

TREAT Mission Supporting Problem Improved Quasi-Static Method in Rattlesnake

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December 1, 2015

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Time-dependent Multigroup Transport

Fluxes ($1 \leq g \leq G$)

$$\frac{1}{\nu^g} \frac{\partial \Psi^g(\vec{r}, \vec{\Omega}, t)}{\partial t} = \sum_{g'=1}^G \int_{4\pi} d\Omega' \left[\Sigma_s^{g' \rightarrow g}(\vec{r}, \vec{\Omega}' \cdot \vec{\Omega}, t) + \frac{\chi_p^g}{4\pi} \nu_p \Sigma_f^{g'}(\vec{r}, t) \right] \Psi^{g'}(\vec{r}, \vec{\Omega}', t)$$

$$- \operatorname{div} [\vec{\Omega} \Psi^g(\vec{r}, \vec{\Omega}, t)] - \Sigma^g(\vec{r}, t) \Psi^g(\vec{r}, \vec{\Omega}, t) + \sum_{i=1}^I \frac{\chi_{d,i}^g(\vec{r})}{4\pi} \lambda_i C_i(\vec{r}, t)$$

+ IC + BC

In operator notation:

$$\frac{1}{\nu} \frac{\partial \Psi}{\partial t} = (H + P_p - L)\Psi + S_d$$

Precursors C_i ($1 \leq i \leq I$)

$$\frac{dC_i}{dt} = \sum_{g=1}^G \nu_{d,i} \Sigma_f^g(\vec{r}, t) \Phi^g(\vec{r}, t) - \lambda_i(\vec{r}, t) C_i(\vec{r}, t)$$

Flux Factorization

Factorization

Decomposition of the multigroup flux into the **product** of a time-dependent **amplitude** (p) and a space-/time-dependent multigroup **shape** (ψ):

$$\Psi^g(\vec{r}, \vec{\Omega}, t) = p(t)\psi^g(\vec{r}, \vec{\Omega}, t)$$

and, for the scalar flux,

$$\Phi^g(\vec{r}, t) = p(t)\varphi^g(\vec{r}, t)$$

with, obviously,

$$\varphi^g(\vec{r}, t) = \int_{4\pi} d\Omega' \psi^g(\vec{r}, \vec{\Omega}', t)$$

- Factorization is **not** an approximation
 - When reporting these in the previous equations, one obtains to the so-called **shape** equations.
 - Note that **factorization is not unique**:

$$\Psi = \cancel{p} \times \psi = \frac{\cancel{p}}{a} \times (a\psi)$$

Shape equations

Shape equations

The shape equations are similar to the original transport equations:

$$\frac{1}{v} \frac{\partial \psi}{\partial t} = (H + P_p - \tilde{L})\psi + \frac{1}{p} S_d$$

$$\frac{dC_i}{dt} = \sum_{g=1}^G \nu_{d,i} \Sigma_f^g(\vec{r}, t) p \varphi^g(\vec{r}, t) - \lambda_i(\vec{r}, t) C_i(\vec{r}, t)$$

Differences with original transport equation

- ① An additional removal term based on $\frac{1}{v^g} \frac{1}{p} \frac{dp}{dt} \psi^g$

$$\tilde{L}^g = L^g + \frac{1}{v^g} \frac{1}{p} \frac{dp}{dt}$$

- ② Delayed neutron source term scaled by $\frac{1}{p}$
- ③ **No change** in the precursor equations but we have re-written them to show explicitly $p \times \varphi^g$

Shape equations: Implementation within the MOOSE framework

Shape equations → FEM solver + implicit time integration

$$\frac{1}{\nu} \frac{\psi^{n+1} - \psi^n}{\Delta t} = \left(H^{n+1} + P_p^{n+1} - L^{n+1} - \frac{1}{\nu} \frac{1}{p^{n+1}} \left. \frac{dp}{dt} \right|_{n+1} \right) \psi^{n+1} + \frac{1}{p^{n+1}} S_d^{n+1}$$

Modification to the original transport equation

- ① An additional removal term based on $\frac{1}{\nu g} \frac{1}{p} \frac{dp}{dt} \psi^g$
→ add a new kernel in Rattlesnake (easy)
- ② Delayed neutron source term scaled by $\frac{1}{p}$
→ scale the delayed neutron source kernel (easy)
- ③ nonlinear coupling between shape variable ψ^{n+1} and amplitude variable p^{n+1}
→ employ MOOSE's nonlinear solvers (easy)

Amplitude equations, Point Reactor Kinetics Equations (PRKE)

Principle

To obtain the **amplitude** equation, we multiply the shape equations with a weighting function (initial adjoint flux, Ψ^*), then integrate over phase-space.

