Российский федеральный ядерный центр-
Всероссийский НИИ экспериментальной
физики

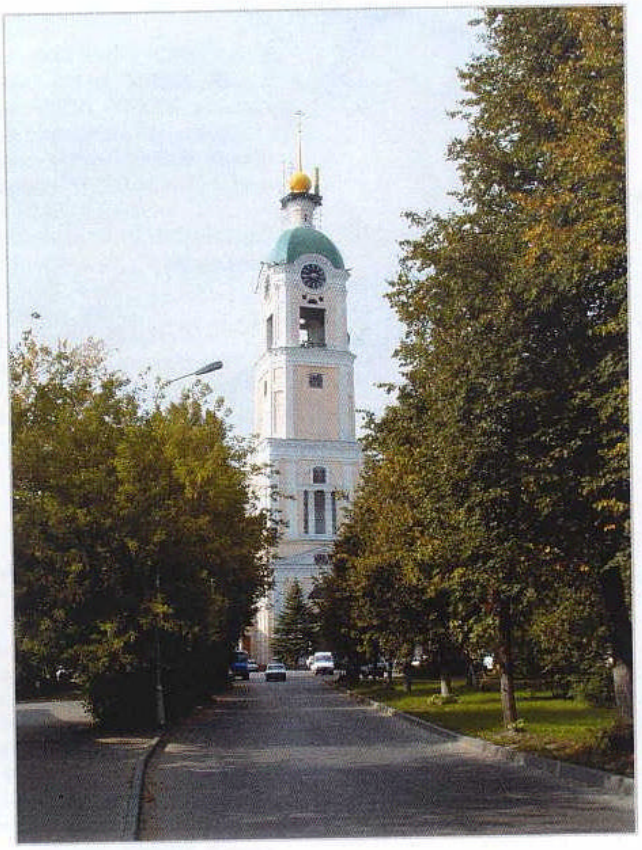
Russian Federal Nuclear Center –
All-Russian Research Institute of
Experimental Physics

Международный семинар

СУПЕРВЫЧИСЛЕНИЯ И МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ

International Seminar

SUPER–COMPUTATIONS AND COMPUTER SIMULATION



ПРОГРАММА
PROGRAM

Sarov
October 6 – 11
2003

The 7th International Seminar
Super-Computations and Computer Simulation

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Sarov
6-10 October, 2003

International Seminar
SUPER-COMPUTATIONS AND COMPUTER SIMULATION
(October 6–11, 2003, Sarov)

October 6, Monday

SEMINAR INAUGURATION

Session Chair – I.D. Sofronov

9.30 – 10.00 Welcome by ***R.I.Il'kaev,*** Director of RFNC–VNIIEF, Academician

Ann Fitz —

10.00 – 10.25 ***Shagaliev R.M.*** (RFNC–VNIIEF, ITMF, Sarov)
78 *AN ADAPTIVE METHOD FOR SOLVING A MULTIDIMENSIONAL TRANSPORT EQUATION USING FRACTIONAL GRIDS IN PHASE SPACE*

10.25 – 10.50 ***Gadzhiev A.D., Kondakov I.A., Pisarev V.N., Starodumov O.I., Shestakov A.A.*** (RFNC–VINIITF, Snezhinsk)
27 *ARTIFICIAL DISSIPATION METHOD OF DISCRETE ORDINATES (DADD SCHEME) FOR NUMERICAL CALCULATIONS OF NEUTRON TRANSPORT EQUATION*

10.50 – 11.15 ***Fortov V.E.,*** [1] ***Konyukhov A.V.,*** [1,2]***, Likhachev A.P.,*** [1]***, Oparin A.M.,*** [2]***, Anisimov S.I.,*** [3]
OW
([1] Institute of Extreme State Thermohpysics, Russian Academy of Sciences
[2] Institute of Computer-Aided Design, Russian Academy of Sciences
[3] Landau Institute of Theoretical Physics, Russian Academy of Sciences)
75 *NUMERICAL STUDY OF SHOCK INSTABILITY IN THERMODYNAMICALLY IMPERFECT MEDIA*
p 81

11.15 – 11.30 *BREAK* Discussion in hall w/ SSA

11.30 – 11.55 ***Yelizarov G.S., Karatanov V.V., Korneev V.V., Levin V.K., Yablonsky S.V.*** (Federal State Unitary Enterprise "NII-KVANT", Moscow)
39 p 45 *FAMILY OF CLUSTER COMPUTER SYSTEMS MVS-1000 OF 1 OR MORE Tflops THROUGHPUT LEVEL*

11.55 – 12.20 ***Kalyaev A.V., Levin I.I.***
(Scientific Research Institute of Multiprocessor Computers, Taganrog)
48 *A MODULE-SCALABLE ARCHITECTURE-PROGRAMMABLE MULTIPROCESSOR SYSTEM*
p 56

12.20 – 12.45 **Baikov E.G., Basalov V.G., Vargin A.M., Vorontsova N.D., Vyalukhin V.M., Ezhov D.V., Zhukov D.A., Kirianov Yu.L., Kosarev S.N., Levkin S.A., Petrova S.N., Popov V.S., Popovidchenko G.A., Sviridov V.A., Stepanenko S.A., Trushkina N.V., Kholostov A.A., Yatsuk V.I.** (RFNC-VNIIEF, ITMF, Sarov)

PROCESSOR COMMUNICATIONS SYSTEM FOR MULTIPROCESSOR ENVIRONMENTS

12.45 – 14.00 *LUNCH*

Session Chair – R.M.Shagaliev

14.00 – 14.25 **De Benedictis E.P.** (Sandia National Laboratories, USA)

ASCI RED STORM AND SUPERCOMPUTER SCALABILITY

14.25 – 14.50 **Lindemuth I.R.**
(Los Alamos National Laboratory, Los Alamos NM USA)

NON-SPLIT ALTERNATING-DIRECTION IMPLICIT METHODS FOR SIMULATING THE BEHAVIOR OF MAGNETIZED PLASMAS

14.50 – 15.15 **Scott H.A.** (LLNL,USA)

NON-LTE RADIATION TRANSPORT, TEMPERATURES AND ENERGY BALANCE

15.15 – 15.40 **Scott H.A.** (LLNL, USA)

SUPERCOMPUTER BLUEGENE/L

15.40 – 16.00 *BREAK*

16.00 – 16.25 **Kamm J.R., Benjamin R.F., Cannon T.M., Davis A.B., Mathews A.R., Rider W.J., Tomkins C.D., Vixie K.R.**
(Los Alamos National Laboratory, USA)

SELECTED VALIDATION ACTIVITIES AT LOS ALAMOS NATIONAL LABORATORY

16.25 – 16.50 **Rider W.J., Kamm J.R.** (LANL, USA),
Greenough J.A. (LLNL, USA)

ORDER-OF-ACCURACY, SOLUTION ACCURACY AND EFFICIENCY IN HIGH-RESOLUTION SHOCK CAPTURING METHODS

16.50 – 17.15 **Zocher M.A.**
(LANL, USA)

ANISOTROPIC FLOW, STRAIN SOFTENING, AND HISTORY DEPENDENCE

start with Gadzhiev
p36

October 7, Tuesday

Session Chair – A.I.Golubev

9.00 – 9.25 ***Merzhievsky L. A.***
(Lavrentiev Hydrodynamics Institute, Siberian Division of Russian Academy of Sciences, Novosibirsk)
56 p64 *CALCULATIONS OF FREE BOUNDARIES AND INTERFACES IN MOVING GRID METHOD*

9.25 – 9.50 ***Bondarenko Yu.A., Sofronov V.N., Kopyshev V.P., Khrustalev V.V.***
(RFNC–VNIIEF, ITMF, Sarov)
18 p28 *NON-UNIQUENESS OF RAREFACTION SHOCK WAVES: EFFECTS OF VISCOSITY, DISPERSION AND INTERPHASE KINETICS*

59 p67 ***9.50 – 10.15*** ***Novikov V.G., Solomyannaya A.D.***
(Keldysh Institute of Applied Mathemtics, Moscow)
CALCULATION OF AN EMISSION SPECTRUM FOR XENON PLASMA

77 p83 ***10.15 – 10.40*** ***Chetverushkin B.N.***
(Institute of Mathematics and Mechanics, Moscow)
KINETIC AND LATTICE BOLTZMANN SCHEMES

10.40 – 11.00 *BREAK*

11.00 – 11.25 ***Khishchenko K.V., Levashov P.R., Fortov V.E.***
(ITES, OIVT, Russian Academy of Sciences, Moscow)
76 p82 *MULTIPHASE MATERIAL EQUATIONS-OF-STATE FOR THE SIMULATION OF HIGH-ENERGY PROCESSES*

32 p41 ***11.25 – 11.50*** ***Gudarenko L.F., Kudelkin V.G.***
(RFNC-VNIIEF, ITMF, Sarov)
THE UPDATED MODEL OF EOS "ROSA" AND ITS SIMPLIFIED VERSION

69 p75 ***11.50 – 12.15*** ***Sapozhnikov F.A., Dremov V.V., Smirnova M.S.***
(RFNC-VNIITF, Snezhinsk)
PARALLEL MOLECULAR DYNAMICS TO STUDY ELASTIC-PLASTIC PROPERTIES OF SOLIDS UNDER HIGH STRAIN RATES

25 p34 ***12.15 – 12.40*** ***Voronin A.B., Voronin B.L., Demin D.A., Demina M.A., Nadykto B.A.*** (RFNC-VNIIEF, ITMF, Sarov)
PRIMARY MICROLEVEL MATERIAL DAMAGE CALCULATIONS WITH MOLECULAR DYNAMICS METHOD

13.00 – 14.00 *LUNCH*

Session Chair – S.M.Bakhrakh

14.00 – 16.00 ***POSTER PRESENTATIONS***

18 p27

1. ***Belyaev S.P., Gorbenko A.D., Degtiarenko L.I., Chistiakova I.N., Yanilkin Yu.V.*** (RFNC-VNIIEF, ITMF, Sarov)
IRREGULAR POINT-BY-POINT PARALLELIZATION METHODS FOR SOLID MECHANICS APPLICATIONS AND IMPLEMENTATION WITHIN TREK++ PACKAGE

79 p84

2. ***Shaporenko A.N., Eremenko A.Yu., Rasskazova V.V.*** (RFNC–VNIIEF, ITMF, Sarov)
SPHERICAL SYMMETRY CALCULATIONS ON 3D IRREGULAR LAGRANGE GRIDS

13 p21

3. ***Bakhrakh S.M., Borliaev V.V., Volodina N.A., Zaitseva M.O., Kovaleva A.D., Kulygina O.N., Ryabchun L.A.*** (RFNC–VNIIEF, ITMF, Sarov)
SMOOTHING ALGORITHMS FOR HIGH-FREQUENCY PERTURBATIONS OF THE VELOCITY FIELDS AS APPLIED TO MULTI-CELL COMPUTATIONS ON A MULTIPROCESSOR

12 p20

4. ***Bakhrakh S.M., Bezrukova I.Yu., Pronevich S.N.*** (RFNC–VNIIEF, ITMF, Sarov)
APPLICATION OF THE PIECEWISE PARABOLIC METHOD TO CONVECTIVE FLOW SIMULATIONS USING LAGRANGIAN-EULERIAN GRID

14 p22

5. ***Bakhrakh S.M., Velichko S.V., Naumov A.O., Ogneva N.E.*** (RFNC-VNIIEF, ITMF, Sarov)
IMPLEMENTATION OF THE ALGORITHM "VORTEX-IN-CELL" FOR NUMERICAL SIMULATION OF TIME-DEPENDENT FLOWS ON MULTIPROCESSOR DISTRIBUTED-MEMORY COMPUTER SYSTEMS

64 p72

6. ***Romanikhin V.P.*** (RFNC–VNIIEF, Sarov)
BREMSSTRAHLUNG SPECTRA COMPUTATIONS FOR LOW-ENERGY ELECTRONS

71 p77

7. ***Sukhikh A.S., Fedianin V.I., Yudintsev V.F.*** (RFNC–VNIIEF, ITMF, Sarov)
SOME ERROR EVALUATION RESULTS FOR ROUND-OFF COMPUTATIONS EXEMPLIFIED BY A LINEAR ALGEBRA APPLICATION

65 p72

8. ***Saveliev V.I.*** (Obninsk Atomic Energy Unuversity)
COMPUTER SIMULATION OF RADIATION GENERATION IN DISCONTINUOUS DIELECTRIC PROPERTY MEDIA

73 p79 9. ***Filippov N.A.*** (Viatskii State University, Kirov)
NUMERAL SYSTEMS AND INTEGER LOGARITHMS

74 p80 10. ***Filippov N.A.*** (Viatskii State University, Kirov)
EQUAL-PRECISION TABLES OF TRIGONOMETRIC FUNCTIONS AND INTEGER LOGARITHMS AS ILLUSTRATED BY TANGENT TABLE

33 p42 11. ***Guk N.A.*** (Dnepropetrovsk NU)
USING NEUROFUZZY TECHNOLOGIES TO PREDICT FINANCIAL INFORMATION

41 p50 12. ***Zaitsev F.S., Lukyanitsa A.A., Shishkin A.G., Trefilov A.B.***
(MSU, Moscow)
APPLICATION OF NEURON NETWORKS TO THE PROBLEMS OF SIMULATIONS AND DATA PROCESSING IN THE AREA OF CONTROLLED THERMONUCLEAR FUSION

31 p40 13. ***Golovanov A.I., Yakushin S.A.*** (Kazan' State University, Kazan', Russia)
FEM CALCULATION OF MULTILAYERED COMPOSITE SHELLS WITH ACCOUNT FOR GEOMETRICAL AND PHYSICAL NONLINEARITY

1 p7 14. ***Averbukh Yu.V.***
(RAS Urals Branch IMM, Ekaterinburg)
PARALLEL COMPUTATIONS IN MODELING APPLICATIONS FOR CHAOTIC DYNAMICS SYSTEMS

46 p55 15. ***Ivanov A.G.***
(RAS Urals Branch IMM, Ekaterinburg)
A PARALLEL PROGRAM OF UNCONDITIONAL MINIMIZATION: ALGORITHM, APPLICATION

3 p9 16. ***Averbukh Yu.V. Baidalin A.Yu., Ismagilov D.R., Kazantsev A.Yu., Poddubnaya S.V.***
(RAS Urals Branch IMM, Ekaterinburg)
3D REPRESENTATION OF THE FUNCTION CALL GRAPH

4 p11 17. ***Averbukh Yu.V., Manakov V.L., Vasev P.A., Komarovsky I.A., Mukhachev A.A., Shinkevich A.N.*** (RAS Urals Branch IMM, Ekaterinburg)
IMPLEMENTATION APPROACHES FOR ON-LINE PARALLEL COMPUTING VISUALIZATION TOOLS

39 p47 18. ***Zharinov A.N., Kumkov S.S.***
(RAS Urals Branch IMM, Ekaterinburg)
NUMERICAL SOLUTION TO THE PROBLEM OF FRONT PROPAGATION IN NONLINEAR CONTROLLED SYSTEMS

60 p68 19. ***Obodan N.I., Makarenko N.B., Guk N.A., Kiselev E.M.***
(Dnepropetrovsk NU)
BEHAVIOR OF A CYLINDER CASING IN THETEMPERATURE FIELD UNDER PARTIAL DESTRUCTION OF THE HEAT PROTECTION LAYER FOLLOWED BY LOCAL COOLING

55
p64

20. ***Maksimov F.A.***
(State Unitary Enterprise «Instrument-Making Design Office», Tula)
ASYMMETRIC FLOW ABOUT A CONE

62
p70

21. ***Ponyatsky V.M.***
(State Unitary Enterprise «Instrument-Making Design Office», Tula)
IDENTIFICATION OF MULTIDIMENSIONAL NON-STATIONARY DYNAMIC OBJECTS WITH KALMAN FILTRATION METHOD

66
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22. ***Sadovoy A.A., Sokolov S.S.***
(RFNC–VNIIEF, ITMF, Sarov)
THE KINETIC MODEL OF DYNAMIC DISTRUCTIONS INCLUDING THE PLASTIC GROWTH OF PORES AND DAMAGES CAUSED BY SHEAR STRAIN

38
p46

23. ***Yel'kinV.M., Mikhailov V.N., Mikhailova T.Yu.***
(RFNC–VNIITF, Snezhinsk)
NUMERICAL SIMULATION OF PLASTIC FLOW LOCALIZATION UNDER SIMPLE SHEAR

20
p30

24. ***Bondar' I.L., Igoshin O.V., Pazhin D.G., Teryushev E.I.***
(RFNC-VNIIEF, ITMF, Sarov)
ACQUISITION AND PROCESSING OF STATISTICAL INFORMATION ABOUT COMPUTATIONS ON DISTRIBUTED COMPUTER COMPLEX UNDER SUPERVISION OF WINDOWS

16.00 – 17.00 ***FAMILIARIZATION WITH POSTER PRESENTATIONS***

17.00 – 17.30 ***DISCUSSION OF PRESENTATIONS***

Tour about the city

First

p11

October 8, Wednesday

p27

Session Chair – Yu.G. Bartenev

51 p66 ***9.00 – 9.25*** ***Kovalenko V.N., Shorin O.N.***
(Keldysh Institute, Moscow)
METAMANAGER: GRID-SERVICE IMPLEMENTATION

50 p58 ***9.25 – 9.50*** ***Kovalenko V.N.,Koriagin D.A.***
(Keldysh Institute, Moscow)
PREDICTION-BASED GRID RESOURCE DISTRIBUTION

44 p53 ***9.50 – 10.15*** ***Zibarov A.V.***
(GDT Software Group, Tula)
FUNCTIONALITY OF PACKAGE GDT AND ITS USE ON MULTIPROCESSOR SYSTEMS

57 p65 ***10.15 – 10.40*** ***Mironov A.A.***
(GDT Software Group, Tula)
CFD CODE ARCHITECTURE FOR HYBRID ECOMPUTER SYSTEMS

10.40 – 11.00 *BREAK*

67 p74 ***11.00 – 11.25*** ***Samofalov V.V., Konovalov A.V., Sharf S.V.***
(RAS Urals Branch IMM, Ekaterinburg)
MULTI-USER OPERATION OF PVFS PARALLEL FILE SYSTEM

10 p77 ***11.25 – 11.50*** ***Stepanenko S.A.***
(RFNC–VNIIEF, ITMF, Sarov)
TOPOLOGICAL REDUNDANCY IN MULTIPROCESSOR ENVIRONMENTS WITH SINGLED-OUT ELEMENTS

80 p84 ***11.50 – 12.15*** ***Yakobovsky M.V., Boldyrev S.N., Krinov P.S., Sukhov S.A.***
(RAS Institute of Mathematics and Mechanics, Moscow)
LARGE-SIZE GRID HANDLING ON DISTRIBUTED COMPUTER SYSTEMS

6 p13 ***12.15 – 12.40*** ***Babaev D.B.***
(GDT Software Group, Tula)
FUNCTIONAL CAPABILITIES OF SCIENTIFICVR VISUALIZER SCIENTIFICVR

12.40 – 14.00 *LUNCH*

chetverushkin
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9 First in morning

Session Chair – V.F.Volgin

2 p8 ***14.00 – 14.25*** ***Averbukh Yu.V., Baidalin A.Yu.***
(RAS Urals Branch IMM, Ekaterinburg)
DEVELOPMENT OF VISUALIZATION TOOLS FOR PARALLEL COMPUTING SOFTWARE

17 p24 ***14.25 – 14.50*** ***Bakhterev M.O.***
(Urals State University, Ekaterinburg)
DISTRIBUTED OPERATING SYSTEM KERNEL DESIGN

8 p16 ***14.50 – 15.15*** ***Babin D.N., Umiarov A.R.***
(MSU, Moscow)
DYNAMIC OBJECT PERSPECTIVE RECOVERY FROM ITS IMAGES

42 p50 ***15.15 – 15.35*** ***Zenkov A.I.***
(RAS Urals Branch IMM, Ekaterinburg)
DEVELOPMENT OF AN APPROACH TO DEVELOPMENT OF SPECIALIZED VISUALIZATION SYSTEMS FOR HIGH-PERFORMANCE RESEARCH COMPUTATIONS

43 p52 ***15.35 – 15.55*** ***Zenkov A.I., Kumkov S.S.***
(RAS Urals Branch IMM, Ekaterinburg)
SPECIALIZED VISUALIZATION TOOLS FOR ANALYSIS OF NUMERICAL SOLUTIONS TO CONFLICT CONTROL PROBLEMS

15.55 – 16.10 *BREAK*

16.10 Sightseeing tour to Diveevo

x

At dinner — "and stop what we're doing?"

October 9, Thursday

Session Chair – V.F.Spiridonov

10 p18 **9.00 – 9.25** ***Barabanov R.A., Butnev O.I., Volkov S.G., Zhogov B.M., Pronin V.A.*** (RFNC–VNIIEF, ITMF, Sarov)

MEDUZA-3D CODE FOR 3D GAS DYNAMICS PROBLEMS USING IRREGULAR GRIDS. RICHTMYER-MESHKOV INSTABILITY SIMULATIONS

16 p24 **9.25 – 9.50** ***Bakhrakh S.M., Volodina N.A., Drennov O.B., Goreva T.A., Mikhailov A.L., Nizovtsev P.N., Shuvalova E.V.*** (RFNC–VNIIEF, ITMF, Sarov)

EXPERIMENTAL AND NUMERICAL (MULTIPROCESSOR) STUDIES OF COATING STABILIZATION EFFECT ON THE BEHAVIOR OF SHEAR INSTABILITY IN METALS

23 p33 **9.50 – 10.15** ***Veselov R.A.*** (RFNC-VNIIEF, ITMF, Sarov)

COMBINATION OF MOVING AND FIXED GRIDS (MIXED GRIDS) USED FOR 2D CALCULATIONS IN GAS DYNAMICS

5 p12 **10.15 – 10.40** ***Artemyev A.Yu., Budnikov V.I., Vershinin V.B., Delov V.I., Linnik D.M., Murugova O.O., Sadchikov V.V., Chernyshev Yu.D.*** (RFNC–VNIIEF, ITMF, Sarov)

3D PROGRAM COMPLEX DZ FOR SOLVING CONTINUUM MECHANICS PROBLEMS IN LAGRANGIAN VARIABLES

10.40 – 11.00 *BREAK*

35 p44 **11.00 – 11.25** ***Derugin Yu.N., Bazin A.A., Velichko O.M., Gorev V.V., Gorev I.V., Gubkova G.N., Zelenskii D.K., Panov A.I., Prudov N.V., Selin V.I., Sizova L.I., Subbotin A.G., Tikhomirov B.P.*** (RFNC–VNIIEF, ITMF, Sarov) ***Kosterin A.V., Chekalin A.N.*** (IMM, Kazan)

3D NUMERICAL CALCULATIONS OF IMPURITY TRANSPORT BY GROUNDWATER

15 p23 **11.25 – 11.50** ***Bakhrakh S.M., Volkov S.G., Kuratov S.E., Naumov A.O., Olkhov O.V.*** (RFNC-VNIIEF, ITMF, Sarov)

USE OF THE ALGORITHM "VORTEX-IN-CELL" FOR NUMERICAL SIMULATION OF HYDRODYNAMIC INSTABILITY

40 p49 **11.50 – 12.15** ***Zhmailo V.A., Sin`kova O.G., Statsenko V.P., Yanilkin Yu.V.*** (RFNC-VNIIEF, ITMF, Sarov)

DIRECT NUMERICAL 3D SIMULATION OF TURBULENT SHEAR MIXING

72 p78 ***12.15 – 12.40*** ***Tishkin V.F., Zmitrenko N.V., Ladonkina M.E.***
(RAS Institute of Mathematics and Mechanics, Moscow)
NUMERICAL SIMULATION OF VELOCITY PULSATIONS IN SHOCK TUBE EXPERIMENTS

13.00 – 14.00 *BREAK*

Session Chair – O.A.Vinokurov

7 p15 ***14.00 – 14.25*** ***Babanov A.V., Zmushko V.V., Rybachenko P.V., Bolshakova A.E.***
(RFNC-VNIIEF, ITMF, Sarov)
MADS++ CODE FOR CONTINUUM MECHANICS CALCULATIONS ON ADAPTIVELY EMBEDDED GRID

30 p40 ***14.25 – 14.50*** ***Glazyrin I.V., Gasilov V.A.***
(RFNC-VNIITF, Snezhinsk; RAS IMM, Moscow)
FEATURES OF 2D MHD APPROACH IMPLEMENTATION ON ADAPTIVE GRIDS

