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Nuclear reactor dynamics - II & III

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### Nuclear reactor dynamics

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### PARTII

Because real life is harder...

- Need of numerical methods
- Factorization approach
- Improvements

## Solution of the transport problem for realistic configurations

The usual "engineering" procedure for too complicated deterministic physicomathematical problems:

- 1. Approximate the model (physics is distorted), e.g. transport  $\rightarrow$  diffusion
- 2. Solve equations of approximate model by algorithms (numerically induced effects are introduced ... discretizations, truncations ... further distortions of physics)

#### Basics of reactor calculations

Split the full problem (too complicate) into a succession of problems trying to separate specific aspects and treat them separately (multi-scale) Well-known technique in engineering

### Basics of reactor calculations: dynamics

Handle numerical stiffness (very important for fast structures)

Reduce the complication of the full problem

# Challenges in the simulation of neutron dynamics

• The Boltzmann equation is a very challenging problem

Example: 3D calculation of a nuclear reactor

- Space: ~  $(10^2)^3 = 10^6$  meshes
- Angle: ~  $10^2$  directions (S<sub>8</sub> in 3D)
- Energy: ~  $10^1 10^2$  groups
- $\rightarrow$  ~ 10<sup>9</sup> 10<sup>10</sup> unknowns for a steady-state calculation
- Time: ∆t ~ 10<sup>-6</sup> s
- $\rightarrow$  ~ 10^6 pseudo-stationary calculation per second in time-dependent evaluation

It yields too much physical detail

In real systems only integral quantities can be observed

## Challenges in the simulation of neutron dynamics

- Need to construct simplified models (multigroup, diffusion...) based on physical assumptions
- Need of numerical algorithms (discretizations, expansions)

Development of approximate models and algorithms

**important**: establish adequateness of approximations for the problem considered (benchmarks) Models and methods for neutron dynamics

- Point kinetics
  - Derivation of the model and physical interpretation
- Quasi-static method
  - Improved quasi-statics (originally developed for fast reactors)
  - Predictor-Corrector quasi-statics
- Multipoint kinetics
  - Features of MPK approach

the neutron distribution is factorized in an amplitude (timedependent) and a shape (time independent)

$$n(r,E,\Omega,t) = P(t)\varphi(r,E,\Omega;\mathbf{X})$$

#### Critical systems

Shape: fundamental eigenfunction of the model

$$\left(\hat{\mathbf{L}}_0 + \frac{1}{k}\hat{\mathbf{M}}_0\right)\varphi = 0$$

Subritical systems

Shape: steady-state solution, dominated by the source

$$\left( \hat{\mathbf{L}}_0 + \hat{\mathbf{M}}_0 \right) \varphi + S_0 = 0$$

The factorized form is introduced into the balance equations

$$\begin{cases} P\hat{\partial}\varphi + \varphi \frac{dP}{dt} = P\hat{B}\varphi + \sum_{i=1}^{6} \lambda_i \left(\frac{\chi_i}{4\pi}C_i\right) + S\\ \frac{\partial(\chi_i C_i/4\pi)}{\partial t} = P\hat{M}_i\varphi - \lambda_i \left(\frac{\chi_i}{4\pi}C_i\right) \end{cases}$$

and is projected on a weighting function w:

$$\begin{cases} \langle w \mid \varphi \rangle \frac{dP}{dt} = \left\langle w \mid \hat{\mathbf{B}}\varphi \right\rangle P + \sum_{i=1}^{6} \lambda_{i} \left\langle w \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle + \left\langle w \mid S \right\rangle \\ \left\langle w \mid \frac{\partial \left(\chi_{i}C_{i}/4\pi\right)}{\partial t} \right\rangle = \left\langle w \mid \hat{\mathbf{M}}_{i}\varphi \right\rangle P - \lambda_{i} \left\langle w \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle \end{cases}$$

Weight w  $\rightarrow$  solution of the adjoint steady-state problem

The procedure is standard for critical reactors, while for subcritical source-driven systems the question on the adjoint source arises

definition can be given on the basis of

physical consideration

and

variational principles

Integral quantities are evaluated and the differential equations for the amplitudes are derived:

$$\begin{cases} \left\langle N_{i} \right\} & \frac{dP(t)}{dt} = \frac{\rho(t) - \tilde{\beta}}{\Lambda} P(t) + \sum_{i=1}^{6} \lambda_{i} \tilde{C}_{i}(t) + \tilde{S} \right) \right\rangle + \left\langle N_{0}^{\dagger} | S \right\rangle \\ \left\langle N \right\} & \frac{dC_{i}(t)}{dt} = \frac{\tilde{\beta}}{\Lambda} P(t) - \lambda_{i} \tilde{C}_{i}(t) & \frac{\chi_{i}}{4\pi} C_{i} \right\rangle \end{cases}$$

