PECOS

Predictive Engineering and Computational Sciences

Outside response of common concepts, terms, approaches, tools, and best practices of VVUQ

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Outline

Code and Solution Verification

Code Verification

- Focuses on identifying failures of the code to correctly implement a desired numerical algorithm
- Analytical solutions to mathematical equations are used to calculate error in a corresponding approximate solution

Solution Verification

- Process of quantifying the numerical errors (e.g. round-off, iterative, and discretization errors) that can cause the numerical solution to be an in- adequate approximation of the correct solution
- One simulates the phenomenon of interest and has no a priori knowledge of the solution; in such cases error can only be estimated

Code Verification

Good Software Hygiene

- Unit Tests
- Regression Tests
- High Level Asserts
- Symmetry Tests
- Jacobian Tests
- Parametric Testing
- Exact Solutions
- Code-to-Code Comparison

Code Verification

Method of Manufactured Solutions (MMS)

- Exact solution typically not known
- Can **manufacture** a solution to generate source term from which one attempts to solve for manufactured solution
- Confirm convergence to solution at expected rate

Pitfalls

- Explosion of terms in source
- Solutions need structure similar to application
  - E.g. Boundary layers
  - Exercise terms important to application
- Software reliability

MASA Library

- Manufactured and Analytical Solution Abstraction Library
- Provides solutions and source terms for many operators
- Sources computed by AD
- Released under LGPL

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]\Bigg(\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 + \\
&\qquad + \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\Bigg) + \\
&-\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]\Bigg(\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 + \\
&\qquad + \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\Bigg) + \\
&+\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]\Bigg(\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 + \\
&\quad + \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\Bigg) + \\
&+\frac{a_{ux}\pi u_x}{2L}\cos\left(\frac{a_{ux}\pi x}{L}\right)\Bigg\{\Bigg(\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 + \\
&\qquad +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\Bigg)\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] + \\
&\qquad + \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)}\Bigg\} + \\
&-\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 \\
&\qquad \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 \\
&\qquad \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!

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

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

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

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

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

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

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

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

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

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

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

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

$$-\frac{a_{vx}\pi v_x}{L}\sin\left(\frac{a_{vx}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot$$
$$\cdot\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]+$$

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

$$+\frac{a_{vz}\pi v_z}{L}\cos\left(\frac{a_{vz}\pi z}{L}\right)\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot$$
$$\cdot\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]+$$

$$+\frac{a_{wx}\pi w_x}{L}\cos\left(\frac{a_{wx}\pi x}{L}\right)\left[u_0+u_x\sin\left(\frac{a_{ux}\pi x}{L}\right)+u_y\cos\left(\frac{a_{uy}\pi y}{L}\right)+u_z\cos\left(\frac{a_{uz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot$$
$$\cdot\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]+$$

$$+\frac{a_{wy}\pi w_y}{L}\cos\left(\frac{a_{wy}\pi y}{L}\right)\left[v_0+v_x\cos\left(\frac{a_{vx}\pi x}{L}\right)+v_y\sin\left(\frac{a_{vy}\pi y}{L}\right)+v_z\sin\left(\frac{a_{vz}\pi z}{L}\right)\right]\left[\rho_0+\rho_x\sin\left(\frac{a_{\rho x}\pi x}{L}\right)+\rho_y\cos\left(\frac{a_{\rho y}\pi y}{L}\right)+\rho_z\sin\left(\frac{a_{\rho z}\pi z}{L}\right)\right]\cdot$$
$$\cdot\left[w_0+w_x\sin\left(\frac{a_{wx}\pi x}{L}\right)+w_y\sin\left(\frac{a_{wy}\pi y}{L}\right)+w_z\cos\left(\frac{a_{wz}\pi z}{L}\right)\right]+$$

