



PECOS

Predictive Engineering and Computational Sciences

Manufactured Solutions for the Favre-Averaged Navier-Stokes Equations with Eddy-Viscosity Turbulence Models

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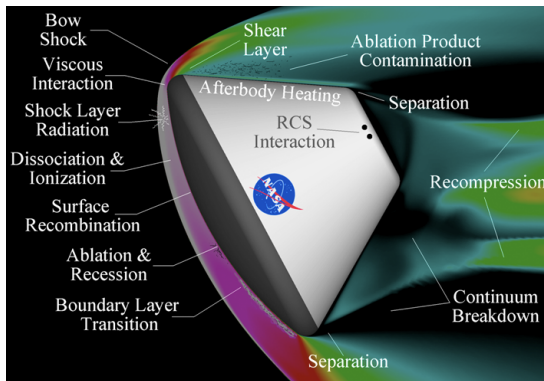
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Outline

- 1 Background: Verification and MMS
- 2 A new Spalart-Allmaras Manufactured Solution
- 3 MASA
- 4 Conclusions

Physics Problem



Atmospheric Entry

- Multiphysics submodels: Flow, Aerothermochemistry, Ablation, Surface chemistry, Radiation, **Turbulence**

Software Quality

Complex Codebase

- Finite Element hypersonic code, fully implicit Navier-Stokes (FIN-S)
- Favre-Averaged Navier Stokes (FANS) + Spalart-Allmaras (SA) turbulence model

General Problem in Scientific Software

- Computer models are being used to inform decision makers
 - ▶ Failures are costly (\$, lives)
- How do you build confidence in the predictions from a codebase?
 - ▶ What constitutes a strong test?

Verification

Verification of Scientific Software

- Verification ensures that the outputs of a computation accurately reflect the solution of the mathematical models.
- Essentially, we are testing if we have correctly instantiated mathematical equations in our code.

Method of Exact Solutions

- Numerically solve a case where the solution is known.

Method of Manufactured Solutions

- Often, analytical solutions either:
 - ▶ Do not exist
 - ▶ Does not fully exercise equations (e.g. symmetric solution, nonlinearities)
- 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, Numpy
(output is machine-generated code)

“Manufactured” Code

[illegible]

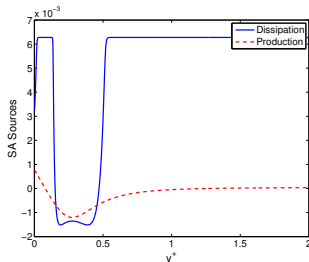
Desired Features of an SA MS

Physically-based MS

- Exercise each term in the PDE in a manner similar to that of a real solution

Shortcoming of other SA MS

- Bond solution: sinusoidal, only satisfies no-slip.
- Eça solutions are shown to have instabilities or near-wall features that disrupt the correct rate of convergence



Governing Equations

FANS + SA

$$\begin{aligned}\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i) &= 0 \\ \frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{u}_i) &= - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (2(\mu + \mu_t) \tilde{S}_{ji}) \\ \frac{\partial}{\partial t} \left[\bar{\rho} \left(\tilde{e} + \frac{1}{2} \tilde{u}_i \tilde{u}_i \right) \right] + \frac{\partial}{\partial x_j} \left[\bar{\rho} \tilde{u}_j \left(\tilde{h} + \frac{1}{2} \tilde{u}_i \tilde{u}_i \right) \right] &= \frac{\partial}{\partial x_j} (2(\mu + \mu_t) \tilde{S}_{ji} \tilde{u}_i) + \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{\text{Pr}} + \frac{\mu_t}{\text{Pr}_t} \right) \frac{\partial \tilde{h}}{\partial x_j} \right] \\ \frac{\partial}{\partial t} (\bar{\rho} \nu_{\text{sa}}) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \nu_{\text{sa}}) &= c_{b1} S_{\text{sa}} \bar{\rho} \nu_{\text{sa}} - c_{w1} f_w \bar{\rho} \left(\frac{\nu_{\text{sa}}}{d} \right)^2 + \frac{1}{\sigma} \frac{\partial}{\partial x_k} \left[(\mu + \bar{\rho} \nu_{\text{sa}}) \frac{\partial \nu_{\text{sa}}}{\partial x_k} \right] + \frac{c_{b2}}{\sigma} \bar{\rho} \frac{\partial \nu_{\text{sa}}}{\partial x_k} \frac{\partial \nu_{\text{sa}}}{\partial x_k}\end{aligned}$$

Calorically perfect gas with *constant* viscosity:

$$\bar{p} = \bar{\rho} R \tilde{T}, \quad \tilde{e} = c_v \tilde{T}, \quad \tilde{h} = c_p \tilde{T},$$