61 70 ***14.50 – 15.15*** ***Pavlenko O.N., Litvinenko I.A.***
(RFNC-VNIITF, Snezhinsk)
SIMULATION OF 3D GAS FLOW WITH PARTICLE-IN-CELL METHOD ON ADAPTIVELY EMBEDDED GRID. SEDOV BLAST CALCULATIONS

Moved to The

p35 ***15.15 – 15.40*** ***Gadzhiev A.D., Seleznev V.N., Shestakov A.A.***
(RFNC–VINIITF, Snezhinsk)
DSn METHOD FOR ARTIFICIAL DISSIPATION AND VDM METHOD FOR ITERATION SPEEDUP IN NUMERICAL CALCULATION OF 2D HEAT TRANSFER EQUATION IN A KINETIC MODEL

36 p45 ***15.40 – 16.05*** ***Dolgoleva G.V.***
(RFNC–VNIIEF, ITMF, Sarov)
NUMERICAL SIMULATION OF RADIATION TRANSPORT AND ITS INTERACTION WITH A SUBSTANCE

16.10 Excursion to Nuclear Weapons Museum and House-Museum of Yu.B. Khariton

October 10, Friday

Session Chair – Yu.N.Deryugin

11 p19 ***9.00 – 9.25*** ***Bartenev Yu.G., Bondarenko Yu.A., Vargina E.M., Golubev A.A., Yeremenko A.Yu., Yerzunov V.A., Kolesov M.A., Maksimov A.S., Panov A.I., Pronevich S.N., Frolova N.V., Tsareva T.V., Shchannikova E.B.***
(RFNC-VNIIEF, ITMF, Sarov)
CURRENT STATE OF THE PARALLEL SPARSE LINEAR SYSTEM SOLVER LIBRARY

~~58~~ 53 p62 ***9.25 – 9.50*** ***Kondrashov V.E.***
(Strategic Stability Institute, RF Minatom, Moscow)
A NEW EVALUATION METHOD FOR SOME MATRICES

19 p30 ***9.50 – 10.15*** ***Bondar' I.L., Davydov A.N., Osipov M.Yu., Teryushev E.I.***
(RFNC-VNIIEF, ITMF, Sarov)
LAN MONITORING SYSTEM

22 p32 ***10.15 – 10.40*** ***Vargin A.M., Kulnev D.V., Semenov G.P., Olesnitsky A.B., Kholushkin V.S., Romanova M.D., Frolova N.V., Barmin A.M., Orazmagomedov R.A., Kiselev A.B.***
(RFNC-VNIIEF, ITMF, Sarov)
THE CONCEPT OF DESIGNING A UNIFIED JOB CONTROL SYSTEM OF THE NON-UNIFORM COMPUTER SYSTEM AT ITMF

10.40 – 10.50 *BREAK*

21 p31 ***10.50 – 11.15*** ***Budnikov V.I., Vargin A.M., Volgin V.F., Butnev O.I., Pletenev F.A., Rudenko V.V., Tarasov V.I., Shagaliev R.M.***
(RFNC-VNIIEF, ITMF, Sarov)
INTERFACE OF PROGRAM COMPLEXES AT ITMF DIVISION OF MATHEMATICS

47 p56 ***11.15 – 11.40*** ***Ivanov A.N., Ivanov N.V.***
(RFNC-VNIIEF, ITMF, Sarov)
CONIDERATION OF THERMAL MOTION OF ATOMS WHEN SOLVING NEUTRON TRANSPORT PROBLEMS USING MONTE CARLO METHOD

58 p66 ***11.40 – 12.05*** ***Morozov V.G., Karpenko I.I., Korepova N.V., Dmitrieva L.V.***
(RFNC–VNIIEF, ITMF, Sarov)
NUMERICAL SHOCK-SENSITIVITY SIMULATION OF PLASTICIZED TATB HE UNDER HEATING

.9
>37

12.05 – 12.20 ***Galkin V.A., Ryzhikov D.A.***
(Obninsk University of Nuclear Power Engineering)
COMPUTER SIMULATIONS IN COAGULATION KINETICS

.8
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12.20 – 12.35 ***Galkin V.A.***
(Obninsk University of Nuclear Power Engineering)
COMPUTATIONAL METHODS FOR SPATIALLY NON-UNIFORM PHYSICAL KINETICS APPLICATIONS CONSERVATION LAW SYSTEMS

12.35 **ADJOURN**

SCHEDULE
of the
visit of a combined US delegation (LANL, LLNL, SNL) to RFNC-VNIIEF for participating in the Conference "Super-Computations and Computer Simulation"

October 5 through 10, 2003

Day One
October 5, 2003.
Sunday

Time	Event
05.30 - 06.30	Meeting at the check-point.
06.30 -08.00	Hotel check-in and rest.
08.00 -09.00	**Breakfast.**
09.00 -10.00	Rest in the hotel.
10.00-19.00	**Tour to Sanacsar Monastery.** Anatoly
19.00-20.00	**Dinner.**
20.00	Rest in the hotel.

Day Two
October 6, 2003.
Monday

Time	Event
08.00 -09.30	**Breakfast.**
09.30-12.00	Conference. Opening Session.
13.00-14.00	**Lunch.**
14.00-17.00	Work of the Conference in accordance with a Program.
17.20-19.00	Rest in the hotel.
19.00-22.00	**Cocktail Party.**
22.00	Rest in the hotel.

Yablonskii_s - b'cond email & open sys. disc.
Vasily Vetzuk - interest in R-B
fellow from Cift-Urals b.cond not right org.
Bartenv Yury Germenokch - discussed funding

Day Three
October 7, 2003.
Tuesday

Time	Event
08.00 -09.00	**Breakfast.**
09.00-12.00	Work of the Conference (continued).
12.00-14.00	**Lunch.**
14.00-17.20	Work of the Conference (continued).
17.30-19.00	**Tour round Historical Sarov**
19.00-22.00	**Dinner at Dr. Mokhovs'** (I. Lindemuth, E. Lindemuth)
19.00-22.00	**Dinner at Dr. Shagalievs'** (D. Kamm, A. Fitzpatrick, M. Zocher, W. Rider, E. De Benedictis, H. Scott)
22.00	Rest in the hotel.

Day Four
October 8, 2003.
Wednesday

Time	Event
08.00 -09.00	**Breakfast.**
09.00-12.00	Work of the Conference (continued).
12.00-14.00	**Lunch.**
14.00-16.20	Work of the Conference (continued).
16.20-19.00	**Tour to Diveevo Convent.**
19.00-20.00	**Dinner.**
20.00	Rest in the hotel.

Day Five
October 9, 2003.
Thursday

Time	Event
08.00 -09.00	**Breakfast.**
09.00-12.00	Work of the Conference (continued).
12.00-14.00	**Lunch.**
14.00-16.10	Work of the Conference (continued).
16.10-17.30	**Visit to the Nuclear Weapons Museum.**
17.30 – 19.00	Rest in the hotel.
19.00-20.00	**Dinner.**
21.00	Rest in the hotel.

Day Six
October 10, 2003
Friday

Time	Event
08.00 -09.00	**Breakfast.**
09.00- 12.30	Conference Closing Session. Conference Wrap-up.
12.30 –14.00	**Lunch.**
14.00-16.00	**Art Shop Tour.**
16.00-17.00	Rest and hotel check-out.
17.20	Departure for Moscow.

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PARALLEL COMPUTATIONS IN MODELING APPLICATIONS FOR CHAOTIC DYNAMICS SYSTEMS

Averbukh Yu.V.
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Currently discrete models like cellular automatons attract the attention of many researchers. One of the reasons is that those systems generate 'Self-Organized Criticality'. Self-Organized Criticality state is characterized by permanently fluctuating energy release process governed by the power statistics with negative index. These phenomena occur in complicated physical and other natural processes.

An important example of natural process where we encounter Self-Organized Criticality includes seismicity in an active tectonic zone. The Gutenberg-Richter law well known in seismology demonstrates on logarithmic scales how the number of earthquakes depends on the earthquake magnitude in a nearly linear way. Forest-fire models are representative for the class of discrete chaotic-dynamics systems in question.

Publications report three forest-fire models whose review would help understanding Self-Organized Criticality laws. The action occurs on a square field composed of $L \times L$ cells. Each cell may be empty or tree-filled. The first model introduces two parameters, p and f. The modeling process proceeds in accordance with the following rules: each empty cell converts to a tree-felled cell at each time with the probability p and each tree-filled cell generates the ignition with the probability f destroying the entire connection region (cluster) of the forest containing this cell. The second model differs from the previous one in that the forest growth and fire process run sequentially, i.e. a cell is selected that generates the tree growth with the probability p, if empty; if it is tree-filled the fire occurs with the probability f. The third model contains the only parameter, ΔP – relative number of cells to be selected. The modeling process proceeds with the following rules. $\Delta P \cdot L^2$ cells are selected; if the selected cell is empty a tree appears there. Then a new cell is selected generating fire, if tree-filled thus destroying the cluster where the selected cell resides. The model studies the forest density, fire-produced yield, cluster distribution over yields. These models are shown to demonstrate in average identical behavior pattern.

Despite of relatively simple rules, these models can be studied only experimentally.

The analysis of system behavior requires a great number of simulation steps on large-size field. This needs parallel computations. A simulation step should be implemented so that the probability of converting from one state to another does not change. The parallelization of three models divides the field into portions each of them handled by a designated processor.

A feature common for each of three models is that the fire should be initiated on a field shared by the processors. This procedure uses the 'wave' parallelization algorithm. For the first model, the choice of cells in each square is independent on other squares and the synchronization is required only after the cell selection is terminated and the fire is running. Therefore the selection efficiency is unity. For the second model, we proved that the cell selection process can not be parallelized. To parallelize the selection process in the third model, we propose the quota method that first counts the number of cells to be chosen by each processor and then each processor selects the cells from the uniform distribution. Quota ate selected in a way

to retain the uniform distribution when each cell is selected. However the resulting model efficiency is low compared to first mode; implementation. Even the first allows to measure efficiently the forest density and fire-produced yield with a parallel solver. We failed to measure the clusters efficiently from the yields at this point.

Among three cellular automatons known as forest fire models, one has a clear parallelization advantage compared to the remaining analogs. Thus the study of chaotic-dynamics systems using parallel solvers generates a problem necessitating the conversion of the given model to another that is similar in behavior pattern and demonstrating a higher parallelism level.

The work was sponsored by the RBRF, grant No. 01-07-90210.

DEVELOPMENT OF VISUALIZATION TOOLS FOR PARALLEL COMPUTING SOFTWARE

Averbukh Yu.V. Baidalin A.Yu.
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Three following tasks are distinguished among parallel computing software visualization applications:

- visual design support and visual programming,
- visual correctness adjustment,
- visual analysis, tuning and performance adjustment.

Note that currently software visualization is important for parallel computing since in the sequential case the applications requiring programming and debugging visualization are actually mitigated with up-to-date programming technologies.

Parallel programming demonstrates various paradigms requiring a variety of representation and interpretation ideologies for the basic entities. For example, program description in terms of Message Passing differs from that of a functionally similar program in terms of Data Parallel.

Publications report that designing software visualization tools should be accomplished in an integrated manner with a unique approach to the development of imaging types for visual programming and correctness/efficiency adjustment. However this was never achieved in actual projects.

This paper considers visualization aspects both theoretically and practically as applied to DVM parallel programming system. The DVM system is characterized by the following features:

- the system relies upon the data parallelism described by incorporating special DVM directives invisible for sequential compilers into the sequential program;
- availability of integrated correctness/efficiency adjustment tools including parallel route assembly and performance predictor;
- DVM debugging is accomplished in off-line mode.

The efficiency data acquisition unity is the interval, i.e. a code fragment run on (system-selected or user-specified) designated processor for which some characteristics (about ten) are measured. The entire debugging data is represented in simple text format. If the system run on hundreds massively parallel solver processors the amount of performance data range from hundreds to thousands kilobytes.

The DVM program debugging specificity is that the interaction descriptions are implicit when data parallelism is used and correctness adjustment should run on a

single processor. At the same time, processor communications description is just crucial for successful representation of parallel programs.

The debugging experience described relates primarily to efficiency adjustment. The development of VisDVM project resulted in a system of performance data representation types: interval *flow chart*, radial graph and interval *wall* to display processor load balance, *tree* and *list* to represent general performance data structure. The system ensured the interaction between two imaging types, the navigation across the data structure and look-up of primary numerical values. Linking the representation types to the source text allows the user to detect rapidly bottlenecks in the program.

To see whether visible design support is feasible, some experimental prototype system were developed. Currently we focus on the development of directive wizards allowing both to assemble an integral directive from individual fragments and to represent a directive as separate components. TracePlayer was developed for the correctness adjustment to reproduce program execution from program route data.

Further DVM improvement envisaging particularly the use of OpenMP connective and MPI as the communications base requires that the visualization system is able of representing new entities. In parallel, the DVM implementers propose to incorporate MPI-level debugging tools into the target system.

Thus the problems emerging from DVM visualization cover a broad class of theoretical and practical software visualization tasks in parallel computing. The existing practices in visual representation tools for DVM can be applied to other software visualization tools.

The work was accomplished under RBRF sponsorship, grants No. 01-07-90210, 01-07-90215.

3D REPRESENTATION OF THE FUNCTION CALL GRAPH

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Ismagilov D.R., Kazantsev A.Yu., Poddubnaya S.V.
(RAS Urals Branch IMM, Ekaterinburg)

3D representation problem in software visualization applications emerged as early as in the mid 80-s. By the mid 90-s, attempts were made in some visual programming systems to develop 3D tools to represent program constructs and to visualize program execution.

After the success of the desktop metaphor, the room metaphor was proposed that had been repeatedly attempted to implement in various human-machine interfaces though on a prototyping level. This metaphor was implicitly used in the efficiency adjustment system, Avatar, to represent performance data of a large-scale parallel program. (The Avatar system uses scattercube metaphor – multiple data output method in a cube; however each cube is actually a room with the walls displaying the performance metrics.) The resulting 3D icon programming system prototype used the room metaphor to create a changing tool for control structures and program data. Icons are placed on the room walls to represent control structures and program function data. The links between the constructs are displayed in space ratherthan on plane unlike traditional 2D diagram and icon visual programming systems.

Intel VTune performance analysis system for large-scale programs focuses on on the call graph visualization used to tune the performance of complicated program ensembles including distributed and parallel programs. The VTune system uses 2D

call graph representation. The analysis of a large-size and structurally complex program with deeply embedded function calls and multiple user functions results in a difficulty caused by 2D display of an extended structure and by the user-evaluation of the final image. Insufficient screen space problem can be resolved by adding one more dimension to the model under development. The resulting 3D picture displayed on the same screen can reproduce much more entities. A 3D image is more easily analyzed and viewed by the user.

Attempts were made to represent the call graph in 3D using several proposed metaphors.

Primarily, the call graph was represented as an ensemble of interconnected rooms. In this case, the rooms are positioned on three levels. We consider the user functions having user functions as children; user functions without children and systems functions. Each level matches a designated level in the resulting image. Each room is a visual function representation. Moreover, the icon on the parent-function room wall in he call graph is also responsible for the function. The graph edges are naturally mapped onto our image – they go from the function icon on the parent wall to the cube-room of the given function. Originally the entire graph is shaded but when the current function installs another the appropriate branch is highlighted. The image is made most realistic by 'from-inside' room image combined with potential 'traveling' inside with our 'building' from one room to another. However the user is unable to have a volume graph visualization. We believe the combination of these two graph representation types gives an optimum result. However the room metaphor is not universal in visualization.

In addition, a 'geocentric' metaphor was offered for 3D call graph representation when the parent function is below and called functions reside on geocentric hemispheres. However since the resulting representation type essentially required virtual reality tools we used embedded sphere implementation. Note that the implemented model contained two function types: systems type and user type. Systems functions lie on the outer hemisphere while user functions reside on the inner portion. The analysis of the resulting model showed a complicated perception and subsequent evaluation of the visualization as well as unresolved self-overlapping problem.

The next representation version of the call graph is based on the embedded sphere metaphor with each of spheres representing both systems and user functions used in the program. The screen permanently displays only a single embedding level – those functions and procedures that are called from the current one thus escaping self-overlapping and insufficient screen space problems. The transition from one function to another is accomplished by simple mouse-clicking on the sphere that represents a user-needed function. The pattern is animated and interactive allowing the user to understand and evaluate better the resulting graphical image.

In addition, a molecule metaphor was offered for the call graph representation. The molecule structure reflects that of the original graph here. Two coupling types are introduced for atoms (representing graph vertices as functions): elastic coupling between bound atoms and electrostatic coupling between all atomic vertices. The electrostatic interaction reflects time characteristics of function calls while te elastic pattern does so for the number of calls. The capability analysis of this metaphor showed that it is more applicable to large-scale system structure representation rather than to imaging the call graphs.

Thus theoretical studies and experimental implementations demonstrated enhanced capabilities of 3D images to represent parallel programming entities.

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IMPLEMENTATION APPROACHES FOR ON-LINE PARALLEL COMPUTING VISUALIZATION TOOLS

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Some supercomputing simulation steps require interactive graphics tools, in particular, to allow the visualization of interim results, state variation of the program, adjustment of parallel computing correctness and/or efficiency. Another important objective is to reduce considerably the amount of transferred data to be visualized. Frequently, the size of transferred files make the computational time compared to that of data transfer and visualization. Operating with parallel solvers with limited data transfer rates over low-performance networks makes the generation of bitmap image inefficient and cost-expensive. Data transfer frequently uses hardware-independent graphics protocols and metafiles in those conditions.

The paper describes some development approaches for on-line visualization tools. These tools are validated within the development of several prototype systems implementing, in particular, the generator of graphics programs; data filtering technology on concurrent processors and automated generation of problem-oriented metafiles.

The creation of parallel interactive program generator should proceed in the context of independently written parallel and visualization programs. Our objective is to convert rapidly from online visualization methods to interactive visualization.

The generator tools would allow the user to implement the interaction between the applications by linking variables/arrays and data transfer moments for those applications. At the early step, the user must open program text files in two parallel windows to be linked. Then transfers are positioned. Once all transfers are designated, sessions should be established (pair event combining a group of input/output operators). The resulting programs can be compiled and launched. Since the generator includes the complete edit-compile-run cycle the compilation yields the only execution-ready task. Recompilation, the use of Java language, tuning to various languages and translators mitigate some portability problems.

Currently, design efforts are underway for the next generator version based on thee-component client-server scheme (where the programs reside on the workstation, on the parallel solver host and on processors).

Consider now the visualization problems of lager-scale and very large-scale parallel computing. The basic task of visualizing great amounts of data is to reduce transferred data for subsequent visualization. The approaches to this problem can divided into two major classes: use of interactive mode and data compaction or filtering.

Clearly, for real applications where the computational time counts several hours and even days and amounts of data handled by the program reach Terabyte scale, no interactivity seen, in the naïve context, can be evoked (communication with the user in the dialog mode), though some methods could be offered to resolve the problem. The second basic approach (more precisely, a class of approaches) is to assemble,

filter and sort data resulting from computations. This approach allows several actions executed sequentially on each parallel solver processor such as obtain mathematical data from executed algorithms, apply filter to process obtained data, transfer filtered data to the computer (possibly, remote) for final visualization.

We can mention many decimation filters, multidimensional projections, plane section, filters oriented to a specific problem and the visualization model. (Data compaction can be also considered as a filter). The parallel program was implemented using MPI library, master-slave scheme and oriented to geometrical data distribution. Filtering is accomplished independently on each processor, which reduces the amount of transfers. It is desirable to examine filter efficiency and parallelization issues when describing the general filtering scheme.

Since the parallelism model is a data parallelism model it seems to be logical to use the DVM system demonstrating good capabilities for the model implementation. Though the DVM compiler additionally restricts the entire program and the data used the system does not actually take any time to implement the parallelism itself when developing the applications in question.

Filtering is the most efficient approach using both interactivity and problem-oriented metafile generation and parallel run of data filtering algorithms. At this point, a series of demos was designed for assembly, filtering, sorting of large amounts of data with subsequent visualization.

Automated metafile generation involves the creation of metaclasses (stub-class) operated by each processor (their methods replace real methods of graphics library by writing all necessary data to the metafile). In addition, a program must be generated to disassemble the metafile resulting from the application run on parallel solver processors.

When reviewing the original VTK C++ library texts we choose progressive upgrade scheme for the ensemble of implemented methods adding new methods as the need occurs.

The approaches to on-line implementation of parallel computing showed the basic feasibility and require further validation through real applications.

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3D PROGRAM COMPLEX DZ FOR SOLVING CONTINUUM MECHANICS PROBLEMS IN LAGRANGIAN VARIABLES

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The 3D complex DZ is based on the technique extended to three spatial variables [1] for computing 2D time-dependent gas dynamics problems in Lagrangian variables (technique D [2]). The original gas dynamics differential equation system is written in Cartesian coordinates. Hexahedrons, whose faces are surfaces of hyperbolic paraboloids, are taken for the unit cells in the difference scheme construction. The complex DZ implements two different schemes approximating equations of motion. Artificial viscosity has been introduced to the difference scheme for the integrated

computation of shock waves. On the whole, the constructed computational gas dynamics difference scheme is explicit, has the second order of approximation both in time and space in the smoothness regions of the solutions on uniform grids. The Courant type necessary condition of the difference scheme robustness has been obtained. The study has been conducted on the hexagonal grid uniform in each direction in the form of right parallelepipeds.

Material elastic-plastic properties are included in the complex DZ using two models [3]: a conservative Wilkins modification, in which the differential-difference equations are derived from the law of reciprocal conversion of kinetic and internal energies, and a much more complex model, which accounts for shear stress relaxation.

The DZ computation of detonation employs several models: the detonation calculation without inclusion of burning kinetics uses the Chapman-Jouguet relation, the principal methods for computing detonation with the inclusion of burning kinetics use Morozov's-Karpenko's and Kopyshev's models.

A program of velocity smoothing has been implemented to suppress short-wave perturbations of velocity. The complex DZ involves two smoothing operators: the fourth-order Chen smoothing operator extended to three dimensions and an algorithm using the artificial scalar viscosity apparatus to avoid degeneracy of hexagonal cells of the computational Lagrangian grid.

A technique for automatic correction of "bad" points of the 3D Lagrangian grid and gas-dynamic quantity re-calculation to the corrected grid has been implemented for local correction of the Lagrangian grid. The technique preserves the Lagrangian representation of the gas-dynamic flow as much as possible due to the local correction. Points at interfaces are corrected using a mixed cell technique, in which adaptive grids are introduced in multimaterial cells.

Besides the discussion of the techniques, the paper presents the complex structure, database with description of principal grid and boundary arrays. The idea of the computation control code is given, the actions in one timestep computation as well as computation interruption conditions and instructions used most frequently in the DZ computations are briefly discussed. Results of benchmark computations are given as numerical examples.

FUNCTIONAL CAPABILITIES OF SCIENTIFICVR VISUALIZER SCIENTIFICVR

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The paper describes the architecture and capabilities of the new ScientificVR® visualizer. Historically, this system emerged from GasDynamicsTool (GDT) package and visualization functions developed for internal use. In February 2000, the idea appeared to implement the visualization unit as a separate software product extending and intensifying its capabilities in parallel with the development of the fifth GDT generation. One of the basic objective s was to design a package architecture that would allow to visualize not only GDT package format but also other visualization formats for abstract data types. The most advanced achievements used in this version include modular scalable architecture, 3D voxel graphics visualization, true-color stereo data representation.

Multifunctional ScientificVR® visualizer is based on a multiplayer modular architecture allowing to add new functions to the installed package by plugging-in external modules. Using specific external modules permits to operate the same package for handling a variety of data in various knowledge domains.

External modules for ScientificVR® can be created both by the package implementers and by the users. Using this architecture allows a significant flexibility in integrated data visualization.

The ScientificVR® visualization system is designed to be more flexible and sophisticated as compared to traditional visualization system architectures. The basic feature of his architecture is unlimited expansion of all five subsystems:

- data loading,
- coordinate conversion,
- functional transforms,
- imaging,
- image output.

This is possible since any subsystem represents an ensemble of plugged-in modules each of them executing a designated function. For example, each plugged-in module for the data loading subsystem ensures the input of data stored in a selected format. Thus adding plugged-in modules to the subsystem allows the loading of data stored in any selected format permitting simultaneous processing of various-origin data (for example, you can create images visualizing experimental and computational data).

If the ensemble of plugged-in system-supplied data does not meet the user requirements for any reason the user can either choose appropriate modules (for example, through the Internet) or create the desired modules independently using any available tools.

