Verification of the Thermal Radiation Diffusion Package In ALEGRA

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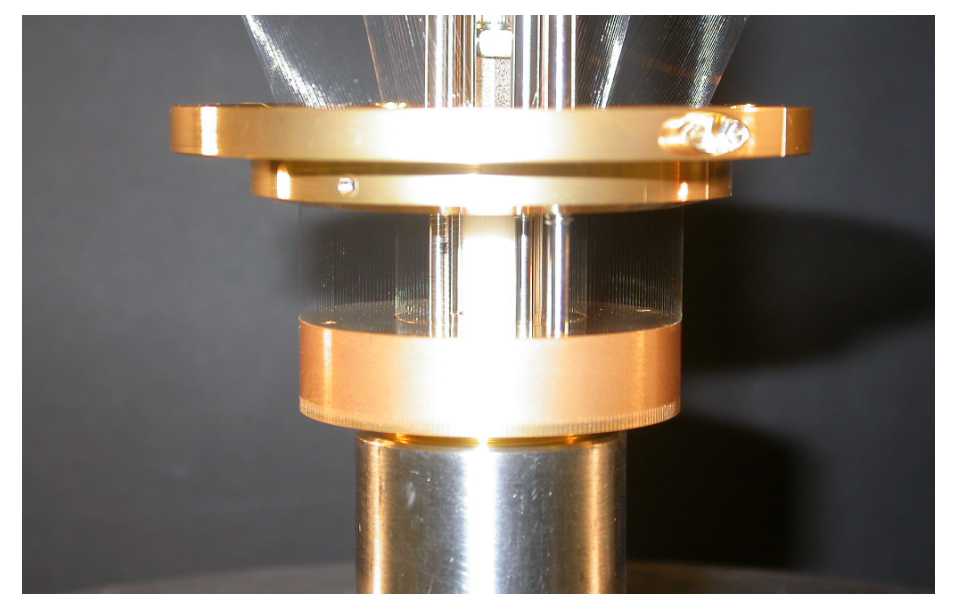
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

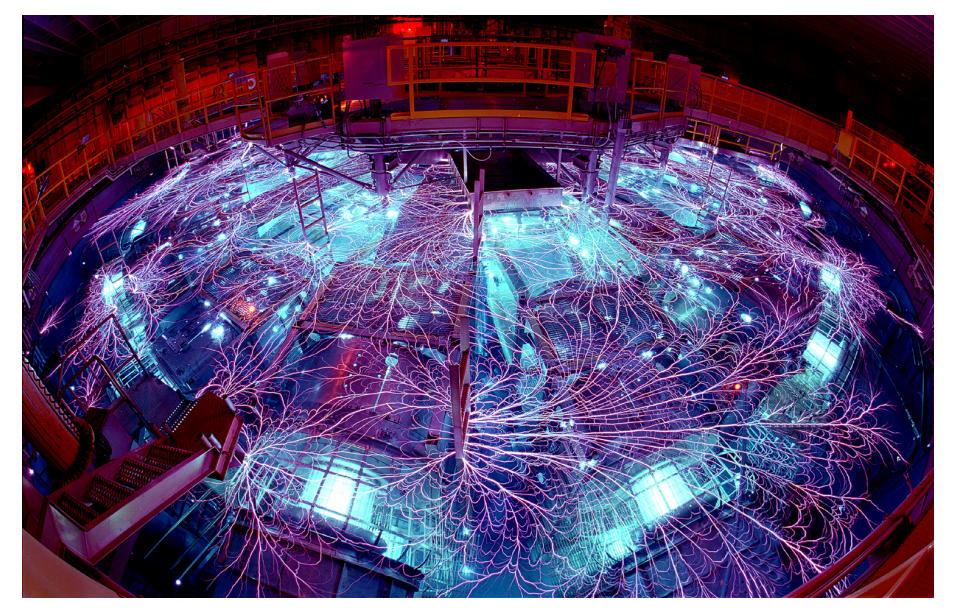
National Nuclear Security Administration

SAND2006-5553C

What is ALEGRA-HEDP?