Notation

For brevity, the adjoint flux product and integration over phase-space will be represented with parenthetical notation:

$$\int_{4\pi} \int_D \Psi^{*g}(\vec{r}, \vec{\Omega}) f^g(\vec{r}, \vec{\Omega}) d^3 r d\Omega = (\Psi^{*g}, f^g)$$

Uniqueness of the factorization

In order to impose uniqueness of the factorization, one requires:

$$K_0 = \sum_{g=1}^G \left(\Psi^{*g}, \frac{1}{\nu^g} \psi^g \right) = \text{constant}$$

PRKE (continued)

PRKE

$$\frac{d\textcolor{red}{p}}{dt} = \left[\frac{\rho - \bar{\beta}}{\Lambda} \right] \textcolor{red}{p} + \sum_{i=1}^I \bar{\lambda}_i \xi_i$$

$$\frac{d\xi_i}{dt} = \frac{\bar{\beta}_i}{\Lambda} \textcolor{red}{p} - \bar{\lambda}_i \xi_i \quad 1 \leq i \leq I$$

PRKE Coefficients

$$\frac{\rho - \bar{\beta}}{\Lambda} = \frac{(\Psi^*, (H + P_p - L)\textcolor{blue}{\psi})}{K_0}$$

$$\frac{\bar{\beta}}{\Lambda} = \sum_{i=1}^I \frac{\bar{\beta}_i}{\Lambda} = \sum_{i=1}^I \frac{(\Psi^*, P_{d,i}\textcolor{blue}{\psi})}{K_0}$$

$$\bar{\lambda}_i = \frac{(\Psi^*, \chi_{d,i} \lambda_i \textcolor{blue}{C}_i)}{(\Psi^*, \chi_{d,i} \textcolor{blue}{C}_i)}$$

These functionals seem daunting to implement but this was relatively straightforward with a couple of options available in MOOSE: (1) element integral postprocessors and (2) save_in kernel attributes)

Coupling between shape and amplitude equations

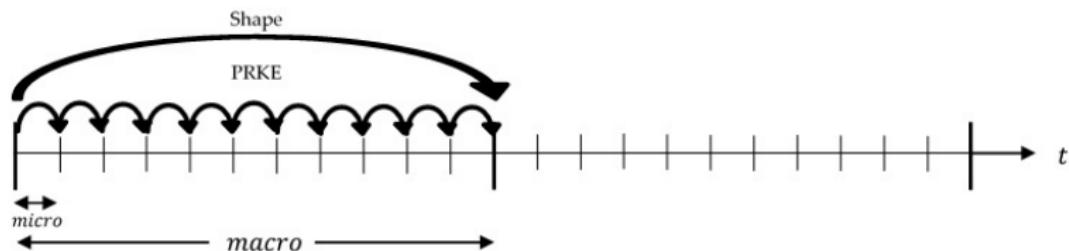
Factorization leads to a **nonlinear** system

The amplitude and shape equations form a system of **nonlinear** coupled equations:

- ① the coefficients appearing in the **PRKEs** depend upon the **shape** solution,
- ② the **shape** equation has a kernel dependent on **amplitude** and its derivative,

Time scales and IQS method solution process

Because solving for the shape can be expensive, especially in two or three dimensions, it is attractive to make the assumption that the shape is weakly time-dependent so the shape can be computed after a multitude of PRKE calculations:



In MOOSE, we employ the available Picard iteration functionality to resolve the nonlinearities

Convergence criteria

Ideally

The normalization constant should not change over time !

$$K_0 = \sum_{g=1}^G \left(\Psi^{*g}, \frac{1}{\nu^g} \psi^g(t=0) \right) = \text{constant}$$

