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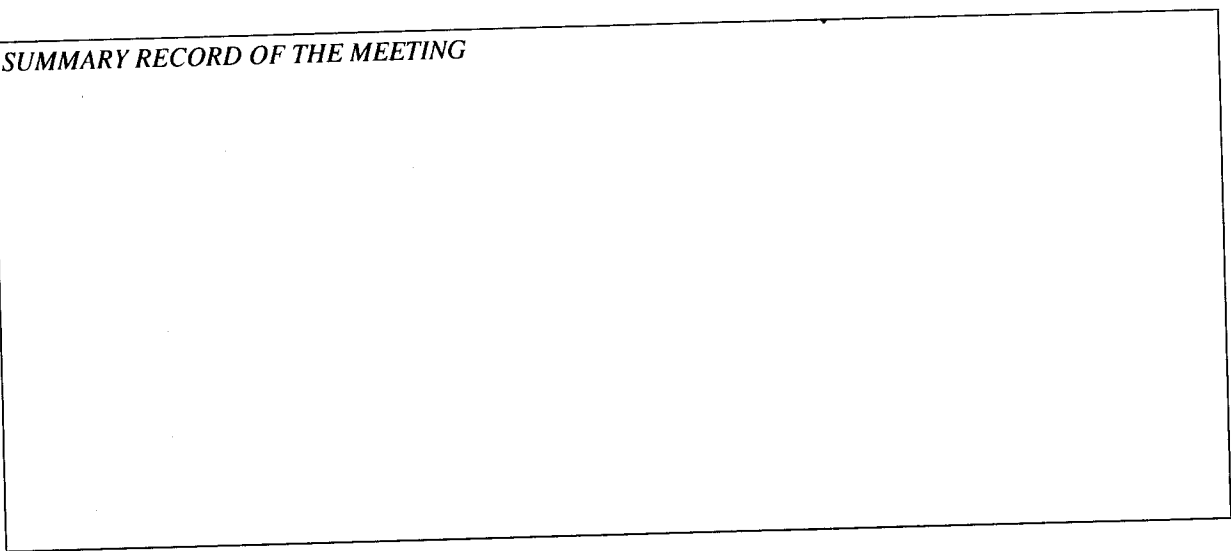
NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

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**TASK FORCE MEETING ON ADAPTING COMPUTER CODES
IN NUCLEAR APPLICATIONS TO PARALLEL ARCHITECTURES**

OECD,Château de la Muette,Paris from 10 to 12 July 1996

SUMMARY RECORD OF THE MEETING



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**Task Force Meeting on Adapting Computer Codes
in Nuclear Applications to Parallel Architectures**

OECD Chateau de la Muette
2 rue André Pascal
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10-12 July 1996

SUMMARY OF MEETING

1. Introduction

1.1 General Items

The Chair Bernadette L. Kirk opened the meeting and welcomed participants to the fourth meeting of the group.

Participants introduced themselves; several members sent apologies for not being able to attend but expressed their willingness in contributing to the work of the group and their interest in attending future meetings. The list of participants is provided as Annex 1.

The proposed agenda was reviewed, presentations by members identified under the different topics and L. Garcia de Viedma suggested to add an additional point: Recommendations to the Nuclear Science Committee. The agenda was approved with this addition. The agenda is provided as Annex 2.

1.2 Objectives of the Meeting

The Secretary of the meeting briefly recalled the main objectives of the meeting :

- discuss the draft state of the art report and propose changes in the light of the most recent developments,
- identify work required to finalise the report, distribute tasks and define a schedule aiming at the publication of the report
- define a work programme for the next year

1.3 Summary of the discussions at the 7th NSC meeting concerning the work programme of the group

L. Garcia de Viedma, representing the NSC recalled first how and why the group was set up. It was set up as one of the tasks of the Working Party on Advanced Computing (WPAC), comprising in addition tasks on quality assurance issues and existing codes, quality assurance standards, and process control software; the NSC had charged the group on supercomputing in nuclear applications to providing advice as to the developments required to adapt existing codes to newly emerging computer architectures and supercomputers, expected developments, their costs and benefits. The NSC expects that the state of the art report is completed by the end of the year; it would be published after NSC has reviewed it.

A proposal presented at the last NSC meeting by Japan concerning future work had been transmitted to the group for discussion and possible approval. The NSC is expecting in addition recommendations for a work programme of the group for the coming year.

