1 Previous DSA Implementation

1.1 Varying Penalty within MFEM for Homogeneous Problems and/or Non-Uniform Meshes

The penalty term (Eq. ??) contains information from the problem. However, as currently implemented, the penalty term is a constant multiplier. To ensure Equation ?? holds within MFEM, we must create a new integrator class based on `DGDiffusionIntegrator` to modify the penalty term according to each of the mesh boundaries. Equation ?? states that the minimum penalty value is 1/4, thus,

$$\kappa_{\text{MFEM}} \left\langle \left\{\!\!\left\{ \frac{D}{h_\perp} \right\}\!\!\right\} [\![\phi]\!], [\![w]\!] \right\rangle \equiv \kappa_e \left\langle [\![\phi]\!], [\![w]\!] \right\rangle \tag{1}$$

$$\kappa_{\text{MFEM}} \left\{\!\!\left\{ \frac{D}{h_\perp} \right\}\!\!\right\} \equiv \kappa_e \geq \frac{1}{4} \tag{2}$$

$$\kappa_{\text{MFEM}} \geq \frac{1}{4} \left\{\!\!\left\{ \frac{h_\perp}{D} \right\}\!\!\right\} \tag{3}$$

Thus, enforcing $\kappa_e = 1/4$, `DGDiffusionIntegrator` would become

$$\frac{1}{4} \left\{\!\!\left\{ \frac{h_\perp}{D} \right\}\!\!\right\} \left\langle \left\{\!\!\left\{ \frac{D}{h_\perp} \right\}\!\!\right\} [\![\phi]\!], [\![w]\!] \right\rangle \tag{4}$$

This method would effectively remove any user input to this integrator, determining the penalty coefficient internally. However, it fixes the penalty value $\kappa_e = 1/4$ rather than $\kappa_e = \max\left(\kappa_e^{IP}, 1/4\right)$. To fully adapt the MIP equations, the maximum $\kappa_e = \max\left(\kappa_e^{IP}, \kappa_{\text{MFEM}}\right)$ should be used where κ_e^{IP} is defined by Equation ??.

2 Older DSA Results

2.1 Diffusion Synthetic Acceleration

Results using the MIP DSA equations using Dirichlet boundary conditions (Eqs. ?? and ??) are solved and some results are compared to unaccelerated solutions in Table ??. The "Adams problem" is defined in Adams [?]. It is a homogeneous 2-D diffusion limit problem with Dirichlet boundary conditions. For the various values of ϵ shown, $\sigma_t = \epsilon^{-1}$, $\sigma_a = \epsilon$, $\sigma_s = \sigma_t - \sigma_a$, and $S_0 = \epsilon$. The Adams problem was discretized with 8^{th} order finite elements, S_8 angular quadrature, and 8^{th} order mesh. Convergence criteria $\epsilon_{\text{conv}} = 10^{-12}$ was used. The penalty term κ^{IP} was not determined exactly the same as [**?**]. Rather, an ad hoc value was used in order to assure convergence. This is the reason for increasing κ^{IP} as ϵ decreases.

Table 1: "Adams" 2-D diffusion limit problem L^2 error between our solution and the reference solution for several values of ϵ. Note 1: did not attempt. Note 2: did not run to convergence. Note 3: converges consistently until some (seemingly arbitrary) point, then becomes erratic.

	without DSA		with DSA			
ϵ	spectral radius	no. iters	no. iters	spectral radius	κ^{IP}	L^2 error
0.1	0.94	474	44	0.53	10^2	0.048
0.05	0.98	1662	note 1	note 1	note 1	0.024
0.01	0.9993	$> 10,000$	49	0.56	10^2	0.0049
10^{-3}	0.9999	$> 10,000$	91 > 91	0.76 0.81	10^3 10^4	0.00049
10^{-4}	note 1	note 1	note 2 note 2 note 2	0.66 (note 3) 0.92 0.95	10^3 10^4 10^5	0.000049
10^{-5}	note 1	note 1	n/a note 2	> 1 0.70 (note 3)	10^3 10^4	0.0000049
10^{-6}	note 1	note 1	n/a note 2	> 1 0.70 (note 3)	10^4 10^5	0.000012

The results shown in Table **??** are varied. As we increase the optical thickness of the problem, we were able to converge toward a solution in a much more reasonable time with DSA than without. Thus, we have observed that we have the diffusion limit. However, this is not without some issues.