Thus, we employ

$$\left| \frac{\sum_{g=1}^G (\Psi^{*g}, \frac{1}{\nu^g} \psi^g(t=t^{n+1}))}{K_0} - 1 \right| = \left| \frac{K_{n+1}}{K_0} - 1 \right| < tol$$

Note that we have seen in practice ...

$$\frac{\|\psi^{g,\ell+1}_{t_{n+1}} - \psi^{g,\ell}_{t_{n+1}}\|}{\|\psi^{g,\ell+1}_{t_{n+1}}\|} < tol \quad \text{or even} \quad \frac{\|\psi^{g,\ell+1}_{t_{n+1}} - \psi^{g,0}_{t_{n+1}}\|}{\|\psi^{g,0}_{t_{n+1}}\|} < tol$$

where ℓ = IQS iteration index over a given macro time step $[t_n, t_{n+1}]$

These empirical criteria must be followed by a renormalization before starting the next time step $[t_{n+1}, t_{n+2}]$

$$\psi^{g,\overset{\text{converged}}{t_{n+1}}} \leftarrow \psi^{g,\overset{\text{converged}}{t_{n+1}}} \times \frac{K_{n+1}^{\text{converged}}}{K_0}$$



Precursors time-discretization

A simple ODE:

$$\frac{dC_i}{dt} = \sum_{g=1}^G \nu_{d,i} \Sigma_f^g(\vec{r}, t) p \varphi^g(\vec{r}, t) - \lambda_i(\vec{r}, t) C_i(\vec{r}, t)$$

Numerical integration: Theta-scheme (already in Rattlesnake)

$$C^{n+1} = \frac{1 - (1 - \theta)\Delta t \lambda}{1 + \theta \Delta t \lambda} C^n + \frac{(1 - \theta)\Delta t \beta (\nu \Sigma_f)^n}{1 + \theta \Delta t \lambda} \varphi^n p^n + \frac{\theta \Delta t \beta (\nu \Sigma_f)^{n+1}}{1 + \theta \Delta t \lambda} \varphi^{n+1} p^{n+1} \quad (1)$$

Reporting this value of C^{n+1} in S_d^{n+1} , one can solve for the shape ψ^{n+1} as a function of ψ^n and C^n (and p^n , p^{n+1} , $dp/dt|_n$ and $dp/dt|_{n+1}$).

Once ψ^{n+1} has been determined, C^{n+1} is updated.

Rattlesnake currently implements both implicit ($\theta = 1$) and Crank-Nicholson ($\theta = 1/2$) as options for precursor evaluation.

Analytical Integration

Analytical Integration

$$C^{n+1} = C^n e^{-\lambda(t_{n+1}-t_n)} + \int_{t_n}^{t_{n+1}} \nu_d \Sigma_f(t') \varphi(t') p(t') e^{-\lambda(t_{n+1}-t')} dt'$$

Assuming a **linear in time variation** over the macro time step $[t_n, t_{n+1}]$ for the **shape** and the **fission cross section**, we get:

$$C^{n+1} = C^n e^{-\lambda \Delta t} + [a_3(\nu_d \Sigma_f)^{n+1} + a_2(\nu_d \Sigma_f)^n] \varphi^{n+1} + [a_2(\nu_d \Sigma_f)^{n+1} + a_1(\nu_d \Sigma_f)^n] \varphi^n$$

where the integration coefficients are defined as:

$$\begin{aligned} a_1 &= \int_{t_n}^{t_{n+1}} \left(\frac{t_{n+1} - t'}{\Delta t} \right)^2 p(t') e^{-\lambda(t_{n+1}-t')} dt' \\ a_2 &= \int_{t_n}^{t_{n+1}} \frac{(t' - t_n)(t_{n+1} - t')}{(\Delta t)^2} p(t') e^{-\lambda(t_{n+1}-t')} dt' \\ a_3 &= \int_{t_n}^{t_{n+1}} \left(\frac{t' - t_n}{\Delta t} \right)^2 p(t') e^{-\lambda(t_{n+1}-t')} dt' \end{aligned}$$

The amplitude **p** is contained in the a_i 's integration coefficients.
 $p(t)$ has been **accurately calculated** at the **micro time** step level.



