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*Author(s):* J. E. Morel

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# Deterministic Transport Methods and Codes at Los Alamos

J. E. Morel
*Transport Methods Group*
*Los Alamos National Laboratory*
*Los Alamos, NM 87545 (USA)*
*jim@lanl.gov*

**Abstract**

A brief history of deterministic transport methods development and deterministic code development at Los Alamos National Laboratory is presented. The current status and capabilities of deterministic transport codes at Los Alamos are discussed together with future research directions.

## 1 Introduction

The purposes of this paper are to

- Present a brief history of deterministic transport methods development at Los Alamos National Laboratory from the 1950's to the present.
- Discuss the current status and capabilities of deterministic transport codes at Los Alamos.
- Discuss future transport needs and possible future research directions.

Our discussion of methods research necessarily includes only a small fraction of the total research actually done. The works that have been included represent a very subjective choice on the part of the author that was strongly influenced by his personal knowledge and experience.

The remainder of this paper is organized in four sections: the first relates to deterministic methods research performed at Los Alamos, the second relates to production codes developed at Los Alamos, the third relates to the current status of transport codes at Los Alamos, and the fourth relates to future research directions at Los Alamos.

## 2 Transport Methods Research at Los Alamos

The purpose of this section is to briefly review the research contributions of Los Alamos National Laboratory in the field of numerical transport methods.

### *2.1 Carlson's Original $S_n$ Method*

The original $S_n$ method was developed by Carlson and his co-workers (Carlson, 1953). The term "$S_N$" referred to "N angular segments." In 1-D slab geometry, $N$ linear segments were used to interpolate $N + 1$ discrete angular flux values. Flux values were always placed at $\mu = -1$, $\mu = 0$, and $\mu = 1$. An equation was obtained for the angular flux value at $\mu = -1$ by collocating at that point. Equations were obtained for the remaining fluxes by integrating the transport equation (with the assumed angular dependence of the flux) over each angular interval associated with a line segment. Lathrop and Carlson later showed that this original approximation was actually equivalent (neglecting boundary conditions) to the modern $S_n$ method with an asymmetric quadrature (Lathrop, 1965).

During the late 50's and early 60's, Carlson and his co-workers developed the "modern" $S_n$ method, which is characterized by:

- Particle conservation and preservation of the constant solution as a central theme for the development of difference equations.
- The use of zero-weighted starting directions in curvilinear coordinates.
- Unified formulations for all geometries.
- Symmetry-preserving and moment-preserving quadratures.
- Use of the multigroup energy treatment.

