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Development of dynamic models for neutron transport calculations

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Summary. — A quasi-static approach within the framework of neutron transport theory is used to develop a computational tool for the time-dependent analysis of nuclear systems. The determination of the shape function needed for the quasi-static scheme is obtained by the steady-state transport code DRAGON. The kinetic model solves the system of ordinary differential equations for the amplitude function on a fast scale. The kinetic parameters are calculated by a coupling module that retrieves the shape from the output of the transport code and performs the required adjoint-weighted quadratures. When the update of the shape has to be carried out, the coupling module generates an appropriate input file for the transport code. Both the standard Improved Quasi-Static scheme and an innovative Predictor-Corrector algorithm are implemented. The results show the feasibility of both procedures and their effectiveness in terms of computational times and accuracy.

PACS 28.20.Gd – Neutron transport: diffusion and moderation.
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1. – Introduction

For several applications in the physics of nuclear systems an accurate transport model may be needed to adequately describe the evolution of the neutron population in perturbed conditions. This may be the case especially when treating advanced systems, such as source-driven subcritical assemblies or some of the Generation IV reactor configurations. In such systems, the use of diffusion models cannot fully account for important physical phenomena.

A direct approach involves the inversion of the transport operator on a very short time scale, thus implying a huge computational effort. To overcome this problem, the quasi-static method can be very appropriate, allowing to obtain high-quality time-dependent predictions with a reasonable computational effort.

In this work, a computational tool coupling the existing transport code DRAGON to a kinetic module is described. The transport code is used for the generation of the shapes needed to evaluate the kinetic parameters of the amplitude model, which is solved on a fast time scale. Two possible implementations of the quasi-static scheme are considered: the Improved Quasi-static Method (IQM) and the Predictor-Corrector Quasi-static Method (PCQM). Some test results are presented and discussed.

2. – Quasi-static approaches to the time-dependent transport problem

The time-dependent analysis of nuclear systems requires the solution of the balance equations for neutrons and delayed neutron precursors:

$$\left\{\begin{array}{l} \dfrac{1}{v}\dfrac{\partial\varphi}{\partial t} = \mathscr{L}(t)\varphi(t) + \dfrac{1}{4\pi}\displaystyle\sum_{i=1}^{I}\chi_i(E)\lambda_i C_i(\boldsymbol{r},t) + S(\boldsymbol{r},E,\boldsymbol{\Omega},t), \\ \dfrac{\chi_i(E)}{4\pi}\dfrac{\partial C_i}{\partial t} = -\dfrac{\chi_i(E)}{4\pi}\lambda_i C_i(\boldsymbol{r},t) + \mathscr{F}_i^d(t)\varphi(t), \qquad i=1,2,\ldots,I, \end{array}\right. \tag{1}$$

where $\varphi(t) \equiv \varphi(\boldsymbol{r},E,\boldsymbol{\Omega},t)$ and $C_i \equiv C_i(\boldsymbol{r},t)$ denote the neutron angular flux and the delayed neutron precursors concentrations, respectively. The general definitions of the operators appearing in eqs. (1) are well known and can be found in ref. [1].

Since the complete solution of system (1) is highly computer-time consuming, various approximate models for neutron kinetics have been developed during the past years [2-6]. In particular, the quasi-static approach is based on the factorization of the neutron flux in the product of an amplitude function A, only depending on time, and a shape function ψ, depending on the phase space variables and, on a slower time scale, on time:

$$\varphi(\boldsymbol{r},E,\boldsymbol{\Omega},t) = A(t)\psi(\boldsymbol{r},E,\boldsymbol{\Omega};t). \tag{2}$$