During the solution to the Adams problem using DSA for $\epsilon = \left\{10^{-4}, 10^{-5}, 10^{-6}\right\}$, the DSA solution was observed to evolve smoothly until it reached a (seemingly arbitrary) point when it begins to behave erratically. The erratic DSA solutions don't begin affecting the scalar flux solution until the magnitude of the DSA solution is on the same order as the maximum scalar flux error between iterations $\left(O\left(10^{-11}\right)\right)$. Thus, the solutions to this problem for $\epsilon = \left\{10^{-4}, 10^{-5}, 10^{-6}\right\}$ are not fully converged. An example output is shown in Figure **??** to demonstrate that the spectral radius became erratic. This example is for $\epsilon = 10^{-4}$ where the spectral radius was consistently about 0.66 until iteration 51.

```
Itr = 50, phi_conv.max =  6.4492988e-11, spectral radius: 0.65659991
L2 error: 4.8937733e-05
Itr = 51, phi_conv.max =  5.7443356e-11, spectral radius: 0.89069149
L2 error: 4.8937729e-05
Itr = 52, phi_conv.max =  4.2847809e-11, spectral radius: 0.7459141
L2 error: 4.893773e-05
Itr = 53, phi_conv.max =  3.8060055e-11, spectral radius: 0.88826141
L2 error: 4.8937731e-05
Itr = 54, phi_conv.max =  2.6113472e-11, spectral radius: 0.68611231
L2 error: 4.8937738e-05
Itr = 55, phi_conv.max =  5.4752064e-11, spectral radius: 2.0966979
L2 error: 4.8937731e-05
Itr = 56, phi_conv.max =  5.4592192e-11, spectral radius: 0.99708007
L2 error: 4.8937735e-05
Itr = 57, phi_conv.max =  2.9092062e-11, spectral radius: 0.53289786
L2 error: 4.8937709e-05
Itr = 58, phi_conv.max =  7.1939399e-11, spectral radius: 2.4728188
L2 error: 4.8937725e-05
Itr = 59, phi_conv.max =  6.8166972e-11, spectral radius: 0.94756105
L2 error: 4.893773e-05
Itr = 60, phi_conv.max =  5.9108274e-11, spectral radius: 0.86711016
```

Figure 1: Partial output for Adams problem showing iteration number (Itr), maximum flux error between iterations (phi_conv.max), spectral radius, and the L^2 error from the reference solution.

The next set of test problems are for a uniform infinite medium using Dirichlet boundary MIP DSA with a zero analytic solution (incidentally it is equivalent the the Adams problem just with a zero volumetric source term). Specifically, $\sigma_t = 1/\epsilon$, $\sigma_a = \epsilon$, $S = 0$, $\psi_{\text{inc}} = 0$, and analytic solution $\phi = S/\sigma_a = 0.0$. The source iteration begins with an initial guess of $\phi = 5$. This problem was discretized with 8^{th} order finite elements, S_8 angular quadrature, and 8^{th} order mesh. Convergence criteria $\epsilon_{\text{conv}} = 10^{-12}$ was used. Table **??** illustrates various solution properties of these test problems.

The erratic behavior is not observed in this problem. As seen in Figures **??** and **??**, the scalar flux and DSA solutions, respectively, show values on the order of 10^{-20}, far beyond the point that the DSA began behaving erratically. This suggests a discrepancy associated with the volumetric source term.

Table 2: 2-D uniform infinite medium diffusion limit problem L^2 error between our solution and the reference solution for several values of ϵ.