### *2.2 Convergence Acceleration Techniques*

The basic source iteration process used to solve the $S_n$ equations can be very slow to converge in problems with little or no absorption. A major area of research in the transport community relates to the development of schemes to accelerate the convergence of the source iteration process. Modern convergence acceleration techniques are generally based on the diffusion-synthetic acceleration (DSA) method or variants of that method. In the 60's and early 70's, the principle of diffusion-synthetic acceleration (DSA) was theoretically understood, but it was unstable in practice for typical engineering calculations. The source of the instabilities was not understood. Reed made a major contribution by theoretically demonstrating that DSA became unstable with sufficiently optically-thick cells and a scattering ratio sufficiently close to unity when the cell-centered diffusion equation was used to accelerate the diamond-differenced transport equation (Reed, 1971). Reed further showed how to stabilize the acceleration. However, the stabilized algorithm was not unconditionally effective, but it was often more effective than other available acceleration techniques. Several years later, Alcouffe demonstrated that consistent differencing between the $S_n$ and diffusion operators would result in an unconditionally stable DSA algorithm (Alcouffe, 1977). In particular, this was theoretically demonstrated for the 1-D slab-geometry transport equation with spatial diamond differencing. Extensions of this work eventually made DSA a practical tool for $S_n$ calculations with spatial diamond differencing. Only the scalar flux component of the scattering source is accelerated in the standard DSA algorithm. In the early 80's, Morel showed that the $P_1$ equations could be used to accelerate both the scalar flux and current in calculations with anisotropic scattering (Morel, 1982). It was demonstrated that this scheme became ineffective in the forward-peaked Fokker-Planck scattering limit, but was nonetheless always significantly more effective than standard DSA. At nearly the same time, Larsen developed a DSA method for the slab-geometry DSA equations with linear-discontinuous spatial discretization (Larsen, 1982). This was the first example of a consistent DSA scheme for an advanced $S_n$ spatial discretization. Since only the slab-geometry $S_n$ equations were considered, efficient solution of the linear-discontinuous diffusion equation was not an issue. However, efficient solution of discontinuous diffusion equations arising from discontinuous multidimensional $S_n$ spatial discretizations remains a significant problem today. Starting in the mid 80's, Los Alamos researchers began to turn their attention to radiative transfer (thermal radiation transport) in the stellar regime. This is the regime of interest in astrophysics and inertial-confinement fusion research. Radiative transfer calculations involve an outer iteration process that is often extremely slow to converge. Morel, Larsen, and Matzen developed a diffusion-based synthetic acceleration technique for these outer iterations that was called the linear multifrequency-grey (LMFG) method (Morel, 1984). This method has proven to be essential for efficient and robust radiative transfer calculations with strong material-radiation coupling. Morel and Manteuffel developed an angular multigrid algorithm for 1-D $S_n$ calculations with highly anisotropic scattering that is efficient even in the Fokker-Planck scattering limit (Morel, 1991a). Such scattering is of central importance for charged-particles. Unfortunately, this scheme was found to be conditionally unstable in multidimensions due to properties of the $S_n$ operator related to ray effects. Effective acceleration for multidimensional transport calculations with highly forward-peaked scattering remains an elusive goal. Adams and Morel developed a diffusion-based upscatter acceleration technique for $S_n$ neutronics calculations with a large number of thermal energy groups (Adams, 1993). Such calculations can be extremely slow to converge in materials with a low absorption cross section, e.g., heavy water. This acceleration scheme is similar in spirit to the LMFG method and is similarly effective. In the early 90's, Morel, Wareing, and Dendy developed a DSA method for the $S_n$ equations in $X - Y$ geometry on rectangular grids with bilinear-discontinuous spatial discretization (Morel, 1993). A multilevel approach to solving the discontinuous acceleration equations was introduced that was unconditionally effective for the rectangular grids considered in the study. The unconditionally efficient solution of discontinuous acceleration equations on multidimensional unstructured grids remains an open problem. In the mid 90's, non-linear $S_n$ spatial discretizations based upon an exponential trial space began to appear. Wareing, Walters, and Morel showed that the linear DSA method could be efficiently applied to the solution of the non-linear $S_n$ equations, thereby avoiding the development and solution of non-linear acceleration equations (Wareing, 1996).

### *2.3 Spatial Discretization Methods*

In the late 60's, Kaye Lathrop first developed the step characteristic method for the slab-geometry $S_n$ equations (Lathrop, 1969). This was the first strictly positive second-order accurate spatial discretization scheme for the $S_n$ equations. Several years later, Bill Reed developed the first linear-discontinuous spatial discretization for the $S_n$ equations (Reed, 1973). This work established a class of schemes that still represent the most advanced available computational technology for $S_n$ spatial discretizations. Furthermore, discontinuous discretization has since been applied to all of the other variables in the $S_n$ equations, e.g., time, angle, and energy. The first linear-characteristic method was developed by Alcouffe, Larsen, Miller, and Wienke (Alcouffe, 1979). Characteristic methods remains a very active area of research today. Walters and O'Dell developed the first high-order nodal scheme for the $S_n$ equations in $X-Y$ geometry (Walters, 1981). Their scheme is based upon a linear representation within the cell together with a linear representation on the cell surfaces. Walters and Wareing developed the first non-linear exponential characteristic method and the first non-linear exponential finite-element method for the $S_n$ equations (Walters, 1994, and Wareing, 1995). These methods are spectacularly accurate for deep penetration problems with coarse cells. Wareing, McGhee, Morel, and Pautz have very recently developed a discontinuous finite-element method for spatially discretizing the $S_n$ equations on 3-D unstructured meshes composed of hexahedra and degenerate hexahedra (wedges, pyramids, and tetrahedra) (Wareing, 1999). General hexahedral meshes appear to present significant problems for discontinuous schemes because such hexahedra often have re-entrant surfaces. Nonetheless, these researchers have shown that there is actually a negligible loss of accuracy and a negligible effect on the source iteration process when using reasonably well-formed spatial meshes. This is a very important result in that it confirms the basic applicability of the $S_n$ method to a popular class of unstructured meshes.