having introduced the definition of the kinetic parameters

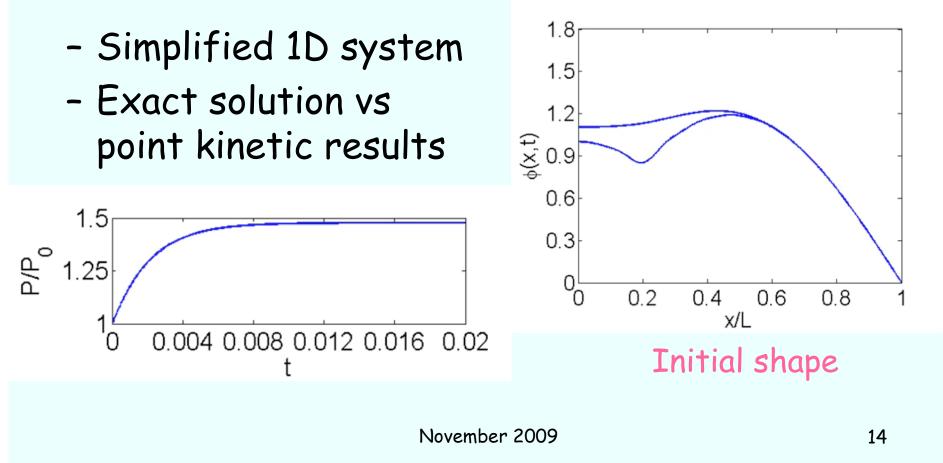
$$\rho(t) = \frac{\left\langle N_{0}^{+} \right| \delta \hat{\mathbf{K}} \varphi \right\rangle}{\left\langle N_{0}^{+} \right| \hat{\mathbf{M}} \varphi \right\rangle} \qquad \tilde{\beta}_{i} = \frac{\left\langle N_{0}^{+} \right| \hat{\mathbf{M}}_{i} \varphi \right\rangle}{\left\langle N_{0}^{+} \right| \hat{\mathbf{M}} \varphi \right\rangle} \qquad \Lambda = \frac{\left\langle N_{0}^{+} \right| \varphi \rangle}{\left\langle N_{0}^{+} \right| \hat{\mathbf{M}} \varphi \right\rangle}$$

- Characteristics of the point kinetic approximation:
  - no space distortion during the transient
  - the evolution is space-time separable
  - any point is representative of the whole system

The approximation is poor when localized phenomena (e.g. control rod insertion) are concerned

### Point kinetics - results

 Transient following extraction of a control device in a critical system



 Results produced with point kinetics underestimate real power evolution

not reliable for safety assessment

- Spatial/spectral effects are neglected
- Need for a more sophisticated method, able to take into account these effects...

Quasi-static method

### A digression on perturbation theory

Is there any connection between reactivity (the driving force of the transient) and the change induced to the multiplication eigenvalue of the system by the perturbation ? A digression on perturbation theory Original eigenvalue problem (quite general)

$$\mathcal{L}\varphi = \omega \mathcal{M}\varphi$$

Perturbed problem

$$\left(\mathcal{L} + \delta \mathcal{L}\right)\left(\varphi + \delta\varphi\right) = \left(\omega + \delta\omega\right)\left(\mathcal{M} + \delta\mathcal{M}\right)\left(\varphi + \delta\varphi\right)$$

A digression on perturbation theory Expanding:

$$\begin{aligned} (\mathcal{L}\varphi) + \delta \mathcal{L}\varphi + [\mathcal{L}\delta\varphi] \\ &= (\omega \mathcal{M}\varphi) + [\omega \mathcal{M}\delta\varphi] + \omega \delta \mathcal{M}\varphi + \delta \omega \mathcal{M}\varphi \end{aligned}$$

Question: is it possible to evaluate  $\delta \omega$ Without evaluating  $\delta \varphi$  ? Adjoint - neutron importance Solve auxiliary problem:

$$\mathcal{L}^+ \varphi^+ = \omega \mathcal{M}^+ \varphi^+$$

Project perturbed equation on ajoint, retain only first-order terms and notice that contributions of terms involving flux perturbations vanish:

$$(\varphi^+, \mathcal{L}\delta\varphi) - (\varphi^+, \omega\mathcal{M}\delta\varphi) = (\mathcal{L}^+\varphi^+, \delta\varphi) - (\omega\mathcal{M}^+\varphi^+, \delta\varphi) (\mathcal{L}^+\varphi^+ - \omega\mathcal{M}^+\varphi^+, \delta\varphi) = 0,$$

