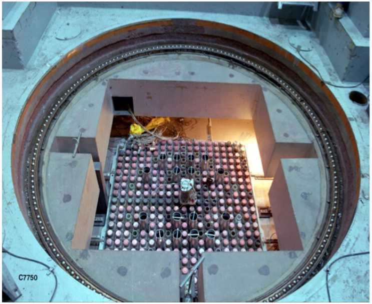


Improved Quasi-Static Method with Step Doubling Adaptation

Zachary M. Prince, Jean C. Ragusa

Department of Nuclear Engineering, Texas A&M University, College Station, TX

November 6, 2016

email: zachmprince@tamu.edu

Outline

1. IQS Theory
   - Time-dependent Multigroup Diffusion
   - IQS Equations
   - IQS method solution process
2. Time Adaptation
   - Theory
   - Solution Process
3. Results
   - TWIGL
   - LRA
   - TREAT
4. Wrap-up

Time-dependent Multigroup Diffusion

Group Fluxes ϕ^g $(1 \le g \le G)$ with Precursors C_i $(1 \le i \le I)$

$$\frac{1}{v^g}\frac{\partial \phi^g}{\partial t} = \frac{\chi_p^g}{k_{eff}} \sum_{g'=1}^{G} (1-\beta)\nu^{g'} \Sigma_f^{g'} \phi^{g'} - \left(-\vec{\nabla}\cdot D^g \vec{\nabla} + \Sigma_r^g\right) \phi^g$$

$$+ \sum_{g' \neq g}^{G} \Sigma_s^{g' \to g} \phi^{g'} + \sum_{i=1}^{I} \chi_{d,i}^g \lambda_i C_i \ , \quad 1 \le g \le G$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{k_{eff}} \sum_{g=1}^{G} \nu^g \Sigma_f^g \phi^g - \lambda_i C_i \ , \quad 1 \le i \le I$$

Flux Factorization

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

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

- Factorization is **not** an approximation.
- Note that $p(t)$ and $\varphi^g(\vec{r},t)$ are not unique.

Shape equations

Shape equations

Implementing factorization and solving for φ^g:

$$\frac{1}{v^g}\frac{\partial \varphi^g}{\partial t} = \frac{\chi_p^g}{k_{eff}} \sum_{g'=1}^{G} (1-\beta)\nu^{g'} \Sigma_f^{g'} \varphi^{g'} - \left(-\vec{\nabla} \cdot D^g \vec{\nabla} + \Sigma_r^g + \frac{1}{v^g}\frac{1}{p}\frac{dp}{dt} \right) \varphi^g$$
$$+ \sum_{g' \neq g}^{G} \Sigma_s^{g' \to g} \varphi^{g'} + \frac{1}{p} \sum_{i=1}^{I} \chi_{d,i}^g \lambda_i C_i \ , \quad 1 \leq g \leq G$$

$$\frac{dC_i}{dt} = p \sum_{g=1}^{G} \nu_{d,i} \Sigma_f^g \varphi^g - \lambda_i C_i, \quad 1 \leq i \leq I$$

Differences with original transport equation

1. An additional removal term based on $\frac{1}{v^g}\frac{1}{p}\frac{dp}{dt}\varphi^g$
2. Delayed neutron source term scaled by $\frac{1}{p}$
3. The delayed fission source in the precursor equation scaled by p

Amplitude equations (PRKE)

Principle

To obtain the amplitude equation, we multiply the shape equations with a weighting function (initial adjoint flux, ϕ^{*g}), then integrate over domain.

Notation

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

$$\int_D \phi^{*g}(\vec{r}) f(\vec{r}) dr^3 = (\phi^{*g}, f)$$

Uniqueness of the factorization

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

$$K_0 = \sum_{g=1}^{G} \left(\phi^{*g}, \frac{1}{v^g} \varphi^g \right) = constant$$

