

Computational Methods in Transport
September 11–16, 2004
Granlibakken Conference Center
Tahoe City, California



Lawrence Livermore National Laboratory
Institute for Pure and Applied Mathematics UCLA

Welcome

Welcome to the Computational Methods in Transport Workshop. The idea for the workshop was born at the SCaLeS (Scientific Case for Large Scale Simulation) meeting held in Washington D.C. in June of 2003. In attendance were a group of scientists, engineers, and computer scientists from a wide variety of disciplines whose charter was to demonstrate, from an applications standpoint, the need for new ultra-scale computing facilities for Office of Science missions. A variety of breakout sessions were formed. One of these sessions dealt with particle transport. Our group consisted of experts from nuclear engineering, astrophysics, combustion, atmospheres, mathematics, etc. The discussions were lively and informative and we all realized what a wonderful opportunity this was to discuss transport issues with persons outside of our disciplines. Conversations flowed between experts who would probably never meet in the normal course of doing research. The workshop you are now attending was created out of my hope that a forum would exist where researchers could discuss successes and failures of their methods across discipline boundaries in an invigorating and relaxing atmosphere that would benefit the transport community at large.

The executive and scientific organizing committees have worked very hard at putting together a conference designed to stimulate discussion and interaction among attendees. My deepest thanks go out to them for their long and hard work. The talks have been selected to give attendees both an overview of transport issues from a wide variety of fields along with talks giving specialized detail. The talks have been made purposefully few in number yet fairly long in length so that speakers could communicate to the audience in a more effective fashion.

Finally, Mark Green (UCLA), Stanley Osher (UCLA), Jim McGraw, and Rob Falgout deserve singular thanks for their guidance and financial support. A special note of thanks goes to the administrative and support people who have made this workshop a reality. Leigh Faulk, Anita Williams, Linda Becker, Janice Amar (UCLA), Karen Lee (UCLA), Linda Oribello, Dave Parker, Linda Null and Fred Allen have performed miracles.

We hope you find the workshop stimulating, challenging, and also relaxing—enjoy!

Frank Graziani

Lawrence Livermore National Laboratory

Organizing Committees

Executive Committee:

Frank Graziani (Lawrence Livermore National Laboratory)

David Keyes (Columbia University)

James McGraw (Lawrence Livermore National Laboratory)

Stanley Osher (IPAM & UCLA)

Scientific Committee:

Marvin Adams (Texas A & M University)

John Castor (Lawrence Livermore National Laboratory)

Frank Evans (University of Colorado at Boulder)

Ivan Hubeny (University of Arizona)

Tom Manteuffel (University of Colorado at Boulder)

Gordon Olson (Los Alamos National Laboratory)

Logistics

Conference sessions will be held in the Mountain-Lake Room. The poster session along with a reception will be held Tuesday afternoon in the Pavilion Room. Breakfast, lunch and dinner will be served in the GranHall room. If weather permits, lunch will be served out on the Garden Deck. Coffee breaks will be held on the Mountain Deck. We will have a number of social hours during the conference. They are free of charge to participants and their guests.

For administrative support, please speak with either Leigh Faulk or Anita Williams in the registration area. If you have specific issues regarding audio/visual equipment, please seek out Dave Parker.

Conference Theme

The transport of particles, be they photons, neutrinos, or charged particles, arises in a myriad of applications. For inertial confinement fusion, whether one is dealing with direct drive through photon or ion beams or dealing with indirect drive via thermal photons in a hohlraum, the accurate transport of energy around and into tiny capsules requires high-order transport solutions for photons and electrons. In astrophysics, the life cycle of the stars, their formation, evolution, and death all require transport of photons and neutrinos. In planetary atmospheres, cloud variability and radiative transfer play a key role in understanding climate. These few examples are just a small subset of the applications where an accurate and fast determination of particle transport is required.

The Computational Methods in Transport Workshop is a workshop devoted to providing a forum where computational transport researchers in a variety of disciplines can communicate across disciplinary boundaries their methods and their successes and failures. Typically, the numerical methods used in a given field are communicated to other researchers in that field. Rarely, however, are those methods communicated outside of that specific field. For example, nuclear engineers and astrophysicists rarely attend the same meetings or read the same literature. This workshop hopes to address this discrepancy. The goal of the Computational Methods in Transport Workshop is to open channels of communication and cooperation so that (1) existing methods used in one field can be applied to other fields and (2) greater scientific resources can be brought to bear on the unsolved outstanding problems.

Our program begins with a keynote address Saturday evening, and it ends on Thursday at lunch. In between, we offer outstanding speakers and provide ample time for discussions. Our hope is that this workshop will provide an excellent venue to network with colleagues and relax in the beautiful surroundings of Lake Tahoe and the High Sierras.

Conference Program

SATURDAY SEPTEMBER 11, 2004

Registration (3:30-6:00)

Social Hour (5:30-6:30)

Dinner (6:30-8:00)

Opening Talk (John Castor) (8:00-8:30)

SUNDAY SEPTEMBER 12, 2004

Review Talks

(Mountain-Lake Room)

<i>Opening Remarks</i>	8:15-8:30	Frank Graziani
<i>An Overview of Radiative Transfer in Atmospheric 3D Clouds</i>	8:30-9:30	Warren Wiscombe
<i>Transition Regime Models from Kinetic Equations</i>	9:30-10:30	David Levermore
BREAK	10:30-11:00	
<i>Radiative Transfer in Astrophysical Applications</i>	11:00-12:00	Ivan Hubeny
LUNCH	12:00-2:00	
<i>Neutron (and Photon) Transport for Nuclear Reactor Applications</i>	2:00-3:00	Ed Larsen
<i>A Coupled Leaf/Canopy Turbid Medium Radiative Transfer Model</i>	3:00-4:00	Barry Ganapol
BREAK	4:00-4:30	
<i>Simulations of High Energy Density Physics Experiments on Massively Parallel Architectures</i>	4:30-5:30	Marty Marinak
Social Hour	5:30-6:30	
DINNER	6:30	