It was agreed that these topics are discussed under their respective agenda items.

The list of papers discussed and distributed at the meeting can be found as Annex 3. Their content is not summarised here, but copies can be obtained on request.

1.4 Review of evolution and trends in advanced computing

B. L. Kirk presented a "Review of Computer Trends and Technologies". F. Diez Sacristan presented "Parallel Vector Processors or Massive Parallel Processors ?" This information will be integrated in a summary form in the general chapter on high performance computer architectures and systems.

2. Review of the Draft State-of-the-Art Report

Topics co-ordinators or their substitutes presented the different chapters discussing high performance computing in nuclear applications and commented the draft version distributed before the meeting. Other members have presented additional experience and developments, a summary of which will be integrated in the respective chapters. Most of the chapters concerned with nuclear applications are already in good shape.

The general chapters, such as executive summary, introduction, and others need still more work to be completed.

Annex 3 lists the papers discussed.

In summary the following actions were agreed on :

Title:

The title of the report should be revised to:
 "High Performance Computing in Nuclear Applications" with subtitle
 "Adaptation of Computer Codes to Parallel Architectures".
 "State of the Art Report of a Task Force of the Nuclear Science Committee"

Foreword:

This part needs to be written; it will include a brief description on how the group was set up and its scope and objectives. It will mention that it is a first international report addressing these issues, that it is not fully comprehensive of all work carried out in the field but that it concentrates on the most promising aspects (action on: E. Sartori, B.L. Kirk and L. Garcia de Viedma)

Executive Summary:

This part will introduce the subject and explain what high performance computing can

achieve, for what it is and for what it is not needed. It will include also a summary of the conclusions of each chapter. The title of the first section should be changed from "Nuclear Reactors and Parallel Computing" to "Nuclear Applications and Parallel Computing"; a slight expansion to reflect this wider scope should also be made. All specific references to computer vendors and specific computer codes should be removed from this part, because it could be considered as advertising and meet with objections from different parties. References to vendors and codes will be relegated to the specific technical chapters, where actual work is described, but all style that might be interpreted as advertising should be avoided. The brief chapter summaries need to be revised in line with the chapters themselves. Proper recommendations should be added as a last section. (Action on: A. Kavenoky, L. Garcia de Viedma, B.L. Kirk, and E. Sartori).

Contributors and Participants:

This table will include the names of those who have contributed written parts to the report, and of those members having attended at least two meetings and contributed in ideas and amendments. Indirect contributions will be acknowledged in the references. The table will acknowledge what chapter each has contributed to. (action on: E. Sartori)

Chapter 1 : Introduction:

This section should give a general background on the importance of computing in general and what the role of parallel computing is in particular. A graph should be added showing the evolution of computing power since nuclear energy was started to be used. It should also give an overall outline of the report and briefly describe the content of each chapter. (action on : B.L. Kirk and E. Sartori)

Chapter 2: High Performance Computers and Computing (in General)

A first part has already been written by L. Garcia de Viedma . The paper by Y. Azmy: "Multiprocessing for Neutron Diffusion and Deterministic Transport Methods" to be published by Progress in Nuclear Energy describes in the chapter: The Basics of Multiprocessing, the different concepts and issues very well. It is suggested that with the approval of the author, this information is used in this chapter. In addition the information provided at the meeting by B.L. Kirk and F. Diez Sacristan should be integrated as well as the section covering this aspect in the discrete ordinates chapter. In summary it should explain in a not too technical language what HPC is all about, the different architectures and issues and discuss in addition aspects of programming languages, their compilers and tools for HPC. The comprehensive table describing today's advanced computer platforms and their characteristics should be omitted as it would become obsolete overnight. (Action on: L. Garcia de Viedma, B.L. Kirk and A. Kavenoky)

Chapter 3:

In the draft, chapter 3 is about "Grand Challenges in Nuclear Applications". The group agreed that this chapter should become Chapter 5. Former Chapter 4 "Assessment of Status and Needs" would be subdivided into two parts: Chapter 3 would deal with the basic equations needed for nuclear applications and their parallel implementation in codes solving them. Chapter 4 would address code systems applying several of these equations to solve very large problems; i.e. fields of work that would benefit considerably from parallel computers. The proposed title for chapter 3 is: Basic Equations and Parallel Computing - Assessment of Status and Needs.

