PECOS

Predictive Engineering and Computational Sciences

MASA: A Tool for the Verification of Scientific Software

Nicholas Malaya

Center for Predictive Engineering and Computational Sciences (PECOS)
Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

July 10th, 2014

Outline

This talk is online:

`https://github.com/manufactured-solutions/presentations/`

Itinerary

- Motivation for Verification
- Introduction to the Method of Manufactured Solutions
- Creating Manufactured Solutions (is hard)
- The MASA Library

Verification Failure Case Study: London Whale

JP Morgan's synthetic credit portfolio

- Developed by "quantitative expert, mathematician and model developer"
- "The model operated through a series of Excel spreadsheets, which had to be completed manually, by a process of copying and pasting data from one spreadsheet to another"
- Bank declared 6 billion in losses and another 600 million in fines.

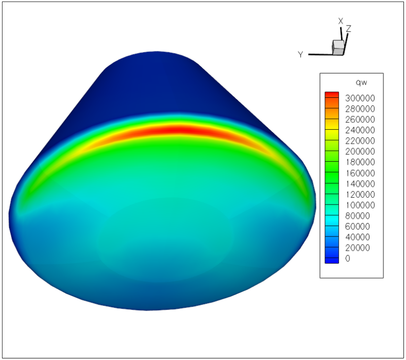
What went wrong?

- After subtracting the old rate from the new rate, the spreadsheet divided by their sum instead of their average
- This error likely had the effect of muting volatility by a factor of two!!

Scientific and Numerical Computing

Simulations have a broad range of applicability

- Computer aided design of Boeing 787
- Global warming
- Earthquake, hurricane, storm surge prediction
- Human treatment and drug discovery



What is verification?

Reality

$$\Downarrow$$

Mathematical Model

$$\frac{d^2x(t)}{dt^2} = \frac{F}{M}$$

$$\Downarrow$$

Numerical Representation

$$\frac{d^2x}{dt^2} = f''(t) \approx \frac{f(t+h)-2f(t)+f(t-h)}{h^2} + O(h^2)$$

Verification

Verification of Scientific Software

- Verification ensures that the outputs of a computation accurately reflect the solution of the mathematical models.

Code Verification

- Ensuring that the code used in the simulation correctly implements the intended numerical discretization of the model.
  - This concept is *not* unique to Scientific Software

What really are we asking?

- Are the errors from the numerical discretization sufficiently small?
- Is the convergence rate consistent with the numerical scheme?

Solution Verification Methods

Method of Exact Solutions

- Numerically solve the governing equations for which the solution can be determined analytically.

Method of Manufactured Solutions

- Often, analytical solutions either:
  - Do not exist (Navier-Stokes)
  - Do not fully exercise equations (e.g. a symmetric solution, nonlinearities)
- Alleviate this using Method of Manufactured Solutions (MMS)
  - Simply put, we “create” our own solutions

Manufactured solution to Laplace's Equation

Laplace's Equation:

$$\nabla^2 \phi = 0$$

In two dimensions:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

"Manufacture" a solution, with two constants:

$$\phi(x,y) = ({\color{red}Ly} - y)^2({\color{red}Ly} + y)^2 + ({\color{red}Lx} - x)^2({\color{red}Lx} + x)^2$$

Calculating the Source Term

We insert our manufactured solution back into the governing equations:

$$\frac{\partial^2((Lx-x)^2(Lx+x)^2)}{\partial x^2}+\frac{\partial^2((Ly-y)^2(Ly+y)^2)}{\partial y^2}=0$$

$$\begin{aligned}&=2(Lx-x)^2-8(Lx-x)(Lx+x)+2(Lx+x)^2\\&+2(Ly-y)^2-8(Ly-y)(Ly+y)+2(Ly+y)^2\\&\neq 0\end{aligned}$$

This does not satisfy Laplace's Equation!

To balance the equation, add the residual to the RHS as a source term.

Example Verification Use Case

To solve Laplace's Equation numerically, we need a discretization scheme.

Let's use a 2nd order finite central difference:

$$\phi_i'' \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} + O(h^2)$$

This requires solving an implicit system of equations:

$$A\vec{\phi} = f$$

You can use your favorite linear solver (e.g. PETSc) to solve the system.

Problem: Solve 2D Laplacian using Finite-Differencing

Outline

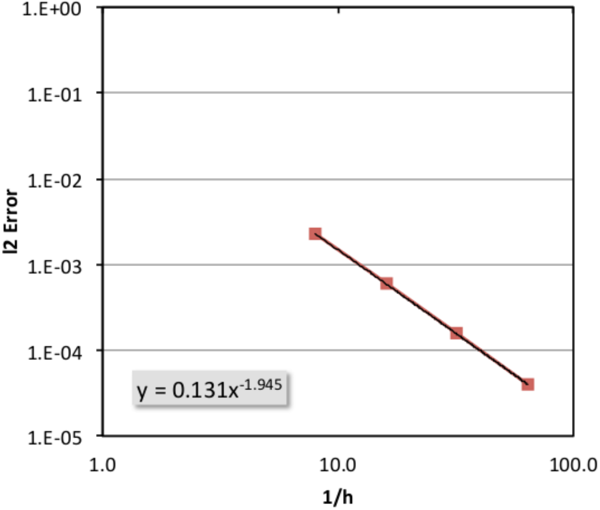
- *Goal:* Write a program in Python
- *Inputs*:
  - # of points in one direction (*npts*)
  - the physical dimension of one side (L_x, L_y)
- *Output*: l_2 error between your numerical solution and an exact solution derived from a manufactured solution

$$l_2 = \sqrt{\frac{\sum_{i=1}^{\text{N}} (\phi_i - \phi_i^{\text{exact}})^2}{N}}$$