ϵ	no. iters	spectral radius	κ^{IP}	L^2 error
0.1	47	0.53	10^3	2.5×10^{-13}
0.01	51	0.56	10^3	3.4×10^{-13}
10^{-3}	104	0.76	10^3	1.6×10^{-13}
10^{-4}	70	0.66	10^3	6.0×10^{-14}
10^{-5}	n/a	> 1	10^3	n/a
	81	0.70	10^4	7.4×10^{-14}
10^{-6}	n/a	> 1	10^4	n/a
	83	0.70	10^5	6.0×10^{-14}

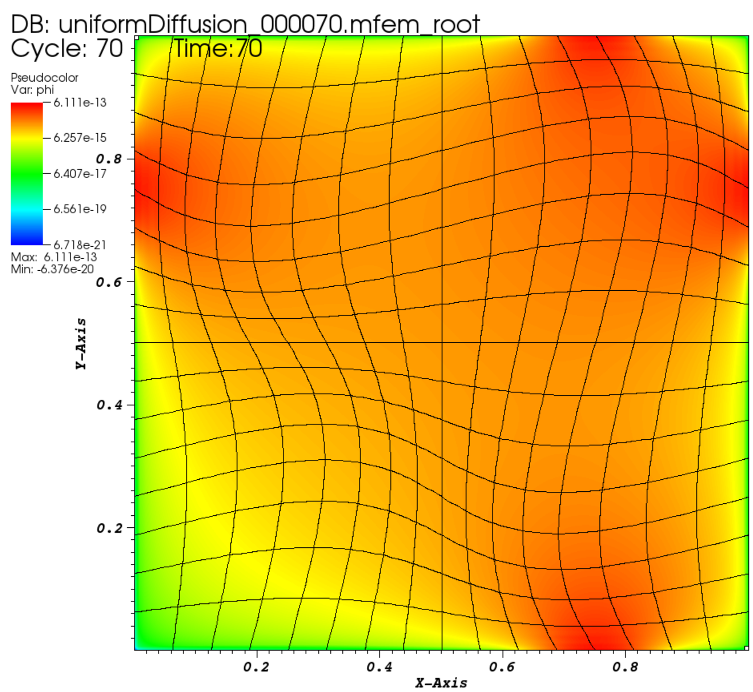

Figure 2: Uniform infinite medium diffusion limit scalar flux solution (log scale) for $\epsilon = 10^{-4}$ of Table **??**.

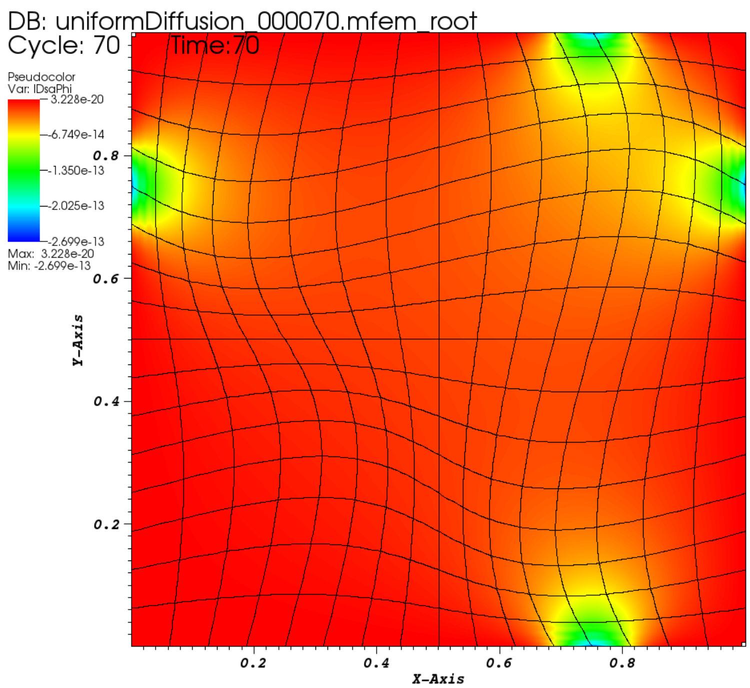

Figure 3: Uniform infinite medium diffusion limit DSA solution for $\epsilon = 10^{-4}$ of Table **??**.