Another feature of ScientificVR® system is functional and coordinate conversion capability.

The functional conversion subsystem consists of plugged-in modules that create derivative data from the source input following a special rule. Functional conversion can be exemplified by scalar field gradient, vector field divergence, scalar vector-vector multiply, scalar or vector argument functions etc.

Imaging subsystem contains plugged-in modules each of them designed for a desired image type generation, for example, 3D voxel graphics, vectors, isolines, isosurfaces, current lines, etc. Images created with plugged-in modules are then combined by the user to obtain the most illustrative data representation.

The package has a wide spectrum of functional capabilities, data representation types, various scalar and vector arrays operations, image representation types. Data representation types include graphics, 2D scalar data color representation, 2D scalar data height representation, isolines, 2D and 3D vectors, current lines and tracers, 3D voxel graphics, isosurfaces, textures.

The ScientificVR® package implements various tools for solid structure rendering. In addition to the capabilities of the geometrical GDT package modeller in geometrical thread rendering format, ScientificVR® is partially compatible with STEP standard (ISO 10303), which permits to imterface with most of the existing CAD systems.

The package demonstrates unlimited image combining capability. For example, density voxel representation can be mapped by pressure isosurfaces with concentration distribution texture painting: the entire pattern can be mapped, in turn,

velocity vectors and/or temperature gradients (the vectors can be painted as implied by the representation of another quantity) etc. This allows the integrated analysis of complex phenomena and the representation of an arbitrary ensemble of parameters.

One of the recent innovations to the visualizer is 3D image stereo representation. To do this, the user can mount a special video card on his computer supporting the display stereo mode and allowing stereo points (for example, ASUS 7100 Deluxe). Stereo imaging is possible for any 3D visualization type such as voxel patterns, isosurfaces, 3D body and vector representations or both.

The resulting stereo images can be written to the AVI file with all additionally available animation capabilities.

The package can produce a variety of animation effects. In addition to traditional AVI files illustrating the time-dependant process history from a single fixed point, we can now make rotating AVI files that can be used to visualize static distributions as well as in combination with time-dependant process history. All animation functions can be used in stereo modes.

ScientificVR® system is flexible and multifunctional which makes it attractive for fast and high-quality visualization

n of data obtained from a variety of sources such as primary sensors, numerical simulation results or theoretical data.

The paper presents multiple examples of how the package can be used to visualize the results of numerical simulation in solid mechanics applications.

MADS++ CODE FOR CONTINUUM MECHANICS CALCULATIONS ON ADAPTIVELY EMBEDDED GRID

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Obtaining numerical results for complex physical processes with a desired accuracy requires important computational resources. In some cases advanced computer technologies can offer these resources though resource requirements often increase too rapidly with growing accuracy requirements. One of the ways to loosen this relationship is to use adaptive grids. MADS code was developed based on the algorithms used in MIMOSA and proved well on regular grids.

The paper considers MADS adaptive grid method applicability to gas dynamics processes with concentrations, detonation and for the calculation of elastic-plastic flows. A specific feature of the method is that it includes embedded grid algorithm with limit split parameter of the original template, ordering the current grid nodes over shock arrival times, saving cell data structures as linked lists, use of fast sort algorithms and the grid for empty number identification. Sequential handling of ordered nodes in detonation domains allows the single-run evaluation of HE burnout at a single timestep. The code implements controlled calculations of detonation and Arrenius kinetics plus control.

One of the important features of the adaptive grid method is the choice way for the grid splitting/coarsening. In elastic-plastic deformation regions, automated grid refining was accomplished for those cells where artificial viscosity (sum of quadratic and linear values) achieved the threshold. Coarsening was prohibited for those cells that experienced plastic deformation in the computational process under the grid rarefaction.

Test computations were used as an example to show the use of adaptive grids may in some cases significantly save computational resources to achieve the desired accuracy. MADS data were compared with the results previously obtained with MIMOSA codes and with experiment.

DYNAMIC OBJECT PERSPECTIVE RECOVERY FROM ITS IMAGES

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This talk reviews computer-aided object tracking and its space location exemplified by the face tracking. A system of typical points much differing from the nearest neighbors is considered instead of the image. Typical points can be said to be local extremums of the color frame function. Finding the sight direction of a driver in disturbed environment requires the capability for establishing the consistency between the typical points of frames obtained from parallel and sequential computations in addition to traditional rendering the face and eyes.

This application allows additional reducing of restrictions. If we have calibrated cameras (stereo cameras) a 3D typical point space location can be recovered from the binocular vision principle. If the typical point displacement is small you can find similarity extremum from a variety of local displacements. Finally, you can initially indicate typical pints in implicit way.

Consider the general case where no similarity and geometrical adjacency exists between the typical points and the number of points differs from one frame to another.

Let two full metric graphs are specified - $G=\langle a_i,v_i\rangle$, $G^*=\langle a^*_i,v^*_i\rangle$ - along with the weighs w_i of G graph vertices. G^* graph differs from G in that its vortex numbers could have been changed, the edge lengths slightly varied, previous vertices disappeared and the new ones emerged. Let G have n vertices and G^* – n* vertices with at least m new ones. We have to find a partial optimum consistency k between the vertices of the two graphs such that the functional

$$\sum_{ij}^{l}\left(\rho(a_i,a_j)-\rho(a^*_{k(i)},a^*_{k(j)})\right)^2-\sum_{i}^{l}\omega_i^2\to\min$$

is minimum.

We propose an algorithm of complexity $N_0+N_1+\ldots+N_m$, ••• s=1,…m

$N_s = C^s_{n^*}\ C_n^{n-n^*+s}\ (n^*-s)^4 \ln(n^*-s)$,

Which yields the polynomial of the number of graph vertices with the exponent of at least 2m+ n – n*+5.

For a small number of new vertices m and disappeared vertices n – n*, the algorithm runs in real time. The application is generalized to the case where the second frame scale changes.

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PROCESSOR COMMUNICATIONS SYSTEM FOR MULTIPROCESSOR ENVIRONMENTS

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The multiprocessor development and operation experience allows to suggest that the most optimum way to build multiprocessors is to apply commonly used processor platforms further referred to as computational modules including a special processor communications system [1, 2]. The communications system parameters essentially determine the hardware performance. The paper examines the communications system design concepts for MP-X multiprocessors, shows basic message passing processes, presents the communications system parameters compared to similar products.

The basic features of the MP-X communications system include:

- Applicability to computational modules designed from various chip types running under various operating systems. The design concepts are presented for the drivers and the adaptation feasibility is illustrated for high-level software;
- Dividing the data paths for transit messages and send-receive of “owned” data establishing the interleaving in the data-receive input path. The communications efficiency is given as a function of double rate data receive capability;
- Multichannel PCI 64/66 interface. Efficiency estimates are presented for the usage of a single or two PCI channels for data receive-send.
- Building arbitrary-topology multiprocessors and tailoring to MP-X architecture (hypercube). The usage scenarios are presented for two-way adapter for classic architectures and two single-way adapters for hypercube multiprocessor architectures;
- Introducing a communications processor allows an optimum communications control distribution between the ‘upper’ and ‘lower’ levels of systems software in particular when handling communications errors as well as for establishing a service subsystem to handle communications environment functioning data. The analysis was conducted for timings of hardware and software-controlled error handling.

- Hardware support of batch data transfer operations. Each-to-all and each-to-all –in-path operations are implemented.
- Communications system design implementation;
- Feasibility for multiway switch implementation.

The communications system channel throughput is240 MB/s, the switch delay does not exceed 250 ns, the throughput of the communication link between the computer and the communications system is 2x512 MB/s. This performance is consistent with the product level of communications systems vendors such as Myricom Corporation [3].

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MEDUZA-3D CODE FOR 3D GAS DYNAMICS PROBLEMS USING IRREGULAR GRIDS. RICHTMYER-MESHKOV INSTABILITY SIMULATIONS

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The paper describes a code for 3D gas dynamics computations using unstructured grids which is the MEDUZA code generalized to a 3D case. Note that currently the authors have implemented a possibility of calculating a fluid motion (solving the system of gas dynamic equations in Lagrangian variables). Further generalization of the mechanisms of maintaining a computational grid and changing the grid topology to a 3D case is supposed.

A 3D analog to the difference scheme of MEDUZA explicit free-Lagrangian code is used to solve the system of gas dynamics equations using a grid composed of tetrahedrons. A single-region model of solving a problem is used. This leads to mixed cells emerging at fluid interfaces that are calculated basing on a multiple-component approach.

The right-hand side of the motion equation is supplemented with the velocity smoothing operator required because of the need in suppressing high-frequency perturbations. The operator is approximated using the grid of tetrahedrons.

The grid cells are polyhedrons (surfaces of integration) with the grid nodes inside; all kinematical and thermodynamic quantities are centered at nodes. The integration surface generation algorithm is based on the use of the centers of masses of tetrahedrons, mass centers of these tetrahedrons' faces and centers of their edges.

To preserve the grid topology, the approach is used, where a point refers to an arbitrarily shaped adjacent tetrahedron and each tetrahedron refers to the four adjacent tetrahedrons and its own four vertices. Such a scheme of preserving the grid topology

allows a number of problems of time step organization to be solved and the code to be made more efficient.

The code that implements the techniques above has been verified using two problems of Richtmyer-Meshkov instability growth due to a shock wave passing across a gas-gas interface. The results obtained are compared with the experimental data and the results of 2D computations.

CURRENT STATE OF THE PARALLEL SPARSE LINEAR SYSTEM SOLVER LIBRARY

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The parallel solver library [1] has been developed significantly with keeping the principal lines of investigation in implementation of the iterative method set for solving large linear systems that appear in the differential equation discretization on regular and irregular grids with an efficient algorithm of execution on parallel computers as well as in development of portable libraries with a convenient and flexible interface for •/•++, Fortran-90 applications.

Beginning from 2002 parallel solvers PMLP came to be used in simulations of some continuum mechanics problems. The transition to Krylov's family PMLP solvers has speeded up the modeling time. In the progress of work the efficiency of single-type solvers PMLP was compared to that of library PETSc in terms of a few components. Currently the works are underway to enhance the parallel solver efficiency and reduce the main memory requirements. For these purposes new preconditioners are being developed and operated ones are being modified.

A convenient user's interface has been developed. It is a shell of both sequential and parallel library part, which significantly facilitated the C/F interface construction and speeded up the library introduction to the production complexes. The C/F interface allowed us to use small object libraries of given properties in program complexes.

To extend the range of the users and simplify the solver introduction in applications, Wizards programs have been developed. The programs allow visual demonstration of the library possibilities and generation of application examples. The studies with the following optimization of a number of the solver library functions allowed us to use the architecture of efficient computer systems in a most efficient manner.

The developers of the library being presented tried to accomplish the above goals in the complex with offering the object-oriented and traditional technology of the library employment, high-quality implementation of the well-known sequential and parallel methods for solving linear systems and shells for studies and research.

Documents in the form of HTML files are available.

The web sites are www.erc.msstate.edu/labs/hpcl/pmlp, www.sarovlabs.com.

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APPLICATION OF THE PIECEWISE PARABOLIC METHOD TO CONVECTIVE FLOW SIMULATIONS USING LAGRANGIAN-EULERIAN GRID

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The paper describes the algorithm implemented within LEGAK complex [1] for qualified computations of convective flows with the piecewise parabolic method [2].

LEGAK complex uses the donor-acceptor method of the first order of accuracy in space. Methods of a higher accuracy order allow significant improvement of the accuracy of computations. Of especial interest among them is the piecewise parabolic method of the third order of accuracy. This method allows more correct localization of hydrodynamic parameter discontinuities.

In contrast to [3], the piece-wise parabolic method has been generalized to a 2D case with the use of a Lagrangian-Eulerian grid and improved, namely: correction of the regridded values of quantities has been introduced, new algorithms have been developed for recalculation of the internal energy and consideration of availability of a Lagrangian line preventing the material spillover. The piecewise parabolic method has been also generalized to a multiple-component case by using it in combination with the donor-acceptor algorithm.

Verification of the method demonstrated its serviceability and significant improvement of the computation accuracy. Richtmyer-Meshkov instability problems have been solved using the method and good agreement with the experimental data [4] has been achieved.

The work was sponsored by RFBR (Project 02-01-010796).

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SMOOTHING ALGORITHMS FOR HIGH-FREQUENCY PERTURBATIONS OF THE VELOCITY FIELDS AS APPLIED TO MULTI-CELL COMPUTATIONS ON A MULTIPROCESSOR

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Many numerical schemes designed for the calculations of time-dependent solid flows on regular grids including LEGAK [1] use smoothing operators for high-frequency perturbations of the velocity field that make the calculations hard when non-used because of the perturbation growth.

With the progress of computer engineering, there is quite natural tendency for the conversion to finer grids and for increasing the number of cells. This increases the perturbation spectrum in the computations. Perturbations emerge that were not observed in the solution for a lower number of cells. The computations result in the need for crash-free computations on ever finer grids.

The paper analyzes and updates smoothing operators implemented in LEGAK package [2].

The study showed that the stabilization of the solution with a great number of points (several thousands columns) requires:

1. Fixed-column grids;
2. Quadratic vector viscosity;
3. Smoothing operator over two axes
4. Smoothing operators where the velocity projection direction is related with fixed columns.
5. Repeated smoothing operator initiation to increase the smoothing ratio without affecting the operator stability.

The work was accomplished under the RBRF sponsorship (project No. 02-01-00796).

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IMPLEMENTATION OF THE ALGORITHM "VORTEX-IN-CELL" FOR NUMERICAL SIMULATION OF TIME-DEPENDENT FLOWS ON MULTIPROCESSOR DISTRIBUTED-MEMORY COMPUTER SYSTEMS

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The algorithm "vortex-in-cell" [1–4] implemented in LEGAK complex for Lagrangian gas dynamics [5, 6] is used for numerical simulation of time-dependent flows. Numerical studies of the algorithm show that it allows consideration of small-scale perturbations using a "rough" enough grid.

The algorithm "vortex-in-cell" has been parallelized within LEGAK complex operated on multiprocessor distributed memory MPI-standard [7] computer systems.

The paper discusses the main principles of the algorithm parallelization, gives examples of computations and data on the parallelization efficiency.

The work was accomplished under partial financial support by RFBR (Project 02-01-00796).

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USE OF THE ALGORITHM "VORTEX-IN-CELL" FOR NUMERICAL SIMULATION OF HYDRODYNAMIC INSTABILITY

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In recent years, approaches to describing time-dependent hydrodynamic flows of compressible fluids using vortices to allow consideration of small-scale perturbations of the main flow have been intensively developing.

Of especial interest are those studies, where vortexes carried by some particles of special kind are considered against the main flow background, i.e. "vortexes-in-cells" [1–4]. Equations describing the evolution of vortexes (their motion, changes of the strength of vortexes) and the velocity field changes (vortex velocities) generated by them are introduced in addition to the principal hydrodynamics equations.

The paper presents the numerical simulation results for the evolution of hydrodynamic flow instabilities: Raleigh-Taylor, Kelvin-Helmholtz and Richtmyer-Meshkov instabilities. Computations were carried out by LEGAK [5] and MEDUZA [6] codes using the algorithm "vortex-in-cell".

The results obtained are in good agreement with the experimental data and the results of direct numerical simulation of unstable flows. The algorithm "vortex-in-cell" allows computations on a much more rough grid than that used for direct numerical simulation.

The algorithm "vortex-in-cell" has been implemented in LEGAK-MP complex [7] to be operated on a multiprocessor distributed-memory system. Data on the efficiency of parallelization of the algorithm "vortex-in-cell" is presented.

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EXPERIMENTAL AND NUMERICAL (MULTIPROCESSOR) STUDIES OF COATING STABILIZATION EFFECT ON THE BEHAVIOR OF SHEAR INSTABILITY IN METALS

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Experimental and numerical (multiprocessor) studies were carried out to understand the coating stabilization effect on the shear instability behavior under incident collision of metal plates [1]. Colliding plates and coating are made of AMZ aluminum alloy. The computations and experiments showed that increasing the coating thickness up to 0.03 mm actually ensures the shear instability stabilization at the interface of colliding plates.

The agreement between theoretical and experimental data is obtained. The computations used the methods from [2] in the multiprocessing mode [3].

The work was accomplished under the RBRF sponsorship (projects No. 02-01-00796, 03-01-06539).

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DISTRIBUTED OPERATING SYSTEM KERNEL DESIGN

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As it can be readily guessed from the title, our paper is devoted to development of an operating system.

Seemingly, why should we devise one more operating system, with having many of them, both commercial and “freely distributed”, developed? However, we believe that there is a reason for spending time and efforts to this kind of development. The

reason is that the well-known and available operating systems do not possess some characteristics (they will be mentioned somewhat later), which would allow us to simplify the development of applications for distributed systems and improve their reliability (the distributed systems are meant). Thus, what, in our opinion, is lacking in the modern operating systems, so that their employment in the matter of the computation arrangement on clusters be more convenient? In fact, these requirements are obvious, and we were not the first to devise them, but for some unknown reason the developers of the operating systems known to us never put forward them together (that is, all of them at a time).

First, this is the support of a tree of resources single for the whole operating system, that is of the structure that would allow some process executed at some system node to use any resource from a file or display to software channel opened by some other process on any system node by mere specification of the resource name. Something of this kind is absolutely necessary, if we want that the users could write applications independent on the node they are executed on and the resources employed by them for their work.

Second, this is the support of the resource protection mechanism, which would allow a fast and simple adjustment of the rights of the user access to the resources. Of course, when this requirement is imposed, there is no need to devise some basically new method for the access security (after all, as a few as two basically different methods are known to the mankind and, to all appearances, there are no other methods), but it is suggested that one should, so to say, cover one of the known methods in an envelope that would allow the method to be used in the context of large distributed systems, in which there may frequently be many administration centers.

Third, this is the support of orthogonal persistence mechanisms, that is all that would allow us to preserve the complete state of distributed application (that is the state of memory of all application processes, their machine contexts, states of files used by the processes, and, finally, states of the channels the processes communicate their messages through). The desire that the operating system support these mechanisms appears in the user immediately when his or her application, which might have been executed for twenty four hours, is suspended unexpectedly at the twenty third hour of its run because some bad man has occasionally pressed an inappropriate button «power» which disabled just the system node one of the application processes was executed on. If the operating system supported the above mechanisms, the user could save the state of his or her application, say, once an hour and would not have to run his or her application from the very beginning after the trouble, that is for the next twenty four hours, but would have only to restore the run from the last time of the state saving and wait only for a couple of hours.

Of course, these are not all requirements than can be imposed on the operating system (for the user's part, we as developers have requirements for the internal system arrangement, for example, it is desirable that it would be possible to debug OS kernel components at the user's level), but this is (we repeat once again) what has been implemented at a time in none of the operating systems known to us and what, we guess, should be present in any operating system designed to support distributed computations.

Presently we are designing the operating system kernel and developing the compiler. In what follows we will say what of the kernel parts have been designed and are ready for implementation, but first answer the question, which has arisen for sure: What is that you do not like in GNU C Compiler? Everything is quite simple – we were unable to gain an understanding of its source code when we were to make some

modifications to the compiler behavior that could not be introduced with options. And as we believe that one of the "internal" requirements is that any person educated enough in the relevant subject area could gain an understanding of the associated operating system component, we decided to write one more compiler from one more dialect of the C language.

But turn back to the operating system kernel. So, what of its subsystems was it possible to devise?

Of course, one of the first tasks was that to develop algorithms and data structures aimed at serving the matter of the processor distribution among different kernel and user tasks (so-called scheduling). We have devised nothing basically new here. In principle, everything is quite standard for the current phase of the operating system development (FIFO scheduling with account for priorities is used for the kernel tasks, scheduling by the «multiple level feedback» algorithm for the user's tasks), excluding, perhaps, the following. We restrict the number of processes that can be run by the user on a single module (processor + memory) to a relatively small number, at the moment this is 128. In our opinion, this restriction in no way harms the operating system ability to support distributed computations and allows the «mfb» algorithm to be modified so, that it becomes possible to distribute the processor among the user's tasks on a fairer basis (a feature of the classic «mfb» is that there is a possibility to create the process group, which can block by its operation that of other processes). As the maximum permissible number of processes operated on one module is small, this "addition" involves no significant computational costs.

Simultaneously with this we devised an interface which would allow the user's processes to interact with the kernel. Of course, we could take standard POSIX and, as one would say, not torment ourselves. However, POSIX in no way satisfies some of our requirements to the operating system, for example, the above-mentioned requirement formulated by us as follows: The developers must have an opportunity to debug the kernel modules at the application level. Moreover, when POSIX was being developed, there was no trace of the distributed systems, while shared-memory multiprocessor computers, which this standard is just aimed at, were employed in the main for the computations. Therefore we embarked on the development, so to say, of our own interface. The idea used as a basis for it is as follows. The application can employ any resource (except memory and central processing unit, which is to be operated through special system invocations) as an asynchronous message passing channel, whereas if the resource can do something more than merely accept some data (for example, like printer) or supply them (for example, like web-chamber), than it is suggested that the process should be given the opportunity to issue special instructions to the resource through another data passing channel designed for this.

Finally, what we are working at the moment is the memory control system, without which, apparently, no further work is possible. Presently we are developing an algorithm, which would allow us to find a free region of the size requested by the process (or of a larger size) for a minimum time [desirably for O(1)] in the virtual address space of the process. Naturally, the work on this search can be brought to the application level, however we believe that this algorithm can exert influence on the type of system invocations needed for the memory manipulation. It is for this reason that we decided to develop it first.

This is what I would like to speak about in more detail.

IRREGULAR POINT-BY-POINT PARALLELIZATION METHODS FOR SOLID MECHANICS APPLICATIONS AND IMPLEMENTATION WITHIN TREK++ PACKAGE

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Quality analysis of parallel programs for distributed-memory computer systems showed that a parallel program should demonstrate the following ensemble of features:

- Fine-grain parallelism;
- Interprocessor communications should be concurrent with processor computations;
- Special measures should be taken to balance the computational load over processors.

The cycle implementation would allow the computations interrupts for processor communications. This approach permits to redistribute the points arbitrary over processors and to compute an arbitrary set of points on a single processor.

The approach proposed here is implemented within 3D TREK++ program package. Currently, computational modules are developed within the package for gas dynamics applications including elastoplasticity and detonation.

The paper presents the performance measurement results for a benchmark. The test problem was scaled so that each processor computes 70*70*70=343000 points. The measurements showed that the parallel efficiency of a gas-dynamic problem was not lower than 0.58 for 70x70x70 cells and not lower than 0.7 for 140*140*140 cells in the range from 1 to 32 processors.

ASCI RED STORM AND SUPERCOMPUTER SCALABILITY

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ASCI Red Storm is a 40 TFLOPS supercomputer under construction for Sandia National Laboratories due to come online in about one year. This supercomputer is under construction by Cray, Inc. and comprises 10,368 AMD Opteron microprocessors on a custom 3D mesh interconnect.

ASCI Red Storm supercomputer was strongly influenced by Sandia's ASCI Red supercomputer. The 9,960 processor ASCI Red demonstrated excellent scalability on key engineering applications with this scalability attributed largely to the balanced interconnect. More specifically, the time ASCI Red required to perform a floating point operation balanced (or was about the same as) the time required to send a floating point number across the network to another processor. The Red Storm supercomputer preserves this balance while being substantially faster.

This talk will elaborate on the scalability principles for this class of supercomputer. Amdahl's Law relating speedup to the amount of serial and parallelizable code was the limiting factor for many years, but has been successfully

addressed in modern supercomputers and codes which achieve ~10,000 way scalability. Two of the principles are:

1. Dividing a problem over 10,000 processors inevitably reduces the problem size on each processor reducing the "area to volume" ratio. This effect can be countered by a high bandwidth, low latency communications network, like in ASCI Red and ASCI Red Storm.

2. As work is distributed over more nodes, the amount of work on each node decreases proportionately. However, the "law of large numbers" is no longer able to smooth out timing instabilities and efficiency can decline. These timing instabilities may be due to hardware (unpredictable cache and TLB hits versus misses) or in the application (the physics in one node is more complex than the physics in another node). To counter this effect requires consistent effort towards stabilizing timing. Red Storm addresses these issues through a Light Weight Kernel (instead of a full operating system) and through the natural properties of the 3D mesh.

In Sandia's view, this leads to an additional term in Amdahl's Law for the speedup of an application $S_{Amdahl}(n)$:

$$S(N) \sim S_{Amdahl}(N)/[1 + f_{comm} \times R_{p/c}]$$

Where S(N) is Sandia's expectation of speedup on N processors, f_{comm} is the fraction of work devoted to communications and $R_{p/c}$ is the ratio of processor speed to communications speed.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy`s National Nuclear Security Administration under contract DE-AC04-94AL85000.