Changes to Rattlesnake

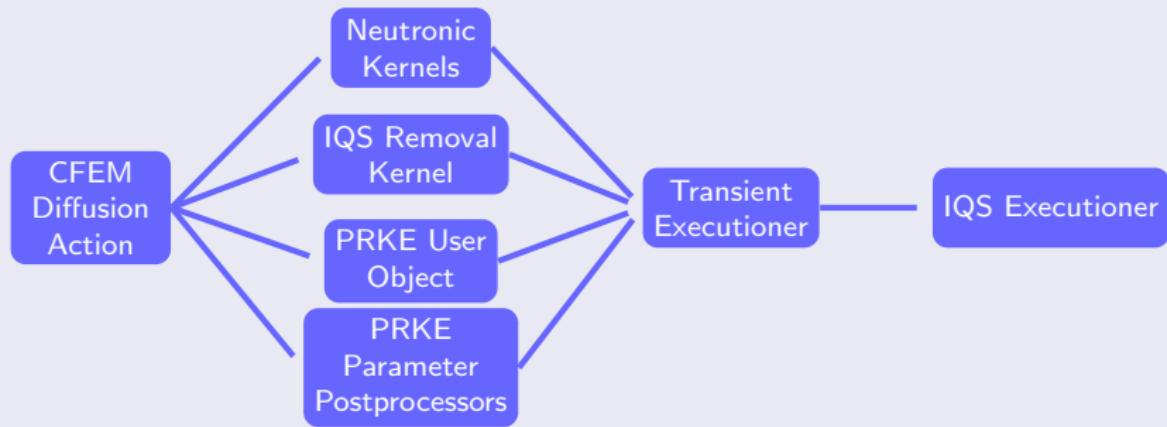
Action Systems

- Continuous FEM Diffusion (**almost complete**)
- Discontinuous FEM Diffusion
- Discontinuous FEM Sn Transport (first-order form)
- Discontinuous FEM Sn Transport (SAAF form)

Four action systems \neq four times the work!

- Action System (adding IQS as an option)
- Post-processors (**element integrals**) for PRKE coefficients: $\rho - \bar{\beta}, \bar{\beta}_i, \bar{\lambda}_i$
Note that the numerator of $\rho - \bar{\beta}$, i.e., $(\Psi^*, (H + P_p - L)\psi)$, is particularly easy thanks to the residual `save_in` option of MOOSE.
- IQS **userobject** (PRKE solve using updated PRKE coefficients)
- IQS **executioner** derived from MOOSE executioner (use of the existing Picard iteration loop in the transient executioner; this can seamlessly enable IQS in multiphysics simulations without any further changes)

