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# Adaptive time step selection in the quasi-static methods of nuclear reactor dynamics

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ABSTRACT

Of the methods available by which to integrate the neutron and delayed neutron precursor balance equations in time, at present the quasi-static methods are among the most practical and favourable. However, the correct application of the quasi-static method requires the use of appropriately determined time steps, for both the reasons of accuracy and efficiency. This work presents a methodology for the adaptive selection of the time steps employed by the quasi-static method, thereby allowing the quasi-static approach to be applied in an efficient manner while maintaining a prescribed level of accuracy. The method is applied to and studied using some numeric test problems.



## 1. Introduction

The solution of the time-dependent neutron and delayed neutron precursor balance equations on the full phase space is among the most computationally intensive operations in the simulation of nuclear fission systems. Aside from the typically large number of unknowns that result from the necessity to describe and, consequently, to discretise the phase space variables, the neutron and delayed neutron precursor balance equations are stiff in time, a property that arises from the vastly different time scales of the physical phenomena represented by the system of integro-differential balance equations.

Various approaches exist to perform the numerical integration in time of the neutron and delayed neutron precursor balance equations. Among these methods is the quasi-static approach, which has become a favourite of reactor physicists thanks to its mathematical elegance, its simplicity, and, when properly applied, its combined accuracy and computational efficiency. The correct application of the quasi-static method is related to the appropriate selection of the time steps, which has direct consequences both on the accuracy of the computed solution and on the efficiency of the method.

Although appreciable effort has been dedicated to the mathematical formulation of the quasi-static equations and to the study of the different algorithmic approaches that can be used to integrate them (Henry, 1958; Ott and Madell, 1966; Ott and Meneley, 1969; Devooght, 1980; Devooght and Mund, 1980; Mika, 1982; Kao and Henry, 1989), significantly less effort has been directed to the study of appropriate methodologies for the selection of the time steps that are involved in the quasi-static approach. Existing time step selection algorithms used in neutronics codes which employ quasi-static solvers (Meneley et al., 1967; Shober et al., 1978) tend to be based on heuristic approaches and experience acquired through application rather than on a well formulated physical-mathematical basis. While such approaches function and while they benefit from experience, the resulting algorithms may become cumbersome, requiring the evaluation of many metrics, which both adds computational burden and potentially imposes criteria which may lead to non-optimal proposals for the time steps.

Instead, an extensive history exists of the development and the application of automated step size selection techniques in numerical solvers of ordinary differential equations (Gear, 1971; Hairer et al., 1987; Hairer and Wanner, 1991). The theory of adaptive time step selection that is developed in the general mathematical context can be extended to the specific case of the equations of nuclear reactor dynamics and to the quasi-static method.

This work presents a methodology for the adaptive selection of the time steps employed in the quasi-static method. First, the quasi-static equations of nuclear reactor dynamics are presented and discussed, with particular focus on the role of the time steps. Next, the fundamental principles of adaptive step size selection in the numerical solution of initial value problems are reviewed in order to provide a basis for that which follows. The two topics are then synthesised into a methodology for the adaptive selection of the time steps employed in the quasi-static method. Finally, the

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methodology is assessed through the application to some numerical test problems.

## 2. Quasi-static method and time scales

The neutron and delayed neutron precursor balance equations for a stationary medium may be written in operator form as

$$\begin{cases} \dfrac{1}{v(E)}\dfrac{\partial}{\partial t}\phi(\mathbf{r},E,\mathbf{\Omega},t) = \left[(\mathcal{L}+\mathcal{M}_p)\phi\right](\mathbf{r},E,\mathbf{\Omega},t) \\ \quad +\displaystyle\sum_{i=1}^{R}\frac{\chi_i(\mathbf{r},E)}{4\pi}\lambda_i c_i(\mathbf{r},t) + S(\mathbf{r},E,\mathbf{\Omega},t), \\ \dfrac{\chi_i(\mathbf{r},E)}{4\pi}\dfrac{\partial}{\partial t}c_i(\mathbf{r},t) = [\mathcal{M}_i\phi](\mathbf{r},E,\mathbf{\Omega},t) - \dfrac{\chi_i(\mathbf{r},E)}{4\pi}\lambda_i c_i(\mathbf{r},t), \\ \quad i=1,\ldots,R, \end{cases} \tag{1}$$

in which the terms have their standard significance: $\phi$ is the angular neutron flux, $\chi_i\lambda_i c_i/4\pi$ is the emissivity of delayed neutrons in precursor family $i$ of a total of $R$ precursor families, $S$ is the independent external neutron source emissivity, $\mathcal{L}$ is the loss operator and $\mathcal{M}_p$ and $\mathcal{M}_i$ represent the prompt and the delayed fission neutron production operators, respectively.