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

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

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

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

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

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

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

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

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

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

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

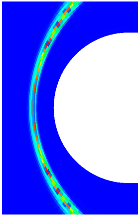
$$-\frac{4}{3}\frac{a_{vy}a_{wz}\pi^2\mu v_yw_z}{L^2}\cos\left(\frac{a_{vy}\pi y}{L}\right)\sin\left(\frac{a_{wz}\pi z}{L}\right)+$$

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

Solution Verification

Goal-Oriented Error Estimation & Adaptivity

- Typically want to control the error in some **functional** of the solution u, say $Q(u)$ and not u
- Error representation: $Q(u) - Q(u^h) = R(u^h; p) + \Delta$
  - p is the solution to the adjoint problem
  - Δ higher-order remainder term
- Use adjoint and residual to drive mesh adaptivity
- Under best conditions rigorous bounds on error, but useful indicator regardless



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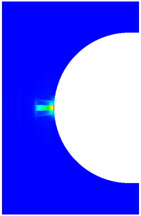

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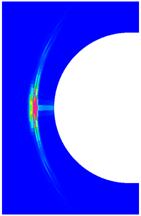
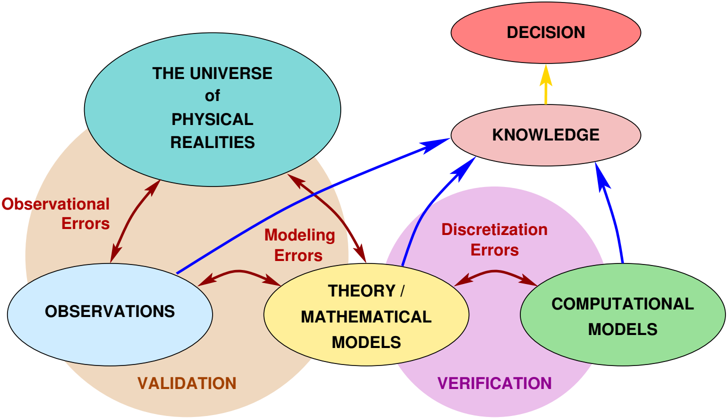


Imperfect Paths to Knowledge and Predictive Simulation



Predictive Simulation: the treatment of model and data uncertainties and their propagation through a computational model to produce predictions of **quantities of interest with quantified uncertainty**.

Models are Imperfect

Mathematical models for complex multi-scale multi-physics systems are not usually posed as general truth statements about physical reality

Examples of Useful Imperfect Models

- Newtonian mechanics
- Continuum mechanics
- Chemical reaction mechanisms
- RANS turbulence models
- Homogenization of complex materials

How do the imperfections of the mathematical models impact the reliability of the simulations in which they are used?

Validation processes are designed to find out

Quantities of Interest

Simulations have a purpose: to inform a decision-making process

- Quantities are predicted to inform the decision
- These are the Quantities of Interest (QoIs)
- Models are not (evaluated as) scientific theories

Acceptance of a model is conditional on:

- its purpose
- the QoIs to be predicted
- the required accuracy

What are Predictions?

Prediction

Purpose of predictive simulation is to predict QoIs for which measurements are **not** available (otherwise predictions not needed)

Measurements may be unavailable because:

- instruments unavailable
- scenarios of interest inaccessible
- system not yet built
- ethical or legal restrictions
- it's the future

How can we have confidence in the predictions?

Posing a “Predictive Validation” Process

Predictive Validation Question

Does the combination of physical models, uncertainty models and supporting data yield acceptable credible predictions of the QoIs?

Validation Activities

- **Inform**: Calibrate to match observations
  - What parameter values, model errors, etc. are plausible given the data?
- **Challenge**: Check that model output consistent with observations
  - Are discrepancies explained by plausible errors/uncertainties (in light of uncertainty models)?
- **Assess**: Determine impact of uncertainty/error on QoI’s
  - Are observed discrepancies between model & data significant to QoI’s?
  - Are the QoI’s sensitive to models & uncertainties to which the observations are not?

