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The Use of High-Performance Computing to Solve Participating Media Radiative Heat Transfer Problems - Results of an NSF Workshop

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EXECUTIVE SUMMARY

Radiation in participating media is an important transport mechanism in many physical systems. The simulation of complex radiative transfer has not effectively exploited high-performance computing capabilities. In response to this need, a workshop attended by members active in the high-performance computing community, members active in the radiative transfer community, and members from closely related fields was held to identify how high-performance computing can be used effectively to solve the transport equation and advance the state-of-the-art in simulating radiative heat transfer. This workshop was held on March 29-30, 1994 in Albuquerque, NM and was conducted by Sandia National Laboratories. The objectives of this workshop were to provide a vehicle to stimulate interest and new research directions within the two communities to exploit the advantages of high-performance computing for solving complex radiative heat transfer problems that are otherwise intractable.

The primary outcome of the workshop is the identification of five major research thrust areas: 1) the development of benchmark solutions, 2) the complex/combined mode problem, 3) the volume rendering problem, 4) the inverse problem, and 5) the solution of the full electromagnetic (EM) equations. Following the workshop, to facilitate communication and teamwork between the participants of the workshop and those recommended by the participants, an E-mail reflector account (hpcinrht@engsci.sandia.gov) was created at Sandia National Laboratories. Using this reflector, research teams were formed to address the five thrust areas identified at the workshop. New research proposals are being generated within these teams, Grand Challenge Application Groups are being formed, and other means of developing cohesive research efforts are being explored.

This document is available for access on the World Wide Web (WWW) at http://www.sandia.gov/html/frame/NSFFinal_with_graphics_1.html and copies have been sent to major research entities, funding agencies and targeted industries in the U.S.

INTRODUCTION

The prediction of radiative transfer in absorbing, emitting and scattering media is critical to advanced development of many important processes at both high and low temperatures, from porous combustors, furnaces and fires to advanced insulation systems for cryogenic superconducting devices. Computational limitations are presently a major factor in dictating the present state-of-the-art since modeling real properties and geometries is very computationally expensive. *Consequently, radiative heat transfer models must be simplified (e.g., spectrally, geometrically, etc.) to keep the computations tractable.* It is expected that high-performance computing will be instrumental in advancing the state-of-the-art by enabling techniques to be employed which include less analytical simplification, more accurate property data, and more realistic geometries. *Potentially, it is possible to modify the computing environment to provide special or specific capabilities that are required for solving realistic radiative heat transfer problems.*

Significant advances have been made recently in computer "horsepower," that is, the ability to perform intense computations rapidly and with large memory capacity. Increases in hardware capabilities, dramatic decreases in effective costs, the development of massively parallel platforms and algorithms, and the ability to link and network high-powered workstations and personal computers are putting the ability to perform intense computations into the hands of most researchers and analysts.

Within the radiative heat transfer community, however, there is a lack of active exploitation of high-performance computing capabilities. The need to do so was apparent at the first symposium on radiative heat transfer solution methods held at the National Heat Transfer Conference in 1992. The symposium participants were asked to solve a 3D problem consisting of a nongray mixture of spherical carbon particles and CO_2 gas contained in a rectangular enclosure. The problem was intended to model a coal-fired furnace. Despite major property and geometry simplifications made in defining the problem, computational times on the order of hours were required to generate results using existing computational techniques. Elimination of any one of the modeling simplifications to make the problem more realistic would render the problem extremely difficult, if not impossible, to solve. Furthermore, it was surprising to find that there existed larger-than-expected variations in the predictions. It was apparent that there exists a need for the radiative heat transfer community to be knowledgeable about high-performance computing and begin exploring its potential in solving problems in the field.

The handling of large amounts of data is an issue which needs to be addressed as part of efforts to exploit high-performance computing. Specifically, very large amounts of data must be efficiently accessible for storage, input/output, and must be readily usable by developers of graphical representation software.

At present, it is not clear if existing hardware and software developed for high-performance computing is designed appropriately to solve radiative heat transfer problems. The high-performance computing community needs to be knowledgeable about the specific aspects of radiative heat transfer and begin exploring the development of computational algorithms and hardware to address them.

It may also be desirable to pursue an object-oriented software approach to solve the radiative transfer equation. Various forms of the same basic equation (generally referred to as the transport equation) are used to model processes in astrophysics, microelectronics, and neutronics. An object-oriented algorithm for solving the general transport equation would benefit researchers in a wide variety of other disciplines.

In summary, although problems involving participating media are often encountered in transport processes, the simulation of complex radiative heat transfer has not effectively exploited current high-performance computing capabilities. There is a need to educate the radiative heat transfer community about the potential of high-performance computing. Similarly, the high-performance computing community needs greater awareness about the barriers to simulating complex radiative

T. W. Tong and R. D. Skocypec, "Summary on Comparison of Radiative Heat Transfer Solutions for a Specified Problem," HTD - 203, Developments on Radiative Transfer, ASME, 1992.

heat transfer. There is also a need for both communities to team and develop interdisciplinary enabling advances.

In response to this need, a workshop attended by members active in the high-performance computing community, members active in the radiative heat transfer community, and members from closely related fields was held to identify how high-performance computing can be used effectively to solve the transport equation and advance the state-of-the-art in simulating radiative heat transfer. This workshop was conducted by Sandia National Laboratories and organized by the authors of this report.

WORKSHOP OBJECTIVES

The objectives of this workshop were to provide a vehicle to stimulate interest and new research directions within the two communities to exploit the advantages of high-performance computing for solving complex radiative heat transfer problems that are otherwise intractable. In particular, the goals were to: (1) educate participants from the radiative heat transfer community about the opportunities of high-performance computing; (2) educate the participants from the high-performance environment about the unique and demanding aspects of radiative heat transfer; and (3) provide a vehicle for the participants to explore interdisciplinary developments in transport modeling, computational algorithms and hardware strategies that will enable a significant improvement in the ability to accurately and efficiently simulate complex radiative heat transfer. It is expected that indirect, but critical, outcomes from this workshop include the generation of new research proposals and the direction of resources by funding agencies.

DISSEMINATION OF WORKSHOP INFORMATION

A summary of the results of this workshop, including the feedback received to date, was presented by the workshop organizers at the 6th AIAA/ASME Thermophysics and Heat Transfer Conference in Colorado Springs, CO during June, 1994. Approximately 80 people attended this session. The results were also presented at the 10th International Heat Transfer Conference in August, 1994. At each presentation, feedback was solicited and has been incorporated into the summary of workshop outcomes. The overall workshop results, including the documentation generated during small group discussions, the general consensus obtained at the workshop, and all subsequent comments, are published in this document. Copies have been sent to major research entities, funding agencies and targeted industries in the U.S. This document is also available for access on the World Wide Web (WWW) at http://www.sandia.gov/html/frame/NSFFinal_with_graphics_1.html.

QUESTIONNAIRE RESPONSES

Approximately two months prior to the workshop, questionnaires on *issues faced by the radiative heat transfer and high-performance computing communities,* were mailed to potential attendees. The questionnaire was developed to provide baseline information to facilitate discussions at the workshop. The questionnaire was divided into three parts, Part I: Issues Faced by the Radiative Heat Transfer Community, Part II: Issues Faced by the High-Performance Computing Community, and Part III: Issues Faced by Both Communities. As a member of the radiative heat transfer and/or high-performance computing community, potential participants were asked to answer all of the questions in either Part I or Part II, all of the questions in Part III, and as much of the remaining part as applied to their experience and expertise.

During presentation of the results at the 6th AIAA/ASME Thermophysics and Heat Transfer Conference in June, 1994 and the 10th International Heat Transfer Conference in August, 1994, members of the community at large were also invited to complete questionnaires. A total of 22 responses were received. Interested parties with a Radiative Heat Transfer (RHT) emphasis submitted 16 responses while 6 responses were submitted by those with a High-Performance Computing (HPC) emphasis. Completion of these questionnaires reflected considerable effort on the part of the participants. The questionnaire results provide valuable insights into the state of the two communities and the issues presently faced by experts in both fields.

An overview of the questionnaire results is presented here. The objectives of this overview are to; 1) summarize the thoughts and ideas of all participants, 2) provide a perspective of the two communities, and 3) identify common themes and key issues. It was not possible to include every detailed comment provided by every member of the group. Only the essential and salient features are included in point form following a statement of the question posed to the participants. In cases where a significant number of participants responded with the same theme, the number of responses is included in braces. An overview of this nature was used at the workshop as a basis to begin workshop discussion.

Summary of Responses

In general, the responses reflect a broad ranges of activities and issues. The most popular responses include:

- Methods - Monte Carlo, Discrete Ordinates
- Platforms - Cray, Workstations
- Languages - FORTRAN 77
- Best Use of HPC - Parallel Platforms

The key features of radiative transfer identified by the questionnaire responses include:

- Complex Geometries
- Action-at-a-Distance Aspect
- Spectral Effects
- Combined Mode Transport

- Scattering
- Nonlinearities

The primary computational difficulties of radiative heat transfer modeling identified by the questionnaire responses include:

- Computational time requirements
- Memory requirements
- Need for platform-specific algorithm development including the lack of code portability
- Lack of compiler maturity for HPC platforms
- Need for grid compatibility in combined mode transport
- Limitation to workstation clusters for industrial applications
- Lack of researcher HPC access and training

Part I: Issues Faced by the Radiative Heat Transfer Community

1. *What radiative heat transfer solution methods and algorithms have you used or are you using in conjunction with high-performance computing? Please be specific about computing platform (e.g. CM5, Paragon, Cray, etc.), programming model (e.g. data parallel, message passing, object-oriented, etc.) and programming language.*

   Methods

   - Monte Carlo (MC) {8}
   - Discrete Ordinates (Sn) {6}
   - Zonal Methods {4}
   - Spherical Harmonics (Pn) {2}
   - Exchange Factor {2}
   - Flux Methods {2}
   - Finite Volume Methods {2}
   - Others including simplified spherical harmonics, integral methods, lattice Boltzmann methods
   - Hybrid methods

   Platforms

   - Massively Parallel (MPP) - Distributed Memory
     - MasPar, nCUBE, Paragon, Meiko CS-2, CM-2 {2}, CM-5 {2}, CM-200
   - Multiple Processor - Shared Memory
     - Sun Dragon, SPARCcenter 2000
   - Serial Mainframe
     - Cray {8}
     - CYBER 205
     - IBM 3090-600J
     - CONVEX

