Space-time kinetics

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Space-time kinetics equations

$$\frac{1}{V_{\mathrm{n},g}}\,\frac{\partial}{\partial t}\phi_g(\boldsymbol{r},t) - \boldsymbol{\nabla}\cdot\mathbb{D}_g(\boldsymbol{r})\boldsymbol{\nabla}\phi_g(\boldsymbol{r},t) + \Sigma_{\mathrm{r}g}(\boldsymbol{r})\,\phi_g(\boldsymbol{r},t)$$
$$= \sum_{\substack{h=1\\h\neq g}}^{G} \Sigma_{g\leftarrow h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t) + \chi_g^{\mathrm{pr}}(\boldsymbol{r})\,(1-\beta)\sum_{h=1}^{G}\nu\Sigma_{\mathrm{f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t)$$
$$+ \sum_{\ell}\chi_{\ell,g}^{\mathrm{del}}(\boldsymbol{r})\,\lambda_\ell\,c_\ell(\boldsymbol{r},t) + q_g(\boldsymbol{r},t)$$

$$\frac{\partial c_\ell(\boldsymbol{r},t)}{\partial t} = \beta_\ell\sum_{h=1}^{G}\nu\Sigma_{\mathrm{f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t) - \lambda_\ell\,c_\ell(\boldsymbol{r},t)\ \ ;\quad \ell = 1, N_d$$

$$\beta = \sum_{\ell}\beta_\ell\ \ .$$

Point kinetics equations 1

$$
\begin{aligned}
\frac{1}{V_{\rm n}(E)}\,\frac{\partial}{\partial t}\phi(E,t) \;&+\; \Sigma(E)\,\phi(E,t) \;=\; \int_0^\infty dE'\,\Sigma_{\rm s,0}(E\leftarrow E')\,\phi(E',t) \\
&+\; \chi^{\rm pr}(E)\,(1-\beta)\int_0^\infty dE'\,\nu\Sigma_{\rm f}(E')\,\phi(E',t) \\
&+\; \sum_\ell \chi_\ell^{\rm del}(E)\,\lambda_\ell\,c_\ell(t)+q(E,t)
\end{aligned}
$$

together with the set of N_d precursor equations:

$$
\frac{\partial c_\ell(t)}{\partial t}=\beta_\ell\int_0^\infty dE\,\nu\Sigma_{\rm f}(E)\,\phi(E,t)-\lambda_\ell\,c_\ell(t)\;\;;\quad \ell=1,N_d\;\;.
$$

Equivalent point kinetics parameters 1

The time-dependent reactivity of the reactor is

$$\bar{\rho}(t) = 1 - \frac{\int_0^\infty dE\, \phi_0^*(E) \left[\Sigma(E)\, \phi(E,t) - \int_0^\infty dE'\, \Sigma_{\mathrm{s},0}(E \leftarrow E')\, \phi(E',t) \right]}{\int_0^\infty dE\, \phi_0^*(E)\, \chi^{\mathrm{ss}}(E) \int_0^\infty dE'\, \nu\Sigma_{\mathrm{f}}(E')\, \phi(E',t)} \ ,$$

the steady-state fission spectrum is

$$\chi^{\mathrm{ss}}(E) = (1-\beta)\, \chi^{\mathrm{pr}}(E) + \sum_\ell \beta_\ell\, \chi_\ell^{\mathrm{del}}(E) \ ,$$

Equivalent point kinetics parameters

the mean neutron generation time of the reactor is

$$\bar{\Lambda}(t) = \frac{\int_0^\infty dE \, \frac{1}{V_\mathrm{n}(E)} \, \phi_0^*(E) \, \phi(E,t)}{\int_0^\infty dE \, \phi_0^*(E) \, \chi^\mathrm{ss}(E) \int_0^\infty dE' \, \nu\Sigma_\mathrm{f}(E') \, \phi(E',t)} \quad ,$$

the average delayed fractions are

$$\bar{\beta}_\ell(t) = \beta_\ell \, \frac{\int_0^\infty dE \, \phi_0^*(E) \, \chi_\ell^\mathrm{del}(E)}{\int_0^\infty dE \, \phi_0^*(E) \, \chi^\mathrm{ss}(E)}$$