MONDAY SEPTEMBER 13, 2004

Atmospheric Physics/Oceanography/Plant Canopies
(Mountain-Lake Room)

<i>3D Radiative Transfer in Cloudy Atmospheres: Diffusion Approximation and Monte Carlo Simulation for Thermal Emission</i>	8:30-9:15	Kuo-Nan Liou
<i>The Spherical Harmonics Discrete Ordinate Method for Atmospheric Radiative Transfer</i>	9:15-10:00	Frank Evans
BREAK	10:00-10:30	
<i>From Simple Plane-parallel to Complex Monte Carlo Calculations of Solar Fluxes and Radiances for Cloudy Atmosphere</i>	10:30-11:15	Alexander Marshak
<i>Effective Transport Kernels for Spatially Correlated Media—Application to the Cloudy Atmosphere</i>	11:15-12:00	Anthony Davis
LUNCH	12:00-2:00	
<i>Computer Challenges In Optical Oceanography</i>	2:00-2:45	Norm McCormick
<i>Stokes Vector–Mueller Matrix Radiative Transfer in an Atmosphere-Ocean System</i>	2:45-3:30	George Kattawar
<i>Vertical and Horizontal Transport of Solar Radiation in Structurally Heterogeneous Canopies: Issues and Caveats</i>	3:30-4:15	Jean-Luc Widlowski
BREAK	4:15-4:30	
<i>Moderated Discussion</i>	4:30-5:30	David Keyes
DINNER	6:00	

TUESDAY SEPTEMBER 14, 2004

Mathematics
(Mountain-Lake Room)

<i>High Order Finite Volume Nonlinear Schemes for the Boltzmann Transport Equation</i>	8:30-9:15	Barna Bihari
<i>Generalized Diffusion Models for Transport in Scattering and Non-scattering Regions</i>	9:15-10:00	Guillaume Bal
BREAK	10:00-10:30	
<i>Computations of Multi-valued Solutions of Nonlinear PDEs</i>	10:30-11:15	Shi Jin
<i>Finite-difference Methods for Solving Multi-dimensional Time-dependent Transport Problems Implemented in the SATURN Package</i>	11:15-12:00	Rashit Shagaliev
LUNCH	12:00-2:00	
POSTER SESSION	2:00-5:00	Pavilion Room
<i>Social Hour</i>	5:30-6:30	
DINNER	6:30	

WEDNESDAY SEPTEMBER 15, 2004

Neutron Transport/Astrophysics/High Energy Density Physics
(Mountain-Lake Room)

<i>Neutron Transport in Nuclear Reactors</i>	8:30-9:15	Marvin Adams
<i>Design, Implementation and Optimization of a Parallel Monte Carlo Particle Transport Code</i>	9:15-10:00	Richard Procassini
BREAK	10:00-10:30	
<i>Neutrino Transport in Core Collapse Supernovae</i>	10:30-11:15	Tony Mezzacappa
<i>Solving the Time-dependent Discrete-ordinates Boltzmann Equation on Parallel Architectures</i>	11:15-12:00	Doug Swesty
LUNCH	12:00-2:00	
<i>Radiative Transfer in Numerical Cosmology</i>	2:00-2:45	Mike Norman
<i>Discrete-ordinates Methods for Radiative Transfer in the Non-relativistic Stellar Regime</i>	2:45-3:30	Jim Morel
BREAK	3:30-4:00	
<i>The Jayenne Implicit Monte Carlo Project: Where We Are, Where We're Heading and the Issues We Face</i>	4:00-4:45	Todd Urbatsch
<i>Parallel Deterministic Methods for Radiation Transport: Lessons Learned and Future Directions</i>	4:45-5:30	Paul Nowak
Social Hour	5:30-6:30	
DINNER	6:30	

THURSDAY SEPTEMBER 16, 2004

Summary
(Mountain-Lake Room)

			Session Chair
<i>Summary I</i>	8:30-8:50	Tom Abel	Frank Graziani
<i>Summary II</i>	8:50-9:10	Bill Martin	
<i>Summary III</i>	9:10-9:30	Des Pilkington	
<i>Summary IV</i>	9:30-10:30	Open/Panel Discussion	
BREAK	10:30-11:00		
<i>Closing Comments</i>	11:00-11:30	Frank Graziani	
LUNCH	12:00-2:00		

Abstracts for Talks

Neutron Transport in Nuclear Reactors

Marvin Adams
Texas A & M University

Upon first inspection, calculation of the neutron distribution in a commercial-scale nuclear reactor appears to be intractable. However, clever people over the course of several decades have created computational methods that produce highly accurate neutron distributions for very low computational cost. Here we describe the reactor-analysis problem and point out some of its daunting challenges. We introduce today's state-of-the-art methods and describe how and why they work so well for the problems they are designed to solve. The overall approach is "divide and conquer"—solving the problem in stages, with each stage building on the previous one. Another key approach is tailoring the approximations to take advantage of the physics of the problem, which yields efficiency at the expense of general applicability. We show that decades of development using these approaches have produced a methodology for today's commercial light-water reactors that provides incredibly accurate solutions for incredibly low computational effort.

Generalized Diffusion Models for Transport in Scattering and Non-scattering Regions

Guillaume Bal
Columbia University

Transport solutions in highly scattering media are known to be well-approximated by solutions to diffusion equations. As several numerical studies show, the presence of non-scattering areas, such as clear layers in optical tomography (a medical imaging technique based on photon propagation in human tissues), hampers the use of classical diffusion. This has resulted in some researchers abandoning diffusion equations to replace them by the numerically much more costly transport equations. I will show that "generalized" diffusion equations can still model transport fairly accurately for a large class of non-scattering inclusions. Such non-scattering areas include clear layers filled with cerebrospinal fluid and hematoma that need to be modeled carefully in optical tomography. Several numerical simulations will also be presented.