   Workstations

   - SGI {2}

- Sun {2}
- RISC 6000 {2}
- Digital

Languages

- FORTRAN 77 {12}, FORTRAN 90 {4}, C {2}, C++

2. *What computational difficulties have you encountered in solving radiative heat transfer problems in the past?*

Computational time {10}

Memory

Representing complex geometries {9}

  - Limited nodes {4}
  - Limited exchange factors {2}

Modeling spectral problems {3}

Modeling scattering {2}

Modeling all lines of sight {2}

Storage {3}

Coupling of solutions with other PDE (i.e. fluid flow) solvers

Competent compilers and debuggers

3. *What are the current, and estimated future, difficulties associated with using high-performance computing to solve radiative heat transfer problems?*

Most responses focused on current difficulties

Programming software

- Difficult to use {6}
- Not portable {4}

Algorithm development

- Spectral problems {2}
- Efficient with correct physics
- Design to reduce communication time

Availability/Accessibility of machines

Operating system not mature

Lack of funding

4. *What are the estimated computing requirements for solving realistic (i.e. 3D, spectral, complex geometry) radiative heat transfer problems (i.e. required Mflops, number of processors, processor speed, processor architecture, CPU time, etc.)?*

Realistic Problem - 3D, Spectral, Complex Geometry

Speed

- Future requirements: 1000Gflops, 100 Gflops
- Present requirements: 500-1000Mflops, 100Mflops, 0.1Mflops

Memory

- Future: 10 Gbyte, 1.0Gbyte
- Present: 1.2 Gbyte, 500Mbytes, 250 Mbytes (furnace), 100 Mbytes, 33Mbytes (5x7x9 grid)

Disc Space required ranges from 10 - 100 Mbytes for source code

Number of Processors: 1, 64, 1000, 2000

Time

- Workstations - hours (can solve 3D spectral problems)
- Massively parallel - minutes

Applications drive hardware developments, not the other way around

5. *What do you see is the best way to exploit high-performance computing to advance the state-of-the-art in radiative heat transfer?*

Develop algorithms specifically designed for parallel platforms {6}

Increased training of Radiative Heat Transfer (RHT) community in high-performance computing/Increased interaction between RHT and HPC communities {3}

Develop Monte Carlo methods dedicated to parallel platforms {3}

Use HPC to obtain highly accurate benchmark solutions {2}

Develop adaptive techniques

Establish greater portability

Develop techniques for distributed processing with high-performance workstations

Develop efficient techniques to couple RHT and PDE solutions

Microtasking

Requires more memory

6. *What are the novel or unique features of the radiative heat transfer problem that need to be addressed?*

Spectral dependency {5}

Communication-at-a-distance aspect, which results in large dense matrices and increased communication time {4}

Large number of variables (and hence memory) inherent in the problem {3}

Directional dependance {3}

Spectral, temperature, and spatial variation of properties {3}

Highly nonlinear nature of the problem {2}

The optimum algorithm depends on the specific nature of the problem

Integral nature of the equations

Accurate calculation of the divergence of the flux

Grid incompatibility for mixed-mode problems

Part II: Issues Faced by the High-Performance Computing Community

1. *What do you see is the best way to exploit high-performance computing to advance the state-of-the-art in problems such as radiative heat transfer that require large amounts of memory and a large matrix of unknowns?*

   In general, large problems: large amounts of memory and large matrix of unknowns
   Use parallel computing {4}
   - Develop efficient, parallel linear algebra routines
   - Develop automatic parallelizing compilers
   - Use parallel solvers, technologies from other applications

   Develop faster linear solvers, better preconditioners
   Use hierarchal methods (such as Hannahan's) not brute force
   Develop efficient, accurate and stable adaptive methods
   Use out-of-core algorithms and data structures
   Use dedicated computers
   Develop innovative MC methods
   Improve access and training

2. *What computing resources are presently available for solving realistic problems (i.e. Mflops, number of processors, processor speed, processor architecture, memory speed, memory latency, storage opacity, I/O speed, etc.)?*

   Realistic Problem - 3D, Spectral, Complex Geometry
   MPP - Distributed Memory
   - nCUBE 2S (10-300 Mflops actual, 1Gbyte memory, 50-200 nsec latency)
   - Meiko CS-2 (Each Processor: 15Mflops scalar, 180 Mflops vector, 128 Mbytes per node)
   - MasPar (8000 processors)
   - Paragon
   - CM5, CM 200

   Multiple Processor - Shared Memory
   - SPARCcenter 2000 (4 processors)
   - Sun Dragon (up to 16 processors)

   Distributed Processor
   - IBM RS 6000 cluster
   - Sun Workstation cluster

   Vector Mainframe
   - Cray C90, XMP, YMP

   Workstations

3. *What future developments in high-performance computing show promise for enhancing our capability to solve large, complex, coupled problems?*

   Parallel Computation {6}

- Robust, standardized parallel languages and software {3}
- More processors {2}
- Higher speed interconnects between processors {2}
- Automatic parallelizing compilers
- Platforms that allow parallelization of coupled problems

Increased processor speed {3}

More memory {3}

Better operating system handling of nonlocal memory references on message-passing architectures

Parallel Virtual Machine (PVM) for workstation clusters

Better graphics

4. *What is your experience with the state-of-the-art compiler technology for high-performance computing?*

Extent of experience

- Considerable {3}
- Moderate {5}
- Limited {2}
- None {2}

Evaluation of current compiler technology

- Technology far behind hardware - limiting factor {3}
- Overall technology "poor" (i.e., bugs are common) {4}
- For C, technology is adequate

5. *How important is it to have massively-parallel machines as opposed to clusters of workstations?*

MPP

- Advantageous for shared data, coupled solutions {2}
- Better I/O
- Latency-bound for > 16 processors
- Better for RHT
- No unique features for RHT

Distributed

- More cost effective, only option for industry {2}
- Effective for MC
- Communication costs dominate

Should have access to both {2}

More experience required to determine preferred platform for RHT

6. *What support tools (debugging utilities, profiling and analysis of the code, etc.) are available to you and do you find them adequate for your application?*

   Response widely varied depending on platform:
   - Favorable
     - PRISM on CM useful for performance monitoring {3}
     - Sun workstation tools (dbx) useful {3}
     - MasPar excellent
   - Unfavorable
     - Paragon - debuggger originally hung up entire system
     - nCUBE - unusable due to poor documentation & bugs
     - Meiko parallel mode tools not available

   Tools barely adequate & need improvement {3}
   Existing tools not user friendly
   Same compilers, debuggers, performance tools for different platforms would speed development

7. *What computer architectures and programming language seem best suited for the needs of the radiative heat transfer community?*

   Architecture
   - Parallel & parallel vector {3}
   - Workstations {3}
   - Single Processor Mainframe

   Languages
   - FORTRAN 90 {4}
   - C, due to data structure {3}
   - High-Performance FORTRAN {2}

   Platform-portable languages needed
   Still significant room for algorithm development

Part III: Issues Faced by Both the Radiative Heat Transfer and the High-Performance Computing Communities

1. *What high-performance computing facilities are available to you and how does a user obtain access to these facilities?*

   Access to National Lab Systems & National Centers Available {9}
   - Proposal required - oversight committee
   - Most proposals accepted

   Access to workstation as a department resource
   - Access to group (network) of workstations {7}

2. *What high-performance computing facilities have you used?*

   Have used Cray machines {10}

Have used large, MPP machines {8}

3. *How does machine architecture affect algorithm design?*

   Algorithms must be developed for a specific architecture {all}
   Defining best platform/algorithm for class of problems is an area of active research

4. *How has high-performance computing enabled you to solve problems that you would otherwise not have attempted to solve?*

   Enabled Solution
   - 3D problems {6}
   - Spectral problems {3}
   - Complex geometries {3}
   - Problems using Monte Carlo
   - Non-trivial problems

   Some 3D, anisotropic scattering, complex geometry problems yet to be solved
   Hasn't helped

5. *What types of problems are you currently working on solving?*

   Focus on 3D problems {7}
   Coupled problems {5}
   3D, spectral, anisotropic scattering {5}
   Specular reflection
   Properties
   Large, complex geometries (furnaces, incinerators)

6. *Are there model modifications or computing approaches that will significantly alter our abilities?*

   Modeling
   - Use of more efficient algorithms (i.e. hierarchal approaches) {3}
   - Examine combined methods to exploit advantages of each
   - Improvements on grid generation

   Computational Approaches
   - Greater use of MPP {3}
   - Modify existing codes for specific architecture {2}
   - More memory
   - Adaptive parallelism
   - Data parallel languages
   - Machines and compilers that deliver significant fraction of their rated performance

7. *Other issues that you think are important to the topic addressed.*

Needs

- Comparison of MC and deterministic techniques
- Experimental and numerical benchmarks for code development
- Greater portability {2}
- More funding support for HPC use in RHT studies
- Better computational methods for large data sets
- Greater interaction with researchers in related fields, i.e., neutron transport, photon transport and imaging
- Better Property Data
- Separate development efforts for MPP machines and for workstation and PC level machines

Don't go overboard with supercomputing, industry can't support cost and may not need the accuracy

Don't divorce approach from turbulence and fluid modeling approaches

WORKSHOP ACTIVITIES

An overview description of the events comprising the workshop is presented here. A detailed agenda is included in the Appendix B.

The workshop was held at the Doubletree Hotel in Albuquerque, NM and began at 8:00 am on March 29, 1994. Introductory comments and description of the workshop objectives were provided by Russell D. Skocypec, Conference Co-Organizer and Manager of the Thermal and Fluid Engineering Department at Sandia National Laboratories. A welcome to the workshop was offered by David J. McCloskey, Director of Engineering Sciences at Sandia National Laboratories.

In order to further the interaction between the two communities, overviews consisting of technical background information and nomenclature were presented by members of both the high-performance computing and the radiative heat transfer communities. Timothy W. Tong of Arizona State University provided the review of radiative heat transfer topics and nomenclature. High-performance computing review and nomenclature was presented by Merle Benson of Sandia National Laboratories. An overview of the questionnaire responses received to date was provided by Louis A. Gritzo of the Thermal and Fluid Engineering Department at Sandia National Laboratories. This overview established the framework for discussion.

