



PECOS

Predictive Engineering and Computational Sciences

Tools and Techniques for Code Verification using Manufactured Solutions

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- 1 Introduction to MMS
- 2 What we have learned
- 3 What we are working on

Introduction to the Method of Manufactured Solutions

Verification of Scientific Software

- Verification ensures that the outputs of a computation accurately reflect the solution of the mathematical models.
- Are we solving our equations correctly?

Method of Exact Solutions

- Numerically solve the equations for a solution that can be determined analytically.

Method of Manufactured Solutions

- Often, analytical solutions either:
 - ▶ Do not exist
 - ▶ Do not fully exercise equations
- Alleviate this using MMS: “create” our own solutions

Generating MMS using Symbolic Packages

MMS Creation Process

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

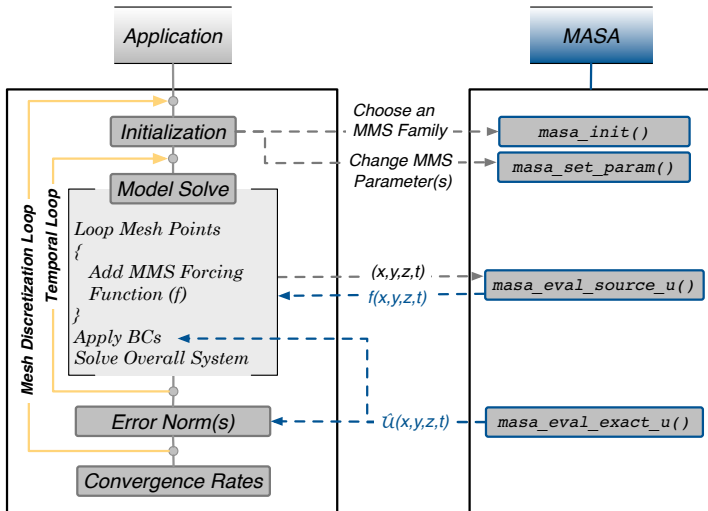
$$\begin{aligned}\hat{u}(x, y, z, t) = & \hat{u}_0 + \hat{u}_x f_s \left(\frac{a \hat{u}_x \pi x}{L} \right) + \hat{u}_y f_s \left(\frac{a \hat{u}_y \pi y}{L} \right) + \\ & + \hat{u}_z f_s \left(\frac{a \hat{u}_z \pi z}{L} \right) + \hat{u}_t f_s \left(\frac{a \hat{u}_t \pi t}{L} \right)\end{aligned}$$

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

Accomplished using packages such as: Maple, Mathematica, SymPy, Macsyma

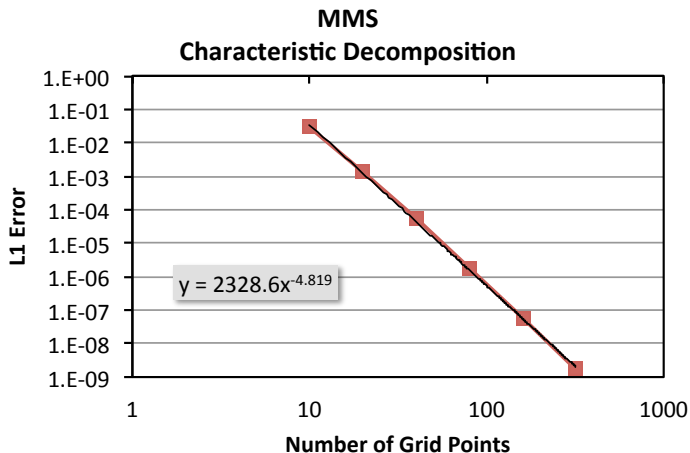
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Generic Verification Approach Using MMS

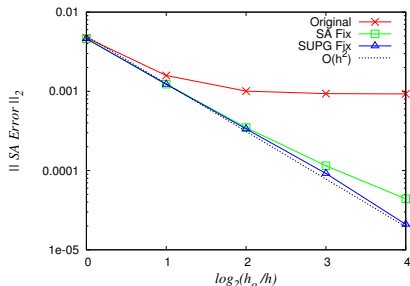


Example: Euler Equations

5th Order Weno Scheme



Detecting Bugs



Verification of FIN-S

- FANS, Spalart-Allmaras
- Model Derivative:

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

- In code:

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

Why is this not more commonly done!?!