The introduction of the factorization formula (2) into the balance equations (1) leads to what is referred to as *shape model*:

$$\left\{\begin{array}{l} \dfrac{1}{v}\dfrac{\partial\psi}{\partial t}A + \dfrac{1}{v}\dfrac{\mathrm{d}A}{\mathrm{d}t}\psi = \mathscr{L}(t)\psi(t)A(t) + \dfrac{1}{4\pi}\displaystyle\sum_{i=1}^{I}\chi_i(E)\lambda_i C_i(\boldsymbol{r},t) + S(\boldsymbol{r},E,\boldsymbol{\Omega},t), \\ \dfrac{\chi_i(E)}{4\pi}\dfrac{\partial C_i}{\partial t} = -\dfrac{\chi_i(E)}{4\pi}\lambda_i C_i(\boldsymbol{r},t) + \mathscr{F}_i^d(t)\psi(t)A(t), \qquad i=1,2,\ldots,I. \end{array}\right. \tag{3}$$

The factorization introduced, eq. (2), is general and thus non-unique. A normalization constraint is introduced requiring the integral of the neutron density, weighted on the adjoint function associated to a reference initial configuration, to be constant:

$$\left\langle \psi_0^\dagger, \frac{1}{v}\psi \right\rangle := \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}E \oint \mathrm{d}\boldsymbol{\Omega}\, \psi_0^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega})\frac{1}{v}\psi(\boldsymbol{r},E,\boldsymbol{\Omega},t) = \gamma_0 \equiv \left\langle \psi_0^\dagger, \frac{1}{v}\varphi_0 \right\rangle, \tag{4}$$

where φ_0 is the neutron flux in the initial configuration. This choice is convenient, since the following step consists in the projection of the shape model over the same weighting

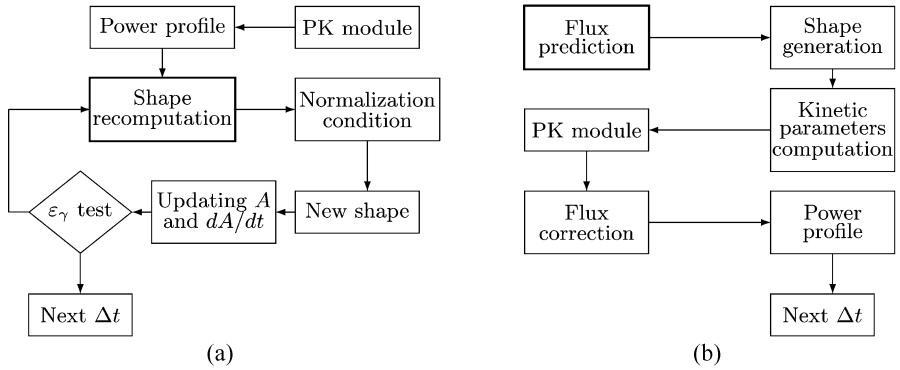


Fig. 1. – Block diagram of the quasi-static algorithms for a single Δt computation. a) IQM; b) PCQM. Bold-edged boxes identify tasks demanded to the DRAGON code.

function, taking advantage of the simplification introduced by condition (4), obtaining the *amplitude model*:

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}A}{\mathrm{d}t} = \dfrac{\rho(t)-\tilde{\beta}(t)}{\Lambda(t)}A(t) + \displaystyle\sum_{i=1}^{I}\lambda_i\tilde{c}_i(t) + \tilde{S}(t) \\ \dfrac{\mathrm{d}\tilde{c}_i}{\mathrm{d}t} = -\lambda_i\tilde{c}_i(t) + \dfrac{\tilde{\beta}(t)}{\Lambda(t)}A(t), \qquad i = 1,2,\ldots,I. \end{array}\right. \tag{5}$$

When the shape function is equal to the steady-state initial neutron flux φ_0, the Point Kinetic equations (PK) are derived.