Section 3.1 Introduction

This introduction should describe in a tabular form the different basic equations and computational methods used to solve them as relevant for nuclear applications. It should point out which ones are used exclusively in nuclear applications and which ones are shared with other areas of technology. A mission researchers in nuclear applications have is to deal with the equations they are exclusively concerned with. Physics and mathematics knowledge is needed for parallelising refined models; existing software engineering tools are helpful but do not provide efficient code. (Action: E. Sartori and other members).

Section 3.2: Stochastic Method - Monte Carlo

The chapter co-ordinated by F. Brown is in very good shape. H. Khalil has been asked to provide F. Brown with the additional information on the VIM code for possible updating. The question was raised whether the work on perturbation in MCNP needs to be mentioned. It was also considered worthwhile to maybe express a bit stronger, that for certain applications parallel use of MC was not as easy as one would like to believe (criticality and time dependence) (Action on: F. Brown and H. Khalil). (Comment received by H. Khalil: the text as it stands does reflect well all relevant aspects)

Section 3.3 Deterministic Transport

This section, it was suggested, should be further subdivided:

Sub-section 3.3.1 Discrete Ordinates (Sn) Method

This part is practically final. The section describing computer architectures should be moved to Chapter 2.

Sub-section 3.3.2 Finite Element Transport Methods

This part will be prepared by C. De Oliveira.

Sub-section 3.3.3 Nodal Transport Methods

This part will be provided by H. Khalil.

Sub-section 3.3.4 Collision Probability Methods

Z. Stankovski has prepared this part. It was suggested that the first part be kept general so it would cover other codes besides Apollo-II. This is possible with a few minor modifications. Work from J. Vujic and R. Roy should also be included.

Section 3.4 Computational Mechanics and Fluidodynamics

This chapter co-ordinated by J. Altes is in good form. After discussion it was agreed that the work presented by J.P. Gregoire should be included. Reactor 3D thermal-hydraulics codes should be briefly mentioned. A section specific to nuclear applications should be added, as well for uniformity reasons, Conclusions, Perspectives and Challenges should be added. (Action on: J. Altes and J.P. Gregoire).

Chapter 4: Nuclear Applications and Parallel Computing - Assessment of Status and Needs

Section 4.1 Introduction

The introduction should indicate more or less the following: commercial codes are unlikely to be rewritten in the near future for massive parallel computers because industry is

often happy with the physics they contain; in addition they contain built-in technological know-how and experience (hard-wired) for today's standard industrial applications. The effort that has been devoted to have the codes licensed and have a QA label has been formidable. Adaptation for use on a few processors run in parallel is considered by some vendors, because it would require less effort than on massive parallel computers and the validation of the modules involved would not need to be repeated. This would shorten response times and has the advantage of tapping unused computer resources overnight. However, available computer power on sequential processors and the methods used in the codes are limiting detailed analysis, especially for new, non-standard designs, advanced fuel cycles and refined modelling. For these new applications hard-wired knowledge from standard applications as integrated in commercial codes is rarely applicable. New codes should therefore be designed to work on the new computer architectures and use more basic principles rather than using hard-wired know how. (Action on: E. Sartori, B.L. Kirk).

Section 4.2 Reactor Safety

Also this chapter is in almost final form. Additional experience as reported by U. Graf, R. Beelman and others should be included. Contacts with the developers of CATHARE should be made in order to update that section (Action on: J. Pena, J.P. Gregoire, E. Sartori).

Section 4.3 Atmospheric Dispersion of Radioactive Materials

A comprehensive review has been prepared by V. Mastrangelo and I. Mehilli covering the characterisation of the wind field and particle dispersion within it. Emphasis goes to small and meso-scale models using congruent co-ordinate systems. A section concerned with radioactivity specific aspects, such as dose calculation will be added (direct contribution from clouds and deposited material). Work and experience from Japan and from the EDF should also be added. It was agreed to remove the list of computer vendors and most powerful computing site because that list becomes so quickly obsolete). (Action on: V. Mastrangelo, I. Mehilli, J.P. Gregoire, E. Sartori)

Section 4.4 Waste Management

Probabilistic performance assessment of nuclear waste repositories can profit very much from parallel computing. If no expert working in the field, available for writing the chapter is found at least the benefit such assessments could gain from parallel processing should be described. (Action on: E. Sartori).

