UNITED STATES
NUCLEAR REGULATORY COMMISSION
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October 6, 1994

MEMORANDUM TO: Margaret Federline, Chief
Performance Assessment and Hydrology Branch

THRU: Norman Eisenberg, Section Leader JJM for NAE
Performance Assessment Section, PAHB

FROM: Richard Codell RC
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SUBJECT: GEOTRAP REVIEW MEETING AND NEA COMPUTER MEETING

GEOTRAP Review Meeting

I attended the GEOTRAP review meeting on August 29, 1994, at NEA headquarters in Paris. The meeting was attended by 16 people representing Belgium, Finland, France, Germany, Sweden, Switzerland, the United States and NEA (see attendance list). I was the only U.S. representative. The U.S. Department of Energy Yucca Mountain and WIPP projects however, have expressed their interest and willingness to participate, and have been communicating their comments to the project. One of the DOE comments alluded to the use of the C-Well results at the Yucca Mountain site which involves hydrological and tracer testing in the saturated zone. Additional national groups not in attendance expressed willingness to participate and sent comments.

The purpose of this meeting was to finalize details of the proposed GEOTRAP project. The working group discussed the format and content of the proposed project, which would be a forum to exercise and compare model and field studies for nuclear waste repositories. Previous international workshops such as HYDROCOIN, INTRACOIN and INTRAVAL focused on a set of standardized modeling exercises and field studies in which all international groups were involved. GEOTRAP will be issue-based, focusing on the issues of spatial heterogeneity and retardation. All parties would approach these issues using examples from their own sites, most likely planned or actual sites of nuclear waste disposal or underground laboratories. Meetings would be scheduled on about nine month intervals, but possibly more frequently at the beginning, as was the case with the DECOVALEX project.

The workshop would limit attendance to a small group from each project consisting of multiple disciplines. Those invited would have done the work and solved problems, but there should be provisions for others attending, including those involved with making decisions about funding projects and those with pressing scientific questions. Teams would report on their own work, with emphasis on its impact on performance assessment. Reports would be produced after each workshop assessing the status of the main issues (e.g., spatial heterogeneity and retardation). GEOTRAP would be coordinated with the NEA-sponsored SEDE and PAAG groups.

One of the proposed features of GEOTRAP is that each of the national groups would have the responsibility to conduct a review of one or two of the other groups' work, in order to gain constructive feed-back to the process. There was some concern aired by the participants that a one or two day review during



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the GEOTRAP meetings would be superficial, and any review conducted outside of the meetings would be a burden to the participants. Many of the participants expressed concern that they were already engaged in advanced work concerning their own nation's repositories, and had little time or resources to engage in extended reviews or preparations for GEOTRAP. In many respects, this is the same criticism leveled at INTRAVAL because many of the participants had insufficient resources to devote to programs other than their own. The use of the term "review" should perhaps be discouraged in favor of "recorded discussions" of the issues, in order to remove the fear of inadequate reviews being misinterpreted by outsiders. Reviews would be informal, but recorded in interim reports from GEOTRAP. There should be in-depth discussions of presentations and feedback to the presenters, but not criticism. The expenditure of resources by the participants must be kept to a minimum because there are significant commitments to ongoing projects and funds are being diverted from research-oriented tasks to field studies. Most agreed however, that GEOTRAP should go forward, because it would be valuable to have interactions among international experts on these important topics, and exposure by the participants to the state-of-the-art. Because GEOTRAP would be an ongoing program and the presentations would be informal, it would enable the participants to become aware of the technologies at early stages of their development.

Many of the participants voiced concerns that the GEOTRAP project was trying to be too many things to too many people. There was a list of 6 common issues; (1) physical media heterogeneity, (2) physical and chemical retardation of radionuclides, (3) boundary and initial conditions, (4) meaning and measurement of data, (5) matching of spatial and temporal scales, and (6) abstracting complex models and data to simpler models suitable for risk assessments. A prevailing sentiment, including that from the DOE Yucca Mountain Project, was that issues (1) and (2) were the main ones, and that all of the others were parts of any complete attack on the problem. The GEOTRAP project should therefore focus on these two main issues, and let the other four fit into the assessments where they make the most sense. The concern here is that GEOTRAP remain focused and avoid the fragmentation of the project into too many sub-topics. Piet Zudema and Jean-Pierre Olivier commented that the proposal for a long-term GEOTRAP commitment should be composed carefully over a period of several years, as a subgroup of PAAG and SEDE. This was not a uniformly held sentiment, however, and Claudio Pescatore urged that there was already significant agreement among the prospective participants to go forward with GEOTRAP.

