Problems and challenges in neutron transport theory and reactor kinetics

P. Ravetto

Politecnico di Torino

Dipartimento di Energetica

Torino, Italy

Introduction

A lot of advances in recent years in neutron transport and computational methods and a lot of new issues

Presentation of a selection of aspects considered relevant

Presentation of some advances in reactor kinetics

Challenges for the neutron transport discipline for reactor physics applications

- High performance computers demand for better models and better algorithms

  - Improve design tools for commercial systems (reliability, safety, improved system performance… better economy)
  - Establish new models and methods for the analysis of advanced innovative systems

Advances in computational methods

Angular discrete methods and spherical harmonics approach, but also…

… Simplified spherical harmonics and second-order models

- Applications of response matrix formulation
- New space discretization schemes
- Wavelet approach for the angular variable

Advances in computational methods

Second-order forms of the transport equation are particularly appealing

Different approaches to derive such equations may be followed

- manipulate simplified spherical harmonics method
- start from integral form of the equation
- use the even-parity formulation (simple in plane geometry…)

Second-order from SP$_N$

The simplified spherical harmonics method (the Gelbard's idea…):

$$\begin{cases} \dfrac{2n+1}{4n+1}\dfrac{df_{2n+1}}{dx}(x) + \dfrac{2n}{4n+1}\dfrac{df_{2n-1}}{dx}(x) + \sigma(x) f_{2n}(x) = q_0(x)\delta_{n0} \\ \dfrac{2n+2}{4n+3}\dfrac{df_{2n+2}}{dx}(x) + \dfrac{2n+1}{4n+3}\dfrac{df_{2n}}{dx}(x) + \sigma(x) f_{2n+1}(x) = 0 \end{cases} \quad (n = 0, 1, \dots, N-1)$$

$$\Downarrow$$

$$\begin{cases} \dfrac{2n+1}{4n+1}\nabla\cdot\mathbf{f}_{2n+1}(\mathbf{r}) + \dfrac{2n}{4n+1}\nabla\cdot\mathbf{f}_{2n-1}(\mathbf{r}) + \sigma(\mathbf{r}) f_{2n}(\mathbf{r}) = q_0(\mathbf{r})\delta_{n0} \\ \dfrac{2n+2}{4n+3}\nabla f_{2n+2}(\mathbf{r}) + \dfrac{2n+1}{4n+3}\nabla f_{2n}(\mathbf{r}) + \sigma(\mathbf{r})\mathbf{f}_{2n+1}(\mathbf{r}) = 0 \end{cases} \quad (n = 0, 1, \dots, N-1)$$

Second-order from SP_N

A second-order form can be obtained by elimination of odd-order terms and diagonalization (standard algebra…):

$$\mathbf{F} = \begin{pmatrix} f_0(\mathbf{r}) \\ f_2(\mathbf{r}) \\ \vdots \\ f_{2N-2}(\mathbf{r}) \end{pmatrix}, \mathbf{Q} = \begin{pmatrix} q_0(\mathbf{r}) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\nabla \cdot \left[\frac{1}{\sigma(\mathbf{r})} \nabla (\mathbb{A}\mathbf{F}) \right] - \sigma(\mathbf{r})\mathbf{F} + \mathbf{Q} = 0,$$

$$\mathbf{F} = \sum_{\beta=1}^{N} \Phi_\beta \mathbf{W}_\beta.$$

Advances in computational methods

Diagonal form of the differential system of equations (A_N approximation):

$$\begin{cases} \nabla \cdot \left(\dfrac{\mu_\alpha^2}{\sigma(\mathbf{r})} \nabla \Phi_\alpha(\mathbf{r}) \right) - \sigma(\mathbf{r}) \Phi_\alpha(\mathbf{r}) + q_0(\mathbf{r}) = 0 \; (\alpha = 1, 2, \ldots, N) \\ q_0(\mathbf{r}) = \sigma_s(\mathbf{r}) \displaystyle\sum_{\beta=1}^{N} w_\beta \Phi_\beta(\mathbf{r}) + S(\mathbf{r}), \end{cases}$$

Note: for homogeneous systems it is equivalent to P_N

Second-order from SP_N

Observations (I):

- w_β and μ_β are the weights and abscissas of the Gauss-Legendre quadrature formula
- The system is a multigroup-like diffusion system of equations, with virtual up-scattering

Second-order from SP_N

Observations (II):

- Moments do not have a physical meaning in the general case, buth their sum is the scalar flux
- Moments are the even-parity fluxes in plane geometry
- The treatment of collision anisotropy is complicated

Second-order from integral transport

Alternatively a second order form can be derived from the integral transport equation

Can give a theoretical background to SP_N

[An exact equation can be derived, even in time-dependent conditions !]

$$\Phi(\mathbf{r}) = \int_{\Re^3} \frac{e^{-|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \underbrace{[\gamma(\mathbf{r}')\Phi(\mathbf{r}') + S(\mathbf{r}')]}_{q(\mathbf{r})} dV'$$

Second-order from integral transport

The kernel is approximated by a superposition of diffusive kernels (Stewart-Zweifel):

$$\frac{e^{-r}}{4\pi r^2} = \int_0^1 \frac{e^{-r/\mu}}{4\pi r \mu^2} d\mu \simeq \sum_{\alpha=1}^{N} p_\alpha \frac{e^{-r/\mu_\alpha}}{4\pi r \mu_\alpha^2},$$