The participants were then divided into 5 small groups and asked to visualize and identify a desired capability 5 years into the future with general ideas on software, hardware and algorithm needs. Small group representatives then presented results from the small group discussion to all workshop participants. The outcome of these small group discussions was a list of concepts and issues which were prioritized by the participants. Given the prioritized list, efforts were devoted to reaching a consensus as to the capabilities to be pursued by integrated high-performance computing and radiative heat transfer research teams. During the discussion, many issues were raised regarding the future direction of radiative heat transfer research and high-performance computing. During this discussion of the future, George Lea from NSF presented an overview of High-Performance Computing and Communications (HPCC) programs. One of the stated NSF HPCC goals is the solution of fundamental problems in science and engineering. The NSF HPCC supports research directed towards these solutions in several ways, one of which is through grand challenge application groups. Supercomputing centers are also made available by NSF for such research endeavors.

After a review of the concepts and issues which resulted from the small group discussions, the participants agreed that the use of high-performance computing to solve radiative heat transfer problems represents the pursuit of a solution to a class of fundamental problems in science and engineering. A framework for the second day of the workshop was then established with the goal of identifying the scope of the problems to be addressed and establishing a mechanism for the creation of grand challenge application teams that integrate expertise from high-performance computing, radiative heat transfer, and related fields.

During the second day of the workshop, efforts were focused on identifying major research thrust areas. Small group meetings were again used for brainstorming with general goals being to identify: 1) what are the appropriate near-term activities, 2) what general direction should be taken to obtain solutions, 3) what are the applications, and 4) what outreach and coupling with other groups should occur. Following the small group meetings, a representative from each group provided a summary to all workshop participants. A discussion period followed during which the presence of high-performance computing was deemed critical for continued developments in radiative transfer. Uncertainties in the future of HPC were also identified which make it increasingly difficult to determine the appropriate direction of radiative heat transfer research. Uncertainties in the future of HPC were highlighted by the two opposing views that; 1) high efficiency shared-memory machines will be common in the next 5 years, and 2) distributed memory machines (with fewer differences in architecture) would be prevalent in the year 2000.

The primary outcome of the workshop is the identification of five major research thrust areas. A summary of these thrust areas was compiled and released for comments. The final draft is included in the next section of this report.

In the course of the closing discussion, it was suggested that an E-mail reflector (i.e. an E-mail address which "reflects" a message to a large group of recipients) should be established. This reflector account has been created at Sandia National Laboratories, the address is **hpcinrht@eng-sci.sandia.gov**. Louis Gritzo (lagritz@sandia.gov) is the point of contact for the reflector. All participants were placed on the reflector and were also requested to provide names of additional interested parties. Additional names were solicited and obtained during presentation of the results at the 6th AIAA/ASME Thermophysics and Heat Transfer Conference in June, 1994 and

L.A. Gritzo, R.D. Skocypec, and T.W. Tong, "White Paper - NSF Workshop on High-Performance Computing in Radiative Heat Transfer" Distributed at the 6th AIAA/ASME Thermophysics and Heat Transfer Conference in June, 1994 and the 10th International Heat Transfer Conference in August, 1994.

the 10th International Heat Transfer Conference in August, 1994. Using this reflector, research teams were formed to address the five thrust areas identified at the workshop.

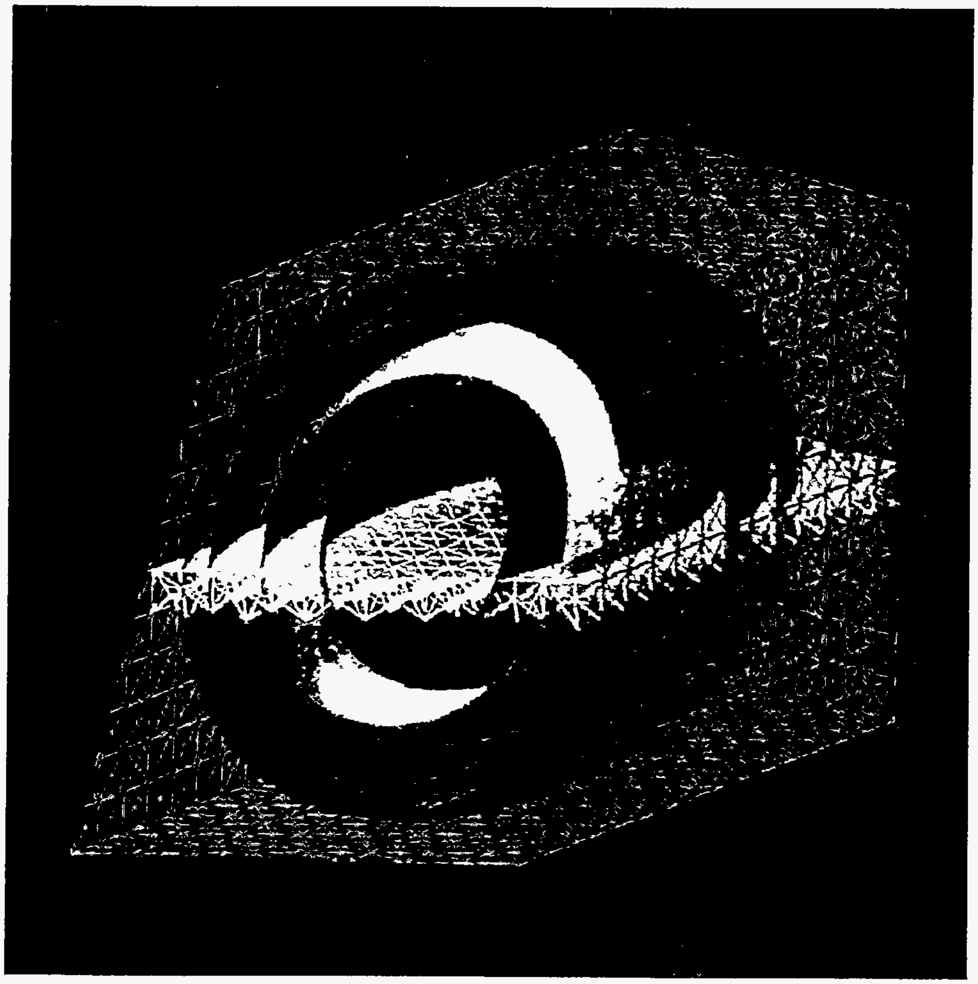
MAJOR RESEARCH THRUSTS

The purpose of this section is to summarize the salient and essential features of the 1-1/2 day workshop. The participants of the workshop, and those recommended by the participants, are encouraged to present their views and feedback to the group via the E-mail reflector system established for this purpose. This section, and the ensuing discussion, is intended to form a framework for the development of interdisciplinary teams to address the "grand challenge" problems identified in these five major research thrusts.

The participants from the radiative heat transfer community felt that the current capabilities for simulating participating-media radiative heat transfer are too limiting. Many important heat transfer problems that have practical engineering relevance can only be treated by neglecting one or more physical aspects. For instance, it is often necessary to reduce the dimensionality of the problem in order to keep the mathematics and computations tractable. For some problems, such a simplification may not be justifiable and its impact on the validity of the solution cannot be assessed unless a more complete solution can be obtained. There is a general consensus that our capabilities for addressing more realistic radiative heat transfer problems could be enhanced significantly by employing high-performance computing techniques.

As a result of large and individual small group workshop discussion, 5 classes of highly challenging, nationally important problems (i.e. research thrusts) relating to the use of high-performance computing in participating media radiative heat transfer were identified. These thrusts represent critical capabilities that are required to analyze transport processes relevant to applications such as advanced manufacturing techniques, design of internal combustion engines, determination of newly engineered materials, laser surgery, etc. These applications require the development of cutting edge technology that will result from addressing the proposed problems. It is anticipated that, with sufficient support, the new capabilities can be developed some number (>3 and <10) of years into the future.

1. Development of Benchmark Solutions



This desired capability consists of the development of benchmark solutions to validate models, and, for validated models, to compare platforms and solution techniques. The solutions are to apply to standard 3D geometries (rectangular boxes and cylinders), and include the effects of shading (i.e. an "L" shaped object). Solutions should be available for both specular and diffuse walls and for both optically thick and optically thin problems.The properties of the media should encompass the influence of scattering (isotropic to highly forward), inhomogeneous media, and spectral characteristics. The solution sets are to include isothermal media, temperature distributions representative of a combustion environment (i.e. a flame temperature in the central region surrounded by a boundary layer), and surface temperature distributions. Output in the form of intensities given at the surfaces and corners (including angular distributions), the flux divergence, and the flux at boundaries was also presented as a requirement of the solution sets. Data from these solutions is to be readily available and should include an estimated uncertainty. Although the need to develop codes which operate on small, inexpensive platforms was frequently mentioned during the workshop, high-performance computing plays an integral role in the development of these benchmark solutions which are required to evaluate the applicability of models developed for lower-performance platforms.

Image courtesy of John McGee, Computer Applications Group C-3, Los Alamos National Laboratory. Image generated as part of joint Sandia/Los Alamos research project.