### Reactivity

## Explicit expression for perturbation of eigenvalue:

$$\delta \omega = \frac{(\varphi^+, \delta \mathcal{L} \varphi) - \omega \left(\varphi^+, \delta \mathcal{M} \delta \varphi\right)}{(\varphi^+, \mathcal{M} \varphi)}$$

$$\delta\omega = \delta\left(\frac{1}{k}\right) = -\frac{1}{k}\frac{\delta k}{k} = -\frac{1}{k}\rho$$

### Conclusions...

- Reactivity introduced by point kinetics has a perturbative meaning
- Perturbation methods are very powerful and very useful in sensitivity analyses
- In fast reactor physics, beside kinetics, PM may be used for: Evaluation of control rod worth Evaluation of nuclide evolution Evaluation of self and mutual shielding of control system

### A further question

Can perturbation analysis be applied to other integral quantities, rather than eigenvalues ?

Consider the problem:

$$\mathcal{B}\varphi = S$$

$$I=(\mathfrak{D},\varphi)$$

### Generalized perturbation theory Perturbed problem:

$$(\mathcal{B} + \delta \mathcal{B}) (\varphi + \delta \varphi) = S + \delta S$$
$$\mathcal{B}\varphi + \delta \mathcal{B}\varphi + \mathcal{B}\delta \varphi = S + \delta S$$

Generalized perturbation theory What is the "best" adjoint problem for the projection?

$$\mathcal{B}^+ \varphi^+ = \mathfrak{D}$$

The perturbation is obtained as:

$$\delta I = (\varphi^+, \delta S) - (\varphi^+, \delta \mathcal{B}\varphi)$$

### Quasi-statics

The factorization procedure is generalized as:

 $n(r,E,\Omega,t) = \underbrace{P(t)\varphi(r,E,\Omega;t)}_{\text{introduced}} \underset{\text{introduced}}{\text{No approximation}}$ 

Amplitude: fast Shape: slowing evolving phenomena evolving phenomena

inserted into the t-d model and projected on a weight

$$\begin{pmatrix}
\left\langle w \mid \frac{\partial \varphi}{\partial t} \right\rangle P + \left\langle w \mid \varphi \right\rangle \frac{dP}{dt} = \left\langle w \mid \hat{\mathbf{B}}\varphi \right\rangle P + \sum_{i=1}^{6} \lambda_{i} \left\langle w \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle + \left\langle w \mid S \right\rangle \\
\left\langle w \mid \frac{\partial \left(\chi_{i}C_{i}/4\pi\right)}{\partial t} \right\rangle = \left\langle w \mid \hat{\mathbf{M}}_{i}\varphi \right\rangle P - \lambda_{i} \left\langle w \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle$$

### Quasi-statics

 Again, the weight is the solution of the adjoint model:

$$\begin{cases} \frac{d}{dt} \left\langle N_{0}^{\dagger} \mid \varphi \right\rangle P + \left\langle N_{0}^{\dagger} \mid \varphi \right\rangle \frac{dP}{dt} = \left\langle N_{0}^{\dagger} \mid \hat{\mathbf{B}}\varphi \right\rangle P + \sum_{i=1}^{6} \lambda_{i} \left\langle N_{0}^{\dagger} \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right)\right\rangle + \left\langle N_{0}^{\dagger} \mid S \right\rangle \\ \left\langle N_{0}^{\dagger} \mid \frac{\partial \left(\chi_{i}C_{i}/4\pi\right)}{\partial t}\right\rangle = \left\langle N_{0}^{\dagger} \mid \hat{\mathbf{M}}_{i}\varphi \right\rangle P - \lambda_{i} \left\langle N_{0}^{\dagger} \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right)\right\rangle \end{cases}$$

and a normalization condition is introduced to make the factorization unique

$$\frac{d}{dt}\left\langle N_{0}^{\dagger}\mid\varphi\right\rangle =0$$

### Quasi-statics

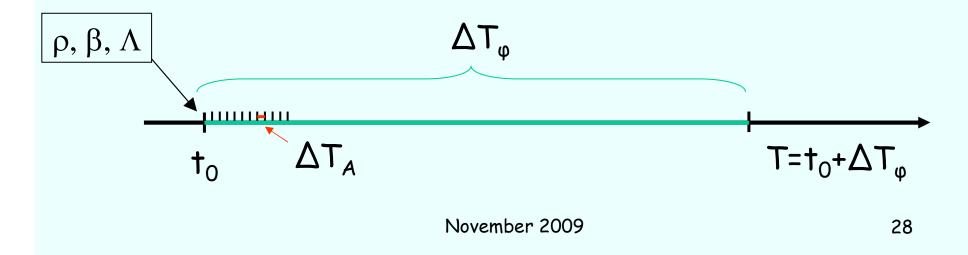
 The final form of the equation for the apmlitude is the well-known point model:

$$\begin{cases} \frac{dP(t)}{dt} = \frac{\rho(t) - \tilde{\beta}}{\Lambda} P(t) + \sum_{i=1}^{6} \lambda_i \tilde{C}_i(t) + \tilde{S} \\ \frac{dC_i(t)}{dt} = \frac{\tilde{\beta}}{\Lambda} P(t) - \lambda_i \tilde{C}_i(t) \end{cases}$$

but the kinetic parameters depend on the shape function, which is the other unknown of the problem