There are already a number of national and international working groups on retardation and spatial variability that would fit nicely in the context of GEOTRAP. There is an NEA-sponsored group, MIRAGE, looking at issues related to retardation. The group is informal, and focused on thermodynamic considerations for sorption and complexation at the laboratory scale rather than direct applications to estimating retardation for performance assessment. It was not clear where MIRAGE was heading, and one of the participants proposed that someone from GEOTRAP track its progress. The next MIRAGE meeting will take place in Brussels, 15-17 November 1994. The MIRAGE project will be addressed at the next PAAG meeting, and there should be discussion on how it might complement GEOTRAP. There are also groups organized to deal with spatial variability, although they are oriented to a specific site in which the participants apply their own models and methods. An example of one of these groups is the continuation of the characterization of the Culebra dolomite at WIPP, which is an offshoot of INTRAVAL.

The participants agreed that there should be an attempt to find a more suitable acronym for the meeting than GEOTRAP, and will entertain alternatives.

The participants proposed that there be a "trial" meeting to test out the format with actual presentations and reviews before there would be any long-term commitment to the concept of GEOTRAP. The trial meeting was scheduled tentatively for 20-22 February 1995 in Germany. The decision to continue GEOTRAP will be based in part on the success of this workshop. The first GEOTRAP workshop must be completed prior to the RWMC meeting so its outcome can be presented.

The project will appoint or contract an individual to prepare a comprehensive background report on the history of the NEA modeling workshops and the needs for and importance of GEOTRAP. This will require an experienced person who was involved significantly in these workshops. They expect this to take about 1/2 year. NEA will also produce an agenda for the first workshop. PAAG and SEDE should support decisions on structure of background and support it.

A tentative agenda for the first GEOTRAP meeting would include the following:

1. Introduction - scope and objectives of workshop. Need for GEOTRAP.

2. Issues and organization. Interaction between site characterization on spatial variability, retardation and performance assessment.

3. Presentations from the teams, focused on how the issues were addressed at their site(s).

4. In-depth discussions of the presentations, with feedback but not criticism.

5. Conclusions:
   - Different perspectives on benefits of international cooperation.
   - Report from program committee on issues, need for project, where to focus further meetings, and modes of operation.
   - Discussion and recommendations.

<u>NEA Meeting on Advanced Computing</u>

I attended the meeting at NEA headquarters "Task Group Meeting on Adapting Computer Codes in Nuclear Applications to Parallel Architectures" on August 30 and 31, 1994, following the GEOTRAP meeting. I was one of five U.S. representatives to the meeting (attendance list attached). However none of the other U.S. or other attendees were experienced with applications to nuclear waste management. The range of applications discussed in this meeting dealt mainly with radiation transport, reactor safety assessments, hydrothermal models and structures. The attendees presented their experiences, successes and problems with applying parallel and vector computers in nuclear applications requiring very large amounts of computing power. Some applications require very fast run execution because they must provide answers on an emergency basis or provide realistic simulations for training; e.g., reactor thermal-hydraulics simulations used for on-line accident analysis and plant simulators. Other types of codes do not have this urgency, but require economical computational power to provide answers to very difficult problems on a time scale of hours to weeks.

The application of parallel computing techniques to waste management problems has occurred only recently. I gave a brief presentation of the modeling needs of Iterative Performance Assessment (IPA), and our plans to use a cluster of workstations for Monte Carlo calculations of repository risk.

Although many of the parallel computer applications are outside the field of the repository risk assessments, many of the same techniques should apply. There are a number of computers specially designed for parallel computation, some with thousands of individual processors. Nevertheless, clusters of workstations tied together with special software (e.g., Parallel Virtual Machine (PVM), and EUROPORT) are popular choices for many of the participants because of the low cost and accessibility of workstations during times of low utilization.

