium electrons in metals under femtosecond laser irradiation", Phys. Rev. B, **60**, 214303-1 – 214303-11 (2002).
2. E. B. Yakovlev, O. N. Sergaeva, V. V. Svirina, M. V. Yarchuk. "Modeling of thin Cr film oxidation under the action of ultrashort laser pulses", Proc. of SPIE, **9065**, 906509-1 – 906509-6 (2013).

ИССЛЕДОВАНИЕ ПРОДУКТОВ ЛАЗЕРНОЙ АБЛЯЦИИ КРЕМНИЯ В РАЗЛИЧНЫХ СРЕДАХ ПРИ ОБЛУЧЕНИИ НАНОСЕКУНДНЫМИ ИМПУЛЬСАМИ ИТТЕРБИЕВОГО ВОЛОКОННОГО ЛАЗЕРА

Д. С. Поляков, В. П. Вейко, А. М. Скворцов, К. Т. Хуинь, Е. С. Чопенко, А. А. Самохвалов
Университет ИТМО, Санкт-Петербург, Россия
polyakovdmitry1988@gmail.com

Интерес к созданию нанокомпозитных структур на основе кремния и кремниевых наночастиц обусловлен перспективностью их применения при создании устройств кремниевой фотоники, энергонезависимой памяти и т.д. Многообещающим методом получения наночастиц кремния является лазерная абляция (в т.ч. под слоем жидкости).[1]

В наших экспериментах облучение образцов монокристаллического кремния наносекундными импульсами волоконного иттербиевого лазера осуществлялось в различных средах (дистиллированная вода, воздух) сериями как одиночных, так и сдвоенных импульсов с регулируемой задержкой.

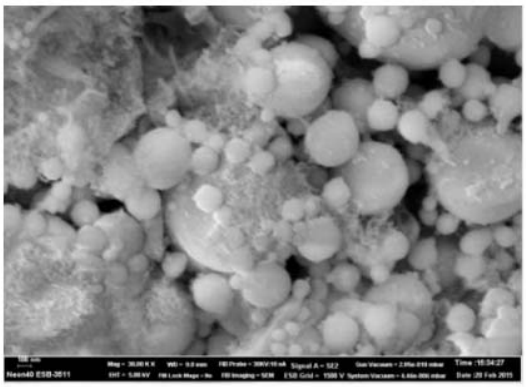


Рисунок 1. СЭМ-изображение наночастиц кремния, полученных при лазерной абляции в воде

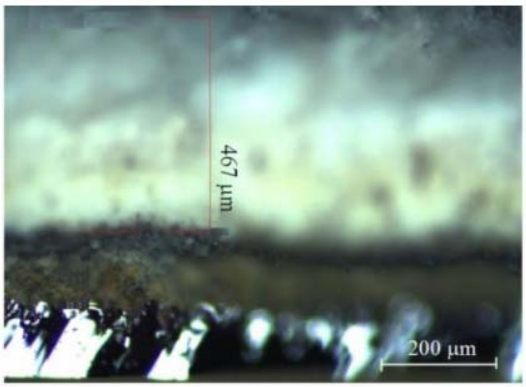


Рисунок 2. Микрофотография скола образца с осажденными частицами, полученными при лазерной абляции на воздухе

После осушения коллоидного раствора, полученного путем абляции под слоем жидкости, наблюдался массив сферических наночастиц с размерами порядка 100 нм, показанный на рис. 1. Характерные размеры полученных частиц, а также энергетическая эффективность их выхода зависят как от плотности мощности импульсов, так и от длительности фрагментации при последующем облучении коллоидного раствора частиц. В результате абляции на воздухе наблюдалась, осажденная из плазменного факела, двухслойная структура (см. рис.2), состоящая из пористого слоя частиц SiO_2 (верхний слой) и Si (нижний слой). В работе исследованы зависимости размеров полученных частиц от режимов обработки. Изучены люминесцентные свойства полученных образцов. Исследована перспективность обратного спекания порошка, полученного при абляции на воздухе (см. рис. 2), для получения слоев SiO_x ($x < 2$) или слоев SiO_2 с нанокластерами Si.

Благодарности: Авторы выражают благодарность Стовпяге А. В. за проведение измерений на электронном микроскопе. Работа выполнена при поддержке гранта РНФ № 14-12-00351

Литература:

1. R. Inartaglia et al., "Optical Properties of Femtosecond Laser-Synthesized Silicon Nanoparticles in Deionized Water", Journal of Physical Chemistry, **115**, 5102-5107 (2011).