Chapter 5: Grand Challenges in Nuclear Applications

Nuclear applications have systematically been omitted from current lists of "Grand Challenges", for two reasons: one, because it might give the wrong impression that there are still large problems to be solved for today's reactors, two, because holders of such lists wish to have a "clean", non controversial list (ethnic cleansing). The definition of "Grand Challenges" is not the same for everybody. The group interprets it as very large problems, that cannot be solved within a reasonable time on today's conventional computers and methods and the solution of which would provide a leap forward and speed up in technological achievements and understanding of phenomena. The group agreed to add such a list specific to nuclear applications. Several areas should be covered, safety: severe accident simulation; radiological impact: real time diagnostics of radioactivity dispersion around a potential accident site; waste management: full scale radioactive waste repository performance assessment over

very long time periods within a few hours. Optimisation of irradiation for cancer therapy: response within a few minutes; reactor simulations: full scale real time simulations of the reactors system. These problems should be described in detail, others once identified should be added. A text justifying the importance and impact of solving these problems should be added. (Action on: E. Sartori and all participants).

Chapter 6: Conclusions and Recommendations

This should be a summary of the conclusions and recommendations of each chapter. General recommendations to NSC should be included. (Action on: L. Garcia de Viedma, B.L. Kirk, E. Sartori)

Appendices:

- Glossary of terms used should be added to help non experts to understand better some of the terminology used.
- List of WWW pages giving update information on the development of high performance computing.

3. Final Phase of the State-of-the-Art Report

The tasks to be accomplished to produce the next draft are described in section 2. New versions of the chapters should be submitted by end of August. A new draft version will be circulated to participants and authors by mid-October for final review. A final draft will be prepared for approval by authors and members of the group and then submitted for review to the Nuclear Science Committee (Action on: L. Garcia de Viedma and E. Sartori).

4. Programme of Work for Next Phase

L. Garcia de Viedma, representing NSC introduced the proposal made by Japan at the last NSC meeting. The working method would be as follows:

- selection of existing representative codes to be parallelised
- arrangement of available parallel computer resources
- using available parallel computer resources
 - . parallelisation of selected codes by participating countries
 - . test run and parallelisation tuning
 - . runs for performance evaluation
- analysis of results from runs
- preparation of report

First of all the group agreed that this proposal would be beneficial to the work carried out by the task force; it will be a good test for portability and an effective way of gauging performance. In general it was felt that there is no lack of available high performance computer resources in the different countries; they are generally available free of charge if a high performance computation project is submitted and approved.

Because parallelisation of codes is a horizontal activity across many fields of application and the members of the group are representative of this diversity it is difficult to identify specific projects in this respect for the whole group. Therefore grouping by area of interest and work distributed to such sub-groups would be an efficient way to proceed.

A first candidate for parallelisation has been identified: it is the code NOABL, used

for determining the wind field over complex terrain. The portability of this module once parallelised as well its scalability will be determined. It will then be integrated as a module of a more general code system for modelling atmospheric dispersion of nuclear materials.

The Group feels that a set of codes that have already been parallelised should also be checked concerning portability, performance and scalability.

The following were identified:

MCNP4 - Monte Carlo for Radiation Transport Problems in General

KENO-Va - Monte Carlo for Criticality Safety

EVENT - 3D finite-elements radiation transport including time dependence

VIM - Monte Carlo for Criticality Safety

VARIANT- 3D nodal transport code

TRAC - Nuclear safety code

several others can be added to the list once they have been identified, however many existing codes are poor candidates for parallelisation. For some of the codes on the list an appropriate arrangement for transfer to other centers needs to be made.

The Group suggests to NSC that the project proposed by Japan be accepted and that contacts are taken up with the proposing parties to clarify few procedural points.

5. Seminars

A seminar on 3D deterministic radiation transport computer programs has been proposed with the co-sponsorship of the Task Force. It is scheduled for 2-3 December 1996 in Paris. Participants agreed to co-operate in shaping the technical programme and to encourage presentation of codes and their parallelisation.

Similar seminars, covering other aspects of nuclear applications should be held in the future.

6. Status of M&C and SNA'97 Conference, Saratoga Springs

Brochures with the announcement (R. Mendelson) have been distributed. Members of the group have been asked to make publicity for it in their work environment and to encourage submission of abstracts describing relevant new work concerning high performance computing in nuclear applications. It was proposed to present a review of the Group's report at the conference. (Action on: B.L. Kirk).