ALEGRA-HEDP is a multiphysics code designed to simulate Z-pinch experiments. Hundreds of tiny wires are heated with megaamps of current. They get very hot, implode on axis and create terawatt X-ray pulses. In order to simulate the experiments, we need a code with magnetohydrodynamics, radiation, thermal conduction, and separate ion and electron temperatures.





Defining Limits of Verification

Before the entire code be verified, each physics component must be verified separately. Here we verify the radiation diffusion package, with coupling to the material energy equation. The relevant equations are:

Radiation Diffusion

$$\frac{1}{c}\frac{\partial E(\nu)}{\partial t} - \nabla\cdot D(E(\nu))\nabla E(\nu) = \sigma_a(\nu)\left[B(T,\nu) - E(\nu)\right] + \frac{S(\nu)}{c}$$

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Material Energy

$$\frac{\partial \rho C_v T}{\partial t} = -\int_0^\infty \sigma_a(\nu)\left[B(T,\nu) - E(\nu)\right] d\nu + Q$$

⑦ ③ ④ ⑤ ⑧

Diffusion Coefficients

$$D_{\mathrm{L2}} = \left[(3\sigma_t(\nu))^2 + \left(\frac{|\nabla E(\nu)|}{E(\nu)}\right)^2\right]^{-\frac{1}{2}} \quad \text{or} \quad D_{\mathrm{POD}} = \frac{1}{3\sigma_t}$$

(2A) (2B)

Boundary Conditions

$$E = f(\mathbf{x},t) \qquad \mathcal{A}E - \mathcal{B}\hat{\mathbf{n}}\cdot\nabla E = \mathcal{C}$$

