A New Semi-Implicit Direct Kinetics Method with Analytical Representation of Delayed Neutrons

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INTRODUCTION

The key physics involved in accurate prediction of reactor fuel element behavior includes neutron transport and thermal hydraulics. For analyzing time- and space-dependent reactor transient powers, space-time neutron kinetics is the most accurate method, if sufficient high-performance computing resources are available. This work seeks to establish a new method for space-time neutron kinetics that is amenable to massively parallel steady-state transport codes, such as Denovo [1] , that can be coupled with massively parallel fuel performance codes, such as the AMP Nuclear Fuel Performance code [2]. Typically, spatial kinetics will be described using factorization or direct kinetics methods [3]. We introduce a new method that shares some features of both while employing its own approximations. One key approximation in this initial approach is neglecting the time-dependent change in the angular flux. This approximation allows the omission of the shape function from the factorization derivation [4] and facilitates a quasi-steady-state derivation of the transport equation for the direct method. The method thus becomes a semi-implicit direct kinetics method featuring an analytic explicit representation of the precursor groups, dependent upon a time-averaged power. The advantages of this method are the ease of implementation in high-fidelity massively parallel transport codes, low amounts of communication required, and low memory requirements.

METHODOLOGY

Consider the time-dependent multigroup Boltzmann transport equation with an explicit representation of delayed neutrons:

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \mathbf{L}\psi = \mathbf{MSD}\psi + (1-\beta)\mathbf{MFD}\psi + \chi \sum_{i=1}^{I} \lambda_i C_i \tag{1}$$

$$\frac{\partial C_i}{\partial t} = \beta_i \mathbf{FD}\psi - \lambda_i C_i, \tag{2}$$

where ψ is the angular flux, t is time, v is velocity, $\mathbf{L}$ is the streaming plus collision operator, $\mathbf{S}$ is the scattering matrix, $\mathbf{F}$ is the fission matrix, $\mathbf{M}$ is the angular prolongation (moment-to-angle) operator, $\mathbf{D}$ is the angular restriction (angle-to-moment) operator, χ is the fission spectrum, i denotes the delayed precursor group, I is the number of precursor groups, λ_i is the group decay constant, β_i is the group delayed neutron fraction, C_i is the group precursor concentration, and $\beta = \sum_i \beta_i$ is the total delayed neutron fraction.

We assume the time derivative of the angular flux is negligible, so that Eq. (1) can be written as

$$[\mathbf{L} - \mathbf{MSD} - (1-\beta)\mathbf{MFD}]\psi = \chi \sum_{i=1}^{6} \lambda_i C_i. \tag{3}$$

The motivation for this assumption is that the neutron velocity is typically large compared with other quantities in the equation, so the impact of this term will typically be small. Additionally, many radiation transport solvers that are not designed specifically for time-dependent calculations do not explicitly store the angular flux because of the large memory requirement, so the angular flux may not be available. Instead of entirely neglecting this term, an alternative is to approximate the time derivative of the angular flux with the time derivative of the angular flux moments $\phi \equiv \mathbf{D}\psi$, as was done in [5]. This approach is not considered further in the current study. The impact of neglecting the angular flux derivative term is that behavior at time scales on the order of the neutron lifetime cannot be correctly captured. However, the behavior at longer times is expected to to be represented well.

Next, we make a further approximation by treating the precursor concentrations in Eq. (3) fully explicitly (i.e., they are evaluated at the beginning of a given time interval) and the angular fluxes in Eq. (2) fully implicitly (i.e., they are evaluated at the end of a given time interval). Under these assumptions, Eq. (3) can be written as

$$[\mathbf{L} - \mathbf{MSD} - (1-\beta)\mathbf{MFD}]\psi^{j+1} = \chi \sum_{i=1}^{6} \lambda_i C_i^j, \tag{4}$$

where the superscript j denotes a quantity at the beginning of time interval j, and $j+1$ denotes the quantity at the end of that interval. This equation represents a fixed-source Boltzmann transport equation with a known source based on the precursor concentration from the previous time step, easily adaptable to work within most neutron transport solver frameworks. Additionally, Eq. (2) is transformed into six independent ordinary differential equations, the analytical solutions for which can be written

$$C_i^{j+1} = C_i^j \exp(-\lambda_i \Delta t^j) + \frac{\beta_i}{\lambda_i}\mathbf{FD}\psi^{j+1}\left[1 - \exp(-\lambda_i \Delta t^j)\right], \tag{5}$$

where $\Delta t^j = t^{j+1} - t^j$. The solution at each time step thus requires a fixed source transport solve plus effectively one exponential evaluation for each delayed precursor group at each spatial point.