- The solution is obtained on a two-scale frame:
  - Evaluation of the kinetic parameters with the shape at time  $t_0$  (if  $t_0=0$ , the initial shape is used)
  - Solution of the point model on time interval  $[t_0,T]$  with a fine time mesh  $\Delta T_{\rm A}$
  - Solution of the shape model (computationally expensive) on  $\Delta T_{o}$ = T-t<sub>0</sub> to update shape function



- Characteristics of the algorithm:
  - The model is non linear

$$\begin{cases} \left\langle N_{0}^{\dagger} \mid \varphi \right\rangle \frac{dP}{dt} = \left\langle N_{0}^{\dagger} \mid \mathbf{B}\varphi \right\rangle P + \sum_{i=1}^{6} \lambda_{i} \left\langle N_{0}^{\dagger} \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle + \left\langle N_{0}^{\dagger} \mid S \right\rangle \\ \left\langle N_{0}^{\dagger} \mid \frac{\partial \left(\chi_{i}C_{i}/4\pi\right)}{\partial t} \right\rangle = \left\langle N_{0}^{\dagger} \mid \mathbf{\hat{M}}_{i}\varphi \right\rangle P - \lambda_{i} \left\langle N_{0}^{\dagger} \mid \left(\frac{\chi_{i}}{4\pi}C_{i}\right) \right\rangle \end{cases}$$

- The normalization condition needs to be fulfilled

### Iterations on the solution of the shape model are performed

- Iterative procedure for the shape update (1)
  - Solution of the shape model with known P and dP/dt:

$$\frac{\varphi^{(n+1)} - \varphi^{(n)}}{\Delta T_{\varphi}} P(T) + \varphi^{(n+1)} \left. \frac{dP}{dt} \right|_{T} = \mathbf{\hat{B}} \varphi^{(n+1)} P(T) + \sum_{i=1}^{6} \lambda_{i} \left( \frac{\chi_{i}}{4\pi} C_{i}^{(n+1)} \right) + S^{(n+1)} \\ \frac{\left( \chi_{i} C_{i}^{(n+1)} / 4\pi \right) - \left( \chi_{i} C_{i}^{(n)} / 4\pi \right)}{\Delta T_{\varphi}} = \mathbf{\hat{M}}_{i} \varphi^{(n+1)} P(T) - \lambda_{i} \left( \frac{\chi_{i}}{4\pi} C_{i}^{(n+1)} \right)$$

- Renormalization of the shape

$$\tilde{\varphi}^{(n+1)} = \frac{\left\langle N_0^{\dagger} \mid \varphi_0 \right\rangle}{\left\langle N_0^{\dagger} \mid \varphi^{(n+1)} \right\rangle} \varphi^{(n+1)} \xrightarrow{\qquad \qquad \text{Check on} \\ \text{error on} \\ \text{shape} }$$

- Iterative procedure for the shape update (2)
  - Computation of kinetic parameters with  $ilde{arphi}^{(n+1)}$
  - Modification of P (continuity of total power)

$$\left\langle \hat{\mathbf{M}}^{(n+1)} \tilde{\varphi}^{(n+1)} \right\rangle P^{(n+1)} = \left\langle \hat{\mathbf{M}}^{(n)} \varphi^{(n)} \right\rangle P^{(n)}$$

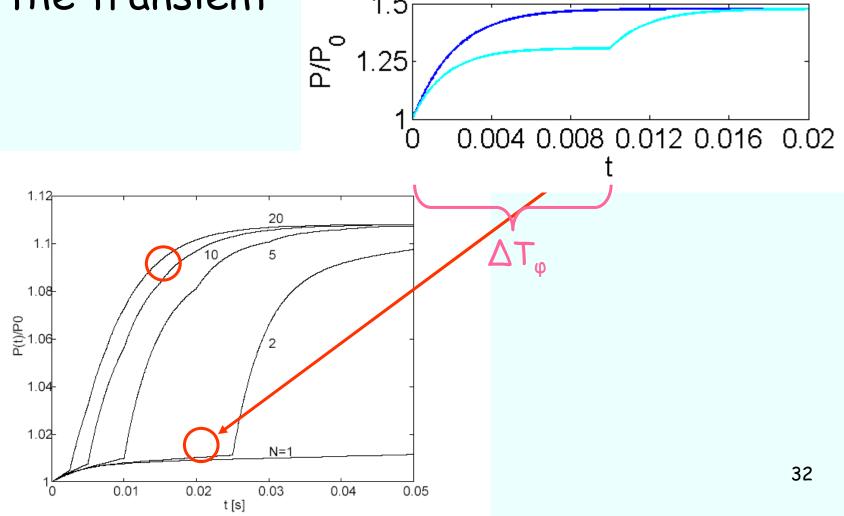
 Modification of dP/dt (fulfillment of point model with updated kinetic parameters)