Break down of IQS Changes



TWIGL benchmark

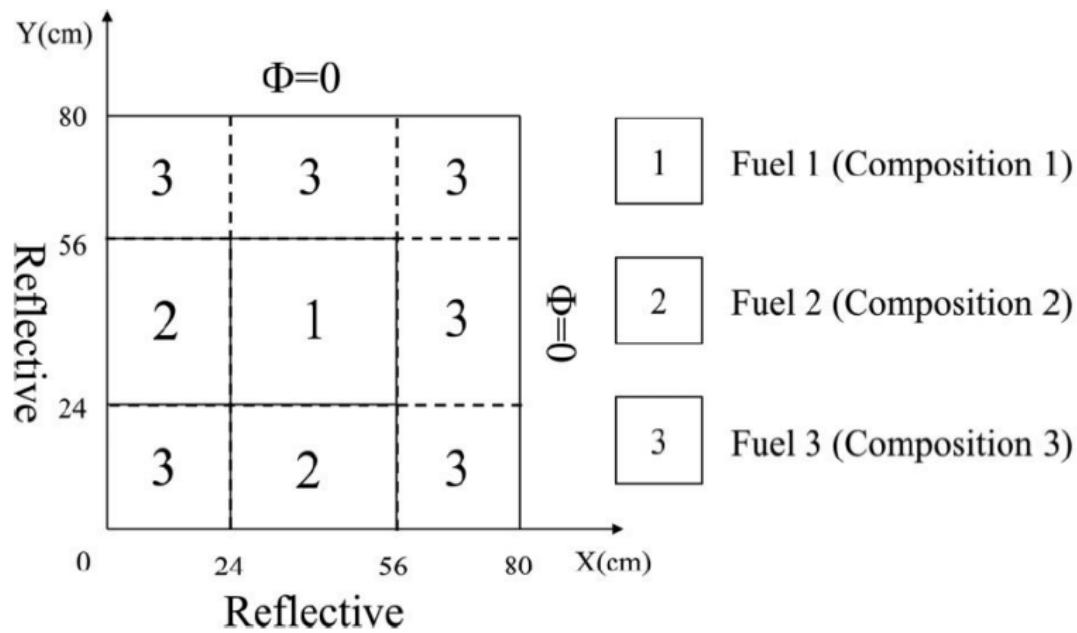
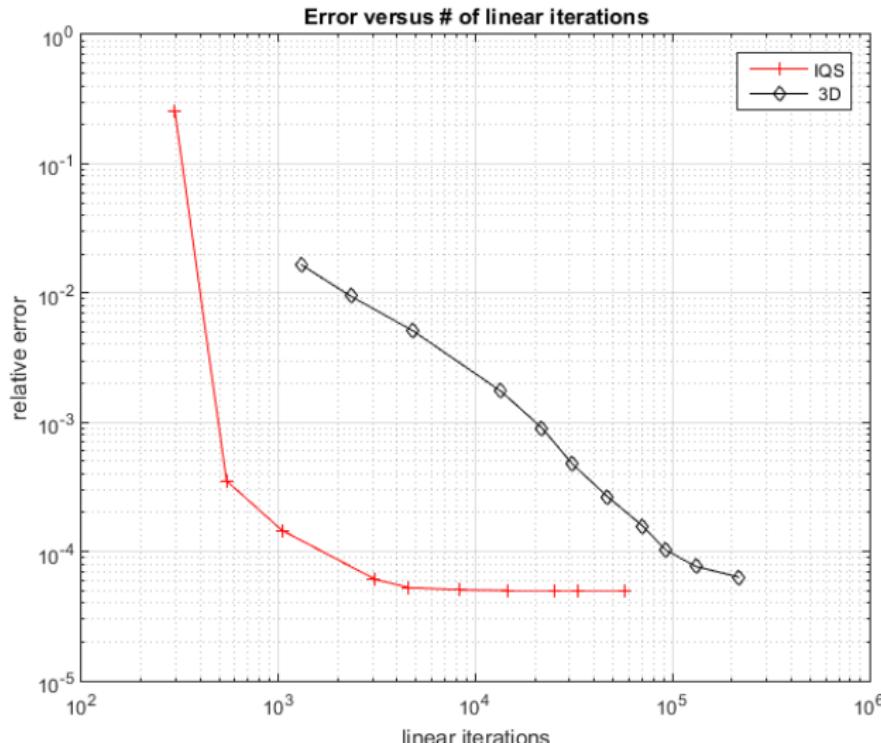


Figure 3. The TWIGL benchmark problem.

TWIGL: Computational Efficacy

Relative error versus # of linear iterations:

Note: saturation due to ref. solution not (yet) accurate enough



TWIGL: Timing

Hot off the press: CPU time

Method	CPU (s)
IQS	205.2
standard	789.5

- IQS is about 4 times faster than the standard approach for the same macro time step size.
- Additional gains are expected when time-step control will be implemented (as larger time steps may be taken for the shape equations)

TWIGL: Shape and flux movies (thermal group)

Conclusion and Outlook

Completed

- Implementation of analytical precursor integration
- IQS for **CFEM Diffusion** action system

In progress

- Rattlesnake documentation
- Time step adaptation/control
- Kinetics benchmarks (neutronics only, e.g., TWIGL, LMW, TREAT)

Next Steps

- DFEM Diffusion action system
- DFEM SN Transport action system
- Dynamics benchmarks (i.e., with feedback, e.g., the LRA test case, TREAT)
- Study of a JFNK-based algorithm to resolve the IQS nonlinearity between the amplitude/shape equations

Questions ?

Thanks

- Yaqi Wang (INL, Rattlesnake code lead)
- Mark DeHart (INL, TREAT M&S lead)
- NEAMS