- *Runs*: Run your snazzy code for npts $= 5, 9, 17,$ and 33 and plot l_2 norm as a function of $1/h$ where $h = \text{length}/(\text{npts} - 1)$

Example Results: What we're hoping for

2nd Order Central Finite-difference Scheme



Useful for Detecting (Subtle) Bugs

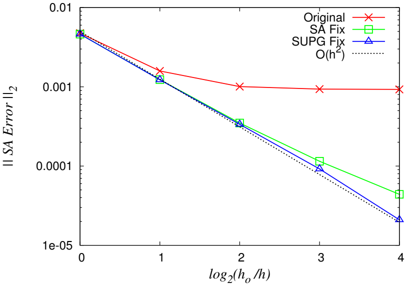
Verification Failure

- FANS, Spalart-Allmaras
- Correct Derivative:

$$\frac{d(sa)}{dx} = \frac{1}{\rho} * \left(\frac{d(\rho * sa)}{dx} - sa \frac{d\rho}{dx} \right)$$

- In code:

$$\frac{d(sa)}{dx} = \frac{1}{\rho} * \frac{d(\rho * sa)}{dx} - sa \frac{d\rho}{dx}$$



A Real Example

MMS Creation Process

- Start by "manufacturing" a suitable closed-form exact solution
- For example, the 10 parameter trigonometric solution of the form: (Roy, 2002)

$$\hat{u}(x,y,z,t) = \hat{u}_0 + \hat{u}_x\, f_s\left(\frac{a_{\hat{u}x}\pi x}{L}\right) + \hat{u}_y\, f_s\left(\frac{a_{\hat{u}y}\pi y}{L}\right) + \\ + \hat{u}_z\, f_s\left(\frac{a_{\hat{u}z}\pi z}{L}\right) + \hat{u}_t\, f_s\left(\frac{a_{\hat{u}_t}\pi t}{L}\right)$$

- Apply this solution to equations of interest, solve for source terms (residual)

Accomplished using symbolic manipulation SymPy, Maple, Mathematica, Macsyma, etc.

Maple MMS: 3D Navier-Stokes Energy Term

$$
\begin{aligned}
Qe = & -\frac{a_{px}\pi p_x}{L}\frac{\gamma}{\gamma-1}\sin\left(\frac{a_{px}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]+\\
& +\frac{a_{py}\pi p_y}{L}\frac{\gamma}{\gamma-1}\cos\left(\frac{a_{py}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]+\\
& -\frac{a_{pz}\pi p_z}{L}\frac{\gamma}{\gamma-1}\sin\left(\frac{a_{pz}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]+\\
& +\frac{a_{\rho x}\pi\rho_x}{2L}\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\left(\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2+\right.\\
& \quad\left.+\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2\right)+\\
& -\frac{a_{\rho y}\pi\rho_y}{2L}\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\left(\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2+\right.\\
& \quad\left.+\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2\right)+\\
& +\frac{a_{\rho z}\pi\rho_z}{2L}\cos\left(\frac{a_{\rho z}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\left(\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2+\right.\\
& \quad\left.+\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2\right)+\\
& +\frac{a_{ux}\pi u_x}{2L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\left\{\left(\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2+\right.\right.\\
& \quad\left.+3\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]+\\
& \quad\left.+\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]\frac{2\gamma}{(\gamma-1)}\right\}+\\
& -\frac{a_{uy}\pi u_y}{L}\sin\left(\frac{a_{uy}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot\\
& \quad\cdot\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]+\\
& -\frac{a_{uz}\pi u_z}{L}\sin\left(\frac{a_{uz}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot\\
& \quad\cdot\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]+
\end{aligned}
$$

But wait, there's more!

$$
-\frac{a_{\rho x}^2\pi^2 k\rho_x\left[2\cos\left(\frac{a_{\rho x}\pi x}{L}\right)^2\rho_x+\sin\left(\frac{a_{\rho x}\pi x}{L}\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\right]\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]}{RL^2\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^3}+
$$

$$
-\frac{a_{\rho y}^2\pi^2 k\rho_y\left[2\sin\left(\frac{a_{\rho y}\pi y}{L}\right)^2\rho_y+\cos\left(\frac{a_{\rho y}\pi y}{L}\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\right]\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]}{RL^2\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^3}+
$$

$$
-\frac{a_{\rho z}^2\pi^2 k\rho_z\left[2\cos\left(\frac{a_{\rho z}\pi z}{L}\right)^2\rho_z+\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\right]\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]}{RL^2\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^3}+
$$