$$\left( \begin{array}{c} \frac{dP}{dt} \\ \frac{dP}{dt} \\ \frac{dC_i}{dt} \\ \end{array} \right)^{(n+1)} = \frac{\rho^{(n+1)} - \tilde{\beta}^{(n+1)}}{\Lambda} P^{(n+1)} + \sum_{i=1}^{6} \lambda_i \tilde{C}_i + \tilde{S} \\ \frac{dC_i}{dt} \\ \frac{dC_i}{dt} \\ \end{array} \right)^{(n+1)} = \frac{\tilde{\beta}^{(n+1)}}{\Lambda} P^{(n+1)} - \lambda_i \tilde{C}_i$$

- Substitution into the shape model and...

### Improved quasi-statics - Results

• Improvement of the dynamic simulation of the transient 1.5



- Characteristics of the method:
  - Spatial and spectral effects can be taken into account
- $\bigcirc$  Solution converges to reference when  $\Delta T_{\phi}$  is reduced
- The method <u>can</u> allow to obtain high quality results with reduced computational time

#### BUT

- O The definition of the interval  $\Delta T_{\phi}$  largely influences the quality of the results (need of adaptive procedure)
- The convergence of the shape is not always ensured
- The iterative procedure of the shape update can be time consuming when large modifications of the shape are involved
- The procedure can become too expensive computationally

Needs for alternative numerical schemes to avoid the non-linearity of the problem

Predictor-corrector quasi-statics

### Predictor-Corrector quasi-statics

- Scheme for the solution of the quasi-static equation, avoiding the non linearity of the model
  - Solution of the balance model on the time mesh  $\Delta T \phi$

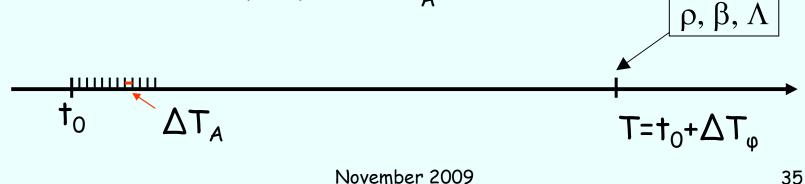
$$\begin{cases} \frac{\partial n}{\partial t} = \hat{\mathbf{B}}n + \sum_{i=1}^{6} \lambda_i \frac{\chi_i}{4\pi} C_i + S \\ \frac{\partial (\chi_i C_i / 4\pi)}{\partial t} = \hat{\mathbf{M}}_i n - \lambda_i \frac{\chi_i}{4\pi} C_i \\ \Delta T_{\varphi} \\ \uparrow_0 \\ T = \dagger_0 + \Delta T_{\varphi} \end{cases}$$

### Predictor-Corrector quasi-statics

- Scheme for the solution of the quasi-static equation, avoiding the non linearity of the model (2)
  - Renormalization if the flux in order to obtain a proper shape function  $\langle N_{0}^{\dagger} | \omega_{0} \rangle$

$$\varphi^{(n+1)} = \frac{\left\langle N_0^{\dagger} \mid \varphi_0 \right\rangle}{\left\langle N_0^{\dagger} \mid n^{(n+1)} \right\rangle} n^{(n+1)}$$