RESULTS

To evaluate the scheme described in the previous section, we examine an infinite homogenous medium problem so that an exact solution can be obtained for comparison. In the creation of this verification program, MATLAB [6] was used.

Point kinetics can be used to obtain an exact solution for the two-group infinite homogeneous medium problem. However, if the adjoint is not solved to obtain appropriately weighted parameters, each energy group must be represented explicitly in order to obtain the exact solution. The difference in using multiple energy groups in the point kinetics equations is the addition of one ODE for each additional energy group, allowing explicit representation of each group's mean generation time. This difference primarily appears in the prompt jump portion of the transient, which showed a 3% difference in the analyses performed in this report. The power equations in this formulation appear as the transport equation, which is greatly simplified for an infinite homogeneous medium.

Two common solution approaches are employed for the point kinetics evaluations: methods that approximate the matrix exponential (such as Padé) and Runge-Kutta methods (such as backward Euler, RK4, RK45, and others) [7]. Although the Runge-Kutta methods are typically quite fast, they can become unstable for stiff systems, such as point kinetics equations, which can necessitate such a small time step that the method is no longer fast. Padé iterative matrix methods are generally slow but highly accurate for such systems, depending upon the approximation order. Alternatively, for problems in which the reactivity is not changing in time, the exact solution at time t can be obtained by evaluating the matrix exponential $e^{\mathbf{A}t}$, where for our problem the matrix $\mathbf{A}$ is a matrix combining Eqs. (4) and (2), i.e.

$$\mathbf{A} = \begin{bmatrix} [\mathbf{L} - \mathbf{MSD} - (1-\beta)\mathbf{MFD}] & \chi\lambda_1 & \cdots & \chi\lambda_6 \\ \beta_1\mathbf{FD} & -\lambda_1 & & \\ \vdots & & \ddots & \\ \beta_6\mathbf{FD} & & & -\lambda_6 \end{bmatrix}. \quad (6)$$

A similar approach was applied to the point kinetics equations in [7].

Infinite Homogeneous Medium Benchmark

The first benchmark considered is an infinite homogenous medium with the delayed neutron parameters given in Table I. The case is intially at steady state and is then perturbed so that there is a 0.5% increase in $\nu\sigma_f$, resulting in a positive reactivity insertion of approximately 0.69β. This perturbation results in a power increase of around a factor of three occurring on the order of the prompt neutron lifetime, followed by an exponential growth on a longer time scale governed by the kinetics parameters. The semi-implicit direct kinetics method (as coded into MATLAB[6]) is compared with the exact solution found using the matrix exponential. The evolution of the power from $t = 0$ to $t = 1.0s$ is shown in Figure 1 and the error at several values of t over a range of Δt values is shown in Figure 2. One important thing to observe in these results is that the error does not approach zero as the time step is reduced. This is an expected result of not correctly capturing the prompt jump portion of the transient as a result of neglecting the time derivative of the angular flux. It is interesting to observe, however, that for a sufficiently small time step, the error does not increase very significantly from $t = 0.1s$ to $t = 10.0s$. This indicates that the primary source of error occurs during the initial prompt jump and that the time discretization performs well beyond that point. The Denovo code [1] was able to reproduce the semi-implicit results as coded into MATLAB within machine precision, verifying the implementation of the method in Denovo.

TABLE I. Delayed Neutron Parameters

Group	β	λ (s^{-1})
1	2.4e-4	1.3e-2
2	1.5e-3	3.2e-2
3	1.3e-3	1.2e-1
4	2.9e-3	3.1e-1
5	1.0e-3	1.4
6	2.5e-4	3.8

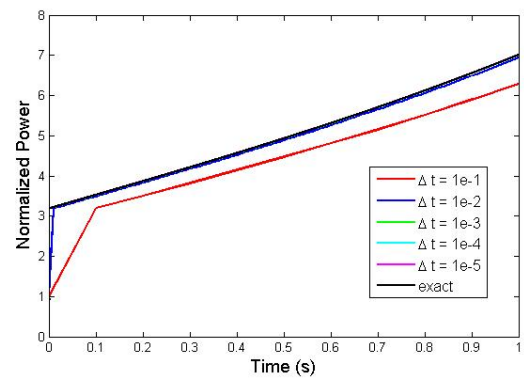

Fig. 1. Semi-implicit direct kinetics vs. two-group point kinetics (in black).