$$
-\frac{4}{3}\frac{a_{ux}^2\pi^2\mu u_x}{L^2}\left[\cos\left(\frac{a_{ux}\pi x}{L}\right)^2 u_x-\sin\left(\frac{a_{ux}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{uy}^2\pi^2\mu u_y}{L^2}\left[\sin\left(\frac{a_{uy}\pi y}{L}\right)^2 u_y-\cos\left(\frac{a_{uy}\pi y}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{uz}^2\pi^2\mu u_z}{L^2}\left[\sin\left(\frac{a_{uz}\pi z}{L}\right)^2 u_z-\cos\left(\frac{a_{uz}\pi z}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{vx}^2\pi^2\mu v_x}{L^2}\left[\sin\left(\frac{a_{vx}\pi x}{L}\right)^2 v_x-\cos\left(\frac{a_{vx}\pi x}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{4}{3}\frac{a_{vy}^2\pi^2\mu v_y}{L^2}\left[\cos\left(\frac{a_{vy}\pi y}{L}\right)^2 v_y-\sin\left(\frac{a_{vy}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{vz}^2\pi^2\mu v_z}{L^2}\left[\cos\left(\frac{a_{vz}\pi z}{L}\right)^2 v_z-\sin\left(\frac{a_{vz}\pi z}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{wx}^2\pi^2\mu w_x}{L^2}\left[\cos\left(\frac{a_{wx}\pi x}{L}\right)^2 w_x-\sin\left(\frac{a_{wx}\pi x}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{wy}^2\pi^2\mu w_y}{L^2}\left[\cos\left(\frac{a_{wy}\pi y}{L}\right)^2 w_y-\sin\left(\frac{a_{wy}\pi y}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{4}{3}\frac{a_{wz}^2\pi^2\mu w_z}{L^2}\left[\sin\left(\frac{a_{wz}\pi z}{L}\right)^2 w_z-\cos\left(\frac{a_{wz}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\right]+
$$

$$
-\frac{a_{vx}\pi v_x}{L}\sin\left(\frac{a_{vx}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot
$$

$$
\cdot\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]+
$$

$$
+\frac{a_{vy}\pi v_y}{2L}\cos\left(\frac{a_{vy}\pi y}{L}\right)\left\{\left(\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2+\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\right.\right.
$$

$$
\left.+3\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]+
$$

$$
\left.+\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]\frac{2\gamma}{\gamma-1}\right\}+
$$

$$
+\frac{a_{vz}\pi v_z}{L}\cos\left(\frac{a_{vz}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot
$$

$$
\cdot\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]+
$$

$$
+\frac{a_{wx}\pi w_x}{L}\cos\left(\frac{a_{wx}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot
$$

$$
\cdot\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]+
$$

$$
+\frac{a_{wy}\pi w_y}{L}\cos\left(\frac{a_{wy}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot
$$

$$
\cdot\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]+
$$

$$
-\frac{a_{wz}\pi w_z}{2L}\sin\left(\frac{a_{wz}\pi z}{L}\right)\left\{\left(3\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]^2+\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]^2+\right.\right.
$$

$$
\left.+\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]^2\right)\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]+
$$

$$
\left.+\left[p_0+p_x\cos\left(\frac{a_{px}\pi x}{L}\right)+p_y\sin\left(\frac{a_{py}\pi y}{L}\right)+p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)\right]\frac{2\gamma}{(\gamma-1)}\right\}+
$$

$$
+\frac{a_{px}^2\pi^2 k p_x\cos\left(\frac{a_{px}\pi x}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]}+
$$

$$
+\frac{a_{py}^2\pi^2 k p_y\sin\left(\frac{a_{py}\pi y}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]}+
$$

$$
+\frac{a_{pz}^2\pi^2 k p_z\cos\left(\frac{a_{pz}\pi z}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]}+
$$

$$
-\frac{2a_{px}a_{\rho x}\pi^2 k p_x\rho_x\cos\left(\frac{a_{\rho x}\pi x}{L}\right)\sin\left(\frac{a_{px}\pi x}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^2}+
$$

$$
-\frac{2a_{py}a_{\rho y}\pi^2 k p_y\rho_y\sin\left(\frac{a_{\rho y}\pi y}{L}\right)\cos\left(\frac{a_{py}\pi y}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^2}+
$$

$$
-\frac{2a_{pz}a_{\rho z}\pi^2 k p_z\rho_z\cos\left(\frac{a_{\rho z}\pi z}{L}\right)\sin\left(\frac{a_{pz}\pi z}{L}\right)}{L^2R\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]^2}+
$$

$$
+\frac{4}{3}\frac{a_{ux}a_{vy}\pi^2\mu u_x v_y}{L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right)\cos\left(\frac{a_{vy}\pi y}{L}\right)+
$$

$$
-\frac{4}{3}\frac{a_{ux}a_{wz}\pi^2\mu u_x w_z}{L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right)\sin\left(\frac{a_{wz}\pi z}{L}\right)+
$$

$$
-\frac{2a_{uy}a_{vx}\pi^2\mu u_y v_x}{L^2}\sin\left(\frac{a_{uy}\pi y}{L}\right)\sin\left(\frac{a_{vx}\pi x}{L}\right)+
$$

$$
+\frac{2a_{uz}a_{wx}\pi^2\mu u_z w_x}{L^2}\cos\left(\frac{a_{wx}\pi x}{L}\right)\sin\left(\frac{a_{uz}\pi z}{L}\right)+
$$

$$
-\frac{4}{3}\frac{a_{vy}a_{wz}\pi^2\mu v_y w_z}{L^2}\cos\left(\frac{a_{vy}\pi y}{L}\right)\sin\left(\frac{a_{wz}\pi z}{L}\right)+
$$

$$
-\frac{2a_{vz}a_{wy}\pi^2\mu v_z w_y}{L^2}\cos\left(\frac{a_{vz}\pi z}{L}\right)\cos\left(\frac{a_{wy}\pi y}{L}\right).
$$