NON-UNIQUENESS OF RAREFACTION SHOCK WAVES: EFFECTS OF VISCOSITY, DISPERSION AND INTERPHASE KINETICS

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The paper examines self-similar solutions for Riemann-type problems for materials with non-convex strictly monotonous equation-of-state where unloading produces rarefaction shock waves. We considered only the case for the barotropic equation-of-state where the pressure is governed by the density only; for simplicity, we chose a single non-convexity fragment. Continuous self-similar rarefaction waves are assumed to be attached to from either side.

The rarefaction wave data available from literature relies upon the assumption that any discontinuous solutions of gas-dynamic equations should be derived from smooth viscous gas-dynamic equations through the limit transition to infinitesimal viscosity coefficient. This is called 'disappearing viscosity method'. For example, reference [1] used the disappearing viscosity method for self-similar problems to prove that a fragment of Raleigh-Michelson straight line connecting the gas parameters (p_1,v_1) and $(p_2,v_2$ on either side of the rarefaction wave on (P,V) plane should touch the adiabat $p=P(v)$ at its extremes (here $v=1/\rho$, $p_1>p_2$, $v_1<v_2$).

Non-convex equations-of-state generally occur in equilibrium process descriptions. We are not aware of sound physical rational indicating that viscosity is the dominating governing process in the vicinity of the phase transition. Instead, arguments can be evoked for the heterogeneous mixture of two phases in favor of

more important dispersion role. Moreover we should not neglect the effect of the phase transition on the rarefaction wave structures.

To smear rarefaction waves, the disappearing viscosity method uses the equation of speed written as $u_t+p_m=(\mu v_{mm})_m$ in Lagrangian variables with positive dispersion coefficient $\mu=const\to+0$. The rarefaction wave $(p_1,v_1)\to(p_2,v_2$, allowed by the disappearing viscosity method in the self-similar solution of the Riemann problem is proved to be determined by the following conditions: the fragment of Raleigh-Michelson straight should touch the adiabat $p=P(v)$ at (p_1,v_1) and pass trough this adiabat without touching at two points (at the interim point (p_3,v_3) and at the point (p_2,v_2))so that the surface areas of two curvilinear triangles are identical. The rarefaction wave obtained with the disappearing normal dispersion method always differs from that obtained with the disappearing viscosity method. Even the velocities of those rarefaction waves differ.

To smear rarefaction waves, we can use artificial interphase kinetics instead of viscosity and dispersion. The material is assumed to be composed of two phases with convex equations-of-state $v=V_1(p)$ and $v=V_2(p)$ for a pure phase, the equilibrium equation-of-state $V(p)=\Theta_0(p)\cdot V_1(p)+(1-\Theta_0(p))\cdot V_2(p)$ is strictly monotonous but has one non-empty non-convexity interval where $\Theta_0(p)$ is a strictly monotonous equilibrium concentration of the first phase. The method of artificial interphase kinetics like /2/ describes the material by the non-equilibrium equation-of-state $v=V(p,\Theta)\equiv\Theta\cdot V_1(p)+(1-\Theta)\cdot V_2(p)$ and the concentration $\Theta(t,m)$ of the first phase is given by the equation of interphase kinetics $\tau\,\Theta_t\,(\Theta-\Theta_0(p))\,(\Theta,p)$ with positive phase relaxation time $\tau\to+0$. It is proved that if the equations-of-state for two pure phases $v=V_1(p)$ and $v=V_2(p)$ do not overlap then rarefaction waves obtained with the artificial interphase kinetics do not match those obtained with the disappearing viscosity for the equilibrium equation-of-state.

Instead, if equations-of-state for two pure phases $v=V_1(p)$ and $v=V_2(p)$ do overlap at the unique point (p_3,v_3), $p_1>p_3>p_2$) in the artificial interphase kinetics method the system would have a different solution: the fragment of Relaigh straight line of the rarefaction wave $(p_1,v_1)\to(p_2,v_2)$ passes through the overlapping point of pure phase equations-of-state and the fragment of Relaigh straight line is tangent to (from below) the equilibrium equation-of-state at the extreme point (p_1,v_1) with a higher pressure. In this case the rarefaction waves obtained with the artificial interphase kinetics method greatly differ from those obtained with both disappearing viscosity and disappearing dispersion.

This proves that accounting various physical processes occurring inside the smeared rarefaction wave results in different rarefaction wave parameters. It is confirmed by 1D gas-dynamic calculations using difference schemes with controlled dissipation and dispersion.

Therefore the non-uniqueness of the rarefaction waves should be solved by answering the question what physical processes ignored by perfect gas dynamics equations dominate in the phase transition region in smeared rarefaction waves for a specific material. The numerical scheme for gas-dynamic calculation must be chosen regarding the answer to this question.

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LAN MONITORING SYSTEM

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The LAN monitoring system is designed for acquisition and storage of information about the state of different LAN components, for example, about servers, active network equipment, etc. as well as for the following analysis of acquired information, acquisition of different statistical information about the network performance and detection of hardware and software failures in real time.

The system is a program complex composed of several logically complete components. The monitoring system components interact on the client-server principle: one singled-out component is the center of the information acquisition and storage and all others communicate with it. To store information, the system uses DB. It stores logical names of all controlled values and the history of their modifications as well as other service information.

The following components have been implemented:

– monitoring system supervisor;
– library for DB manipulation;
– library for manipulation of the data passing protocol for OS Windows;
– library for manipulation of the data passing protocol for OS Linux;
– module for manipulation of protocol ICMP;
– module for manipulation of protocol SNMP;
– module for e-mailing messages;
– module for checking services that employ the text communication protocol (FTP, HTTP, etc.);
– module for acquisition of information about the state of servers and workstations under supervision of WINDOWS NT/2000XP;
– module for acquisition of information about the use of server resources for environment Linux;
– module for mapping the topological network scheme.

ACQUISITION AND PROCESSING OF STATISTICAL INFORMATION ABOUT COMPUTATIONS ON DISTRIBUTED COMPUTER COMPLEX UNDER SUPERVISION OF WINDOWS

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The acquisition and processing of statistical information about task computations allows us to save and, then, analyze different statistical information about the task computation run both on personal computers and clusters operated under the supervision of operating system WINDOWS. The computation data analyzed

includes: processor time, main memory amount, task number, task executor, and many other parameters. The statistical information is acquired both from uniprocessor and multiprocessor tasks developed using program package MPICH.

A program complex composed of a number of components responsible for different functions in the information acquisition has been developed. The components interact on the client-server principle: one separated component is the center of the information acquisition and storage and all the others communicate with it. The system uses DB to store information.

The following components have been implemented:

– information acquisition server;
– code for information acquisition from tasks computed on personal computers;
– code for acquisition of information about multiprocessor task computation;
– code for information acquisition from tasks computed on a cluster;
– server processing requests for the cluster computation;
– monitoring code to supervise and control the task computation on the cluster in real time;
– client code allowing the cluster run both of uniprocessor and multiprocessor tasks;
– some others.

INTERFACE OF PROGRAM COMPLEXES AT ITMF DIVISION OF MATHEMATICS

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Efforts on development and improvement of a number of code complexes for solving computational physics problems are in progress at ITMF's Mathematics Division. Operation of all code complexes is based on a dialog with the user who specifies the job, controls the computation process and analyses the results. It is known that the interface part of any code complex for numerical simulation may total 50-60% of the code as a whole and requires significant labor input to develop and maintain it.

Efforts on developing codes for a unified interface for computational complexes operated at ITMF are aimed at lowering the labor costs required to develop and improve the code complexes, improving the technological effectiveness of computations and their result analysis.

Unification of data storage methods, i.e. creation of unified data structures and formats, is an important stage of such code development efforts. Development of codes common for several different complexes is possible basing on the adopted method for storing data.

The following information processes take place, when a typical computation within the institute's research area is carried out:

- specification of a job for computations;
- accumulation of results during computations;
- use of common libraries during computations;

- visualization of computation results, both intermediate and final;
- representation of time dependences and integral values;
- comparison between the results of computations by various codes, or for various problems;
- result recording, archiving and storing.

The paper describes the codes and libraries developed within the unified interface of computational complexes. Initial data specification codes and codes for processing and viewing the results of computations are in focus.

To conclude, the paper considers a number of issues concerning introduction and operation of codes comprising the unified interface.

THE CONCEPT OF DESIGNING A UNIFIED JOB CONTROL SYSTEM OF THE NON-UNIFORM COMPUTER SYSTEM AT ITMF

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Job control is one of the important attributes of computational systems. Intensive development of the ITMF Computer Center equipped with high-performance multi-processor clusters having various platforms (OS, job control languages, job managers) generates the problems of rational and quick execution of production computations. So, the development and implementation in codes of the specialized software – the unified job control system (UJCS) – is an urgent task.

UJCS should provide

– the centralized scheduling and control of job computations;
– allocation and control of resources necessary for execution of jobs;
– job monitoring;
– storage and processing of statistical data, both on jobs and computational resources of the non-uniform computer system (NUCS) as a whole;
– protection against unauthorized access;
– user authorization.

UJCS should include:

– a subsystem for centralized performance of job input and log-in operations;
– a subsystem for generating a central queue of jobs (job scheduler);
– a planning-and-budgetary subsystem;
– a transport system providing communications between the control and executive servers;
– a manager of resources of computer clusters.

The job control system presented is designed basing on Web-technology that provides starting the jobs interactively, viewing their status, statistical data and the results obtained. The use of the job control system has to increase the efficiency of computer systems in use, significantly facilitate and automate the computation processes in the computational environment of the ITMF's non-uniform computer system.

COMBINATION OF MOVING AND FIXED GRIDS (MIXED GRIDS) USED FOR 2D CALCULATIONS IN GAS DYNAMICS

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The calculations in gas dynamics can use moving or fixed regular grids. Clearly, many applications are not tailored to pure lagrangian or Eulerian scheme while a combination of Eulerian and Lagrangian variable approximation may turn to be appropriate. The practices show that the computational domain can be split into subdomains in most applications so that each subdomain is best fitted by the moving or fixed grid for large time intervals. The idea to use combined Eulerian-Lagrangian approximations was proposed by V. Nokh in 1964 [1]. RAMZAS-KP [2] uses orthogonal regular rectangular moving and fixed Eulerian grids. We call the computations on these grids 'combined-grid computations'.

The interaction algorithms for the moving and fixed portions were studied and validated by calculating light gas implosion by a heavy shell. The shell was approximated with the moving spherical Eulerian-Lagrangian grid while a fixed rectangular cylindrical Eulerian grid was applied to the inner gas portion. Some cells of the inner rectangular Eulerian fragment are not involved in the computations being fictitious. We call boundary cells those containing the interface between the fragments while the remaining cells will be referred to as computational. As the interface moves the computational cells can convert to boundary ones, the boundary cells becoming non-computational and vice versa. All these changes are tracked at each timestep.

Several algorithm versions were proposed and implemented for the interaction of the grid fragments. The ways were examined to improve the computational accuracy on mixed grids.

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'KONTUR M' ALGORITHM FOR FINDINGAND VISUALIZATION OF3D OBJECT CROSS SECTIONS

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In recent years, methods and technologies are rapidly evolving for 3D modeling which results from a considerable growth of computer performance allowing more rapid and accurate calculations of complex 3D geometry applications.

3D geometry is specified in various ways determined by the class of applications to be computed such as theoretically multiplex, functionally topological or primitive-

set-based. RFNC–VNIITF uses a variety of techniques. The algorithm proposed here is applied to physical objects whose surface is defined through theoretically multiplex operations and with pseudo 3D methods. The geometry description looks like an ensemble of analytical object description strings.

More precisely, consider two specific numerical simulation fields requiring 3D geometries to be adequately specified and analyzed:

1. 3D geometry specification for Monte Carlo simulation.
2. 3D geometry specification and subsequent difference grid generation in numerical 3D simulation difference schemes.

3D geometry specification is known to take a considerable portion as compared to the entire simulation time. The model can actually consist of hundreds or thousands objects. If no adequate visualization exists for the 3D geometry specification and correctness check this task turns to be highly complicated. The integrity and correctness of 3D geometry specification are verified through mathematical methods, however they are insufficient. The major development goal of these algorithms is to allow the following:

1. 3D geometry specification.
2. Analysis of the specified 3D geometry.
3. 3D geometry editing.
4. Computational data analysis within the specified 3D geometry.

The basic subtasks include:

1. Location and visualization of profiles and cross section interiorities.
2. Location and 3D visualization of object surfaces.
3. Cross section visualization combined with that for a part of a 3D object.

This paper presents the numerical 'KONTUR M' algorithm for finding and visualization of cross sections for analytically specified 3D objects by generating a special adaptive 2D grid and grid isolines. This research pursues the paper that reported KONTUR and ASL algorithm at the 'Graphicon 2002' conference in 2002/*/. The algorithms restrictions are considered. The algorithm is implemented within the visual system. The algorithm results are illustrated by analytically specifying 3D geometries.

*Mogilenskikh D.V. *'KONTUR' algorithm for finding and visualization of plane cross sections for 3D objects // Proceedigs of the 12-th International Computer Graphics and Computer Vision Conference 'Graphicon 2002', Nizhny Novgorod September 16-21, 2002, P. 230-238.*

PRIMARY MICROLEVEL MATERIAL DAMAGE CALCULATIONS WITH MOLECULAR DYNAMICS METHOD

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The progress in advanced technologies, the improvement of existing power systems and designing fusion devices require that structural materials run through their life cycles under various environments including the exposure to fast particles. The particles produced by the accelerators, fission and fusion reactors interact with exposed materials and structural elements, knock out atoms thus changing the structure of used materials.

Radiative material damage capability covers a wide range of physical processes including elastic and inelastic interactions of bombarding emitted particles with solid atoms, cascades of atomic collisions, atomic diffusion, defect structure evolution resulting in changing macroscopic properties of exposed materials.

Unfortunately, dangerous changes caused by radiation leading to material damage still represent non-finalized problem. This is due to the complexity of physical processes occurring in materials where rigid rays penetrate.

Given the results of [1–2], the general pattern of radiative material damage is as follows.

High-energy particles interacting with material shift the atoms from the nodes of crystal lattice partially transmitting their energy. If this energy exceeds the threslold energy E of atomic shift from the equilibrium state the atom is knocked out from the lattice node. Those atoms are called 'primary knocked out atoms'. Further collisions of primary knocked out atoms with other lattice atoms produce secondary particles generating, in turn, tertiary particles etc. This results in a cascade of moving atoms. The region of exposed solid where the cascade passed forms a great number (up to several thousands) of Frenckel pairs (vacancies and interstitial atoms) and locally heats the material. Cascade motion around the collision sites of high-energy particles and material atoms forms a structurally complex region composed of depletion and enrichment zones. All together they produce the so-called primary material damage.

This paper describes the improvement of parallel gas dynamics code capabilities [3] for energy dispersion calculation of high-energy particles. The problem setup is given along with the particle interaction potentials. Computer simulation results are reviewed for the primary radiative damage of metals. In particular, pressure and temperature fields are given for various times obtained by averaging microscopic theoretical characteristics over the ensemble of particles.

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DSn METHOD FOR ARTIFICIAL DISSIPATION AND VDM METHOD FOR ITERATION SPEEDUP IN NUMERICAL CALCULATION OF 2D HEAT TRANSFER EQUATION IN A KINETIC MODEL

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FENIX program package [1] is designed for numerical simulation in complex geometry and high-strain solid mechanics and kinetics applications. FENIX energy

transport simulation runs in radiant heat conduction, multigroup P_1, quasidiffusion and kinetic approximations.

The numerical method for the calculation of the transport equation in kinetic approximation is based on $DDAD$ scheme proposed for neutron transport calculations [2]. $DDAD$ scheme is a modified version of DS_n method increasing the method efficiency in optically thick environments while retaining the second accuracy order over spatial coordinates. To speed up the iteration convergence over the transport equation non-linearity, diagonal matrix selection method (VDM) is implemented. A similar method in 1D plane case was proposed in [3]. This method was used n 2D case for DDAD scheme. The program implements domain calculations, the calculations involving iteration-initiated exchange of boundary conditions, parallel computations over energy groups and photon flight directions like in neutron transport calculations from [4].

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ARTIFICIAL DISSIPATION METHOD OF DISCRETE ORDINATES (DADD SCHEME) FOR NUMERICAL CALCULATIONS OF NEUTRON TRANSPORT EQUATION

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DS_n scheme is one of the crucial methods for the transport equation calculation [1]. Second order accurate DS_n scheme (DD-•••••) is known to yield the oscillating solution in optically thick media [2]. This defect is caused by the linear interpolation of αN expression used in describing used in DD scheme to describe

the absorption of particles in the transport equation. This approximation generates, in first approximation, an anti-dissipation additive of the form $-\frac{\alpha}{8}h^2\frac{\partial^2 N}{\partial x^2}$.

Reed [2] recommends to apply a three-point scheme in optically thick media $(\alpha h \geq 2)$ and a two-point DD scheme for $\alpha h < 2$. The three-point scheme does not include αN interpolation as DD scheme does thus preventing the generation of anti-dissipation additive mentioned above. However the combined scheme is difficult for numerical implementation. Our paper offers another approach: remove the antidissipation by subtracting it from the residual term while remaining within the two-point DS_n scheme. This is achieved through specially selected artificial dissipation. The new method retains the second order accuracy. The resulting method was called $DDAD$ scheme (*Diamond Difference with Artificial Dissipation*).

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COMPUTATIONAL METHODS FOR SPATIALLY NON-UNIFORM PHYSICAL KINETICS APPLICATIONS CONSERVATION LAW SYSTEMS

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The paper considers kinetic physics computer models exemplified by cluster generation in spatially uniform and non-uniform geometry applications for Smolukhovsky equations. The computational structure is shown for the applications requiring parallel computing systems to achieve the desired accuracy of physical interpretation. We describe the classes of functionals transferred between the parallel computers, the Monte Carlo process is proved to statistically converge to the exact solution.

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COMPUTER SIMULATIONS IN COAGULATION KINETICS

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Smoluchowski equation

The direct numerical simulations in the coagulation kinetics that can be described with Smoluchowski equation are addressed. The convergence of the Monte Carlo simulation to the exact solution is justified within the computational experiment. Issues of optimal partition of the mass variable domain and functional forms in parallel computations are considered.

The evolution of physical systems composed of a statistically large amount of elements colliding during their motion is modeled with *Bolzmann type spatially heterogeneous equation* [1]

$$\frac{\partial u^{(\omega)}(z,t)}{\partial t} + div_z\left(v^{(\omega)}u^{(\omega)}(z,t)\right) = S^{(\omega)}\left(u^{(\cdot)}(z,t)\right) \tag{1}$$

$$\omega \in \Omega, \quad t \in R_1^+, \quad z \in R_n,$$

where function u to be found describes the physical system states at each time $t \geq 0$ at points with spatial coordinates $z = (z_1, z_2, \ldots, z_n)$ and parameter set $\{\omega\} = \Omega$ describes possible states of the physical system elements. $v^{(\omega)}$ is the *free transport velocity*.

In 1916, when studying the coagulating particle evolution in electrolytes, M.Smoluchowski, an outstanding Polish physicist, wrote the kinetic equation of coagulation for the function of particle distribution by mass. The direct simulations are analyzed in refs. [2, 3, 4]. The model proved efficient in simulations of the defect development in power reactor materials [2] and phase transitions in the problem of nuclear reactor layoff-resumption [3].

For the kinetic coagulation theory models of form (1), where phase space $\Omega \in R_1^+$ is nonnegative real numbers (particle masses), the Smoluchowski equation is written as

$$\frac{\partial u(t)}{\partial t} = \frac{1}{2}\int_0^{\omega} \Phi(\omega - \omega', \omega') u^{(\omega-\omega')} u^{(\omega')} d\omega' - u^{(\omega)} \int_0^{\infty} \Phi(\omega, \omega') u^{(\omega')} d\omega' \cdot \tag{2}$$

The rate (kernel) Φ of particle collisions is considered as a known function that is subject to the conditions $\Phi(\omega, \omega') = \Phi(\omega', \omega) \geq 0$ with $\omega, \omega' \in R_1^+$. The Smoluchowski equation looks similarly in the particle coagulation theory with discrete masses

$$\frac{\partial u(t)}{\partial t} = \frac{1}{2}\sum_{\omega'=1}^{\omega-1} \Phi(\omega - \omega', \omega') u^{(\omega-\omega')} u^{(\omega')} - u^{(\omega)} \sum_{\omega'=1}^{\infty} \Phi(\omega, \omega') u^{(\omega')}, \ \omega \in \Omega = N \cdot \tag{3}$$

In addition to the results for the spatially homogeneous case, of interest are a number of issues requiring a significant further development. This is primarily true for the issues of the mathematical justification of the Smoluchowski equation, relation between the solutions to Cauchy problems and actual coagulation processes, including the exact physical meaning of the solution to equation (2). A significant advance has been already made on this way. Adjacent to the aforementioned fundamental problem are the challenges of the direct Monte Carlo simulations of the coagulation processes. Smoluchowski equation (2) is written reasoning from the considerations of collisions similar to those in the derivation of Bolzmann equation of the kinetic gas theory. However, there are models based on A.A.Vlasov's ideas for the plasma theory that lead to other kinetic equation forms. Hence, of undoubtful interest is the study of spatially homogeneous coagulation models in the framework of Vlasov's approach in the continuous particle growth model.

Direct simulation of coagulation

Consider a model that describes the coagulation process at the level of system particle interaction (merging). Let there be N particles in the system, with the particles being numbered with real numbers from 1 to N. Each of the particles has mass $x_i \geq 0$. At time t the system state is given with vector $(x_1(t), x_2(t), \ldots, x_N(t))$. Determine the state at time $t + \tau$. Assume that no more than one particle pair interacts for time $\tau > 0$ in the system. Detemine this pair in random manner assuming that the probability of selection of each particle pair is the same. The particle pair is selected as a current state of the Markovian chain in an appropriate matrix space. The selected particles numbered i and j coagulate with probability P. The probability P relates to

kernel $\Phi(x, y)$ appearing in Smoluchowski equation (2), number N of particles, and step τ as follows:

$$P = \tau(N) N \Phi(x_i, x_j), \quad P \le 1$$

Note that this expression sets the limitation on the timestep. After the expiration of time τ, the system state is determined with vector

$$(x_1(t+\tau),..., x_N(t+\tau)) = \begin{cases} (x_1(t), x_2(t),..., x_{i-1}(t), x_i(t) + x_j(t), x_{i+1}(t),..., x_{j-1}(t), 0, x_{j+1}(t),..., x_N(t)), \\ (x_1(t),..., x_N(t)), \end{cases}$$

where the first vector value is taken on with probability P and the second with probability $(1-P)$.

An important justification of this model is the following theorem.

Theorem. Let the initial vector of states $x(t)$ of the coagulating system be composed of statistically independent random masses $x_i(t),\ 1 \le i \le N$. Let the relative number of particles of mass i with $t = 0$ satisfy the following expression:

$$\frac{N_i(0)}{N} = \frac{1}{N} \sum_{\substack{l=1 \\ x_l(t)=i}}^{N} 1 \to u^{(i)}(0),$$

where $u^{(i)}(0)$ are the initial data of the Cauchy problem.

Then with probability 1

$$\frac{N_i(t)}{N} = \frac{1}{N} \sum_{\substack{l=1 \\ x_l(t)=i}}^{N} 1 \xrightarrow[N \to \infty]{} u^{(i)}(t), \quad t \ge 0,$$

where $u^{(i)}(t)$ is the solution to the Smoluchowski equation.

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FEATURES OF 2D MHD APPROACH IMPLEMENTATION ON ADAPTIVE GRIDS

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A code designed for 2D simulations of magnetogasdynamic flows with using an adaptive grid is discussed. The algorithms embedded in the code are written for an arbitrary movable coordinate system. This allows calculation of flow with severe strains inside the flow region, with the boundaries varying weakly, which enables setting magnetic field conditions on them. The numerical simulations show that the schemes are fairly accurate and cost-efficient. Examples of the calculations are given which demonstrate the algorithm features.

FEM CALCULATION OF MULTILAYERED COMPOSITE SHELLS WITH ACCOUNT FOR GEOMETRICAL AND PHYSICAL NONLINEARITY

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A FEM-base algorithm for nonlinear static calculation of multilayered shells of small and medium thickness with different loading types is presented. The computational model involves a quadratic isoparametric nine-node finite element (FE) of an arbitrary-geometry shell with five degrees of freedom in each node constructed using the method of double deformation approximation by super-convergence points.