2.1.1 Strong Scatter with Discontinuous Boundary Conditions with DSA

This test problem was solved without DSA in Woods et al. [?]. Implementing the Dirichlet boundary condition DSA reduced the number of source iterations to 37 ($\rho \approx 0.54$) using $\kappa_{\mathrm{MFEM}} = 1/2 \cdot h_\perp / D = 150$ where $h_\perp = \{0.1, 0.02\}$. The modified convergence criteria was used where $\epsilon_{\mathrm{conv}} = 10^{-12}$. Figures **??** and **??** illustrate the solution and the natural log of the solution, respectively. This problem did not display any erratic convergence behavior.

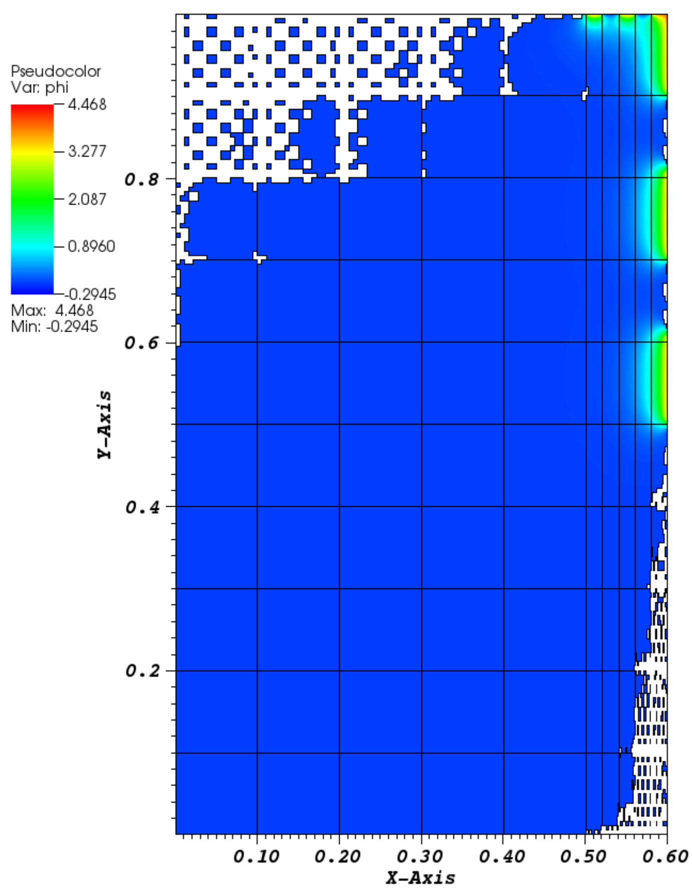

Figure 4: Strong scatter with discontinuous boundary conditions problem solved with DSA. White regions indicate negative fluxes.