This condition will be the criteria for solution convergence

Point Reactor Kinetics Equation

PRKE

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

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

PRKE Coefficients

$$\frac{\rho - \bar{\beta}}{\Lambda} = \frac{\sum_{g=1}^{G} \left(\phi^{*g}, \sum_{g'=1}^{G} \frac{\chi_p^g}{k_{eff}} \nu_p^{g'} \Sigma_f^{g'} \varphi^{g'} + \sum_{g' \neq g}^{G} \Sigma_s^{g' \to g} \varphi^{g'} - \left(-\vec{\nabla} \cdot D^g \vec{\nabla} + \Sigma_r^g \right) \varphi^g \right)}{\sum_{g=1}^{G} \left(\phi^{*g}, \frac{1}{v^g} \varphi^g \right)}$$

$$\frac{\bar{\beta}}{\Lambda} = \sum_{i=1}^{I} \frac{\bar{\beta}_i}{\Lambda} = \frac{1}{k_{eff}} \frac{\sum_{i=1}^{I} \sum_{g=1}^{G} (\phi^{*g}, \beta_i \nu^g \Sigma_f^g \varphi^g)}{\sum_{g=1}^{G} \left(\phi^{*g}, \frac{1}{v^g} \varphi^g \right)}$$

$$\bar{\lambda}_i = \frac{\sum_{g=1}^{G} (\phi^{*g}, \chi_{d,i}^g \lambda_i C_i)}{\sum_{g=1}^{G} (\phi^{*g}, \chi_{d,i}^g C_i)}$$

IQS

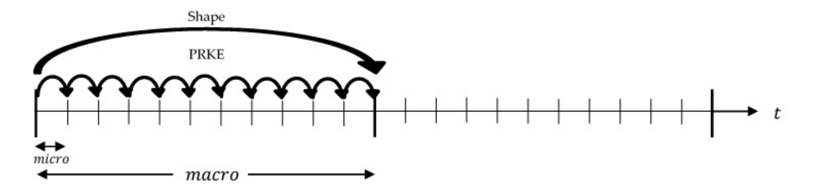
Factorization leads to a nonlinear system

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

1. the coefficients appearing in the PRKE's 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:



Convergence criteria

Ideally

The normalization constant should not change over time !

$$K_0 = \sum_{g=1}^{G} \left(\phi^{*g}, \frac{1}{v^g} \varphi_0^g \right) = constant$$

Thus, we employ $$\left| \frac{\sum_{g=1}^{G} \left(\phi^{*g}, \frac{1}{v^g} \varphi_{n+1}^g \right)}{K_0} - 1 \right| = \left| \frac{K_{n+1}}{K_0} - 1 \right| < tol$$

Note that we have seen in practice ...

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

where ℓ is the 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 $[t_{n+1}, t_{n+2}]$

$$\varphi_{n+1}^{g,converged} \times \frac{K_{n+1}^{converged}}{K_0} \rightarrow \varphi_{n+1}^{g}$$

IQS Predictor-Corrector

IQS P-C linearizes the system and avoids iterations on the shape:

1. Evaluate multigroup diffusion equation to get predicted flux $\phi_{n+1}^{g,pred}$
2. Scale predicted flux to obtain shape:

$$\varphi_{n+1}^{g} = \phi_{n+1}^{g,pred} \frac{\sum_{g=1}^{G}\left(\phi^{*g}, \frac{1}{v^g}\phi_0^g\right)}{\sum_{g=1}^{G}\left(\phi^{*g}, \frac{1}{v^g}\phi_{n+1}^{g,pred}\right)} = \phi_{n+1}^{g,pred}\frac{K_0}{K_{n+1}}$$

3. Compute PRKE parameters at t_{n+1}
4. Evaluate PRKE along micro step using interpolated parameters to obtain p_{n+1}
5. Scale φ_{n+1}^{g} to obtain corrected flux:

$$\phi_{n+1}^{g,corr} = p_{n+1} \times \varphi_{n+1}^{g}$$

Advantage: No IQS nonlinear iteration is necessary
Disadvantage: Assumes $\sum_{g=1}^{G}\left(\phi^{*g}, \frac{1}{v^g}\varphi_{n+1}^{g}\right)$ is inherently constant

Time Adaptation

Time Adaptation Theory

Motivation

- The concept of time adaptation is to have the behavior of some aspect of the evaluation determine the size of the time step.
- The computational efficiency of IQS is best demonstrated when time adaptation is applied.
- Step doubling adaptation was chosen because it is relatively simple and it utilizes the behavior of the solution to determine step size.