⑨ ⑩

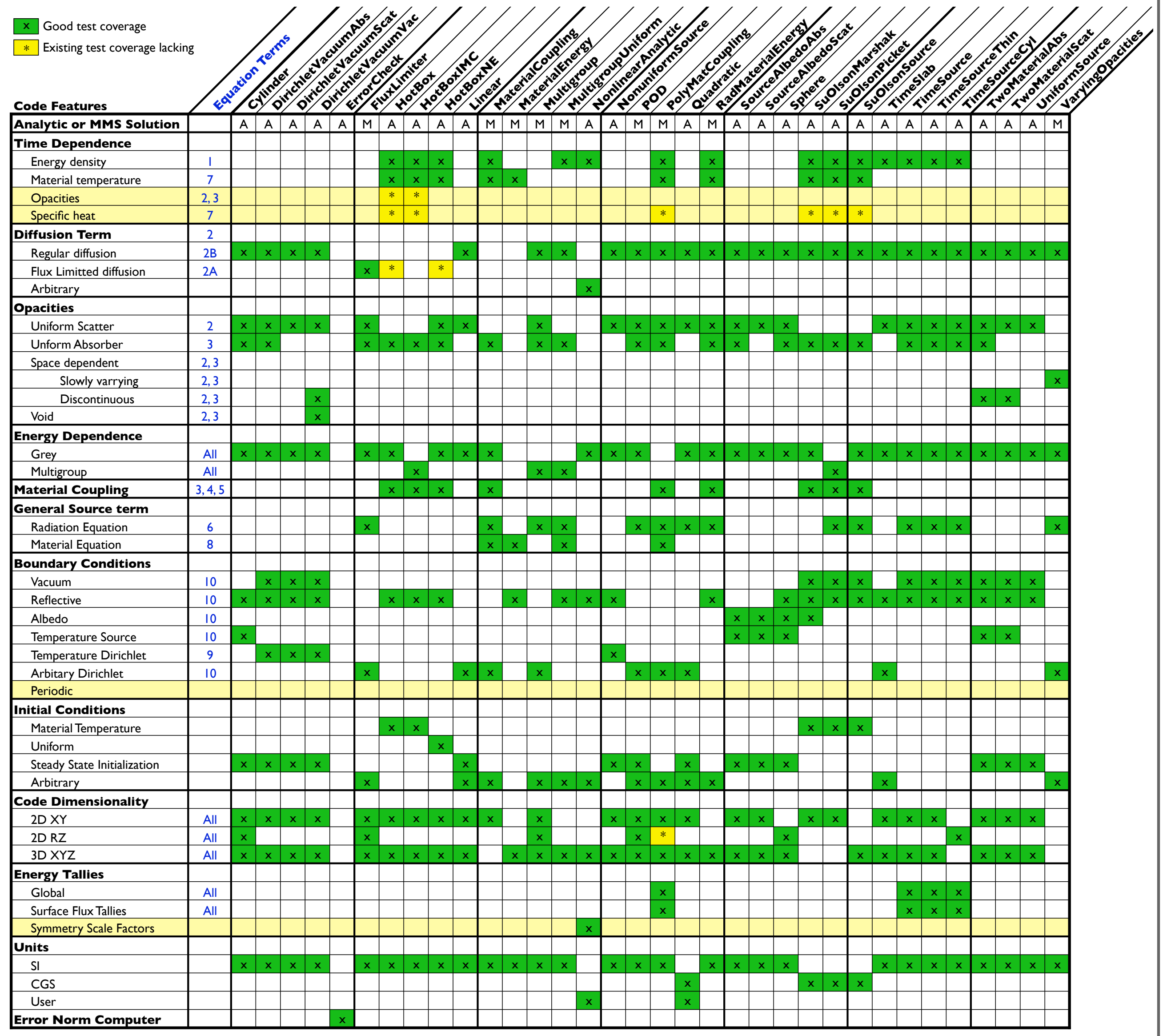
The Test Suite Philosophy

Over thirty different test problems have been developed to test various components of the code. Each test problem is designed to isolate one code feature or term in the equations. Additionally, there are some more comprehensive tests to test the interaction of various features.

All the tests are one dimensional, but may be of Cartesian, cylindrical or spherical geometry, which are run in the 2D-XY, 2D-RZ, and 3D-XYZ versions of the code.

Many of the tests are simple forward solutions of the diffusion equation, but many of the tests for the nonlinear portions of the code are generated using the Method of Manu-

