

The Early Days of the S_n Method*

K. D. Lathrop

Stanford Linear Accelerator Center,
Stanford University, Stanford, CA 94309

From the beginning at Los Alamos National Laboratory (LANL), solutions to the transport equation were very important. Many long-forgotten approximate solution techniques, including one by Feynman¹, were developed to help design nuclear weapons. Most of these methods were based on the methods of mathematical physics familiar to the project physicists and predated the use of computers, but continued research and pressing need produced two new and powerful computer-based systems: Monte Carlo and the S_n Method. The healthy and long-term competition between the two Los Alamos groups responsible for these quite different approaches was both stimulating and synergistic.

In 1953, Bengt Carlson described² a finite difference approximation to the transport equation in which the angular variable was represented by n piecewise continuous linear segments. He christened the representation the angular segmentation, or S_n , method. In the next ten years Carlson and his coworkers, without changing the name, developed a much improved general-geometry discrete ordinates system. This system, for which the best early description is Reference 3, was an integrated whole based on a set of

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compatible themes. Using the multigroup formulation as a starting place, these themes included the following:

1. particle-conserving difference equations
2. accurate but simple finite difference approximations for speed of evaluation
3. a unified formulation for all geometries
4. minimum-angle quadratures with symmetries based on the symmetries of the geometry involved.

The discrete ordinates method was first suggested by Wick⁴ in 1943, but the detailed development was due to Chandrasekhar⁵. The great disadvantage of the method was the difficulty of extending it to curved geometries and treating the angular derivatives of the transport operator. Carlson invented an elegant representation for these angular derivatives in terms of a given set of angular quadrature weights and directions by assuming a space-angle finite difference scheme with undetermined coefficients and then determining the coefficients by satisfying particle conservation in detail. In addition to its practical advantages, this scheme facilitated experimentation with different quadrature schemes. Carlson's innovative use of particle conservation was partially stimulated by the need of LANL designers to have accurate, detailed particle balances for their iterated designs of fast, leaky assemblies. Carlson, Lee and Lathrop^{6,7} experimented with quadrature schemes and evolved workable recipes for reducing the required number of directions by one-half in cylindrical and higher dimensional geometries. "Singular" quadrature directions in which the angular derivative terms do not appear were used to initialize the angular variable just as readily as the spatial boundary conditions could be applied. Using a simple

central difference approximation then reduced the whole process of inverting the differential transport operator to evaluating a set of simple, stable, recursion relations. Hence, data storage requirements were minimal.

With source iteration, the S_n system was nearly perfect for fast numerical evaluation. Using a technique invented by Carlson and Bell⁸, the source iteration was accelerated by enforcing whole-system particle balance (re-balance) at each iteration, and this was possible because of the construction of the difference equations. Unlike numerical approximations to the diffusion equation, convergence of S_n iterations did not worsen as the spatial mesh size decreased.

The effectiveness, efficiency and generality of the discrete S_n method rather quickly led to its application in one-, two- and three- dimensional computer codes^{9, 10}, some of which were heavily used around the world.

Not until the mid 1960's was it realized¹¹ (at approximately the same time at Bettis Atomic Power Laboratory and LANL) that use of discrete directions in two-dimensional geometries leads to anomalous spatial variations or ray effects¹². This late recognition was in part because two-dimensional calculations were not widely used earlier and in part because earlier two-dimensional calculations were more often for distributed sources rather than for the isolated sources in absorbers that most clearly display anomalous results. Ray effects can be eliminated, at additional computational cost by adding a zero-sum angular source which converts the discrete ordinates equations to spherical harmonic equations¹³.

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