C-code output

```
 RHO = rho_0 + rho_x * sin(a_rhox * PI * x / L) + rho_y * cos(a_rhoy * PI * y / L) + rho_z * sin(a_rhoz * PI * z / L) + rho_t * sin(a_rhot * PI * t / L);
  U = u_0 + u_x * sin(a_ux * PI * x / L) + u_y * cos(a_uy * PI * y / L) + u_z * cos(a_uz * PI * z / L) + u_t * cos(a_ut * PI * t / L);
  V = v_0 + v_x * cos(a_vx * PI * x / L) + v_y * sin(a_vy * PI * y / L) + v_z * sin(a_vz * PI * z / L) + v_t * sin(a_vt * PI * t / L);
  W = w_0 + w_x * sin(a_wx * PI * x / L) + w_y * sin(a_wy * PI * y / L) + w_z * cos(a_wz * PI * z / L) + w_t * cos(a_wt * PI * t / L);
  P = p_0 + p_x * cos(a_px * PI * x / L) + p_y * sin(a_py * PI * y / L) + p_z * cos(a_pz * PI * z / L) + p_t * cos(a_pt * PI * t / L);
  M1 = A_mu * pow(P / R / RHO, 0.3e1 / 0.2e1);
  M2 = P / R / RHO + B_mu;
  MU = M1 / M2;
  Q_e = (0.3e1 * a_ux * u_x * cos(a_ux * PI * x / L) + a_vy * v_y * cos(a_vy * PI * y / L) - a_wz * w_z * sin(a_wz * PI * z / L)) * PI * RHO * U * U / L / 0.2e1 + (a_ux * u_x * cos(a_ux * PI
* x / L) + 0.3e1 * a_vy * v_y * cos(a_vy * PI * y / L) - a_wz * w_z * sin(a_wz * PI * z / L)) * PI * RHO * V * V / L / 0.2e1 + (a_ux * u_x * cos(a_ux * PI * x / L) + a_vy * v_y * cos(a_vy *
PI * y / L) - 0.3e1 * a_wz * w_z * sin(a_wz * PI * z / L)) * PI * RHO * W * W / L / 0.2e1 + (0.4e1 * a_ux * a_ux * u_x * sin(a_ux * PI * x / L) + 0.3e1 * a_uy * a_uy * u_y * cos(a_uy * PI * y
/ L) + 0.3e1 * a_uz * a_uz * u_z * cos(a_uz * PI * z / L)) * MU * PI * PI * U * pow(L, -0.2e1) / 0.3e1 + (0.3e1 * a_vx * a_vx * v_x * cos(a_vx * PI * x / L) + 0.4e1 * a_vy * a_vy * v_y *
sin(a_vy * PI * y / L) + 0.3e1 * a_vz * a_vz * v_z * sin(a_vz * PI * z / L)) * MU * PI * PI * V * pow(L, -0.2e1) / 0.3e1 + (0.3e1 * a_wx * a_wx * w_x * sin(a_wx * PI * x / L) + 0.3e1 * a_wy *
a_wy * w_y * sin(a_wy * PI * y / L) + 0.4e1 * a_wz * a_wz * w_z * cos(a_wz * PI * z / L)) * MU * PI * PI * W * pow(L, -0.2e1) / 0.3e1 + (a_ux * u_x * cos(a_ux * PI * x / L) + a_vy * v_y *
cos(a_vy * PI * y / L) - a_wz * w_z * sin(a_wz * PI * z / L)) * PI * P / (Gamma - 0.1e1) / L - (0.2e1 * a_rhox * a_px * rho_x * p_x * cos(a_rhox * PI * x / L) * sin(a_px * PI * x / L) + 0.2e1
* a_rhoy * a_py * rho_y * p_y * sin(a_rhoy * PI * y / L) * cos(a_py * PI * y / L) + 0.2e1 * a_rhoz * a_pz * rho_z * p_z * cos(a_rhoz * PI * z / L) * sin(a_pz * PI * z / L)) * PI * PI * k *
pow(L, -0.2e1) / R * pow(RHO, -0.2e1) + (U * U + V * V + W * W) * a_rhot * PI * rho_t * cos(a_rhot * PI * t / L) / L / 0.2e1 - a_pt * PI * p_t * sin(a_pt * PI * t / L) / (Gamma - 0.1e1) / L -
(a_uy * u_y * sin(a_uy * PI * y / L) + a_vx * v_x * sin(a_vx * PI * x / L)) * PI * RHO * U * V / L - (a_uz * u_z * sin(a_uz * PI * z / L) - a_wx * w_x * cos(a_wx * PI * x / L)) * PI * RHO * U
* W / L + (a_vz * v_z * cos(a_vz * PI * z / L) + a_wy * w_y * cos(a_wy * PI * y / L)) * PI * RHO * V * W / L + (a_px * a_px * p_x * cos(a_px * PI * x / L) + a_py * a_py * p_y * sin(a_py * PI
* y / L) + a_pz * a_pz * p_z * cos(a_pz * PI * z / L)) * PI * PI * k * pow(L, -0.2e1) / R / RHO - (0.4e1 * a_ux * a_ux * u_x * u_x * pow(cos(a_ux * PI * x / L), 0.2e1) - 0.4e1 * a_ux * a_vy *
u_x * v_y * cos(a_ux * PI * x / L) * cos(a_vy * PI * y / L) + 0.4e1 * a_ux * a_wz * u_x * w_z * cos(a_ux * PI * x / L) * sin(a_wz * PI * z / L) + 0.3e1 * a_uy * a_uy * u_y * u_y *
