Improved Quasi-Static Method with Step Doubling Time Adaptation

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INTRODUCTION

The imminent restart of the Transient Reactor Testing Facility (TREAT) at Idaho National Laboratory (INL) has brought significant attention to the development of transient reactor modeling. TREAT was designed to subject fuels and other reactor components to various degrees of neutron pulses, from minor transients to accident scenario. Inherently, this task requires predicting pulse responses due to various control rod movements; which is a complicated endeavor. Originally, this was done using an iterative process of rod movements and measuring the resulting response. With the advances in computer modeling, the current goal, preceding the restart, is to use simulation to characterize responses before experiments take place. However, neutron transient modeling is extremely computationally expensive due to the required implicit time-stepping. Therefore, methods that mitigate computation time, with minimal detriment to accuracy, are highly desired. This paper will describe the improved quasi-static method (IQS), which hopes to decrease computation time significantly from traditional "brute force" transient methods.

IQS is a spatial kinetics method that involves factorizing the flux solution into time-dependent amplitude and space- and time-dependent shape [1, 2]. The impetus of the method is the assumption that shape is weakly time-dependent, so expensive space-dependent evaluations are only required on large time steps. While inexpensive amplitude evaluations are performed on much smaller time steps to retain accuracy. IQS has been tested extensively on kinetics benchmarks with constant time steps. However, to test it's viability for TREAT simulations, evaluating IQS's performance with time adaptation is required. The rest of this paper will briefly describe the derivation of IQS, the time adaptation technique used, and results from a kinetic benchmarks.

THEORY

In this Section, we recall the equation for the IQS method, starting from the standard multi-group transport equations with delayed neutron precursors in operator form:

$$\frac{1}{v^g}\frac{\partial \Psi^g}{\partial t} = \sum_{g'=1}^{G}\left(H^{g'\to g} + P_p^{g'\to g}\right)\Psi^{g'} - L^g\Psi^g + S_d^g \tag{1}$$

$$\frac{dC_i}{dt} = \sum_{g=1}^{G} P_{d,i}^g \Psi^g - \lambda_i C_i\,, \quad 1 \le i \le I \tag{2}$$

Factorization is an important step in the derivation of the IQS method. The factorization approach leads to a decomposition of the multigroup flux into the product of a time-dependent amplitude (p) and a space-/time-dependent multigroup shape (ψ):

$$\Psi^g(\boldsymbol{r},\Omega,t) = p(t)\psi^g(\boldsymbol{r},\Omega,t) \tag{3}$$

To obtain the amplitude equations, the multigroup equations are multiplied by a weighting function, typically the initial adjoint flux (ϕ^*), and then integrated over phase-space. For brevity, the inner product over space will be represented with parenthetical notation ($(\Psi^{*g}, f^g) = \int_{4\pi}\int_D \Psi^{*g}(\boldsymbol{r},\boldsymbol{\Omega}) f^g(\boldsymbol{r},\boldsymbol{\Omega}) d^3r d^2\Omega$). In order to impose uniqueness of the factorization, one requires $\sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\psi^g\right)$ to be constant. And after some manipulation, the standard point reactor kinetics equations (PRKE) for the amplitude solution are obtained:

$$\frac{dp}{dt} = \left[\frac{\rho-\bar{\beta}}{\Lambda}\right]p + \sum_{i=1}^{I}\bar{\lambda}_i\xi_i \tag{4}$$

$$\frac{d\xi_i}{dt} = \frac{\bar{\beta}_i}{\Lambda} - \bar{\lambda}_i\xi_i \quad 1 \le i \le I \tag{5}$$

Where the functional coefficients are calculated using the space-/time-dependent shape function as follows:

$$\frac{\rho-\bar{\beta}}{\Lambda} = \frac{\sum_{g=1}^{G}\left(\Psi^{*g}, \sum_{g'}(H^{'\to g}g + P_p^{g'\to g} - L^{g'}\delta_{g'g})\psi^{g'}\right)}{\sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\psi^g\right)} \tag{6}$$

$$\frac{\bar{\beta}}{\Lambda} = \sum_{i=1}^{I}\frac{\bar{\beta}_i}{\Lambda} = \sum_{i=1}^{I}\frac{\sum_{g=1}^{G}(\Psi^{*g}, P_{d,i}^g\psi^g)}{\sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\psi^g\right)} \tag{7}$$

$$\bar{\lambda}_i = \frac{\sum_{g=1}^{G}(\Psi^{*g}, \chi_{d,i}^g\lambda_i C_i)}{\sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\psi^g\right)} \tag{8}$$

IQS Predictor-Corrector (IQS P-C)

This version of IQS first solves the flux diffusion (represented by Equations and 2) to get a predicted flux. The predicted flux at this step is then converted to shape by rescaling as follows:

$$\psi_{n+1}^g = \underbrace{\Psi_{n+1}^g}_{\text{predicted}}\frac{K_0}{K_{n+1}} \tag{9}$$

Where:

$$K_{n+1} = \sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\Psi_{n+1}^g\right) \tag{10}$$

$$K_0 = \sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\psi_{n+1}^g\right) = \sum_{g=1}^{G}\left(\Psi^{*g}, \frac{1}{v^g}\Psi_0^g\right) \tag{11}$$

The PRKE parameters are then computed with this shape using Equations 6 - 8 and interpolated over the macro step, then the PRKE is evaluated. With the newly computed amplitude, the shape is rescaled and the corrected flux is evaluated:

$$\underbrace{\Psi_{n+1}^g}_{\text{corrected}} = p_{n+1}\times\psi_{n+1}^g \tag{12}$$

