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Stability analysis of the Backward Euler time discretization for the pin-resolved transport transient reactor calculation

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ABSTRACT

Three-dimensional, full core transport modeling with pin-resolved detail for reactor dynamic simulation is important for some multi-physics reactor applications. However, it can be computationally intensive due to the difficulty in maintaining accuracy while minimizing the number of time steps. A recently proposed Transient Multi-Level (TML) methodology overcomes this difficulty by use multi-level transient solvers to capture the physical phenomenal in different time domains and thus maximize the numerical accuracy and computational efficiency. One major problem with the TML method is the negative flux/precursor number density generated using large time steps for the MOC solver, which is due to the Backward Euler discretization scheme. In this paper, the stability issue of Backward Euler discretization is first investigated using the Point Kinetics Equations (PKEs), and the predicted maximum allowed time step for SPERT test 60 case is shown to be less than 10 ms. To overcome this difficulty, linear and exponential transformations are investigated using the PKEs. The linear transformation is shown to increase the maximum time step by a factor of 2, and the exponential transformation is shown to increase the maximum time step by a factor of 5, as well as provide unconditionally stability above a specified threshold. The two sets of transformations are then applied to TML scheme in the MPACT code, and the numerical results presented show good agreement for standard, linear transformed, and exponential transformed maximum time step between the PKEs model and the MPACT whole core transport solution for three different cases, including a pin cell case, a 3D SPERT assembly case and a row of assemblies ("striped assembly case") from the SPERT model. Finally, the successful whole transient execution of the stripe assembly case shows the ability of the exponential transformation method to use 10 ms and 20 ms time steps, which all failed using the standard method.

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1. Introduction

Three-dimensional, full core modeling with pin-resolved detail has become the state of art computational simulation for nuclear reactors. However, the computational intensiveness has become challenging, especially for time-dependent transient analysis since it is difficult to maintain accuracy when using large time steps to minimize the number of transport solutions. As a result, several innovative methods have been investigated to more efficiently solve the time-dependent Boltzmann equation. One of the most popular and widely used methods has been the quasi-static method which originated with Henry (1958) and Henry and Curlee (1958) and continued with Ott and Meneley (1969) who proposed the Improved Quasi-Static (IQS) method in 1969. The

* Corresponding author. *E-mail addresses:* angzhu@umich.edu (A. Zhu), yunlin@umich.edu (Y. Xu), downar@umich.edu (T. Downar). underlying premise of the Quasi-Static method is that the flux can be factorized into an amplitude and a shape function since the amplitude of the flux changes much more rapidly than the flux shape. In the IQS method the shape function is solved by a modified time-dependent Boltzmann equation with a known amplitude function, and the amplitude function is calculated using the PKEs which are formed by integrating the time-dependent Boltzmann equation with the known shape function. The shape and amplitudes functions are iteratively solved with a shape constraint function until the convergence is satisfied. Recently, Ban et al. (2012) adopted the nodal/PKEs based IQS method and innovated a new fine/coarse mesh based IQS method by introducing a coarse mesh wise rather than whole core amplitude function, which was named Multigrid Amplitude Function (MAF) and was later implemented in a transport based transient solver (Tsujita et al., 2013; Shaner et al., 2013).

In addition to the IQS/MAF method, a new factorization method called Predictor–Corrector Quasi-Static method (PCQM)







(Kao and Henry, 1989) has recently become popular. Instead of solving the shape and amplitude functions, the PCQM computes the flux directly in the predictor step and the flux is corrected using the amplitude function evaluated at the corrector step. Several studies (Dulla et al., 2006, 2008; Caron et al., 2015) have applied the PCQM to the nodal/PKEs scheme and have shown improved accuracy and computational efficiency over traditional IQS method by avoiding the iteration between shape and amplitude function in the PCQM method.

Recently, a Transient Multi-Level (TML) method was proposed by Zhu et al. (2015a) and the PCQM iteration scheme is used for coupling of both the 3D-Transport/3D-CMFD level and the 3D-CMFD/PKEs level. At each level, the original flux equation is solved in the coarse predictor step and then is factorized as an amplitude and a shape function in the corrector step, where the predicted solution is corrected using multiple fine steps. In the first level 3D-Transort/3D-CMFD coupling, the angular and sub-pin flux shape function in the Boltzmann transport equation are assumed to vary slowly over time and the CMFD cell wise amplitude function is solved using multiple steps of the CMFD transient equation. In the second level, the CMFD scalar flux calculated in the last step is further corrected by a whole core amplitude function generated by solution of the Point Kinetics Equations (PKEs). The numerical results in Zhu et al. (2015a) show a considerable reduction of the computational time can be achieved while maintaining a high level of numerical accuracy.