Both the shape and amplitude models are non-linear, since the kinetics parameters in (5) depend on the shape and the product of the two unknowns appears explicitly in (3). The improved quasi-static method (IQM) takes advantage of the different time scales appearing in the transient evolution. First, the amplitude equations are solved over a large time interval Δt, using a finer time mesh δt. Then, the shape model is solved on the same Δt, updating the kinetic parameters and iterating the solution by modifying the derivative of the amplitude function. This allows to reduce the error on the normalization condition (4), defined as

$$\varepsilon_\gamma = \frac{|\gamma-\gamma_0|}{\gamma_0}, \qquad \gamma = \left\langle \psi_0^\dagger, \frac{1}{v}\psi \right\rangle. \tag{6}$$

The block diagram for IQM is sketched in fig. 1a, enlightening the presence of the normalization iterations. The non-linearity of IQM can represent a relevant problem, since the convergence of the γ parameter is a critical aspect. For this reason, a different approach to quasi-statics has been recently proposed to overcome this issue, the predictor-corrector quasi-static method (PCQM) [1,7]. The two time-scale approach to the time-dependent problem is still used, but the shape update procedure is carried out first to obtain improved kinetic parameters. To do so, the neutron balance equations (1) are solved on the coarse time step Δt and the obtained predicted flux is renormalized in order to obtain a shape fulfilling condition (4). The kinetic parameters evaluated with the new shape are

then used for the solution of eqs. (5), to provide the power evolution on the fine mesh δt. The block diagram for PCQM is given in fig. 1b.

3. – Description of the work

The quasi-static algorithms described in the previous section require the solution of a time-dependent balance equation for neutrons and precursors. Once the time derivative is approximated by a suitable numerical scheme, both the neutron balance equations (1) and the shape model (3) can be recast into a pseudo-stationary form. In this work, a first-order implicit-Euler scheme is adopted. The shape model for IQM can be written as

$$\left[\mathscr{L}(t) - \frac{1}{v\Delta t} - \frac{1}{vA(t)}\frac{\mathrm{d}A}{\mathrm{d}t}\right]\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) + \tilde{Q}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = 0, \tag{7}$$

where the generalized source $\tilde{Q}$, including the contribution of precursors, takes the form

$$\begin{aligned}\tilde{Q}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = {} & \frac{S(\boldsymbol{r}, E, \boldsymbol{\Omega}, t)}{A(t)} + \frac{\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t - \Delta t)}{v\Delta t} + \sum_i \lambda_i \frac{\chi_i}{4\pi}\frac{1}{A(t)} \\ & \cdot\left[C_{i,0}(\boldsymbol{r})e^{-\lambda_i \Delta t} + \int_{t-\Delta t}^{t} \mathrm{d}\tau \mathscr{F}_i^d(\tau)\varphi(\boldsymbol{r}, E, \boldsymbol{\Omega}, \tau)e^{-\lambda_i(t-\tau)}\right],\end{aligned} \tag{8}$$

and a time-absorption term, depending on the value of the amplitude and its derivative, appears on the left-hand side of (7).

In PCQM, the form of the pseudo-stationary equation is

$$\left[\mathscr{L}(t) - \frac{1}{v\Delta t} + \frac{\Delta t}{2}\sum_i \lambda_i \mathscr{F}_i^d(t)\right]\tilde{\varphi}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) + \tilde{Q}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = 0, \tag{9}$$

where the generalized source $\tilde{Q}$ is now defined as

$$\begin{aligned}\tilde{Q}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = {} & S(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) + \frac{\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t - \Delta t)}{v\Delta t} \\ & + \sum_i \lambda_i \left[\frac{\chi_i}{4\pi}C_{i,0}(\boldsymbol{r})e^{-\lambda_i \Delta t} + \frac{\Delta t}{2}\mathscr{F}_i^d(t)\tilde{\varphi}(\boldsymbol{r}, E, \boldsymbol{\Omega}, t)\right].\end{aligned} \tag{10}$$

This feature of both approaches is well suited for the use of a steady-state solver instead of a full dedicated time-dependent code. This possibility allows to use well-assessed and optimized flux solvers to be coupled to an external module dealing with the quasi-static algorithms [8].

In this work, the open-source stand-alone steady-state neutron transport solver DRAGON, developed by the École Polytechnique de Montréal, is used [9]. The code is coupled to a kinetic module, implementing the quasi-static schemes described before, through an interface module which manages the input/output data. Equations (7) and (9) are solved introducing *virtual* cross-sections and sources in the transport solver. The quasi-static procedure is established through linked computational modules.