Equivalent point kinetics parameters 3

and

$$\bar{\beta}(t) = \sum_{\ell} \bar{\beta}_\ell(t) = 1 - (1-\beta)\,\frac{\int_0^\infty dE\,\phi_0^*(E)\,\chi^{\rm pr}(E)}{\int_0^\infty dE\,\phi_0^*(E)\,\chi^{\rm ss}(E)}$$

and where the neutron population, precursor concentration and external source are

$$n(t) = \int_0^\infty dE\,\frac{1}{V_{\rm n}(E)}\,\phi_0^*(E)\,\phi(E,t) \quad ,$$

$$\bar{c}_\ell(t) = c_\ell(t)\int_0^\infty dE\,\phi_0^*(E)\,\chi_\ell^{\rm del}(E)$$

and

$$\bar{q}(t) = \int_0^\infty dE\,\phi_0^*(E)\,q(E,t) \quad .$$

Point kinetics equations (classical form) 1

$$\begin{aligned} \frac{d}{dt} n(t) &= \frac{\bar{\rho}(t) - \bar{\beta}(t)}{\bar{\Lambda}(t)} \, n(t) + \sum_{\ell} \lambda_\ell \, \bar{c}_\ell(t) + \bar{q}(t) \\ \frac{d}{dt} \bar{c}_\ell(t) &= \frac{\bar{\beta}_\ell(t)}{\bar{\Lambda}(t)} \, n(t) - \lambda_\ell \, \bar{c}_\ell(t) \; ; \;\; \ell = 1, N_d \end{aligned}$$

Point kinetics equations (classical form) 2

Point kinetics equations are written in matrix form as

$$
\begin{aligned}
\boldsymbol{x}(0) &= \boldsymbol{x}_0 \\
\frac{d}{dt}\boldsymbol{x}(t) &= \mathbb{A}\,\boldsymbol{x}(t) + \boldsymbol{S}
\end{aligned}
$$

$$
\boldsymbol{x}(t) = [\, n(t) \quad \bar{c}_1(t) \quad \bar{c}_2(t) \quad \ldots \quad \bar{c}_{N_d}(t)\,]^\top \ , \quad \boldsymbol{S} = [\, \bar{q} \quad 0 \quad 0 \quad \ldots \quad 0\,]^\top
$$

$$
\mathbb{A} = \begin{bmatrix}
\dfrac{\bar{\rho} - \bar{\beta}}{\bar{\Lambda}} & \lambda_1 & \lambda_2 & \ldots & \lambda_{N_d} \\
\dfrac{\bar{\beta}_1}{\bar{\Lambda}} & -\lambda_1 & 0 & \ldots & 0 \\
\dfrac{\bar{\beta}_2}{\bar{\Lambda}} & 0 & -\lambda_2 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\dfrac{\bar{\beta}_{N_d}}{\bar{\Lambda}} & 0 & 0 & \ldots & -\lambda_{N_d}
\end{bmatrix} .
$$

Point kinetics equations (classical form) 3

Steady-state equation:

$$\mathbb{A}\,\boldsymbol{x} = \boldsymbol{0}$$

$$c_\ell(0) \equiv c_{\ell,0} = \frac{\bar{\beta}_\ell}{\bar{\Lambda}\,\lambda_\ell}\,n_0 \quad ; \quad \ell = 1, N_d \quad .$$

Each side of the point kinetics equation is multiplied by the integrating factor $\mathrm{e}^{-\mathbb{A}t}$ and integrated in time. We obtain the analytical solution of the point-kinetics equations as

$$\boldsymbol{x}(t) = \mathrm{e}^{\mathbb{A}t}\,\boldsymbol{x}_0 + \left(\mathrm{e}^{\mathbb{A}t} - \mathbb{I}\right)\,\mathbb{A}^{-1}\,\boldsymbol{S}$$

where we made use of the identity

$$\int_0^t dt'\,\mathrm{e}^{-\mathbb{A}t'}\left[\frac{d}{dt'}\boldsymbol{x}(t') - \mathbb{A}\,\boldsymbol{x}(t')\right] = \mathrm{e}^{-\mathbb{A}t}\,\boldsymbol{x}(t) - \boldsymbol{x}(0) \quad .$$