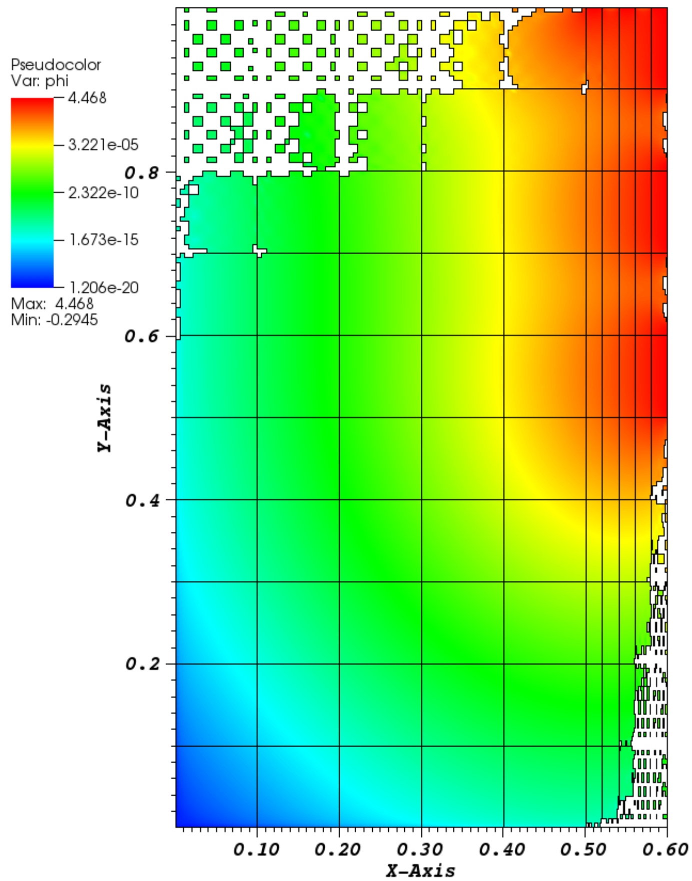

Figure 5: Log of strong scatter with discontinuous boundary conditions problem solved with DSA. White regions indicate negative fluxes.

2.1.2 Material Discontinuity Stress Test with DSA

Adding DSA to the material discontinuity stress test of Woods et al. [?] reduces the spectral radius to $\rho \approx 0.994$ using $\kappa_{\text{MFEM}} = 450$. A discussion of κ_{MFEM} is necessary. Both $\kappa_{\text{MFEM}} = 400$ and $\kappa_{\text{MFEM}} = 500$ caused the source iteration to diverge. This parameter is supposed to vary based on $h_{\perp}^{\pm}$ and $D^{\pm}$. Homogeneous problems on a regular mesh can have a global κ_{MFEM} but this heterogeneous problem will require multiple κ_{MFEM} values at the various material interfaces. For now, this global value allows the source iteration to converge and is still much faster than without DSA altogether.

This problem was solved using S_4 level-symmetric quadrature and 8^{th} order finite elements. The modified convergence criteria was used where $\epsilon_{\text{conv}} = 10^{-12}$. An error occurred causing the calculation to stop every 900 iterations (about 55 minutes). Restarting the simulation from a restart file allowed this problem to converge according to the convergence criteria. This problem converged in 4027 iterations. Figures **??** and **??** illustrate the scalar flux solution and the log of the scalar flux, respectively.

