PECOS

Predictive Engineering and Computational Sciences

MASA: A Tool for the Verification of Scientific Software

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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.

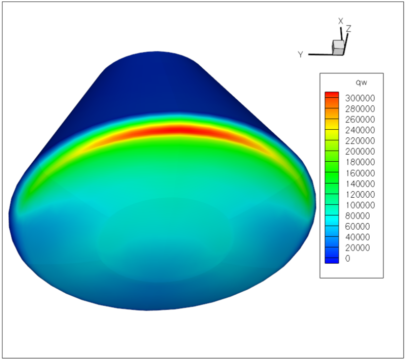
What went wrong?

- 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:

$$\phi(x, y) = (Ly - y)^2 (Ly + y)^2 + (Lx - x)^2 (Lx + x)^2$$

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

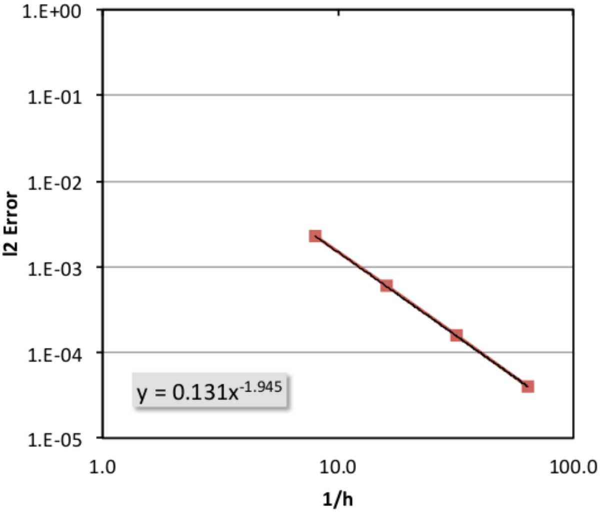
- *Goal:* Write a program in Python
- *Inputs*:
  - # of points in one direction (*npts*)
  - the physical dimension of one side (L_x, L_y)
- *Output*: l_2 error between your numerical solution and an exact solution derived from a manufactured solution

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

- *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

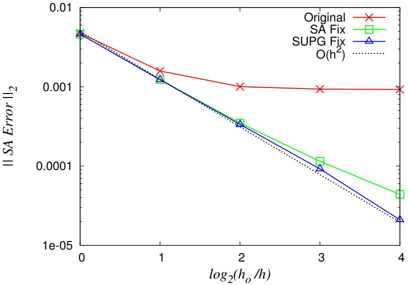
Verification Failure

- FANS, Spalart-Allmaras
- 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!

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

LCOV - code coverage report

			Hit	Total	Coverage
Current view:	top level - build/src				
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

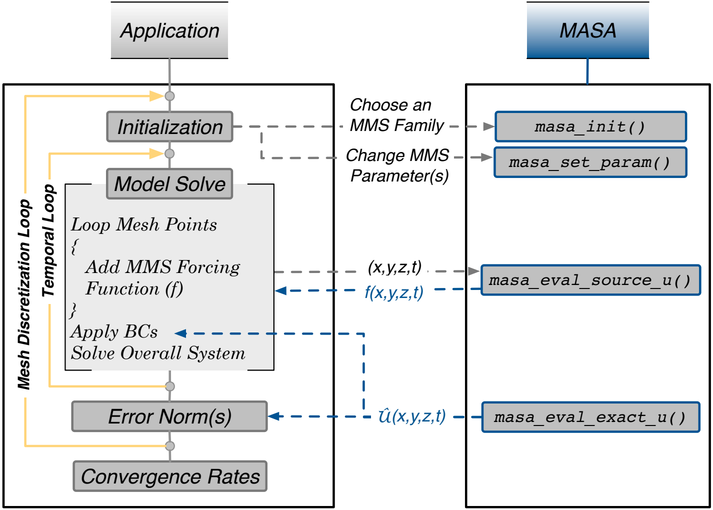
Testing

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

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.

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