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VARIATIONAL METHODS IN THE KINETIC MODELING OF NUCLEAR REACTORS: RECENT ADVANCES

S. Dulla, P. Picca, P. Ravetto
Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129 Torino - Italy
sandra.dulla@polito.it; paolo.picca@polito.it; piero.ravetto@polito.it

ABSTRACT

The variational approach can be very useful in the study of approximate methods, giving a sound mathematical background to numerical algorithms and computational techniques. The variational approach has been applied to nuclear reactor kinetic equations, to obtain a formulation of standard methods such as point kinetics and quasi-statics. more recently, the multipoint method has also been proposed for the efficient simulation of space-energy transients in nuclear reactors and in source-driven subcritical systems. The method is now founded on a variational basis that allows a consistent definition of integral parameters. The mathematical structure of multipoint and modal methods is also investigated, evidencing merits and shortcomings of both techniques. Some numerical results for simple systems are presented and the errors with respect to reference calculations are reported and discussed.

Key Words: neutron kinetics, variational methods, point models, modal methods

1. INTRODUCTION

The kinetic analysis of nuclear reactors requires the solution of the time-dependent transport equation or some of its approximations coupled with the balance equations for precursors by means of suitable numerical techniques. To obtain accurate results in the simulation of spatial and spectral transients a large computational effort may be needed. Various methods have been developed over the years. The quasi-static method, associated to a point kinetic model for the amplitude function, has proved to be rather efficient in providing good results, although in some cases a large number of expensive shape recomputations may be required [1–4]. Some methods have been proposed to overcome the shortcomings of the point kinetic model used for the computation on the fast scale of the amplitude functions between two shape recalculations. All the alternative methods developed can be given a unifying variational formulation [5].

In more recent times a variational consistent formulation of the multipoint method has been developed [6]. The method can be considered as an effective nodal approach that allows the use of coupled balance equations on few very large macroregions in phase space. Coupling among macroregions is physically due to spatial motion and energy transfer through collisions. Its application to source-driven system evaluations has led to excellent results [7]. Also the possibility of its inclusion in a quasi-static framework has been investigated. In the present work the variational approach will be used to derive possible alternatives in reactor kinetics models. The comparisons among different techniques will evidence potentialities and shortcomings.

2. DESCRIPTION OF THE WORK

A variational formulation of a kinetic model in general transport theory can be obtained by considering a general functional where proper Lagrange multipliers are introduced [6], and the contributions of initial and boundary conditions are also included:

$$\begin{aligned} H[\varphi,\mathscr{E}_i,\varphi^\dagger,\mathscr{E}_i^\dagger,\vartheta,\Gamma,\Lambda] &= G[\varphi] + \int_0^t dt \int d\mathbf{x}\varphi^\dagger \left[-\frac{1}{v}\frac{\partial\varphi}{\partial t} + \left(-\hat{\mathbf{L}}\varphi + \hat{\mathbf{M}}_p\varphi\right) \right. \\ &\left. + \sum_{i=1}^R \mathscr{E}_i + S \right] + \sum_{i=1}^R \int_0^t dt \int d\mathbf{x}\mathscr{E}_i^\dagger \left[\frac{1}{\lambda_i}\frac{\partial\mathscr{E}_i}{\partial t} + \mathscr{E}_i - \hat{\mathbf{M}}_i\varphi \right] \\ &+ \int d\mathbf{x}\Gamma(\mathbf{x})\left[\varphi(\mathbf{x},t=0) - \varphi_0(\mathbf{x})\right] + \sum_{i=1}^R \int d\mathbf{x}\Lambda_i(\mathbf{x})\left[\mathscr{E}_i(\mathbf{x},t=0) - \mathscr{E}_{i,0}(\mathbf{x})\right] \\ &+ \int_0^t dt \int_{\partial V} d\mathscr{A} \int dE \int_{\Omega_{in}} d\Omega\vartheta \left\{ \varphi(\mathbf{r}_s,E,\mathbf{\Omega}_{in},t) \right. \\ &\left. - f(\mathbf{r}_s,E,\mathbf{\Omega}_{in},t) - \left[\hat{\mathbf{R}}\varphi\right](\mathbf{r}_s,E,\mathbf{\Omega}_{in},t) \right\}. \end{aligned} \tag{1}$$

A general number R of families of delayed neutron precursors is here considered.