pow(sin(a_uy * PI * y / L), 0.2e1) + 0.6e1 * a_uy * a_vx * u_y * v_x * sin(a_uy * PI * y / L) * sin(a_vx * PI * x / L) + 0.3e1 * a_uz * a_uz * u_z * u_z * pow(sin(a_uz * PI * z / L), 0.2e1) -
0.6e1 * a_uz * a_wx * u_z * w_x * sin(a_uz * PI * z / L) * cos(a_wx * PI * x / L) + 0.3e1 * a_vx * a_vx * v_x * v_x * pow(sin(a_vx * PI * x / L), 0.2e1) + 0.4e1 * a_vy * a_vy * v_y * v_y *
pow(cos(a_vy * PI * y / L), 0.2e1) + 0.4e1 * a_vy * a_wz * v_y * w_z * cos(a_vy * PI * y / L) * sin(a_wz * PI * z / L) + 0.3e1 * a_vz * a_vz * v_z * v_z * pow(cos(a_vz * PI * z / L), 0.2e1) +
0.6e1 * a_vz * a_wy * v_z * w_y * cos(a_vz * PI * z / L) * cos(a_wy * PI * y / L) + 0.3e1 * a_wx * a_wx * w_x * w_x * pow(cos(a_wx * PI * x / L), 0.2e1) + 0.3e1 * a_wy * a_wy * w_y * w_y *
pow(cos(a_wy * PI * y / L), 0.2e1) + 0.4e1 * a_wz * a_wz * w_z * w_z * pow(sin(a_wz * PI * z / L), 0.2e1)) * MU * PI * PI * pow(L, -0.2e1) / 0.3e1 + (a_ux * u_x * cos(a_ux * PI * x / L) +
a_vy * v_y * cos(a_vy * PI * y / L) - a_wz * w_z * sin(a_wz * PI * z / L)) * PI * P / L - a_ut * PI * u_t * RHO * U * sin(a_ut * PI * t / L) / L + a_vt * PI * v_t * RHO * V * cos(a_vt * PI *
t / L) / L - a_wt * PI * w_t * RHO * W * sin(a_wt * PI * t / L) / L + (U * U + V * V + W * W) * a_rhox * PI * rho_x * U * cos(a_rhox * PI * x / L) / L / 0.2e1 - (U * U + V * V + W * W) *
a_rhoy * PI * rho_y * V * sin(a_rhoy * PI * y / L) / L / 0.2e1 + (U * U + V * V + W * W) * a_rhoz * PI * rho_z * W * cos(a_rhoz * PI * z / L) / L / 0.2e1 - (a_rhox * a_rhox * rho_x *
sin(a_rhox * PI * x / L) + a_rhoy * a_rhoy * rho_y * cos(a_rhoy * PI * y / L) + a_rhoz * a_rhoz * rho_z * sin(a_rhoz * PI * z / L)) * PI * PI * k * P * pow(L, -0.2e1) / R * pow(RHO, -0.2e1) -
(0.2e1 * a_rhox * a_rhox * rho_x * rho_x * pow(cos(a_rhox * PI * x / L), 0.2e1) + 0.2e1 * a_rhoy * a_rhoy * rho_y * rho_y * pow(sin(a_rhoy * PI * y / L), 0.2e1) + 0.2e1 * a_rhoz * a_rhoz *
rho_z * rho_z * pow(cos(a_rhoz * PI * z / L), 0.2e1)) * PI * PI * k * P * pow(L, -0.2e1) / R * pow(RHO, -0.3e1) - (0.3e1 * a_rhox * a_uz * rho_x * u_z * cos(a_rhox * PI * x / L) * sin(a_uz *
PI * z / L) - 0.3e1 * a_rhox * a_wx * rho_x * w_x * cos(a_rhox * PI * x / L) * cos(a_wx * PI * x / L) + 0.3e1 * a_rhoy * a_vz * rho_y * v_z * sin(a_rhoy * PI * y / L) * cos(a_vz * PI * z / L)
+ 0.3e1 * a_rhoy * a_wy * rho_y * w_y * sin(a_rhoy * PI * y / L) * cos(a_wy * PI * y / L) + 0.2e1 * a_rhoz * a_ux * rho_z * u_x * cos(a_rhoz * PI * z / L) * cos(a_ux * PI * x / L) + 0.2e1 *
a_rhoz * a_vy * rho_z * v_y * cos(a_rhoz * PI * z / L) * cos(a_vy * PI * y / L) + 0.4e1 * a_rhoz * a_wz * rho_z * w_z * cos(a_rhoz * PI * z / L) * sin(a_wz * PI * z / L)) * MU * (0.3e1 * B_mu
* R * RHO + P) * PI * PI * W / (B_mu * R * RHO + P) * pow(L, -0.2e1) / RHO / 0.6e1 - a_pz * PI * p_z * Gamma * W * sin(a_pz * PI * z / L) / (Gamma - 0.1e1) / L - (0.3e1 * a_px * a_uy * p_x *
u_y * sin(a_px * PI * x / L) * sin(a_uy * PI * y / L) + 0.3e1 * a_px * a_vx * p_x * v_x * sin(a_px * PI * x / L) * sin(a_vx * PI * x / L) - 0.2e1 * a_py * a_ux * p_y * u_x * cos(a_py * PI * y
/ L) * cos(a_ux * PI * x / L) + 0.4e1 * a_py * a_vy * p_y * v_y * cos(a_py * PI * y / L) * cos(a_vy * PI * y / L) + 0.2e1 * a_py * a_wz * p_y * w_z * cos(a_py * PI * y / L) * sin(a_wz * PI *