$p_\beta = w_\beta/2$ and μ_β are the weights and abscissas of a quadrature formula (without need of restriction to Gauss-Legendre)

Second-order from integral transport

Consider integral equations for moments f_β

$$f_\beta(\mathbf{r}) = \int_V q(\mathbf{r}') \frac{e^{-|\mathbf{r}-\mathbf{r}'|/\mu_\beta}}{4\pi\mu_\beta^2|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}', \quad \beta = 1, 2, \ldots, N$$

to obtain a more general form of the A_N approximation:

$$\begin{cases} \mu_\beta^2 \nabla^2 f_\beta(\mathbf{r}) - f_\beta(\mathbf{r}) + q(\mathbf{r}) = 0, \quad \beta = 1, 2, \ldots, N. \\ \Phi(\mathbf{r}) = \sum_{\alpha=1}^{N} p_\alpha f_\alpha(\mathbf{r}), \end{cases}$$

Second-order from integral transport: the exact equation

Consider the integral time-dependent equation:

$$\Phi(\mathbf{r},t) = \int_V q(\mathbf{r}', t - |\mathbf{r}-\mathbf{r}'|)\frac{e^{-|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\,d\mathbf{r}'$$

and the auxiliary equation:

$$f(\mathbf{r},\mu,t) = \int_V q(\mathbf{r}', t - |\mathbf{r}-\mathbf{r}'|)\frac{e^{-|\mathbf{r}-\mathbf{r}'|/\mu}}{4\pi\mu^2|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}'$$

Second-order from integral transport: the exact equation

Use D'Alambert equality:

$$\left(\nabla^2 - k^2\frac{\partial^2}{\partial t^2}\right)\frac{g(\mathbf{r}', t - |\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} = -4\pi g(\mathbf{r}', t)\delta(\mathbf{r}-\mathbf{r}')$$

Second-order from integral transport: the exact equation

A second-order integro-differential equation is obtained for the time-dependent situation…and exact ! (A_∞ formulation)

$$\begin{cases} \mu^2\nabla^2 f(\mathbf{r},\mu,t) - \left(1+\mu\frac{\partial}{\partial t}\right)^2 f(\mathbf{r},\mu,t) + q(\mathbf{r},t) = 0, \\ \Phi(\mathbf{r},t) = \int_0^1 f(\mathbf{r},\mu,t)\,\mathrm{d}\mu \end{cases}$$

Exact second order integro-differential transport equation

Wave term is appearing

When discretized (A_N), a system of telegrapher's equations is obtained

Observations

In steady-state A_∞ allows to extend analytical Case-like approach to general geometry (benchmarks)

Second-order forms are suitable for response matrix formulations

Equations can be cast into a form involving only boundary values of the unknown, leading to a boundary element numerical scheme (BEM)

The boundary element approach

$$\frac{\mu_\alpha^2}{\sigma}\nabla_{\mathbf{r}}^2\tilde{\Phi}_{\alpha\beta} - \sigma\tilde{\Phi}_{\alpha\beta} + \sigma_s w_\alpha \sum_{\nu=1}^{N} \tilde{\Phi}_{\nu\beta} + \delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}') = 0$$

$$\tilde{\Phi}_{\alpha\beta}(|\mathbf{r}-\mathbf{r}'|) = \sum_{m=1}^{N} g_{m\beta} C_\alpha^{(m)} \frac{e^{-\kappa_m|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

Multiply second-order equations by Green functions, integrate over volume and apply Green identity…..

The boundary element approach

…. to obtain the equation:

$$c(\mathbf{r})\Phi_\beta(\mathbf{r}) + \sum_{\alpha=1}^{N} \int_\Sigma \left[\tilde{\Phi}_{\alpha\beta}(|\mathbf{r} - \mathbf{r}'_\Sigma|) J_{n',\alpha}(\mathbf{r}'_\Sigma) + \tilde{J}_{n',\alpha\beta}(\mathbf{r}, \mathbf{r}'_\Sigma)\Phi_\alpha(\mathbf{r}'_\Sigma)\right] d\Sigma' \quad = \quad \Psi_\beta(\mathbf{r})$$

with:

$$J_{n,\alpha}(\mathbf{r}_\Sigma) = -\frac{\mu_\alpha^2}{\sigma}\frac{\partial \Phi_\alpha}{\partial \mathbf{n}}(\mathbf{r}_\Sigma),$$

$$\tilde{J}_{n,\alpha\beta}(\mathbf{r}, \mathbf{r}_\Sigma) = \frac{\mu_\alpha^2}{\sigma}\frac{\partial \tilde{\Phi}_{\alpha\beta}}{\partial \mathbf{n}'}(|\mathbf{r} - \mathbf{r}'_\Sigma|),$$

$$\Psi_\beta(\mathbf{r}) = \sum_{\alpha=1}^{N} \int_V \tilde{\Phi}_{\alpha\beta}(|\mathbf{r} - \mathbf{r}'|) S(\mathbf{r}') dV'$$

The boundary element approach

Note:

- Volume solution can be reconstructed from boundary values
- Valid for all points…

… if applied at any boundary point…

The boundary element approach

… a boundary formulation is obtained

unknowns appear only at boundary points!

