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Adaptive modal methods to integrate the neutron diffusion equation

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1 Introduction

The distribution of the neutrons inside a reactor core along time can be described by the time dependent multigroup neutron diffusion equation. A finite element method (FEM) is used to discretize the neutron diffusion equation to get a system of semi-ordinary differential equations

$$\begin{aligned} V^{-1}\frac{\mathrm{d}\Phi}{\mathrm{d}t} + L\Phi &= (1-\beta)M\Phi + \sum_{k=1}^{K}\lambda_k^d X C_k, \\ \frac{\mathrm{d}C_k}{\mathrm{d}t} &= \beta_k M_1 \Phi - \lambda_k^d C_k, \qquad k = 1,\ldots,K. \end{aligned} \tag{1}$$

The FEM has been implemented by using the open source finite elements library `Deal.ii`. This system of ordinary differential equations is, in general, stiff. Several approaches have been studied to integrate this time-dependent equation such as the backward differential method, the quasi-static method or the modal method. In this work, we use this last approach that assumes that the solution can be described by the sum of amplitude functions multiplied by shape functions of modes. The shape functions are obtained from the solution of the λ-modes problem

$$L\psi_m = \frac{1}{\lambda_m} M\psi_m. \tag{2}$$

Generally, the eigenfunctions are updated in the time-dependent equations with a fixed time-step size to obtain accurate results [1]. This implies to select a suitable time step before the simulation. In this work, we propose an adaptive time-step control that selects an appropriate step size from a given tolerance. The time selection for the backward method and the quasi-static method is usually based on the local error in the time discretization. In the modal approach, different types of errors are studied for updating the time-step selection.

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2 The updated modal method

The modal methodology supposes that $\Phi(\vec{r},t)$ admits the following expansion

$$\Phi(\vec{r},t)=\sum_{m=1}^{q} n_m(t)\psi_m(\vec{r}), \tag{3}$$

where $n_m(t)$ are the amplitude coefficients and $\psi_m(\vec{r})$ are the shape functions obtained when problem (2) is solved. Moreover, the matrices L and M of the problem (2) can be expressed as $L=L_0+\delta L$, $M=M_0+\delta M$, respectively, where L_0 and M_0 are the matrices at $t=0$ and in steady-state (M_0 is divided by $k_{eff}=\lambda_1$).
Taking into account these considerations and multiplying by the adjoint eigenfunctions associated with the λ-modes problem, $\psi_l^{\dagger,i}$, over the Eq. (1), one can obtain the system of ODE's

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{N}=\mathbf{T}\mathbf{N}, \tag{4}$$

where

$$\mathbf{N}=\begin{pmatrix} n_1\cdots n_q & c_{11}\cdots c_{q1} & \cdots & c_{1K}\cdots c_{qK}\end{pmatrix}^T,$$

$$\mathbf{T}=\left(\begin{array}{c|ccc} \Lambda^{-1}((1-\beta)I-[\lambda]^{-1}-A^L+(1-\beta)A^M) & \Lambda^{-1}\lambda_1^d & \cdots & \Lambda^{-1}\lambda_K^d \\ \hline \beta_1(I+A^M) & -\lambda_1^d I & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \beta_K(I+A^M) & 0 & \cdots & -\lambda_K^d I \end{array}\right),$$

and

$$\begin{aligned} \Lambda_{lm}&=\langle\psi_l^\dagger, V^{-1}\psi_m\rangle, & A_{lm}^L&=\langle\psi_l^\dagger,\delta L\psi_m\rangle,\\ A_{lm}^M&=\langle\psi_l^\dagger,\delta M\psi_m\rangle, & c_{lk}&=\langle\psi_l^\dagger, XC_k\rangle, \end{aligned}$$

The initial conditions values are

$$\begin{aligned} &n_1(0)=1, && n_m(0)=0,\ m=2,\dots,q,\\ &c_{1k}(0)=\frac{\beta_k}{\lambda_k^d}, && c_{mk}(0)=0,\ m=2,\dots,q, \quad k=1,\dots,K, \end{aligned}$$

that are obtained from the equations in the critical state. The ODE is solved with the CVODE module from the open source library SUNDIALS.

In realistic transients, the flux can be suffered extremely spatial variations. Obtaining accurate approximations implies a high number of modes. That means a high computational cost [2]. A solution is a modal methodology where the modes are updated in a certain time interval $[t_i,t_i+\Delta t_i]=[t_i,t_{i+1}]$. In each interval $[t_i,t_{i+1}]$, the neutron diffusion equation can be integrated through the solution of the λ-modes problem associated at time t_i.