The physically and geometrically nonlinear deformation is studied with the step method within "modernized Lagrangian set-up". For layered shells from composite materials relations have been constructed to calculate stiffness and geometric stiffness matrices in the analytical integration over thickness [1]. The transversal shear stiffness matrix modification with independent estimation of the transversal shear stresses in the form of quadratic parabolas within each layer that vary continuously through package thickness [2] is used. The linear variation in the geometry and displacements over thickness is assumed.

To include the physical non-linearity, the principal concepts of the plastic flow theory, ideally elastic-plastic body model are employed. The elastic and plastic deformation zones are segregated using the Hill plasticity criterion for orthotropic material written with account for the squeezing stress smallness.

In view of the fact that the relationships between the stress and strain increments are determined independently for each layer and differ from layer to layer because of different mechanical characteristics in each layer, we can write

$$\begin{aligned} \{\Delta\sigma'_k\} &= [A_k]\{\varepsilon'\} + [C_k]\{\gamma'\} \\ \{\Delta\tau'_k\} &= [C_k]^T\{\varepsilon'\} + [B_k]\{\gamma'\} \end{aligned} \qquad (1)$$

where $\{\varepsilon'\}^T = \{\varepsilon'_{11}, \varepsilon'_{22}, \varepsilon'_{12}\}$, $\{\gamma'\}^T = \{\gamma'_{13}, \gamma'_{23}\}$ are the Green strain increment tensor components, $\{\Delta\sigma'\}^T = \{\Delta\sigma'_{11}, \Delta\sigma'_{22}, \Delta\sigma'_{12}\}$, $\{\Delta\tau'\}^T = \{\Delta\sigma'_{13}, \Delta\sigma'_{23}\}$ are the Payola-Kirchhoff stress increment tensor

components oriented relative to the local Cartesian coordinate system with unit vectors $\vec{p}_i$ $(i = 1,2,3)$. The coordinate system is introduced at each quadrature point of the element so, that unit vector $\vec{p}_3$ is directed perpendicularly to the shell surface. $[A_k]$, $[C_k]$, $[B_k]$ are blocks of the matrix of elastic-plastic constants

$$[D'^{(ep)}_k(\varsigma)] = [D'^{(ep)}_{k,1}] \cdot N_1(\varsigma) + [D'^{(ep)}_{k,2}] \cdot N_2(\varsigma) + [D'^{(ep)}_{k,3}] \cdot N_3(\varsigma). \qquad (2)$$

Here $[D'^{(ep)}_{k,1}], [D'^{(ep)}_{k,2}], [D'^{(ep)}_{k,3}]$ are the elastic-plastic constant matrices calculated for the *k*-th layer at three points, whose elements depend on the stressed-strained state at the points at the current loading step, N_1, N_2, N_3 are quadratic polynomials. Matrix $[D'^{(ep)}]$ results from turning matrix

$$[D^{(ep)}] = [D^{(e)}] - \frac{[D^{(e)}]\{\partial\Phi(\sigma)/\partial\sigma\}\{\partial\Phi(\sigma)/\partial\sigma\}^T[D^{(e)}]}{\{\partial\Phi/\partial\sigma\}^T[D^{(e)}]\{\partial\Phi/\partial\sigma\}}, \qquad (3)$$

written in the orthotropy axes. To improve the accuracy, an iterative procedure of the initial stress method type is employed at the loading step.

Examples of solved test problems are given.

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THE UPDATED MODEL OF EOS "ROSA" AND ITS SIMPLIFIED VERSION

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The paper presents ROSA-M model to be used in semi-empirical equations of states (EOS) of metals that is a modification to the model currently used in ROSA type equations of state. The given modification objective is to extend the model applicability to include high temperatures and high pressures.

The model applicability has been extended by introduction of the temperature dependence of electron Grueneisen coefficients and by using the potential components in a range of high pressures of TFPK model. Besides, the new functional dependences of Grueneisen coefficients of electrons and nuclei on the zero-temperature densities have been proposed in the updated model in order to reduce the number of parameters and simplify the procedure of fitting them.

A simplified version of the model that uses a more simple functional dependence of Grueneisen coefficient of nuclei on the zero-temperature densities at has been also presented. The Grueneisen coefficient of electrons is taken constant and independent

on density and temperature. This model version is less applicable than the updated model of EOS ROSA, however, it has a considerably less number of parameters and, thereby, simplifies the procedure of fitting them.

The equations of state for aluminum have been developed using both models. The results of computations using the state equations developed are compared with each other and with the available data of experiments.

USING NEUROFUZZY TECHNOLOGIES TO PREDICT FINANCIAL INFORMATION

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Using the up-to-date economical-mathematical methods to predict the equity market behaviors is a promising direction in the financial analysis. This problem is solved using conventional approaches, such as fundamental market factor analysis, classic technical analysis, regressive and correlative analysis. However, all these methods are general, possess no flexible system of adjustment to a specific market, to a specific equity. This paper suggests an approach, where the method of technical analysis is employed for the analysis rules and a neuron network based on the fuzzy logic principles for the computational method. This allowed us to develop a self-learning system for a problem which is hard to formalize.

A set of rules known as Elder's mechanical trade system has been used as a basis for the fuzzy neutron network. The following production rules are used to predict the equity behavior:

IF the moving mean constructed from the price list increases and the force indicator of the market participants speculating for a price fall is below zero, THEN this is an evidence of potential price increase.

IF the moving mean constructed from the price list decreases and the force indicator of the market participants speculating for the price advance is above zero, THEN this is an evidence of potential price decrease.

To represent these rules, fuzzy sets L_1, L_2, H_1, H_2, G, P with sigmoid type membership functions $f(x) = \frac{1}{1+\exp^{-b(x-c)}}$ are constructed that describe the notions of the moving mean increase (decrease), position of the speculators' force indicator above (below) zero. The membership function form has been selected with account for the specificity of the mechanical trade system used, besides, this function form is differentiable over the entire abscissa axis and the possibility to change coefficients b and c during the neuron network learning allows the fuzzy sets to be described more accurately.

The neuron network is composed of five strata:

Stratum 1: the stratum neutron outputs determine the membership function values for the network input data: x_1 is the moving mean value, x_2 is the force indicator of the market participants speculating for the price fall, x_3 is the force indicator of the market participants speculating for the price advance;

Stratum 2: its outputs determine the precondition truth degree of each rule α_i in the system knowledgebase, the stratum neurons can implement the t-norm to model the logic "AND" operation, $\alpha_1 = L_1(x_1) \wedge L_2(x_2)$, $\alpha_2 = H_1(x_1) \wedge H_2(x_3)$;

Stratum 3: the stratum neurons normalize the precondition truth degrees for each rule

$$\beta_1 = \frac{\alpha_1}{\alpha_1 + \alpha_2 + \alpha_3},\ \beta_2 = \frac{\alpha_2}{\alpha_1 + \alpha_2 + \alpha_3},\ \beta_3 = \frac{\alpha_3}{\alpha_1 + \alpha_2 + \alpha_3};$$

Stratum 4: the stratum neurons determine the partial outputs of the conditional part of the rules

$$z_1 = G^{-1}(\alpha_1) = c_5 - \frac{1}{b_5}\ln\frac{1-\alpha_1}{\alpha_1},\quad z_2 = P^{-1}(\alpha_2) = c_5 + \frac{1}{b_5}\ln\frac{1-\alpha_2}{\alpha_2};$$

Stratum 5: the only neuron determines the network output in accordance with the centroid method

$$z_0 = \frac{\alpha_1 z_1 + \alpha_2 z_2}{\alpha_1 + \alpha_2}.$$

The system parameters for the membership functions are corrected using the gradient method. The reasonable error function is the mean-square deviation of form $E_k = \frac{1}{2}(z_0{}^k - y^k)^2$.

The suggested approach has been implemented as a program in environment Delphi 5. The analysis of the code results infers the following:

the prediction quality depends on the price list form;

the prediction quality becomes higher significantly when the indicator parameters are corrected;

the neuron network learning rate depends on the learning norm and reasonable error;

when the price variations are slight, the learning should be performed at a certain step, so that there would be possible to take into account a greater variety of data.

The system constructed provides an adequate prediction in about 65% cases under the condition of the neuron network parameter pre-adjustment.

STREAMLINE VISUALIZATION AND METHODS FOR COMPLEX VISUALIZATION OF DISCRETE VECTOR FIELDS

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The paper describes methods for post-processing and visualization of results of 2D numerical simulations of continuum mechanics problems with difference methods, in particular, the methods for processing and visualization of vector fields.

The description is made by the example of the simulation methods using 2D regular difference grids.

Contents of the paper:

1. Numerical algorithm for determination of streamlines (SL) – post-processing of accumulated results and acquisition of further information. The vector field SL are found using a 2D analog of Fong's algorithm employed in ref. [1]. The algorithm is represented by steps:

Step 1 (Initialization of SL). Initialization of the basic point (BP) on the domain of definition of the vector field.

Step 2 (Localization of BP). Determination of BP cell membership.

Step 3 (Fong's interpolation). SL are found using bilinear interpolation approaches [1].

Step 4 (Construction of SL):

- Method for empirically setting the length of unit displacement of SL from BP along vector.
- Method based on a single linear interpolation along the cell edge.

Additions and comments on the algorithm have been considered:

- SL construction stop.
- Intersection of SL with each other.
- SL numerical construction accuracy.
- SL construction in the opposite direction.
- Collision of the streams, uncertainty.

2. SL visualization functions – graphic representation methods.
3. Methods of complex visualization to enhance information yield – using SL visualization functions simultaneously with other visualization functions.

The paper presents several methods for the vector field SL pseudo-dynamics animation.

The algorithm has been implemented in the system of scientific visualization of 2D numerical simulation results and experiments VIZI2D [2]. The paper is illustrated.

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3D NUMERICAL CALCULATIONS OF IMPURITY TRANSPORT BY GROUNDWATER

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The paper considers 3D groundwater migration applications and propagation of soluble impurities produced by typical local sources through groundwater.

The model equation includes filtering equations for saturated-unsaturated porous medium and mass transport equations. The general problem naturally divides into two subproblems. The first – filtering problem is to find the time-dependent velocity field

of the bearing flow. The second- mass transfer problem – determines the impurity motion dynamics regarding the resulting velocity field.

A unique irregular grid is generated composed of parallelepipeds with an oblique quadrangle at the base to calculate the problem numerically.

The discretization of differential equations uses the finite-difference method. The filtering equation is approximated by implicit operator method where the difference analog of grad operator relates to the grid nodes and the conjugate div operator is defined in the centers of the grid cells. The equation for water-soluble impurities is numerically solved using the process-splitting method. The entire process splits into four steps: impurity transport calculation, diffusion calculation including dispersion, sorption consideration, accounting chemical reactions in the vapor volume and at the fluid-matrix interface. The transport equation is solved both with the method of characteristics and the difference methods – FCT method and third order accurate TVD method. The diffusion and dispersion are calculated with an implicit method similar to that for the filtering equation. Sorption and chemistry kinetics are determined with implicit and explicit difference schemes.

The method is implemented in C++.

The paper presents the results of test and methodical computations for some problems.

The work was accomplished under the ISTC Project # 1565.

NUMERICAL SIMULATION OF RADIATION TRANSPORT AND ITS INTERACTION WITH A SUBSTANCE

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Radiation transport by photons and its interaction with a substance is one of the governing processes during simulations of many physical problems.

The paper describes various approximations used when numerically simulating the processes above, discusses the difficulties of implementing these approximations, demonstrates the results of their operation as applied to describing the radiation transport processes and radiation interaction with a substance using the particular numerical examples.

FAMILY OF CLUSTER COMPUTER SYSTEMS MVS-1000 OF 1 OR MORE Tflops THROUGHPUT LEVEL

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This paper presents the possibilities to develop efficient computer systems using the modern system-structural concept of the super-computer construction. The concept is as follows. The commercially promising microprocessors most powerful at the moment are used as a basis for high-speed computational modules within one or more shared main memory processors. The modules are integrated with high-speed communication networks for inter-processor data communication and general-system control of appropriate software. This concept of the multi-processor computer system

(MCS) construction is currently dominating and will continue to be valuable, at least, in the coming years. These systems ensure a high reliability ("viability" in failure of separate modules and devices), high possibilities of scalability (in firmware makeup), and portability (succession) of software stock.

The typical CS includes:

- several ready computational (processor) modules, like those used in personal computers and workstations;
- a communication network integrating the modules;
- OS Linux on each module;
- •, •++ type high-level languages and library MPI for development of parallel application programs.

It is conventional to call these CS as "clusters". The notion "cluster" is defined as a set of computers integrated within some network to solve one problem.

The development of the clusters within a hundred or more and then thousand processors suggests that, irrespective of all existing prerequisites and potential capabilities of individual software and hardware, the achievement of a high and ultrahigh throughput (of Tflops level) in a wide range of applications is an intricate scientific-technical problem.

Selection of efficient technical approaches requires significant experience in development and implementation of computationally intensive application algorithms on multiprocessor CS, in making and operation of these CS.

The insufficient experience of the CS and application algorithm developers can lead to inadequate employment of the system throughput and reliability as well as to difficulties in the CS maintenance.

In 1997–2003 RASU FSUE "NII-KVANT" jointly with RAS M.V.Keldysh IAM and other institutions developed MCS-1000 type supercomputers that include up to a thousand of processors. Several tens of relatively cheap clusters with 8 to 32 processors, medium-class facilities with more powerful communication networks, and 32 to 128 processors were manufactured and supplied to the customers, and in July 2001 the 768-processor supercomputer based on microprocessors Alpha21264 and network Myrinet of 1-Tflops throughput (trillion floating-point operations per second) was commissioned.

The modern state of the microprocessor and communication tool technologies allows development of cluster type supercomputers with significantly higher technical and economic characteristics and up to10 Tflops throughput level.

NUMERICAL SIMULATION OF PLASTIC FLOW LOCALIZATION UNDER SIMPLE SHEAR

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The numerical simulation algorithm for localization of plastic flow when loading a thermovisco-plastic material using the simple shear scheme has been developed. The code solves the connected system of equations in partial variables describing the continuum flow. A determinant relation known from literature as "power relation" that relates the plastic deformation rate to the flow stress and temperature and the cumulative plastic deformation was used as an equation closing the system of continuum equations. The determinant relation describes the dependence of the flow

stress on the strain rate, as well as the strain hardening and the thermal weakening of material in a quite simple form. When numerically solving the system of equations describing the continuum flow with simple shear, partial variables in a spatial coordinate are calculated using interpolation cubic spline-functions. The explicit computational scheme was used to integrate the functions in time.

Numerical simulation of the experiments on dynamic ($\dot{\varepsilon} \sim 10^3 c^{-1}$) torsion of thin-wall piped steel samples [1, 2] using the Kolsky facility resulted in a full pattern of evolution of the plastic flow localization process. The calculated dependences for the shear band width evolving in time and the localized temperature and plastic deformation are in good agreement with the experimental data. A good agreement with the experiment has been also achieved for the distribution of temperature over a sample in stage of the developed localization process.

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NUMERICAL SOLUTION TO THE PROBLEM OF FRONT PROPAGATION IN NONLINEAR CONTROLLED SYSTEMS

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The paper addresses an independent nonlinear control problem

$dx/dt = f(x) + g(x)u, \quad x \quad R^2, \quad u \quad P(x),$

with continuous functions f and g. Limitations $P(x)$ on control u can be dependent, including discontinuously, on phase variable x. It is necessary to construct sets of attainability $G(t; M)$ on a given grid of times $\{t_i\}$ for a given initial set M.

The problems of fire spread can be formalized within this problem class. In this case the limitation $P(x)$ on control u determines the flame spread rate at a given point. This kind of set-up can also appear in the problems of acoustic oscillation spread in heterogeneous plates (for example, in spray uniformity diagnostics). If some quantity of regions are selected on a plane, where $P(x) = \{0\}$ is taken, then the problem will correspond to the problem of obstacle bypassing for shortest time.

Previously, formulations of control and differential game problems were considered [1], where the limitations on control depended on the phase vector in continuous manner. In the available literature it was impossible to detect any papers devoted to the study of problems with the discontinuous dependence of the limitations on controls.

The suggested algorithm for construction of the sets of attainability is oriented to sequential construction of their boundaries (fronts), beginning with that of the set M. A new front is constructed in two steps. First, the previous front is broken into regular

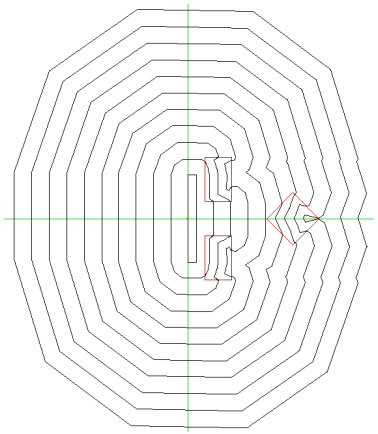

Fig. 1: General view of the fronts

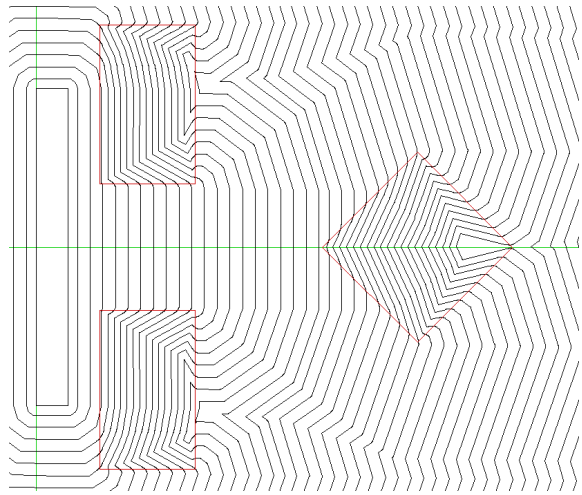

Fig. 2: Overcoming the regions by the fronts at a slow propagation speed

arcs which develop in time. Then from the resultant arc set a closed broken line, the new front, is formed. This entails a nontrivial computational geometry problem.

Fig. 1 presents the result of the front calculation for problem

$dx/dt = u, \quad x \quad R^2, \quad u \quad P(x).$

The discontinuous nature of set $P(x)$ as a function of x corresponds to a fast speed of the front propagation on the entire plane except three regions, which are seen in the figure as an “oblique” square and two rectangles with sides parallel to the coordinate axes. The front propagation speed is slow inside these three regions. The set $P(x)$ is a decagon inscribed in a circle of radius 0.5, if x belongs to any of the specified regions, and a decagon inscribed in a circle of radius 1.0 outside the regions. The initial set M the spread begins with is a vertical rectangle with vertex coordinates (0.1, 0.5), (0.1, -0.5), (0.0, -0.5), (0.0, 0.5).

The coordinates of the rectangular region vertices are (0.2, 0.2), (0.2, 0.7), (0.5, 0.7), (0.5, 0.2), those of the square region vertices are (0.9, 0.0), (1.2, 0.3), (1.5, 0.0), (1.2, -0.3). The computation was performed with step 0.0001 within time interval [0, 2.0]. The figure displays each thousandth front.

Fig. 2 depicts a more detailed pattern of the overcoming the regions by the fronts at a slow propagation. Here each two hundredth front is displayed.

A more detailed description of the front construction algorithm for the last problem can be found in ref. [3]. Ref. [3] also presents the results of the calculation for several other examples.

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DIRECT NUMERICAL 3D SIMULATION OF TURBULENT SHEAR MIXING

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The simplest shear flow is considered – 1D time-dependent plane mixing layer. Many more complex flows approach it under some conditions: time-independent plane mixing layer, initial portion of plane and cylindrical jets, initial mixing phase in cylindrical vortex etc.

The direct 2D simulation data for the turbulence at the interface between two plane –parallel fluid flows were earlier reported in [1]. Papers [2, 3] pursued the research efforts launched in [1] based on 2D and 3D simulation.

Numerical arrays of hydrodynamic values from 3D computations are used for to find the moments of those values. Spectral analysis was conducted for the rate pulsations of the turbulent mixing zone to study its approach to Khlmogorov spectrum.

Some 3D computational data are compared with the measurements and with semi-empirical turbulence mixing theory data including Reinolds tensor anisotropy.

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APPLICATION OF NEURON NETWORKS TO THE PROBLEMS OF SIMULATIONS AND DATA PROCESSING IN THE AREA OF CONTROLLED THERMONUCLEAR FUSION

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Presently, a new methodology is forming in research that is based on computer simulations and computational experiment. The mathematical model in combination with powerful computer engineering allows relatively cheaply, fast, fairly deeply and comprehensively studying some object or effect.

The computational experiment is closely related to the full-scale experiment. On the one hand, the actual experiment serves the base for construction and refinement of a computational model. On the other hand, simulations allow us to study the object or effect characteristics in extreme situation unachievable in the actual experiment and obtain data on quantities inaccessible to direct measurement.

However, in many modern problems the mathematical model itself and its computer implementation prove extremely involved. A large-scale computational experiment becomes hard to perform because of a large amount of computations. The problem appears to replace the original mathematical model with the approximate one that would allow the research to be accomplished in a short time.

Besides, the computational experiment generates a large data amount that frequently exceeds the full-scale measurement amount. Therefore the computed data processing problems become particularly important.

The solution of the above-mentioned problems with the classic methods proves impossible in many cases, new approaches have to be developed and used. One of the areas is employment of neuron networks. This paper addresses the development of the technique for application of neuron networks to the problem of computer simulations and experimental data processing in the area of controlled thermonuclear fusion (CTF).

The application of the neuron networks to the problem of replacement of the original mathematical model with the approximate one, to solution of inverse problems, data analysis and visualization is discussed. The technique efficiency is demonstrated by examples.

The studies infer the practicability of using the neuron network approaches in the area of CTF for solving problems of computer simulations and experimental data processing. The technique developed can be useful in other areas as well, particularly when the classic methods are inapplicable.

DEVELOPMENT OF AN APPROACH TO DEVELOPMENT OF SPECIALIZED VISUALIZATION SYSTEMS FOR HIGH-PERFORMANCE RESEARCH COMPUTATIONS

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Any high-performance research computations involve manipulations of large numerical arrays. A feature of the arrays is the basic impossibility for the scientist to

manipulate them directly. A method to overcome this problem is the visualization of the final data. Recently, this method has become essentially a standard for the representation of the results of research and is used more and more frequently as an efficient tool for the research itself. The visualization itself came to be studied a long time ago, essentially from the time when the computer graphics appeared. At the moment there are several models of the scientific visualization, however, the issues of construction of the visualization systems and development of possible criteria for their assessment continue to be inadequately elucidated. This paper makes an attempt to describe one of possible approaches.

The effort leans on quite an extensive experience in construction of different visualization systems that has been gained by RAS Urals Branch IMM Team of Research Visualization as well as on a number of theoretical works pertaining to the visualization theory and program engineering discipline. The approach is based on the notion of the cognitive computer graphics, that is the graphics, which not only illustrates the computed data, but also is an efficient tool of the scientist during his or her studies. To detect the cognitiveness criteria, the notion of the classic visualization pipeline undergoes some modification, the notions of the original numerical data language, visualization language, and visualization metaphor as a method to transform constructs of one language to the ones of another are added to it. Also, possible approaches to selection of the visualization language and visualization metaphors are presented. The paper justifies the selection of the language of geometric three-dimensional bodies as a visualization language for a prototype system.

The practical part of the effort consisted in development of the toolkit for implementation of the approach to construction of specialized visualization systems, that is a set of software components and their descriptions that would allow fast and cost-efficient generation of the visualization systems specialized for solution of specific problems. The toolkit is composed of two parts. The first part is responsible for construction of chains of initial data transformations into a 3D scene. The chain of the transformations is an ordered module set, where the output of the previous module is transferred to the input of the next. The modules can be both operating system executables and packages in the Java language. The modules solving type visualization problems can significantly speed up the 3D scene generation in the transformation chains for a specific problem.

The second toolkit part is a “visualizing” program that maps the generated scene and allows different manipulations of it. The program has a fairly developed functionality and can be effectively improved further. It employs technologies Java3D, XML, editable command history technology, etc. The 3D scene is described by invocation of the transformation chains corresponding to the format of the opened data. The scene description format is fairly flexible and extendable. There are both textual and binary versions of it.

The approach and software discussed in this paper have been extensively employed for optimal control problems by RAS Urals Branch IMM for more that two years. The works to use the approach for a new problem class are presently underway.