reduction of dimensionality

$$c(\mathbf{r}_\Sigma)\Phi_\beta(\mathbf{r}_\Sigma) + \sum_{\alpha=1}^{N} \int_\Sigma \left[\tilde{\Phi}_{\alpha\beta}(|\mathbf{r}_\Sigma - \mathbf{r}'_\Sigma|) J_{n',\alpha}(\mathbf{r}'_\Sigma) + \tilde{J}_{n',\alpha\beta}(\mathbf{r}_\Sigma, \mathbf{r}'_\Sigma)\Phi_\alpha(\mathbf{r}'_\Sigma) \right] d\Sigma'$$

$$= \quad \Psi_\beta(\mathbf{r}_\Sigma)$$

The boundary element approach

- BEM is obtained by discretization of the boundary
- Physical connection between boundary terms and source volume terms → response matrix formulation

$$\left|j^{+}\right\rangle = \mathbb{G}\left|j^{-}\right\rangle + |b\rangle$$

Advances in computational methods

The method of characteristics

- The solution is “tracked” along a set of rays (characteristics)
- Geometrical flexibility (heterogeneous, unstructured)
- Full-core transport calculations

Advances in computational methods

The inversion of the transport operator by source iteration

- Advances in synthetic approaches (Multi-D, anisotropic scattering…)
- Preconditioning and Krylov approaches
- Extension to schemes applying the method of characteristics

Advances in computational methods

Cross section generation

- Improved computational methods call for "good" data !
- Need of physically consistent averaging-homogenization procedures
- Need to accurately treat anisotropy
- Need of adjustment by integral parameter measurement

Advances for new systems

Generation IV systems with new geometrical and material configurations

- Pebble-bed reactors
- Molten-salt reactors
- Fast systems (sodium and lead – cooled)

New physical phenomena (interaction of neutronics with fluid-dynamics), new models, new numerics

Accelerator-driven systems

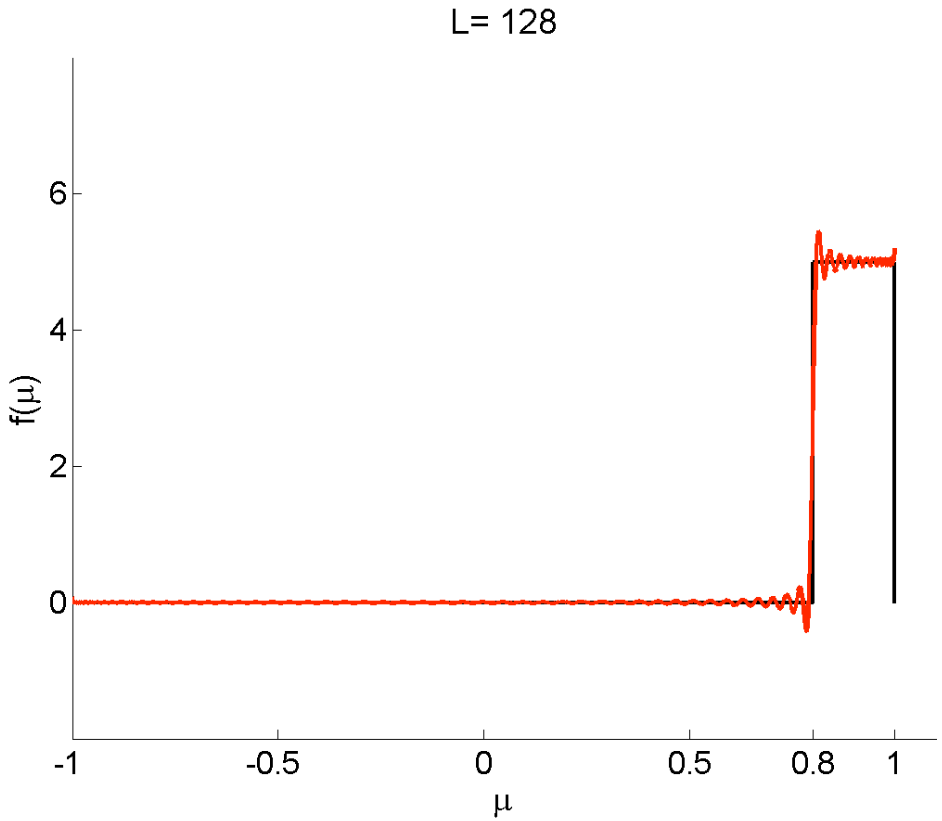
Angular schemes to handle anisotropy effects and mitigate ray-effects

Source effects and integral parameters

Propagation phenomena

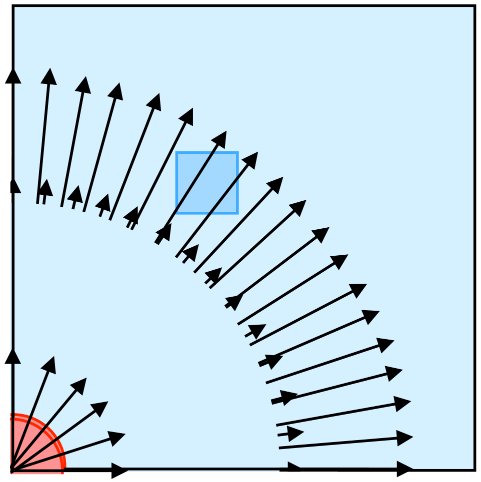
Anisotropy effects

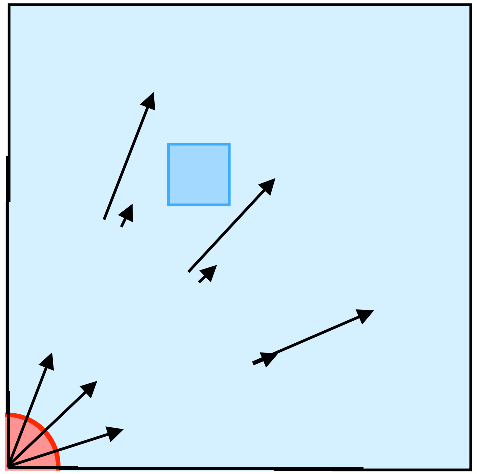
High-order Legendre expansions may be needed to avoid unphysical behaviours