The differential equations that are needed to integrate have the same form than the problem without updating (Eq. (4)). The initial conditions for $n_m^{i,\lambda}$ at time t_i must be defined to solve

the differential problem in the interval $[t_i, t_{i+1}]$. For the expansion (3) at $t = t_i$, one could approximate the value of $n_m^{i,\lambda}(t_i)$ as

$$n_m^{i,\lambda}(t_i) \approx \frac{\langle \psi_m^{\dagger,i}, M^i \Phi(t_i) \rangle}{\langle \psi_m^{\dagger,i}, M^i \psi_m^i \rangle},$$

where $\Phi(t_i)$ is obtained from the previous modal step.
The concentration of precursors at time t_i can be computed as

$$c_{l,k}^{i,\lambda}(t_i) = \sum_{m=1}^{q} a_{lm} c_{m,k}^{i-1,\lambda}(t_i), \quad \text{where,} \quad a_{lm} = \frac{\langle \psi_l^{\dagger,i}, M^{i-1} \psi_m^{i-1} \rangle}{\langle \psi_m^{\dagger,i-1}, M^{i-1} \psi_m^{i-1} \rangle}.$$

The λ-modes problem is solved with the block inverse-free preconditioned Arnoldi method, (BIFPAM) (see more details in [5]).

3 Adaptive time-step control

The modes can be updated with fix time-step, but it implies several limitations such as selecting a time-step previously that leads to obtain results with unpredictable errors. In this work, we study an adaptive time-step control. Its implementation requires to define an error estimation due to the modal expansion assumption and a suitable constraint to select the time-step based on the error estimation.

Estimation error The modal error comes (essentially) from the assumption in the modal expansion because the eigenvalue functions do not form a complete basis. Therefore, if there are large variations in the flux along the time, the modal method will obtain large errors. The first estimation is based in the difference between eigenfunctions. The *modal difference error* is defined as

$$\varepsilon_{md} = \max_m \|\psi_m^{i-1} - \psi_m^i\|.$$

The *modal residual error* is computed thought the residual error as

$$\varepsilon_{mr} = \max_m \|L^i \psi_m^{i-1} - \lambda_m^{i-1} M^i \psi_m^{i-1}\|.$$

Finally, we assume that the flux will change according to the changing on the absorption cross-section Σ_{a1}. We define the *cross-section perturbation error* as

$$\varepsilon_{sa} = \sum_c \|\Sigma_{a1}^{i-1}(c) - \Sigma_{a1}^i(c)\|,$$

where c is a cell of the reactor.

Control Algorithm Two strategies based on the error in the previous step are proposed. The *Fixed Error Control* strategy defined as

$$\Delta t_i = \begin{cases} \Delta t_{i-1} * 2, & \varepsilon < min_{le}, \\ \Delta t_{i-1}, & min_{le} < \varepsilon < max_{le}, \\ \Delta t_{i-1} \,/\, 2, & max_{le} < \varepsilon. \end{cases}$$

The *Adaptive Error Control*, based on the control algorithms defined for differential methods. The step Δt_i is computed as

$$\Delta t_i = \Delta t_{i-1} \min\{2.0, \max\{0.5, \sqrt{3.0/\varepsilon}\}\},$$

4 Numerical results

The Langenbuch reactor [4] is chosen to study the performance of the adaptive modal methodology proposed with a local perturbation. This reactor has two sets of control rods that define the transient (Fig. 1.a). It starts with the withdrawal of one bar of C1 at 10cm/s. The rest of C1 is inserted at 3cm/s over $7.5 < t < 47.5$s. C2 is inserted at 3cm/s over $7.5 < t < 47.5$s. The evolution of the global power is represented in Figure 1. The solutions are compared with the solutions obtained with a backward differential method [3] (Fig. 1.b).