However, one major challenge of the TML method is that the flux/precursor number density generated by the transport step can be negative when using large time steps in the Backward Euler discretization. This imposes significant limits on the performance of the TML method and is the focus of the research described in this paper. The stability issue is first investigated using PKEs and found to be about 10 ms for typical reactivity insertion accidents (RIA), such as the SPERT (Special Power Excursion Reactor Test) test 60 (Durgone, 1965). Two transformation methods are proposed in this paper to overcome this problem, including both linear and exponential transformation methods. The exponential transformation is a legacy method (Reed and Hansen, 1970; Ferguson and Hansen, 1973; Buckner and Stewart, 1976), which has successfully accelerated the diffusion type transient problem.

The paper is organized as follows. Section 2 provides a detailed description of the transient solvers developed in MPACT Team (2013), including both the 3D-transport and the PKEs transient formulations. In Section 3, the stability issue for Backward Euler discretization with large time step is investigated using PKEs models. Section 4 is devoted to the two transient transformation methods and their stability analysis using PKEs model. Section 5 then describes the application of linear and exponential transformations to the MPACT transport transient solver. Finally, Section 6 provides numerical stability results using the PKEs and MPACT for the standard, linear and exponential transformation methods, using a pin cell, a 3D SPERT (Cao et al., 2015) assembly and a row of SPERT assemblies in a "stripe" model.

2. Transient methodology

The transient capability was recently added to the MPACT (Zhu et al., 2015b) code and the detail formulation of the equations for the transient solvers are presented in this section, including the 3D-transport transient equations and the PKEs.

2.1. 3D-transport transient equation

The 3D transport transient solver begins with the continuous 3D Boltzmann equation and the neutron precursor equations:

$$\begin{split} & \frac{1}{\nu(E)} \frac{\partial \varphi(\mathbf{r}, \Omega, E, t)}{\partial t} = -\Omega \cdot \nabla \varphi(\mathbf{r}, \Omega, E, t) - \Sigma_t(\mathbf{r}, E, t) \varphi(\mathbf{r}, \Omega, E, t) \\ & + \int_0^\infty \int_0^{4\pi} \Sigma_s(\mathbf{r}, \Omega \cdot \Omega', E' \to E, t) \varphi(\mathbf{r}, \Omega', E', t) d\Omega' dE' \\ & + \frac{1}{4\pi} (\chi_p(\mathbf{r}, E, t)(1 - \beta(\mathbf{r}, t)) S_F(\mathbf{r}, t) + \chi_d(\mathbf{r}, E, t) S_d(\mathbf{r}, t)) \end{split}$$
(1)

$$\frac{dC_k(\mathbf{r},t)}{dt} = \beta_k(\mathbf{r},t)S_F(\mathbf{r},t) - \lambda_k(\mathbf{r},t)C_k(\mathbf{r},t), k = 1, 2, ..., 6$$
(2)

where φ and C_k are the angular flux and the delayed neutron precursor density, and S_F and S_d are the total fission source and the delayed neutron source which are defined as:

$$S_F(\mathbf{r},t) = \frac{1}{k_{eff}^s} \int_0^\infty \nu \Sigma_f(\mathbf{r}, E', t) \phi(\mathbf{r}, E', t) dE'$$
(3)

$$S_d(\mathbf{r},t) = \sum_{k=1}^6 \lambda_k(\mathbf{r},t) C_k(\mathbf{r},t)$$
(4)

In the above equations, the S_F value is adjusted by the eigenvalue determined in the steady-state calculation used to initialize the transient.

For a given time step size Δt_n at time step *n*, Eq. (1) can be discretized using the Backward Euler method as:

$$\frac{\varphi^{n}(\mathbf{r},\Omega,E) - \varphi^{n-1}(\mathbf{r},\Omega,E)}{\nu(E)\Delta t_{n}} = R^{n}(\mathbf{r},\Omega,E)$$
(5)

with R^n denoting all the right hand side terms of Eq. (1) at time step *n*.