Ray effects

Mitigation of ray effects may be crucial to correctly interpret source-driven experiments





Source-dominated systems

Need of a new approach:

- No reference reactor
- Appearance of phenomena that were "hidden" in nearly critical fission-dominated reactors
- Possible inadequacy of standard numerical methods

Angular schemes: finite elements and wavelets

An angular expansion is introduced:

$$\phi(\mathbf{r}, E, \Omega) = \sum_{k=-N}^{N} f_k(\mathbf{r}, E) u_k(\Omega)$$

The description of anisotropic emission is improved and ray effects are mitigated

With proper choices of the formulation, a discrete-ordinate-like system of equations can be obtained for components $f_k(\mathbf{r}, E)$

Accurate benchmarks

Novel methods require accurate and reliable benchmarks, for verification, validation and qualification of physical models, algorithms and codes

- Analytical benchmarks
- Numerical benchmarks
- Experimental benchmarks

The role of analytical solutions

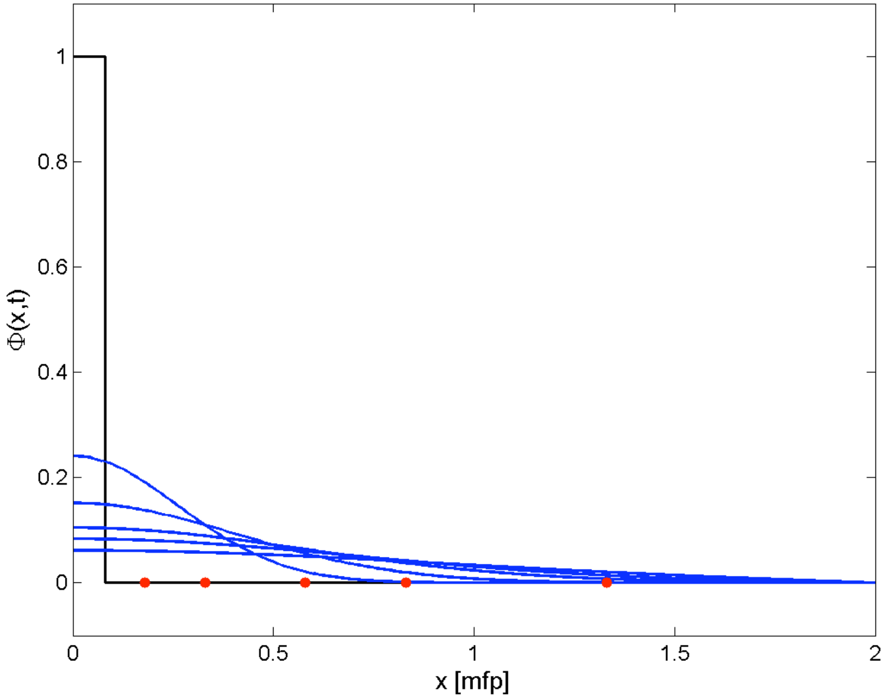
- Retain a high educational value
- Allow full insight into the physical problem
- Give the possibility to compare different models and algorithms and to establish reliable limits of validity
- Allow to discriminate physical and numerical effects

An example: pulse propagation

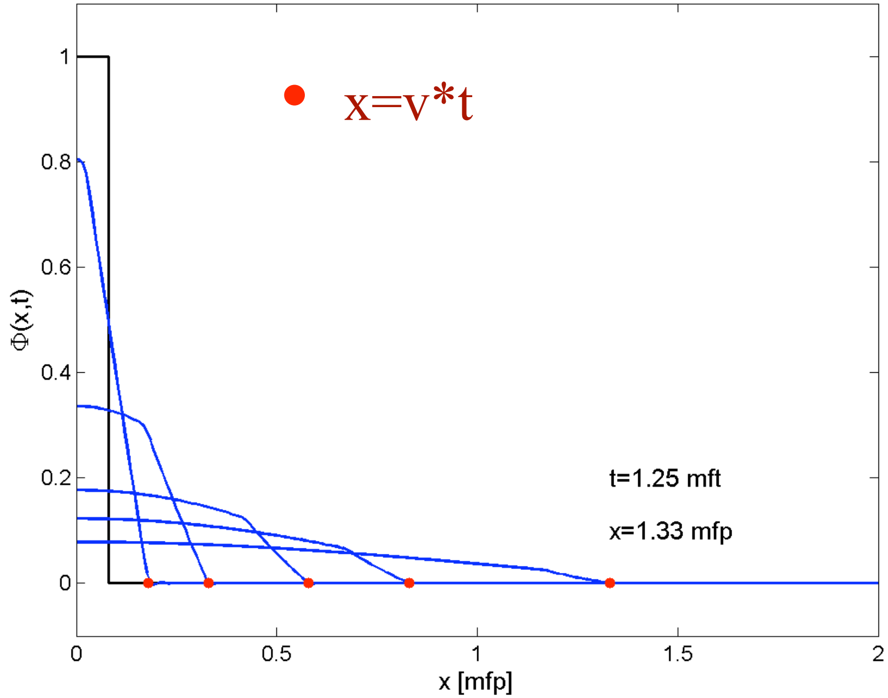
- Appearance of time-dependent ray effects connected to angular discretization
- Inadequateness of diffusion theory due to the infinite-velocity limit (no ray effects)
- Space and time ray effects in multi-D
- Spatial distortions due to space discretizations

