IQS Notes
TAMU

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Contents

1 Time-dependent diffusion

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} = \nu_p \sigma_f \Phi - (-\nabla\cdot D\nabla\Phi + \sigma_a \Phi) + \lambda C \tag{1}$$

$$\frac{dC}{dt} = \nu_d \sigma_f \Phi - \lambda C \tag{2}$$

2 IQS

2.1 Factorization

Factorization into amplitude and shape functions:

$$\Phi(\vec{r},t) = p(t)\varphi(\vec{r},t) \tag{3}$$

Factorization is not unique:

$$\Phi(\vec{r},t) = \frac{p(t)}{f(t)}\left(f(t)\varphi(\vec{r},t)\right)$$

2.2 Equations for the shape φ

$$\frac{1}{v}\frac{\partial \varphi}{\partial t} = \nu_p \sigma_f \varphi - (-\nabla\cdot D\nabla\varphi + (\sigma_a + \alpha(t))\varphi) + \frac{1}{p}\lambda C \tag{4}$$

where

$$\alpha(t) = \frac{1}{v}\frac{1}{p(t)}\frac{dp}{dt}$$

Very little change in the precursor equation:

$$\frac{dC}{dt} = \nu_d \sigma_f p\varphi - \lambda C \tag{5}$$

2.3 Equations for the amplitude p

These are simply obtained by integration of the shape equations over the entire space. We use the following short-cut notation:

$$\langle f, g\rangle = \int_{\text{domain}} f(\vec{r})g(\vec{r})d^3r$$

The starting point is the shape equation (re-written below before division by p occurred).

$$\frac{1}{v}p\frac{\partial \varphi}{\partial t} + \frac{1}{v}\varphi\frac{dp}{dt} = \nu_p \sigma_f p\varphi - p\left(-\nabla\cdot D\nabla\varphi + \sigma_a\varphi\right) + \lambda C \tag{6}$$

Before carrying out the integration over space, we multiply the equation by a time-independent weighting function (a common choice for this function is the initial adjoint flux, $\Phi_0^\dagger$).

After a bit of algebra, we obtain

$$\frac{dp}{dt} = \left(\frac{\rho}{\Lambda} - \frac{\beta}{\Lambda} - \theta\right) p + \lambda\xi \tag{7}$$

$$\frac{d\xi}{dt} = \frac{\beta}{\Lambda} p - (\lambda + \theta)\,\xi \tag{8}$$

with the following definitions

$$\frac{\rho}{\Lambda} = \frac{\langle \Phi_0^\dagger, [\nu\sigma_f - (-\nabla\cdot D\nabla + \sigma_a)]\,\varphi\rangle}{\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle} \tag{9}$$

$$\frac{\beta}{\Lambda} = \frac{\langle \Phi_0^\dagger, \nu_d\sigma_f\varphi\rangle}{\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle} \tag{10}$$

$$\theta = \frac{\langle \Phi_0^\dagger, v^{-1}\frac{\partial\varphi}{\partial t}\rangle}{\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle} = \frac{\frac{d}{dt}\langle \Phi_0^\dagger, v^{-1}\varphi\rangle}{\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle} \tag{11}$$

The total time derivative expression for θ is due to the fact that v and the initial adjoint function are both independent of time.

We have also defined

$$\xi = \frac{\langle \Phi_0^\dagger, C\rangle}{\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle}$$

which gives

$$\langle \Phi_0^\dagger, \frac{dC}{dt}\rangle = \langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle\frac{d\xi}{dt} + \xi\frac{d}{dt}\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle$$

and explains the presence of the θ term in the PRKE equation for the precursor concentrations.

2.4 Normalization choice

We choose to have the following quantity constant in time

$$\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle = K_0 \tag{12}$$

even though the shape itself may still be allowed to change in time.

This makes the factorization **unique** and lets $\theta = 0$, yielding the standard form of the PRKE equations (note that in the PRKE approximation, i.e., when the shape is assume independent of time, we automatically have $\theta = 0$).

$$\frac{dp}{dt} = \left(\frac{\rho}{\Lambda} - \frac{\beta}{\Lambda}\right) p + \lambda\xi \tag{13}$$

$$\frac{d\xi}{dt} = \frac{\beta}{\Lambda} p - \lambda\xi \tag{14}$$

2.5 IQS solution procedure

In the IQS method, the shape is solved for on macro time steps $[t^n, t^{n+1}]$ (one solve for the shape over that time step) while the PRKE equations are solve on micro time steps: $t^n, t^{n+1/M}, \dots, t^{n+m/M}, \dots, t^{n+1}$ (for a total of M solves during one macro time step).