Time Adaptation

The time adaptation used for quantifying IQS's ability is step doubling. The step doubling technique involves estimating the local truncation error for a certain time step by taking the difference between a solution with one full step and a solution with two half steps. If the step is small enough, the error will be smaller than a user driven tolerance and the magnitude of the next step will be calculated based on the error. If the step is too large, the step will be repeated with a smaller step calculated with the resulting error. The error of the time step is approximated by Equation 13, where φ_1^g and φ_2^g are the solutions with the full step and half step, respectively. φ is changed to ϕ for regular flux evaluation and IQS P-C. If $e_n > e_{max}$ the time step is repeated; if $e_n < e_{max}$ the system moves to the next time step. The next Δt is calculated using Equation 14, where μ is the convergence order of the time integration scheme being used. e_{max} and e_{tol} are user defined parameters; e_{max} is usually less than e_{tol} to better guarantee that the calculated Δt_{new} will pass the error criteria so time steps won't be repeated.

$$e_n = \frac{\left\| \sum_{g=1}^{G} \int_{4\pi} \Psi_2^g d^2\Omega - \sum_{g=1}^{G} \int_{4\pi} \Psi_1^g d^2\Omega \right\|_{L^2}}{\max\left(\left\| \sum_{g=1}^{G} \int_{4\pi} \Psi_2^g d^2\Omega \right\|_{L^2}, \left\| \sum_{g=1}^{G} \int_{4\pi} \Psi_1^g d^2\Omega \right\|_{L^2} \right)} \quad (13)$$

$$\Delta t_{new} = \Delta t_{old} \left(\frac{e_{tol}}{e_n} \right)^{\frac{1}{\mu+1}} \quad (14)$$

RESULTS AND ANALYSIS

This section describes results of the TWIGL benchmark that tests the IQS implementation and shows its effectiveness on computation speed and accuracy. The benchmark was solved with regular diffusion (brute force) and IQS P-C with backward-Euler time discretization. The performance for each method are represented by the number of macro time steps and solves with step doubling time adaptation.

TWIGL Benchmark

This benchmark problem originates from the Argonne National Lab Benchmark Problem Book. It is a 2D, 2-group reactor core model with no reflector region, the geometry, material properties, and transient perturbation can be seen in [3]. Figure 1 shows the IQS solution as compared with the Brute Force solution with minimal time steps. Table I shows the results for time adaptation. The results show that IQS performs exceptionally well compared to brute force for this highly transient example.

CONCLUSIONS

The purpose of this paper was to show IQS's performance with step doubling time adaptation. The TWIGL benchmark was used to quantify the method's performance. The results from the TWIGL example shows significant improvement from the traditional brute force method. This improvement was anticipated because the shape for TWIGL changes very little through the transient, so the PRKE in IQS does most of the work. In conclusion, IQS shows impressive performance for complex neutronics problems with time adaptation. However, to rigorously test IQS, more complex problems including TREAT models and transport problems need to be applied.

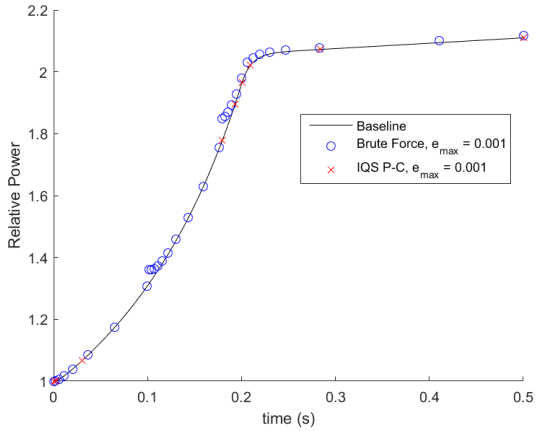

Fig. 1: Power level comarison of TWIGL benchmark between IQS and Brute Force using $e_{max} = 0.001$

		Brute Force			IQS P-C		
Test	e_{max}	Error	Steps	Solves	Error	Steps	Solves
1	0.05	0.00012677	9	29	0.03380433	4	9
2	0.01	3.5555e-05	5	40	0.00263068	5	12
3	0.005	4.0364e-05	5	40	0.00160486	6	21
4	0.001	0.00294822	5	36	1.7527e-05	10	35
5	0.0005	0.00099778	6	55	1.4185e-05	16	74
6	0.0001	0.00019510	7	65	6.2903e-06	19	78
7	5.0e-05	0.00018372	12	163	1.5247e-06	24	92
8	1.0e-05	8.0564e-05	379	5729	9.8321e-07	48	210

TABLE I: TWIGL step doubling results

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REFERENCES

1. K. OTT, "Quasi-static treatment of spatial phenomena in reactor dynamics," *Nuclear Science and Engineering*, **26**, 563 (1966).
2. S. DULLA, E. H. MUND, and P. RAVETTO, "The quasi-static method revisited," *Progress in Nuclear Energy*, **50**, *8*, 908 – 920 (2008).
3. P. BY THE BENCHMARK PROBLEM COMMITTEE OF THE MATHEMATICS and C. D. OF THE AMERICAN NUCLEAR SOCIETY, *Argonne Code Center: Benchmark Problem Book: Numerical Determination of the Space, Time, Angle, or Energy Distribution of Particles in an Assembly*, 3 ed. (1968).