Calculation of an exponential matrix 1

A straightforward technique consists to obtain the N_d+1 eigenvalues and eigenvectors of linear system

$$(\mathbb{A}-\omega_i\,\mathbb{I})\,\boldsymbol{p}_i=\boldsymbol{0}\ \text{ where }\ 1\le i\le N_d+1$$

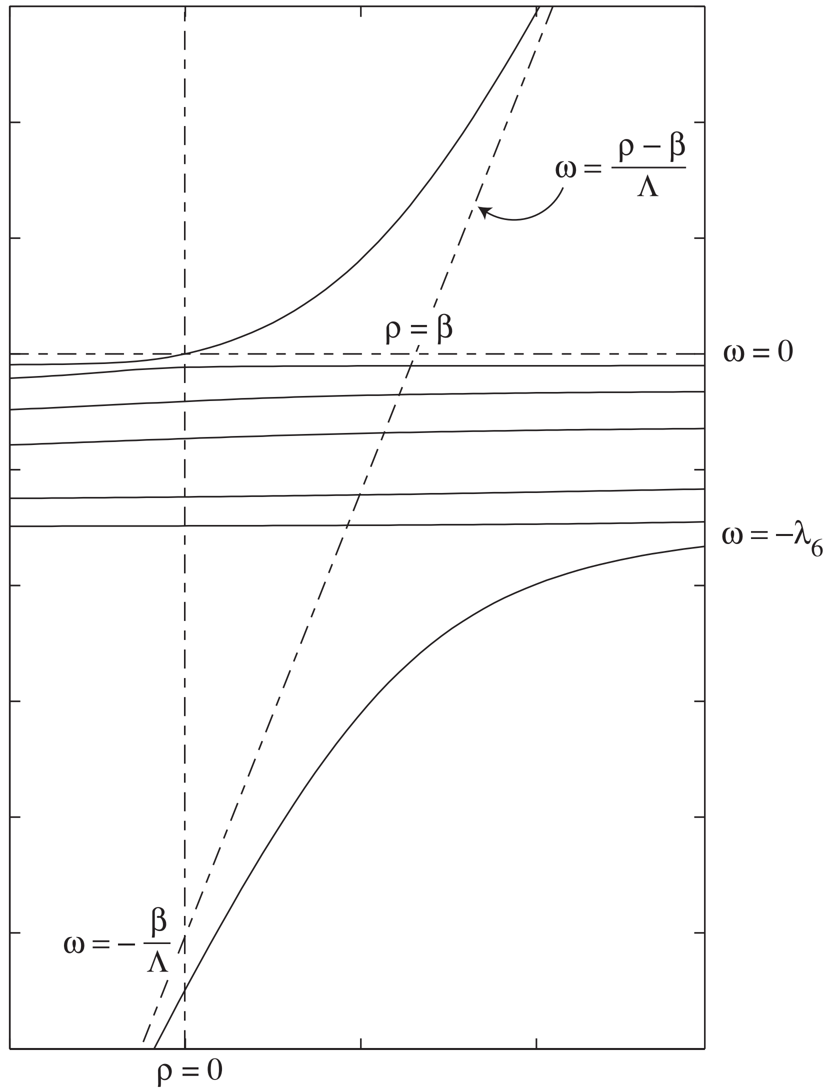
The eigenvalues are the root of the characteristic polynomial

$$\det\left(\mathbb{A}-\omega\,\mathbb{I}\right)=0$$

which can be obtained as the roots of the “inhour equation”:

$$\bar\rho-\bar\beta-\bar\Lambda\,\omega+\sum_\ell\frac{\bar\beta_\ell\,\lambda_\ell}{\lambda_\ell+\omega}=0\ \ .$$