High Order Finite Volume Nonlinear Schemes for the Boltzmann Transport Equation

Barna Bihari and Peter Brown
Lawrence Livermore National Laboratory

The Boltzmann Transport Equation (BTE) is a linear integro-differential equation to be solved for a scalar unknown, usually called the particle flux. Finite volume schemes, on the other hand, are typically used to solve equations of high speed fluid dynamics where conservation is crucial. Application of these schemes to the BTE ensures not only conservation, but also provides for a more natural handling of boundary conditions, material properties and source terms, as well as an easier parallel implementation and post processing. The finite volume scheme also lends itself to an efficient implementation of high order spatial discretizations.

Material interfaces and time-dependent large source terms can introduce severe oscillations even with second order fixed stencil schemes. Slope limiting, or essentially non-oscillatory (ENO) spatial interpolations eliminate these oscillations, and make higher-than-second-order spatial accuracies possible. A newer variation of these nonlinear schemes is the Weighted ENO (WENO) scheme that makes the stencil transition less abrupt and boosts the accuracy in smooth regions. For unsteady problems, the resulting nonlinear spatial discretization yields a set of ODE's in time, which in turn is solved via high order implicit time-stepping with error control. For the steady-state case, we need to solve the non-linear system, typically by Newton-Krylov iterations. Both of these approaches require a preconditioner in order to obtain a reasonable rate of convergence.

We will discuss the advantages of using an ENO/WENO method, as well as the various issues introduced by such nonlinear methods originally designed for computing shocked fluid flows. There will be several numerical examples presented to demonstrate the accuracy, non-oscillatory nature and efficiency of these high order methods, in comparison with other fixed-stencil schemes. Parallel-efficiency, scalability, boundary conditions and convergence acceleration aspects will be addressed as well.

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

Effective Transport Kernels for Spatially Correlated Media— Application to the Cloudy Atmosphere

***Anthony Davis
Los Alamos National Laboratory***

We are motivated here by the important problem of partitioning the absorption of solar radiation inside the atmosphere-surface system over vast (>100 km) domains, a basic step towards climate forecasting, in the presence of clouds. It is shown under very general conditions that the effective transport kernel is never exponential and always decays more slowly. However, for this strong statement about effective medium theory to have a significant impact, we need to be in a situation where the unresolved (and assumed random) variability has spatial correlations that range at least to the actual mean-free-path which, incidentally, is always larger than predicted by the mean density and cross-section. The cloudy atmosphere ranges from totally- to semi-opaque, so deviations from exponential decay in the transport kernel will matter. The observed variability in a wide variety of cloud scenarios leads to power-law kernels, hence to a “Levy-flight” or “anomalous diffusion” model for the multiple scattering. It will be shown that recent advances in differential absorption spectroscopy in oxygen lines agree with specific predictions of this unconventional model for bulk photon transport through the atmosphere. It is not clear that the anomalous diffusion model can be applied to the estimation of detailed layer-by-layer solar energy deposition. However, it can certainly help in conveying statistical meaning to the new observational diagnostics of absorption in the complex atmospheric medium, namely, photon path lengths from oxygen line spectroscopy.

The Spherical Harmonics Discrete Ordinate Method for Atmospheric Radiative Transfer

***Frank Evans
University of Colorado at Boulder***

This talk will describe the SHDOM algorithm for computing radiative transfer in three-dimensional cloudy atmospheres. SHDOM is the most widely used deterministic (i.e., non-Monte Carlo) model used for 3D transport in atmospheric physics. It uses a source function iteration approach in which the source function is represented by a spherical harmonics series at each grid point, while integration of the source function to compute intensity is carried out along discrete ordinates. The choices made in the algorithm design to maximize computational speed and minimize memory use will be described. The advantages and disadvantages of SHDOM compared to Monte Carlo methods will also be discussed.

A Coupled Leaf/Canopy Turbid Medium Radiative Transfer Model

Barry Ganapol
University of Arizona

Applications of radiative transfer are commonly concerned with participating scattering and absorbing media that are geometrically well defined and have well characterized physical properties. This is not the case for radiative transfer describing reflection from a vegetation canopy in response to passive sunlight. Here one is faced with a medium under continuous morphological transition resulting from seasonal and inter-annual variation, biogenic and anthropologic stresses as well as the ubiquitous biodiversity of nature. Canopy reflectance modeling is a necessary component of scientific investigation that establishes diagnostic links between investigative conjecture and spectral data collected in the laboratory and field or through remote sensing from air-born or satellite detectors. Various approaches have been proposed to model canopy reflectance. Turbid canopy reflectance models, such as SAIL and THREEVEG, and leaf radiative transfer models like PROSPECT and LIBERTY, have been developed to address fundamental issues in remote sensing and ecology. In this presentation, the coupling of a within-leaf radiative transfer model (called LEAFMOD) to a canopy radiative transfer model (called CANMOD) will be described for estimating biochemical content of vegetation through spectral profiles of reflected light or for detecting background spectral signatures. The governing philosophy in the development of the coupled leaf/canopy radiative transfer model, called LCM2, is that nature averages over our ignorance of the exact geometrical canopy configuration and leaf structure and that "simple" is most appropriate here. Features of the model include a consistent radiative transfer characterization of photon scattering within a homogeneous leaf, which then directly couples leaf chemical information to the canopy reflectance. With an average leaf thickness, specific absorptivities, a scattering profile and concentrations for the major biochemical constituents, LEAFMOD (in the forward mode) provides leaf hemispherical reflectances and transmittances and the directional distribution of the radiance exiting the leaf surfaces. In this way, a leaf scattering characterization (or leaf phase function) can be constructed that will serve as input to a vegetation canopy model. This presentation will concentrate on the transport methods used in the LCM2 model. In particular, a new 1D/SN algorithm based on Romberg acceleration convergence of the inner iteration will be presented. In addition, the inclusion of linear polarization in an FN solution format will be discussed.