7. Recommendations to NSC

- The Task Group recommends that the NSC reviews the final report, comments on it and approves its publication (end 1996).
- The proposal made by Japan through the NSC can be adopted by the group without a need of setting up a new task force.

The parallelisation of one important module NOABL, needed for the wind field calculation in atmospheric dispersion simulations will be parallelised and the speedup and scalability determined. Codes that have already been parallelised will be made available for an

international exercise on gauging the speedup and scalability on different architectures.

The Group recommends that the NSC approves this activity.

- The Group will organise seminars and sponsor conferences on specialist topics and methods that can best profit from parallel computing. A first seminar concerns 3D deterministic transport codes and will be held from 2-3 December 1996 in Paris. The NSC is asked to approve participation in this seminar.
- The group will monitor progress achieved in member countries concerning use of advanced computing in nuclear applications. The summarised results will be submitted to NSC and where badly needed action is identified, proposals will be submitted. The Group proposes that a revised State-of-the-Art report is produced within 3 years, because this area is changing very fast and although particular effort has been devoted to keep the present report general enough to be valid for some time updates will be needed to reflect new issues and challenges.

8. Date and Place of Next Meeting

Participants have suggested that the next meeting be held in conjunction with the M&C and SNA'97 conference in Saratoga Springs in October 1997; the duration shall be one day. This will be sufficient as a large number of new developments in the field will be presented at the conference.

The Chair thanked all participants for attending and providing essential contributions to the success of the meeting.

ANNEX 1

List of Participants

NSC Task Force Meeting on Adapting Computer Codes in Nuclear
Applications to Parallel Computing Architectures

OECD Headquarters - Paris, 10-12 July 1996

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ANNEX 2

Organisation for Economic Cooperation and Development (OECD)

Nuclear Energy Agency (NEA)

Nuclear Science Committee

Task Force Meeting on Adapting Computer Codes
in Nuclear Applications to Parallel Architectures

OECD Chateau de la Muette
2 rue André Pascal
75016 Paris

10-12 July 1996

AGENDA

1. INTRODUCTION

1.1 Introductory Remarks
Introduction of Participants
Approval of the Agenda

1.2 General Introduction: objectives of the meeting

1.3 Summary of the discussions held at the 7th NSC Meeting concerning the work
programme of the Task Force

1.4 Short review of evolution since the last meeting of high performance computing
in general and in nuclear research in particular, expected trends

2. REVIEW OF THE DRAFT STATE-OF-THE-ART REPORT

2.1 Chapter Presentation by the Group Leaders on Adapting Codes with different techniques
to the new computer architectures

- * Monte Carlo Methods
- * Deterministic Transport Methods
- * Collision Probability Methods

- * Finite Elements Method
- * Nodal Transport Methods
- * Computational Mechanics and Fluid Dynamics
- * Adaptation of Nuclear Safety/Accident Analysis Codes to new Architectures
- * Atmospheric Dispersion of Nuclear Materials
- * System Assessment in Radioactive Waste Management

2.2 General Chapters

- * Introduction: history , scope and objectives of the report
- * Needs for high performance computing in Nuclear Applications
 - . status of High Performance Computing in General, Hardware, Programming Languages, Compilers, Tools
 - . Expected future trends
 - . basic equations/methods for nuclear applications (overview)
- * grand challenge problems in nuclear applications (future perspectives)
- * Conclusions and Recommendations (Efforts needed, costs, benefits)
- * Appendices

3. FINAL PHASE FOR THE STATE OF THE ART REPORT

- * Identification and distribution of tasks
- * Schedule for finalizing the report
- * Final review of text and publication

4. PROGRAMME OF WORK FOR NEXT PHASE

- * proposals for joint adaptation or new development of parallelised codes
- * selection of proposals, method of work, resources needed
- * schedule
- * updating of state of the art report; needs, frequency

5. SEMINARS

- * proposal for a seminar on 3D deterministic transport codes, autumn 1996
- * other proposals

6. STATUS of M&C+SNA'97, Saratoga Springs

7. RECOMMENDATIONS TO THE NSC

8. DATE AND PLACE OF NEXT MEETING

ANNEX 3

NSC Task Force Meeting on Adapting Computer Codes in Nuclear
Applications to Parallel Computing Architectures

OECD Headquarters - Paris, 10-12 July 1996

List of Distributed and Discussed Papers

1. Agenda NEA/NSC/DOC(96)-19
2. List of Participants
3. E. Sartori: Circular letter to participants, 1 July 1996
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