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SUMMARY OF THE FIFTH MEETING OF THE NSC TASK FORCE ON HIGH PERFORMANCE COMPUTING IN NUCLEAR APPLICATIONS

Sheraton, Saratoga Springs
6 October 1997
7-10 p.m.

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Or. Eng.

OECD Nuclear Energy Agency

Fifth Meeting of the NSC Task Force on High Performance Computing in Nuclear Applications

Sheraton, Saratoga Springs 6 October 1997 7-10 p.m.

SUMMARY

1. WELCOME

Bernadette L. Kirk (Chair) opened the meeting and welcomed participants. She explained that this meeting would be shorter than previous ones, as the Secretary of the group had to leave before the originally scheduled date for the meeting (10 October).

2. PARTICIPANTS

The meeting was attended by 20 participants, who introduced themselves. Some attended the meeting for the first time. The list of participants is provided in the Annex. Several members could not attend and sent apologies for their absence.

3. OBJECTIVES OF THE MEETING

The Chair had given an overview of the activities of the group during the session on "Parallel and Distributed Computing" the same morning at the Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications. She recalled when and why the group was set up. The group's objectives include the preparation of a State-of-the-Art-Report (SOAR) on "High Performance Computing in Nuclear Applications" and to provide the OECD/NEA NSC with guidance as to where efforts should be concentrated in Member countries for the advancement of the development of high performance computing in nuclear applications. Another objective is to co-ordinate benchmark exercises in high performance computing and the organisations of seminars, conferences and training courses.

4. STATUS OF THE STATE-OF-THE-ART REPORT

A new draft version of the report was distributed for participants to review and to provide comments and amendments where required (deadline end of October). Some sections require further work, in particular:

a) A foreword needs to be written (*action on E. Sartori, review by B. Kirk*).

b) The Executive Summary should be reviewed by participants. It was felt that in the present form it is too long and should be entitled "Overview". An Executive Summary of about two pages should be prepared (*action on B. Kirk and E. Sartori*).

c) The table with Contributors and Participants should be complemented with a table describing who contributed to which chapter and a general acknowledgement should be prepared listing all those who in some way have contributed.

d) Chapter 1 has been kept very general. Members of the group should express their opinion whether or not the general style is found appropriate.

e) Chapter 2 needs to be reviewed by participants and checked to what extent it duplicates other parts of the text.

f) An introduction needs to be added to Chapter 3, outlining the overall organisation of the chapter and listing the basic equations and different approximations used in radiation transport (*action on E. Sartori and B. Kirk*). Ray Alcouffe has pointed out that a section on the Diffusion Operator (Elliptic Differential Solvers) should be added. He agreed to provide the text of that section (*action on Ray Alcouffe*) Section 3.3.2 on Finite Elements (and Spherical Harmonics) transport methods is missing. K. Kobayashi volunteered to contact Cassiano de Oliveira and to provide a joint text on that subject (*action on K. Kobayashi and C. de Oliveira*).

g) Chapter 4 needs an introduction describing the objectives and outline of the chapter (code systems using different types of basic equations for solving large system analysis problems: safety, waste management, atmospheric dispersion of nuclear materials). A section on large charged particle transport problems should be added to this chapter (*Greg Valdez agreed to prepare this text*).

h) Instead of "'Grand Challenge' Problems in Nuclear Applications", Chapter 5 will be entitled "Additional Challenging Problems in Nuclear Applications". It should contain a list of problems requiring special efforts to develop, especially those for which time constraints are crucial and for which high speed computing is badly needed. Examples are:

   - medical applications with radiation;
   - nuclear methods in oil-well logging;
   - severe accidents analysis;
   - material science (molecular dynamics?) for nuclear applications;
   - problems requiring particularly large computations to enable progress in research (*action on all participants to provide concrete examples*).

i) Chapter 6 should include reference to the effect improved and refined modelling has on safety margins and increased accuracy, and the impact this may have in keeping nuclear energy competitive (*action on B. Kirk and E. Sartori*).