Test Suite Coverage



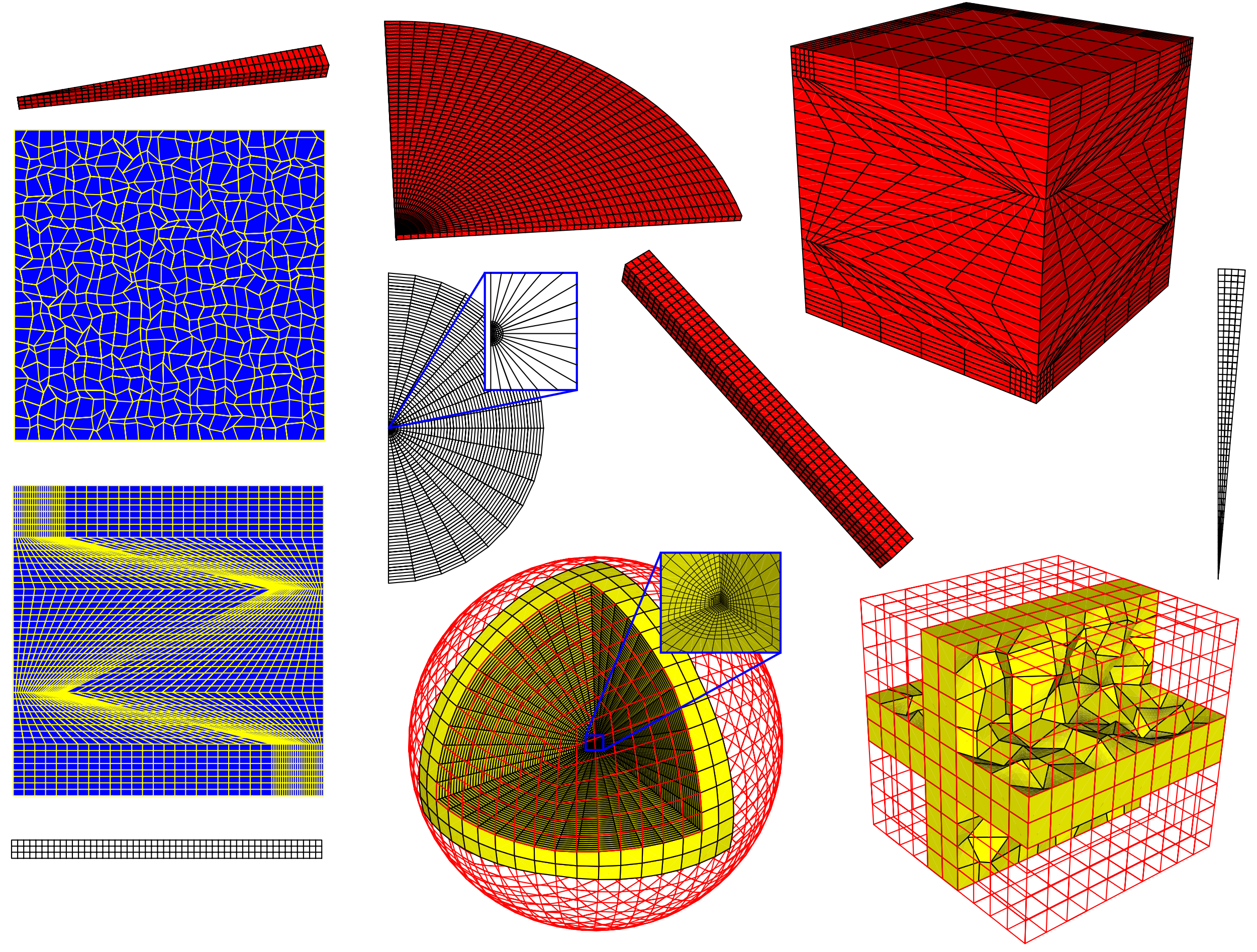
🟩 x Good test coverage

🟨 * Existing test coverage lacking

Code Features	Equation Terms	Cylinder	DirichletVacuumAbs	DirichletVacuumScat	DirichletVacuumVac	ErrorCheck	FluxLimiter	HotBox	HotBoxIMC	HotBoxNE	Linear	MaterialCoupling	MaterialEnergy	Multigroup	MultigroupUniform	NonlinearAnalytic	NonuniformSource	POD	PolyMatCoupling	Quadratic	RadMaterialEnergy	SourceAlbedoAbs	SourceAlbedoScat	Sphere	SuOlsonMarshak	SuOlsonPicket	SuOlsonSource	TimeSlab	TimeSource	TimeSourceThin	TimeSourceCyl	TwoMaterialAbs	TwoMaterialScat	UniformSource	VaryingOpacities
Analytic or MMS Solution		A	A	A	A	A	M	A	A	A	A	M	M	M	M	A	A	M	M	A	M	A	A	A	A	A	A	A	A	A	A	A	A	A	M
Time Dependence																																			
Energy density	1							x	x	x		x			x	x			x		x				x	x	x	x	x	x	x				
Material temperature	7							x	x	x		x	x						x		x				x	x	x								
Opacities	2, 3							*	*																										
Specific heat	7							*	*										*						*	*	*								
Diffusion Term	2																																		
Regular diffusion	2B	x	x	x	x						x			x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Flux Limitted diffusion	2A						x	*		*																									
Arbitrary																x																			
Opacities																																			
Uniform Scatter	2	x	x	x	x		x			x	x			x			x	x	x	x	x	x	x	x				x	x	x	x	x	x	x	
Unform Absorber	3	x	x				x	x	x	x		x		x	x			x	x		x	x		x	x	x	x		x	x	x	x			
Space dependent	2, 3																																		
Slowly varrying	2, 3																																		x
Discontinuous	2, 3				x																											x	x		
Void	2, 3				x																														
Energy Dependence																																			
Grey	All	x	x	x	x		x	x		x	x	x				x	x	x		x	x	x	x	x	x		x	x	x	x	x	x	x	x	x
Multigroup	All								x					x	x											x									
Material Coupling	3, 4, 5							x	x	x		x							x		x				x	x	x								
General Source term																																			
Radiation Equation	6						x					x		x	x			x	x	x	x					x	x		x	x	x				x
Material Equation	8											x	x		x				x																
Boundary Conditions																																			
Vacuum	10		x	x	x																				x	x	x		x	x	x	x	x	x	
Reflective	10	x	x	x	x			x	x	x			x		x	x	x				x			x	x	x	x	x	x	x	x	x	x	x	
Albedo	10																					x	x	x	x										
Temperature Source	10	x																				x	x	x								x	x		
Temperature Dirichlet	9		x	x	x												x																		
Arbitary Dirichlet	10						x				x	x		x				x	x	x								x							x
Periodic																																			
Initial Conditions																																			