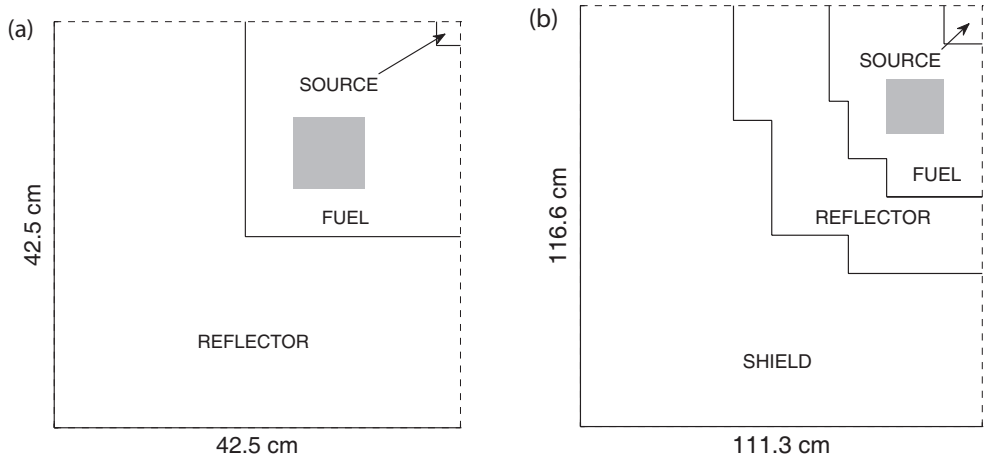


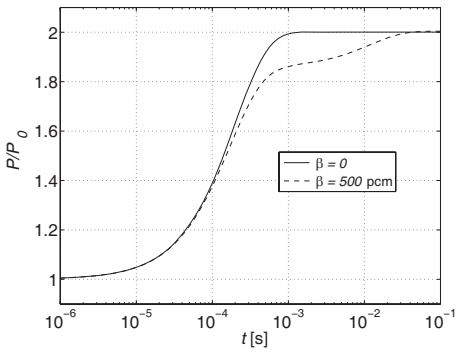
Fig. 2. – Representation of one quarter of the two reactor domains. a) 2D square test reactor; b) 2D MASURCA-like reactor. The shaded areas identify the regions where cross-section perturbations are introduced. The neutron transport calculations are performed by imposing reflective boundary conditions on the dashed edges, while vacuum boundary conditions are imposed on the solid edges.

4. – Results

In this section some test calculations are presented in order to demonstrate the feasibility of the procedure and the efficiency of the computational tool in the prediction of the reactor power evolution, induced by source and cross-section perturbations inserted into the system. However, it must be highlighted that, in order to obtain a fully consistent model with eqs. (8) and (10), the steady-state transport solver must accept angular-dependent sources and provide angular fluxes as output, for the computation of the kinetic parameters. In this work, the DRAGON code solves the transport equation using the collision probability method, with a 10^{-6} maximum tolerance on the error on the eigenvalue and the flux. This module provides as output the scalar fluxes and accepts as input only isotropic source distributions. These aspects constitute an inconsistency in the formulation of the quasi-static algorithm and could introduce relevant errors when problems with a high anisotropy of the neutron shape are concerned (*e.g.*, high-energy neutrons). However, the results in the current section show that for some cases accurate power predictions can be obtained.

The dynamic code takes into account the presence of delayed neutrons. The choice of macro Δt and micro δt time-step sizes is provided by the user. In the following calculations $\delta t = 10^{-6}\,\mathrm{s}$, while parametric studies on the value of Δt are performed. In figs. 2a and 2b, a picture of the two systems analyzed is presented. They are adopted for one-group and three-group calculations, respectively.