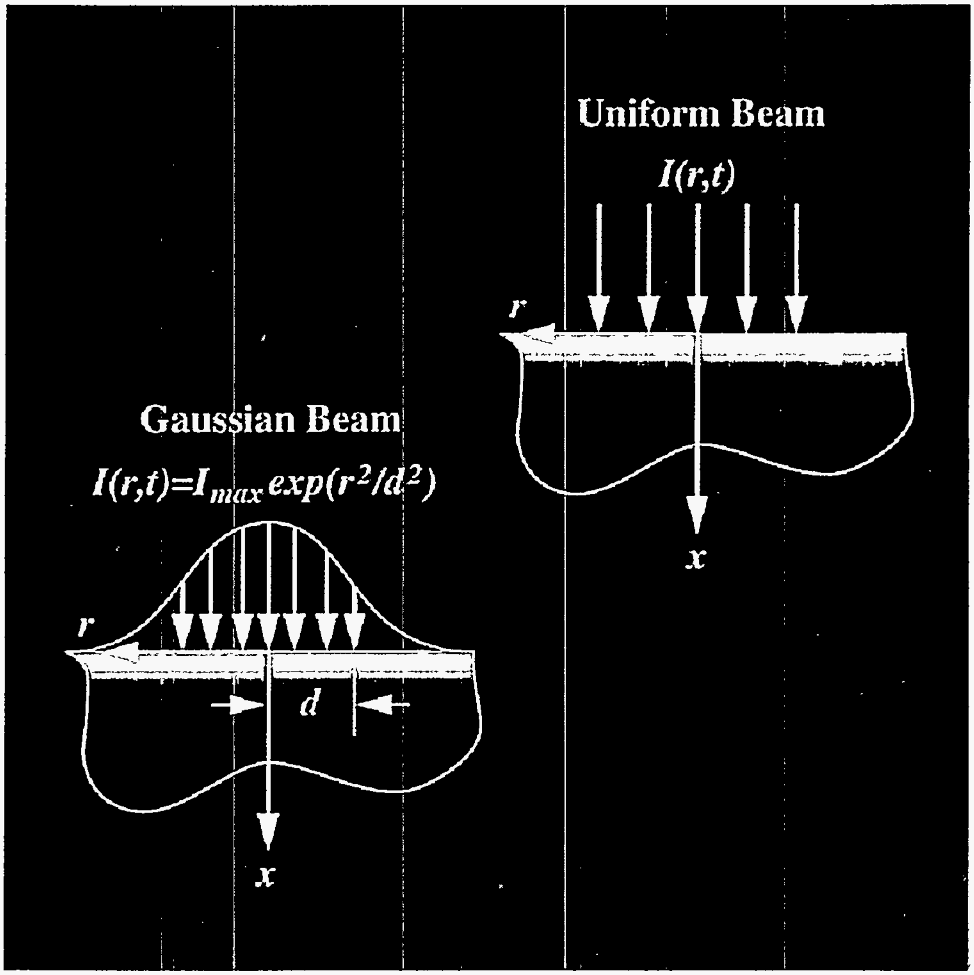
2. Complex/Combined-Mode Problem

The capability to obtain radiative heat transfer solutions which are coupled with other methods of energy and/or momentum transfer (i.e. other heat transfer modes and or subsonic/supersonic fluid flow) stimulated the most interest from the attendees. The ability to address 3D complex geometries was cited as being imperative to applying this capability to practical applications. Inhomogeneous (both spatially and temporally) media, anisotropic scattering, and spectral dependence should also be included. The ability to address the interaction of radiative heat transfer with chemically reacting (including nonequilibrium) flows, turbulent flows, conditions which include phase change and mass transfer, and environments which include the production/ destruction of species were also presented as essential features of this capability. Some of the applications discussed (none tractable today) include modeling gas turbines, coal furnaces, and fuel fires. High-performance computing (the need for large memory, fast interconnect networks, and parallel algorithms), and outreach to the fluid mechanics and combustion communities will be required to obtain this capability (i.e. the formation of multi-disciplinary teams representative of a “Grand Challenge” problem). Heterogeneous computing was discussed as being potentially well-suited for these problems since functional decomposition appears to be a very viable candidate and Monte Carlo techniques are ideal for large parallel platforms.

3. Volume Rendering Problem

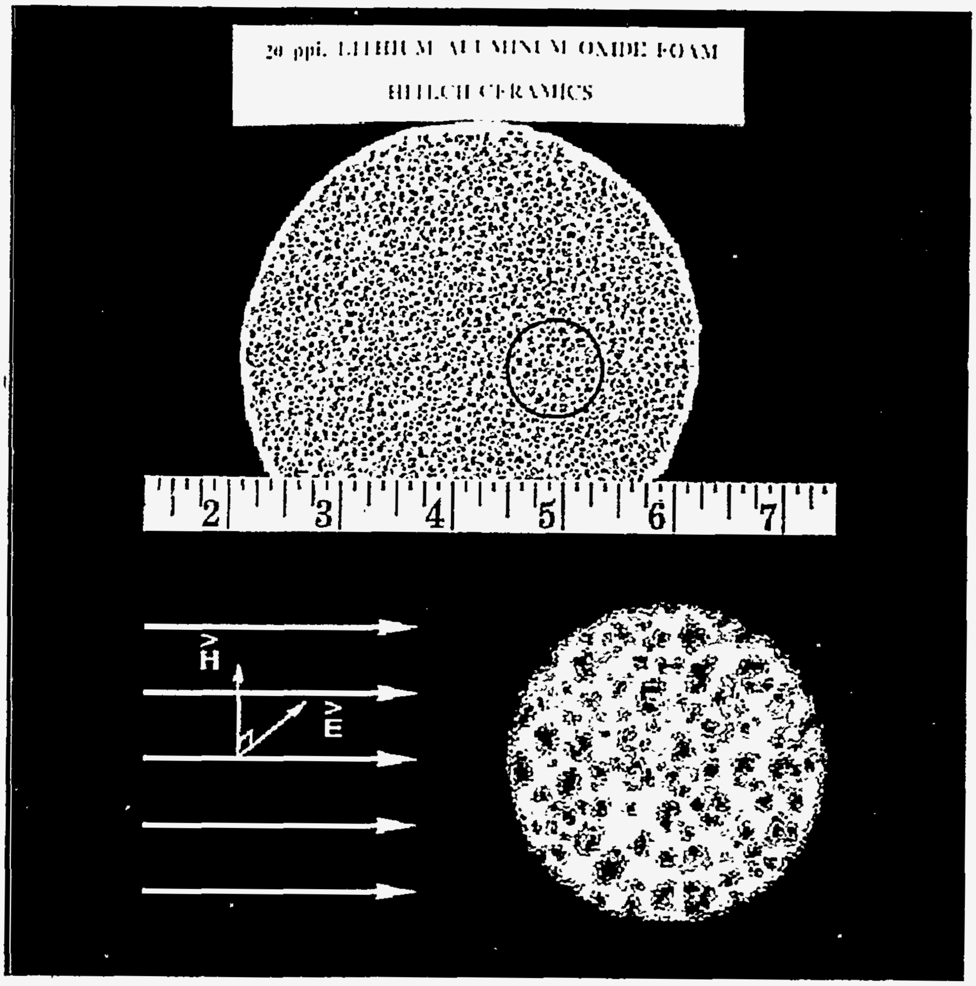
The ability to perform realistic simulations of radiation through non-transparent media (light through smoke, for instance) for cases which include angular and spectrally-varying properties of the surfaces and media is the focus of this desired capability. Again, the ability to address 3D geometries was deemed essential. Shadowing, time varying, translucent, and specular surfaces, fluorescence, polarization and scattering were also cited as important features. One of the principle challenges of this problem is to perform real time (30 frames per second) rendering of images. The visualization technology provided by the capability would allow simulations of interest to safety analyses (smoke filled rooms, foggy environments), military (including remote sensing, underwater vision) and commercial (headlamps, entertainment, virtual reality) interests.

4. Inverse Problem



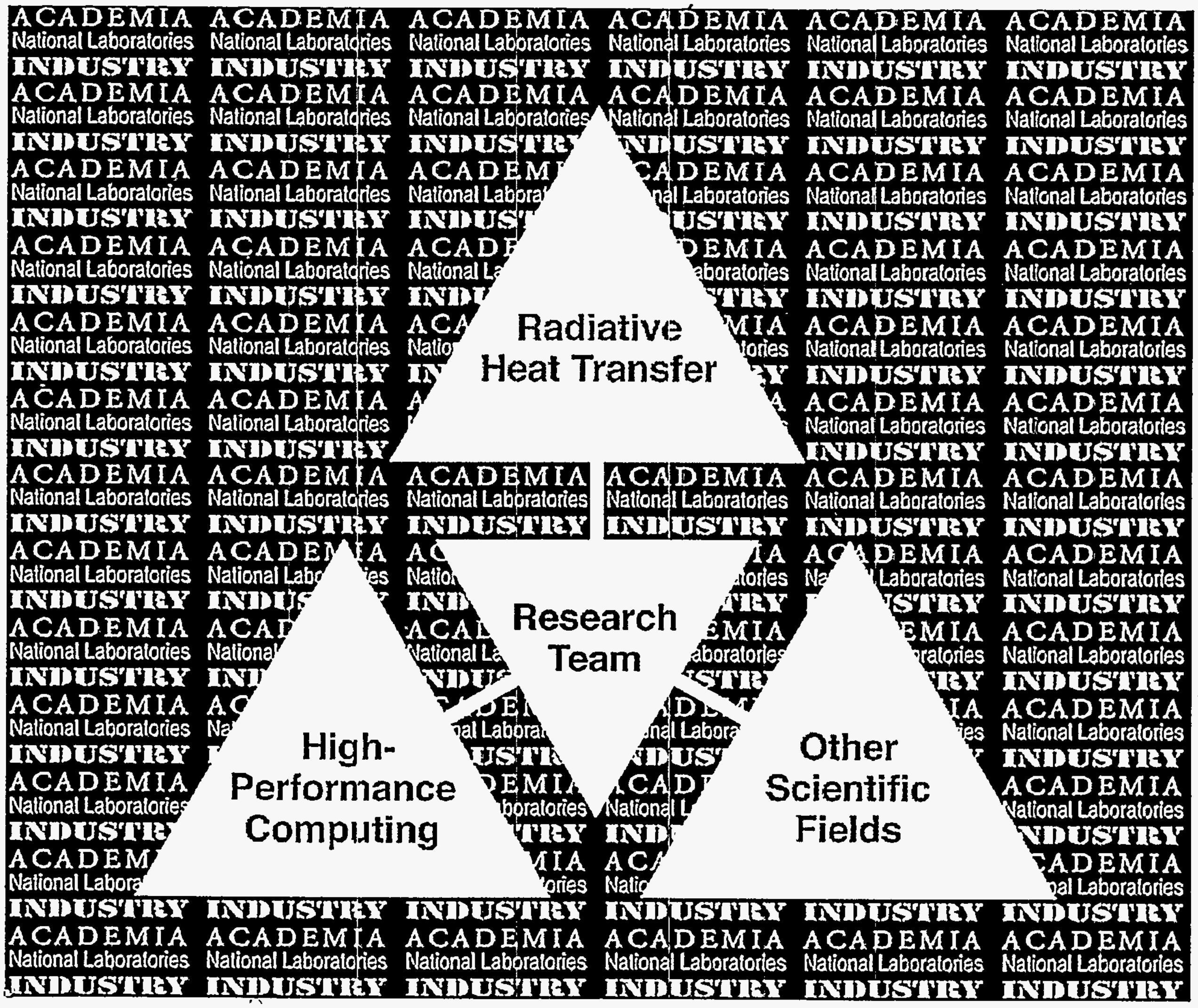
The ability to, given the flux distribution, determine the spatial resolution of other parameters (radiative properties, source or temperature distribution) in the Radiative Transfer Equation (RTE) is the thrust of this desired capability. The three important classes of inverse problems identified include radiative property determination, design optimization, and process control. The treatment of noisy data, non-uniqueness, and sensitivities/uncertainties for both constrained and unconstrained complex 3D systems (furnaces measurement systems, etc.) comprise additional technical issues raised at the workshop. A typical application to design optimization would include beginning with a basic furnace shape and optimizing the placement of the burners and adjusting the media properties (air-fuel ratio) to get an even temperature distribution. Large-scale (numerical) optimization with the added technical challenge of expensive function evaluations was cited as a requirement for all inverse problem solutions. Applications in process control impose the additional challenge of requiring rapid solutions. The investigation of a large and primarily new realm of algorithm design, as well as systems and platform implementation issues are key aspects of this challenge.