*2.4 Angular Quadrature and Angular Discretizations*

In the mid 60's, Lathrop and Carlson published a report on multidimensional quadrature sets that remains a standard reference today (Lathrop, 1965). Over twenty years later, Walters developed multidimensional Chebychev-Legendre product quadrature sets and demonstrated their mathematical properties (Walters, 1988). Soon afterward, Morel developed the Galerkin quadrature technique, which is essential for performing $S_n$ calculations in multidimensions with highly forward-peaked scattering, e.g., charged-particle scattering (Morel, 1989). One year later, Walters and Morel investigated linear-discontinuous differencing of the angular derivative term in 1-D spherical geometry (Walters, 1990). It was found that in many problems, diamond differencing yielded a more accurate solution on meshes of intermediate angular refinement than the LD method. This surprising behavior was traced to the effect of the starting direction flux in the diamond method, which can be very accurately calculated since it satisfies the slab-geometry equation. A starting direction flux does not appear in the LD scheme. This difficulty was circumvented by modifying the LD scheme to use a continuous-quadratic approximation in the first angular cell together with the standard LD treatment for all the other cells. This approximation used a starting flux value, and was found to be uniformly more accurate than the diamond scheme. Very recently, Dahl, Ganapol, and Morel developed a least-squares-based method for generating positive scattering sources (Dahl, 1999). The method developed by these researchers seems to work quite well for neutral-particle calculations, but more rigorous methods are required for charged-particle calculations. Positive scattering sources are essential in non-linear exponential-based transport calculations. The generation of accurate strictly positive scattering sources is surprisingly difficult. An fully satisfactory technique has not yet been developed.

*2.5 Ray Effect Mitigation*

Ray effects are non-physical anomalies that often appear in optically-thin multidimensional $S_n$ calculations because the solution propagates along a finite set of directions defined by the angular quadrature set. Ray effects may represent the most significant deficiency of the $S_n$ method. Lathrop developed the first "fictitious source" method for mitigating ray-effects in multidimensional $S_n$ calculations (Lathrop, 1971). His approach was based upon a set of polynomials on the unit sphere that are orthogonal under quadrature integration. One year later, Reed developed a fictitious source based upon projection operators that converted $S_n$ solutions to true $P_{n-1}$ solutions (Reed, 1972). Five years later, Miller and Reed refined Reed's projection technique so that it achieved spherical-harmonic equivalence with minimal perturbations of the $S_n$ equations (Miller, 1977). They also developed the first fictitious source for the $S_n$ equations in $R-Z$-geometry. It now appears likely that efficient computation of $P_{n-1}$ solutions via the $S_n$ equations with fictitious sources is not possible without a major modification to the standard source-iteration process. Thus there is little or no research activity in this area today.

*2.6 Discrete Asymptotic Analysis*

As previously noted, radiative transfer became of considerable interest at Los Alamos in the mid 80's. Both optically thin and diffusive regions routinely appear in radiative transfer problems in the stellar regime. A diffusive solution can vary arbitrarily slowly over an arbitrary number of mean-free-paths. Thus it would clearly be desirable to obtain accurate $S_n$ solutions in diffusive regions whenever the spatial variation of the exact solution is resolved by the mesh independent of the optical thickness of the cells. Larsen, Morel, and Miller showed that such desirable behavior can be obtained if an $S_n$ spatial discretization scheme has the correct asymptotic behavior (Larsen, 1987). Their discrete asymptotic analysis has become a standard tool for designing $S_n$ spatial discretization schemes for radiative transfer applications. The diffusion limit considered by Larsen, et al., is actually a linearized version of the true non-linear limit associated with radiative transfer. Morel, Wareing, and Smith recently demonstrated a full non-linear asymptotic analysis and applied it to the $S_n$ radiative transfer equations with linear-discontinuous spatial differencing (Morel, 1996).