z / L) - 0.3e1 * a_pz * a_vz * p_z * v_z * sin(a_pz * PI * z / L) * cos(a_vz * PI * z / L) - 0.3e1 * a_pz * a_wy * p_z * w_y * sin(a_pz * PI * z / L) * cos(a_wy * PI * y / L)) * (0.3e1 * B_mu
* R * RHO + P) * MU * PI * PI * V / (B_mu * R * RHO + P) * pow(L, -0.2e1) / P / 0.6e1 + a_py * PI * p_y * Gamma * V * cos(a_py * PI * y / L) / (Gamma - 0.1e1) / L - (0.3e1 * a_rhox * a_uy *
rho_x * u_y * cos(a_rhox * PI * x / L) * sin(a_uy * PI * y / L) + 0.3e1 * a_rhox * a_vx * rho_x * v_x * cos(a_rhox * PI * x / L) * sin(a_vx * PI * x / L) - 0.2e1 * a_rhoy * a_ux * rho_y * u_x
* sin(a_rhoy * PI * y / L) * cos(a_ux * PI * x / L) + 0.4e1 * a_rhoy * a_vy * rho_y * v_y * sin(a_rhoy * PI * y / L) * cos(a_vy * PI * y / L) + 0.2e1 * a_rhoy * a_wz * rho_y * w_z *
sin(a_rhoy * PI * y / L) * sin(a_wz * PI * z / L) - 0.3e1 * a_rhoz * a_vz * rho_z * v_z * cos(a_rhoz * PI * z / L) * cos(a_vz * PI * z / L) - 0.3e1 * a_rhoz * a_wy * rho_z * w_y * cos(a_rhoz
* PI * z / L) * cos(a_wy * PI * y / L)) * MU * (0.3e1 * B_mu * R * RHO + P) * PI * PI * V / (B_mu * R * RHO + P) * pow(L, -0.2e1) / RHO / 0.6e1 + (0.4e1 * a_rhox * a_ux * rho_x * u_x *
cos(a_rhox * PI * x / L) * cos(a_ux * PI * x / L) - 0.2e1 * a_rhox * a_vy * rho_x * v_y * cos(a_rhox * PI * x / L) * cos(a_vy * PI * y / L) + 0.2e1 * a_rhox * a_wz * rho_x * w_z * cos(a_rhox
* PI * x / L) * sin(a_wz * PI * z / L) + 0.3e1 * a_rhoy * a_uy * rho_y * u_y * sin(a_rhoy * PI * y / L) * sin(a_uy * PI * y / L) + 0.3e1 * a_rhoy * a_vx * rho_y * v_x * sin(a_rhoy * PI * y /
L) * sin(a_vx * PI * x / L) - 0.3e1 * a_rhoz * a_uz * rho_z * u_z * cos(a_rhoz * PI * z / L) * sin(a_uz * PI * z / L) + 0.3e1 * a_rhoz * a_wx * rho_z * w_x * cos(a_rhoz * PI * z / L) *
cos(a_wx * PI * x / L)) * MU * (0.3e1 * B_mu * R * RHO + P) * PI * PI * U / (B_mu * R * RHO + P) * pow(L, -0.2e1) / RHO / 0.6e1 - a_px * PI * p_x * Gamma * U * sin(a_px * PI * x / L) / (Gamma
- 0.1e1) / L + (0.4e1 * a_px * a_ux * p_x * u_x * sin(a_px * PI * x / L) * cos(a_ux * PI * x / L) - 0.2e1 * a_px * a_vy * p_x * v_y * sin(a_px * PI * x / L) * cos(a_vy * PI * y / L) + 0.2e1 *
a_px * a_wz * p_x * w_z * sin(a_px * PI * x / L) * sin(a_wz * PI * z / L) + 0.3e1 * a_py * a_uy * p_y * u_y * cos(a_py * PI * y / L) * sin(a_uy * PI * y / L) + 0.3e1 * a_py * a_vx * p_y * v_x
* cos(a_py * PI * y / L) * sin(a_vx * PI * x / L) - 0.3e1 * a_pz * a_uz * p_z * u_z * sin(a_pz * PI * z / L) * sin(a_uz * PI * z / L) + 0.3e1 * a_pz * a_wx * p_z * w_x * sin(a_pz * PI * z /
L) * cos(a_wx * PI * x / L)) * (0.3e1 * B_mu * R * RHO + P) * MU * PI * PI * U / (B_mu * R * RHO + P) * pow(L, -0.2e1) / P / 0.6e1 - (0.3e1 * a_px * a_uz * p_x * u_z * sin(a_px * PI * x / L)
* sin(a_uz * PI * z / L) - 0.3e1 * a_px * a_wx * p_x * w_x * sin(a_px * PI * x / L) * cos(a_wx * PI * x / L) + 0.3e1 * a_py * a_vz * p_y * v_z * cos(a_py * PI * y / L) * cos(a_vz * PI * z /
L) + 0.3e1 * a_py * a_wy * p_y * w_y * cos(a_py * PI * y / L) * cos(a_wy * PI * y / L) + 0.2e1 * a_pz * a_ux * p_z * u_x * sin(a_pz * PI * z / L) * cos(a_ux * PI * x / L) + 0.2e1 * a_pz *
a_vy * p_z * v_y * sin(a_pz * PI * z / L) * cos(a_vy * PI * y / L) + 0.4e1 * a_pz * a_wz * p_z * w_z * sin(a_pz * PI * z / L) * sin(a_wz * PI * z / L)) * (0.3e1 * B_mu * R * RHO + P) * MU *
PI * PI * W / (B_mu * R * RHO + P) * pow(L, -0.2e1) / P / 0.6e1;
```