5. Solution of Full Electromagnetic (EM) Equations



Since the RTE is related to Maxwell's equations, it is of scientific and practical interest to know the limits of applicability of the RTE's assumptions. This challenge involves developing a solution technique for the full EM equations and assessing the realm of applicability of the RTE. The effects of near field solutions, polarization, noncontinuous media, complex geometries, dependent scattering, and photon-phonon interactions are to be considered. This capability would allow the expansion of radiative transfer techniques to include applications such as thin films, dense porous media (insulation), nanoscale systems, composites, catalytic reactor design, radiative therapy, and manufacturing (i.e. fiber-wound materials). Outreach to existing EM research communities would form one basis for applying high-performance computing to this challenging problem.

RESEARCH TEAMS



To facilitate the formation of Grand Challenge Applications teams, the conference organizers requested via the E-mail reflector and at presentations at the 6th AIAA/ASME Thermophysics and Heat Transfer Conference and the 10th International Heat Transfer Conference, that all interested parties identify the degree to which they would like to participate. Recipients were asked if they were willing to: (a) lead/organize a team [higher interest], (b) actively contribute to a team effort [interest], or (c) support an effort as time permits [lower interest]. A listing of the teams formed to date is provided below. E-mail addresses of team members are listed in Appendix C.

1. The Development of Benchmark Solutions of the RTE

(a) lead/organize: Pei-feng Hsu and Zhiqiang Tan

(b) actively contribute:
- Walter Yuen
- Richard Buckius
- Jack Howell
- Ray Viskanta
- Jim Maltby
- Lou Gritzo
- Tim Tong
- Craig Saltiel
- Joseph Kolibal
- Al Crosbie
- Pat Burns
- Jeff Farmer
- Brent Webb
- John Chai
- Dean Dobranich

(c) support:
- Merle Benson
- Chuck Koelbel
- Yildiz Bayazitoglu
- Terry J. Hendricks
- Pinar Menguc

(d) international contributors:
- Pedro Coelho
- Sergey Surzhikov
- Andrei V. Galaktionov
- Leonid A. Dombrovsky
- Chih-Yang Wu

2. Complex/Combined-Mode Problem

(a) lead/organize: Walter Yuen

(b) actively contribute:
- Richard Buckius
- Jack Howell
- Ray Viskanta
- Tim Tong
- Jim Maltby
- Lou Gritzo
- S.H. Chan
- Craig Saltiel
- Joseph Kolibal
- Peter Jones
- Al Crosbie
- Shawn Burns
- Pat Burns
- Jeff Farmer
- Yildiz Bayazitoglu
- Brent Webb

John Chai
Dean Dobranich

(c) support: Merle Benson
Terry J. Hendricks

(d) international contributors: Pedro Coelho
Sergey Surzhikov
W. Malalasekera
Leonid A. Dombrovsky

3. Volume Rendering Problem

(a) lead/organize: None identified at this time

(b) actively contribute: Richard Buckius
Craig Saltiel
Joseph Kolibal
Al Crosbie

(c) support: Merle Benson
Jack Howell
Al Crosbie
Yildiz Bayazitoglu
John Chai

(d) international contributors: Sergey Surzhikov

4. Inverse Problems

(a) lead/organize: Pinar Menguc and Ted Bergman

(b) actively contribute: Walter Yuen
Richard Buckius
Ray Viskanta
Tim Tong
Lou Gritzo
Craig Saltiel
Joseph Kolibal
Al Crosbie
Pat Burns
Jeff Farmer
Brent Webb
Eric Thacher
John Chai
Dean Dobranich

(c) support: Merle Benson
Jim Maltby
Chuck Koelbel
Terry J. Hendricks
Yildiz Bayazitoglu

(d) international contributors: Sergey Surzhikov
Andrei V. Galaktionov
W. Malalasekera

Leonid A. Dombrovsky

5. Solution of Full Electromagnetic (EM) Equations
(a) lead/organize: Tim Tong and Daniel Mackowski
(b) actively contribute: Merle Benson
Walter Yuen
Richard Buckius
Jack Howell
Lou Gritzo
Craig Saltiel
Joseph Kolibal
Yildiz Bayazitoglu
Al Crosbie
Dean Dobranich
(c) support: Chuck Koelbel
Costas P. Grigoropoulos
Pinar Menguc
(d) international contributors: Sergey Surzhikov

NSF FY95 PROGRAM SOLICITATION: OPPORTUNITIES IN SUPPORT OF MULTIDISCIPLINARY RESEARCH

a component of the U.S. High Performance Computing and Communications Program

This program solicitation is also on STIS, under nsf95-5a (BIO), nsf95-5b (CISE), nsf95-5c (ENG), nsf95-5d (MPS), nsf95-5e (SBE).

REVISED PREPROPOSAL DEADLINE: February 27, 1995

Proposal Deadline: June 9, 1995

NATIONAL SCIENCE FOUNDATION - OPPORTUNITIES IN SUPPORT OF MULTIDISCIPLINARY RESEARCH

The National Science Foundation (NSF) announces opportunities in support of multidisciplinary, group-oriented research for Fiscal Year 1995 in connection with the U.S. High Performance Computing and Communications (HPCC) Program, including the new Information Infrastructure Technology and Applications (IITA) component and the National Information Infrastructure (NII). This activity builds on the success of the Grand Challenge Application Groups and the joint Engineering--Computer & Information Science & Engineering--Education & Human Resources (ENG-CISE-EHR) National Challenge Groups competitions to include five distinct but interrelated components:

GRAND CHALLENGES:

to prepare the groundwork for the HPCC goal of sustained teraflop computing on important application problems utilizing parallel, distributed and heterogeneous computing systems and high-performance networks;

NATIONAL CHALLENGES:

to demonstrate the solution of problems beneficial to a broad spectrum of society which contain an extensive information processing component, and which could benefit greatly by building an underlying information infrastructure;

ENABLING TECHNOLOGIES:

to accelerate progress in developing those technologies that will enable the community to take full advantage of high-performance computing and communications systems in solving problems represented by the Grand Challenges and National Challenges.

Computer Science Challenges: focus is on the development of computing technology ranging from computer architecture through systems software to algorithms.

Mathematical Sciences Challenges: focus is on advances in the mathematical sciences ranging from algorithms through the development of tools to the essential use of computation in extending mathematical frontiers.

Problem Solving Environments: focus is on the development of computational environments that take advantage of unique characteristics of specific problems in order to shorten the problem solving cycle..

A total of fifteen to twenty proposals are expected to receive funding. These will augment the portfolio of sixteen Grand Challenge Applications Groups awarded in FY 1992 and FY 1993, three National Challenges awarded in FY 1994, and the six awards in FY 1994 under the ENG-CISE-EHR National Challenge Groups competition.

Activities supported under this solicitation are expected to achieve significant progress on one or more of the following:

1. Fundamental problems in science, engineering and information processing whose solution could be advanced by applying high-performance computing and communications techniques and resources;
2. Enabling technologies which facilitate those advances;
3. Research in computer science and/or mathematics contributing to the preceding two activities.

The emphasis will be on support for cross-disciplinary groups requiring and/or contributing HPCC capabilities.

Only areas of science and engineering represented by the following participating NSF Directorates are eligible for funding under this solicitation: Biological Sciences (BIO), Computer and Information Science and Engineering (CISE), Engineering (ENG), Mathematics and Physical Sciences (MPS), and Social, Behavioral, and Economic Sciences (SBE).

Description of the Five Program Components.

GRAND CHALLENGES.

This program component will support multidisciplinary groups of scientists, engineers, mathematicians and computer scientists to apply emerging high-performance computing and communications systems to advance the solution of computationally intensive, complex science and engineering problems. Grand Challenge Applications Groups are expected to employ testbed systems exploiting new and emerging computer and communications architectures to prepare the groundwork for the HPCC goal of sustained teraflop computing on important application problems. Projects funded through this effort will focus on the fusion of disciplinary research with emerging high-performance computing and communications environments and architectures, within the framework of the HPCC program goals. It is anticipated that projects will include aspects of design of models, algorithms and software, as well as problem solving environments, to fully realize the potential of parallel, distributed and heterogeneous computing systems and of high-performance networks on Grand Challenge problems and on enabling technologies.

NATIONAL CHALLENGES.

This program component will support multidisciplinary groups of scientists, engineers, mathematicians and computer scientists to apply emerging high-performance computing and communications systems to advance the solution of National Challenge problems. These are large-scale, distributed applications having high social and economic impact that have been identified as containing an extensive information processing component and which could benefit greatly by building an underlying information infrastructure. Example application areas include Digital Libraries, Education, Manufacturing, Crisis Management, Health Care Delivery, Environmental Research, Civil Infrastructure, and Government Information Delivery. Although primarily information intensive, many of these challenges will require computational modeling and tools for high-performance computing that are being developed or need to be developed under other components of the HPCC program.

ENABLING TECHNOLOGIES.

Computer Science Challenges.

This program component will provide support to accelerate progress in developing the high-performance computing technology needed by the interdisciplinary communities represented by the Grand Challenges and National Challenges. It is expected that efforts supported under this component will span the spectrum from basic research to the development of prototypes appropriate for evaluation by the scientific, engineering and industrial communities. Teams of computer scientists and engineers will be supported to address issues which range from computer architecture to networking and communications to systems software to algorithms. Examples of areas which would be considered for support include the following:

Innovative approaches to computing systems architectures, including all aspects of high-performance memory systems and wide band I/O;

Network interface architectures and operating systems for effective, seamless, low-overhead communications among collections of workstations;

Information access technologies that enable efficient search of large distributed information repositories, make the distributed information resources understandable, and are designed to be made available over data networks;

Development of environments, system software and algorithms to support the effective utilization of parallel architectures and communications networks;

Foundations for building NII applications from re-usable objects that provide services, such that the applications are affordable, interoperable, easy-to-use and have an appropriate level of security and dependability.