Inhour equation with precursors



Inhour equation with precursors

We reproduce here a simple Matlab script for solving the inhour equation

$$\bar{\rho} - \bar{\beta} - \bar{\Lambda}\,\omega + \sum_{\ell} \frac{\bar{\beta}_\ell\,\lambda_\ell}{\lambda_\ell + \omega} = 0$$

```
function y = inhour(lambda, L, beta, rho)
% Find the roots of the inhour equation
% function y = inhour(lambda, L, beta, rho)
% (c) 2007 Alain Hebert, Ecole Polytechnique de Montreal
  [nn, dd]=residue(lambda.*beta,-lambda,[]) ;
  y=sort(roots(conv([-L, rho-sum(beta)],dd)+[0 0 nn])) ;
```

The script parameters are defined as

- `lambda`= array of dimension N_d containing the decay constants λ_ℓ for the delayed neutrons
- `L`= neutron generation time $\bar{\Lambda}$
- `beta`= array of dimension N_d containing the delayed fractions $\bar{\beta}_\ell$
- `rho`= reactivity $\bar{\rho}$
- `y`= array of dimension $N_d + 1$ containing the roots ω_i of the inhour equation.

Calculation of an exponential matrix 1

The analytical solution also requires the knowledge of the matrix $\mathbb{P}$ whose columns are the eigenvectors of square matrix $\mathbb{A}$. This matrix is equal to

$$\mathbb{P} = \{p_{i,j} \; ; \; i = 1, N_d + 1 \text{ and } j = 1, N_d + 1\}$$

where

$$p_{1,j} = 1 \text{ and } p_{i+1,j} = \frac{\bar{\beta}_i}{\bar{\Lambda}\,(\lambda_i + \omega_j)} \quad .$$

Calculation of an exponential matrix 1

Similarly, we can show that

$$\mathbb{P}^{-1} = \{y_{i,j} \; ; \; i = 1, N_d + 1 \text{ and } j = 1, N_d + 1\}$$

where

$$y_{i,1} = \left[1 + \sum_{\ell} \frac{\bar{\beta}_\ell \, \lambda_\ell}{\bar{\Lambda} \, (\lambda_\ell + \omega_i)^2}\right]^{-1} \text{ and } \; y_{i,j+1} = y_{i,1} \, \frac{\lambda_j}{\lambda_j + \omega_i} \quad .$$

Theorem

If $\mathbb{P}$ is the matrix whose columns are the eigenvectors of square matrix $\mathbb{A}$, and if ω_i are the corresponding eigenvalues, then

$$\mathrm{e}^{\mathbb{A}t} = \mathbb{P} \, \mathrm{diag}(\mathrm{e}^{\omega_i t}) \, \mathbb{P}^{-1} \quad .$$

The theta finite-difference scheme 1

A finite difference relation is used for time discretization of neutron flux and precursor equations, written as

$$
\begin{aligned}
(1-\Theta)\ \frac{\partial}{\partial t}\phi_g(\boldsymbol{r},t)\bigg|_{t_{n-1}} + \Theta\ \frac{\partial}{\partial t}\phi_g(\boldsymbol{r},t)\bigg|_{t_n} &= \frac{\phi_g(\boldsymbol{r},t_n)-\phi_g(\boldsymbol{r},t_{n-1})}{\Delta t_n} \\
(1-\Theta)\ \frac{\partial}{\partial t}c_\ell(\boldsymbol{r},t)\bigg|_{t_{n-1}} + \Theta\ \frac{\partial}{\partial t}c_\ell(\boldsymbol{r},t)\bigg|_{t_n} &= \frac{c_\ell(\boldsymbol{r},t_n)-c_\ell(\boldsymbol{r},t_{n-1})}{\Delta t_n}
\end{aligned}
$$

where $\ell = 1, N_d$.

Setting $\Theta = 0$, $\Theta = 1$ and $\Theta = 1/2$ yield the explicit scheme, the fully implicit scheme and the Crank-Nicholson scheme, respectively.