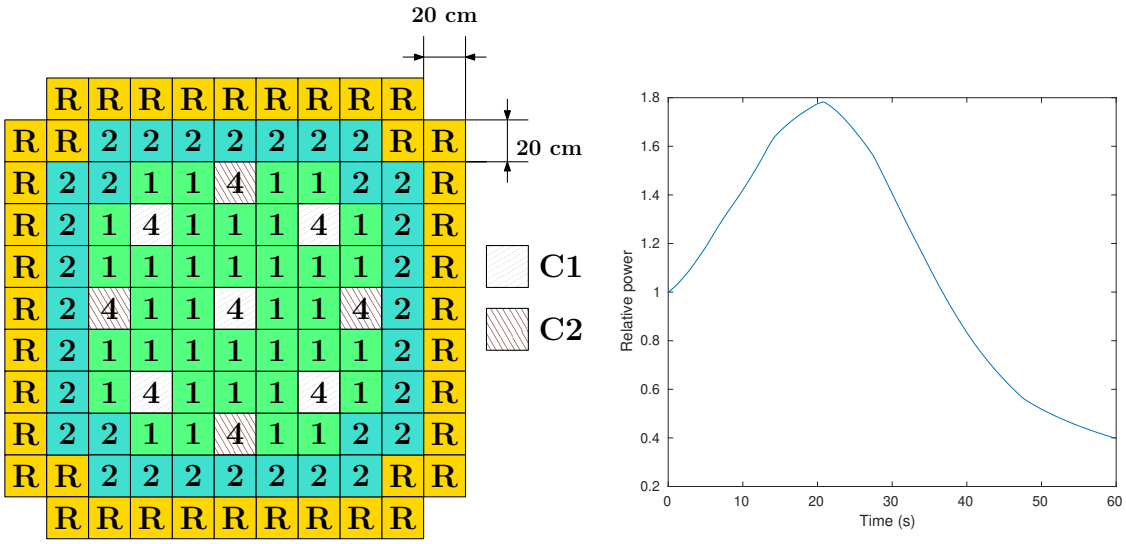

Figure 1: Geometry and global power of the Langenbuch transient.

Table 1 shows that better approximations are obtained if the step of updating is smaller. However, the computational times in these cases are also higher. Moreover, one can observe that using a high number of modes in the expansion gives more accurate results. A combination between a reasonable number of modes and a not small time-step is the most effective option. However, these parameters are dependent on the transient.

N. eigs. (q)	Updated	Error	CPU Time
1	1.0s	4.9e-03	38min
1	5.0s	1.8e-02	9min
3	5.0s	1.5e-02	10min
3	10.0s	3.5e-02	6min

Table 1: Performance of the Updated modal method with fixed time-step.

The global error is represented along the time (Fig. 2). It is observed that the large errors are produced when the local perturbation is applied and before to the updating of the modes. Fig. 2 represents the radial profile of the error at $t = 2.1$ in the case with 3 eigenvalues and time-step equal to 5 s. It is observed that this is focused around the control rod that is withdrawal at this moment. The same conclusions are deduced with other settings.

Error time-step	Control	Error	CPU Time
ε_{md}	Fixed	9e-03	53.0min
ε_{md}	Adaptive	9e-03	100.2min
ε_{mr}	Fixed	7e-03	8.0min
ε_{mr}	Adaptive	1e-02	6.0min
ε_{sa}	Fixed	8e-03	7.2min
ε_{sa}	Adaptive	1e-02	6.3min

Table 2: Errors and CPU time obtained with the adaptive time-step modal method.

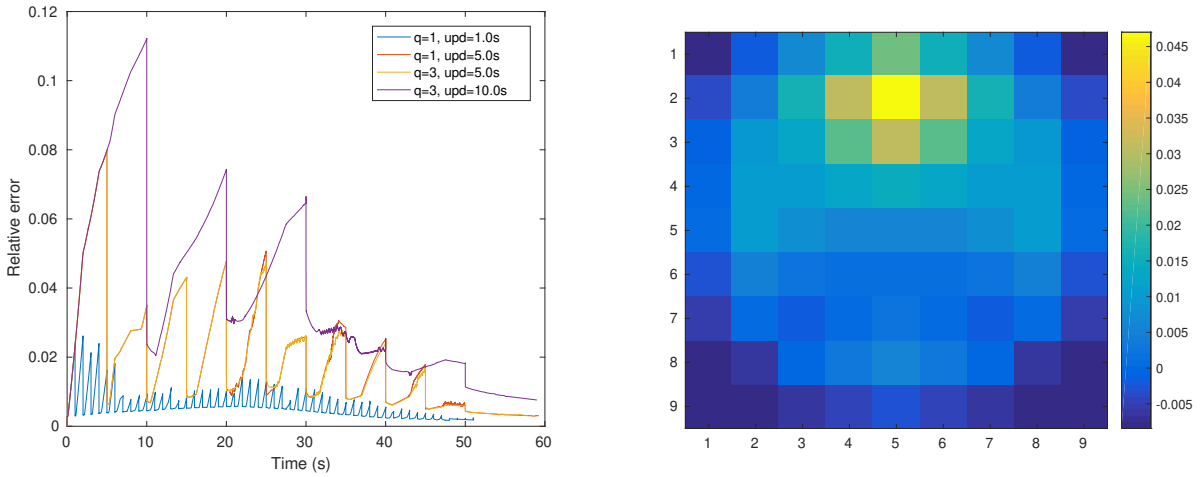

Figure 2: Error in the Langenbuch transient with fixed time-step.

Table 2 shows the error and CPU times obtained with the different error estimations and control errors obtained with 3 eigenvalues. First, one can observed that the modal difference error (md) is not a very efficient technique because it needs to compute the modes for estimating the error (that is very expensive). Regarding to other error estimations, there are not big differences between them. If now, the type of control error is compared the adaptive gives similar approximations than the fixed control but in less time.

Finally, we compare the error between the adaptive time-step modal method and the fixed time-step modal method with 3 eigenvalues and the same initial time-step (5.0 s). More accurate results are obtained with the adaptive method in less time. Moreover, if this error is analyzed over the time in both cases, an error more distributed is obtained by using the adaptive time-step control.

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