Manufactured Analytical Solutions Abstractions Library

Goal: Provide a repository and standardized interface for MMS usage

High Priority:

- Extreme fidelity to generated MMS
- Portability
- Traceability
- Extensible

Low Priority:

- Speed/Performance

Verifying the "Verifier"

Precision is not negotiable.

MASA Testing

- Error target $< 1e\text{-}15$
  - Absolute error on local machines
  - Relative error (other)
  - On all supported compiler sets
- -O0 not sufficient
  - -fp-model precise (Intel)
  - -fno-unsafe-math-optimizations (GNU)
  - -Kieee -Mnofpapprox (PGI)
- "make check"
  - Run by Buildbot every two hours

```
[nick@magus trunk]$ make check
-----------------------------------------
Initializing MASA Tests
-----------------------------------------
PASS: init.sh
PASS: misc
PASS: fail_cond
PASS: catch_exception
PASS: register
PASS: poly
PASS: uninit
PASS: vec
PASS: purge
PASS: heat_const_steady
PASS: euler1d
.           .
.           .
.           .
-----------------------------------------
Finalizing MASA Tests
-----------------------------------------
===================
All 65 tests passed
===================
```

Software Library Snapshot

Software Environment

- Built with: Autotools, C++
- Supports Intel, GNU, Portland Group compilers
- C/C++/Fortran/Python interfaces
- Python interfaces generated with SWIG

Testing

- GIT: version control
- Buildbot: automated testing
- GCOV: line coverage
  - 15,826 lines of code
  - 13,195 lines of testing
  - 98%+ line coverage

LCOV - code coverage report

Current view:	top level - build/src		Hit	Total	Coverage
Test:	MASA	**Lines:**	3077	3132	98.2 %
Date:	2011-04-27	**Functions:**	946	1277	74.1 %

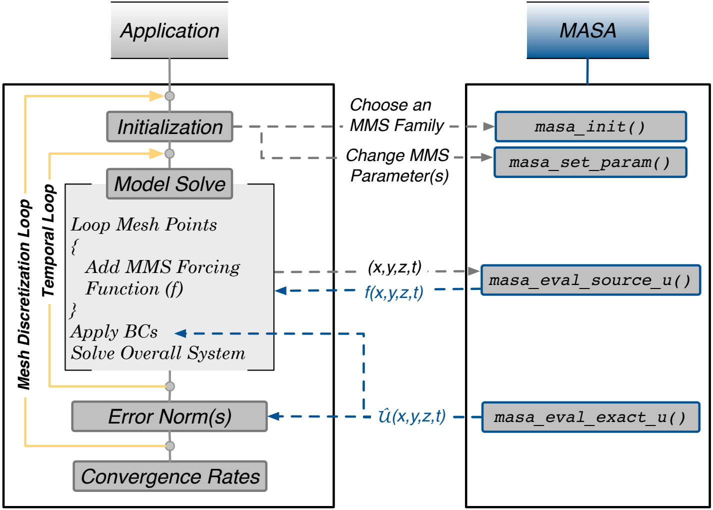
Filename	Line Coverage		Functions	
ablation.cpp	100.0 %	167 / 167	94.4 %	34 / 36
axi_cns.cpp	100.0 %	73 / 73	58.3 %	14 / 24
axi_euler.cpp	100.0 %	71 / 71	58.3 %	14 / 24
cmasa.cpp	100.0 %	98 / 98	100.0 %	71 / 71
cns.cpp	100.0 %	328 / 328	54.4 %	37 / 68
cp_normal.cpp	100.0 %	68 / 68	87.5 %	21 / 24
euler.cpp	100.0 %	426 / 426	54.3 %	50 / 92
euler_chem.cpp	100.0 %	118 / 118	57.7 %	15 / 26
euler_transient.cpp	100.0 %	72 / 72	60.0 %	12 / 20
fans_sa.cpp	100.0 %	402 / 402	54.3 %	38 / 70
heat.cpp	100.0 %	318 / 318	69.2 %	72 / 104
masa.f90	83.3 %	10 / 12	80.0 %	4 / 5
masa_class.cpp	94.4 %	184 / 195	70.0 %	35 / 50
masa_core.cpp	98.3 %	340 / 346	91.4 %	222 / 243
masa_internal.h	86.7 %	111 / 128	69.1 %	221 / 320
masa_map.cpp	100.0 %	25 / 25	100.0 %	6 / 6
radiation.cpp	88.8 %	71 / 80	62.5 %	10 / 16
rans_sa.cpp	100.0 %	93 / 93	96.3 %	52 / 54
smasa.h	100.0 %	1 / 1	50.0 %	2 / 4
sod.cpp	91.0 %	101 / 111	80.0 %	16 / 20