Radiative Transfer in Astrophysical Applications

Ivan Hubeny
University of Arizona, Tucson

Astrophysics is the field where radiative transfer plays an extremely important, even sometimes crucial, role. Radiation is almost exclusively the only information about a distant object we have. Yet, the radiation is not only a passive probe of the physical state of the object, but in many cases an active energy and momentum balance agent. However, a treatment of radiation involves a highly non-linear, highly coupled, highly non-local, multi-dimensional, and sometimes even time-dependent problem, which poses enormous numerical challenges.

In this review, I will summarize various numerical techniques used to deal with a non-local and non-linear coupling of radiation and matter. Efficient methods can either be constructed purely mathematically, by formulating the problem essentially exactly, and using various pre-conditioners to invert resulting huge matrices. The methods can also be developed using our physical insight, by realizing that some parts of the coupling are more important than others, which leads to techniques in which an important part of the coupling is treated directly, while the rest is treated iteratively. In fact, the most successful techniques are those which combine both approaches, and which can be generically called physics-based pre-conditioning techniques. The group of methods developed in astrophysics called the Accelerated Lambda Iteration (ALI) method, are a typical example of such techniques. In this talk, I will discuss the method in a general context, and show its various applications.

Stokes Vector–Mueller Matrix Radiative Transfer in an Atmosphere-Ocean System

George Kattawar
Texas A&M University

Since the genesis of radiative transfer, polarization has in large part been ignored due to the complexity it introduced into the equation of transfer. It was often felt that no significant errors were introduced by neglecting it. We will present a brief introduction of the Stokes vector–Mueller matrix approach and show why one should include it into the radiative transfer calculations. In addition to the fact that it is the only correct way to do radiative transfer, we will present cases to show the errors that will be incurred by neglecting it. We will also show the many new and exciting things that have evolved using this approach. The virtues of having this new information have led to applications ranging from better target detection both on-land and in the ocean to detection of precancerous skin

lesions. There is also a possibility that Mueller matrix imaging may be used for remote detection of anthrax spores. Both linear and circular polarization conveys different pieces of information about a target and we will show how each can be used to enhance the surface features of targets. Emphasis will be placed on how a Monte Carlo calculation can be used to compute the effective multiple scattering Mueller matrix (MSMM); however, often times a forward scheme will not be realistic and thus to improve statistics, a backward Monte Carlo scheme has to be used. This scheme requires using biased sampling to perform the calculation. We will show how effective this scheme is in calculating the MSMM and discuss future applications.

Computations of Multi-valued Solutions of Nonlinear PDEs

Shi Jin
University of Wisconsin

Many physical problems arising from high frequency waves, dispersive waves or Hamiltonian systems require the computations of multi-valued solutions, which cannot be described by the viscosity methods. In this talk I will review several recent numerical methods for such problems, including the moment methods, kinetic equations and level set methods. Applications to the semi-classical Schrödinger equation and Euler-Poisson equations with applications to modulated electron beams in Klystrons, and general symmetric hyperbolic systems will be discussed.

Neutron (and Photon) Transport for Nuclear Reactor Applications

Ed Larsen
University of Michigan

This talk will review the basic physical and computational characteristics of neutron transport problems for nuclear reactor cores (and coupled neutron-photon transport for nuclear reactor shields). The underlying physical nature of these problems (in terms of how they differ from other types of particle transport problems) will be outlined, and the basic computational methods that have been developed during the past 50 years for solving these problems will be characterized. The talk will include a discussion of some current popular research topics and significant open problems. The overall goal of the talk is to introduce the audience to the types of neutron and photon transport problems in the practical arena of nuclear engineering, and the types of computational methods that currently exist and are on the drawing board for solving these problems.

Transition Regime Models from Kinetic Equations

***Dave Levermore
University of Maryland***

This talk will survey some recent advances in the development of transition regime models from kinetic equations. The classes of stationary-balance models and quasi-stationary-balance models will be presented for linear kinetic equations. These models share elements with both traditional moment closures and expansions. They also include a natural framework for developing boundary conditions. Generalizations of these ideas to nonlinear kinetic settings include entropy-based moment closures, and hierarchies of fluid dynamical systems for the classical Boltzmann equation that dissipate entropy and include dispersive terms with higher order space derivatives.

3D Radiative Transfer in Cloudy Atmospheres: Diffusion Approximation and Monte Carlo Simulation for Thermal Emission

***Kuo-Nan Liou
(Y. Chen and Y. Gu)
University of California, Los Angeles***

Clouds, which occupy more than 50% of the sky, are generally finite and inhomogeneous. They are the most important element in modulating the energy budget of the Earth-atmosphere system and hence climate. The potential effects of cloud geometry and inhomogeneity on the transfer of radiation must be carefully studied in order to understand their impact on the radiative properties of the atmosphere. Moreover, incorporation of these effects on radiative transfer in climate and general circulation models (GCMs) remains one of the most difficult problems due to the complexity of cloud formation treatment in the model and the associated radiative transfer calculations. All GCMs at present consider clouds to be plane-parallel and homogeneous with respect to radiation calculations.

We developed a solution for the 3D diffusion radiative transfer equation in Cartesian coordinates utilizing a four-term spherical harmonics expansion for the scattering phase function and intensity, intended for potential incorporation in climate models. The general second-order partial differential equation derived from the diffusion approximation has been solved by employing an efficient full multigrid method, which can simulate the transfer of solar and thermal infrared radiation in inhomogeneous cloudy atmospheres with different boundary conditions, including sharp discontinuity. The correlated k-distribution method has been used for the sorting of gaseous absorbing lines in association with multiple-

scattering atmospheres for the calculation of fluxes covering the entire solar and thermal infrared spectra. Comparison of the broadband fluxes and heating rates computed from this approach to those from the equivalent plane-parallel and 3D Monte Carlo models shows excellent agreement. For thermal emission, we developed a 3D Monte Carlo model for specific application to broadband infrared radiative transfer that differs from the conventional use of point source. The model domain consists of a variable structure based on cubic grid cells in which the emissivities for gases and cloud particles are parameterized.

