Block quasi-Newton solver for transport equations

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A new quasi-Newton algorithm has been developed for systems in which the Jacobian is known to have a block multi-diagonal structure, as occurs in transport equations where the fluxes depend primarily on only the local values and their gradients. A primary goal of this work is to minimize the number of numerically expensive local flux calculations (e.g., diffusivities). Secondary design considerations were 2nd order temporal and spatial error, good numerical stability, and a modular design. A test suite has also been developed to allow validation of the solver.

Like the most common quasi-Newton algorithm, the Broyden method, our new quasi-Newton approach uses flux evaluations from previous iterations to approximate the Jacobian. Assuming that the diffusivity evaluations dominate the computation time, the approximate Jacobian is free. Our approximation of the Jacobian, which we call the hyper-secant approximation, requires the solution of a small, dense linear system per radial grid point per iteration. Unlike the Broyden Jacobian, the hyper-secant approximation converges toward the finite-difference Jacobian after sufficiently many iterations.

We will present numerical studies of spatial and temporal accuracy as well as stability for time steps exceeding the CFL limit by many orders of magnitude.