An example: pulse propagation

Diffusion

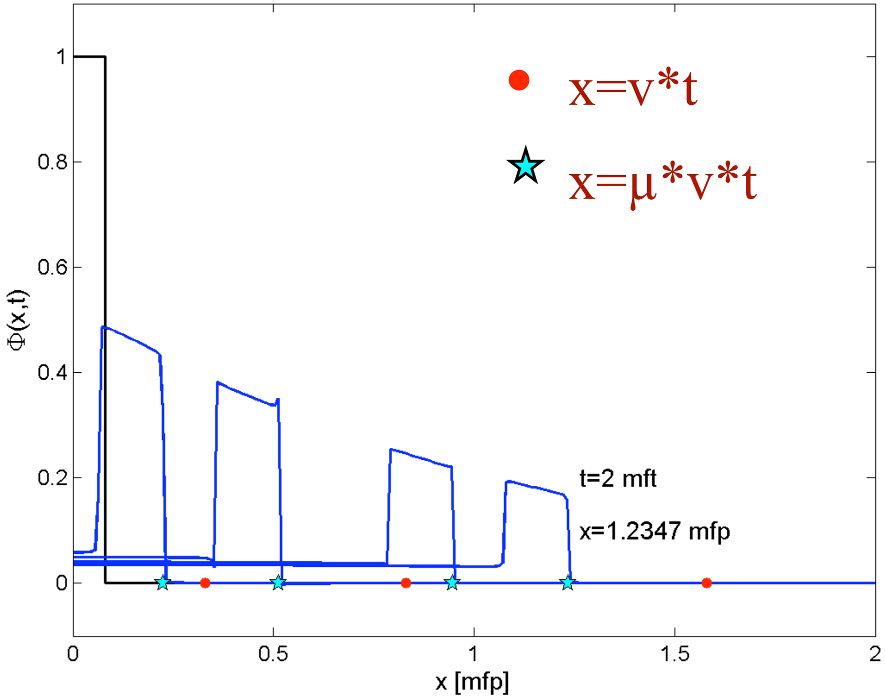


Exact transport

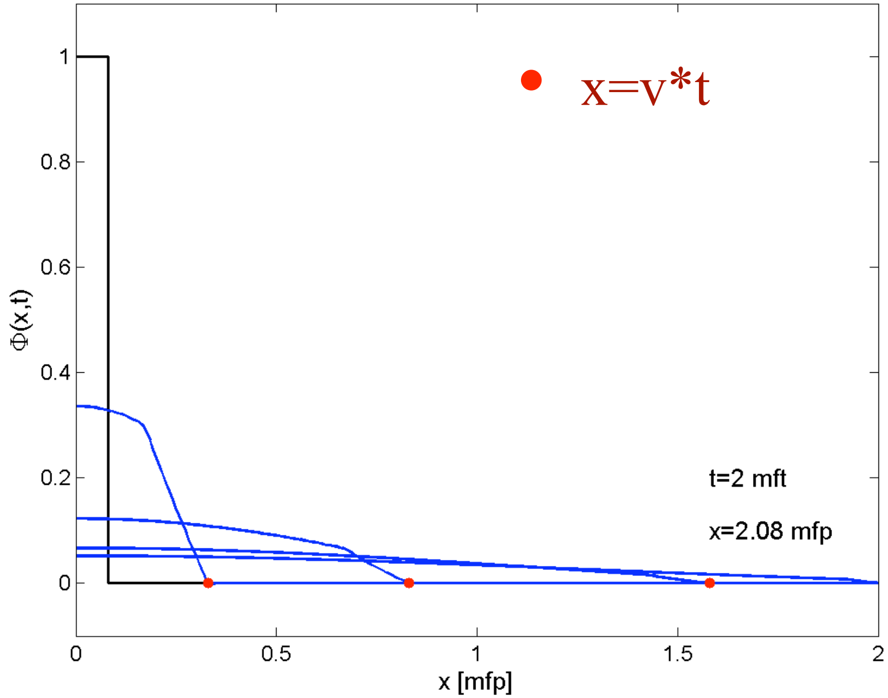


An example: pulse propagation

P_1

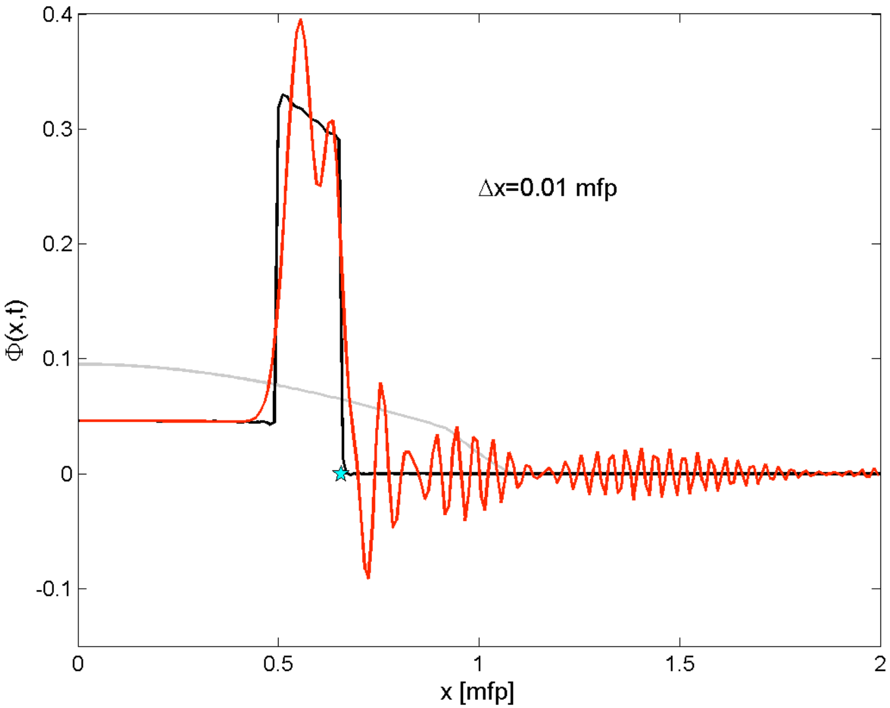


Exact transport

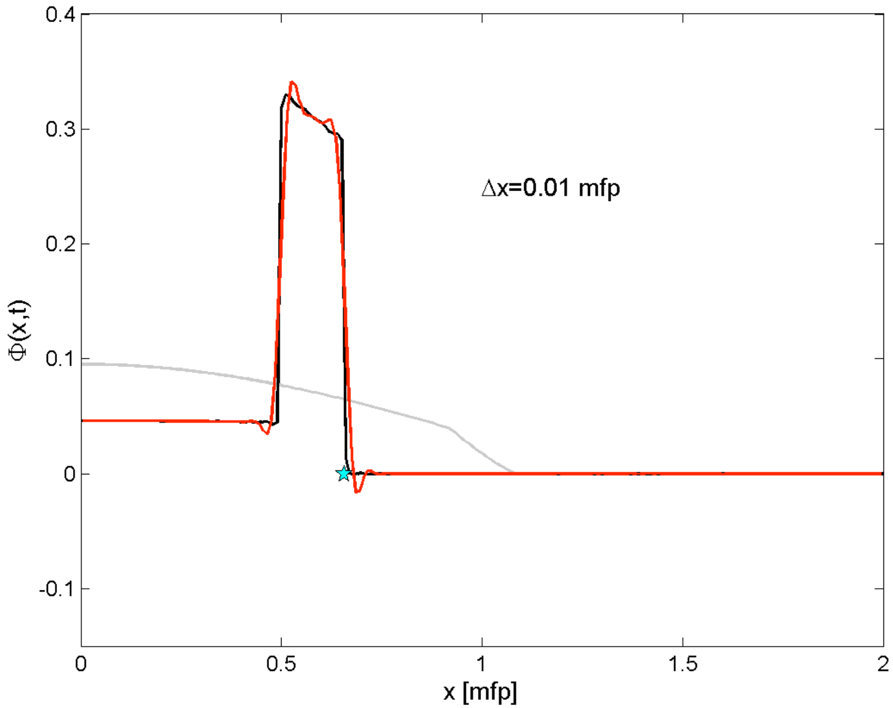


An example: pulse propagation

P_1 – diamond difference



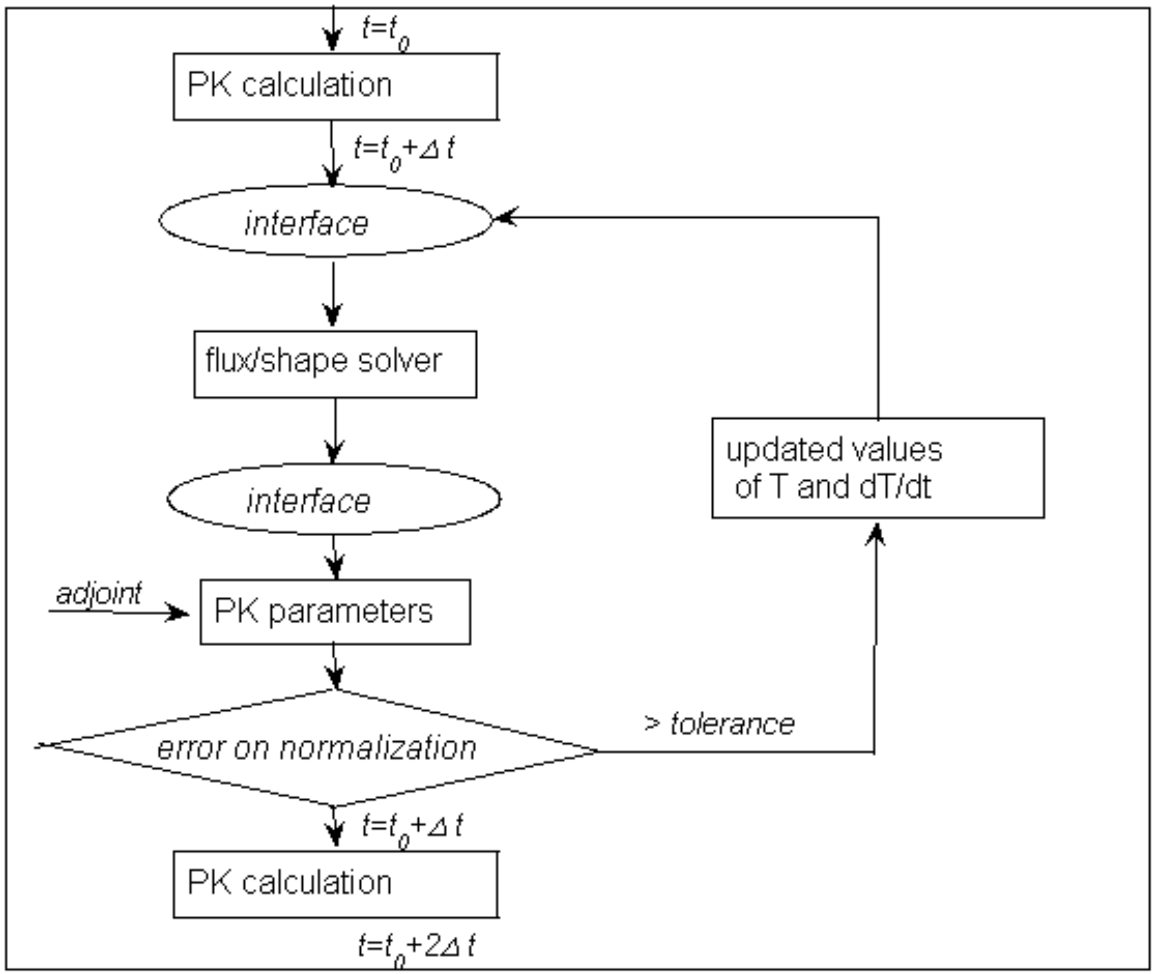
P_1 – linear discontinuous



Time-dependent problems

- Many dynamic problems for innovative systems involve important transport effects:
  - Accelerator-driven systems (high energy neutrons, high streaming due to the source)
  - Pulsed experiment interpretation (wavefront propagation effects)
  - Gas reactors (voids)
  - High heterogeneity configurations

Time-dependent problems



Time-dependent problems: enhanced quasi-static schemes

- Predictor-corrector quasi-statics