Local Truncation Error

We can estimate the local truncation error of the latest solve with a Taylor series expansion:

$$\|LTE_n\|_{L^2} = \Delta t_n^{p+1} \left\| \frac{\phi_n^{(p+1)}}{(p+1)!} + \Delta t_n \frac{\phi_n^{(p+2)}}{(p+2)!} + \ldots \right\|_{L^2}$$

Where p is the time discretization method's order and y_n is the solution at time $= t_n$. Δt_n was the latest solves time step and Δt_{n+1} is the next solves time step that has a desired error $\|LTE_{n+1}\|_{L^2}$. It can be

Step Doubling Theory

New Step Size

Using the definitions of the local errors:

$$\Delta t_{n+1}^{p+1} \simeq \Delta t_n^{p+1} \theta \frac{\|LTE_{n+1}\|_{L^2}}{\|LTE_n\|_{L^2}}$$

Where $\theta \equiv 1 + O(\Delta t_n)$. $\|LTE_{n+1}\|_{L^2}$ is some user defined relative error tolerance (e_{tol}) and $e_n \equiv \frac{\theta}{\|LTE_n\|_{L^2}}$ is a method's approximation to the last step's local error. Therefore in practice:

$$\Delta t_{new} = \Delta t_{old} \left[\frac{e_{tol}}{e_n}\right]^{1/(p+1)}$$

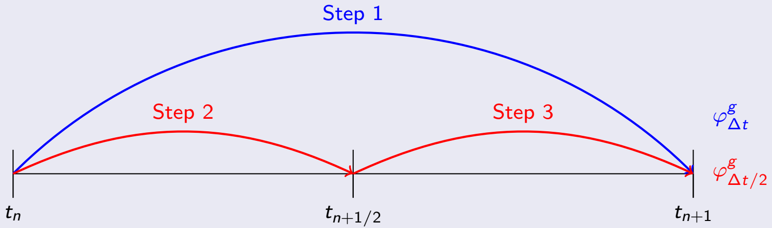
Step Doubling

Step doubling approximates the local error (e_n) by taking the difference in the local error of a solution with Δt ($\phi_{\Delta t}$) and $\Delta t/2$ ($\phi_{\Delta t/2}$):

$$e_n = \frac{\left\|\phi_{\Delta t/2} - \phi_{\Delta t}\right\|_{L^2}}{\max\left(\left\|\phi_{\Delta t/2}\right\|_{L^2}, \|]\phi_{\Delta t}\|_{L^2}\right)}$$

Step Doubling Solution Process

Solution Process with IQS

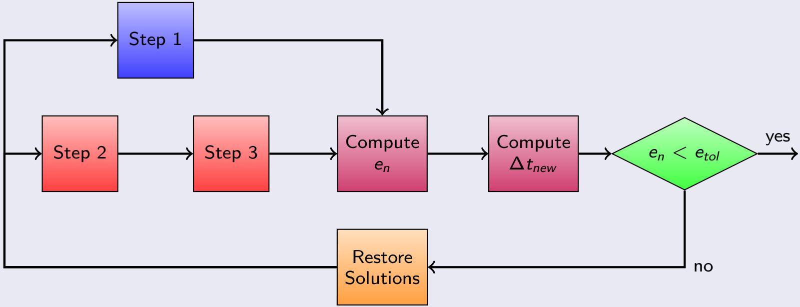


$$e_n = \frac{\left\| \sum_{g=1}^{G} \left(\varphi^g_{\Delta t/2} - \varphi^g_{\Delta t} \right) \right\|_{L^2}}{\max \left(\left\| \sum_{g=1}^{G} \varphi^g_{\Delta t/2} \right\|_{L^2}, \left\| \sum_{g=1}^{G} \varphi^g_{\Delta t} \right\|_{L^2} \right)}$$