The final version of the SOAR Report should be published by the end of 1997.

5. PROCEEDINGS OF SPECIALISTS' MEETING ON 3-D DETERMINISTIC TRANSPORT CODES – STATUS OF BENCHMARK

The proceedings of the Specialists' meeting have been sent for printing.

The benchmark specification for the new 3-D radiation transport problems with and without scattering (prepared by K. Kobayashi) has been distributed and the deadline for providing the results is 31 October 1997. This benchmark will be the subject of a master thesis under the supervision of K. Kobayashi. Participants agreed that the results they provide can be used in that context. Prof. Kobayashi's student will assemble and synthesise the results provided by participants and will include it into a first draft to be sent to participants, which will include the reference solutions. This report will be commented on by participants.

One issue discussed concerned comparability of results. In particular it was recommended that participants provide information of the volume of the mesh used for which results were requested. In at least one case the reference solution will provide the point values and codes are providing normally cell averaged values. This additional information should help explain some discrepancies that may show up among the results of participants. In addition it was suggested that participants should provide contour plots about sections through the given geometry for the problem. This would be integrated in the final report as appendices and will provide insight into the behaviour of the different methods and codes used.

The list of benchmarks proposed at the 3-D meeting should be expanded to include the one on pressure vessel dosimetry proposed by A. Haghighat. Igor Suslov volunteered to provide a benchmark specification with irregular geometry for consideration by the Group and the NSC (*action on I. Suslov*).

Finally it was suggested that a benchmark on 3-D radiation transport should be defined involving about 25 million meshes in order to compare code performance on parallel machines. This proposal will be provided at the next meeting (*action on R. Baker and R. Alcouffe*).

6. PORTABILITY AND PERFORMANCE OF SELECTED, PARALLELISED COMPUTER CODES

The project proposed at the previous meeting with the objective of determining and measuring portability, scalability and performance of parallelised codes did not meet with enthusiasm as it would draw from participants additional (in most cases not funded) resources. Instead it was agreed that at the next meeting participants should share their experience in implementing Message Passing Interface (MPI) in their codes. Codes that have been parallelised should be sent, where possible, to the distribution centres such as RSICC and NEADB for distribution to interested parties. Both the RSICC and NEADB would arrange that experience gained in portability and performance are fed back to the authors and to the group. E. Sartori reported on the progress made in parallelising modules of an atmospheric dispersion program, a collaboration between the CNAM France, IKE Germany and the OECD/NEA. The parallelised modules will be generally released.

7. RECOMMENDATIONS AND CONCLUSIONS

Participants have expressed concern that lack of funds provided to high performance computing in Member countries in the field of nuclear applications prevents the achievement of major progress and/or breakthroughs. They recommend that the NSC undertake action to ensure that responsible parties in this area are made aware that high performance computing in nuclear applications needs funding. This technology would substantially contribute to refined modelling, reduction of uncertainties, improved determination of margins. Increased availability of high performance computing would also play a role in making/keeping nuclear energy competitive.

8. NEXT MEETING

It was agreed that the next meeting should discuss the results of the 3-D deterministic transport benchmarks, share experience in the implementation of MPI and review progress in the field which will subsequently be reported to the NSC. The date and place suggested for the next meeting was 4-5 August in Paris. These dates are preliminary and may need to be revised because of the holiday season in Europe. An alternative date could be 25-26 August 1998.

14 October 1997

OECD Nuclear Energy Agency

Tentative List of Participants in the Fifth Meeting of the NSC Task Force on High Performance Computing in Nuclear Applications

Sheraton, Saratoga Springs ⁓ 6 October 1997 ⁓ 7-10 p.m.

