ASME V&V 40 Subcommittee Verification Working Group: Challenge Problems for Computational Modeling of Medical Devices

Marc Horner, Ph.D.
ANSYS, Inc.

Ismail Guler
Boston Scientific

Danny Levine
Zimmer Biomet
Session Overview

Overview of the ASME V&V 40 Standard
Verification Overview
Code Verification Challenge Problems
Calculation Verification Challenge Problems
- A note on the GCI
Overview of the ASME V&V 40 Standard
The V&V40 standard outlines a process for making risk-informed determinations as to whether CM&S is credible for decision-making for a specified context of use.
The question of interest describes the specific question, decision or concern that is being addressed.

Context of use defines the specific role and scope of the computational model used to inform that decision.
Model risk is the possibility that the model may lead to a false/incorrect conclusion about device performance, resulting in adverse outcomes.

- **Model influence** is the contribution of the computational model to the decision relative to other available evidence.

- **Decision consequence** is the significance of an adverse outcome resulting from an incorrect decision.
Model credibility refers to the trust in the predictive capability of the computational model for the COU.

Trust can be established through the collection of V&V evidence and by demonstrating the applicability of the V&V activities to support the use of the CM for the COU.

Goals for each credibility factor are based on model risk.
Credibility Assessment

1. Establish Risk-Informed Credibility
   - Define COU
   - Assess model risk
   - Establish credibility goals

2. Credibility Activities
   - Establish plan
   - Execute plan

3. Assess Credibility
   - Computational model credible for COU?
     - Yes: Documentation and evidence
     - No: Continue with credibility assessment

4. References:
   - ASME V&V10
   - ASME V&V20
### Current Subcommittee Work Items

<table>
<thead>
<tr>
<th>NUMBER</th>
<th>TITLE</th>
<th>LEADER(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>V&amp;V 40.1</td>
<td>Using (Historical) Clinical Data as a Comparator</td>
<td>Paul Briant, Exponent</td>
</tr>
</tbody>
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| V&V 40.2 | End-to-End Example                                                    | Sudeep Sastry, WL Gore  
Brandon Lurie, WL Gore                                                      |
| V&V 40.3 | Patient-Specific Models                                               | Mark Goodin, Simutech  
Shumin Cheng                                                              |
| V&V 40.4 | Verification Best Practices (Code and Calculation)                    | Marc Horner, ANSYS  
Ismail Guler, Boston Scientific                                         |
| V&V 40.5 | Mock Submission: V&V 40 Practice in Regulatory Applications           | Tina Morrison, US FDA  
Brent Craven, US FDA                                                       |
| V&V 40.6 | V&V 40 Revisions                                                      | V&V 40 Chair                                                             |
Verification Overview
What is computational modeling & simulation (CM&S)?

Adapted from ASME V&V 10
What is model verification & validation (V&V)?

Verification is “solving the equations right”.

Validation is “solving the right equations”.

Adapted from ASME V&V 10
What are the uncertainties inherent in CM&S?

Adapted from ASME V&V 20
Goal: The fundamentals of code and calculation verification are thoroughly reviewed in the ASME V&V 10, 10.1, and 20 standards. However, the computational models used in the evaluation of medical devices can be quite complex and have their own subtleties. The objective of the ASME V&V 40.4 working group is to explore, learn, and employ code and calculation verification best practices on representative examples from the medical device space.
## ASME V&V 40 “code verification” credibility factors

<table>
<thead>
<tr>
<th>Activity</th>
<th>Credibility Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Verification</strong></td>
<td></td>
</tr>
<tr>
<td>Code</td>
<td>Software quality assurance</td>
</tr>
<tr>
<td></td>
<td>Numerical code verification</td>
</tr>
<tr>
<td>Calculation</td>
<td>Discretization error</td>
</tr>
<tr>
<td></td>
<td>Numerical solver error</td>
</tr>
<tr>
<td></td>
<td>Use error</td>
</tr>
<tr>
<td><strong>Validation</strong></td>
<td></td>
</tr>
<tr>
<td>Computational model</td>
<td>Model form</td>
</tr>
<tr>
<td></td>
<td>Model inputs</td>
</tr>
<tr>
<td>Comparator</td>
<td>Test samples</td>
</tr>
<tr>
<td></td>
<td>Test conditions</td>
</tr>
<tr>
<td>Assessment</td>
<td>Equivalency of input parameters</td>
</tr>
<tr>
<td></td>
<td>Output comparison</td>
</tr>
<tr>
<td><strong>Applicability</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Relevance of the quantities of interest</td>
</tr>
<tr>
<td></td>
<td>Relevance of the validation activities to the COU</td>
</tr>
</tbody>
</table>
Code verification – Observed order of accuracy

\[ f_h = f_{\text{exact}} + C \cdot h^p + O(h^{p+1}) \]