$$\Delta t_{new} = S_f \Delta t \left[\frac{e_{tol}}{e_n} \right]^{1/(p+1)}$$

Step Doubling Solution Process

Programming Visualization

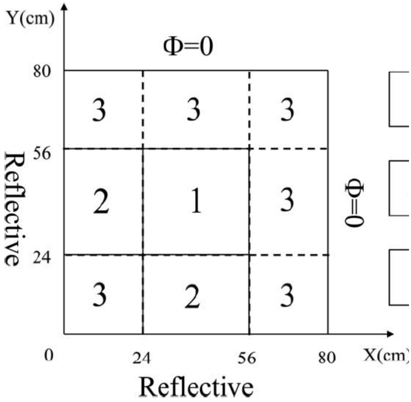


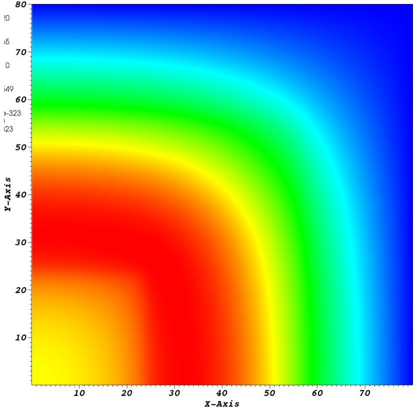
Each Step undergoes:

- Shape evaluation
- PRKE evaluations
- Multiphysics evaluations
- Iterations for convergence of amplitude, shape, and multiphysics

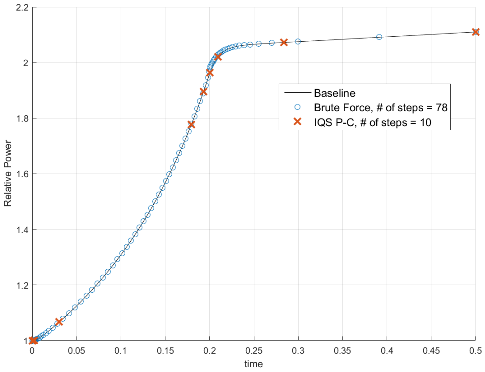
Results

TWIGL Benchmark





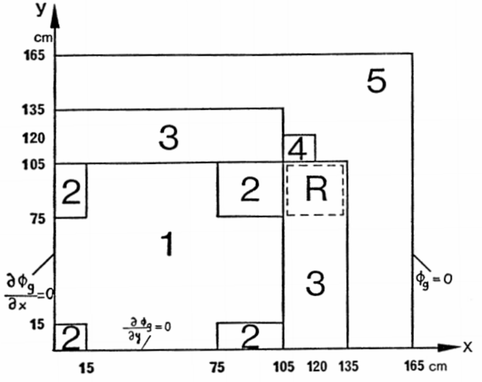
TWIGL Results

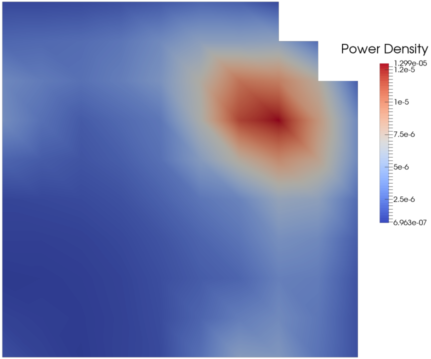


Brute Force				
Test	e_{tol}	Error	Steps	Solves
1	0.05	0.00012677	9	29
2	0.01	3.5555e-05	11	35
3	0.005	4.0364e-05	11	31
4	0.001	0.00294822	33	122
5	0.0005	0.00099778	39	131
6	0.0001	0.00019510	78	236
7	5.0e-05	0.00018372	112	342
8	1.0e-05	8.0564e-05	263	794

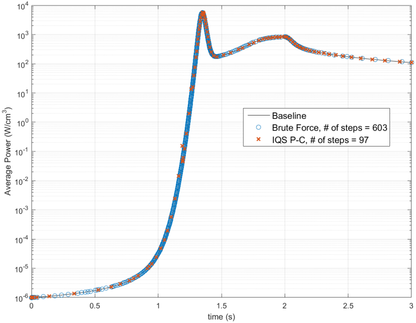
IQS P-C				
Test	e_{tol}	Error	Steps	Solves
1	0.05	0.03380433	4	9
2	0.01	0.00263068	5	12
3	0.005	0.00160486	6	21
4	0.001	1.7527e-05	10	35
5	0.0005	1.4185e-05	16	74
6	0.0001	6.2903e-06	19	78
7	5.0e-05	1.5247e-06	24	92
8	1.0e-05	9.8321e-07	48	210