We applied the 3D radiative transfer models to the 3D cirrus cloud fields constructed from remote sensing on the basis of a unification of satellite and ground-based cloud profiling radar observations over the DOE ARM-SGP site. Two cases, which illustrate substantial horizontal and vertical variability in ice crystal size distribution, have been chosen for the analysis of 3D fluxes and heating rates in terms of mean and variance in different spatial scales. Pertinent results are presented and physically discussed.

Simulations of High Energy Density Physics Experiments on Massively Parallel Architectures

***Marty Marinak
Lawrence Livermore National Laboratory***

High energy density experimental facilities access extreme conditions of temperature and pressure, allowing us to probe states of matter relevant to astrophysics and planetary and stellar interiors. Laboratory experiments now yield detailed measurements of radiation transport and opacities, equations-of-state and material dynamics at high pressure, and implosions and hydrodynamic instabilities. Developing an understanding of material properties and processes occurring at high energy densities is also the central challenge for inertial confinement fusion (ICF). Current high energy lasers, such as Omega at the University of Rochester Laboratory of Laser Energetics, and others worldwide, and pulsed power machines such as the Z facility at Sandia National Laboratories, conduct experiments at pressures of up to 40 Mbar and temperatures of 200 eV. The National Ignition Facility (NIF) should reach Gbar pressures and temperatures of tens of keV, enabling exploration of new regimes, including attainment of thermonuclear ignition. The design of high energy density experiments and interpretation of the experimental results rely heavily upon complex codes which treat a full spectrum of physical processes. These codes model heating from intense laser beams, particle beams, or strong electric currents. They model energy transport by soft x-rays over a spectrum of frequencies. Thermal energy transport by electrons and ions is modeled, either in the local or non-local limits,

possibly in the presence of evolving magnetic fields. Modeling of thermonuclear burn in ICF capsules necessitates transporting charged particle and neutron products as well. These processes act while the plasma is in motion, often evolving under the action of one or more hydrodynamic instabilities. Thus the transport algorithms employed must be sufficiently economical and efficient to allow highly resolved simulations to proceed on hydrodynamic timescales. The transport algorithms must also scale efficiently for distributed parallel processing to facilitate simulations of targets in three dimensions. We examine various transport methods employed in high energy density physics simulations. Special emphasis will be placed on methods that have proven practical for everyday use while representing the important physical processes. The propagation and deposition of laser energy are considered in the context of ray tracing models, which include the ponderomotive pressure and scattering effects. We discuss models for electron thermal transport ranging from the local limit to a non-local treatment that employs a delocalization kernel to retain the main features caused by kinetic effects. We examine approaches for modeling of magnetic fields in 3D, considering the complications that arise from wide variations in the Hall parameter and from the Nernst convective term. We outline various methods for calculating thermal x-ray transport and discuss the significance of non-LTE effects. The effectiveness of the methods will be examined through comparisons of simulations with experiments. Results from large-scale simulations run on over 1000 processors, using a combination of massively parallel processing and symmetric multiprocessing, will be described.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

From Simple Plane-parallel to Complex Monte Carlo Calculations of Solar Fluxes and Radiances for Cloudy Atmospheres

***Alexander Marshak
NASA Goddard Space Flight Center***

In my presentation, I will describe several approximation methods with different levels of complexity; they will be gradually applied to simple examples of horizontally inhomogeneous clouds. Understanding of photon horizontal transport and radiative smoothing can help to improve accuracy of the methods. The accuracy of the methods will be compared with the full Monte Carlo calculations. The specifics of Monte Carlo in cloudy atmospheres will also be discussed. A special emphasis will be put on the strong forward scattering peak in the phase functions.

Computer Challenges In Optical Oceanography

Norm McCormick
University of Washington

A major simplification in many optical ocean calculations is that the plane parallel medium (1-D) approximation is usually sufficient because of the large extent of the solar radiation field and the relatively layered structure of seawater. In this approximation the polar and azimuthal angle variables can be uncoupled [1]. Traditional methods of solving radiative transfer problems for seawater include Monte Carlo, invariant imbedding, and discrete ordinates (both traditional, and so-called analytic, in which the angle dependence of the radiation is represented in the form of an eigenmode expansion). For an analysis of coupled atmosphere-ocean systems, Fresnel reflection effects cause the air-water boundary condition to be more complicated than that for traditional neutral particle transport theory. Waves induced by wind and tidal motion also create difficulties when describing transfer across the interface. Furthermore, near the surface, polarization effects sometimes are important. A brief review of the classical procedures for solving ocean optics problems will be presented, followed by a discussion of some challenges remaining for the development of seawater optical monitoring systems.

[1] S. Chandrasekhar, *Radiative Transfer* (Dover, New York, 1960), section 48.1.

Neutrino Transport in Core Collapse Supernovae

Tony Mezzacappa
Oak Ridge National Laboratory

Neutrino production, transport, and interaction is arguably the single-most important component of a core collapse supernova model. Neutrinos are believed to be responsible for powering these supernovae, in part or entirely, and their production and transport set the stage for the radiation magneto-hydrodynamics of stellar core collapse and bounce, which provides the initial conditions for the post-stellar-core-bounce dynamics. Neutrino transport is governed by multidimensional, phase-space, integro-partial differential kinetic equations. The solution of these equations dominates the computational challenge in simulating this supernova class. We present the neutrino transport and neutrino radiation hydrodynamics equations involved, and their finite differencing, and discuss their solution. We use the spherically symmetric (spatially one-dimensional) case to illustrate the equations and the issues involved, but give the general formalism for the spatially multidimensional case as well. We conclude by briefly discussing the implications of the now experimentally measured nonzero neutrino masses.