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SPECIALIZED VISUALIZATION TOOLS FOR ANALYSIS OF NUMERICAL SOLUTIONS TO CONFLICT CONTROL PROBLEMS

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Many practical problems, such as problems of pursuit of one object by another, perturbation spread in solids, generation of oscillations in the presence of noise, equity market prediction, etc. can be formalized within the theory of differential games (theory of conflict control) [1, 2]. The conflict control problem solution implies construction of a function of optimal guaranteed result (function of the worth of game) as well as the player strategies implementing this optimal result (optimal strategies). Unfortunately, the analytical solution construction is possible only in an extremely narrow problem class. Since the early 1980s RAS Urals Branch IMM has been extensively developing numerical methods for solving differential games [3–5], including those for massively parallel computers [6].

Concurrent with the development and improvement of the numerical algorithms, NMM has been developing specialized computed data visualization programs [7, 8]. The visualization programs can be used to rapidly and visually analyze the numerical solution obtained, find its singularities (worth of game function non-smoothness, optimal strategy degeneracy point) and study the solution structure in the vicinity of the singularities.

The paper demonstrates the recent versions of the programs being developed, shows an approximate session of their execution. Also, the solution visualization demonstration for specific examples with explanation of the singularities that may be of interest to specialists in the area of conflict control is being planned.

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FUNCTIONALITY OF PACKAGE GDT AND ITS USE ON MULTIPROCESSOR SYSTEMS

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The cluster-architecture multiprocessor computer stock has been extensively developed recently. Thanks to a relatively straightforward ideology and implementation as well as low cost these systems become more and more popular and there are grounds to believe that it is these systems that the bulk of the computations in the area of numerical simulations of physical processes will fall on in the foreseeable future. As the cluster architecture differs from that of the conventional personal computers, it is necessary to adapt the existing codes and packages to the new cluster architecture. The principal modification consists in the computational algorithm parallelization, with this being true both in the SMP and distributed-memory version. The parallelization procedures for the distributed-memory clusters can lead to a change in the functionality of the existing packages developed originally for sequential computations or SMP parallel computations.

The paper reviews the functionality of package GDT, gives examples of its use on different cluster system types. Ways of possible APP-cluster system construction unification through development of hybrid computer complexes and standardization of separate modules are discussed. Computation capability and scalability are exemplified for several multiprocessor computer system types. Potentials of the package development and use for computations of ultralarge tasks (more than a billion of 3D cells) for industrial and research applications are discussed.

ANISOTROPIC FLOW, STRAIN SOFTENING, AND HISTORY DEPENDENCE

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This presentation is intended to be illustrative of some of the mathematical difficulties which may be encountered in an attempt to predict the response of a material domain subject to some arbitrary thermo-mechanical loading history. For this purpose, the difficulties encountered in three rather challenging domain behaviors shall be presented as illustrative: those associated with anisotropic flow, strain softening, and history dependence.

The vast majority of computational codes which are currently being used to predict plastic behavior rely on use of the Jaumann-Noll stress rate. In a very

important paper which appeared in 1979, Dienes1 described a shortcoming, inherent in the application of the Jaumann-Noll stress rate, to a problem involving a hypothetical isotropic hypoelastic material subjected to shear. This shortcoming results in non-physical material behavior being predicted. While the results of Dienes appear rather alarming at first, recognition of the fact that real material do not behave hypoelastically, but tend to flow plastically, serves to remove the sense of alarm since it is observed that for plastic materials the non-physical behavior disappears. It is for this reason that the vast majority of computational codes continued to rely on the Jaumann-Noll stress rate after the publication of Dienes's paper. Unfortunately, it can be shown that if the material flows anisotropically, the non-physical behavior which is associated with the use of the Jaumann-Noll stress rate does not disappear, and other, more costly, computational techniques must be adopted. The mathematical difficulties associated with anisotropic flow shall be described, and one possible approach to overcoming these difficulties shall be presented.

When ductile metals are loaded to capacity, the following sequence of events is often observed. Localized regions of large deformation and plastic flow begin to form on a microscopic level. Then as the deformation proceeds, these localized deformation regions spawn damage in the form of voids, which with further loading grow and coalesce to produce cracks and ultimate failure. The formation of these localized regions of deformation and damage formation introduces a physical length scale to the problem within which localized material softening occurs. The presence of this localized softening phenomenon has important ramifications for the analyst who wishes to predict the deformation and damage evolution process. In dynamic loading problems, the impact is manifested in an ill-posedness of the initial boundary value problem as the governing equation becomes elliptic. Classical rate-independent material models applied to this problem are inadequate in that the numerical results exhibit an unacceptable mesh sensitivity. To adequately model the above described processes, a material model must introduce an appropriate characteristic length scale to the mathematical formulation which will remove the potential numerical ill-posedness. This might be accomplished through the use of higher order temporal derivatives which are associated with rate-dependent methods, or through non-local schemes which introduce higher order spatial derivatives. The mathematical difficulties associated with strain softening shall be described, and one possible approach to overcoming these difficulties shall be presented.

Some materials, such as those which are characterized as viscoelastic, respond to stimuli in a history-dependent manner. That is, these materials possess memory. The second law of thermodynamics dictates that materials of this type must have their constitutive equations cast in integral form, and that their current response depends on their entire history. Modeling the behavior of such materials therefore represents a tremendous computational challenge. The mathematical difficulties associated with predicting the behavior of materials possessing memory shall be discussed, and one possible approach to overcoming these difficulties shall be presented.

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A PARALLEL PROGRAM OF UNCONDITIONAL MINIMIZATION: ALGORITHM, APPLICATION

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The solution to many practical problems can be reduced to the search for the minimum of a scalar function of several variables. Frequently it is useful to do this at the step of the initial investigation into the problem, where the domain the desired parameters are in is unknown (even approximately).

As a rule, in actual problems the function is represented not as a relation, but is a result of some numerical procedure (for example, differential equation integration). Therefore information about the function gradient values is unavailable. Hence, it is impossible or hard to use the gradient search methods. For this reason this paper considers the direct search method, i.e. a method that explicitly uses the function values at points only.

The algorithm under discussion has been developed on the basis of Hook-Jives method. The general ideology of the method consists in interchange of the search about a base point, which determines the function decrease direction, and the search according to a sample, which corrected motion in the decrease direction proceeds in.

The original Hook-Jives method employs a sequential algorithm both in the search about the base point and that about the sample. In the algorithm, the coordinates of the current point for the calculation depend on the function value at the previous point. This does not allow parallelization. In addition, the algorithm has some anisotropy: the function argument increase direction is preferred.

When making parallelization, three versions of the algorithm for the search for the minimum of a function of many variables were developed. The algorithms differ in the search depth. The algorithms with a deeper search increase the probability of the global minimum determination.

The parallelization proceeds according to the processor farm scheme. The master task implements the function minimum search algorithm with calling, when necessary, working tasks to calculate the function values. The working task accepts the order from the master, calculates the function values at the order points, finds their minimum, and sends the result to the master. To make the search efficiency higher, Monte Carlo elements have been introduced to the program.

The parallel program is written in the C language for operating system Router. The program was debugged and run on computers MVS-100/1000. The minimum argument dimension in actual problems is on the order of one hundred.

The parallel program has been used to solve different problems. In particular, the program was debugged on the problem of brachistochrone in the central gravitational field. An optimal path field was obtained for different relative positions of the initial point, gravitational center, and final point.

One of the interesting problems, which have been solved using the program, is that of chemical reaction rate constant identification. Here the program minimized one of the discrepancy functions (non-smooth or even discontinuous) in order to find the vector of parameters consistent with the measurements taken.

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CONIDERATION OF THERMAL MOTION OF ATOMS WHEN SOLVING NEUTRON TRANSPORT PROBLEMS USING MONTE CARLO METHOD

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The paper describes the procedure allowing consideration of thermal atomic motion in Monte Carlo neutron transport computations. The procedure is based on the method of “maximum cross-section” and uses thermal cross-sections calculated for basic temperatures and elementary (cold) scattering indicatrices for simulation of trajectories. In a limit case of zero basic temperature, elementary (cold) cross-sections are used. For the procedure to be efficient, the “maximum cross-section” value should not noticeably differ from the original cross-section within the range of energies determined by the energy of neutron and the medium temperature. The behavior of thermal cross-sections is more smoothed than the behavior of cold ones and, therefore, their use allows the procedure efficiency to be improved, especially in the range of energies characterized by resonance behavior of cold cross-sections. Besides, the majority of neutron/material interaction processes are of the threshold level and these thresholds are within the range of high energies, where the thermal motion effect becomes small. Within the range of low and medium energies, the main processes are elastic scattering and absorption. During absorption all the effects of thermal motion are considered when calculating thermal cross-sections. The only problem is in the elastic scattering process. The paper shows that the maximum value of cold cross-sections of elastic scattering within some range of energies is required for the thermal motion to be considered precisely. These cross-sections have a rather smooth behavior, especially for light atoms. In view of this circumstance, it is possible to neglect some details of the elastic scattering cross-section behavior and assume it to be equal to the cross-section value within the neutron energy under consideration. Such approximation allows significant improvement of the procedure efficiency. The model problems demonstrate the accuracy of the proposed method of considering the thermal atomic motion.

A MODULE-SCALABLE ARCHITECTURE-PROGRAMMABLE MULTIPROCESSOR SYSTEM

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Presently, the re-configurable computers become often more efficient than the conventional-architecture parallel systems. However, as the re-configurable computers are problem-specific, they can not be an alternative to the multiprocessor systems constructed from the multi-purpose processors because of the overheads

required for the structure readjustment. This motivates the development of the parallel pipeline architecture-programmable computer systems, which would allow development of virtual specialized computers within the multi-purpose frame architecture, whose structure is adequate to an application problem (problem fragment) to be solved. The virtual problem-specific architecture is synthesized within the multi-purpose multiprocessor system through adjustment of the system components to certain large mathematical operations. The implementation of the programmable architecture reconfigurable computers on the basis of the PLIS technology will allow us to make the reconfigurable devices without involvement of a large amount of funds in a very short time as well as will ensure the device functionality improvement during its operation without any modernization of the elemental base.

The programmable-architecture computers employ an original principle of the structural-procedural computation arrangement. The computer program is a determined sequence of frames, each of which implements the computational pipeline using the operand thread method. The task frame components are mapped into the system structure in the natural manner. The information subgraphs describing the operational structure of the task frames are mapped onto a set of uniprocessors connected by a spatial commutation system. The addressing and commutation functions are implemented by hardware in the distributed-memory controller and commutator.

In contrast to a number of reconfigurable computers that require continuous loading of program and numerical information from the host computer, not a single frame corresponding to a specialized computer, but the whole program which is a sequence of frame calls is loaded into the programmable-architecture computer. Then the computer operates independently. The data processing rate can be made faster significantly because of the availability of many distributed-memory channels.

The reconfigurable computer with the structural-procedural computation implementation ensures an efficient implementation of data processing algorithms and linear growth in throughput with increasing number of base modules. The base modules are constructed on the basis of the same architecture principles as the system as a whole. Such approach ensures a natural implementation of the structural-procedural parallel programs for different parallelization types. The base modules communicate data using a spatial commutation system. The commutation system of the base module implements not only data communications between the base module components, but also those between the base modules.

Scientific Research Institute of Multiprocessor Computers (Taganrog) has developed a module-scalable programmable-architecture computer system containing up to eight base modules, each of which contains 64 uniprocessors. The scaled throughput of the base module is $2.5 \cdot 10^{10}$ operations/s. The scaled peak throughput of the system is 10^{11} operations per second.

Two system architecture programming levels have been implemented in the multiprocessor system. The first is the user's (system programmer's) level, at which macrooperations are created by the processor tuning to certain arithmetic operations and the processors are integrated into the computational structure using the commutation system. The second is the circuit level, at which the uniprocessor command system can be changed by the PLIS technology tools with implementation of a specialized operation set.

SELECTED VALIDATION ACTIVITIES AT LOS ALAMOS NATIONAL LABORATORY

Kamm J.R., Benjamin R.F., Cannon T.M., Davis A.B., Mathews A.R., Rider W.J., Tomkins C.D., Vixie K.R.
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Predictive capability is the goal of contemporary computational physics. The quantitative comparison between experiments and simulations, i.e., *meaningful* code validation, remains a significant limitation. Major advances in experimental and computational capabilities have elevated simulation science to the boundary of a higher standard for code validation; however, we cannot proceed without a collection of improved tools for quantitatively comparing experimental data with computational results. A recently begun activity, "Physics-Based Analysis of Dynamic Experimentation and Simulation," underway at Los Alamos National Laboratory, addresses this problem. This talk describes this effort, which has the goal of developing and implementing new physicsbased statistical analysis methods adapted specifically to code validation.

We discuss the ideals behind this approach, namely, methods that are balanced between appropriate simplicity (to allow extraction of information from measured data) and adequate complexity (to ensure that the extracted information is meaningful). To qualify as physics-based, we seek analysis methods for which no observable scale, statistical moment, or histogram feature is ignored or given special preference. We favor parametric statistical representations that capture the essential nonlinear processes, e.g., instabilities or cascades—methods that are inherently "physics friendly". These criteria, all firmly based in contemporary nonlinear science, will guide us in designing new validation metrics, i.e., quantitative gauges with which to compare experimental data and simulation results.

We illustrate our strategy with a preliminary investigation on shock-induced fluid mixing using fractals, wavelets, and structure function analysis. We further describe some recent results that compare numerical simulations with high explosives experiments conducted at the Los Alamos proton radiography facility. We speculate on specific regimes and phenomena to which our evolving analysis techniques might apply.

PREDICTION-BASED GRID RESOURCE DISTRIBUTION

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A new computing paradigm – Grid – emerged and is progressing as a tool for meaningful usage of various computer system types residing at arbitrary point in the global telecommunications network. Grid is designed not only to open the remote access to computers, software and data but also to integrate multiple spatially distributed resources into the unique operating system so that running applications could have access to any desired ensemble of resources.

Grid is an open dynamically organized multi-user computing environment where all the resources have the owner and the access in the shared mode is available for

multiple authorized users. The owners and users operating with resource allocation/usage rules form a virtual Grid structure. [1].

In Grid context, it is for the first time that the objective is to ensure the given servicing quality (QoS) in a globally distributed environment comparable with the level achieved in a closed corporate structure but for much larger scales.

Whether this goal can be achieved depends on the software that should first support Grid functioning and second, should allow developing applications for this environment. Globus – GT is de facto standard for this software (www.globus.org). The recent GT-3 release supporting the open Grid service infrastructure (OGSI) [2] increased Globus development capabilities oriented primarily to science and engineering applications. Now the scope of application is extended to business and industry applications from a variety of fields. In this connection, the priority focuses on the multi-user Grid operation mode. One of the aspects of this problem is to coordinate the access to the resources of multiple independently executing distributed applications.

Research efforts conducted for several years by Keldysh Institute concentrates on the management of computing resources. In 2001, Metamanager software package was implemented to function as proxy and to support the global queue of jobs distributing them over available resources. Currently, this research progresses towards assured servicing quality by ensuring an improved scheduling mechanism.

Scheduling resource allocation to jobs is a classic problem and was resolved for various computer architectures; however it is specific as applied to Grid environment, which is caused by:

- large amount of scheduling objects (jobs and resources);
- global distribution of objects;
- lack of direct access to resources.

The latter is due to that Grid is organized based on off-line principle where the resource owners allocate only apart of resources to be used within Grid retaining the rest for internal (local) jobs and local managers control the execution of all jobs on the resources.

Under these conditions, we proposed the communications principles for two traffic control levels (global-local) and developed the approach allowing global scheduling within Metamanager. The approach relies upon the prediction of resource allocation/deallocation for a period of time in future (this prediction can be obtained by modeling the operation of local managers). The modeling results are sent from each node to Metamanager in a form such that the latter can see whether the resources can be used for its (global) jobs. We hope the implementation of this scheme, the use of new interface to local managers interim resource redundancy) along with scheduling algorithm BackFill would allow handling not only traditional but multiprocessor tasks with simultaneous resource allocation on several Grid nodes.

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METAMANAGER: GRID-SERVICE IMPLEMENTATION

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The Metamanager is a system for task management in the heterogeneous network – Grid. Grid Network consists of nodes composing a virtual configuration [1]. A node means a group pf computers controlled by the Local Resource Management System (LRMS). The basic goal of the Metamanager is distribute the tasks over accessible resources in terms of access authorization, job priorities and resource loading.

To implement the Metamanager, a special component – agent - is installed on each accessible resource. The agent can model the situation on a designated resource for an advanced time period and transfer received schedule (the LRMS modeling result) to the Metamanager. Given received information, Metamanager can apply various scheduling algorithms to distribute the jobs over resources considering their loading.

Metamanager is a distributed system consisting of several components:

- Client utilities. These are needed to send the job to Metamanager, to receive sent job data, to cancel the job and to deliver the results;
- Agents residing on the computational nodes sending local job of the LRMS;
- Scheduler communicating with clients and agents and accomplishes the scheduling.

Metamanager is implemented with Globus development system that is de facto standard for constructing Grid applications. Recently emerged Globus 3.0 implements the open infrastructure of Grid services [2].

Grid services are designed to hide the network communications level from the applications programmer. There exists Grid service development technology allowing the programmer to concentrate on algorithmic aspects of the Grid service operation thus automating the routine functioning. The programmer should describe the interface of a grid service to be created to implement it later. Then the existing utilities from the service interface are used to build up automatically the interface description in the cross-platform language WSDL together with so-called stubs to ensure the network communications of the Grid service and its client. The resulting classes are emplaced in a Web container to be accessible through the network. The Grid service client gets the access to a Grid service instance through the special programming interface (API) and calls the desired method. And the client stubs use the existing description of the Grid service to generate the request and send this request to the server through SOAP protocol. This request is processed and returned to the client.

The scheduler and client utilities as well as the scheduler and agents communicate through the Grid services.

The Grid service designed for agent handling receives the schedule from the agent to write this schedule to the Metamanager database. To reduce the network traffic, the agents do not send the entire schedule but only those schedule changes that occurred as compared to the previous send operation. However this requires the numbering of

updates to prevent possible message lost and a mechanism for forced reception of the complete schedule after various failure types.

The amount of data needed for the Metamanager is great therefore the database is used to store it. Since the schedule come from the agents at arbitrary time a synchronization mechanism is provided to keep the database consistent and up-to-date. This is achieved by using the event queue mechanism: the entire information to be placed into the database is written to the queue. The Metamanager having completed the scheduling cycle updates the database in accordance with incoming information removing the messages from the queue and starts a new scheduling cycle based on the changes occurred.

Thus the Metamanager allows to distribute automatically the jobs over multiple accessible resources considering the actual situation on the Grid nodes. Moreover, the Metamanager is an easily expanded portable system since it is implemented using Grid services.

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KONTUR_ISO ALGORITHM FOR FINDING AND VISUALIZATION OF 3D SPACIAL-TYPE OBJECT CROSS SECTIONS BY GENERATING ISOLINES

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This paper pursuits the representation study of algorithms for finding and visualization of 3D object cross sections specified in various ways. KONTUR_ISO algorithm yields good results for some classes of 3D objects. KONTUR and ASL [*] algorithms were presented earlier. 3D numerical simulation is the scope of application for our research. Emphasize two specific simulation fields requiring the calculation of problems such as:

1. Define 3D geometry for Monte Carlo simulation.
2. Define 3D geometry and generate difference schemes in numerical difference simulation methods.

Conceptually, this algorithm is a counterpart of the algorithms from [*]. It is inferior in application generality while having some significant advantages in finding object cross sections. The illustrative evidence was obtained by running the algorithm in VIZI systems developed at RFNC-VNIITF, in particular, in:

1. VIZI_Prizma for analyzing and visualization of 3D geometries and physical properties for Monte Carlo numerical simulation complex, PRIZMA.
2. VIZI_Surf for defining, editing and visualization of 3D geometries.
3. VIZI3D analysis and scientific visualization of 3D simulation data.

Method background

1. In KONTUR_ISO, the analytical description of a 3D object surface is converted to the discrete form. The surface is represented as a regular topologically 2D grid that will be referred to as ***pseudo-three-dimensional***. This is a major feature differing our algorithm from others where the surface remains analytically described.
2. In KONTUR_ISO, the cross section surface remains analytically described in canonical form and should have the fixed-sign feature. This also differs our algorithm from others where the cross section surface is represented in a discrete way as additional 2D grid.

A NEW EVALUATION METHOD FOR SOME MATRICES

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The paper formulates and validates (both theoretically and numerically) a new spectrum evaluation method for some matrices using divergence criterion of Gauss exception procedure. The basic example explaining the method details considers a tridiagonal Teplitrz matrix M of order $m>2$ produced by three numbers (generally complex numbers) a, b, c, $ac\neq 0$ where the elements a fill the first subdiagonal, b do so for the pivot diagonal and c – the first superdiagonal. Let λ be a spectral variable. Then we can show that the divergence region R_d of Gauss exception for matrix M-λE is a straight line $\Lambda=b\pm 2(ac)^{0.5}$ without one of extreme points and the M matrix spectrum fills this line everywhere as m grows without going beyond with filling density increasing at the extremities of Λ. The reasoning of this basic result uses papers [1] and [2].

The generalization is given by the case where the first and the final rows of M matrix are interpreted as boundary condition coefficients thus violating Teplitz pattern of M matrix. Then two spectrum points can escape from Λ and go out from the straight line determined by Λ extremities. To see whether it is true, we have to use the convergence region R_c of Gauss exception for M-λE. matrix. We are able to analyze the case where M first has the rows with the elements a_1, b_1, c_1 followed by a_2, b_2, c_2. It is possible to evaluate the spectrum of four and five-diagonal Teplitz matrices, but the analysis will be more complicated.

The method is useful in that it allows to obtain very accurate matrix spectrum data without actual evaluation.

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NON-SPLIT ALTERNATING-DIRECTION IMPLICIT METHODS FOR SIMULATING THE BEHAVIOR OF MAGNETIZED PLASMAS

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The numerical solution of the multi-dimensional, non-ideal, resistive magnetohydrodynamic (MHD) equations for applications ranging from soft x-ray generation to controlled thermonuclear fusion has been of interest for more than four decades, beginning with the pioneering work of Hain and Roberts [1]. A now more-or-less "standard" set of MHD equations includes addition of the Lorentz force, resistive diffusion, radiative and anisotropic thermal transport, and Faraday's law to the usual hydrodynamic equations. Although some still look at MHD as simply a "bell-and-whistle" for hydrodynamics, an understanding of the complexity of the equations leads to the realization that the usual hydrodynamics is a rather trivial subset of MHD. In MHD, the "Courant conditions" faced by explicit methods can vary by many orders of magnitude over the spatial domain, and the dominant Courant condition in one part of the domain can be due to a different process than the dominant condition in another part of the domain. The severe Courant conditions force explicit methods to operate at a time-step size much smaller than the physical time-scales of interest. Although the usual approach to overcoming severe time-step limitations is operator splitting coupled with implicit methods, the strong coupling between several physical processes in MHD introduces the possibility of introduction of severe errors by operator splitting unless a very small time step, perhaps one even smaller than the explicit Courant limit, is used. As discussed in several papers by Briley and MacDonald [e.g., 2], the usual operator splitting involves intermediate steps which do not approximate the governing equations and these intermediate steps can lead to difficulties.

To make the accurate solution of a useful set of MHD equations feasible at a time long before parallel supercomputers were invented, a generalization of the Douglas-Gunn/Peaceman-Rachford implicit approach was developed [3]. In this approach, all physical processes in all spatial directions are solved simultaneously through a series of linearized block-tri-diagonal steps that are iterated to obtain a satisfactory level of convergence for implicit, non-linear terms. Now more than three decades old, this technique, presently implemented in a computer code named MHRDR (Magneto-Hydro- Radiative Dynamics Research), still finds use for specialized problems in MHD (e.g., the dense plasma focus, the inverse z-pinch) and has been ported to many modern computer platforms by the University of Nevada at Reno in collaboration with Los Alamos. The MHRDR code was the first US computer code to predict that the VNIIEF MAGO plasma formation system [4] has nearly ideal properties as a target plasma for Magnetized Target Fusion (MTF) [5]. Various aspects of the method will be described, along with its successes and limitations.

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ASYMMETRIC FLOW ABOUT A CONE

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The paper presents results of the simulations of flow about a cone and axisymmetric body at the angle of attack with generation of an asymmetric flow pattern on the leeward side. The simulation uses the Navier-Stokes equations in the thin layer approximation with the method of establishment.