Modifications

In the original formulation, S_{sa} is given by,

$$S_{sa} = \Omega + \frac{\nu_{sa}}{\kappa^2 d^2} f_{v2}$$

This definition is modified to:

$$S_{m0} = \frac{\nu_{sa}}{\kappa^2 d^2} f_{v2}$$

S_{sa} is given by,

$$S_{sa} = \Omega + S_m$$

where,

$$S_m = \begin{cases} S_{m0}, & S_{m0} \geq -c_{v2}\Omega \\ \frac{\Omega(c_{v2}^2\Omega + c_{v3}S_{m0})}{((c_{v3} - 2c_{v2})\Omega - S_{m0})}, & \text{otherwise.} \end{cases}$$

Our SA Manufactured Solution

- Parameters colored in red (values appear in paper appendix)
- Using our understanding of incompressible flow physics to inform our modeling assumptions for this MS

Streamwise Velocity

- The mean streamwise velocity is given by,

$$\tilde{u} = \frac{u_{\infty}}{A} \sin \left(\frac{A}{u_{\infty}} u_{eq} \right)$$

The van Driest equivalent velocity can be written as,

$$u_{eq} = u_{\tau} u_{eq}^{+},$$

- Must specify both u_{τ} and u_{eq}^{+}

Completing Streamwise Velocity Specification

Correlations

- Friction velocity can be determined from the skin friction coefficient
- The incompressible 1/7th power law is used for the skin friction coefficient. Thus,

$$c_{f,\text{inc}}(Re_x) = C_{cf} Re_x^{-1/7}$$

- To complete the manufactured solution, u_{eq}^+ is set using the velocity profile model of Cebeci and Bradshaw (1980):

$$u_{eq}^+ = \frac{1}{\kappa} \log(1 + \kappa y^+) + C_1 \left[1 - e^{-y^+/\eta_1} - \frac{y^+}{\eta_1} e^{-y^+/\eta_1} \right]$$

Wall-normal velocity and SA State

- From an order of magnitude analysis of the continuity equation, the mean wall-normal velocity is set to,

$$\tilde{v} = -\eta_v \frac{du_\tau}{dx} y$$

- SA model designed such that $\nu_{sa} = \kappa u_\tau y$ in the inner region of the boundary layer. Specifically, the SA state variable is given by,

$$\nu_{sa} = \kappa u_\tau y - \alpha y^2,$$

Thermodynamic State

Specifying Temperature, Pressure and Density

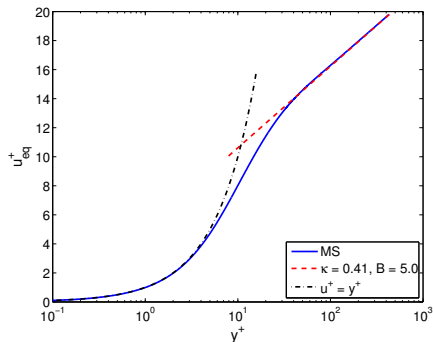
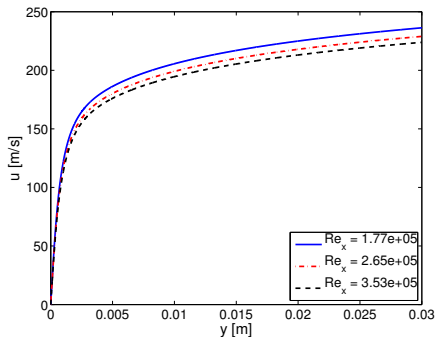
- Mean temperature uses White's(91) temperature-velocity relation:

$$\tilde{T} = T_{\infty} \left[1 + r_T \frac{\gamma - 1}{2} M_{\infty}^2 \left(1 - \left(\frac{\tilde{u}}{u_{\infty}} \right)^2 \right) \right]$$

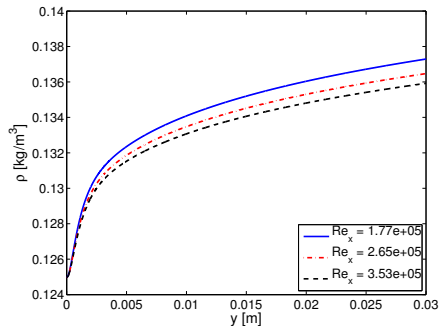
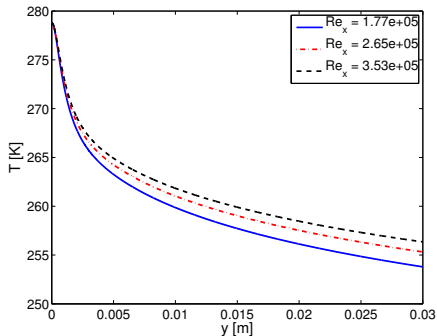
- Pressure is assumed to be a constant, p_0
- Density is computed from the ideal gas equation:

$$\bar{\rho} = \frac{p_0}{R\tilde{T}}$$

Manufactured Velocity Profiles

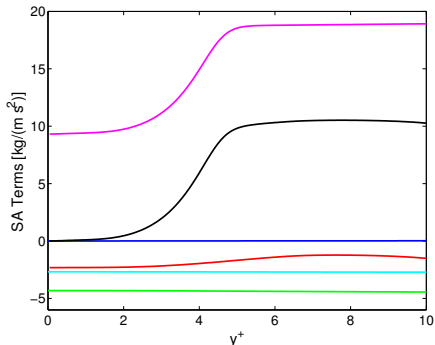
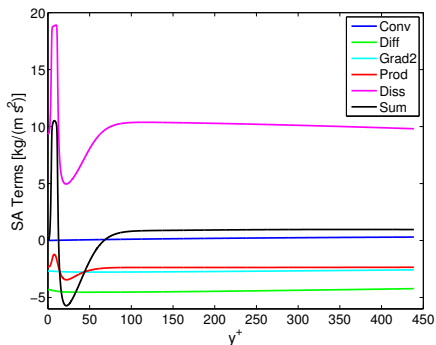


Manufactured Temperature and Density Profiles



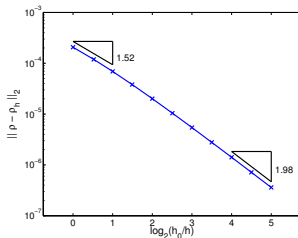
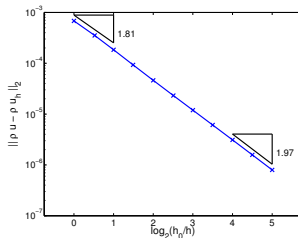
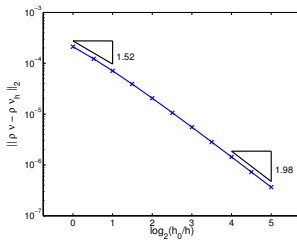
- T and ρ designed to provide moderate variation

SA Equation Budgets

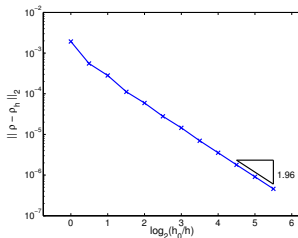
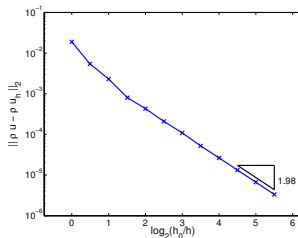
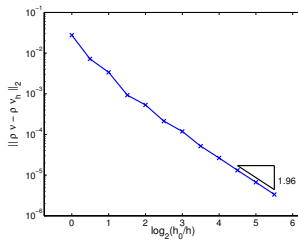


- Inside viscous sublayer, source term is small relative to other terms
- Production and dissipation terms go to constants at the wall
- Source term is largest in buffer region

Convergence Rates: Low Re_x

(a) $\bar{\rho}$ (b) $\bar{\rho}\tilde{u}$ (c) $\bar{\rho}\nu_{sa}$

Convergence Rates: $Re_x = 3.5 * 10^5$

(d) $\bar{\rho}$ (e) $\bar{\rho} \tilde{u}$ (f) $\bar{\rho} \nu_{sa}$

Manufactured Analytical Solutions Abstractions Library

Goal: Provide a repository and standardized interface for MMS usage

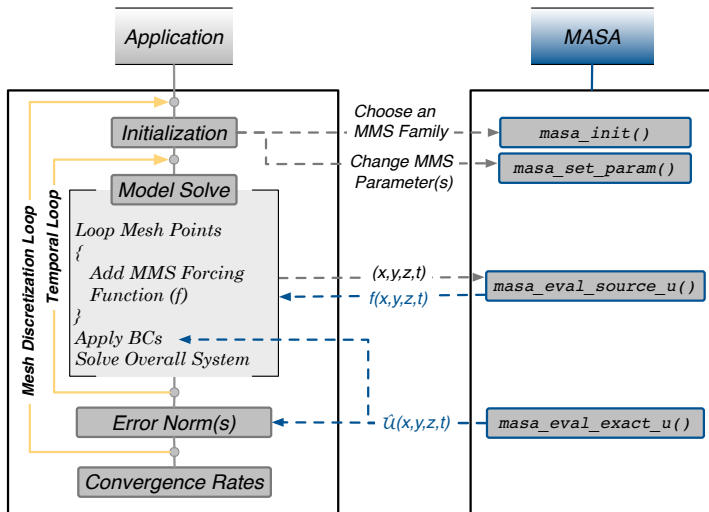
High Priority:

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

Low Priority:

- Speed/Performance

General Verification Approach Using MMS and MASA



Verifying the “Verifier”

Precision is not negotiable: **users must trust MASA output!**

MASA Testing

- Error target $< 1e-15$
 - ▶ Relative error
 - ▶ 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: unittest  
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

LCOV - code coverage report

| | | | |
|--|----------------|-------|----------|
| Current view: top level - buildbot | Hit | Total | Coverage |
| Test: MASA | 3077 | 3120 | 98.6% |
| Date: 2011-04-27 | Functions: 946 | 1277 | 94.3% |

| Filename | Line Coverage | Functions |
|------------|-------------------|------------------|
| buildbot.c | 100.0 % 107 / 107 | 94.4 % 34 / 36 |
| buildbot.h | 100.0 % 71 / 71 | 98.6 % 17 / 18 |
| buildbot.c | 100.0 % 71 / 71 | 98.6 % 17 / 18 |
| buildbot.c | 100.0 % 98 / 98 | 100.0 % 11 / 11 |
| buildbot.c | 100.0 % 328 / 328 | 100.0 % 10 / 10 |
| buildbot.c | 100.0 % 68 / 68 | 87.5 % 21 / 24 |
| buildbot.c | 100.0 % 426 / 426 | 94.3 % 30 / 32 |
| buildbot.c | 100.0 % 118 / 118 | 97.7 % 15 / 16 |
| buildbot.c | 100.0 % 72 / 72 | 100.0 % 12 / 12 |
| buildbot.c | 100.0 % 402 / 402 | 94.3 % 26 / 28 |
| buildbot.c | 100.0 % 218 / 218 | 98.3 % 71 / 73 |
| buildbot.c | 83.3 % 10 / 12 | 100.0 % 4 / 5 |
| buildbot.c | 94.4 % 104 / 105 | 100.0 % 10 / 10 |
| buildbot.c | 98.3 % 340 / 345 | 91.4 % 221 / 243 |
| buildbot.c | 86.7 % 111 / 126 | 94.1 % 211 / 225 |
| buildbot.c | 100.0 % 25 / 25 | 100.0 % 6 / 6 |
| buildbot.c | 88.0 % 71 / 80 | 100.0 % 10 / 10 |
| buildbot.c | 100.0 % 93 / 93 | 96.3 % 52 / 54 |
| buildbot.c | 100.0 % 1 / 1 | 100.0 % 1 / 1 |
| buildbot.c | 91.0 % 101 / 111 | 88.0 % 16 / 20 |

Generated by: [LCOV version 1.8](#)

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:

$$\begin{aligned}\rho(x) &= \rho_0 + \rho_x \sin\left(\frac{a_{ux}\pi x}{L}\right) \\ u(x) &= u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) \\ p(x) &= p_0 + p_x \cos\left(\frac{a_{ux}\pi x}{L}\right)\end{aligned}\quad (3.26)$$

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:

$$\begin{aligned}\text{rho}_1 &= \rho_0 + \rho_x \sin\left(\frac{a_{ux}\pi x}{L}\right) \\ U_1 &= u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) \\ P_1 &= p_0 + p_x \cos\left(\frac{a_{ux}\pi x}{L}\right)\end{aligned}$$

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_z |
| a_px | a_py | a_pz | a_rhox | a_rhoy | a_rhoz | a_uu |
| 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

- `mass_eval_2d_exact_u()`
- `mass_eval_2d_exact_v()`
- `mass_eval_2d_exact_p()`
- `mass_eval_2d_exact_rho()`
- `mass_eval_2d_grad_u()`
- `mass_eval_2d_grad_v()`
- `mass_eval_2d_grad_p()`
- `mass_eval_2d_grad_rho()`

3.2.3.3 3D Steady Euler

Initialization:

- `euler_3d`

Functions:

- `mass_init()`
- `mass_eval_3d_source_rho_u()`
- `mass_eval_3d_source_rho_v()`
- `mass_eval_3d_source_rho_w()`
- `mass_eval_3d_source_rho_e()`
- `mass_eval_3d_source_rho()`
- `mass_eval_3d_exact_u()`
- `mass_eval_3d_exact_v()`
- `mass_eval_3d_exact_w()`
- `mass_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**

Conclusions

New SA Model

- Generated a new, physically-based, MS
- Great care goes into constructing MS

MASA

- Open-source, extensible repository for MS and software verification

Getting the word out

- AIAA journal paper (in preparation)
- Engineering with Computers (submitted)
- Download MASA 0.40 at:
<https://red.ices.utexas.edu/projects/>

Thank you!

Questions?

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