The operator G appearing in expression (1) represents the *detector*, from which the physical quantity of interest for the analysis is constructed. Its definition plays a crucial role in the development of approximate kinetic models, having an influence on the determination of the weight functions to be adopted. For instance, if the total power production at a certain instant τ is requested, the first term in the r.h.s. of Eq. (1) assumes the form:

$$G[\varphi] = P_{th}(\tau) = \int_V d\mathbf{r} \int dE \oint d\Omega\gamma(\mathbf{r},E)\Sigma_f(\mathbf{r},E,\tau)\varphi(\mathbf{r},E,\mathbf{\Omega},\tau), \tag{2}$$

where γ is the energy release per fission.

On taking the variation of the functional with respect to variations of the functions and of the Lagrange multipliers, one obtains direct and adjoint equations, with associated boundary and initial conditions. Variations of the Lagrange multipliers provides the initial balance kinetic equations and variations of the neutron flux and precursors allows to obtain balance equations for the multipliers, which constitute the corresponding adjoint time-dependent model:

$$\begin{cases} -\dfrac{1}{v}\dfrac{\partial\varphi^\dagger(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} = \left[-\hat{\mathbf{L}}^\dagger(t)\varphi^\dagger + \hat{\mathbf{M}}_p^\dagger(t)\varphi^\dagger\right](\mathbf{r},E,\mathbf{\Omega},t) \\ \qquad\qquad + \displaystyle\sum_{i=1}^R \left[\hat{\mathbf{M}}_i^\dagger\mathscr{E}_i^\dagger\right](\mathbf{r},E,t) + Q^\dagger(\mathbf{r},E,\mathbf{\Omega},t) \\ -\dfrac{1}{\lambda_i}\dfrac{\partial\mathscr{E}_i^\dagger(\mathbf{r},E,t)}{\partial t} = -\mathscr{E}_i^\dagger(\mathbf{r},E,t) + \dfrac{1}{4\pi}\displaystyle\oint d\Omega\varphi^\dagger(\mathbf{r},E,\mathbf{\Omega},t), \qquad i=1,...,R, \end{cases} \tag{3}$$

where the adjoint source $Q^\dagger$ is strictly connected to the definition of the operator G [6] and the adjoint solution may be physically interpreted as proper neutron importance.

Starting from this general variational formulation of the problem, approximate models can be obtained consistently by introducing additional hypotheses on the behaviour of the physical quantities and corresponding importances. A well-known approach is based on the assumption of trial (time)-(phase-space) factorized expressions for all unknowns, neutron flux and delayed neutron emissivities as well as corresponding adjoints:

$$\begin{aligned}
\varphi(\mathbf{x},t) &= \sum_{j=1}^{J} \left(N_j(t)u_j(\mathbf{x})\right) \phi(\mathbf{x};t) = \sum_{j=1}^{J} N_j(t)\phi_j(\mathbf{x};t),\\
\mathscr{E}_i(\mathbf{x},t) &= \sum_{j=1}^{J} \left(E_{i,j}(t)u_j(\mathbf{x})\right) \epsilon_i(\mathbf{x};t) = \sum_{j=1}^{J} E_{i,j}(t)\epsilon_{i,j}(\mathbf{x};t),\\
\varphi^\dagger(\mathbf{x},t) &= \sum_{j=1}^{J} \left(N_j^\dagger(t)u_j(\mathbf{x})\right) \phi^\dagger(\mathbf{x};t) = \sum_{j=1}^{J} N_j^\dagger(t)\phi_j^\dagger(\mathbf{x};t),\\
\mathscr{E}_i^\dagger(\mathbf{x},t) &= \sum_{j=1}^{J} \left(E_{i,j}^\dagger(t)u_j(\mathbf{x})\right) \epsilon_i^\dagger(\mathbf{x};t) = \sum_{j=1}^{J} E_{i,j}^\dagger(t)\epsilon_{i,j}^\dagger(\mathbf{x};t).
\end{aligned} \tag{4}$$