Collaboration and partnerships with researchers focused on applications such as those addressed by Grand Challenge or National Challenge groups are encouraged as appropriate.

Mathematical Sciences Challenges.

This program component will support multidisciplinary groups of mathematical scientists, computer scientists, scientists, and engineers to develop the advances in mathematical sciences necessary for the full use of high-performance computing and communications systems, or to apply high-performance computing technology to problems of significant mathematical interest. Areas of interest include:

Algorithm design and analysis;

New computational paradigms;

Mathematical investigations that require high-performance computing to open areas of mathematical research that are otherwise inaccessible;

New mathematical and statistical tools that provide better access to high-performance resources.

Collaboration and partnerships with researchers focused on applications such as those addressed by Grand Challenge or National Challenge groups are encouraged.

Problem Solving Environments.

This program component will support research to accelerate the development of Problem Solving Environments (PSEs) for computational and information science. It represents a specific thrust that combines elements of computer science and scientific computing. PSEs are systems that provide all of the computational facilities necessary to solve a particular class of problems, including solution methods, support for selection of solution methods, facilities to simplify setting up a particular problem and viewing the results, all couched in a language appropriate for the target class of problems. In particular, this component aims to foster research in these areas:

PSE foundations: Research in general and abstract properties of PSEs to derive design principles and methodologies for PSEs. This work will include study of generic features of scientific problem solving for large domains, and their efficient mapping onto high-performance computer hardware and software;

Key technologies for PSEs: Research on computational and computer-scientific technologies specifically applicable to PSE development;

Construction of PSEs: PSE prototypes for important classes of scientific and engineering problems. These will be complex enough to exhibit the general features and difficulties of the process.

It is anticipated that the groups supported will consist of computer scientists, computational scientists, and application scientists or engineers.

Supported Activities.

Proposers are encouraged to provide innovative, collaborative approaches to formulating solutions to multidisciplinary challenge problems and to research on the underlying computing and communication technologies. Items that are appropriate for support include: research time for individual investigators, postdoctoral researchers, graduate students, HPCC equipment, testbed development, access to high-performance computing systems, networking and communications, HPCC educational activities, and salary for technical support personnel.

These opportunities, originally created through the cooperation of disciplinary sub-activities within NSF, are supported by the Foundation and coordinated by a cross-directorate group working with disciplinary program officers and other federal agencies participating in the HPCC program. This Federal interagency HPCC program seeks to expand U.S. technological leadership, speed the pace of innovation, and spur gains in U.S. productivity and competitiveness through advances in high-performance computing and communications. The program responds to the opportunities for advances inherent in the use of advanced computer models incorporating the basic science of parallel processing and the improved productivity derived by the interaction of people who are spatially separated sharing networked access to information processing and computing resources.

Additional information on NSF HPCC activities in conjunction with the interagency HPCC effort can be obtained from the NSF HPCC Coordinators listed as contacts in this document.

Criteria for Review.

All proposals to NSF are subject to the review criteria described in the NSF brochure, Grant Proposal Guide (GPG), NSF 94-2. Single copies of this brochure are available at no cost from the NSF Forms and Publications Unit, (703) 306-1130, or via e-mail: pubs@nsf.gov. Brochures are also available through NSF's online Science and Technology Information System (STIS). To access the system, follow the instructions on the STIS flyer (NSF 94-4). To get an electronic copy of the flyer, send an e-mail message to stisfly@nsf.gov. The review criteria in GPG deal with: quality of scientific effort proposed; competence of investigators; relevance of research; and impact on infrastructure.

The following criteria that reflect the objectives of the interagency HPCC program will also be considered in evaluation of proposals received under this solicitation:

potential for impact in a critical area of science and engineering or of high-performance computing required by science and engineering;

potential for impact in an information intensive societal application or of high-performance information processing required by that application;

degree of interaction between focused scientific, engineering, or information applications and computational activities and the degree to which that interaction has broad implications for high-performance computing and processing beyond the specific problem area or discipline being studied;

development of new computational techniques or software for, or new fundamental understanding of, high-performance systems with potential benefit for the broader scientific community and/or society;

potential for impact on the development of computational techniques, environments, or paradigms;

extent to which the group is integrated with a common focus;

record of accomplishment and potential for advancing frontiers of high-performance parallel, distributed or heterogeneous computing environments;

extent to which the research proposed provides a testbed for new high-performance computing, information processing and communications systems;

educational activities to increase the participation and training of students and researchers in high-performance computing and communications;

innovative involvement of educators;

extent that women and underrepresented minorities are involved at all levels of the group;

degree of cost sharing and extent of university commitment;

innovative partnerships with national laboratories and private industry.

Proposal Submission, Review and Award Processes.

Review of proposals will be coordinated across the Foundation involving all programs related to the proposed project. Proposals reviewed under this solicitation that overlap other inter-agency or NSF Strategic Initiatives will be referred to those activities for joint consideration.

Preproposals and proposals will be reviewed in one of the five components discussed above. The review process for each component will be similar in structure and be coordinated by the HPCC Coordinating Committee. When necessary, preproposals or proposals spanning more than one program component will be reviewed by each of the appropriate components.

A combination of mail, panel, or site visit review will be used as needed. Awards are planned to be jointly funded between the programs involved. Awards are planned to be in the range of $300,000 to $800,000 per year for a period of three to five years. The number and size of awards will be based on the quality and potential impact of the proposals reviewed, and the availability of funds.

Preproposals.

In order to minimize the work of the research and reviewer communities on potential proposals that may be inappropriate or less likely to be competitive, submission of a preproposal by e-mail is required. A preproposal is a prerequisite to, but does not obligate the submission of, a full-length proposal and must be received by February 27, 1995. The e-mail submission should be in plain text, i.e. ascii, format addressed to:

Internet: hpccgrps@nsf.gov

The preproposal must contain the following information in the indicated order, with a page being limited to approximately 300 words. Preproposals that do not comply will be returned without review.

1 Page: Title of group activity, List of PI and Co-PIs with departmental and institutional affiliations, Mailing and e-mail addresses, phone and FAX numbers of PI only, Indication of which of the five components is most appropriate, i.e. Grand Challenges, National Challenges, Computer Science Challenges, Mathematical Sciences Challenges, Problem Solving Environments.

(The ultimate responsibility for assigning a preproposal to a program component will reside at NSF. When appropriate, a preproposal that spans two components will be reviewed by both components.)

1 Page: Abstract

4 Pages: Outline of project plan, Evidence of multidisciplinary interactions.

1 Page: Estimated first year budget (not binding on final proposal)

1 Page: List of individuals with whom the PI or Co-PIs have had a close working relationship in the last 48 months

Following Biographical sketch as per GPG with a limitation of Pages, 2 pages per PI and Co-PIs

Since preproposals are not formal proposals, participant or institutional agreements are not necessary at this stage.

Preproposals will be reviewed by panels. The outcome of this review process will determine which groups will be invited to submit formal proposals. Groups not receiving an invitation are not prohibited from formally applying; however, they should do so only after carefully weighing the reviewer comments on their preproposal.

It is anticipated that the results from the preproposal review will be announced via e-mail during the week of April 10, 1995.

Final Proposal Deadline.

Fifteen copies of final proposals, including one copy bearing original signatures and institutional approval, must be mailed to:

HPCC Coordinator NSF, Room 1105, 4201 Wilson Blvd., Arlington, VA 22230

It is essential that this precise address be used.

Only one copy of NSF Form 1225, Information about Principal Investigator/Project Director should be sent attached to the original signed copy.

Proposals must be:

i) received by NSF no later than June 9, 1995; or ii) postmarked no later than five (5) days prior to the deadline date; or iii) sent via commercial overnight mail no later than two (2) days prior to the deadline date to be considered for an award.

Proposals submitted in response to this solicitation must be prepared and submitted in accordance with the guidelines provided in the NSF brochure, GPG (94-2); in particular, page formatting requirements given on page 3 will be strictly enforced, and proposals not complying will be returned without review.

However, the following are exceptions to the guidelines and specific to this activity only:

> the project description is limited to 15 pages (single spaced) including one page describing cost sharing;
>
> each PI and Co-PI may use up to an additional 2 pages each to describe results under prior NSF support, focusing on those results relevant to the proposed project.

Proposals not conforming to these guidelines will be returned to the proposer without review.

The review process will be concluded by late July, 1995, with announcement of awards planned for September, 1995.

Additional Requirements.

It is anticipated that prior to any awards additional information may be required on some or all of the following topics as appropriate.

> Milestones for the full period of the award.
>
> Publicity, documentation, support and dissemination of software developed under the award.
>
> University policy on software licensing and distribution.
>
> Plans for making results available to the broader community.
>
> Management plan.
>
> Role of databases and degree of interoperability with other appropriate databases.

Inquiries.

Inquiries relative to this solicitation should be addressed via electronic mail to: hpccgrps@nsf.gov.

Written inquiries may be made to

HPCC Coordinator NSF, Room 1105, 4201 Wilson Blvd., Arlington, VA 22230

Related Activities and Contact Persons.

For details on the U.S. High Performance Computing and Communications Program see the supplement to the President's Fiscal Year 1995 Budget entitled "Technology for the National Information Infrastructure" Copies can be obtained from the Directorate for Computer and Information Science and Engineering, NSF, 4201 Wilson Blvd., Room 1105, Arlington, VA, 22230.

General information on the HPCC program may be obtained from the NSF coordinator; particulars on a specific directorate's involvement from the relevant directorate level coordinator; and advice on specific projects from the appropriate disciplinary program manager. The NSF directorates are: BIO (Biological Sciences), CISE (Computer & Information Science & Engineering), EHR (Education and Human Resources), ENG (Engineering), GEO (Geosciences), MPS (Mathematical and Physical Sciences), and SBE (Social, Behavioral and Economic Sciences)

NSF HPCC Coordinator: Robert Voigt, (703) 306-1900, rvoigt@nsf.gov

BIO HPCC Coordinator: Peter Arzberger, (703) 306-1469, parzberg@nsf.gov

CISE HPCC Coordinator: Oscar Garcia, (703) 306-1928, ogarcia@nsf.gov

EHR HPCC Coordinator: Nora Sabelli, (703) 306-1651, nsabelli@nsf.gov

ENG HPCC Coordinator: Lawrence Goldberg, (703) 306-1339, lgoldber@nsf.gov

GEO HPCC Coordinator: Clifford Jacobs, (703) 306-1521, cjacobs@nsf.gov

MPS HPCC Coordinator: Alvin Thaler, (703) 306-1880, thaler@nsf.gov

SBE HPCC Coordinator: William Bainbridge, (703) 306-1756, wbainbri@nsf.gov

The only Directorates participating in this solicitation are: BIO, CISE, ENG, MPS, and SBE.