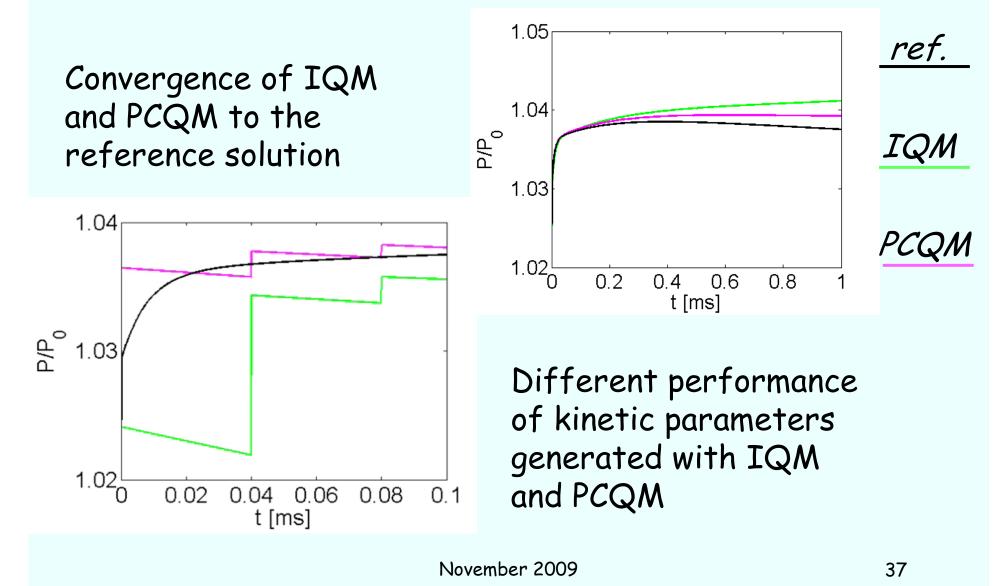
- Evaluation of kinetic parameters and point kinetic solution with time mesh  $\Delta T_A$ 



#### Predictor-Corrector quasi-statics

- Characteristics of PC quasi-statics
- Output is a set of the set of
- Kinetic parameters used for point-kinetic calculations are more suitable to describe the transient during ΔTφ and can provide more accurate results
- The computational effort can be effectively reduced with respect to IQM
- When transients with large power effects and small shape modifications are involved, PCQM can fail in reducing computational time (point-like transients)

# P-C quasi-statics - Results

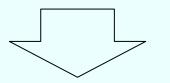


# Further improvements

- The factorization procedure can be improved, subdividing the domain in several regions of the phase space
- This approach can be very effective when loosely coupled systems are concerned

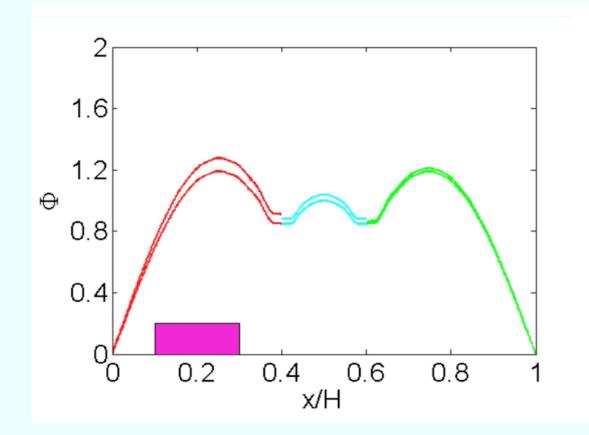
Multipoint method

- The method can be viewed as an extension of the point kinetic model
- The domain considered in the phase space is subdivided in K (reasonably small) regions (points)
- The neutron density in each region is factorized in a product of amplitude and shape



• K point-like systems for the amplitudes  $P_K$  are obtained, all coupled by integral coefficients obtained by the projection technique

• Example of the multipoint phylosophy



Initial neutron density

Localized perturbation

Different regions are affected differently by the perturbation...

... and are simulated with different amplitude functions

Balance equations in discretized form and phase-space subdivision:

$$\begin{cases} \frac{1}{v_m} \frac{d\phi_{nm}}{dt} = \sum_{n'} \sum_{m'} k_{nm,n'm'} \phi_{n'm'} + \\ \sum_{i=1}^{6} \lambda_i \chi_{i,m} C_{i,n} + S_{nm} \\ \frac{dC_{i,n}}{dt} = \beta_i \sum_{m'} f_{nm'} \phi_{nm'} - \lambda_i C_{i,n} \quad i = 1, 2, ..., 6 \end{cases}$$

$$\phi_{nm}(t) = \phi(\mathbf{r}_n, V_m, t) \qquad C_{i,n}(t) = C_i(\mathbf{r}_n, t)$$
  
$$\phi_{nm}(t) = A_{NM}(t)\varphi_{nm}(t) \qquad \mathbf{r}_n, V_m \in \Gamma_{NM}$$

Regionwise inner products  $\langle w | g \rangle = \left| \sum_{n} \sum_{m} \right|_{NM} w_{nm} g_{nm}$ 

Introduce factorization (shape equations known amplitudes):

Project on weight (amplitude equation - known shape):

$$\begin{cases} \frac{dA_{NM}}{dt} = \sum_{N'} \sum_{M'} K_{NM,N'M'} A_{N'M'} + \\ \sum_{i=1}^{6} \lambda_i C_{i,NM} + S_{NM} \\ \frac{dC_{i,NM}}{dt} = \beta_i \sum_{M'} F_{i,NM,M'} A_{NM'} - \lambda_i C_{i,NM} \\ i = 1, 2, ..., 6, \end{cases}$$