Validation Expectations are Model Dependent

Interpolation “models”: simple fit to data

- Test for missing dependencies
- Test accuracy of fitting function
- Check that use is in the range of training data

Physics-based models: formulated from theory

- This is what allows extrapolation
- Check that used in domain of applicability
- May include less reliable components:
  - Embedded (semi-) empirical models
  - Simplifying assumptions
  - Inadequacy models
  - A validation assessment is needed for these

Predictive Validation and Uncertainty

Treating Uncertainty is Integral to Predictive Validation

- Uncertainty in data and parameters limit the sensitivity of the validation process
- Uncertainty from model inadequacy enables assessment of impact of inconsistencies with data on QoI's

Need Mathematical Treatment of Uncertainty

- We represent with Bayesian probability
- Probabilistic "models" of knowledge/uncertainty
  - Data & its uncertainty
  - Prior knowledge
  - Knowledge of model inadequacy
- Bayesian inference for calibration & model selection

Outline

An Abstract Setting for Predictions

Consider a model of the form:

$$\mathcal{R}(u, \tau(\theta); \xi) = 0$$

- $\mathcal{R}$ Physics-based system model (e.g. momentum conservation)
- u System state
- $\tau(u; \theta, \xi)$ embedded model (e.g constitutive) with parameters θ
- ξ scenario parameters

- Observables given by $d(u, \tau(\theta); \xi)$
- QoIs given by $q(u, \tau(\theta); \xi)$
- $\mathcal{R}$, d and q considered reliable (no uncertainties)

τ may be inadequate and θ, ξ may be uncertain

Data Uncertainty and Model Inadequacy

$$
\begin{aligned}
0 &= \mathcal{R}(u, \tau(\theta) + \epsilon_{\text{mod}}; \xi) \\
D &= d(u, \tau(\theta) + \epsilon_{\text{mod}}; \xi) + \epsilon_{\text{exp}} \\
Q &= q(u, \tau(\theta) + \epsilon_{\text{mod}}; \xi)
\end{aligned}
$$

Predictive Uncertainty

$$
\begin{aligned}
0 &= \mathcal{R}(u, \tau(\theta); \xi) \\
D &= d(u, \tau(\theta); \xi) + \epsilon_{\text{exp}} + \tilde{\epsilon}_{\text{mod}} \\
Q &= ?
\end{aligned}
$$

Kennedy & O'Hagen

Uncertainty in predictions, **q**, arise from uncertain parameters, $\boldsymbol{\theta}$, $\boldsymbol{\xi}$ **AND** model inadequacy ϵ_{mod}

Some Caveats:

- all sources of uncertainty have been identified
- the data are accurate with well characterized uncertainties
- computational models are reliable (verified)
- numerical solutions are well resolved

A Processes for Predictive Validation

1.Inform models τ^m and ϵ_{mod}

- Use data for observables D_c from scenarios ξ_c
- Bayesian inference to calibrate θ_i for models τ_i^m and meta-parameters for $\epsilon_{\mathrm{mod}i}$ for model classes i
- Bayesian model selection among model classes i

2. Challenge selected models

- Use data for observables D_v from scenarios ξ_v (include D_c from ξ_c)
- Are physics $+$ uncertainty models consistent with observations? (Bayesian hypothesis testing?)
- Uncertainty models **must** account for all discrepancies between physics models and observations

A Processes for Predictive Validation

3. Asses validity of predictions

- Does scenario ξ_p exercise τ^m outside the conditions in which it has been challenged? (requires characterization of relevant "conditions")
- Are prediction quantities q sensitive to uncertainties to which observed quantities are not?
- Are prediction uncertainties in q too large for decision maker

Entitled to make predictions **only** if answers to questions in (3) are "**no**"