Related Computational Science and Engineering Activities.

The HPCC program at NSF is coordinated across all disciplinary research directorates to encourage joint review and support of proposals with ongoing computational science and engineering programs. All NSF disciplines continue to support base activities in computational science and engineering research within their disciplinary research programs in addition to their involvement with this Opportunities in Support of Multidisciplinary Research. The opportunities described herein represent one, but not the only approach to support HPCC activities.

Selected Computational Science and Engineering Contacts.

Computational Biology, BIO: Peter Arzberger, (703) 306-1469, parzberg@nsf.gov

Computational Neuroscience, BIO: Karen Sigvardt, (703) 306-1416, ksigvard@nsf.gov

Information, Robotics & Intelligent Systems, CISE: Y.T. Chien, (703) 306-1930, ytchien@nsf.gov

New Technologies, CISE: Richard Hirsh, (703) 306-1970, rhirsh@nsf.gov

Numeric, Symbolic & Geometric Computation, CISE: Kamal Abdali, (703) 306-1911, kabdali@nsf.gov

Theory of Computing, CISE: Dana Latch, (703) 306-1911, dlatch@nsf.gov,

Operating Systems & Software Systems, CISE: Krishna Kavi, (703) 306-1912, kkavi@nsf.gov

Programming Languages & Compilers, CISE: Krishna Kavi, (703) 306-1912, kkavi@nsf.gov

Computer Systems, CISE: Yechezkel Zalcstein, (703) 306-1914, zzalcste@nsf.gov

Experimental Systems, CISE: Michael Foster, (703) 306-1936, mfoster@nsf.gov

Networking & Communications Research, CISE: Darleen Fisher, (703) 306-1949, dlfisher@nsf.gov

Computational Engineering, ENG: George Lea, (703) 306-1339, glea@nsf.gov

Computational Chemistry, MPS: Richard Hilderbrandt, (703) 306-1844, rhilderb@nsf.gov

Computational Materials, MPS: G. Bruce Taggart, (703) 306-1834, gtaggart@nsf.gov

Computational Mathematics, MPS: Michael Steuerwalt, (703) 306-1878, msteuerw@nsf.gov

Computational Physics, MPS: Richard Isaacson, (703) 306-1899, isaacson@nsf.gov

The National Science Foundation (NSF) provides awards for research in the sciences and engineering. The awardee is wholly responsible for the conduct of such research and preparation of the results for publication.

The Foundation, therefore, does not assume responsibility for such findings and their interpretation. The Foundation welcomes proposals on behalf of all qualified scientists and engineers, and strongly encourages women, minorities and persons with disabilities to compete fully in any of the research and research-related programs described in this document.

In accordance with Federal statutes and regulations and NSF policies, no person on grounds of race, color, age, sex, national origin, or disability shall be excluded from participation in, denied the benefits of, or be subject to discrimination under, any program or activity receiving financial assistance from the National Science Foundation.

Grant Administration.

Grants awarded as a result of this solicitation are administered in accordance with the terms and conditions of NSF GC-1, "Grant General Conditions," or FDP-II, "Federal Demonstration Project General Terms and Conditions," depending on the grantee organization. Copies of these documents are available at no cost from the NSF Forms and Publications Unit, phone (703) 306-1130, or via e-mail pubs@nsf.gov. More comprehensive information is contained in the NSF Grant Policy Manual (NSF 88-47) (including the 7 changes issued through April, 1993), for sale through the Superintendent of Documents, Government Printing Office, Washington, DC 20402. The telephone number at GPO is (202) 512-1800.

Facilitation Awards for Handicapped Scientists and Engineers provide funding for special assistance or equipment to enable persons with disabilities (investigators and other staff, including student research assistants) to work on an NSF project. See program announcement NSF 91-54, or contact the Facilitation Awards Coordinator, Directorate for Education and Human Resources, Washington, DC 20550, (703) 306-1636.

The Foundation has TDD (Telephonic Device for the Deaf) capability, which enables individuals with hearing impairment to communicate with the Division of Personnel and Management about NSF programs, employment, or general information. The telephone number is (703) 306-0090.

This program is described in the Catalog of Federal Domestic Assistance categories: 47.074, BIO; 47.070, CISE; 47.041, ENG; 47.049, MPS; and 47.075, SBE.

Electronic Dissemination.

You can get information fast through STIS (Science and Technology Information System), NSF's online publishing system, described in NSF 94-4 the "STIS flyer" (elsewhere in this publication). To get more copies of the flyer, call the NSF Publications Section at (703) 306-0214. For an electronic copy, send an e-mail message to stisfly@nsf.gov.

Ordering by Electronic Mail.

If you are a user of electronic mail and have access to the Internet, you may order publications electronically by sending requests to pubs@nsf.gov. In your request, include the NSF publication number and title, number of copies, your name, and a complete mailing address. Publications should be received within three weeks after placement of your order.

Privacy Act and Public Burden Statements.

The information requested on this proposal material is solicited under the authority of the National Science Foundation Act of 1950, as amended. It will be used in connection with the selection of qualified proposals and may be used and disclosed to qualified reviewers and staff assistants as part of the review process and to other government agencies. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records" and NSF-51, "Reviewers/Proposals File and Associated Records" 56 Federal Register 54907 (October 23, 1991). Submission of the information is voluntary. Failure to provide full and complete information, however, may reduce the possibility of your receiving an award.

Public reporting burden for this collection of information is estimated to average 120 hours per response, including the time for reviewing instructions. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to:

Herman G. Fleming Reports Clearance Officer Division of Contracts, Policy & Oversight National Science Foundation Arlington, VA 22230

and to:

Office of Management and Budget Paperwork Reduction Project (3145-0058) Washington, DC 20503

NSF 95-5 (new) OMB 3145-0058 P.T. 34 K.W. 1004000

CONCLUSIONS AND FUTURE ACTIVITIES

The workshop was successful in educating participants from the radiative heat transfer community about the opportunities of high-performance computing and educating the participants from the high-performance environment about the unique and demanding aspects of radiative heat transfer. Through the identification of the key concepts and issues, the identification of the five research thrust areas, the formation of research team frameworks, and the creation of an E-mail reflector to facilitate communication and teamwork, the workshop has provided a vehicle for the participants to explore interdisciplinary developments in transport modeling, computational algorithms and hardware strategies that will enable a significant improvement in the ability to accurately and efficiently simulate complex radiative heat transfer. As the teams formed at this workshop have the opportunity to create Grand Challenge Application Groups and explore other means of developing cohesive research efforts, the generation of new research proposals, the direction of resources by funding agencies, and technical developments which are consistent with industry needs and applications are expected.

The future role of the workshop organizers is to; 1) solicit comments regarding the outcome of the workshop, 2) serve as a proactive conduit of information, and 3) participate as team members. As research teams become active and accomplishments occur, it is hoped that future symposia and workshops will be held which focus on one or more of the research thrusts.

ACKNOWLEDGEMENTS

The authors wish to thank the National Science Foundation for sponsoring the workshop. Special appreciation is extended to George Lea, Bud Peterson, and Mike Chen of the NSF for their support and assistance. The authors thank Merle Benson, Don Wagy, John Zepper, and Dean Dobranich of SNL for their assistance and contributions. The authors also wish to express their appreciation to the workshop participants for their time, effort, and valuable contributions.

APPENDIX A - LIST OF ATTENDEES

Merle Benson
Scientific Computing Systems
Sandia National Labs, NM

Richard Buckius
Department of Mechanical & Industrial Engineering
University of Illinois at Urbana-Champaign

Pat Burns
Department of Mechanical Engineering
Colorado State University

Richard Casey
Information Technology
Arizona State University

Mike Chen
Department of Mechanical Engineering & Applied Mechanics
University of Michigan

Al Crosbie
Thermal Radiative Transfer Group
University of Missouri-Rolla

Robert Ferrell
Thinking Machines Corp

Joe Grcar
Computational Mechanics Department
Sandia National Labs, CA

Lou Gritzo
Thermal and Fluid Engineering
Sandia National Labs, NM

John Gustafson
Ames Laboratory
Iowa State University

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APPENDIX B - AGENDA

<u>March 28, 1994</u>

5:00	Preregistration *Reception Foyer, First Floor*
7:00 - 9:00	Informal Reception (hors d'oeuvres, cash bar) *Reception Foyer*

<u>March 29, 1994</u>

7:00	Registration *Reception Foyer*
8:00	Welcome, Background, Workshop Objectives, Introductions/Desired Outcomes *ULAM Salon I, First Floor*
	Technical Background, Nomenclature Overview
	Radiative Heat Transfer (Tim Tong, Arizona State University) High-Performance Computing (Merle Benson, Sandia National Labs)
	Break
	Present-Day Approach, Consensus on Identification of Technical Barriers
	Overview Questionnaire Results Common Themes Regarding Critical Technical Issues (Lou Gritzo, Sandia National Labs)
11:30	Lunch *Reception Foyer*
	Define 5-Year Goal In small groups, visualize and identify a desired capability 5 years into the future, with general ideas on software, hardware and algorithm needs.
1:30	Small Group Presentations to Large Group (10 minutes each) *ULAM Salon I*
	Break
	Large Group Discussions to Reach Consensus on 5-Year Goal, Summary Statements
5:00 - 5:30	Expense Vouchering for Supported Participants *Reception Foyer*
6:00	Social Hour (cash bar) *Reception Foyer*
7:00	Dinner *Reception Foyer*

March 30, 1994

8:00	Review Objectives of the Day *ULAM Salon I*
	Define Strategies on How to Achieve 5-Year Goal In small groups, identify research strategies and technical developments that must occur (software, hardware, algorithms) to overcome the technical barriers and achieve the 5-year goal. *Reception Foyer*
	Break
10:15	Small Group Presentations to Large Group (15 minutes each) *ULAM Salon I*
11:30	Lunch *Reception Foyer*
	Large Group Discussions to Reach Consensus on How to Achieve 5-Year Goal *ULAM Salon I*
	Break
	Summary Statements, Research Opportunities, Discussion of Next Steps, Closing Remarks
4:00	Adjourn