There are several classes of computations for which parallel computers are being applied. An important class of problems involves Monte Carlo computations. Cluster computers are ideally suited to Monte Carlo computations in which communications between individual workstations would be minimized. Monte Carlo problems are said to "scale" well; i.e. increasing the number of processors decreases the solution time nearly proportionately.

The other class of computations for which parallel computers are being applied are large multidimensional problems in radiation transport and hydrodynamics. Usually, the computational domain (e.g., the N finite difference cells or finite elements) are divided among a smaller number of processors. This is known as "coarse-grained" or "domain decomposition". Within a single time step, each processor works only on its domain. When all possible computations within the domains are completed, then messages are passed among the domains as many times as is necessary to complete the time step. The two problems that are key to efficient operation of this class of problem are the ability to pass messages quickly among the domains, and the partitioning of the problem so that each of the domain problems are solved at approximately the same time so there is a minimum of waiting. The links among clusters of computers (e.g., Ethernet or Internet) are often the critical path for computational efficiency. Computers specially designed with multiple processors in close physical proximity and shared memories for fast message passing avoid the slow communication links. Both Monte Carlo and domain decomposition require consideration of "load balancing" so that computers or processors are not sitting idle. This is especially the case with clusters of dissimilar computers.

There were remarkable speed-ups in computing results for a class of problems, especially those using Monte Carlo techniques. In some cases, where Monte Carlo techniques were not applicable, improvements were less dramatic. In many cases the computer programs would have to be essentially rewritten to take full advantage of the power of parallel computation. Since many of the codes were highly complicated and have been used successfully on non-parallel computers, there was an understandable reluctance to retrofit these codes to parallel architecture.

Among computers specially designed for modern high-speed computations, there are two dominant philosophies: Parallel Vector Processors (PVP) and Massively Parallel Processors (MPP). PVP computers rely on a relatively few processors, but each one has high computational power capable of vector computations; i.e., up to a few hundred calculations can be completed simultaneously in each processor, providing the results do not depend on other numbers in the same vector. The Cray supercomputers such as those we have used for IPA Phases 1 and 2 and certain of the INTRAVAL calculations are in this category. The technology is mature, and software is in a state of high development, including compilers and debugging tools. The outlook for PVP computers is limited however because there are physical limitations on how much the individual processors can be speeded up. MPP computers do not theoretically have the same limitations because for suitable problems, increasing the number of processors increases the speed of the solution, limited mainly by the problem of message passing. The future therefore lies with MPP computers, but practical considerations such as the state of compiler development, and other tools, favors PVP computers for many present applications.

I was able to learn a great deal from attending the computer meeting that I feel would be applicable to our computational needs in the Division of Waste Management. I see applications of advanced parallel architectures to both the Monte Carlo aspect of waste management problems such as the propagation of uncertainty, and domain decomposition for multi-dimensional groundwater flow and transport problems. The amount of computational power being applied to the problems presented in this meeting is truly astounding, and it appears that we have not begun to tap the resources already available at relatively low cost. For example, workstations such as the IBM RISC-6000 and the Digital Equipment Corporation Alpha are available now for a cost of a few tens of thousands of dollars, yet have the computational power approaching that of current Cray mainframe computers that we have been using for IPA (There is an IBM RISC-6000 in NMSS, but I met some resistance when I proposed to demonstrate its suitability). Workstation cluster computation such as we are proposing for IPA was a popular topic at this meeting, especially when coupled with fast workstations such as the RISC-6000 and Alpha.

It would be interesting to compare the computational effort (e.g., total floating point calculations) for our most recent Phase 2 IPA to several of the calculations discussed at this meeting. The other attendees expressed considerable interest in adding Waste Management to the working group, including the comparison of computational effort involved. The meeting organizers encouraged NRC and other participants to take part in future meetings, and to report on the progress of parallel computer applications to repository risk assessments. The next meeting will take place in Portland Oregon in May of 1995, to coincide with an ANS meeting.

I would be glad to brief you on either of the two meetings I attended. I also have available a number of handouts from the meetings.

Attachments:
1. Attendance list for GEOTRAP meeting
2. Attendance list for computer meeting

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# GEOTRAP REVIEW MEETING

August 29, 1994

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## on Adapting Computer Codes in Nuclear Applications to Parallel Architectures

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