- \( f_{\text{exact}} \): exact solution to mathematical model
- \( f_h \): approximate numerical solution (\( f_i = f_{h_i} \))
- \( h \): characteristic element size for a given mesh
- \( p \): order of accuracy for the numerical method
- \( C \): a constant which does not depend on "\( h \)"
- \( H.O.T \): higher order terms

Mesh with smallest element size in group considered

\[ h_1 < h_2 \]

\[ \hat{p}_1 = \frac{\ln(|E_2/E_1|)}{\ln r} \]

(observed order of accuracy)

\[ E_i = f_i - f_{\text{exact}} \]

(discretization error)

ASME V&V 20-2009
**ASME V&V 40 “calculation verification” credibility factors**

<table>
<thead>
<tr>
<th>Activity</th>
<th>Credibility Factor</th>
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<tbody>
<tr>
<td><strong>Verification</strong></td>
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<td>Code</td>
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<td>Model inputs</td>
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<td>Output comparison</td>
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<td><strong>Applicability</strong></td>
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<td>Relevance of the quantities of interest</td>
</tr>
<tr>
<td></td>
<td>Relevance of the validation activities to the COU</td>
</tr>
</tbody>
</table>
Systematic mesh refinement

\[ r_{ij} = \frac{h_i}{h_j} \]

\[ r = r_{32} = r_{21} = 2 \]

\[ r = \frac{h_3}{h_2} = \frac{h_2}{h_1} = 2 \]

(mesh refinement factor)
Calculation verification – Richardson extrapolation

\[ f_h = f_{\text{exact}} + C \cdot h^p + O(h^{p+1}) \]

- \( f_{\text{exact}} \): exact solution to mathematical model
- \( f_h \): approximate numerical solution \( (f_i = f_{h_i}) \)
- \( h \): characteristic element size for a given mesh
- \( p \): order of accuracy for the numerical method
- \( C \): a constant which does not depend on "h"
- \( H.O.T \): higher order terms

mesh with smallest element size in group considered

\( h_1 < h_2 < h_3 \)

\[ \hat{p}_1 = \ln \left( \frac{f_3 - f_2}{f_2 - f_1} \right) / \ln r \]  
(observed order of accuracy)

\[ \overline{f}_1 = f_1 + \frac{f_1 - f_2}{r^{\hat{p}_1} - 1} \]  
(Richardson extrapolation estimate of exact solution)

\[ (E_1)_i = f_i - \overline{f}_1 \]  
(discretization error)
**Calculation verification – Grid convergence index (GCI)**

\[
(GCI)_1 = \frac{(F_s)_1}{r_{p_1} - 1} |f_2 - f_1| \quad \text{(Roache’s grid convergence index for fine mesh solution)}
\]

\[
\left| \frac{\hat{p} - p_f}{p_f} \right| \leq 0.1 \quad \Rightarrow \quad F_s = 1.25 \quad \& \quad p = p_f
\]

\[
\left| \frac{\hat{p} - p_f}{p_f} \right| > 0.1 \quad \Rightarrow \quad F_s = 3.0 \quad \& \quad p = \min(\max(0.5, \hat{p}), p_f)
\]

(GCI is an uncertainty estimate (an uncertainty bar or uncertainty band, not an error estimate).

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2) ASME V&V 20-2009
## Benchmark calculation verification data (courtesy of Kenny Aycock)

<table>
<thead>
<tr>
<th>#</th>
<th>coarse</th>
<th>medium</th>
<th>fine</th>
<th>r</th>
<th>p, theor.</th>
<th>p, obs.</th>
<th>Richardson Extrapolation</th>
<th>FS</th>
<th>GCI</th>
<th>GCI(%)</th>
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<tr>
<td>1</td>
<td>376</td>
<td>392</td>
<td>400</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>408</td>
<td>1.25</td>
<td>10</td>
<td>2.5</td>
</tr>
<tr>
<td>2</td>
<td>1000</td>
<td>2000</td>
<td>2250</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2333</td>
<td>1.25</td>
<td>104.2</td>
<td>4.630</td>
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<tr>
<td>3</td>
<td>600</td>
<td>584</td>
<td>573.8</td>
<td>1.26</td>
<td>2</td>
<td>1.95</td>
<td>555.9</td>
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<td>21.69</td>
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<td>0.051</td>
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<td>5</td>
<td>660</td>
<td>680</td>
<td>663</td>
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<td>100</td>
<td>110</td>
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<td>diverging</td>
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</tbody>
</table>
Code Verification Challenge Problem
ASME V&V 40.4 Code Verification Best Practices Working Group Members