Discrete-Ordinates Methods for Radiative Transfer in the Non-Relativistic Stellar Regime

Jim Morel

Los Alamos National Laboratory

We give an overview of discrete-ordinates or SN methods for radiative transfer in the non-relativistic stellar regime. We first describe the basic equations of radiative transfer, which consist of a transfer equation for the angular intensity and a material temperature equation. The transfer equation considers emission, absorption, and Thompson scattering. If required, Compton scattering is separately treated via operator splitting. The material temperature equation includes absorption and emission terms. If required, heat conduction is treated via operator splitting. A Newton-like method is used to solve the nonlinear equations. The associated linearization procedure enables the material temperature to be eliminated from the transfer equation. We next describe discretization and solution techniques for the linearized transfer equation. The SN method generally refers to an angular discretization of the transfer equation that is based upon collocation at a discrete set of directions that also serve as quadrature points for evaluating directional integrals. Temporal discretization techniques include the traditional backward-Euler and Crank-Nicholson methods. For illustrative purposes, we assume the backward-Euler method. The standard multi-group method is almost exclusively used for energy or frequency discretization. Spatial discretization requires considerable care and is almost always based upon some type of discontinuous method. The rather severe requirements placed upon spatial discretization schemes are discussed and an example of a good 1-D scheme is given. The basic source iteration technique for solving the transfer equation is described next, followed by a description of two traditional diffusion based techniques for accelerating the convergence of the source iterations. We next discuss the application of Krylov methods to the solution of the transfer equation, and the recasting of traditional acceleration techniques as pre-conditioners. Finally, we discuss a simplified non-relativistic model for material-motion corrections to the Eulerian-frame transfer equation for use in radiation-hydrodynamics calculations.

Parallel Deterministic Methods for Radiation Transport: Lessons Learned and Future Directions

Paul Nowak

Lawrence Livermore National Laboratory

We consider the solution of time-dependent, energy-dependent, discrete ordinates, and nonlinear radiative transfer problems on three-dimensional unstructured spatial grids. The class of simulations we consider are those in which radiation flows through a moving background media, where the spatial grid moves with the fluid in some regions and the grid may be “relaxed” in other regions. This class of problems is characterized by tens of thousands of radiation variables per spatial zone and upwards of millions of zones, thus requiring large parallel computing platforms with distributed memory. We discuss the use of spatial decomposition using message passing between “nodes,” and threading algorithms within a node. We also present an energy group “batching” approach that greatly enhances cache performance. Our conclusion, after considering cache performance, storage limitations and dependencies inherent in the physics, is that a model that uses a combination of message-passing and threading is superior to one that uses message-passing alone. We present numerical evidence to support this conclusion.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

Radiative Transfer in Numerical Cosmology

Mike Norman

UC San Diego

In this talk I review the computational challenges and numerical methods that have been developed to simulate the transport of ionizing radiation in numerical cosmology as motivated by the grand challenge problem of cosmological reionization. A key goal is to develop models that accurately reproduce the ionization history of the intergalactic medium over cosmic time. Recent evidence from NASA’s WMAP satellite indicate that an early generation of stars began the process some 100–200 Myr after the Big Bang. Ray-tracing, moment methods, and Monte Carlo methods are reviewed with examples. I conclude by discussing our plans for incorporating radiative transfer into adaptive mesh refinement hydrodynamic cosmological simulations and estimate the resources required to carry them out.

Design, Implementation and Optimization of a Parallel Monte Carlo Particle Transport Code

Richard Procassini

(Janine Taylor, Gregory Greenman, Matthew O'Brien and Dermott Cullen)

Lawrence Livermore National Laboratory

The design, implementation and optimization of a parallel, Monte Carlo particle transport code is presented. MERCURY [1] is a modern Monte Carlo code being developed at the Lawrence Livermore National Laboratory (LLNL). It is capable of modeling the transport of neutrons, gammas, and five light ions through a variety of problem geometries, both combinatorial and mesh based. A key requirement which has driven the design and development of MERCURY is the ability to run on various massively parallel computing platforms. To this end, we have designed and implemented a multifaceted approach to parallelism in MERCURY. This parallel programming model employs both distributed memory message passing and shared memory threading techniques. This allows us to model particle transport through very large meshes or geometries (spatial parallelism), as well as very large particle counts (particle parallelism). Following a detailed discussion of the parallel implementation of MERCURY, we assess the parallel performance of the code on two criticality problems. Particle induced load imbalance will be shown to degrade the parallel efficiency of spatially decomposed calculations. We will present the latest results of our efforts to minimize the load imbalance by (a) varying the number of replicated domains in spatial and particle decomposed calculations and (b) varying the size of each domain via spatial re-decomposition.

[1] R. J. Procassini and J. M. Taylor, *MERCURY User Guide (Version b.6)*, Lawrence Livermore National Laboratory, Report UCRLTM204296 (2004). UCRLABS205670 Page 1.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

Finite-difference Methods for Solving Multi-dimensional Time-dependent Transport Problems Implemented in the SATURN Package

Rashit Shagaliev

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***Russian Federal Nuclear Center—All-Russian Scientific
Research Institute of Experimental Physics***

This talk briefly describes the numerical methods for time-dependent problems implemented in SATURN code complex. This system of codes is intended for solving 2D and 3D, both linear and nonlinear, spectral transport problems encountered in physics of high densities and energies in multiple-group approximation.

The main principles forming the basis for the numerical methods of solving 2D time-dependent transport problems used in SATURN are, as follows:

1. Two types of spatial grids are used in SATURN to approximate the transport equation in space variables, they are:

—Regular non-orthogonal grids of convex quadrangles;

—Irregular non-orthogonal grids of arbitrary-shape convex polygons.

Several conservative finite-difference schemes have been proposed for the 2D transport equation approximation using the grids above: namely, schemes of the DS_n-method type, schemes that introduce closing relations based on moment equations, adaptive methods with refined grids in phase space, etc. All of these schemes have a common feature in that with the use of non-orthogonal grids they preserve some important features of DS_n-schemes, such as the transport equation approximation within a single cell of phase space and, consequently, a possibility to resolve systems of grid equations using point-to-point computations. At the same time, they slightly differ from each other in the accuracy of approximating on essentially non-orthogonal grids, in monotonicity of grid solutions, and in some other features. This talk gives a more detailed formulation of the schemes mentioned above and presents some results of their computational investigations.