- Alternative factorizations

Enhanced quasi-static schemes: Predictor-Corrector

The flux equation is solved on a coarse time scale and the shape is obtained by renormalization (predictor step)

The new shape is then used to evaluate the kinetic parameters for the amplitude equations (corrector step)

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

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

Alternative factorizations: multipoint

Starting from the balance equations

$$\begin{cases} \dfrac{1}{v}\dfrac{\partial\varphi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} = \left[-\widehat{\mathbf{L}}(t)\varphi + \widehat{\mathbf{M}}_{\mathrm{p}}(t)\varphi\right](\mathbf{r},E,\mathbf{\Omega},t) + \sum_{i=1}^{R}\mathscr{E}_i(\mathbf{r},E,t) + S(\mathbf{r},E,\mathbf{\Omega},t) \\ \dfrac{1}{\lambda_i}\dfrac{\partial\mathscr{E}_i(\mathbf{r},E,t)}{\partial t} = -\mathscr{E}_i(\mathbf{r},E,t) + \left[\widehat{\mathbf{M}}_i\varphi\right](\mathbf{r},E,\mathbf{\Omega},t), \quad i=1,\dots,R \end{cases}$$

Introduce factorization as

$$\varphi(\mathbf{x},t) = \sum_{j=1}^{J}\left(N_j(t)u_j(\mathbf{x})\right) \;\; \phi(\mathbf{x};t) = \sum_{j=1}^{J}N_j(t)\phi_j(\mathbf{x};t),$$

$$\mathscr{E}_i(\mathbf{x};t) = \sum_{j=1}^{J}\left(E_{i,j}(t)u_j(\mathbf{x})\right) \;\; \epsilon_i(\mathbf{x};t) = \sum_{j=1}^{J}E_{i,j}(t)\epsilon_{i,j}(\mathbf{x};t),$$

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

Alternative factorizations: multipoint

Multipoint factorization in phase space Γ

$$\varphi(\mathbf{x},t) = \sum_{j=1}^{J} \left(N_j(t)u_j(\mathbf{x})\right) \quad \phi(\mathbf{x};t) = \sum_{j=1}^{J} N_j(t)\phi_j(\mathbf{x};t),$$

A coupled system of first-order differential equations is obtained for the amplitudes