When designing new aircraft, the angle of attack range becomes wider. On the leeward side the flow separation and vortex structures form. With originally symmetric problem set-up the computational domain size typically reduces. However, when considering flow even about a geometrically simple body like cone, the symmetry of the flow pattern can be broken at certain parameters in the separation zone. The asymmetry of flow about the cone appears in a certain range of the cone apex angle and angle of attack, Mach and Reynolds numbers as a consequence of the symmetric flow instability. Asymmetric flow forms significant side forces.

The paper presents the methods used in the simulation and the results in regard to the flow structure in the separation zones, position of the separation lines, and estimated side forces.

CALCULATIONS OF FREE BOUNDARIES AND INTERFACES IN MOVING GRID METHOD

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The method of moving difference grids is commonly used to calculate high-velocity processes in physics and mechanics. One of basic difficulties to be resolved while developing the grid algorithms is to evaluate the history of computational domain boundaries that can be both interfaces and free outer boundaries. There exist some examples illustrating how the chosen algorithm for the calculation of boundary motion influence the computational data. Remind that related mathematical applications from this class are very complex problems involving unknown moving boundaries.

This paper describes the computational algorithm to calculate the motion of interfaces and free boundaries used to solve the dynamic deformation and failure of solids. The algorithm allows not only to describe the behavior of originally selected boundaries but also to introduce and remove new free boundaries and interfaces as the material destruction proceeds. The algorithm capabilities and applicability are illustrated by the calculation of high-velocity impact and jet formation.

CFD CODE ARCHITECTURE FOR HYBRID ECOMPUTER SYSTEMS

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The classic build-up scheme for the CFD package is that consisting of three components: preprocessor – solver – postprocessor. This scheme is uncoupled all components operating independently. This frequently leads to complications such as data communications between the package components, inability to govern the computing process at the calculation time, lack of control over the computational data until the calculations are completed. Overcoming these difficulties requires the integration of all package components. There exist a variety of methods for this integration. Compiling all package components as a single execution module is the most commonly used way. The disadvantages of this scheme include its low flexibility, tailoring to a specific hardware and software platform, poor package portability to other platforms.

Our paper offers an alternative approach to the construction of the integrated package. The package is assembled from several communicating modules. The communications protocol has two levels. The lower level encompasses the transport protocol. The transport protocols were developed based on TCP/IP and MPI. For the upper level, the communications protocols are designed for several parallel solvers allowing the integration of an arbitrary number of solvers for joint calculation of large-scale problems (hundreds million cells or more) along with the communications protocol for solvers and control module and that for the communications between the control module and the application interface. All modules are implemented to run under three operating systems: Win32, Linux, Solaris. Solaris version supports two hardware platform types: UltraSPARC and x86. Thus the work resulted in a package whose components are able of jointly running on three platforms; for example, the end user interface can run in Win32 and the solvers can operate in SPARC-Solaris cluster or in PC-Linux. This architecture allows the user to operate the cluster remotely, fro example, through Internet combining the advantages of a convenient interface and the performance of the cluster.

The paper gives the testing results and some examples of package applications implemented in various versions of computing environments.

NUMERICAL SHOCK-SENSITIVITY SIMULATION OF PLASTICIZED TATB HE UNDER HEATING

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TATB-based HE is able of withstanding the temperatures up to 280•C Increasing the shock-sensitivity of TATB-based HE is an important issue.

In this paper, the detonation kinetics model developed under the guidance of V. G. Morozov [1, 2] was first applied to the simulation of detonation generation and motion in a TATB HE pre-heated to 180•C.

The heating is simulated by applying initial internal energy to tungsten-wired plate and to surrounding plasticized TATB layers.

The computations yielded the following results: no detonation is initiated in the triggering assembly at the initial plasticized TATB density of 1.91g/cm^3 and the shock wave propagates through the HE. Applying the initial internal energy when modeling the heating forms a time-independent shock affecting the entire HE specimen including 'non-heated' 1.91 g/cm^3 region.

The paper presents the numerical simulation results: 2D pressure and density patterns, burnout as a function of time in the case of shock propagation through 'cool' TATB HE and shock propagation patterns across the heated HE.

The theoretical results agree with X-ray experiments.

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CALCULATION OF AN EMISSION SPECTRUM FOR XENON PLASMA

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The method for calculation spectral absorption and emission coefficients for plasmas of multicharged ions is developed. It is based on intermediate coupling scheme and is realized on multi processors computation system MVS-1000M. To verify the model and algorithms the emission spectrum of xenon plasma is modeled, which is comparing with experimental data of laboratory CYMER (where the dense plasma focus was used). The main problem is to define the experimental temperature, because plasma is in non-equilibrium state and plasma properties can depend on radiation field.

In calculations the transparent case was assumed and it was shown that for experimental density $\rho \sim 10^{-6}$ g/cm^3 (it was obtained by numerical simulation) the coronal equilibrium approximation may be used. It means that the main processes are impact ionization and radiative recombination.

The influence of different approximations and plasma parameters were analyzed. As can see from experimental data (Fig.1) the main line clusters corresponds to transitions 5p-4d for different initial states of ions $4p^6 4d^N$(N=8-10). The strongest transitions 4f-4d for all ions are placed at λ<12 nm. The calculated spectrum at temperature T=35 eV and density $\rho=10^{-6}$ g/cm^3 is close to experimental one (see Fig.2, where calculated spectrum was shifted by 0.5 nm to the right). The additional broadening 0.05 eV was also included in calculations in accordance with experimental resolution. As can see from figures we have satisfactory agreement of calculation results with experiment, nevertheless it is evident that re-absorption effects are essential for spectral lines $\lambda \sim 11$ nm. It should be also noted that at the considered temperature there are excited ion states $4p^5 4d^{N+1}$, and auto-ionizing states, which produce 4d-4p lines that are absent in experimental picture. This may be connected with the not sufficient accuracy of calculations in accounting for auto-ionizing states.

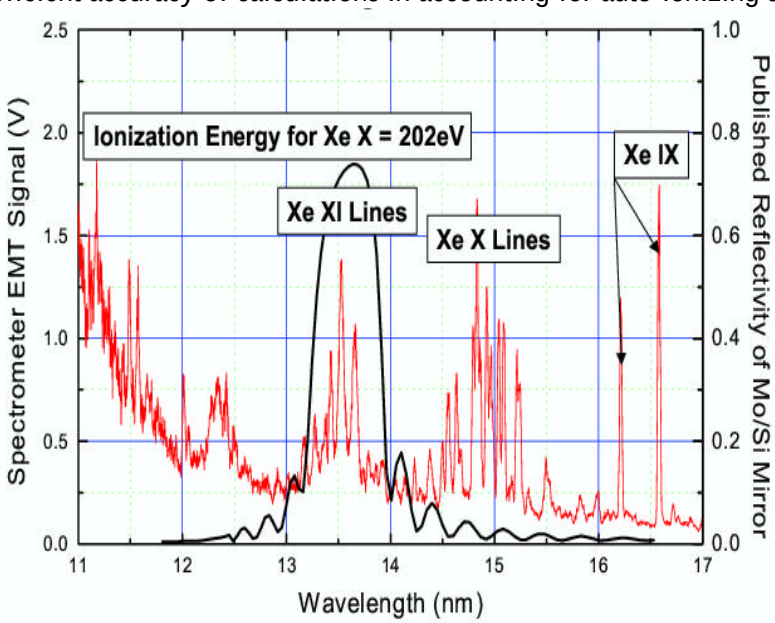

Fig.1.

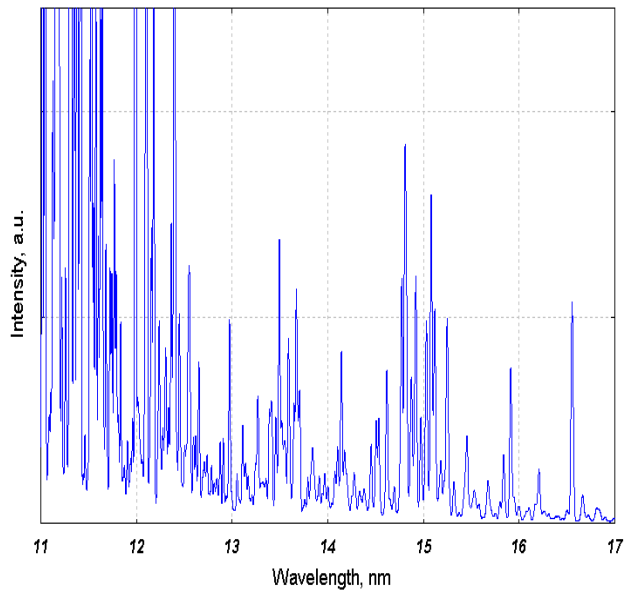

Fig.2.

BEHAVIOR OF A CYLINDER CASING IN THETEMPERATURE FIELD UNDER PARTIAL DESTRUCTION OF THE HEAT PROTECTION LAYER FOLLOWED BY LOCAL COOLING

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The effect of residual stress on structural survivability is well known. The resulting unloading-produced field of self-balanced (contracting and tensile) stresses can both increase and reduce the limit loads. It is also known that in the event of local failure of heat protection in systems in the temperature field a local cooling source is used. This engineering choice results in a field of residual stresses contributing to the destruction.

This paper considers the behavior of a cylinder shell with damaged heat-protection layer in a temperature field resulting in heating the damaged zone. Forced cooling of the heated zone produces residual stresses (compressing in around the hot spot and tensile inside it). The heating zone may generate surface defects that can lead to unsealing (material breakdown) and subsequent destruction because of tensile stress. Heat protection zone may demonstrate the heat-protection layer detachment, which leads to the heating zone growth. Thus we have to determine peak allowed hot spot temperature that does not produce those effects.

The stress-strain state of the shell heated according the law $T(\alpha_1,\alpha_2)=\begin{cases}0, & on\,\Omega_1\\ T_0, & on\,\Omega_2\end{cases}$, where Ω_1, Ω_2 are the domains of damaged and undamaged zones separated by the boundary • is determined with the finite-element method using COSMOS package. To determine the stress-strain state at the time where the temperature reaches $\bullet_0$, we use the method of extension over the temperature parameter. Residual stresses $\sigma^{\cdots}$ are calculated at the time where the temperature in Ω_2 reaches $\bullet_0$.

If the cooled zone has a through fissure we must study the destruction process. The destruction model is chosen to be represented by Cherepanov-Reiss criterion that states that the destruction occurs whenever the invariant J integral calculated along the damage boundary reaches its critical value that is the material constant. The fissure growth condition is obtained by varying the total strained shell energy regarding the energy required to generate a new defect surface through the growth process using the varied surface defect parameter (coordinate). The total energy is defined as $\bullet = \bullet_0 - 2\gamma(\alpha_1 - \bullet_1) + 2\gamma(\alpha_1 - \bullet_2)$ where γ is the specific destruction energy needed to generate the stratification surface unit. Zero variation requirement of $\bullet$ functional obatained by varying $\bullet_1$, $\bullet_2$ coordinates with a fixed temperature as given by the energy balance equation yields the daqmage growth equation: $\delta_{x_1} \bullet = 0$; $\delta_{x_2} \bullet = 0$.

Varying over the damage boundaries $\bullet_1$ and $\bullet_2$ for the functional with variable boundaries allows to write the defect growth equation as $\bullet^{\bullet +} - \bullet^{\bullet -} - 2\gamma = 0$ with $\alpha_1 = \bullet_1$, $\alpha_1 = \bullet_2$, where $\bullet^{\bullet \pm}$ is the value of $\bullet$ functional for boundary bypass of the defect localized by the coordinates $\alpha_1 = \bullet_1$, $\alpha_1 = \bullet_2$.

As given by Cherepanov criterion [1] for brittle failure, the requirement $\bullet^{\bullet +} - \bullet^{\bullet -} = J$ is met where J is the invariant integral calculated at the fissure front with $\alpha_1 = \bullet_1$, $\bullet_2$. The final defect growth condition is as follows: $J = J_*$ where $J_* = 2\gamma$ is the limit value of J integral depending on structure manufacturing technology.

Heating the damaged shell can also result in ripping of the heat protection layer from the base, which leads to subsequent growth of the heating zone. The defect growth requirement then takes the form $\max(\bullet_{\bullet_1}^{+} - \bullet_{\bullet_1}^{-}, \bullet_{\bullet_2}^{+} - \bullet_{\bullet_2}^{-}) = J_*$.

The approach developed here was used to analyze numerically how the heating temperature $\bullet_0$ that leads to the bearing shell failure after the damaged zone depends on the damaged zone size in the event of shell material defect (fissure) resulting from the upper surface damage or the life cycle. The numerical evaluation of J_* (the threshold value of J integral) was accomplished using a steal-3 plate ($\bullet = 1{,}95 \cdot 10^{11}$ $\bullet/m^2$, $\sigma_{\bullet} = 38 \cdot 10^7$ $\bullet/m^2$) with the cross section $b \times \delta = 30 \times 0{,}13$ (mm) having a central fissure with l = 5 mm that had been stretched till the failure. COSMOS package was used to determine the theoretical value of invariant J integral at the failure time that was taken to be the value of J_*. The resulting value is $J_* = 1{,}06$ kg/mm.

The strain plot of the two-layer shell shows the solution corresponding to the defect growth requirement beyond the point $J = J_*$ where the avalanche layer break occurs.

The critical heating temperature where the protection layer separates depends on the zone size in non-monotonic way; the separation temperature minimum in shell systems corresponds to ‘average’ failures.

Thus the hot spots emerging in shell systems due to the heat protection layer damage can be the source of the system destruction caused both by residual stresses resulting from local fast cooling and by the change of the stress-strain state where the value of J integral reaches J_*.

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SIMULATION OF 3D GAS FLOW WITH PARTICLE-IN-CELL METHOD ON ADAPTIVELY EMBEDDED GRID. SEDOV BLAST CALCULATIONS

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The paper presents the PIC method on a cubic adaptively embedded grid for numerical simulation of 3D high-strain gas flows. The computational algorithm is described, the simulation results are given for Sedov blast calculations. The numerical solution analysis showed that the adaptively embedded grid allows to reproduce the shock jump from the explosion domain that is 200 times smaller than the computational domain. Though the cubic grid is used the computations retain the spherical solution. A good agreement is observed between our data and the analytical solution.

The calculations are presented for the interaction between the explosion-produced spherical wave and a dense spherical body. The results obtained with the 3D code agree well with the data for a similar problem in 2D geometry.

IDENTIFICATION OF MULTIDIMENSIONAL NON-STATIONARY DYNAMIC OBJECTS WITH KALMAN FILTRATION METHOD

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When studying an aircraft control system, an important problem is to study its elements. Dynamic object models are identified from measured information signals. The Kalman filtration method is considered as a basic method for the parameter identification.

The dynamic object identification problem is posed in finding the model in the form of a linear differential equation system. The well-known parametric identification methods, such as MNK, Kalman filtration, imply setting the model structure as a difference equation.

The Kalman filtration algorithm for the dynamic object identification in the form of a multidimensional linear model is

$$\begin{cases} \mathbf{Q_o}(\mathrm{k}+1/\mathrm{k}) = \bullet\ (\mathrm{k}+1/\mathrm{k})\,\mathbf{Q_o}(\mathrm{k}); \\ \mathbf{Q_o}(\mathrm{k}) = \mathbf{Q_o}(\mathrm{k/k-1}) + \mathbf{L}(\mathrm{k})\left[\mathbf{y}^{\mathrm{T}}(\mathrm{k}) - \mathbf{y_o}^{\mathrm{T}}(\mathrm{k})\right]; \\ \mathbf{y_o}(\mathrm{k}) = \left[\bullet_{\mathbf{o}}^{\mathrm{T}}(\mathrm{k})\,\mathbf{Q_o}(\mathrm{k}/\mathrm{k}-1)\right]^{\mathrm{T}}, \end{cases}$$

where y(k) is the vector of dynamic object output variables of dimension px1 at time $k\Delta t$; $\mathbf{y_o}(k)$ is the vector of estimated dynamic object output variables of dimension px1; p is the number of the object output variables; u(k) is the vector of the dynamic object input variables of dimension qx1; q is the number of the object input variables; $\bullet\ (\mathrm{k}+1/\mathrm{k})$ is the state transition matrix (reflecting the dynamic object parameter change nature) of dimension n_Mxn_M; $\mathbf{Q_o}(\mathrm{k}) = (\mathbf{Ao}_1 \vdots \ldots \vdots \mathbf{Ao}_{\mathrm{na}} \vdots \mathbf{Bo}_1 \vdots \ldots \vdots \mathbf{Bo}_{\mathrm{nb}} \vdots \mathbf{Co}_0 \vdots \mathbf{Co}_1 \vdots \ldots \vdots \mathbf{Co}_{\mathrm{nc}})^{\mathrm{T}}$ is the estimated parameter matrix of dimension ($n_M = na \times p + nb \times q + (nc+1) \times l$); $\mathbf{Q_o}(\mathrm{k/k-1})$ – is

the matrix of the predicted parameters; $\mathbf{A}_0, \mathbf{A}_1, \ldots, \mathbf{A}_{na}, \mathbf{B}_0, \mathbf{B}_1, \ldots, \mathbf{B}_{nb}, \mathbf{C}_0, \mathbf{C}_1, \ldots, \mathbf{C}_{nc}$ are the matrices of the model coefficients of dimension *p*x*p*, *p*x*q*, and *p*x*l*, respectively; $\bullet\ \mathbf{o}(k) = \left(-\mathbf{yo}^T(k-1), \ldots, -\mathbf{yo}^T(k-na), \mathbf{u}^T(k-1), \ldots, \mathbf{u}^T(k-nb), \mathbf{e}^T(k), \ldots, \mathbf{e}^T(k-nc)\right)^T$ is the vector of the data with estimated output signal of dimension n_Mxp; $\mathbf{L}(k)$ is the filter coefficient matrix of dimension n_Mx1:

$$\begin{cases} \mathbf{P_Q}(k+1/k) = \bullet\ (k/k-1)\,\mathbf{PP_Q}(k)\bullet\ ^{\bullet}(k/k-1) + \mathbf{C_Q}(k)\,\mathbf{R1_Q}\,\mathbf{C_Q}^T(k); \\ \mathbf{L}(k) = \mathbf{P_Q}(k/k-1)\bullet_{\mathbf{o}}(k)\left[\bullet_{\mathbf{o}}^T(k)\,\mathbf{P_Q}(k/k-1)\bullet_{\mathbf{o}}(k) + \mathbf{R2_Q}\right]^{-1}; \\ \mathbf{PP_Q}(k) = \mathbf{P_Q}(k/k-1) - \mathbf{L}(k)\bullet_{\mathbf{o}}^T(k)\,\mathbf{P_Q}(k/k-1), \end{cases}$$

where $\mathbf{P_Q}(k+1/k)$ is the predicted parameter error dispersion matrix of dimension n_Mxn_M; $\mathbf{PP_Q}(k)$ is the estimated parameter error dispersion matrix of dimension n_Mxn_M; $\mathbf{C_Q}(k)$ is the matrix of coefficients of dimension n_Mxn_M; $\mathbf{R1_Q}(k)$ is the forming noise level of dimension n_Mxn_M; $\mathbf{R2_Q}(k)$ is the measurement noise level.

The non-stationarity both of the dynamic object and information signals is accounted for by identification of the linear difference model system parameters on time intervals $\Delta T_i = i\Delta t$. The intervals can therewith be both fixed and current.

Upon the identification of the parameters $\mathbf{Q_o}(k)$ the transition is made from the linear difference equation system to the parameters of the desired linear differential equation system.

The estimations of the designed algorithm accuracy in identification of both type dynamic flights by test signals and dynamic object characteristics by telemetric measurements demonstrated efficiency of the Kalman filtration algorithms.

ORDER-OF-ACCURACY, SOLUTION ACCURACY AND EFFICIENCY IN HIGH-RESOLUTION SHOCK CAPTURING METHODS

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In this work, we examine the error in numerical simulations of shock problems for the Euler equations of gas dynamics. We first consider standard integration schemes, such as PLMDE and WENO. The result of this study forms the basis for the development of new hybrid high-resolution methods that incorporate the best elements of each of the standard methods. We show that calculation of the error gives clear evidence that the new methods are both more accurate and more efficient than the standard methods, i.e., the new methods are truly higher-resolution. We discuss the basic philosophy of the standard methods (WENO and PLMDE) and describe in detail the new hybrid scheme.

Finally, we conclude with some perspectives on the challenge provided by compressible turbulent mixing and the problems associated with assessing the accuracy of such flows.

BREMSSTRAHLUNG SPECTRA COMPUTATIONS FOR LOW-ENERGY ELECTRONS

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The knowledge of secondary photon emission fields generated in solids exposed to accelerated electrons is needed for the calculation of many applications in nuclear device engineering. In particular, this problem emerges in adjusting of X-ray sensors for plasma diagnostics on “Globus-M” fusion installation. The problem is caused by a very soft X-ray of fusion plasma, which necessitates the application of bremsstrahlung of electron beam with energies lower than 10 keV for sensor adjusting. Spectra of such sources are hard to measure with the reuired accuracy so that they are obtained computationally by calculating electron-photon transport.

The paper describes a special-purpose program simulating the accelerated electron beam interaction with the target material using Monte Carlo method that allowed to calculate both bremsstrahlung and characteristic X-ray components.

The program has the following basic features:

1. electron beam energy range 100eV-32keV;
2. arbitrary-Z monoatomic target material;
3. elastic and plastic electron scattering on atoms are included;
4. bremsstarhlung photon emission through statistical and polarization channels is considered;
5. electron-photon cascades are simulated in the target body;
6. photoelectric absorption of X-ray photons by the target and filter atoms is considered.

To test the basic program blocks, the simulation results were compared with the existing experimental data. In particular, angular and energy distributions were obtained for the 20keV electron beam at the aluminum foil outlet.

The simulation algorithm for bremsstrahlung and characteristic radiation was checked by calculating the bremsstrahlung spectrum of 20 keV electron beam in a thick copper target with a normal surface- impacting bwam.

COMPUTER SIMULATION OF RADIATION GENERATION IN DISCONTINUOUS DIELECTRIC PROPERTY MEDIA

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The paper presents the problem geometry and computer model for the (transient) radiation generation for a relativistic charge passing across the interface between media with different dielectric properties. The radiation generation dynamics is described by Maxwell-Vlasov system in multidmensional phase space. Numerical simulation methods within the finite-difference scheme for Maxwell-Vlasov system (a system with dioscontinuous partial derivatives for six-dimensional disribution function) generally require singificant computational capabilities and are only possible using parallel algorithms on massively parallel computer clusters.

The calculation and analysis of Maxwell-Vlasov systems for the physical phenomemnon of inteest (radiation generation) are given for the finite-oreder phase space. Parallel computing startegy is discussed for massively parallel computer clusters. The algorithm uses the interleaving scheme and SPMD (Single Program-Multiple Data) method.

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THE KINETIC MODEL OF DYNAMIC DISTRUCTIONS INCLUDING THE PLASTIC GROWTH OF PORES AND DAMAGES CAUSED BY SHEAR STRAIN

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The problem of destruction of various physical objects subject to shockwave loading is of practical interest and it is extensively studied in problems of dispersion of fragments of nuclear active materials, when simulating emergences at nuclear power plants, in problems of fragmentation of comets entering into the planet atmosphere, in problems of jet formation in a shaped charge, in various penetration problems, etc. Today, the most consistent pattern of dynamic destruction is developed, qualitatively, using mesoscopic approach. When solving practical problems, however, one manages to obtain quantitative results, mainly, within continual models.

The paper presents the kinetic model of dynamic destructions, including the plastic growth of pores and damages on shear plastic flows, which uses two scalar parameters of damage. There has been made an attempt to combine two mechanisms of elastic-plastic material destruction within the model basing on generation of micro-defects (simulated by formation and development of micropores at tension stresses [1,2]) and basing on generation of micro-damages in the plastic material flow region [3]. The model has been implemented within 2D DMK code complex [4] and allows correct description of complex processes of solid destruction using the kinetic approach.

The model capabilities are demonstrated using the results of 2D computations of a thick barrier breaking through by a rod and a thin barrier breaking through by a bullet. Results for the first problem demonstrate the model abilities to describe the destruction process on shear flows and the processes of visco-plastic formation and growth of pores, results for the second problem demonstrate the developed method abilities to solve the problems with the predominant influence of shear strains.

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MULTI-USER OPERATION OF PVFS PARALLEL FILE SYSTEM

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The project was accomplished under RBRF sponsorship, grants 01-07-90215, 00-15-96042.

The interest to parallel input-output on computer clusters is determined by the following:

- the existence of actual applications whose input-output system requirements greatly differ from the 'standard';
- available computer cluster architecture input-output redundancy capabilities. Indeed, the computational nodes of the existing clusters generally have local hard disks used only for the initial system boot and swap.