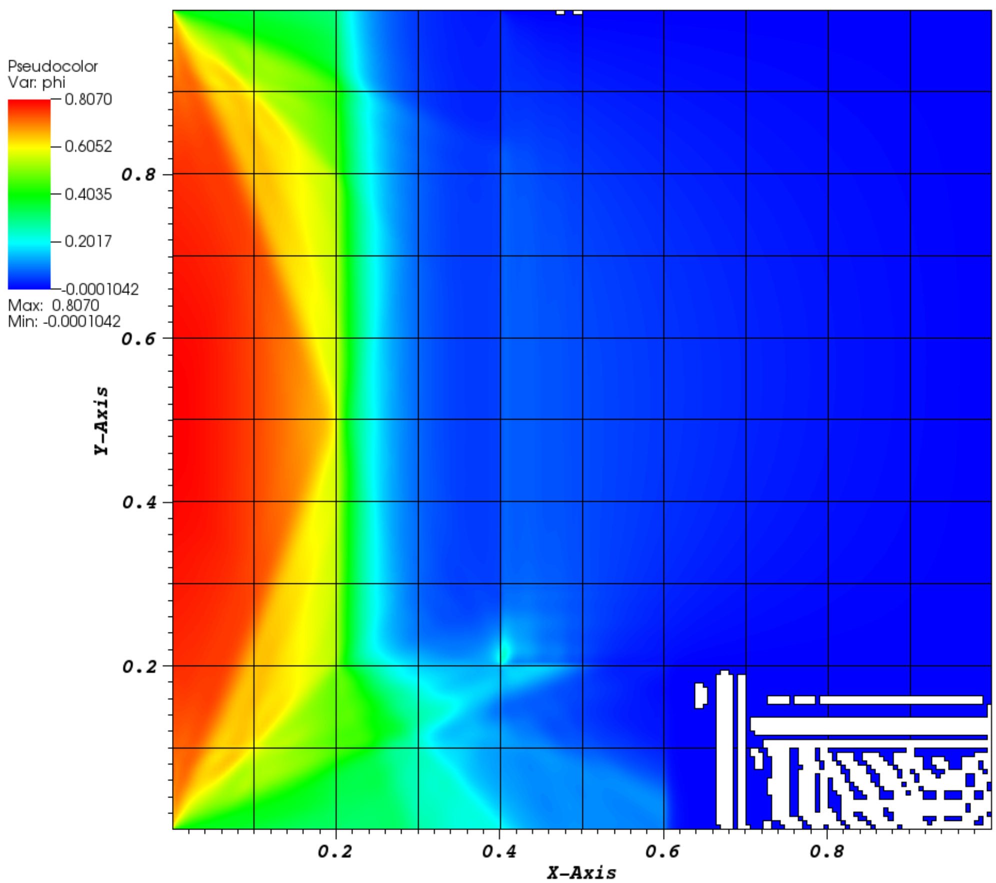

Figure 6: Material discontinuity stress test solved with DSA. White regions indicate negative fluxes.