Material Temperature								x	x																x	x	x								
Uniform										x																									
Steady State Initialization		x	x	x	x						x						x	x		x		x	x	x								x	x	x	
Arbitrary							x				x	x		x	x	x		x	x	x	x							x							x
Code Dimensionality																																			
2D XY	All	x	x	x	x		x	x	x	x	x	x		x			x	x	x	x		x	x		x	x		x	x	x		x	x	x	
2D RZ	All	x					x							x				x	*					x							x				
3D XYZ	All	x	x	x	x		x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x			x	x	x	x		x	x	x	
Energy Tallies																																			
Global	All																		x										x	x	x				
Surface Flux Tallies	All																		x										x	x	x				
Symmetry Scale Factors																x																			
Units																																			
SI		x	x	x	x		x	x	x	x	x	x	x	x	x		x	x	x		x	x	x	x				x	x	x	x	x	x	x	x
CGS																				x					x	x	x								
User																x				x															
Error Norm Computer						x																													

In the chart above, the code features are identified with equation terms. The code features that each test uses are highlighted. Yellow boxes with stars indicate incomplete coverage of some sort. For example, the HotBox problem ensures that equilibrium is maintained with the material, so the flux limiter and opacities could vary, but do not.

Each of these tests is run and analyzed automatically on regular meshes, skewed meshes, and randomized meshes. Regular meshes that are not aligned to the coordinate system are also used. Convergence rates for each mesh type are computed and plotted. A history of errors and convergence rates is kept to alert the developer to problems in the code. Nearly 1000 different simulations make up the test suite.



A Few Test Problems

Many of the test problems are simple solutions to the diffusion equation. At least half of all the problems in the suite found bugs in the code, even though it otherwise appeared to be working correctly.

Time Dependent Test of Energy Tallies

(TimeSource)

This test turns on volume source at time zero, exciting just one eigenmode, and allows a time dependant solution to be found analytically. Not only does this test the diffusion part of the code, many of the energy tallies for users can be computed. In a finite slab with no absorption, we have

$$\frac{\partial E}{\partial t} - \frac{c}{3\sigma}\frac{\partial^2 E}{\partial x^2} = S\cos L_1 x$$

where L_1 is the first root of

$$\cos L_1 x_0 - \frac{2L_1}{3\sigma}\sin L_1 x_0 = 0$$

The solution is:

$$E(x,t) = \frac{3\sigma S}{cL_1^2}\left[1 - e^{-\frac{cL_1^2}{3\sigma}t}\right]\cos L_1 x$$