### 2.7 *Charged-Particle Transport*

In the late 70's, Antal and Lee applied the $S_n$ method to the transport of ions in a plasma (Antal, 1977). In the early 80's, Wienke developed an $S_n$ method for electron transport under the influence of both scattering and electromagnetic fields (Wienke, 1982). This work was highly advanced for its time. A few years later, Morel developed a discretization for the angular Fokker-Planck operator in 1-D slab and spherical geometries (Morel, 1985a). This discretization rigorously preserved both the zero'th and first moments of the operator as well as its positivity. Later that same year, Morel developed multigroup-Legendre coefficients for the continuous slowing down operator with diamond differencing that enabled standard $S_n$ codes to model that operator with second-order accuracy (Morel, 1985b). Previous treatments compatible with existing $S_n$ codes were only first-order accurate. One year later, the linear-discontinuous method was first applied to the continuous slowing down operator by Lazo and Morel (Lazo, 1986).

### 2.8 *Second-Order $S_n$ Methods*

Discrete Ordinates solution techniques for the second-order form of the transport equation became of interest at Los Alamos in the early 90's because they could be applied on unstructured 3-D spatial meshes and because they could be solved on massively parallel computers using well-established solution techniques originally developed for the diffusion equation. Morel and McGhee formulated a source iteration process with anisotropic scattering for the even-parity $S_n$ equations and demonstrated its equivalence to the source iteration process for the standard form of the $S_n$ equations (Morel, 1995). This equivalence implies that any convergence acceleration technique applicable to the first-order $S_n$ equations should have an equivalent counterpart for the even-parity equations. Very recently, Morel and McGhee investigated the computational utility of a little-known second-order form of the transport equation that has the standard angular flux as its unknown rather than an even-parity or odd-parity component of the flux (Morel, 1999). This equation, which was termed the SAAF (self-adjoint angular flux ) equation, was shown to offer several significant advantages relative to the even-parity and odd-parity equations. This is particularly so for $S_n$ calculations with reflective boundary conditions.

### 2.9 *Parallel Solution Techniques*

The first massively parallel 3-D unstructured-mesh $S_n$ calculations were performed on the Connection Machine at Los Alamos in 1990 and documented in a paper by Morel, McGhee, Olvey, and Claiborn (Morel, 1991b). The even-parity form of the $S_n$ equations was solved using techniques originally developed for the diffusion equation in conjunction with source iteration and DSA. The first massively parallel algorithm for solving the standard first-order $S_n$ equations via a direct (as opposed to iterative) solution of the source iteration equations was developed by Baker and Koch (Baker, 1998). This algorithm scales well and, most importantly, is as fast as the best scalar algorithm on a single processor. It now appears that direct parallel approaches for solving the source iteration equations on rectangular meshes are decidedly superior to iterative parallel approaches. This result is contrary to the prevailing thought that existed when parallel $S_n$ methods were first being developed in the early 90's.

## 3 Discrete Ordinates Codes at Los Alamos

A list of most of the discrete ordinates codes developed at LANL from the 60's through the 90's follows. All of these codes used an $S_n$ angular discretization with anisotropic scattering in conjunction with the multigroup-Legendre energy treatment.