This approach allows to reconstruct various well-assessed kinetic models, such as point kinetics [5] and quasi-statics [8, 9], if the sums appearing in expressions (4) are reduced to a single term and introducing phase-space trial functions consistently with the model under investigation (e.g., time-independent for point kinetics).

More in general, starting again from Eqs. (4) and plugging equations (4) into the functional H, it is possible to obtain balance equations of all the different functions by setting all variations to zero. Specifically, when variations with respect to the time functions $N_j^\dagger$ are considered, first-order kinetic equations are obtained, that can be recast into matrix form as:

$$\frac{d}{dt}\left|X\right\rangle = \hat{M}\left|X\right\rangle + \left|S\right\rangle, \tag{5}$$

where the unknown and source vectors, respectively, are:

$$\begin{aligned}
\left|X\right\rangle^t &= \left|N_1, N_2, ..., N_K, E_{1,1}, ..., E_{1,K}, E_{2,1}, ..., E_{R,K}\right\rangle^t\\
\left|S\right\rangle^t &= \left|\tilde{S}_1, \tilde{S}_2, ..., \tilde{S}_K, 0, ..., 0\right\rangle^t,
\end{aligned} \tag{6}$$

having assumed J trial functions.

The general structure here devised is suitable to be adapted for the derivation of multipoint kinetic model if the phase-space trial functions are defined each on a specific subdomain Γ_j, or, in other terms, the function u_j appearing in Eq. (4) is defined as:

$$u_j(\mathbf{x}) = \begin{cases} 1 & \text{on } \Gamma_j \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

Starting from this subdivision of the system in few subdomains, various multipoint formulations can be obtained, each one differing from the others according to the assumption made on the factorization adopted for the adjoint and thus on the definition of the proper functional [6]. In

particular, when dealing with subcritical source-driven systems it is possible to define a multifunctional multipoint model (MPK-2), based on the assumption of several adjoint functions, as many as the subdomains defined. The different adjoints are obtained operating on G and thus on the adjoint source of the steady-state adjoint problem to be solved. A similar approach is not feasible for systems departing from a critical state, where a single-functional multipoint model (MPK-1) is adopted. The coupling characteristics of the two multipoint approaches are rather different and lead to significantly different results for subcritical systems, as will be shown in the following section.

On the other hand, the phase-space shapes ϕ_j appearing in Eq. (4) can be selected as time-constant functions suitable to describe the expected behaviour of the neutron population. A classic choice refers to the modes associated to the reference reactor, preliminarily determined by the solution of an eigenvalue problem. In such a case a modal method is obtained. The variational formulation of the modal approach follows the same steps as the previous procedure, outlined above, leading to the definition of a balance equation for the adjoint in the form of (3). When a time-independent adjoint is considered, the problem reduces to the evaluation of the solution of the adjoint eigenvalue problem, to be used for the projection step.

The modal and nodal approaches, when taken in their lower order (i.e., one mode or one node), lead to standard point kinetic models for an initially critical system, obviously allowing different interpretations, evidencing different physical characteristics of the point assumption. When dealing with subcritical systems, in which the initial reference configuration is source-driven, the multipoint approach reduces to the corresponding point kinetics if a single region is considered, while the nodal approach still refers to the critical, source-free configuration for the definition of the evolution modes. This difference may play an important role in the accuracy of the time-dependent prediction of such methods and they may also turn out to serve as alternative tools for the interpretation of experiments [10].