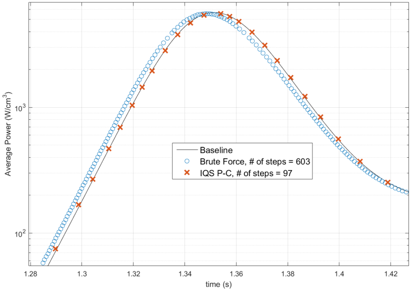
LRA Benchmark





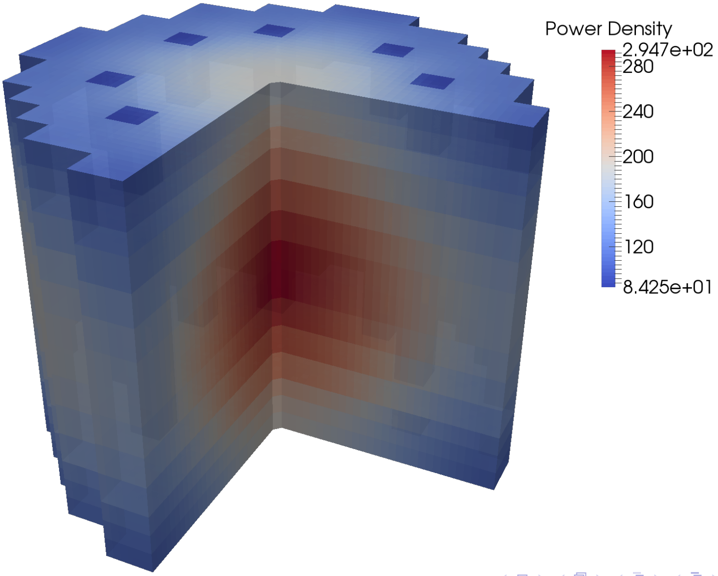
LRA Results



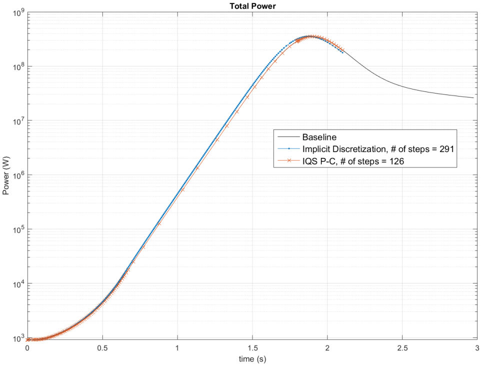


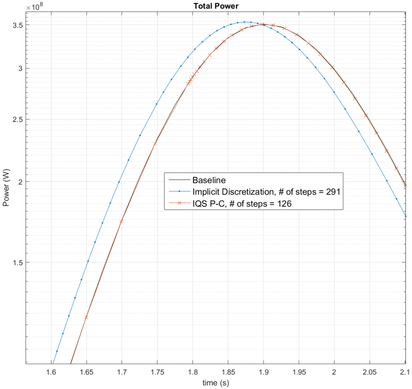
	Brute Force			IQS P-C		
Event	Power (W/cm^3)	Error	Steps	Power (W/cm^3)	Error	Steps
Max Power	5567.3	0.019454	423	5568.3	0.019274	47
End (3 s)	109.66	2.3650e-4	603	109.65	3.0622e-4	97

TREAT: Transient-15



TREAT Results





Wrap-up

Conclusion and Outlook

Completed

- Application and verification of step doubling IQS for pure neutronics
- Application of step doubling IQS with simple temperature feedback

In progress

- Verification of IQS with temperature feedback
- Exploration of IQS techniques for multiphysics feedback
- Application of step doubling IQS for full core TREAT model

Next Steps

- Implementation of IQS into Newton iteration process
- IQS application to SAAF-S_N and transport benchmarks

Questions ?

Thank you

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