Generated by: LCOV version 1.9

Python API example: What you need from MASA

```
import masa

masa.masa_init("3d Navier Stokes transient sutherland","navierstokes_3d_transient_sutherland")

# evaluate source terms at some point in spacetime
x = 1.1
y = 1.3
z = 0.8
t = 1.2

# source terms
rho_field  = masa.masa_eval_4d_source_rho(x,y,z,t) # rho
rhou_field = masa.masa_eval_4d_source_u  (x,y,z,t) # rho*u
rhov_field = masa.masa_eval_4d_source_v  (x,y,z,t) # rho*v
rhow_field = masa.masa_eval_4d_source_w  (x,y,z,t) # rho*w
e_field    = masa.masa_eval_4d_source_e  (x,y,z,t) # e

# analytical terms
mms_rho_field  = masa.masa_eval_4d_exact_rho(x,y,z,t) # rho
mms_rhou_field = masa.masa_eval_4d_exact_u  (x,y,z,t) # rho*u
mms_rhov_field = masa.masa_eval_4d_exact_v  (x,y,z,t) # rho*v
mms_rhow_field = masa.masa_eval_4d_exact_w  (x,y,z,t) # rho*w
mms_p_field    = masa.masa_eval_4d_exact_p  (x,y,z,t) # pressure
```

General Verification Approach Using MMS and MASA



Available Solutions in MASA 0.43.1

Equations	Dimensions	Time
Euler	1,2,3, axi	Transient, Steady
Non-linear heat conduction	1,2,3	Transient, Steady
Navier-Stokes	1,2,3, axi	Transient, Steady
N-S + Sutherland	3	Transient, Steady
N-S + ablation	1	Transient, Steady
Burgers	2	Transient, Steady
Sod Shock Tube	1	Transient
Euler + chemistry	1	Steady
RANS: Spalart-Allmaras	1	Steady
FANS: SA	2	Steady
FANS: SA + wall	2	Steady
Radiation	1	Steady
SMASA: Gaussian	1	Steady

Future Solution Development

The sky is the limit

- Einstein's field equations (General Relativity)
- Schrodinger equation (Quantum Mechanics)
- Black-Scholes (Finance)
- etc.

Enter Automatic Differentiation

- AD numerically evaluates the derivative of a function
  - applies chain rule repeatedly
- Superior error characteristics (round-off)
- Slow (but we barely care)
- Several libraries: Theano, NAG, Sacado, etc.

MASA PDE Examples

Source Terms: Euler

```
// Arbitrary manufactured solutions
U.template get<0>() = u_0 + u_x * sin(a_ux * PI * x / L)
                          + u_y * cos(a_uy * PI * y / L);
```

$$\nabla \cdot (\rho u) = 0$$

$$\nabla \cdot (eu) + p\nabla \cdot u = 0$$

```
// Mass, momentum and energy
Scalar   Q_rho   = raw_value(divergence(RHO*U));
RawArray Q_rho_u = raw_value(divergence(RHO*U.outerproduct(U)) +
                   P.derivatives());
 Scalar  Q_rho_e = raw_value(divergence((RHO*ET+P)*U));
```

Importing New Solutions

Requirements

- Latex documents can be loaded directly into MASA documentation
  - Model document detailing analytical solution and source terms
  - Interface documentation detailing parameters and functions
- Source and analytical terms in C/C++/Fortran90/AD
  - Can be integrated into your local MASA copy automagically (perl!)
  - Submit a patch
    - (unit tests would be nice)
- Willingness to share
- Publish these solutions!

- Success of MASA depends on use as a community tool

Snapshot

Release

- MASA 0.43.2 current release
- `https://github.com/manufactured-solutions/MASA`
- Open source, LGPL V2.1, free

Publications

- “MASA: a library for verification using manufactured analytical solutions”
- A transient manufactured solution for the compressible Navier-Stokes equations with a power law viscosity
- Manufactured Solutions for the Favre-Averaged Navier-Stokes Equations with Eddy-Viscosity Turbulence Models
- ”A linear regression model for verification of linear problems using Bayesian calibration“ (in prep)

Conclusions

Summary

- MMS is not a difficult concept, but can be tricky and time consuming
- Must have a high degree of confidence in your verification suite
- MASA is an open source library designed to:
  - Increase use of existing MMS in the community
  - Provide a standardized interface and toolset to the community
  - Serve as an example of high quality verification software
  - Available at: `https://github.com/manufactured-solutions/MASA`

Thank you!

Have a well verified day.

nick@ices.utexas.edu