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: **users must trust output!**

MASA Testing

- Error target $< 1e-15$
 - ▶ 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 62 tests passed
=====
```

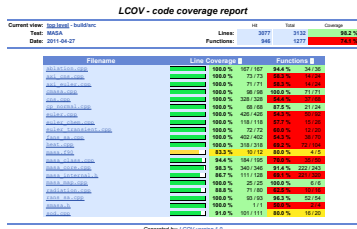
Portability

Software Environment

- Built with: Autotools, C++
- Supports Intel, GNU, Portland Group compilers
- C/C++ interfaces
- Fortran interfaces
 - iso_c_bindings**
 - Fortran 2003 Standard

Testing

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



Traceability

Doxygen provides code and model documentation

3.2 Euler Equations

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where $\phi = \rho, u, v, w$ or p , and $f_n(\cdot)$ functions denote either sine or cosine function. Note that in this case, ϕ_x, ϕ_y and ϕ_z are constants and the subscripts do not denote differentiation.

Although ? provide the constants used in the manufactured solutions for the 2D supersonic and subsonic cases for Euler and Navier-Stokes equations, only the source term for the 2D mass conservation equation (3.20) is presented.

Source terms for mass conservation (Q_ρ), momentum (Q_u, Q_v and Q_w) and total energy (Q_e) equations are obtained by symbolic manipulations of compressible steady Euler equations above using Maple 13 (?) and are presented in the following sections for the one, two and three-dimensional cases.

3.2.2.1 1D Steady Euler

The manufactured analytical solutions (3.52) for each one of the variables in one-dimensional case of Euler equations are:

$$\begin{aligned}\rho(x) &= \rho_0 + \rho_s \sin\left(\frac{a_{\rho s} \pi x}{L}\right) \\ u(x) &= u_0 + u_s \sin\left(\frac{a_{us} \pi x}{L}\right) \\ p(x) &= p_0 + p_s \cos\left(\frac{a_{ps} \pi x}{L}\right)\end{aligned}\quad (3.26)$$

The MMS applied to Euler equations consists in modifying the 1D Euler equations (3.20) – (3.22) by adding a source term to the right-hand side of each equation:

$$\begin{aligned}\frac{\partial(\rho u)}{\partial x} &= Q_\rho \\ \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(p)}{\partial x} &= Q_u \\ \frac{\partial(\rho u v)}{\partial x} + \frac{\partial(p v)}{\partial x} &= Q_v\end{aligned}\quad (3.27)$$

so the modified set of equations (3.27) conveniently has the analytical solution given in Equation (3.53).

Source terms Q_ρ, Q_u and Q_v , are obtained by symbolic manipulations of equations above using Maple and are presented in the following sections. The following auxiliary variables have been included in order to improve readability and computational efficiency:

$$\begin{aligned}\text{rho}_1 &= \rho_0 + \rho_s \sin\left(\frac{a_{\rho s} \pi x}{L}\right) \\ U_1 &= u_0 + u_s \sin\left(\frac{a_{us} \pi x}{L}\right) \\ P_1 &= p_0 + p_s \cos\left(\frac{a_{ps} \pi x}{L}\right)\end{aligned}$$

where the subscripts refer to the 1D case.

The mass conservation equation written as an operator is:

$$\mathcal{L} = \frac{\partial(\rho u)}{\partial x}$$

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3.2 Euler Equations

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| | | | | | | |
|-------|-------|-------|--------|--------|--------|------|
| k | u_0 | u_x | u_y | u_z | v_0 | L |
| v_0 | v_x | v_y | v_z | w_0 | w_x | w_y |
| rho_0 | rho_x | rho_y | rho_z | p_0 | p_x | p_y |
| a_px | a_py | a_pz | a_rhox | a_rhoy | a_rhoz | a_us |
| a_uy | a_uz | a_vx | a_vy | a_vz | a_wx | a_wy |
| a_wz | mu | Gamma | | | | |

Table 3.6: Parameters used by the 3D Steady Euler

- `masa_eval_2d_exact_u()`
- `masa_eval_2d_exact_v()`
- `masa_eval_2d_exact_p()`