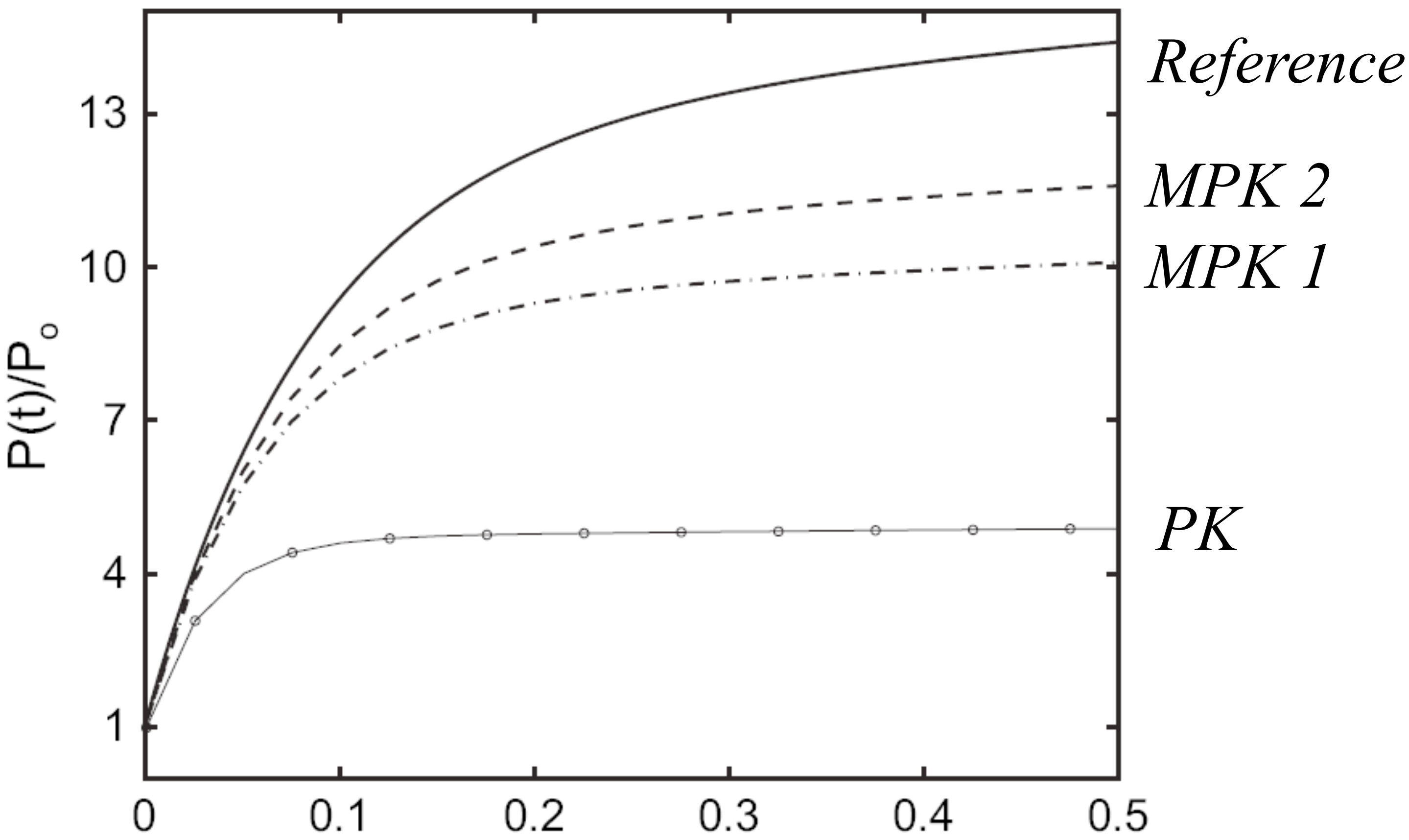
Alternative factorizations: multipoint

System for amplitudes

$$
\begin{cases}
\displaystyle\sum_{k=1}^{J}\left\langle \phi_j^\dagger \middle| \frac{1}{v}\phi_k \right\rangle \frac{\mathrm{d}N_k}{\mathrm{d}t} + \sum_{k=1}^{J}\left\langle \phi_j^\dagger \middle| \frac{1}{v}\frac{\partial \phi_k}{\partial t} \right\rangle N_k = \sum_{k=1}^{J}\langle \phi_j^\dagger | (-\widehat{\mathbf{L}}\phi_k + \widehat{\mathbf{M}}_{\mathrm{p}}\phi_k)\rangle N_k \\
\displaystyle\quad + \sum_{i=1}^{R}\sum_{k=1}^{J}\langle \phi_j^\dagger | \epsilon_{i,k}\rangle E_{i,k} + \langle \phi_j^\dagger | S\rangle, \quad j = 1,\ldots,J, \\
\displaystyle\frac{1}{\lambda_i}\sum_{k=1}^{J}\langle \epsilon_{i,j}^\dagger | \epsilon_{i,k}\rangle \frac{\mathrm{d}E_{i,k}}{\mathrm{d}t} + \frac{1}{\lambda_i}\sum_{k=1}^{J}\left\langle \epsilon_{i,j} \middle| \frac{\partial \epsilon_{i,k}}{\partial t}\right\rangle E_{i,k} = -\sum_{k=1}^{J}\langle \epsilon_{i,j}^\dagger | \epsilon_{i,k}\rangle E_{i,k} \\
\displaystyle\quad + \sum_{k=1}^{J}\langle \epsilon_{i,j}^\dagger | \widehat{\mathbf{M}}_i\phi_k\rangle N_k, \quad i = 1,\ldots,R;\ j = 1,\ldots,J,
\end{cases}
$$

Alternative factorizations: multipoint

Improved results with respect to point kinetics



Concluding remarks

- Exciting new problems in reactor physics

- Exciting work for physicists, numerical analysts and code developers

Reactor physics offers
many interesting professional opportunities
to young researchers and students !