2. The KM-method of accelerating convergence of simple iterations and some modifications of this method are successfully used in the SATURN package for a higher efficiency of solving systems of multiple-group grid transport equations in optically dense nonlinear problems. This talk gives a brief description of the KM-method and some examples of its estimated efficiency.

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3. Finding solutions to many multidimensional time-dependent transport problems results in a large computational burden. To solve such problems on modern multiprocessor platforms, a combined parallelization algorithm is implemented in SATURN that includes a capability of spatial small-block decomposition of a problem using non-orthogonal grids in combination with decomposition in energy and angular variables. This talk describes specific features of the algorithm. Issues of generalizing the methods and algorithms described to a 3D case are considered. Examples of computations by SATURN in combination with hydrodynamic codes for 2D non-linear application problems of laser thermonuclear fusion are presented.

***Solving the Time-dependent Discrete-ordinates
Boltzmann Equation on Parallel Architectures***

***Doug Swesty
SUNY-Stony Brook***

The solution of the time-dependent discrete-ordinates form of the Boltzmann equation arises in wide variety of transport and radiation-hydrodynamic problems. In this talk I will describe one approach to the numerical solution of this equation on massively parallel architectures. Instead of using a more traditional source-iteration method, we employ Krylov subspace algorithms to solve the full linear system arising from the implicitly-discretized Boltzmann equation. This approach offers numerous advantages and a few drawbacks. The approach is also easily extensible, via Newton-Krylov methods, to non-linear cases where radiation-heating or radiation-hydrodynamic effects are included in the problem. The success of this full linear system method lies in the development of pre-conditioners which aid the convergence of the iterative Krylov-subspace algorithms. I will discuss some preconditioning strategies that are useful for broad classes of problems.

The Jayenne Implicit Monte Carlo Project: Where We Are, Where We're Heading, and the Issues We Face

Todd Urbatsch

***(Thomas M. Evans, Michael W. Buksas, Jeffery D. Densmore, and
Aimee L. Hungerford; CCS-4, Transport Methods Group)***

Los Alamos National Laboratory

The Jayenne Implicit Monte Carlo (IMC) Project is an object-oriented, C++ software effort for producing codes and packages that simulate nonlinear thermal radiative x-ray transport using the Fleck and Cummings IMC method. The stand-alone, radiation-only code Milagro is the part of the Jayenne Project used to verify the underlying classes, which are then used to construct IMC packages that interface to application codes. Milagro is parallel, using either mesh replication or mesh decomposition, multi-geometry, multi-mesh, gray or multi-group in frequency, and reproducible. The Jayenne software is designed using leveled, acyclic object dependencies, such that all objects can be thoroughly unit-tested and used confidently by higher level objects. Independent variables, such as space and frequency, are used as template parameters so that physics and numerics classes remain unchanged regardless of whichever mesh type they use, whether it is 2-D or 3-D, whether it is AMR or structured, or whether the simulation is gray or multi-group. Curvilinear geometries are represented by 3-D Cartesian approximations for speed and ease of tracking and tallying: the at-top "RZ-Wedge" for cylindrical geometry and the "Sphyramid" mesh for 1 spherical geometry. Jayenne also has the Random Walk treatment of Fleck and Canfield for speeding up IMC in diffusive regimes.

We continue to face many issues in the Jayenne IMC Project. Issues with memory and speed drive most of our research. For instance, replicating the mesh on each processor provides the fastest transport but the most egregious memory consumption; decomposing the mesh saves memory but approaches serial runtimes regardless of processor count. Furthermore, IMC has a mix of traditional Monte Carlo work in its tracking and deterministic work in its loops over the entire mesh to calculate the source at the beginning of the time step and the tallies at the end of the time step. This dual nature of IMC precludes any one usual parallel scheme from being optimal. Always fighting the memory and speed battle, we additionally find that we are often faced with unresolved transport boundary layers, which can affect accuracy greatly. Another issue we have with IMC is that estimating statistical error for nonlinear Monte Carlo transport is not easy; in fact we do not do it. Usually unable to afford replicate runs, we rely on expert knowledge and trial-and-error for selecting the number of particles. Lastly, at a national laboratory we are constantly faced with the age-old tension between

doing methods research and developing and maintaining production software, although it is clear that both are necessary.

The Monte Carlo Team of the Transport Methods Group at LANL is performing some exciting methods, algorithms, and software research. The bulk of our methods research is in hybrid Monte Carlo methods. Over the last several years, we have developed (spatially) Discrete Diffusion Monte Carlo (DDMC) methods for linear static diffusion, equilibrium diffusion, and now for full time-continuous non-equilibrium thermal diffusion. The latter is a prospective cell-based alternative to the Random Walk technique. We are also researching Residual Monte Carlo methods (a la J. Halton) for low-order approximations, where, for the Discrete Equilibrium Diffusion Monte Carlo hybrid method, we have obtained speedups on the order of a billion. Our hope is that residual Monte Carlo methods will be a competitive alternative to deterministic linear solvers. Low-memory, time-dependent particle tracking is another research area in which we are looking to reduce the Monte Carlo memory requirements. In the area of algorithms research, specifically parallel schemes, we are pursuing general domain replication/decomposition and “OpenMPI” strategies. Finally, we are involved peripherally with a separate project, which is developing a multi-physics software process, library, and infrastructure, in which we, for one, will be able to better select the data decompositions that are most efficient for IMC.2.