As a preliminary assessment, a transient induced by doubling the external neutron source intensity is considered for the system in fig. 2a. The transport problem being linear, the final value of the power must be consequently doubled. Results are presented in fig. 3. The presence of delayed neutrons is taken into account by considering one family of precursors only, with $\beta = 500\,\mathrm{pcm}$ and $\lambda = 100\,\mathrm{s}^{-1}$. This value of the decay constant, even if not realistic, allows to analyze whether the code is treating correctly



Δt [ms]	IQM	PCQM
5.00	2.000275	2.000333
2.50	2.000371	2.000469
1.25	2.000480	2.000480
1.00	2.000540	2.000539

Fig. 3. – Doubling of the external source. The values in the table refer to the power levels at the end of the transient, in the case without delayed neutrons. The macro time-steps and the micro time-steps are uniform.

the presence of precursors and the consequent different time scales, adopting a reduced transient duration. The convergence to the asymptotic solution can be clearly seen.

The study of test transients involving delayed neutron precursors points out a main difference between IQM and PCQM: the presence of delayed neutrons requires to adapt the macro time-step along the evolution of the transient to capture the change of the neutron shape. If an adaptive technique is considered, it can be assumed that, once the spatial transient is extinguished, the following evolution up to equilibrium with the delayed neutron precursors (last Δt) could be well retraced by a PK calculation with the last available kinetic parameters. In IQM this is automatically fulfilled, since the amplitude calculation is performed before the shape update. On the other hand, PCQM requires as a first step the solution of the flux problem, which can lead to significant errors when the last Δt is too large. To overcome this problem, the PCQM should be hybridized with a PK module that performs the calculation along the last Δt.

A second test calculation carried out for the system in fig. 2a is a transient induced by a step-wise fission cross-section perturbation, leaving the reactor in a subcritical state. The same data for precursors as in the previous case are assumed. Since after a transient the system settles on a new steady-state, an asymptotic transport calculation is carried out to determine the *exact* value of the flux and of the power at the end of the transient. It is clear from figs. 4 and 5 that a correct evaluation of the power evolution requires the analysis up to the time when delayed neutrons reach equilibrium. Moreover, a full PK treatment is not sufficient to predict the power level at the end of the transient, while both IQM and PCQM can provide accurate results.

In fig. 6 a test calculation for the system in fig. 2b is presented. For the sake of simplicity, no delayed neutrons are considered, in order to reduce the time interval on which the analysis is carried out. It can be observed that IQM requires a certain number of shape updates to provide a satisfactory power prediction. This is due to the error introduced in the shape recomputation process. On the other hand, PCQM can produce reliable results even considering just one macro time-step, provided it is short enough. Nevertheless, in most calculations, the shape recomputation error introduced in the IQM does not affect dramatically the power prediction, as it is usually of the order of the relative error on the power itself.

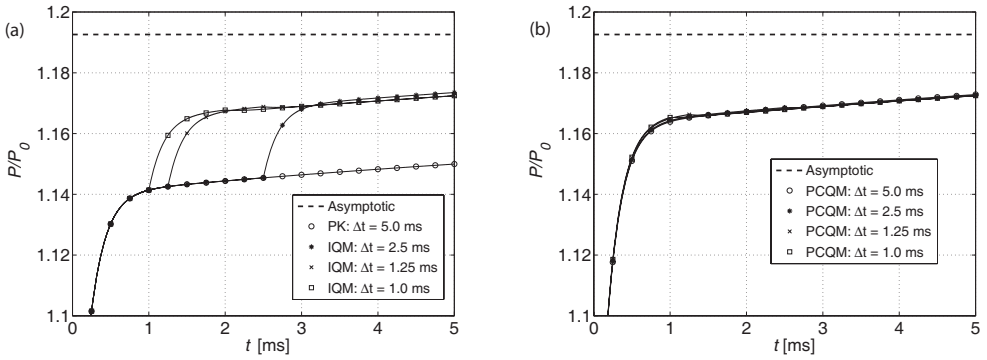


Fig. 4. – Power evolution induced by a uniform fission cross-section perturbation ($\delta\nu\Sigma_f/\nu\Sigma_f = +10\%$). a) Comparison of the power evolution for IQM; b) the same for PCQM. The time interval is subdivided into uniform macro time-steps. The initial multiplication factor is 0.96884. The reactivity insertion is $\Delta\rho = +574\,\mathrm{pcm}$. The graph is zoomed in the region $[0, 5\,\mathrm{ms}]$, to evidence the prompt-jump.