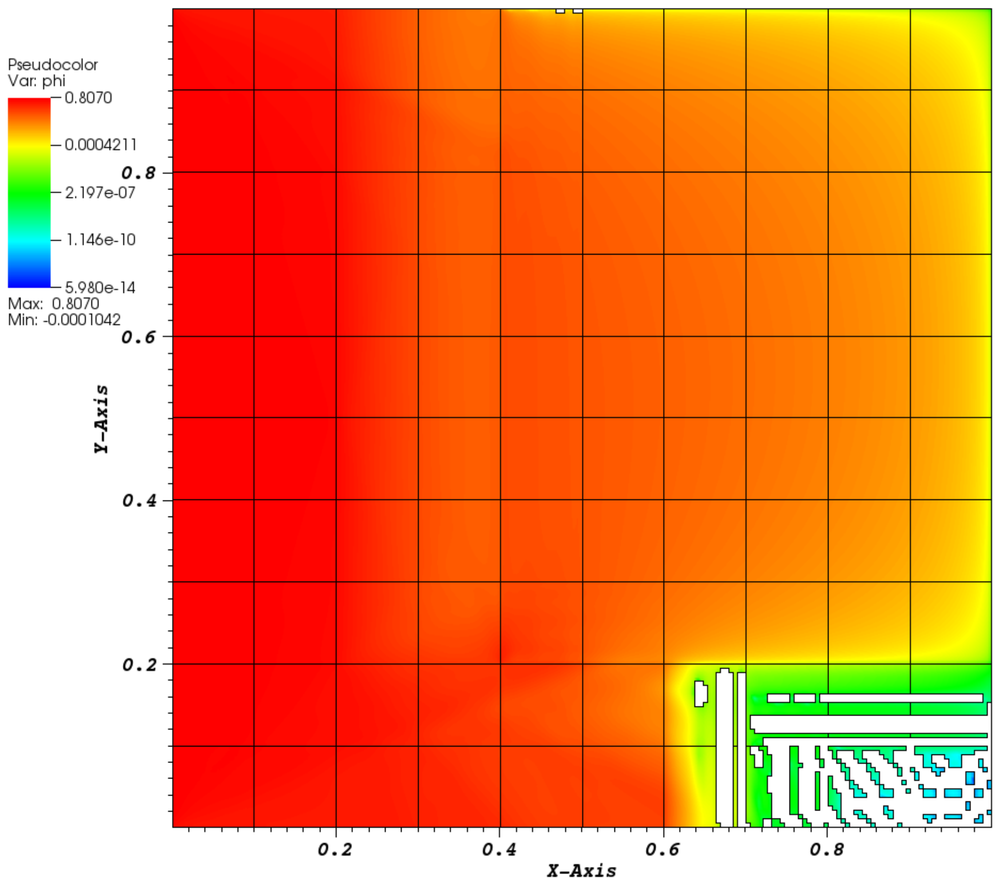

Figure 7: Log of material discontinuity stress test solved with DSA. White regions indicate negative fluxes.

This problem converged in significantly more iterations than the other test problems described above. Figure **??** illustrates the magnitude of the error between two successive iterations of scalar flux. Clearly, the slowest region to converge is within the highly scattering region near the very low and very high absorption regions.

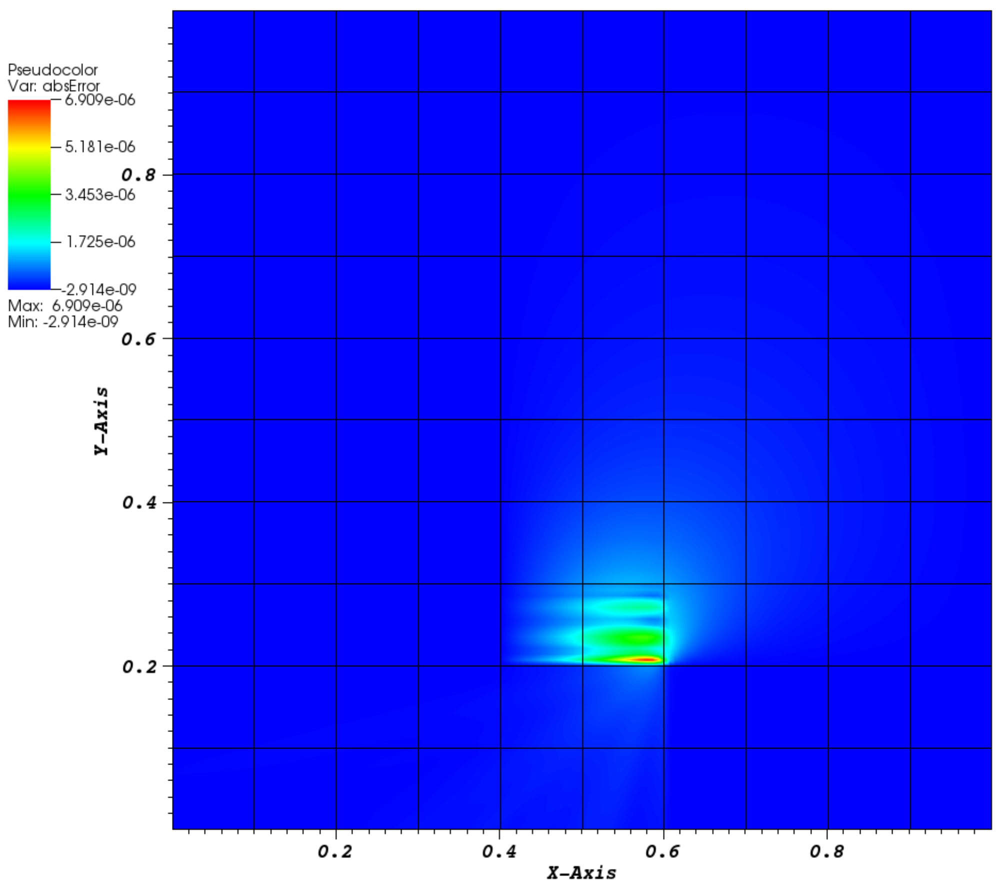

Figure 8: Magnitude of scalar flux error between successive iterations for material discontinuity stress test. This calculation was performed with S_8 level-symmetric quadrature.