Normalization condition (its application may require iteration):

$$\frac{d}{dt} \left[ \sum_{n} \sum_{m} \right]_{NM} w_{nm} \frac{1}{v_m} \varphi_{nm}(t) = \frac{d}{dt} \gamma_{NM} = 0$$

Kinetic effective parameters and source are introduced

### Multipoint effective terms

$$K_{NM,N'M'} = \frac{1}{\gamma_{NM}} \left[ \sum_{n} \sum_{m} \sum_{m} \right]_{NM} \left( w_{nm} \left[ \sum_{n'} \sum_{m'} \right]_{N'M'} k_{nm,n'm'} \varphi_{n'm'} \right) \text{ coupling terms} \right]$$
effective source
$$S_{NM} = \frac{1}{\gamma_{NM}} \left[ \sum_{n} \sum_{m} \right]_{NM} w_{nm} S_{nm}$$

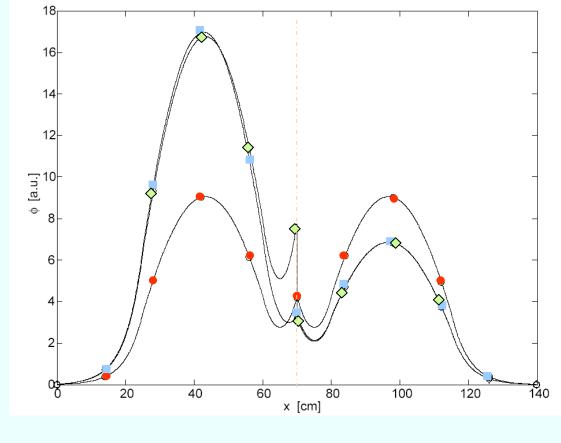
$$C_{i,NM} = \frac{1}{\gamma_{NM}} \left[ \sum_{n} \sum_{m} \right]_{NM} w_{nm} \chi_{i,m} C_{i,n} \quad \text{effective delayed concentration} \right]$$

$$F_{i,NM,M'} = \frac{1}{\gamma_{NM}} \left[ \sum_{n} \sum_{m} \right]_{NM} w_{nm} \chi_{i,m} \beta_{i} \left[ \sum_{m'} \right]_{M'} f_{nm'} \varphi_{nm'}$$
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#### Multipoint features

Multipoint can be used in quasi-statics Graph to show features of multipoint:

Circle (•) : PK Square (•): exact Diamond (> ): 2-point

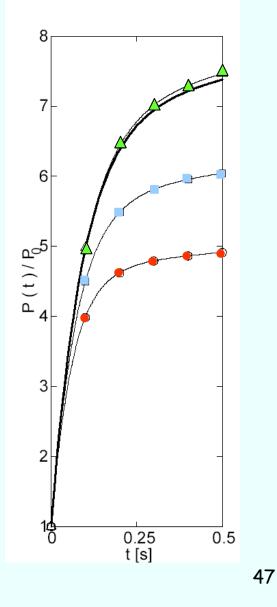


#### Effect of choice of points

Different subdivision of the phase space has influence on the accuracy of the results