3. RESULTS

Numerical results in various configurations are here presented, to show the different features of the kinetic models, together with the advantages or shortcomings for some specific physical situations. Multipoint and modal approaches are assessed and compared to point kinetics and to *reference* results, obtained by the inversion of the full balance model.

As a first step, one dimensional diffusion calculations in one energy group are performed. The objective is to study how multipoint and modal approaches can deal with spatial transients for both critical and subcritical systems. One family of delayed neutron precursors is now assumed. The relatively simple configuration allows to compare easily approximate models results with reference calculations, being the mathematical problem self-adjoint.

An initially critical system is perturbed by a localized asymmetrical decrease of the absorption cross section, amounting to a change of the effective multiplication constant of 1257 pcm. A single-functional multipoint option (MPK-1) is employed, with two different subdivision of the geometrical space into two portions: an optimized one, trying to separate and evidence the perturbed region (case a) and a more crude and less efficient option. The perturbation localization and the domain subdivisions are sketched in Fig. 1. To have the same number of degrees of

Table I. Percentage error on the system power at various time instants for a transient in a critical system.

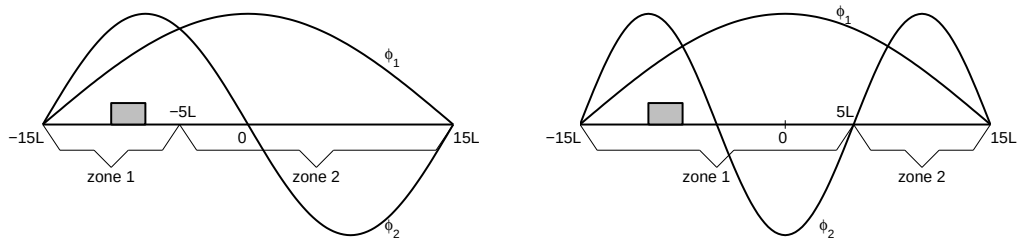
time [ms]	modal (case c)	modal (case d)	MPK-1 (case a)	MPK-1 (case b)	PK
0.5	−0.14	−0.14	−0.13	−0.15	−0.14
1	−0.24	−0.24	−0.23	−0.25	−0.25
10	−0.60	−0.64	−0.92	−0.96	−0.95
50	−1.58	−1.80	−3.42	−3.53	−3.53
100	−2.65	−3.07	−6.28	−6.44	−6.46
500	−11.00	−12.91	−26.53	−27.13	−27.17
1000	−21.35	−24.89	−47.51	−48.41	−48.47

freedom, two modes are considered for the modal method, namely the fundamental spatial eigenfunction of the Helmholtz operator plus the second (odd - case c) or third (even - case d) higher harmonics, to study the effectiveness of the use of different modes. The spatial behavior of the modes is again represented in Fig. 1. In Table I the percentage relative error on the total power is reported at various instants with respect to a *reference* highly accurate numerical solution. As one can see, the modal approach yields better results at all time, and little is gained by multipoint with respect to standard point kinetics (PK). In addition, the importance of an appropriate choice of the evolution modes and of the space subdivision can play a role in the accuracy of the results obtained. This effect can be of large importance, as it is shown in the following exercises concerning a subcritical case.

Table II. Comparison of matrices $\hat{M}$ adopting the single- and multi-functional option for MPK. Values are renormalized to the highest absolute element in the matrix.

MPK-1				MPK-2			
-0.98	1.0	$4 \cdot 10^{-5}$	0	-0.66	1.0	$1 \cdot 10^{-3}$	$-2 \cdot 10^{-4}$
0.17	-0.20	0	$6 \cdot 10^{-6}$	0.09	-0.62	$-1 \cdot 10^{-4}$	$1 \cdot 10^{-4}$
$8 \cdot 10^{-4}$	0	$-6 \cdot 10^{-6}$	0	$7 \cdot 10^{-3}$	0.01	$-1 \cdot 10^{-4}$	0
0	$5 \cdot 10^{-3}$	0	$-6 \cdot 10^{-6}$	$6 \cdot 10^{-3}$	0.06	0	$-1 \cdot 10^{-4}$

As a second exercise, a subcritical configuration is considered, having the same geometrical characteristics as the critical system previously considered. The external source is symmetrically



(a) MPK-1 (case a) and modal (case c).