5. – Conclusions

A computational tool that can perform time-dependent neutronic transport calculations using a quasi-static approach is developed. The DRAGON code is used as a transport solver to generate direct and adjoint fluxes, to be used for the calculation of the kinetic parameters introduced into the amplitude model. A coupling module provides the input information for the DRAGON code by suitable modifications of cross-sections and sources as needed, in order to take into account the evolution of neutron and precursor concentrations.

Test calculations show the feasibility of the procedure and the accuracy of the results, both for the classical IQM and for the innovative PCQM. Some considerations are highlighted concerning the possibility to hybridize the two algorithms when dealing with a long transient analysis. The results presented show that both algorithms can reproduce

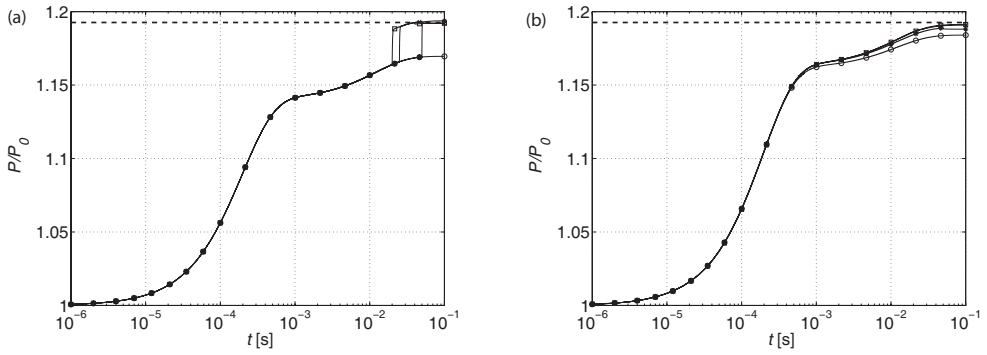


Fig. 5. – Comparison of the power evolution for the whole transient analysis adopting the IQM (a), markers as in fig. 4a. b) The same but adopting the PCQM, markers as in fig. 4b. The time interval is subdivided into uniform macro time-steps, the same for both IQM and PCQM.

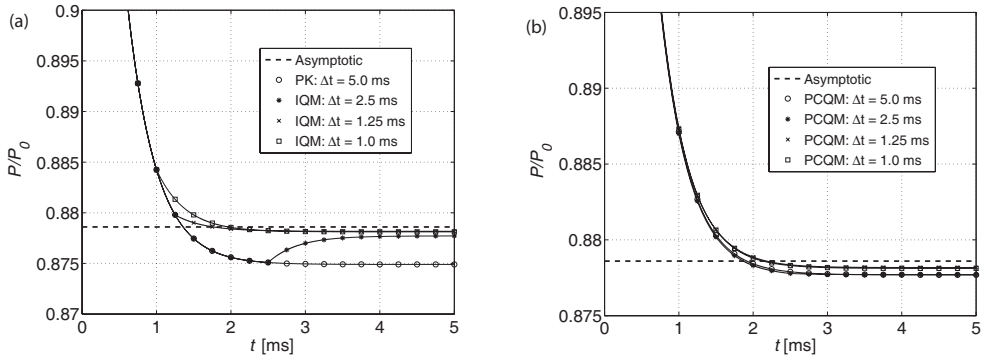


Fig. 6. – Power evolution induced by a uniform capture cross-section perturbation ($\delta\Sigma_c/\Sigma_c = +20\%$). a) Comparison of the power evolution for IQM; b) the same for PCQM. The initial multiplication factor is 0.97240. The reactivity insertion is $\Delta\rho = -371$ pcm. The view is zoomed in the region $[0, 5\,\mathrm{ms}]$, where only the prompt neutron equilibrium is reached.

the power level at the end of the transient rather accurately: it must be reminded that PCQM is computationally more advantageous than IQM.

Further development should be directed towards handling angular distributions for sources and fluxes. This step will lead to a fully consistent computational tool for transport nuclear reactor kinetics.

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