Because of the factorization approximation, we are actually solving a nonlinear problem over the macro time step. Convergence is said to be reached when the new shape $\varphi(\vec{r}, t^{n+1})$ satisfies the normalize condition $\langle \Phi_0^\dagger, v^{-1}\,\varphi\rangle = K_0$.

The process over $[t^n, t^{n+1}]$ is as follows. Let the nonlinear iteration index be ℓ.

1. Set $\ell = 0$
2. Estimate the shape at the end time $\varphi^{n+1,\ell}$ (could be extrapolation, or just assume equal to begin time shape function)
3. Using the begin time and end time shape to compute ρ/Λ and β/Λ at the micro time steps (this is a bit costly, so in reality we only do this for a certain multiple of the micro time steps, assuming a linear variation in time of the shape and using the exact values of the XS at the evaluation instants).
4. Solve the PRKE equations using data from 3.
5. Compute $\alpha(t^{n+1}) = \frac{1}{v}\frac{1}{p(t^{n+1})}\left.\frac{dp}{dt}\right|_{t^{n+1}}$
6. Compute the shape at the end time $\varphi^{n+1,\ell+1}$
7. Check for convergence in K_0. If so, EXIT
8. Otherwise $\ell \leftarrow \ell + 1$ and GO BACK to 3.

3 Homogeneous perturbation in an homogenous domain

In this Section I consider a “simple” test case which I was hoping to test the implementation of IQS.

3.1 Problem description

Consider an initially critical homogeneous slab reactor solved with 1-g diffusion theory. The initial flux/shape is therefore a cosine. We can make the reactor critical simply by dividing the ν's with $\mathrm{k_{eff}}$.

At time $t = 0$, the σ_a is subjected to a variation that is linear in time (and this, at all times, the domain remains homogenous, i.e., no spatially varying cross sections).

Because the initial flux only contains the steady-state fundamental mode and because the modification is homogeneous, no other modes are excited and the flux function only changes in magnitude. That is, the shape function remains constant and the flux amplitude is actually given by the solution of the PRKE.

3.2 Brute force temporal discretization

A backward Euler time discretization yields, for the flux,

$$\frac{1}{v}\frac{\Phi^{n+1}-\Phi^{n}}{\Delta t} = (\nu_p\sigma_f)^{n+1}\Phi^{n+1} - \left(-\nabla\cdot D\nabla + \sigma_a\right)^{n+1}\Phi^{n+1} + \lambda C^{n+1} \tag{15}$$

For a constant shape, this becomes:

$$\frac{\varphi_0}{v}\frac{p^{n+1}-p^{n}}{\Delta t} = (\nu_p\sigma_f)^{n+1}\varphi_0 p^{n+1} - \left(-\nabla\cdot D\nabla + \sigma_a\right)^{n+1}\varphi_0 p^{n+1} + \lambda\varphi_0\xi^{n+1} \tag{16}$$

What equations should be satisfied by p^{n+1} and ξ^{n+1}? Simply the PRKE discretized with backward Euler over $[t^n, t^{n+1}]$ (one step!). This can be easily verified if you take the above equation, multiply it by $\Phi_0^\dagger$ and integrate over the entire domain.

We numerically observed that the brute-force solve yielded the same results as the PRKE solve when using the initial shape in the PRKE parameters.

3.3 IQS approach with NO subcycling for the PRKE

If the shape and the amplitude functions are solved using the same time step, then we have

$$\frac{1}{v}\frac{\varphi^{n+1}-\varphi^{n}}{\Delta t} = (\nu_p\sigma_f)^{n+1}\varphi^{n+1} - \left(-\nabla\cdot D\nabla + (\sigma_a+\alpha)\right)^{n+1}\varphi^{n+1} + \frac{1}{p^{n+1}}\lambda C^{n+1} \tag{17}$$

where

$$\alpha^{n+1} = \frac{1}{v}\frac{1}{p^{n+1}}\frac{p^{n+1}-p^{n}}{\Delta t}$$

This form of α is due to the fact that we assumed here to employ only one time interval for the PRKE (no subcycling). Note that by letting $\varphi^{n+1} = \varphi^n = \varphi_0$, we can re-arrange Eq. (17) as Eq. (15).

3.4 IQS approach with subcycling for the PRKE

Now, Eq. (17) tells you also something quite important. If you solve Eq. (17) for φ^{n+1}, you obtain a solution (we verified if the PRKE are done with the same time step as the shape, that the shape solution remains constant). Now, Eq. (17) is a linear system ($A\varphi^{n+1} = b$), so if I change slightly the entry of matrix A, I should get another solution for φ^{n+1}. Well, subcycling the PRKE gives us a better value for α (it is more accurate since we solve the PRKE on a finer time grid), so we automatically see that φ^{n+1} cannot remain constant equal to its initial value. Where's the flaw ????