Vertical and Horizontal Transport of Solar Radiation in Structurally Heterogeneous Canopies: Issues and Caveats

***Jean-Luc Widlowski
Joint Research Center***

Vegetation canopies are inherently 3-D, with various levels of clumping occurring at different scales: the within-crown, the tree, and the canopy level. As such their reflectance anisotropy in the optical domain is not accurately simulated by adopting a purely turbid medium representation. For example, the local reflection maximum in the retro-reflection direction—known as the ‘hot spot’—is precisely due to the finite size of the scatterers in the canopy layer, as well as the spectral contrast with the underlying background. Structurally homogeneous canopy representations (i.e., plane-parallel vegetation layers containing uniformly distributed finite-sized scatterers with specified distributions of their orientation: 1-D), thus constitute the simplest canopy representation capable of matching multi-spectral space borne reflectance measurements under almost any view and illumination geometry. In fact, at large spatial resolutions, 1-D canopy representations may generate reflectance fields that are undistinguishable from those generated over 3-D surface types. However, when

the spatial resolution of the observing sensor becomes finer, then horizontal photon migration in conjunction with multi-directional canopy sampling issues start to affect the aptitude of 1-D canopy representations to match multi-angular and multi-spectral reflectance observations over 3-D target surfaces. In any case, the interpretation of the state variables of such radiatively equivalent 1-D models is far from simple, and the canopy reflectance modeling community is only just beginning to address these issues. The quantitative documentation of horizontal and vertical transport phenomena at high spatial resolutions requires (1) the availability of structural (and to a lesser extent also spectral) information on 3-D vegetation canopies, (2) a sophisticated 3-D Rayleigh-Taylor model capable of representing the local radiation transfer within such a heterogeneous environment, and (3) the usage of suitable variance reduction and/or software parallelization techniques in order to keep the computation times within acceptable levels. Recently, the implementation of the 'photon spreading' technique within a parallelized Monte Carlo ray tracing model has allowed us to perform the forward simulation of fluxes and bi-directional reflectance fields over structurally heterogeneous scenes at very high spatial resolutions. Initial results of these efforts will be presented, and a number of issues and caveats related to these forward and inverse modeling problems will be documented.

An Overview of Radiative Transfer in Atmospheric 3D Clouds

Warren Wiscombe
NASA Goddard Space Flight Center

Poster Titles

Nonlinear Yvon-Mertens Method for the Transport Equation

Dmitriy Anistratov and Loren Roberts

NC State University

A Piecewise Linear Finite Element Discretization of the Diffusion Equation

Marvin Adams, Texas A&M University

Brian Yang and Mike Zika, Lawrence Livermore National Laboratory

Symbolic Implicit Monte Carlo Radiation Transport in the Difference Formulation: A Piecewise Constant Discretization

Eugene D. Brooks III, Michael Scott McKinley, Frank Daffin, Abraham Szoke

Lawrence Livermore National Laboratory (UCRL-ABS-203979)

Continuously Varying Material Properties and Tallies for Monte Carlo Calculations

Forrest Brown, Los Alamos National Laboratory

William R. Martin, University of Michigan

Deterministic Transport in RAGE

Michael Clover

Los Alamos National Laboratory

An Evaluation of the Difference Formulation for Photon Transport in a Two Level Atomic System in Slab Geometry

F. C. Daffin, M. S. McKinley, E. D. Brooks III and A. Szoke

Lawrence Livermore National Laboratory

Finite Element Transport using Wachspress Rational Basis Functions on Quadrilaterals in Diffusive Regions

Gregory Davidson

Oregon State University

Transport Needs in Astrophysics

Chris Fryer

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Implicit Monte Carlo Diffusion: And Acceleration Technique for Monte Carlo Photonics

Nick Gentile

Lawrence Livermore National Laboratory

KM-method for Iteration Convergence Acceleration in Solution of the 2D Time-dependent Multi-group Transport Equation and its Modifications

A. V. Gichuk, L. P. Fedotova, R. M. Shagaliev

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Mathematical Simulation of the Radiative Transfer in Statistically Inhomogeneous Clouds

Evgueni Kassianov

Pacific Northwest National Laboratory

The Integrated TIGER Series Version 5.0

Thomas W. Laub

Sandia National Laboratories

Backward Error Compensation for Transportation Equations with Application to the Level Set Method

Yingjie Liu, Georgia Institute of Technology

Collaborator: Todd Dupont, University of Chicago

Central Schemes on Overlapping Cells

Yingjie Liu

Georgia Institute of Technology

Positive Discrete Ordinates Techniques

Kirk Mathews

Air Force Institute of Technology

Implicit Riemann Solvers for the Pn Equations

Ryan McClarren, University of Michigan/Sandia National Laboratories

Thomas Brunner, Sandia National Laboratories

James Paul Holloway, University of Michigan

Thomas Mehlhorn, Sandia National Laboratories

GILE-BOLTZTRAN: A Neutrino Radiation Hydrodynamics Code for Core-collapse Supernovae Simulations

Bronson Messer

University of Chicago

Variance Reduction Techniques for the Symbolic Implicit Monte Carlo Method

Jerome Metral

Commissariat a l'Energie Atomique

Perturbation Technique in 3D Cloud Optics: Theory and Results

Igor N. Polonsky, Anthony B. Davis and Michael A. Box

Los Alamos National Laboratory

A Moment-preserving Non-analog Method for Charged Particle Transport

Anil K. Prinja

The University of New Mexico

Non-LTE Radiation Transport in High Radiation Plasmas

H. A. Scott

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Algorithms for Parallelization of 2D Transport Equation on Arbitrary Non-orthogonal Grids

R. M. Shagaliev, A. V. Alekseyev, I. M. Belyakov, A. V. Gichuk, A. A. Nuzhdin, V. Yu. Rezhikov

Russian Federal Nuclear Center—All-Russian Scientific Research Institute of Experimental Physics (RFNC-VNIIEF)

Solution of 2D Photon Transport and Radiation-medium Interaction Problems Using Space-adaptive Algorithm

R. M. Shagaliev, A. V. Alekseyev, I. M. Belyakov, A. V. Gichuk, V. V. Evdokimov, A. N. Moskvina, A. A. Nuzhdin, N. P. Pleteneva, T. V. Shemyakina

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Fully Implicit Solution of Large Scale Non-equilibrium Radiation Diffusion with High Order Time Integration

Carol Woodward

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Conference Notes

Conference Notes