Theta scheme with point kinetics

$$\frac{\boldsymbol{x}^{(n+1)} - \boldsymbol{x}^{(n)}}{\Delta t_n} = \Theta \ \mathbb{A} \ \boldsymbol{x}^{(n+1)} + (1 - \Theta) \ \mathbb{A} \ \boldsymbol{x}^{(n)} + \boldsymbol{S}$$

where $\boldsymbol{x}^{(n)} \equiv \boldsymbol{x}(t_n)$.

The theta scheme can be applied to the point-kinetics equations and used to study its stability characteristics. It can also be applied to the space-time kinetics equations for solving full-core problems.

Above equation with $\boldsymbol{S} = \boldsymbol{0}$ may be written as

$$\boldsymbol{x}^{(n+1)} = \mathbb{R} \, \boldsymbol{x}^{(n)}$$

where $\mathbb{I}$ is the identity matrix and where the iterative matrix is defined as

$$\mathbb{R} = \left[\frac{\mathbb{I}}{\Delta t_n} - \Theta \, \mathbb{A} \right]^{-1} \left[\frac{\mathbb{I}}{\Delta t_n} + (1 - \Theta) \, \mathbb{A} \right] \ .$$

Theta scheme with point kinetics 2

The eigenvalue problem associated to the above iterative scheme is written

$$\gamma_i \, \boldsymbol{p}_i - \mathbb{R} \, \boldsymbol{p}_i = \boldsymbol{0}$$

where γ_i is the i–th eigenvalue of matrix $\mathbb{R}$ and $\boldsymbol{p}_i$ is the corresponding eigenvector. We can easily show that these eigenvectors are identical to those of the inhour equation and that the corresponding eigenvalues are related using

$$\gamma_i = \frac{1 + (1 - \Theta) \, \omega_i \, \Delta t_n}{1 - \Theta \, \omega_i \, \Delta t_n} \quad .$$

The eigenvectors of matrix $\mathbb{R}$ are linearly independent, so that the initial condition $\boldsymbol{x}_0$ can be expressed as a linear combination:

$$\boldsymbol{x}_0 \equiv \boldsymbol{x}^{(0)} = \sum_i c_i \, \boldsymbol{p}_i \quad .$$

Stability condition

After a progression of n time-steps, we have

$$\boldsymbol{x}^{(n)} = \mathbb{R}\,\boldsymbol{x}^{(n-1)} = \mathbb{R}\sum_i c_i\,\gamma_i^{n-1}\,\boldsymbol{p}_i = \sum_i c_i\,\gamma_i^{n}\,\boldsymbol{p}_i \quad .$$

We apply a negative reactivity $\rho < 0$ to a point kinetics problem and verify that the numerical solution given by previous equation vanishes as t increases. The stability will be guaranteed if $|\gamma_i| < 1$ for all values of i.

If $\rho < 0$, we observe from inhour figure that all eigenvalues ω_i are negative. γ_i equation leads to condition $|\gamma_i| < 1$ if

$$-\left(1 + \Theta\,|\omega_i|\,\Delta t_n\right) < 1 - (1-\Theta)\,|\omega_i|\,\Delta t_n < 1 + \Theta\,|\omega_i|\,\Delta t_n$$

which is satisfied if $\frac{1-2\Theta}{2}\,|\omega_i|\,\Delta t_n < 1 \; ; \;\; \forall\, i$.

Stability condition

We conclude that

- the explicit scheme ($\Theta = 0$) is stable if the time-step size is set below a threshold value written as

$$\Delta t_n < \frac{2}{\max_i(|\omega_i|)} \quad .$$

- the fully implicit and Crank-Nicholson schemes are unconditionally stable. The practical choice of Θ for production calculations is selected in interval $1/2 \le \Theta \le 1$.