The quasi-static method for the solution of the neutron and delayed neutron precursor balance equations is based on a separation-projection technique in which the neutron flux is factorised into the product of an amplitude function $T$ and a shape function $\psi$ (Henry, 1958), that is

$$\phi(\mathbf{r},E,\mathbf{\Omega},t) = T(t)\psi(\mathbf{r},E,\mathbf{\Omega},t). \tag{2}$$

The factorisation, which is rendered unique by imposing an appropriate normalisation condition, has the objective of reducing the time stiffness of the original problem by allowing each of the two functions to characterise separately the dominant physics on its respective time scale, with the amplitude being characterised by the faster and the shape being characterised by the slower. The introduction of this factorisation into Eq. (1), followed by the projection onto the adjoint solution of the reference system ultimately results in the amplitude equations

$$\begin{cases} \dfrac{d}{dt}T(t) = \dfrac{\rho(t)-\widetilde{\beta}(t)}{\Lambda(t)}T(t) + \displaystyle\sum_{i=1}^{R}\lambda_i\widetilde{c}_i(t) + \widetilde{s}(t), \\ \dfrac{d}{dt}\widetilde{c}_i(t) = \dfrac{\widetilde{\beta}_i(t)}{\Lambda(t)}T(t) - \lambda_i\widetilde{c}_i(t), \quad i=1,\ldots,R, \end{cases} \tag{3}$$

and the shape equations

$$\begin{cases} \dfrac{1}{v(E)}\dfrac{\partial}{\partial t}\psi(\mathbf{r},E,\mathbf{\Omega},t) = \left[\left(\mathcal{L}+\mathcal{M}_p - \dfrac{1}{v}\dfrac{1}{T}\dfrac{d}{dt}T\right)\psi\right](\mathbf{r},E,\mathbf{\Omega},t) \\ \quad +\dfrac{1}{T(t)}\left[\displaystyle\sum_{i=1}^{R}\frac{\chi_i(\mathbf{r},E)}{4\pi}\lambda_i c_i(\mathbf{r},t) + S(\mathbf{r},E,\mathbf{\Omega},t)\right], \\ \dfrac{\chi_i(\mathbf{r},E)}{4\pi}\dfrac{\partial}{\partial t}c_i(\mathbf{r},t) = T(t)[\mathcal{M}_i\psi](\mathbf{r},E,\mathbf{\Omega},t) - \dfrac{\chi_i(\mathbf{r},E)}{4\pi}\lambda_i c_i(\mathbf{r},t), \\ \quad i=1,\ldots,R, \end{cases} \tag{4}$$

with the effective delayed neutron precursor amplitudes $\widetilde{c}_i$, the neutron generation time $\Lambda$, the effective delayed neutron fractions $\widetilde{\beta}_i$, the dynamic reactivity $\rho$ and the effective independent neutron source strength $\widetilde{s}$ that appear in Eq. (3) given by the standard weighted integral definitions (Bell and Glasstone, 1970).

Despite the various algorithmic approaches that exist to advance the solution, the principle which is common to all quasi-static methods is that the integration of the neutron flux in time is performed on a multi-scale discretisation of the time domain. The shape equations are solved every shape time step, $\Delta t_\psi$, while the integral kinetics parameters are updated on the reactivity time steps, $\Delta t_\rho \leqslant \Delta t_\psi$, and the amplitude equations are solved on the amplitude time steps, $\Delta t_T \leqslant \Delta t_\rho$. The solution of the neutron flux at any generic time $t$ can be reconstructed through Eq. (2), perhaps interpolating the amplitude and/or the shape as required. A fundamental consideration for the use of the quasi-static method is related to the selection of the aforementioned time steps, as their selection has implications both on the accuracy of the solution and on the efficiency of the method. This is especially true for the shape time steps and the reactivity time steps, though perhaps less so for the amplitude time steps.

The shape time step determines the duration for which the temporally continuous shape function is assumed to be accurately representable by a set of discrete values and interpolation rules. Therefore, an appropriate shape time step is one for which the variation of the shape across the time step is small in magnitude or for which the solution is insensitive to the variation of the shape. The temporal evolution of the shape depends on the type of transient and the sensitivity of the solution to changes of the shape depends on the physical characteristics of the system. In addition to the previous consideration that is strictly related to the mathematical hypotheses of the quasi-static method, the selection of the shape time step also needs to take into consideration the properties of the numerical method according to which the flux or the shape equations are integrated.

The reactivity time step couples the scalar coefficients of the amplitude equations to the phase-space-dependent operators and source emissivity of the neutron and delayed neutron precursor balance equations. Consequently, the limitations on the selection of the reactivity time step are associated to the methods by which the flux or shape equations and the amplitude equations are integrated in the implemented quasi-static algorithm. Namely, it is the method of integration applied to the flux or shape equations that determines the assumed evolution of the integral kinetics parameters across the shape time step, while it is the method by which the amplitude equations are integrated that may impose practical limitations on the functional dependence of the integral kinetics parameters permitted as input.

The amplitude time step is a purely mathematical construct that is utilised to integrate the amplitude equations across a specified reactivity time step. In virtue of their structure as a system of coupled first-order ordinary differential equations, the amplitude equations benefit from the existence of many numerical, both general mathematical (Gear, 1971) and application-specific (Ganapol, 2013), and analytical (Akcasu et al., 1971; Hetrick, 1971) methods that allow to determine the amplitude to a high degree of accuracy. Thus, in the overall framework of the quasi-static method, the amplitude time steps are not of particular interest, other than requiring that they satisfy the requirements for the accuracy imposed on the solution of the amplitude equations.

## 3. Adaptive step size control in initial value problems

Adaptive step size control for the numerical integration of initial value problems is based on the estimation and on the control of the local error (or, alternatively, the local truncation error) introduced by the numerical method. Consider the initial value problem of Cauchy in the independent variable $t$, to be solved numerically. It can be demonstrated that the local error of a numerical method of order $q$ is (Gear, 1971)

$$e(t,h) = \Theta(t)h^{q+1} + \mathcal{O}(h^{q+2}), \tag{5}$$

where $\Theta$ is the norm of the principal error function and $h$ is the step size. In general, it is not possible to provide an exact expression for the local error; consequently, an appropriate bound must be estimated. By assuming that all step sizes used in the integration