Outline

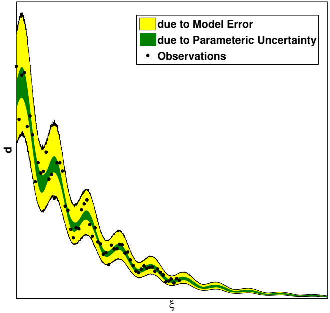
Tools for Calibration

- **Bayesian model calibration**
- Bayesian model selection

Determine:

- Values of the parameters that are consistent with the calibration data
- Includes learning about the model error.

$$\underbrace{\pi(\boldsymbol{\theta}|D_{cal})}_{\text{posterior}} = \frac{\overbrace{\pi(D_{cal}|\boldsymbol{\theta})}^{\text{likelihood}}\,\overbrace{\pi(\boldsymbol{\theta})}^{\text{prior}}}{\underbrace{\pi(D_{cal})}_{\text{evidence}}}$$



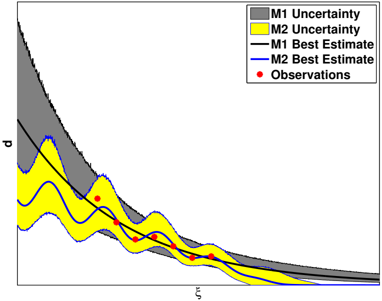
Tools for Calibration

- Bayesian model calibration
- **Bayesian model selection**

Identify:

- The most plausible error structure for model error
- The best among a set of approximate or phenomenological models.

$$\underbrace{\pi(\mathrm{M}_i|D_{cal},\mathcal{M})}_{\text{posterior plausibility}} = \frac{\overbrace{\pi(D_{cal}|\mathrm{M}_i,\mathcal{M})}^{\text{evidence}}\ \overbrace{\pi(\mathrm{M}_i|\mathcal{M})}^{\text{prior plausibility}}}{\pi(D_{cal}|\mathcal{M})}$$



Tools for Validation

- **Bayesian model selection**
- Consistency metric

- Reject models that are less consistent with the calibration data
- Keep the models that best trades-off the principle of parsimony with the goodness-of-fit

$$\mathrm{M}_1 \succ \mathrm{M}_2 \quad \Longleftrightarrow \quad \pi(\mathrm{M}_1 | D_{cal}, \mathcal{M}) > \pi(\mathrm{M}_2 | D_{cal}, \mathcal{M})$$

$$\underbrace{\frac{\pi(D_{cal}|\mathrm{M}_1)}{\pi(D_{cal}|\mathrm{M}_2)}}_{\text{Bayes factor}} \underbrace{\frac{\pi(\mathrm{M}_1, \mathcal{M})}{\pi(\mathrm{M}_2, \mathcal{M})}}_{\text{prior odds}} > 1$$

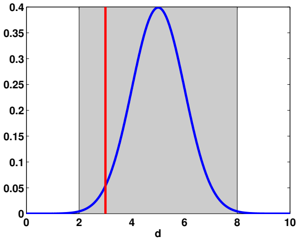
$$\underbrace{\ln[\pi(D_{cal}|\mathrm{M}_1)]}_{\text{log evidence}} = \underbrace{E\left[\ln[\pi(D_{cal}|\boldsymbol{\theta}, \mathrm{M}_1)]\right]}_{\text{data fit}} - \underbrace{\mathrm{KL}\left(\pi(\boldsymbol{\theta}|D_{cal}, \mathrm{M}_1) \,||\, \pi(\boldsymbol{\theta}|\mathrm{M}_1)\right)}_{\text{model complexity}}$$

$$\left(\text{model complexity} \;\; ; \;\; \text{goodness of fit} \;\; ; \;\; \text{prior} \right)$$

Tools for Validation

- Bayesian model selection
- **Consistency metric**

Need a quantitative characterization of consistency of model predictions with validation data.