1-D Fast Reactor Transient

The next benchmark selected for this effort was the Argonne National Laboratory benchmark problem 16-A1, which is a 1-dimensional spatial-kinetics benchmark for a sodium fast reactor [8]. The problem features seven material regions of fuel blankets, fuel regions, sodium regions, and two energy groups, cross sections for which are provided in the benchmark. Meshing information is also provided in the benchmark, as the mesh used is nonuniform. In order to approximate the quadrature given in the benchmark, a Gauss-Legendre product quadrature was used, with four azimuthal and four polar octants. The convergence criterion was 1e-6, the scattering order used was

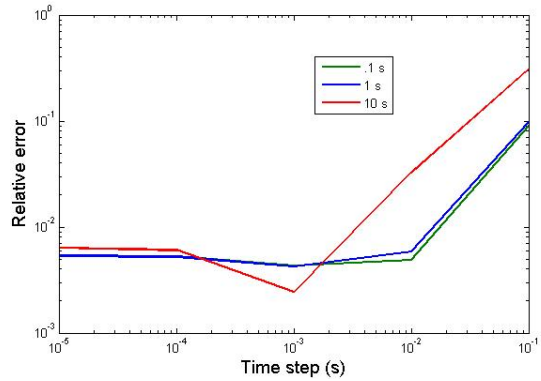

Fig. 2. Relative error of semi-implicit decoupled direct kinetics at t = 0.1, 1.0 s, and 10.0s

P_0, and the solver used was a Krylov solver. The perturbation considered is a change in the material densities in the leftmost fissile regions, which constitutes an increase in the fission cross sections, as well as a decrease in the material density in the rightmost fuel region. The second flux solution, at t=0.01 s, consists of several intermediary transport, or shape, solutions, which are run as fixed-source problems. This problem is run using the analytically determined spatially dependent precursors as the fixed source. The comparison of the perturbed steady-state fluxes with the flux at some short time (t = 0.01s) after the perturbation is shown in Figure 3. The fluxes from the semi-implicit direct kinetics method used with the Denovo[1] code at t = 0.01 seconds were within 5% of the fluxes given in the 16-A1 benchmark. These differences are primarily attributable to the neglect of the time-dependent angular flux change term in the kinetics equations [4].

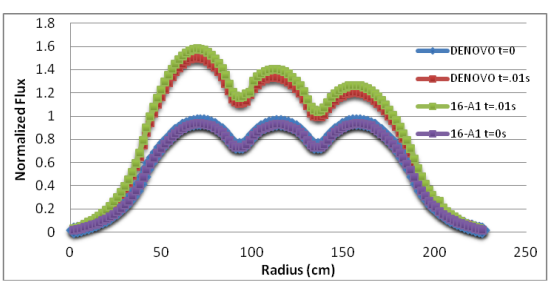

Fig. 3. 16-A1 benchmark 1-D fast reactor.

CONCLUSIONS

A previous paper [4] demonstrated that this kinetics method could be rapidly implemented within a traditional steady-state radiation transport code and was able to produce reasonable results for unperturbed and perturbed fluxes against the 16-A1 benchmark. This paper has shown that the method is capable of reproducing an exact multigroup point kinetics solution with an average error on the order of 0.5%. This paper has also shown the appropriate time step size to use with the semi-implicit direct kinetics method derived in the paper. In future work, the time derivative of the angular flux will be approximated with moments, which will be exact for the infinite homogenous medium problem [5]. Future work will include scaling studies that are under way on a cluster owned by the University of Tennessee Nuclear Engineering department, as well as the Kraken supercomputer operated by the National Institute of Computational Sciences. Because of the low error of the approximation, as well as the ease of implementation, this method can be favorable for rapid implementation in traditional steady-state massively parallel transport codes, which are particularly well suited to coupling with thermal-hydraulic codes [2].

ACKNOWLEDGMENTS

This project staff acknowledges funding support for James Banfield through a grant to the University of Tennessee–Knoxville from the DOE Office of Nuclear Energy's Nuclear Energy University Programs. This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

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