One important tally is the net energy leaked off the mesh:

$$P_{\mathrm{nl}}(t) = \frac{2S}{L_1}\left[1 - e^{-\frac{cL_1^2}{3\sigma}t}\right]\sin L_1 x_0$$

Flux Limiter Test

(FluxLimiter)

Flux limited diffusion is a nonlinear problem, even with very nice material properties, which makes finding an analytic solution very difficult. This test uses the Method of Manufactured Solutions (MMS). In MMS, the solution for the energy density is inserted into the equations, and the source to support that solution is computed. Here, we limit the problem to steady-state and uniform, constant opacities. First we specify the solution as

$$E(r) = E_0 \mathrm{e}^{-\kappa r^2}$$

Solving for the source in the diffusion equation gives

$$S = c\left[\sigma_a E - \frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r} r^{\alpha-1} D_{\mathrm{L2}}\frac{\partial E}{\partial r}\right]$$

Inserting the assumed solution finally gives us

$$S = c\left[\sigma_a - \frac{8r^2\kappa^3(1-\alpha) + 16r^4\kappa^4 - 18\alpha\kappa\sigma_t^2 + 36r^2\kappa^2\sigma_t^2}{(9\sigma_t^2 + 4\kappa^2 r^2)^{\frac{3}{2}}}\right] E(r)$$

Because the gradient is zero at the origin, the flux limiter is inactive there. As *r* increases, so does the ratio of the gradient to energy density ratio. The entire range of the flux limiter can be tested in one simulation by setting the parameters, including the size of the mesh, carefully. We use:

$$r_{\max} \approx 1 \qquad \kappa = 5 \qquad \sigma_t = \frac{1}{30} \qquad \sigma_a = \frac{33}{1000}$$

(α is 1, 2, or 3 for Cartesian, cylindrical, or spherical geometry.)

Nonlinear Radiation-Material Coupling

(MaterialCoupling)

In general, the material coupling is also nonlinear, and analytic solutions are very difficult to obtain. The Su-Olson tests introduced a non-physical specific heat to linearize the equations, but this choice makes the linearization terms in most linearized methods independent of material temperature. This MMS test uses a constant specific heat. The assumed solutions are:

$$E(r,t) = a\left[T_0\left(1 + \frac{\mathrm{e}^{-\tau t}}{2}\right)\right]^4\left[1 + \frac{\mathrm{e}^{-\tau t}}{2}\cos\omega r\right]$$

$$T(r,t) = T_0\left[1 - \frac{\mathrm{e}^{-\tau t}}{2}\cos\omega r\right]$$

These solutions are inserted into the coupled equations to find the sources. It is important in this problem for each term in the equations to have roughly the same magnitude. This solution decays to an equilibrium solution. Given the other parameters, the natural length and time scales can be computed and used in the solution, minimizing the dependence on the sources In SI Units, the parameters are:

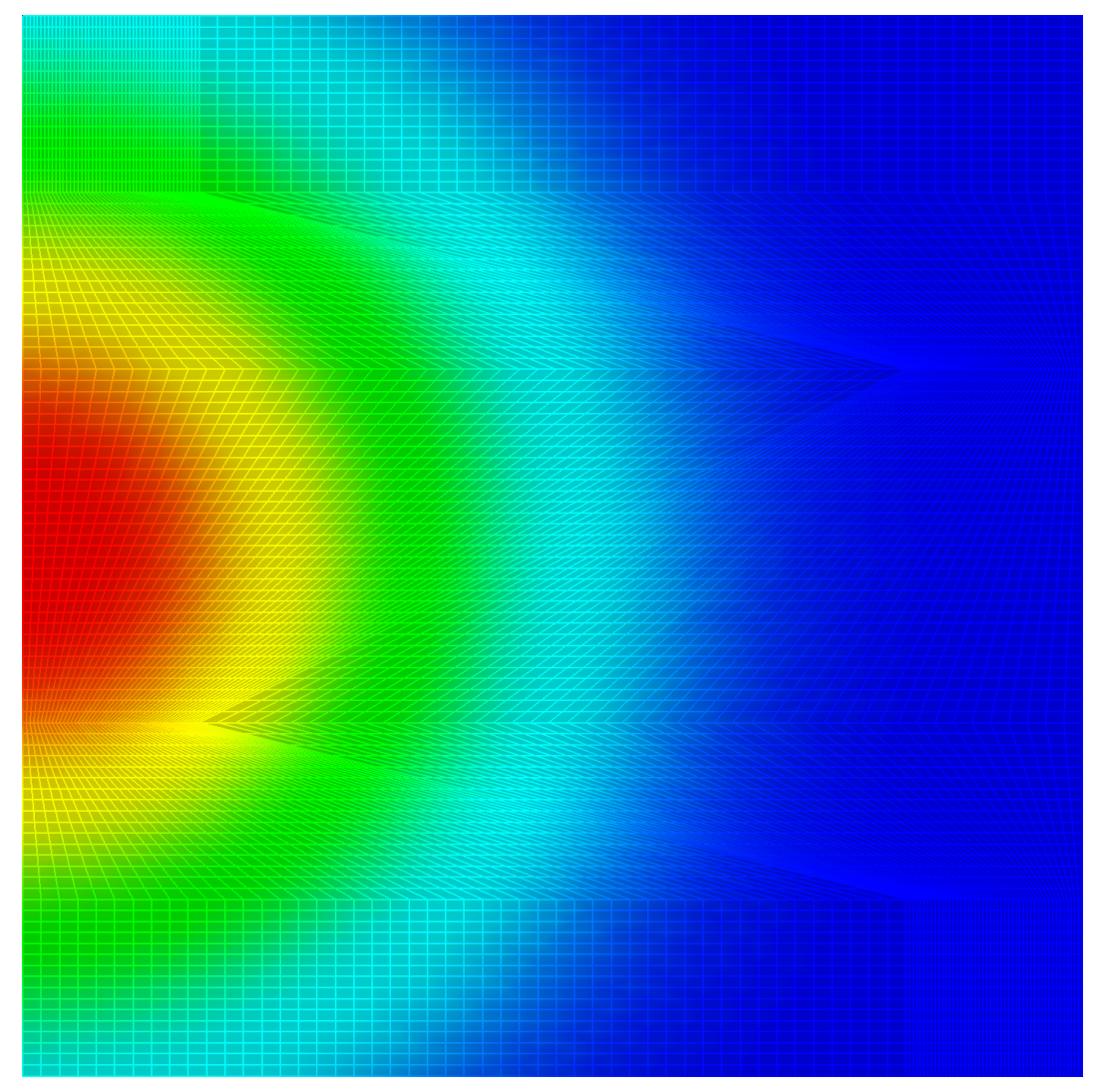
$$\rho = 2 \quad C_v = 3 \quad \sigma = 4 \quad T_0 = 10^5$$

$$\omega = \sqrt{\frac{15\tau\sigma}{c}} = 21.3503497 \qquad \tau = \frac{241 c\sigma a T_0^3}{16\rho C_v} = 2.27761040\times 10^9$$