FRANCE

* MASTRANGELO, Victor Laboratoire de Physique Conservatoire National des Arts et Metiers 292 rue S. Martin 75141 PARIS CEDEX 03	Tel: +33 (0)1 40 24 55 74/21 59 Fax: +33 (0)1 40 27 29 54 Eml: mastrang@cnam.fr
* STANKOVSKI, Zarko DRN/DMT/SERMA CE SACLAY 91191 GIF sur YVETTE CEDEX	Tel: +33 (0)1 69 08 40 64 Fax: +33 (0)1 69 08 94 90 Eml: zstankovski@cea.fr

GERMANY

* ALTES, Juergen Inst.f.Sicherheitsforschung und Reaktortechnik (ISR) Forschungszentrum Juelich D-52425 JUELICH Postfach 1913	Tel: +49 (2461) 61 46 51 Fax: +49 (2461) 61 31 33 Eml: j.altes@kfa-juelich.de
* GRAF, Udo Gesellschaft fuer Anlagen- und Reaktorsicherheit Forschungsgelaende D-85748 GARCHING	Tel: +49 (89) 32004 395 Fax: +49 (89) 32004 301 Eml: gra@grs.de

JAPAN

AIKAWA, Hiroshi Deputy Director, Center for Prom. Computations Sci.&Engr. JAERI 2-2-54 Nakameguro, Meguro-ku TOKYO 153	Tel: +81 (3) 5723 2501 Fax: +81 (3) 5723 2537 Eml: aikawa@koma.jaeri.go.jp
ASAI, Kiyoshi Director of CCSE JAERI 2-2-54 Nakameguro Meguro-ku Tokyo 153	Tel: +81 (3) 5723 2500 Fax: +81 (3) 5723 2539 Eml: asai@koma.jaeri.go.jp
IMAMURA, T. CCSE JAERI 2-2-54 Nakameguro Meguro-ku Tokyo 153	Tel: Fax: Eml: imamura@koma.jaeri.go.jp

KABURAKI, Hideo
Center for Promotion of
Computational Science & Engeneering
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun
Ibaraki 319-11
Tel: +81 (29) 282 6826, 5976
Fax: +81 (29) 282 6070
Eml: kaburaki@sugar.tokai.jaeri.go.

KOBAYASHI, Keisuke
Dept. of Nuclear Engineering
Kyoto University
Yoshida
KYOTO 606-01
Tel: +81 (75) 753 58 32
Fax: +81 (75) 753 58 45
Eml: a51836@sakura.kudpc.kyoto-u.ac

MEXICO
DEL VALLE GALLEGOS, Edmundo
Comision Nacional de Seguridad
Nuclear y Salvaguardias
Dr. Barragan 779
Col. Doctores
Mexico, D.F.
Tel: +52 (5) 590 5162
Fax:
Eml: cnsns1@servidor.unam.mx

RUSSIAN FEDERATION
SUSLOV, Igor R.
Institute of Physics and
Power Engineering
Bondarenko Sq. 1
249020 OBNINSK
Kaluga Region
Tel: +7 (08439) 98491
Fax:
Eml: suslov@chadwick.engr.utk.edu

SPAIN
* GARCIA DE VIEDMA, Luis
Deputy Director, Computing
Consejo de Seguridad Nuclear
C/Justo Dorado, 11
28040 MADRID
Tel: +34 (1) 3460 124, 178
Fax: +34 (1) 3460 588
Eml: lgva@csn.es

PENA, Jorge
Computing Centre
Consejo de Seguridad Nuclear
C/ Justo Dorado, 11
28040 MADRID
Tel: +34 (1) 346 0123
Fax: +34 (1) 346 0588
Eml: jpg@csn.es

UNITED KINGDOM
* DE OLIVEIRA, Cassiano R.E.
Appl. Mod. & Computation Grp.
Centre Environmental Techn.
Imperial Col.Sci.Tech. & Med.
Prince Consort Road
LONDON SW7 2BP
Tel: +44 (171) 594 9319
Fax: +44 (171) 594 6540
Eml: c.oliveira@ic.ac.uk