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APPENDIX D - GLOSSARY OF RADIATIVE HEAT TRANSFER

Absorption coefficient $\sigma_{a\lambda}$ - a radiative property that characterizes the medium's ability to absorb radiant energy

Albedo ω - ratio of the scattering coefficient to the extinction coefficient

Blackbody - an object that absorbs all radiant energy that arrives at it

Blackbody emissive power e_b - total radiant energy emitted by a blackbody, a flux quantity, i.e. energy per unit time per unit area

Configuration factor F_{m-n} - a geometric factor that represents the fraction of radiant energy leaving surface m and arriving at surface n

Equation of transfer - an integral-differential equation that governs the propagation of the radiation intensity in a participating medium

Extinction coefficient $\sigma_{e\lambda}$ - the sum of the scattering and absorption coefficients

Gray - independent of wavelength

In-scattering - represented by the integral term in the equation of transfer

Intensity i - radiant energy in a given direction

Inverse problem - a terminology generally refers to performing an experiment to measure transmitted, reflected or scattered radiation intensity and use the data to deduce information about the system

Mie theory - a mathematical solution for the scattering of radiation by isotropic and homogeneous spherical particles

Monochromatic - a description pertaining to the values of a quantity at individual wavelengths

Multiple scattering - see in-scattering

Net radiative heat flux q^r - net rate of radiant energy transferred in the positive and negative directions per unit area

Non-gray - spectrally dependent

Optical thickness τ_o - the integral of the extinction coefficient over the physical thickness of a medium

Optically thick - the optical thickness is much greater than one

Optically thin - the optical thickness is much less than one

Participating media - media that participate in the radiative heat transfer process by means of any of the following mechanisms: absorption, scattering, and emission of radiant energy

Planck's law - a mathematical function that describes the spectral radiation intensity emitted by a blackbody

Radiant energy Q^r - energy pertaining to radiative heat transfer

Radiation intensity - see intensity

Radiative properties - properties that pertain to the radiative characteristics of a surface or a medium

Radiative transfer equation - see equation of transfer

RTE - see equation of transfer

Scattering albedo - see albedo

Scattering coefficient $\sigma_{s\lambda}$ - a radiative property that characterizes a medium's ability to scatter radiation

Scattering phase function Φ - a mathematical function that describes the angular distribution of the scattered radiation intensity

Selective surface - a surface that has radiative properties that are spectrally dependent

Single scattering albedo - see albedo

Spectral - see monochromatic

Total - integrated over all wavelengths

Transfer equation - see equation of transfer

View factor - see configuration factor

APPENDIX E - GLOSSARY OF HIGH-PERFORMANCE COMPUTING

Adaptive:(adj.)

Taking local surroundings or history into account. An adaptive mesh-generating algorithm generates a finer mesh near discontinuities such as boundaries and corners; an adaptive routing algorithm may send identical messages in different directions at different times, depending on the local density of the message traffic.

Asynchronous:(adj.)

Not guaranteed to enforce coincidence in clock time. In an asynchronous communication operation, the sender and receiver may or may not both be engaged in the operation at the same instant in clock time.

Broadcast: (v.)

To send a message to all possible recipients. Broadcast can be implemented as a repeated send, but is more efficiently implemented by using spanning trees and having each node in the tree propagate the message to its descendents.

Decomposition:(n.)

A division of a data structure into substructures that can be distributed separately, or a technique for dividing a computation into subcomputations that can be executed separately. The most common decomposition in parallel computing include:

Functional Decomposition: Breaking a calculation into qualitatively different subcalculations, such as the transformation, shading, z-buffering, and rendering portions of a polygon display algorithm.

Geometric Decomposition: Breaking a calculation into sections that correspond to some physical subdivision of the system being modeled, such as tiling a mesh. to achieve good load balance, such sections may be either distributed according to some regular rule or scattered randomly.

Iterative Decomposition: Breaking down a calculation in which one or more operations are repeatedly applied to one or more data values by executing those operations on those data simultaneously. In a "deterministic" decomposition, the data to be processed are fixed, and the same operations are applied to each. In a "speculative" decomposition, different operations are applied simultaneously to the same input until at least one has completed.

Distributed Computer:(n.)

A computer made up of many smaller and potentially independent computers, such as a network of workstations. The architecture is increasingly studied because of its cost-effectiveness and flexibility. Distributed computers are often heterogeneous.

Distributed Memory: (n.)

Memory that is physically distributed among several modules. A distributed-memoarchitecture may appear to users to have a single shared memory and a single address space, or may appear as disjoint memory made up of many address spaces.

Domain:(n.)

The part of a larger computing resource allocated for the sole use of a specific user or group of users.

Heterogeneous:(adj.)

Containing components of more than one kind. A heterogeneous architecture may be one in which some components are processors, and others memories, or it may be one that uses different types of processors together.

Homogeneous:(adj.)

Made up of identical components. A homogeneous architecture is one in which each element is the same; processor arrays and multicomputers are usually homogeneous.

Kernel:(n.)

A process providing basic services. A "service" kernel can run on every processor to support minimal operating system services, while a "routing" kernel can handle or forward incoming messages.

Latency:(n.)

The time taken to service a request, deliver a message, and so on, which is independent of the size or nature of the operation. The latency of a message-passing system is the minimum time to deliver a message, even one of zero length that does not have to leave the source processor; the latency of a file system is the time required to decode and execute a null operation.

Load Balance: (n.)

The degree to which work is evenly distributed among available processors. A program executes most quickly when it is perfectly load balanced, that is, when every processor has exactly the same amount of work to do.

Locality:(n.)

The degree to which that computations done by a processor depend only on values held close to that processor, or the degree to which computations done on a point in some data structure depend only on values near that point. Locality can be measured by the ratio of local to nonlocal data accesses, or by the distribution of distances of, or times taken by, nonlocal accesses.

Message Passing:(n.)

A style of interprocess communication in which processes send discrete message to one another. Some computer architectures are called "message-passing" architectures because they support this model in hardware, although message passing has often been used to construct operating systems and network software for uniprocessors and distributed computers.

MIMD:(adj.)

Multiple Instruction, Multiple Data; a category in which many instructions streams are concurrently applied to multiple data sets. A MIMD architecture is one in which heterogeneous processes may execute at different rates.

Monte Carlo:(adj.)

Making use of randomness. A simulation in which many independent trials are run independently to gather statistics is a "Monte Carlo Simulation". A search algorithm that uses randomness to try to speed up convergence is a "Monte Carlo Algorithm".

Multitasking:(n.)

Executing many processes on a single processor. This is usually done by time-slicing the execution of individual processes and performing a context switch each time a process is swapped in or out. Most operating systems support multitasking, but it can be expensive if the need to switch large caches or execution pipelines makes context switching expensive.

Multicast:(n.)

To send a message to many, but not necessarily all, possible recipient processes.

Multiprocessor:(n.)

A computer in which processors can execute separate instructions streams, but have access to a single address space. Most multiprocessors are shared-memory machines, constructed by connecting several processors to one or more memory banks through a bus or switch.

Nonblocking:(adj.)

An operation that does not block the execution of the process using it. Usually applied to communication operations, where it implies that the communicating process may perform other operations before the communication has completed.

Operating System:(n.)

That software responsible for providing standard services and supporting standard operations, such as multitasking and file access.

Optimal:(adj.)

Cannot be bettered. An optimal mapping is one that yields the best possible load balance; and optimal parallel algorithm is one that has the lowest possible time-processor product.

Parallelization:(n.)

Turning a serial computation into a parallel one. This may be done automatically, by a "parallelizing complier", or (more usually) by rewriting the program that it uses some parallel paradigm.

Performance Model:(n.)

A formula that predicts the speed, efficiency, memory requirements, or other execution characteristics of a program on a particular architecture.

Private Memory:(n.)

Memory that appears to the users to be divided between many address spaces, each of which can be accessed by only one process. Most operating systems rely on some memory protection mechanism to prevent one process form accessing the private memory of another; in disjoint-memory machines, the problem is usually finding a way to emulate shared memory using a set of private memories.

RISC:(adj.)

Reduced Instruction Set Computer; a computer that provides only a few simple instructions but executes them extremely quickly, RISC machines typically rely more on instruction prefetch and caching to achieve high-performance than CISC machines. The term is also applied to software designs that give users a small number of simple, efficient operations.

Routing:(n.)

The act of moving a message from its source to its destination. A "routing algorithm" is a rule for deciding, at any intermediate node, where to send a message next; a "routing technique" is a way of handling the message as it passes through individual nodes.

Scalable:(adj.)

Capable of being increased in size, or more accurately, capable of delivering an increase in performance proportional to an increase in size. A scalable architecture is one that can be used as a design for arbitrarily large machines, or one whose increase in performance is linear in the amount of hardware invested.

Shared Memory:(n.)

Memory that appears to the user to be contained in a single address space and that can be accessed by any process. In a uniprocessor or multiprocessor there is typically a single memory unit, or several memory units interleaved to give the appearance of a single memory unit.

SIMD:(adj.)

Single Instruction, Multiple Data; a category in which a single instruction stream is concurrently applied to multiple data sets. A SIMD architecture is one in which homogeneous processes synchronously execute the same instructions on their own data, or one in which an operation can be executed on vectors of fixed or varying size.

Spanning Tree:(n.)

A tree containing a subset of the links in a graph which reaches every node in that graph. A spanning tree can always be constructed so that its depth (the greatest distance between its root and any leaf) is no greater than the diameter of the graph. Spanning trees are frequently used to implement broadcast operations.

Switch:(n.)

A physical communication medium containing nodes that perform only communications functions.

Synchronous:(adj.)

Occurring at the same clock time. For example, if a communication event is synchronous when there is some moment at which both the sender and the receiver are engaged in the operation.

Virtual Memory:(n.)

A system that stores portions of an address space that are not being used in some medium other than main high-speed memory, such as a disk or slower solid-state memory. When a reference is made to a value not presently in main memory, the virtual memory manager must swap some values in main memory for the values required. Virtual memory is used by almost all uniprocessors and multiprocessors, but is not available on some processor arrays and multicomputers.

Definitions taken from IEEE Parallel & Distributed Technology February 1993.

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