The Boltzmann equation is coupled to the precursor equations by integrating Eq. (2) and the precursor equations with a second order approximation for the fission source is written as in Eq. (6):

$$C_{k}^{n}(\mathbf{r}) = \Omega_{k}^{0}(\tilde{\lambda}_{k}^{n})C_{k}^{n-1}(\mathbf{r}) + \frac{1}{\lambda_{k}^{n}} \Big[\beta_{k}^{n}(\mathbf{r})S_{F}^{n}(\mathbf{r})\Omega_{k}^{n}(\tilde{\lambda}_{k}^{n}) + \beta_{k}^{n-1}(\mathbf{r})S_{F}^{n-1}(\mathbf{r})\Omega_{k}^{n-1}(\tilde{\lambda}_{k}^{n}) + \beta_{k}^{n-2}(\mathbf{r})S_{F}^{n-2}(\mathbf{r})\Omega_{k}^{n-2}(\tilde{\lambda}_{k}^{n}) \Big]$$

$$(6)$$

where $\tilde{\lambda}_k^n = \lambda_k^n \Delta t_n \ E(x) = e^{-x}, \ \kappa_0(x) = 1 - e^{-x}, \ \kappa_1(x) = 1 - \frac{\kappa_0(x)}{x}, \\ \kappa_2(x) = 1 - \frac{2\kappa_1(x)}{x}$

$$\Omega_{k}^{0}(\tilde{\lambda}_{k}^{n}) = E(\tilde{\lambda}_{k}^{n}), \Omega_{k}^{n}(\tilde{\lambda}_{k}^{n}) = \frac{\kappa_{2}(\tilde{\lambda}_{k}^{n}) + \gamma \kappa_{1}(\tilde{\lambda}_{k}^{n})}{(1+\gamma)} \\
\Omega_{k}^{n-1}(\tilde{\lambda}_{k}^{n}) = \left(\kappa_{0}(\tilde{\lambda}_{k}^{n}) - \frac{\kappa_{2}(\tilde{\lambda}_{k}^{n}) + (\gamma-1)\kappa_{1}(\tilde{\lambda}_{k}^{n})}{\gamma}\right) \\
\Omega_{k}^{n-2}(\tilde{\lambda}_{k}^{n}) = \frac{\kappa_{2}(\tilde{\lambda}_{k}^{n}) - \kappa_{1}(\tilde{\lambda}_{k}^{n})}{(1+\gamma)\gamma}$$
(7)

Thus, the delayed neutron source can be expressed as:

$$S_d^n(\mathbf{r}) = \omega^n(\mathbf{r})S_F^n(\mathbf{r}) + S_d^{n-1}(\mathbf{r})$$
(8)
where $\omega^n = \sum_{k=1}^6 \beta_k \Omega_k^n(\tilde{\lambda}_k^n)$ and

$$\begin{split} \tilde{S}_{d}^{n-1}(\mathbf{r}) &= \sum_{k=1}^{6} \lambda_{k} \Omega_{k}^{0}(\tilde{\lambda}_{k}^{n}) C_{k}^{n-1}(\mathbf{r}) + S_{F}^{n-1}(\mathbf{r}) \sum_{k=1}^{6} \beta_{k}^{n-1}(\mathbf{r}) \Omega_{k}^{n-1}(\tilde{\lambda}_{k}^{n}) \\ &+ S_{F}^{n-2}(\mathbf{r}) \sum_{k=1}^{6} \beta_{k}^{n-2}(\mathbf{r}) \Omega_{k}^{n-2}(\tilde{\lambda}_{k}^{n}) \end{split}$$

By inserting the delayed neutron source terms Eq. (8) into Eq. (1) and expressing all the terms of R^n explicitly, and applying an isotropic assumption to $\partial \varphi / \partial t$, the final solution can be simplified as:

$$\Omega \cdot \nabla \varphi^{n}(\mathbf{r}, \Omega, E) + \Sigma_{t}^{n} \varphi^{n}(\mathbf{r}, \Omega, E) = \int_{0}^{\infty} \int_{0}^{4\pi} \Sigma_{s}^{n}(\mathbf{r}, \Omega \cdot \Omega', E')$$
$$\rightarrow E) \varphi^{n}(\mathbf{r}, \Omega', E') d\Omega' dE' + \frac{\chi^{n}(\mathbf{r}, E) S_{F}^{n}(\mathbf{r})}{4\pi} + \frac{S_{tr}^{n}(\mathbf{r}, E)}{4\pi}$$
(9)

where the transient source is defined in Eq. (10) by using the correlation $\chi(\mathbf{r}, E) = \chi_p(\mathbf{r}, E)(1 - \beta(\mathbf{r})) + \chi_d(\mathbf{r}, E)\beta(\mathbf{r})$:

$$S_{tr}^{n}(\mathbf{r}, E) = A(\mathbf{r}, E)\phi_{g}^{n} + B(\mathbf{r}, E)S_{F}^{n} + C(\mathbf{r}, E)$$
(10)

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