(b) MPK-1 (case b) and modal (case d).

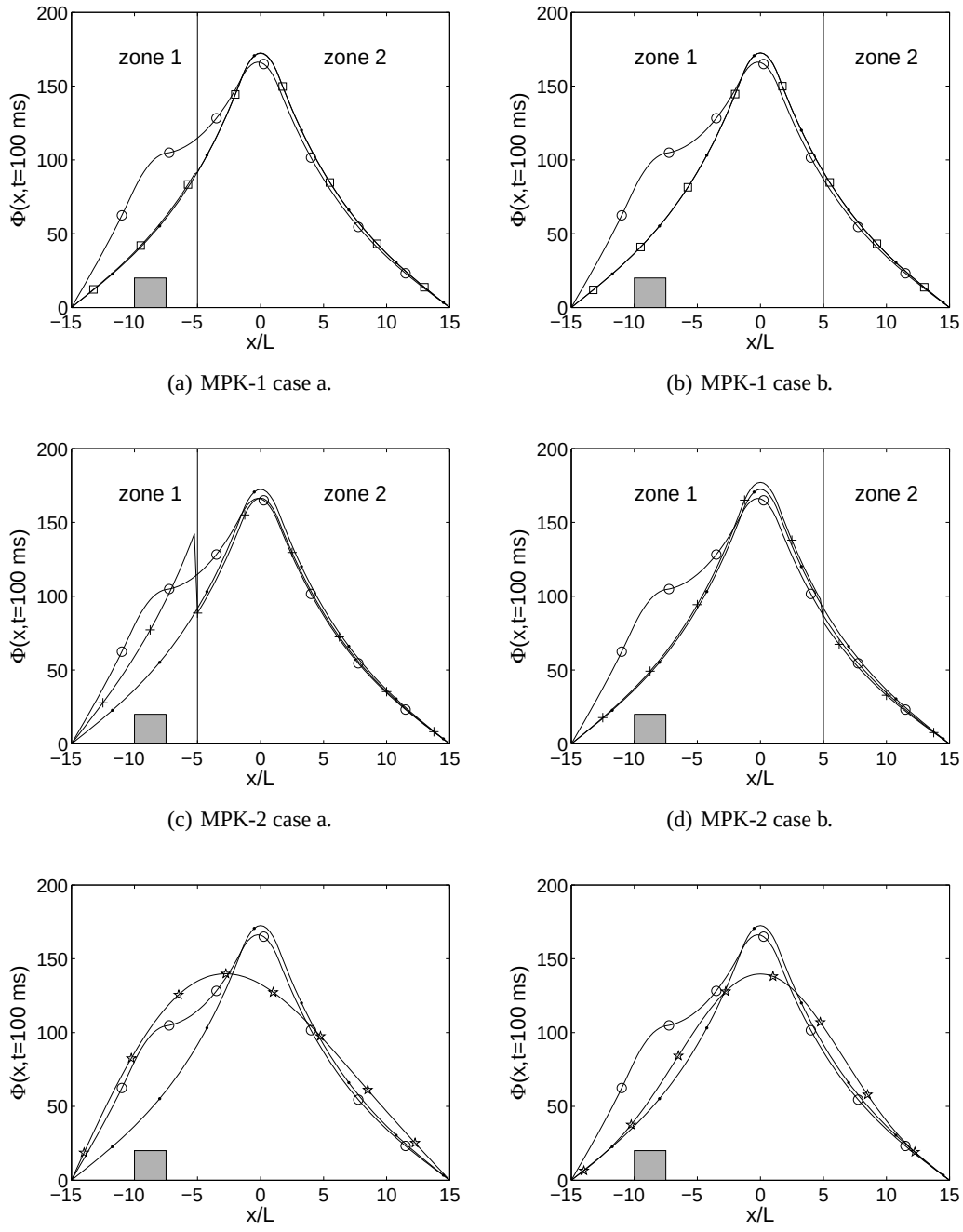
Figure 1. Configuration of critical system with a localized perturbation in absorption (shaded in grey). The characteristics of the two different options for multipoint and modal calculations are presented.