Christopher Basciano¹, Jeff Bodner², Constantine Butakoff³, Carlos Corrales⁴, Chris Delametter⁵, Swapnil Dindorkar⁶, Jun Ding⁷, Beatriz Eguzkitza³, Mark Goodin⁸, Sharath Gopal⁹, Ismail Guler¹⁰, Marc Horner¹¹, Kranthi Kolli¹², Sanjeev Kulkarni⁶, Anup Paul¹³, Sudeep Sastry¹⁴, Travis Schauer¹⁰, Jaykumar Teli⁶

¹Becton Dickinson, ²Medtronic, ³Barcelona Supercomputing Center, ⁴Baxter, ⁵Siemens, ⁶Neilsoft, ⁷Abbott, ⁸SimuTech Group, ⁹Eli Lilly, ¹⁰Boston Scientific, ¹¹ANSYS, Inc., ¹²Weill Cornell Medical College, ¹³Stress Engineering Services, ¹⁴WL Gore
The following is a brief summary of a code verification challenge problem, which was hosted by the ASME V&V40 Code Verification sub-group in 2015.

**Problem Description:**
- Steady-state, laminar flow of a blood analogue in a pipe

**Geometry:**
- Pipe Diameter: 3mm
- Pipe Length: 4 cm

**Material Properties:**
- Density: 1.06 g/cm$^3$
- Viscosity: 0.035 g/cm-s

**Boundary Conditions:**
- Inlet flow rate: 3.75 cm$^3$/s
- Outlet pressure: 93 mm Hg

**Analytical Solution**

$$v_z = \frac{2R^2}{\mu} \frac{dP}{dz} \left(1 - \frac{r^2}{R^2}\right)$$
**ANSYS - Solution Strategy**

**Solver:** ANSYS Fluent v 18.2

**Geometry:** Axi-symmetric

**Numerical Settings:**
- Pressure-velocity coupling scheme: Coupled
- Gradient: Green-Gauss node based
- Momentum disc.: Second-order upwind
- Pressure disc.: Second-order
- Residuals: 2e-012*

**Iterations:**
- Run until all d.o.f.s are converged

<table>
<thead>
<tr>
<th>Residual Setting</th>
<th>Relative Error at point-1 [%]</th>
<th>Relative Error at point-2 [%]</th>
<th>Relative Mass Flow Rate Error [%]</th>
<th>P_{obs,vel-p1}</th>
<th>P_{obs,vel-p2}</th>
<th>P_{obs,Q}</th>
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<tr>
<td>1.00E-06</td>
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<td>1.94</td>
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<td>0.00183</td>
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<td>1.99</td>
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<td>0.00076</td>
<td>0.00183</td>
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<td>1.30E-12</td>
<td>0.00114</td>
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<td>0.00183</td>
<td>2.00</td>
<td>1.99</td>
<td>2.00</td>
</tr>
</tbody>
</table>
## ANSYS - Observed Order of Convergence

### FLUENT axi-sym model

<table>
<thead>
<tr>
<th>Solution Source</th>
<th>$x=1$ cm</th>
<th>$x=2$ cm</th>
<th>$x=3$ cm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$P_{avg}$</td>
<td>$v_{x,avg}$</td>
<td>$v_{x,\text{max}}$</td>
</tr>
<tr>
<td>Mesh 1/2</td>
<td>3.31</td>
<td>4.82</td>
<td>1.26</td>
</tr>
<tr>
<td>Mesh 2/3</td>
<td>5.67</td>
<td>6.37</td>
<td>4.71</td>
</tr>
<tr>
<td>Mesh 3/4</td>
<td>1.94</td>
<td>2.00</td>
<td>1.88</td>
</tr>
<tr>
<td>Mesh 4/5</td>
<td>1.97</td>
<td>2.00</td>
<td>1.94</td>
</tr>
<tr>
<td>Mesh 5/6</td>
<td>1.99</td>
<td>2.00</td>
<td>1.98</td>
</tr>
<tr>
<td>Mesh 6/7</td>
<td>1.97</td>
<td>2.00</td>
<td>2.00</td>
</tr>
</tbody>
</table>

*images from D’Souza et al. ASME V&V Symposium (2015)*
Boston Scientific - Solution Strategy

Flow characteristics:
- Circular rigid tube
- Steady
- Single phase
- Laminar
- Incompressible
- Newtonian fluid

\[ D = 3 \text{ mm} \quad \text{(diameter of pipe)} \]
\[ L = 4 \text{ cm} \quad \text{(length of pipe)} \]