- `masa_eval_2d_exact_rho()`
- `masa_eval_2d_grad_u()`
- `masa_eval_2d_grad_v()`
- `masa_eval_2d_grad_p()`
- `masa_eval_2d_grad_rho()`

3.2.3.3 3D Steady Euler

Initialization:

- `euler_3d`

Functions:

- `masa_init()`
- `masa_eval_3d_source_rho_u()`
- `masa_eval_3d_source_rho_v()`
- `masa_eval_3d_source_rho_w()`
- `masa_eval_3d_source_rho_e()`
- `masa_eval_3d_source_rho_x()`
- `masa_eval_3d_exact_u()`
- `masa_eval_3d_exact_v()`
- `masa_eval_3d_exact_w()`
- `masa_eval_3d_exact_p()`

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Available Solutions in MASA 0.40

| 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

Single Physics

- Additional RANS models ($k-\omega$, $k-\epsilon$, etc.)
- Shocks

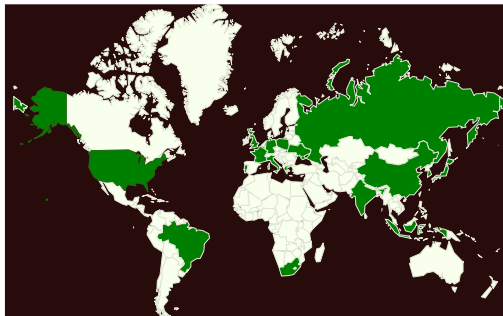
Multiphysics

- Turbulence with chemistry
- Flow with improved transport

Importing New Solutions in MASA 0.40

- Model document detailing analytical solution and source terms
- Latex documents can be loaded directly into MASA documentation
- Source and analytical terms in C/C++/Fortran90
- **Willingness to share**

Public Library



Current Release

- MASA 0.40.2
- <https://red.ices.utexas.edu/projects/software>
- Open source, LGPL V2.1, free

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_{px}\pi \rho_x}{2L} \cos\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]^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 + \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 + \\
 & - \frac{a_{py}\pi \rho_y}{2L} \sin\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] \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 + \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 + \\
 & + \frac{a_{pz}\pi \rho_z}{2L} \cos\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] \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 + \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 + \\
 & + \frac{a_{ux}\pi u_x}{2L} \cos\left(\frac{a_{ux}\pi x}{L}\right) \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. \\
 & + 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 \left. \left[\rho_0 + \rho_x \sin\left(\frac{a_{px}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{py}\pi y}{L}\right) + \rho_z \sin\left(\frac{a_{pz}\pi z}{L}\right) \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_{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_{px}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{py}\pi y}{L}\right) + \rho_z \sin\left(\frac{a_{pz}\pi z}{L}\right) \right] \cdot \\
 & \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_{wz}\pi u_z}{L} \sin\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] \left[\rho_0 + \rho_x \sin\left(\frac{a_{px}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{py}\pi y}{L}\right) + \rho_z \sin\left(\frac{a_{pz}\pi z}{L}\right) \right] \cdot \\
 & \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}$$

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Combinatorial Explosion

Explosion in source term size

- Complexity increases with more sophisticated mathematical models
 - ▶ Sutherland viscosity model has over 1,612,000 characters
- Large memory requirements (128 GB not sufficient for Sutherland)
- Computational intensity
- **segfaults**

Hierarchic MMS

- Decompose each equation into sub-terms
- Each term is operated on individually by the manufactured solution
- Resulting expressions are re-combined to regain source term

The Hierarchic MMS

Consider the full 3D Navier-Stokes energy equation:

$$\mathcal{L} = \frac{\partial(\rho e_t)}{\partial t} + \nabla \cdot (\rho \mathbf{u} e_t) + \nabla \cdot \mathbf{q} + \nabla \cdot (p \mathbf{u}) - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u})$$

Decompose:

$$\mathcal{L}_1 = \frac{\partial(\rho e_t)}{\partial t}$$

$$\mathcal{L}_2 = \nabla \cdot (\rho \mathbf{u} e_t)$$

$$\mathcal{L}_3 = \nabla \cdot \mathbf{q}$$

$$\mathcal{L}_4 = \nabla \cdot (p \mathbf{u})$$

$$\mathcal{L}_5 = -\nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u})$$

Hierarchic MMS extensions:

- Expand each component of divergence
- Transient and steady cases ($\mathcal{L}_1 = 0$)
- Sutherland model only requires altering \mathcal{L}_5
- Navier-Stokes \rightarrow Euler and additional terms
- Can assist in debugging

[illegible]

Reduced source term C-output

[illegible]

Shortcomings

Symbolic Shortcomings

- Hierarchic decomposition is an improvement, but is it enough?
 - ▶ Even with factorization, source terms still massive
 - ▶ Generating manufactured solutions was a full time job at PECOS
- Everything we have discussed has been generated outside of MASA
 - ▶ Not thrilled with Maple, Mathematica

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: NAG, Sacado, etc.

“Dual Numbers” - [Clifford 1873],[Study 1891]

- A new element ϵ
- Closed under addition and multiplication:

$$\left\{ \sum_{i=0}^m a_i \epsilon^i : a_i \in \mathbb{R}, m < \infty \right\}$$

- Take the quotient with $\epsilon^2 \equiv 0$

$$\mathbb{D}[\mathbb{R}] \equiv \{a + b\epsilon : a, b \in \mathbb{R}\}$$

- Used with quaternions to represent rotations and translations
- Arithmetic:

$$(a + b\epsilon) + (c + d\epsilon) = ((a + c) + (b + d)\epsilon)$$

$$(a + b\epsilon) - (c + d\epsilon) = ((a + c) - (b + d)\epsilon)$$

$$\begin{aligned} (a + b\epsilon) \times (c + d\epsilon) &= (ac) + ad\epsilon + bc\epsilon + bd\epsilon^2 \\ &= ((ac) + (ad + bc)\epsilon) \end{aligned}$$

“Hyper-dual Numbers” - [Fike 2009]

- Add two new elements ϵ_1, ϵ_2 to \mathbb{R}
- Take the quotient with $\epsilon_1^2 \equiv \epsilon_2^2 \equiv 0$

$$\mathbb{H}[\mathbb{R}] \equiv \{a + b\epsilon_1 + c\epsilon_2 + d\epsilon_1\epsilon_2 : a, b, c, d \in \mathbb{R}\}$$

- Arithmetic:

$$\begin{aligned} (a + b\epsilon_1 + c\epsilon_2 + d\epsilon_1\epsilon_2) + (e + f\epsilon_1 + g\epsilon_2 + h\epsilon_1\epsilon_2) &= \\ ((a + e) + (b + f)\epsilon_1 + (c + g)\epsilon_2 + (d + h)\epsilon_1\epsilon_2) &= \\ (a + b\epsilon_1 + c\epsilon_2 + d\epsilon_1\epsilon_2) - (e + f\epsilon_1 + g\epsilon_2 + h\epsilon_1\epsilon_2) &= \\ ((a - e) + (b - f)\epsilon_1 + (c - g)\epsilon_2 + (d - h)\epsilon_1\epsilon_2) &= \\ (a + b\epsilon_1 + c\epsilon_2 + d\epsilon_1\epsilon_2) \times (e + f\epsilon_1 + g\epsilon_2 + h\epsilon_1\epsilon_2) &= \\ (ae) + (af + be)\epsilon_1 + (ag + ce)\epsilon_2 + (ah + de + bg + cf)\epsilon_1\epsilon_2 &= \end{aligned}$$

“Hyper-Dual Numbers”

- With $\epsilon_1^2 \equiv \epsilon_2^2 \equiv 0 \equiv (\epsilon_1 \epsilon_2)^2 = 0$
- Where $X \equiv x + \epsilon_1 + \epsilon_2$, we find:

$$f(X) = f(x) + f'(x)\epsilon_1 + f'(x)\epsilon_2 + f''(x)\epsilon_1\epsilon_2$$

- The Taylor series truncates exactly at the second-derivative term
- Using hyper-dual numbers results in first- and second-derivative calculations that are exact, regardless of step size
- methods for computing exact higher derivatives can be created by using more non-real parts (ϵ_3 , for instance)

Data Type Independence: Generic Programming

- Template arguments can be data types
- Class data members can depend on template argument
- Methods and functions can as well

Example