located in the center of the system and spans over a 12-cm interval. The initial value of k_{eff} is 0.97. The localized perturbation of the absorption introduces a 1311 pcm reactivity. As pointed out in the previous section, for subcritical systems it is possible to give a multi-functional formulation of the multipoint method (MPK-2), which proves to be more effective since a better coupling of the macroregions is produced. The role of the coupling can be clearly seen observing the matrices characterizing the time-system of kinetic equations. Also in this case two spatial point are considered and only one family of delayed neutron precursors, leading to a 4-by-4 matrix (two points for neutrons and two points for precursors). The comparison is given in Table II for the space subdivision corresponding to case a: obviously, the off-diagonal terms are responsible for the coupling among the points.

The power evolution produced by the different multipoint and modal approaches are summarized in Table III, where percentage errors with respect to reference results are reported. The difference in the performances of the two multipoint options is rather relevant, leading to the obvious choice of the adoption of the multi-functional version (MPK-2). Comparing these results with the ones obtained with the modal approach, both methods prove to yield significantly better results with respect to point kinetics, if the choice of the space subdivision and the definition of the evolution modes is made on a physically significant basis (case a and c). The importance of this aspect is well evidenced by the comparison with less efficient choices (case b and d), where the power prediction obtained are very close to point kinetics results. The reconstructed space distribution for the various cases described are given in Figure 2.

4. CONCLUSIONS

The present work assesses the performance of different kinetic approaches that can be derived by a unifying procedure based on a variational principle, formulated for the time-dependent neutron and delayed precursor concentrations equations. Besides standard methods such as point kinetics



(a) MPK-1 case a.

(b) MPK-1 case b.

(c) MPK-2 case a.

(d) MPK-2 case b.

(e) modal case c.

(f) modal case d.

Figure 2. Flux distributions at $t = 100$ ms obtained with different kinetic approaches. Grey area identifies perturbed region; vertical line indicates separation between macroregions. Reference ($\circ$); modal ($\star$); MPK-1 ($\square$); MPK-2 ($+$); PK ($\bullet$).

Table III. Percentage error on the system power at various time instants for a transient in a subcritical system.

time [ms]	modal (case c)	modal (case d)	MPK-1 (case a)	MPK-1 (case b)	MPK-2 (case a)	MPK-2 (case b)	PK
0.1	0.03	−0.26	−0.11	−0.19	−0.02	−0.24	−0.18
0.5	−0.004	−1.40	−0.97	−1.08	−0.28	−1.27	−1.07
1	−0.10	−2.70	−2.10	−2.23	−0.64	−2.44	−2.22
5	−1.12	−8.86	−8.09	−8.33	−2.79	−8.18	−8.33
100	−2.69	−12.11	−11.45	−11.72	−4.51	−11.48	−11.73

and quasi-statics, modal and nodal approaches can be based on a variational formulation. In this work, a particular attention is given to the multipoint method and its parenthood with the modal approach is investigated. While the variational technique allows a consistent and unambiguous definition of the integral kinetic parameters, the problem of the optimization of the multipoint phase-domain subdivision is yet unresolved and may constitute the objective of a further work. Numerical results are presented for both critical and subcritical source-driven systems, discussing merits and shortcoming of the methods presented.

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