Bold: exact Circle (•) : PK Square (•): 2-point Triangle (^): 2-point

and A are characterized by different subdivisions of the spatial domain



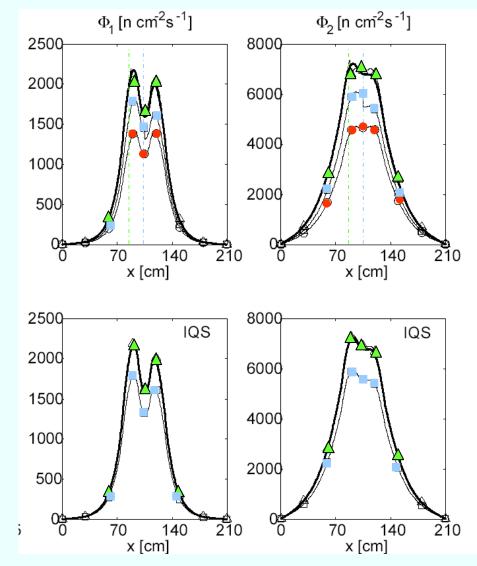
#### Effect of choice of points

 The different subdivision of the spatial domain are evidenced

Bold: exact Circle (•): PK Square (•): 2-point Triangle (▲): 2-point

 Update of shape functions through quasi-static procedure

Continuity of fluxes



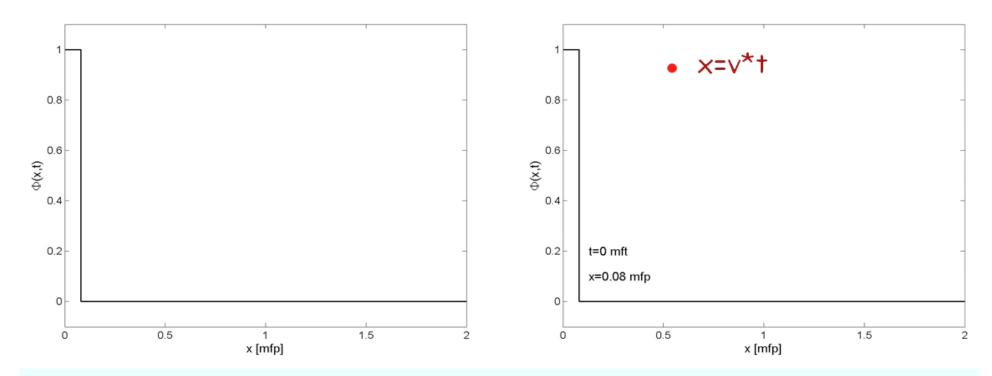
# Hard problems in kinetics

- Propagation phenomena or
- Is there anything better than diffusion ?
- ...do we need something better than diffusion ?

- Appearance of time-dependent ray effects connected to angular discretization
- Inadequateness of diffusion theory due to the infinite-velocity limit (no ray effects)
- Space and time ray effects in multi-D
- Spatial distortions due to space discretizations

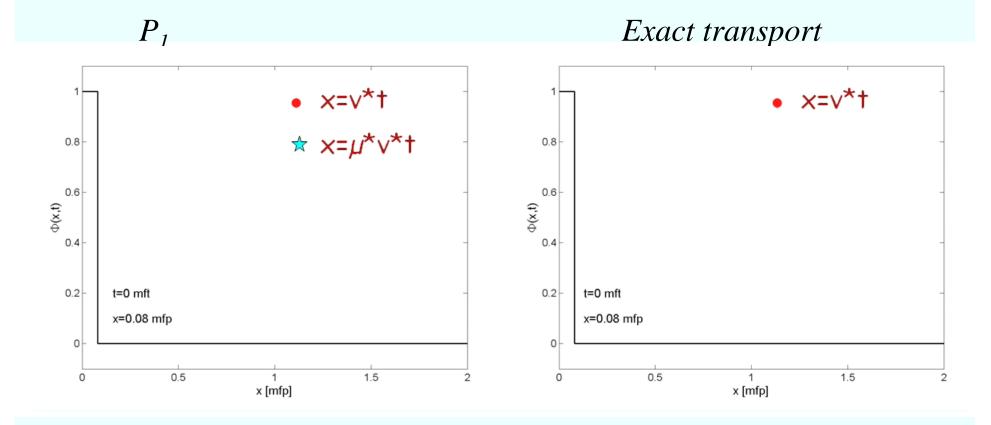
Diffusion

Exact transport



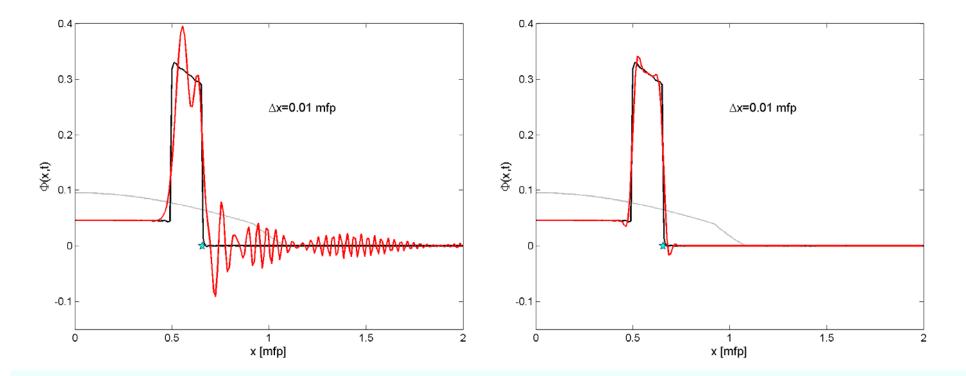
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#### $P_1$ – diamond difference

 $P_1$  – linear discontinuous



#### Enhanced quasi-static schemes: Alternative factorizations

Rather than assuming the standard amplitude-shape factorization:

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

a privileged variable in phase space is identified and treated separately in the factorization

$$\phi(\mathbf{r}, E, \Omega, t) = \phi(\mathbf{X}, t) = T(x_1, t)\psi(\mathbf{X}, t)$$