```
template <typename T>
class NumericVector {
T* data;
};
```

This is how MASA provides arbitrary precision, e.g.

```
masa_eval_source< double >()
```

Constructing higher rank objects

Templated classes can be instantiated with plain data types

- or with other instantiated templated types
- or with other instantiations of themselves

Example

```
NumericVector<float> floatvec;  
NumericVector<complex<double> > complexdoublevec;  
NumericVector<NumericVector<float> > floatmatrix;
```

MASA PDE Examples

Manufactured Solution

```
// 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);

U.template get<1>() = v_0 + v_x * cos(a_vx * PI * x / L) +
                    v_y * sin(a_vy * PI * y / L);

ADScalar RHO = rho_0 + rho_x * sin(a_rhox * PI * x / L) +
                rho_y * cos(a_rhoy * PI * y / L);

ADScalar P = p_0 + p_x * cos(a_px * PI * x / L) +
              p_y * sin(a_py * PI * y / L);
```

MASA PDE Examples

Source Terms: Euler

```
// Gas state
ADScalar T = P / RHO / R;
ADScalar E = 1. / (Gamma-1.) * P / RHO;
ADScalar ET = E + .5 * U.dot(U);

// 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));
```

MASA PDE Examples

Source Terms: Navier-Stokes

```
// Gas state
ADScalar T = P / RHO / R;
ADScalar E = 1. / (Gamma-1.) * P / RHO;
ADScalar ET = E + .5 * U.dot(U);

// Constitutive laws
Tensor GradU = gradient(U);
Tensor Tau = mu * (GradU + transpose(GradU) -
    2./3. * divergence(U) * RawArray::identity());
FullArray q = -k * T.derivatives();

Scalar Q_rho = raw_value(divergence(RHO*U));
RawArray Q_rho_u = raw_value(divergence(RHO*U.outerproduct(U) - Tau) +
    P.derivatives());
Scalar Q_rho_e = raw_value(divergence((RHO*ET+P)*U + q - Tau.dot(U)));
```

Operator-Overloaded Multi-precision

Example

```
template <typename T, typename S>
struct ShadowNumber {
    T _val;
    S _shadow;
};
```

- Simultaneous calculation with multiple floating point representations, to estimate rounding error.

Example

```
ShadowNumber<float, double>          shadowed_float;
ShadowNumber<double, long double>    shadowed_double;
```


Future AD work

Future Work

- Automatic Latex Generation
- Latex Parser – MMS generator
- Complex multiphysics
- Inverse Problems

Stochastic MASA and QUESO Verification

Initial Effort

- Conjugate Prior(s)
 - ▶ Posterior is in the same family as the prior
- Initial problem: Gaussian
- QUESO: multilevel Monte Carlo
 - ▶ {5k, 50k, 500k} samples
- Tricky: sampling posterior
 - ▶ Convergence rates can be bounded

| | |
|----------------------|-----------|
| 5k Posterior Mean | = 2.19617 |
| 50k Posterior Mean | = 2.18629 |
| 500k Posterior Mean | = 2.1789 |
| SMASA Posterior Mean | = 2.17749 |

| | |
|--------------------------|------------|
| 5k Posterior Std.Dev. | = 0.31234 |
| 50k Posterior Std.Dev. | = 0.313286 |
| 500k Posterior Std.Dev. | = 0.303793 |
| SMASA Posterior Std.Dev. | = 0.301511 |

Future work: expand AD to inverse problems.

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://red.ices.utexas.edu/projects/software>

Conclusions

Thank you!

Have a well verified day.

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