At this point, the 'heroic' era n this field finished; API standards formed de facto for the application programmer: MPI-IO as a part of MPI 2 and POSIX API for lower-performance demanding users. In this context, we decided to orient to extending the existing stable parallel file system in accordance with the operational realities of a real computing center [1] rather than to zero-departure development. After the analysis of freeware soft, we made he decision in favor of expanded PVFS (Climson University and Argonne National Laboratory products) [2].

PVFS is debugged to meet the industrial level and is used for real applications as reported by publications. Its design bottleneck is the failure handling on one of the nodes – this function is actually ignored. The operation practices of massively parallel supercomputers including that for the 768-processor MVS-1000M system shows that a meaningful failure handling is highly desirable for hundreds thousands computing nodes.

Having analyzed typical error situations and users demands, we recognized that it is most important to support failure-resistant writing. We would like to emphasize the following significant modifications we made to PVFS:

- incorporation of new redundant I/O nodes which allows the user to continue writing (transparently) when the write-in node is inaccessible. After the basic node is recovered, data migration is accomplished;
- logging of operations and metaoperations to enhance the failure resistance (open file logs on I/O devices) or ensuring recovery correctness (for example, you have to log 'ftruncate' if redundant I/O devices are running [2]).

Testing shows that we had succeeded in avoiding the situations where the reliability measures considerably decrease the efficiency – the degradation was a few per cent only and the performance can be even improved in some cases.

Another objective of our research in parallel I/O is to develop service tools. If those tools do not exist, the application programmer has to keep in mind the coupling of multiple factors to imagine the entire parallel I/O dynamics in parallel with computations. Similar problems occur when improving an outside file system, though well structured. Visualization is a standard choice for those problems. To visualize the parallel file system operation, we implemented performance data grabber, postprocessing tools and an ensemble of scenarios for IBM DataExplorer that generates 3D images. The visualyzer capability to render the system behavior dynamics allowed to detect the abnormal behavior pattern of one of the I/O nodes and to fix the migration error.

For more PVFS improvement data including benchmarks, refer to http://paralle.uran.ru/pvfs/.

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PARALLEL MOLECULAR DYNAMICS TO STUDY ELASTIC-PLASTIC PROPERTIES OF SOLIDS UNDER HIGH STRAIN RATES

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The recent decade demonstrated a dramatic progress in molecular dynamics methods in parallel with that of computer systems. Researchers turned from relatively simple computations on systems consisting of several hundreds molecules with simple Lennard-Johns type interaction potential to the simulation of dynamic processes on systems including several hundred millions molecules and to the simulation of relatively small systems where the molecular interaction is described by first-principle or semi-empirical quantum mechanics methods. The solution of quantum mechanics problem is included into molecular dynamics calculations.

The authors of this paper wrote the program package MOLOKH representing an ensemble of programs allowing the simulation of material behavior with classic parallel molecular dynamics method and permitting to obtain any available data from the model in real time.

Parallel classic molecular dynamics is used to study elastic–plastic properties of solids. These research efforts include the examination of monocrystal and polycrystal behavior under loading and slabbing mechanism under specimen tensile in rarefaction waves.

To study these processes, we used a specimen consisting of $2*10^7$ atoms with the body-centered or face-centered cubic lattice in the form of a parallelepiped with the size $n_1a \times n_2a \times n_3a$, where a is the lattice constant. Various boundary condition types are used. The equation of motion was numerically integrated using Leap Frog algorithm. Molecular interactions were described with Lennard-Johns potentials and the interstitial atom model.

Our initial goal was to see how the copper monocrystal microstructure response depends on the orientation towards the shock front. The microstructure behavior pattern was also shown to be greatly influenced by the initial specimen temperature.

The studies of the polycrystal specimen include the determination of how the dynamic strength yield depends on average grain sizes, initial temperature and strain rates.

The simulation of b.c.c. iron monocrystal shock compression showed structural changes that can be explained by the polymorphic transition to dense compacted structure. This structural transition actually occurs in iron at approximately 12 GPa

and is well known as $\alpha \rightarrow \varepsilon$ transition. The pressure obtained from the simulation (30 GPa) exceeds the experimental value and we have to choose an appropriate atomic interaction potential able of giving a good description for more than one phase.

The goal of the next series of computations was to track the material behavior under tensile stress. Several computations were run with a model consisting of two f.c.c. specimens with different lengths colliding at a given velocity. The boundary conditions were chosen to be periodic or reflected along the axes perpendicular to the motion direction and free along the axes parallel to the motion direction. The interaction between two rarefaction waves generated after the shock waves had reached free surface resulted in a negative pressure region in the longer specimen. The tensile load can lead to a breakdown.

We found the initial breakdown step to form vacancies in the form of spherical voids despite of 1D motion pattern. Merging the voids results in fissuring. In the case of a polycrystal specimen the void generation centers lie on the grain boundaries while shock-produced packing defects are the centers in a monocrystal.

NON-LTE RADIATION TRANSPORT, TEMPERATURES AND ENERGY BALANCE

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Temperature and energy density are both fundamental quantities in the theory of X-ray radiation transport. However, the relationship between temperature and energy density in matter that is not in local thermodynamic equilibrium (LTE) is neither simple nor unique. Evolution of internal degrees of freedom and the dependence on radiation intensities of these degrees of freedom both affect this relationship.We discuss the evolution of temperature in the context of a collisional-radiative model driving a radiation transport calculation. We derive two extensions to a traditional radiation transport treatment to account for these effects.

We present two numerical studies. The first examines a radiatively-cooled low density Ti plasma and quantitatively demonstrates the effect of the internal degrees of freedom. The second evolves a Lu plasma in a Z-pinch configuration. Accounting for the effects of strong line radiation using an approximate numerical treatment dramatically improves both the stability and accuracy of the calculation.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract W-7405-ENG-48.

TOPOLOGICAL REDUNDANCY IN MULTIPROCESSOR ENVIRONMENTS WITH SINGLED-OUT ELEMENTS

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The paper proposes the redundancy method for multiprocessor environments. Processor elements not involved in a given problem computation are used as backup ones. They can be enabled for solving "a less important" problem that will be removed, if there is need in backup processors.

Some probability estimates for fault-free operation of the redundancy method proposed are given.

SOME UNCERTAINTY EVALUATION RESULTS FOR ROUND-OFF COMPUTATIONS EXEMPLIFIED BY A LINEAR ALGEBRA APPLICATION

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A 2D heat conduction application with the known exact solution was used as an example for successful of the formula parameters for relative round-off computation error. This formula for the relative error, d, of the result obtained in N arithmetic operations is

$d = 10^K \cdot \sqrt{N} \cdot C_1 \cdot \Delta_1$,

Here Δ_1 is the relative limit error of a single round-off operation, a constant determined by the length of the basic computer word.

For example, for HP Work Station X400 computer, that ran single and double-precision computations, the length m of a single word for REAL*4 allocation is equal to 32 binary digits and $\Delta_1 = 10^{-7}$; the length m of a double word for REAL*8 allocation is equal to 64 binary digits and $\Delta_1 = 10^{-16}$. Expression $\sqrt{N}$ for large N is defined by the probability addition mechanism for relative errors of arguments in round-off arithmetic operations and the value 10^k is determined by the features of the numerical scheme and specific computation that can dramatically increase the accumulated error. One of these features is that the algorithms contain neighboring value subtract operations increasing the relative result error. Finally, the coefficient C_1 corrects the overestimate of both theoretical value $\sqrt{N}$ and Δ_1. The paper indicates that large-scale computations can achieve the parameter values such as $K \approx 6 \div 7$; $C_1 \approx 0.001 \div 0.1$. The formula allows to evaluate a priori the number m of binary digits of the basic computer word required to retain the needed accuracy n computations with large N. For example, 96-bit words (m_1=96, $\Delta_1 = 10^{-25.5}$) should be reasonably designated to allocate the numbers. This estimation is one of the results obtained from the presented research efforts. The value of N mentioned here can be easily achieved for rapidly progressing computer systems.

NUMERICAL SIMULATION OF VELOCITY PULSATIONS IN SHOCK TUBE EXPERIMENTS

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The paper presents Richtmyer-Meshkov instability problem setup and results for the conditions corresponding to the experiment [1]. This experiment measured longitudinal velocity pulsations along with turbulent mixing zone width, which yields extensive data for comparison with the theoretical results.

The problem physics corresponds to the pressure 10^{-4} GPa = 1 bar in a low pressure chamber. The pressure behind the shock wave in SF_6 is 2.152 bar, density is $1.209 \cdot 10^{-2}$ g/cm^3 , shock velocity is 195.2 m/s, flow velocity behind the shock wave is 97.76 m/s, initial densities of SF_6 and air in the low pressure chamber are $6.037 \cdot 10^{-3}$ and $1.198 \cdot 10^{-3}$ g/cm^3, respectively. The velocity of the shock wave penetrating air is 428.7 m/s and the interface velocity is 130.1 m/s. SF_6 and air properties were taken to be as follows. The two materials are inviscid perfect gases with adiabat indices γ=1.094 (SF_6) and γ=1.4 (air), their molecular weight ratio is taken to be 5.04 (SF_6/air).

The basic goal of the computations was to see how longitudinal velocity component pulsations $<w^2> - <w>^2$ depend on time at sensor locations (Doppler anemometers).

The physical meaning of the problem and research objectives indicate the following environment can be examined as initial input. In $z_{min} \le z \le z_{SW} < 0$ SF_6 state behind the shock wave was taken to have M=1.45. In $z_{SW} < z < 0$, SF_6 is at rest at 10^{-4} GPa, in $0<z<z_{max}$, $z_{max}=300$ mm, air is at rest at 10^{-4} GPa. Here $|z_{SW}|$ can have a relatively small value to ensure low time of shock arrival to the contact discontinuity point (for example, 1%) as compared to the entire computational time that is about 2500μs in terms of physical variables. As the shock passes across SF_6 /air interface discontinuity decay occurs resulting in that the rarefaction wave starts moving to the left (towards lower z values) having the leading front (left) and the trailing front (right) and the shock wave goes to the right to be reflected twice from the edge $z=300$ mm of the mixing zone generated due to the contact discontinuity conversion. By 2500-2700 μs, the shock wave impacts the mixing zone for the third time. The value of z_{min} should be such that the leading front of the rarefaction wave arrives to this boundary at most at 2000-2500 μs so that reflections at the interface, if any, do not produce perturbations able of degrading the solution of interest. The tube geometry $x_{min} \le x \le x_{max}$, $y_{min} \le y \le y_{max}$ is characterized by $x_{min}=y_{min}=0$ and $x_{max}=y_{max}=80$ mm. Thus the walls $x=x_{min}$, $x=x_{max}$, $y=y_{min}$, $y=y_{max}$ and $z=z_{max}$ are taken to be rigid (the boundary value of the corresponding normal velocity constant is zero). The wall $z=z_{min}$ is “permeable” and density, pressure and longitudinal velocity derivatives over z are zero here. Until any perturbations arrive from the computational region, these conditions allow to reproduce the conditions behind the initial shock in SF_6 at each time.

The computations allow the following conclusions.

To reproduce experimental data in an acceptable way, it is sufficient to run computations in the region of size $0 \le x \le 80$ mm, $0 \le y \le 80$ mm, $-100 \le z \le 300$ mm; note that prior to the shock arrival to the interface no numerical perturbations occur in the interface zone. The cross section size of the shock tube does not greatly influence the

computational results. Definition type and density perturbation value impact significantly the computational data. To make the theoretical data closer to experiment, it is necessary to reduce the grid timestep (up to $h=0.333$ mm) with the average value of initial density perturbations in the transient layer up to 20% of the density difference of the gases at rest.

The computations can be run for the tube cross section of 4 x 4 cm, which would allow to reduce the total amount of grid cells.

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NUMERAL SYSTEMS AND INTEGER LOGARITHMS

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Encoding real 1D numbers is accomplished in three steps. The first step finds the quantization law from the given encoding accuracy of all numbers. The second step finds the suite of intracode for all high bits from the accepted amount of digits. The third step adds an appropriate multiplier (digit) to each high bit and generates the code to be fond from the resulting values. This demonstrates three types of numeral systems: defining the accuracy by the absolute uncertainty ΔZ constant for all numbers Z to be encoded yields arithmetic progression quantization. The suite of high bits for 'a' digits is composed of $\bullet^{\pm j}$ components where $\pm j$ = …-2, -1, 0, +1. +2,…– are high bit numbers placing a decimal point in each this suite after a^0 to separate the integer and fractional parts for integer 'a' The third step multiplies each $\bullet^{\pm j}$ by the corresponding digits $k_j \in \{0, 1, 2, \ldots(\bullet\text{-}l)\}$ and sums the result. This yields an additive numeral system code. defining the accuracy by the constant relative uncertainty yields geometric progression quantization with the denominator C, the suite components of high bits are composed of $\bullet\hat{}(\bullet^j)$ from j=0 through m. Then $(\bullet^j)$ are multiplied by the appropriate k_j values and all resulting $\bullet\hat{}k_j(\bullet^j)$ are intermultiplied. This yields a multiplicative numeral system code.

Defining the encoding accuracy for all Z by an arbitrary curve gives nonlinear non-uniform quantization where the representative and reference values like the differences of the latter (quantization steps) will not have analytical relations regarding real measure units. Thus no suite of high bits exists for nonlinear non-uniform quantization. The only existing relationship is that between each Z_i value to be encoded and the quantization step number I**.**, i.e. we deal only with quantitative relationships between all manifolds $\{Z_i \Leftrightarrow$ i**.**$\}$. Hence no numeral system exists for nonlinear non-uniform quantization whose importance is emphasized in the presentation 'Irregular grids…' by I.D. Sofronov at the conference 2002. You can encode the numbers i**.** as such in additive quantization system as follows: I**.** = $\Sigma \mathrm{sign}(i) k_j a^j$ from j=0 through j=m. However quantazing the same range of Z over the geometric progression with a relative constant uncertainty equal to the least maximum relative uncertainty of the original nonlinear quantization yields the values of Z denominated with the neighboring values of the geometric progression members

encoded in the multiplicative numeral system with a relative uncertainty that does not exceed the specified nonlinear quantization over the entire range of Z.

Moreover if you attempt to find the logarithm of the final codes over the base equal to the denominator of the accepted geometric progression you will obtain the integer logarithms allowing simplified and faster computations.

EQUAL-PRECISION TABLES OF TRIGONOMETRIC FUNCTIONS AND INTEGER LOGARITHMS AS ILLUSTRATED BY TANGENT TABLE

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Existing tables of trigonometric functions are generated to be not only interconvertible but to satisfy the accuracies of both the function and angle values. However they can be represented in a more cost-efficient way, i.e. with less lines (number codes), which is crucial for designing a supercomputer from the readings of one-place and two-place computation data. Moreover these tables in addition to the values of trigonometric functions can output their integer logarithms. The most illustrative example is given by the table of tangents and corresponding angles since the values of this function vary from zero to infinity.

How this table can be generated for the first quadrant is described below. As given by [1, 2], you choose the values on the tangent axis (Y-axis) to represent those of geometric progression members with the zero member corresponding to tg45° = 1 and the denominator is = $(100 + |\delta_{max}|)/(100 - |\delta_{max}|)$ where $\delta_{max,\pm l}$ = const=δ_{max} is the maximum relative percent uncertainty of any representative ±i value of $tg_{\bullet,\pm l} = tg_{\bullet\bullet}C^{\pm l}$ for the geometric progression member.

Each pair - $tg_{\bullet,l}$, $tg_{g,l+l}$ (for $tg_{\bullet,i} \geq l$) and $tg_{\bullet,-i}$, $tg_{\bullet,-(i-l)}$ (for $tg_{\bullet,-i} < l$) is separated by a reference (boundary) value of the numerical norm scale $tg_{o,i} = tg_{\bullet,i}\ 100 / (100 + |\delta_{max}|)$. Tracing a straight line from each of them to the right parallel to X-axis representing angles α to intersect the tangential curve and then dropping a perpendicular to X axis gives a suite of reference values for α_{oi}. Any tangent to be found for any α will be determined with a relative uncertainty (that does not exceed δ_{max}) by the representative value of $tg_{\bullet\pm l}$ according to the following bilateral discrete inequality: $tg\alpha \approx tg_{\bullet,l}$ with $(\alpha_{oi} \leq \alpha \leq \alpha_{oi+l})$ for $\alpha \geq 45°$ and $tg\alpha \approx tg_{\bullet,-l}$ with $(\alpha_{o,-i} \leq \alpha < \alpha_{o,-(i-l)})$ for $\alpha < 45°$. Here the suite $\alpha_{0,\pm i}$ does not compose the geometric progression.

Quantizing α axis over the geometric progression for δ_{max}, i.e. finding $\alpha_{o,\pm l}$ and then $\alpha_{\bullet,\pm l}$ and racing perpendiculars from those points to the intersection points of the tangential and horizontals to the intersection point of Y axis will give all $tg_{\bullet,\pm i}$ and $tg_{o,\pm i}$. Now find $tg^{-l}\alpha \approx \alpha_{\bullet\pm i}$ with $(tg\alpha_{oi} \leq tg\alpha < tg\alpha_{oi+l})$. Since $tg_{\bullet,\pm l}$ in the first case and $\alpha_{\bullet,\pm i}$ in the second case are the geometric progression members their ±i integer logarithms.

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NUMERICAL STUDY OF SHOCK INSTABILITY IN THERMODYNAMICALLY IMPERFECT MEDIA

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[3] Landau Institute of Theoretical Physics, Russian Academy of Sciences

The authors of [1–4] develop the linear shock stability theory finding that Hugoniots can contain areas where shock waves are unstable to relatively small perturbations in a broad class of environments (in particular, for the environments having phase transitions and well pronounced ionization). It was shown that two shock instability types are possible: •••• ••••••••, ••• ••••• ••• •••• ••: crimping (absolute) instability characterized by the exponential growth of the periodic shock front perturbation amplitude in time and acoustic instability resulting that the front is the source of sound and entropy downstream perturbations. In the latter case "ripples" at the shock surface exists as long as possible without growing and increasing (this shock response to small perturbations could be called neutral instability). Papers [1, 2] first formulated the criteria for both instability types.

Later, some papers (see, in particular, [5, 6]) showed the shock wave portions meeting absolute shock instability criterion reside inside the portions of non-unique shock discontinuity representation. The latter means that the original shock wave may behave like the arbitrary discontinuity decaying to form an ensemble of other wave components moving with different velocities without catching up each other. In this context, the authors of [6] suggested the absolute instability does not actually occur because of the shock decay resulting in irreversible transition to one of possible wave configurations. The review of these configurations was given in [6], however what configuration is actually selected still remains open.

Despite of nearly fifty years of shock instability study and multiple theoretical publications dealing with linear analysis of this problem there are little experimental evidence of the above mentioned linear predictions considering essentially the decay of unstable shock wave (see, for example, [7, 8]). On the one hand, this may be due to that required thermodynamic conditions are difficult to implement experimentally for the predictions to be true. Another reason may result from poor data describing the history of the shock instability indicating the form it can take within an experiment and how this experiment should be instrumented to interpret nonlinear phenomena in a reliable way. This information could be obtained from a numerical experiment, however we are aware of little publications (see [9, 10] and related references) devoted to the simulation of the shock wave instability; moreover the reported results are fragmentary.

This study is the first one from a series of parametric numerical studies of the shock behavior along Hugoniots containing shock instability portions. The paper studies the shock instability in a model environment with the equation-of-state proposed in [9] and in solid deuterium with the equation-of-state from SESAME library [8]. 2D codes used in simulation were developed from numerical algorithms for Euler equations yielding high-quality description of discontinuous flows. Duplicating the computations using various numerical methods to control potential

impact of the scheme characteristics on the choice of solution in non-unique representation region showed no impact.

Two-wave structure generation was analyzed in the event of the initial shock decay on the lower branch in the non-unique shock representation region overlapping the absolute instability region. The transition from incomplete to complete shock wave was obtained. The paper first considered the case where the initial shock wave decays in stable and acoustically unstable components. The propagation direction of sonic waves produced by the shock front agrees well with linear theory predictions.

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MULTIPHASE MATERIAL EQUATIONS-OF-STATE FOR THE SIMULATION OF HIGH-ENERGY PROCESSES

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Thermodynamically full model is presented for semi-empirical equations-of-state including polymorphic phase transitions, melting and vaporization. For some materials, (metals, carbon) and compounds (alkali metal halogenides), this model served the base to generate the equations-of-state and compute thermodynamic characteristics of various in a wide temperature and pressure range. Various theoretical data were compared with the existing experimental and theoretical results showing a high adequacy degree of high-energy state descriptions.

A method was developed to represent multiphase equations-of-state as the tables of thermodynamic functions and derivatives on grids adapted to phase transition

boundaries (melting, vaporization and sublimation). To fill-in the tables, the plane of variables 'specific volume-temperature (V, T)' is covered with two rectangular grids with the nodes (V_i^s, T_j) and (V_i^l, T_j) for solid and fluid (liquid and gas), respectively, that encompass the parameter range of interest. The timestep sizes are chosen such that the phase boundaries pass only through the cell vertices instead of crossing the cell edges. For his grid generation technique, any stable state of fluid, gas or two-phase compounds such as 'crystal-fluid', 'fluid-vapor', 'crystal-vapor' is matched by the point (V, T) residing either inside of or at the edge of the triangular or quadrangular cell with all its vertices owned by the stability region of the same phase state. For each node, the function value $f_{i,j} = f(V_i, T_j)$ is applied, where f is one the thermodynamic quantities used in the computations, for example, specific internal energy, pressure or adiabatic sound speed. Then is found f at an arbitrary point (V, T) by linearly interpolating over the vertices of the cell receiving the point. A similar approach can be used to describe metastable states.

This technique for table filling allows to use efficiently the resulting multiphase equations-of-state in the numerical simulation of time-dependent hydrodynamic processes in condensed media at high energy concentrations.

KINETIC AND LATTICE BOLTZMANN SCHEMES

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Recently, foreign publications report multiple research efforts dealing with the application of Lattice Boltzmann schemes (LBS). They are successfully used on multiprocessors. The paper tracks the relation between kinetically conjugate schemes and LBS, both used to simulate various physical instabilities on fine space-time grids.

AN ADAPTIVE METHOD FOR SOLVING A MULTIDIMENSIONAL TRANSPORT EQUATION USING REFINED GRIDS IN PHASE SPACE

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The paper presents the main ideas of the adaptive method for finite-difference approximation to a time-dependent multidimensional transport equation with the use of adaptive refined grids in phase space.

The approximation to the transport equation on the grids above is performed separately in spatial, angular and energy variables. For spatial approximation to the transport equation both regular (of a matrix structure) and irregular arbitrary non-orthogonal grids are used, with the transport equation being approximated using AM-S method. The adaptive AM-A method for angular approximation to the transport equation using refined grids has been developed that makes it possible to numerically solve the systems of grid transport equations with the known right-hand parts using the algorithm of successive "point-by-point" computation.

Issues of approximating the transport equation in energy variables using adaptive grids and issues of improving the efficiency of the iteration process of finding solutions to systems of many-group grid transport equations, both on a single

processor and using the algorithm of fine-grain parallelization implemented in Saturn-3 complex are considered.

SPHERICAL SYMMETRY CALCULATIONS ON 3D IRREGULAR LAGRANGE GRIDS

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The authors have developed some techniques for 3D Lagrangian grid arrangement in sphere symmetry calculations. 3D Lagrangian gas dynamics was used for several test computations with newly designed grid types. Test computations examined how spherical symmetry is retained and how the perturbations behave at the shell interfaces in single-domain approximation. The tests include shock and entropy implosion applications. The computational results are compared with the exact solutions of the existing problems.

LARGE-SIZE GRID HANDLING ON DISTRIBUTED COMPUTER SYSTEMS

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Currently the simulation of physical and technology processes is commonly run on multiprocessors using unstructured 2D and 3D grids. The grids containing relatively great amount of nodes allow highly accurate space approximation near complicated shape body surfaces while requiring much computational cost, which results in using multiprocessors. Usually, a computer system running simulation and computational data analysis is a distributed system consisting of one or more multiprocessors, a file server and workstations, which implies additional requirements for user-supplied software configuration. To process large amount of grid data on distributed systems, we offer special software library and visualization package based on client-server technology, which makes it applicable both for local networks and Grid systems. Special-purpose library of interest allow reasonable splitting of 2D and 3D large-size unstructured grids, compaction and distributed input/output of grids and grid functions.