Space-time kinetics with $\Theta = 1$

$$\frac{1}{V_{\mathrm{n},g}\,\Delta t_n}\,\phi_g(\boldsymbol{r},t_n) - \boldsymbol{\nabla}\cdot\mathbb{D}_g(\boldsymbol{r})\boldsymbol{\nabla}\phi_g(\boldsymbol{r},t_n) + \Sigma_{\mathrm{r}g}(\boldsymbol{r})\,\phi_g(\boldsymbol{r},t_n)$$

$$= S_g^{\mathrm{imp}}(\boldsymbol{r},t_n) + \sum_{\substack{h=1\\h\neq g}}^{G}\Sigma_{g\leftarrow h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t_n)$$

$$+ \left\{\chi_g^{\mathrm{ss}}(\boldsymbol{r}) - \sum_{\ell}\chi_{\ell,g}^{\mathrm{del}}(\boldsymbol{r})\,\frac{\beta_\ell}{1+\lambda_\ell\,\Delta t_n}\right\}\sum_{h=1}^{G}\nu\Sigma_{\mathrm{f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t_n)$$

$$c_\ell(\boldsymbol{r},t_n) = \frac{1}{1+\lambda_\ell\,\Delta t_n}\left[c_\ell(\boldsymbol{r},t_{n-1}) + \beta_\ell\,\Delta t_n\sum_{h=1}^{G}\nu\Sigma_{\mathrm{f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t_n)\right]$$

Space-time kinetics with $\Theta = 1$ 2

with the fixed source defined as

$$
\begin{aligned}
S_g^{\rm imp}(\boldsymbol{r},t_n) &= \frac{1}{V_{{\rm n},g}\,\Delta t_n}\,\phi_g(\boldsymbol{r},t_{n-1}) \\
&+ \sum_\ell \chi_{\ell,g}^{\rm del}(\boldsymbol{r})\,\frac{\lambda_\ell}{1+\lambda_\ell\,\Delta t_n}\,c_\ell(\boldsymbol{r},t_{n-1}) + q_g(\boldsymbol{r},t_n)
\end{aligned}
$$

Space-time kinetics with $\Theta = 0$

$$\frac{1}{V_{\mathrm{n},g}\,\Delta t_n}\,\phi_g(\boldsymbol{r},t_n) = S_g^{\mathrm{exp}}(\boldsymbol{r},t_n)$$

$$c_\ell(\boldsymbol{r},t_n) = (1-\lambda_\ell\,\Delta t_n)\,c_\ell(\boldsymbol{r},t_{n-1}) + \beta_\ell\,\Delta t_n\sum_{h=1}^{G}\nu\Sigma_{\mathrm{f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r},t_{n-1})$$

Space-time kinetics with $\Theta = 0$ 2

with the fixed source defined as

$$\begin{aligned}
S_g^{\rm exp}(\boldsymbol{r}, t_n) &= \frac{1}{V_{{\rm n},g}\,\Delta t_n}\,\phi_g(\boldsymbol{r}, t_{n-1}) + \boldsymbol{\nabla}\cdot\mathbb{D}_g(\boldsymbol{r})\boldsymbol{\nabla}\phi_g(\boldsymbol{r}, t_{n-1}) \\
&- \Sigma_{{\rm r}g}(\boldsymbol{r})\,\phi_g(\boldsymbol{r}, t_{n-1}) + \sum_{\substack{h=1\\h\neq g}}^{G} \Sigma_{g\leftarrow h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r}, t_{n-1}) \\
&+ \left[\chi_g^{\rm ss}(\boldsymbol{r}) - \sum_\ell \beta_\ell\,\chi_{\ell,g}^{\rm del}(\boldsymbol{r})\right] \sum_{h=1}^{G} \nu\Sigma_{{\rm f}h}(\boldsymbol{r})\,\phi_h(\boldsymbol{r}, t_{n-1}) \\
&+ \sum_\ell \chi_{\ell,g}^{\rm del}(\boldsymbol{r})\,\lambda_\ell\,c_\ell(\boldsymbol{r}, t_{n-1}) + q_g(\boldsymbol{r}, t_{n-1}) \ \ .
\end{aligned}$$