“quarter model with two symmetry planes”

\[ \mu = 0.035 \text{ dyn} \cdot \text{s} / \text{cm}^2 \quad \text{(dynamic viscosity of fluid)} \]
\[ \rho = 1.06 \text{ g} / \text{cm}^3 \quad \text{(density of fluid)} \]

\[ \text{Re} = \frac{\rho \cdot \bar{u} \cdot D}{\mu} = \frac{4 \cdot \rho \cdot Q}{\pi \cdot \mu \cdot D} \approx 482 \]
Boston Scientific – Discretization Error ($v_{\text{axial}}$)

$$E_{u} = \bar{u}_h - \bar{u} \quad \text{(discretization error)}$$

**COMSOL (FEM)**

**FLUENT (FVM)**

- $y = 813.3870x^{1.9044}$
- $y = 532.4538x^{1.9965}$
Boston Scientific – Observed Order of Accuracy ($v_{axial}$)

\[ \hat{p}_1 = \frac{\ln \left( \frac{|E_2|}{|E_1|} \right)}{\ln r} \]  
(observed order of accuracy)

COMSOL (FEM)  
FLUENT (FVM)

- Observed order of convergence, $p$
- Mesh level, $m$ (m & m+1)

- $\bigcirc$ $u_{avg}$ at $x = 1$ cm
- $\Box$ $u_{avg}$ at $x = 2$ cm
- $\triangle$ $u_{avg}$ at $x = 3$ cm
Flow characteristics:
- Circular rigid tube
- Pulsatile
- Single phase
- Laminar
- Incompressible
- Newtonian fluid

\[ R = 4 \text{ mm} \] (radius of pipe)
\[ L = 4 \text{ cm} \] (length of pipe)

\[ p_{inlet} = p_0 \cos(\omega t) \]
\[ v = 0 \]
\[ w = 0 \]

\[ \Delta p = p_0 - p_{outlet} = 3 \text{ Pa} \]
\[ f = 60 \text{ beats/min} = 1 \text{ Hz} \]
\[ \omega = 2\pi f \]

\[ \mu = 0.035 \text{ dyn} \cdot \text{s} / \text{cm}^2 \] (dynamic viscosity of fluid)
\[ \rho = 1.06 \text{ g} / \text{cm}^3 \] (density of fluid)
Analytical Solutions Generated in MATLAB

\[ u_z(r, t) = \text{Re} \left\{ \frac{A^*}{i\omega \rho} \left[ 1 - \frac{J_0(i^{3/2} \alpha r / R)}{J_0(i^{3/2} \alpha)} \right] e^{i\omega t} \right\} \]
Womersley flow 3D
14/05/2019

Constantine Butakoff
Kostantyn.butakov@bsc.es

Mariano Vazquez
Beatriz Eguzkitza
Guillaume Houzeaux
Our Mesh (Crossection)

Level 0
10,179 elements

Level 1
81,432 elements

Level 2
651,456 elements
Simulations

Velocity evolution. Error in last 5s: 0.00068 ± 0.00007 cm/s, max=0.00139 cm/s

Blue – analytical, Orange – simulated in the finest mesh

10 seconds of simulation

Residuals in the order of 1e-14

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Elements</th>
<th>CPU</th>
<th>Time</th>
<th>Timestep</th>
</tr>
</thead>
<tbody>
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<td>14m</td>
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<tr>
<td>Medium</td>
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<td>16</td>
<td>5h</td>
<td>0.005</td>
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<tr>
<td>Finest</td>
<td>651,456</td>
<td>96</td>
<td>14h</td>
<td>0.00125</td>
</tr>
</tbody>
</table>
Obtained profiles (finest mesh)

Axial component of the velocity across the pipe radius in the time interval 0-10s

- Time: 0.0s
- Time: 0.25s
- Time: 0.5s
- Time: 0.75s
L2 Error (whole mesh)

![Graph showing Velocity X component error for different mesh resolutions](image)

Table 3: Order of the ALYA's numerical scheme at different time steps between 9 and 10 seconds

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Time</th>
<th>9s</th>
<th>9.25s</th>
<th>9.5s</th>
<th>9.75s</th>
<th>10s</th>
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<tbody>
<tr>
<td>Slope</td>
<td></td>
<td>1.88</td>
<td>1.62</td>
<td>1.95</td>
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<td>1.88</td>
</tr>
<tr>
<td>Richardson Extrapolation</td>
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<td>1.82</td>
<td>1.26</td>
<td>2.09</td>
<td>2.16</td>
<td>1.82</td>
</tr>
</tbody>
</table>
Contact

• marc.horner@ansys.com

• Ismail.Guler@bsci.com

• danny.levine@zimmerbiomet.com
  – Parasolid and STEP versions of hip stem geometry available.
  – Also available:
    • Spreadsheet for GCI mesh metric calculation
    • Python script for GCI mesh metric calculation
Thank you!