UNITED STATES OF AMERICA
ALCOUFFE, Raymond
Los Alamos National
Laboratory
MS B-226
LOS ALAMOS, NM 87545
Tel: +1 (505) 667 5956
Fax: +1 (505) 665 4080
Eml: rea@lanl.gov

AZMY, Yousry
Oak-Ridge National Laboratory
Ms-6363
P.O.Box 2008
OAK-RIDGE, Tennessee 37831
Tel: +1 (423) 574 8069
Fax: +1 (423) 574 9619
Eml: yya@ornl.gov

BAKER, Randal S.
Los Alamos National Laboratory
Radiation Transport Group
XTM, MS B226
LOS ALAMOS, NM 87545
Tel: +1 (505) 667 3041
Fax: +1 (505) 665 5538
Eml: rsb@lanl.gov

BOHNHOFF, Bill
Sandia National Lab.
Albuquerque
New Mexico 87102
Tel: +1 (505) 844 0092
Fax: +1 (505) 845 7841
Eml: wjbohnh@sandia.gov

* BROWN, Forrest B.
P.O. Box 9049
NISKAYUNA, NY 12309-9049
Tel: +1 (518) 395 7370
Fax: +1 (518) 395 6171
Eml: brownf@rpi.edu

* CODELL, Richard
U.S. Nuclear Regulatory Comm.
Mail Stop T7D13
WASHINGTON, DC 20555
Tel: +1 (301) 415 8167
Fax: +1 (301) 415 5399
Eml: rbc@nrc.gov

HAGHIGHAT, Alireza
Nuclear Engineering Dept.
Pennsylvania State University
231 Sackett Building
University Park, PA 16802
Tel: +1 (814) 865 0039 OR 1341
Fax: +1 (814) 865 8499
Eml: haghigha@gracie.psu.edu

(Chair)
KIRK, Bernadette L.
Radiation Safety Information Computational Center
Oak Ridge National Laboratory
Post Office Box 2008
OAK RIDGE, TN 37831-6362
Tel: +1 (423) 574 6176
Fax: +1 (423) 574 6182
Eml: blk@ornl.gov

KUCUKBOYACI, Vefa
Penn State University
Nuclear Engineering Dept.
231 Sackett bld
University Park, PA 16802
Tel: +1 (814) 865 2858
Fax: +1 (814) 865 8499
Eml: vefa@gracie.nuce.psu.edu

PETROVIC, Bojan
Nuclear Engineering Dept.
Pennsylvania State University
231 Sackett Building
University Park, PA 16802
Tel: +1 (814) 865 0045
Fax: +1 (814) 865 8499
Eml: petrovic@gracie.nuce.psu.edu

PEVEY, Ronald
Nuclear Engineering dept.
University of Tennessee
Knoxville, TN 37996
Tel: +1 (423) 974 7573
Fax: +1 (423) 974 0668
Eml: rpevey@utk.edu

SJODEN, Glenn E.
USAF Academy
P.O. Box 242
Colorado 80840-0242
Tel: +1 (719) 333 3995/4470
Fax: +1 (719) 333 2114
Eml: sjoden@gracie.nuce.psu.edu

VALDEZ, Greg D.
Sandia National Laboratories
MS 1179
Albuquerque,
New Mexico 87185-1179

Tel: +1 (505) 845 7798
Fax: +1 (505) 845 7841
Eml: gdvalde@sandia.gov

International Organisations (Secretary)
SARTORI, Enrico
OECD/NEA Data Bank
Le Seine-Saint Germain
12 boulevard des Iles
F-92130 ISSY-LES-MOULINEAUX

Tel: +33 (0)1 45 24 10 72
Fax: +33 (0)1 45 24 11 10
Eml: sartori@nea.fr

* Regret not to be able to attend this time