- DTF-IV - The first modern $S_n$ code: 1-D geometries, diamond differencing with fixup, steady state source problems and eigenvalues problems. Used in 60's and early 70's.
- TWOTRAN - 2-D geometries, rectangular mesh, diamond differencing with fixup, steady state source problems and eigenvalue problems. Used in late 60's and 70's.
- TRANZIT - Time-dependent version of TWOTRAN. Used in late 60's and 70's.
- THREETRAN - 3-D cartesian geometry, rectangular mesh, diamond differencing with fixup, steady state source problems and eigenvalue problems. Used in middle to late 70's. This code was not very practical because of computer memory limitations that existed during this time period.
- ONETRAN - Successor to DTF. 1-D geometries, linear-discontinuous spatial differencing. Used in 70's and 80's.
- TIMEX - Time-dependent version ONETRAN.
- TRIPLET - 2-D Cartesian geometry, semi-structured triangular mesh, arbitrary-order discontinuous finite-element spatial discretization, source problems and eigenvalue problems. Used in 70's and 80's. Highly advanced for its time.
- TRIDENT - An $R-Z$ geometry version of TRIPLET.
- ONEDANT - 1-D geometries, diamond-differencing with fixup, DSA, steady-state source problems and eigenvalue problems. Used in early 80's and 90's.
- TWODANT - 2-D geometries, diamond-differencing with fixup, DSA, steady-state source problems and eigenvalue problems. Used in early 80's and 90's.
- THREEDANT - 3-D geometries, diamond-differencing with fixup, DSA, steady-state source problems and eigenvalue problems. Used in 90's.

## 4 Current Status of Codes

Group XTM at Los Alamos currently has a large number of deterministic research codes for both neutronics and radiative transfer. Most of XTM's programmatic efforts relate to the development of transport software packages for multiphysics computer codes. XTM's research codes can be described as follows:

- PARTISN: A parallel 3-D rectangular-mesh neutral-particle $S_n$ code with DSA that solves the standard first-order transport equation and provides time-dependent, steady-state, and eigenvalue solutions. This code also has options for more advanced spatial and temporal discretizations. It is written in F90.

- DANTE: A parallel 3-D unstructured hybrid finite-element-mesh $S_n$/$P_n$/$SP_n$ code with several advanced diffusion-based acceleration techniques that solves various second-order forms of the transport equation, e.g., even-parity, odd-parity, and SAAF, and provides time-dependent, steady-state, and eigenvalue solutions This codes uses a continuous finite-element approximation in the spatial variables. It has options for both neutral-particle calculations and radiative transfer calculations. It is written in F90.

- PERICLES: A serial 3-D unstructured hybrid finite-element-mesh neutral/charged-particle $S_n$ code with DSA that solves the standard first-order form of the transport equation and provides steady-state, and eigenvalue solutions. This codes uses a discontinuous finite-element approximation in the spatial variables and for the continuous-slowing-down operator in charged-particle transport calculations. It is written in F90.

- ATTILA: A serial 3-D unstructured-tetrahedral-mesh neutral/charged-particle $S_n$ code with DSA that solves the standard first-order form of the transport equation and provides steady-state, and eigenvalue solutions. This codes uses a linear-discontinuous finite-element approximation in the spatial variables and for the continuous-slowing-down operator used in charged-particle transport calculations. It also has special options for oil-well logging tool calculations. ATTILA is written in F90.

## 5 Future Directions in Research and Code Development

Research in the following areas is either in progress or planned for the near future:

- Massively parallel techniques for solving the first-order $S_n$ equations on unstructured-meshes and rectangular block-adaptive meshes.

- Spatial discretization schemes and associated DSA and multifrequency-grey acceleration schemes for the first-order $S_n$ radiative transfer equations on unstructured meshes.

- Compatible transport and hydrodynamic discretization schemes for strongly coupled radiation-hydrodynamics calculations.

- Massively parallel techniques for solving the diffusion equation on unstructured and cell-by-cell adaptive meshes.

- Multilevel techniques for solving discontinuous finite-element discretizations of the $P_1$ equations on structured and unstructured meshes.

- Investigation of optimal spherical-harmonic interpolation points on the unit sphere. This work will feed back into the development of positive scattering source representations.

- Investigation of special multidimensional $S_n$ quadrature sets designed to be compatible with angular multigrid solution techniques for problems with highly anisotropic scattering.

- Application of the discontinuous finite-element method to the spatial discretization of the $P_n$ equations, and the development of an efficient solution technique for the resulting discrete equations.

- Investigation of angular adaptive mesh refinement techniques.

- Use of object-oriented, templated, generic programming techniques to build a library of reusable software modules for transport code development.

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