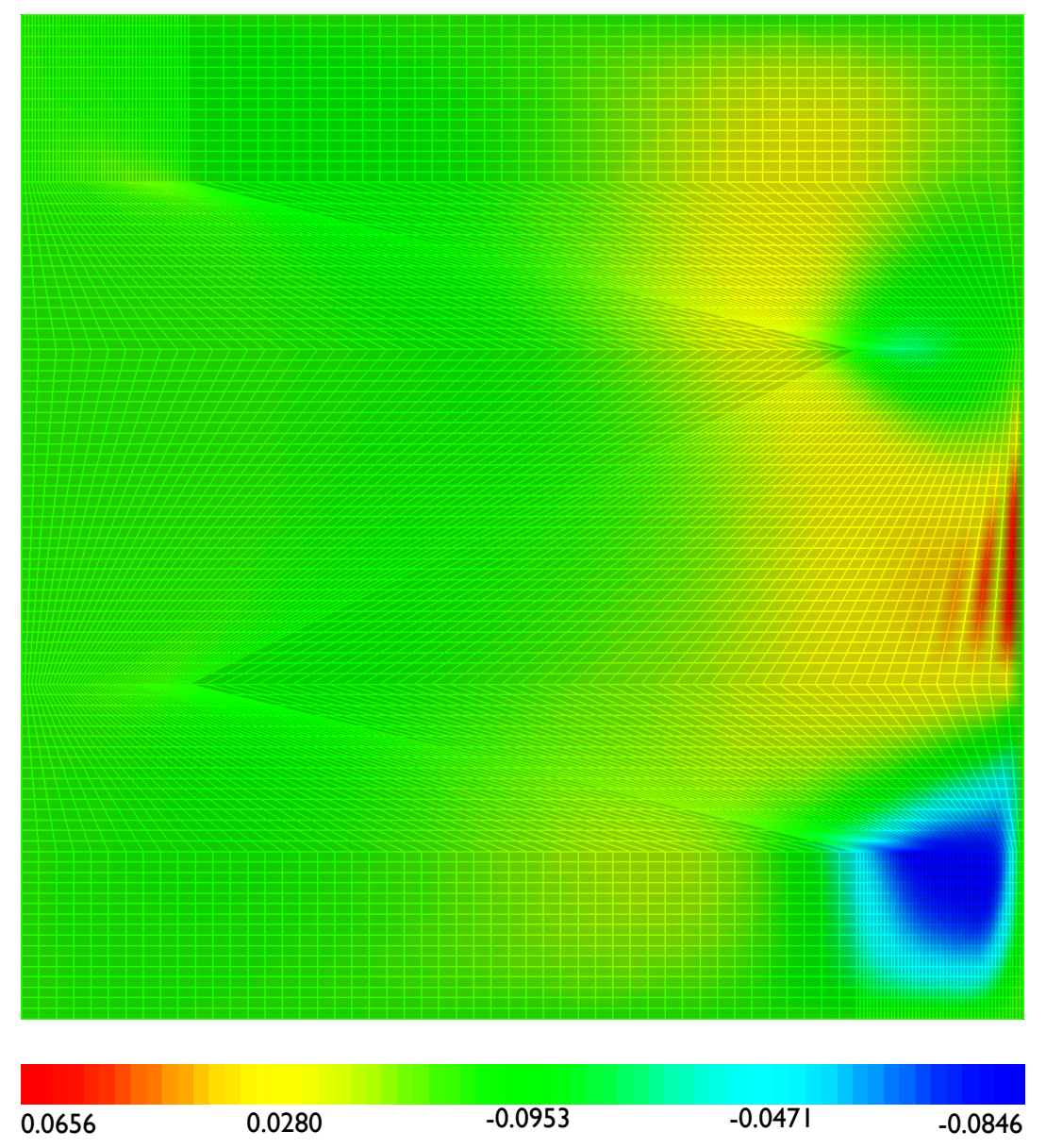
Verification Tools

Running MMS tests can be difficult due to the arbitrary nature of the source terms and boundary conditions. ALEGRA has a **Run Time Compiler** (RTC) that interprets C-like code at execution time. Arbitrary boundary conditions and source terms are implemented in terms of the RTC, easily allowing new MMS tests to be built without needing to recompile the code with special terms for that problem. The RTC is also used to compute the expected solution and relative errors in the code. This has been extremely valuable for debugging the problem input decks as well as the code.

Energy Density for FluxLimiter on a 2D Z-Mesh



Relative Error for FluxLimiter



Tampa is a collection of Python scripts used to manage execution and analysis of the simulations in the suite. XML configuration files are read, and the problem automatically set up on different types and resolution of meshes.