Consistent

- This is different from accuracy which assess whether observations and model predictions are "close enough"
- To entitle prediction, uncertainty models must plausibly account for all discrepancies between physics models and observations.

Outline

Data Reduction Modeling

Assessing uncertainties in data is **NOT** primarily statistical

Why is it needed?

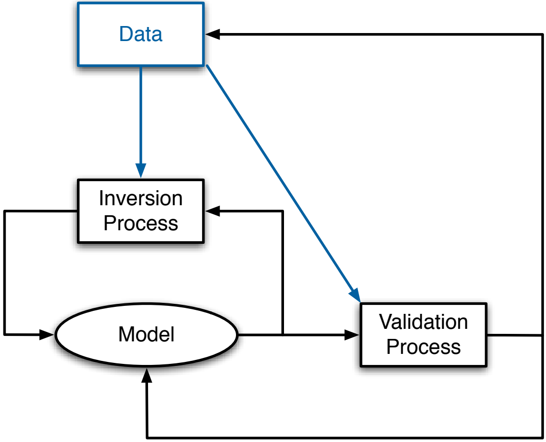
- Very likely that quantities we wish to measure are not directly measurable in an experiment
- Have to infer the values from other measurements using a mathematical model
- Estimate/recover uncertainties in legacy experimental data

Impact on Validation and UQ

- Our philosophy: All mathematical models must be validated
- Must incorporate uncertainty of both the measured data and the data reduction model into the final uncertainty quantification of the data

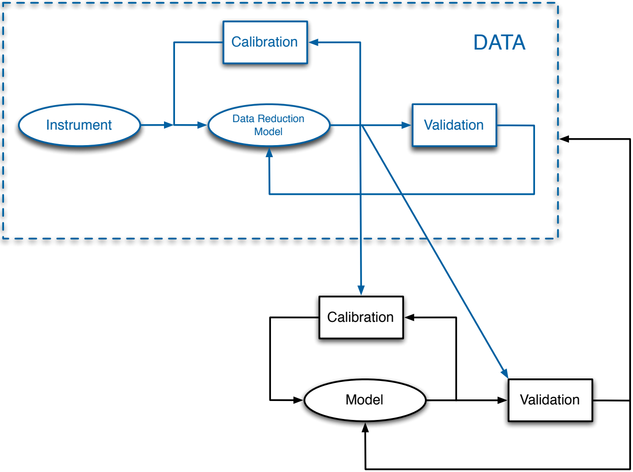
Data Reduction Modeling

Traditional calibration schematic:



Data Reduction Modeling

Incorporation of data reduction model:



Challenges

Complexity of Analysis

- DRM's may be complex multi-physics models in their own right
- Need very reliable validation and uncertainty analysis
- Logical dependencies of measurements

Cooperation of Experimental and Computational Scientists

- As data consumers, computational scientists must be able to properly characterize uncertainty in the data, <u>including</u> any data reduction models
- Requires many details of experimental procedures - some data producers may be reluctant to share such details or may simply be unavailable (legacy data)

Outline

Final Remarks

Verification

- Techniques of code verification are well established but not as widely used as they should be
- Techniques of solution verification can be further developed
  - Strengthen *a posteriori* error estimates of QoI's for complex problems
- Bigger issue is adoption, e.g.:
  - Few application codes support adjoints
  - Even error estimates based on grid refinement are often not used
- Distinct from Validation and UQ

Final Remarks

Validation and UQ

- Involve much larger conceptual & research issues
  - Unobserved prediction QoI's (predictive validation)
  - Importance of reliable physics models enabling extrapolation
  - Critical role of inadequacy models esp. for "embedded models"
  - Need observational data with well characterized uncertainties, but in many problems, this is not available...
  - Uncertainty modeling: mathematically encoding the often qualitative generally incomplete physical information that we have
    - Priors, model inadequacy and data uncertainties

Important, but I did not Discuss

- Algorithms & software
- Decision making
- Rare events
- Education & socialization