Simulation governance:
New technical requirements for software tools in computational solid mechanics

Barna Szabó and Ricardo Actis
Engineering Software Research and Development, Inc.
St. Louis, Missouri USA
Outline

- Simulation governance: Response to the prediction challenge in engineering practice
- The main elements of simulation governance in mechanical design and certification
  - Application of design rules
  - Formulation of design rules
- Example: Safe life design problem
- New technical requirements for FEA software tools:
  - Support for verification and virtual experimentation
  - Collection, management and interpretation of calibration data and other empirical evidence
- Conventional FEA software products do not meet these requirements
  - Fundamental problems with implementation
- Conclusions
Simulation governance

Formulation of design rules

- Simulation governance is an open-ended process by which mathematical models are ranked and progressively improved over time in the light of new experimental data.
- Standards are required for the collection, management and interpretation of experimental data.
- Control of numerical and modeling errors is essential.
- The relative performance of mathematical models is objectively evaluated.
- Provides a framework for innovation.

Application of design rules

- Simulation governance is essentially verification.
- Standardization should be used whenever possible.

New technical requirements for software tools.
Mathematical models

- We understand a mathematical model to be a transformation of data $D$ that characterizes some physical reality into the data of interest denoted by $F$.

- Data $D$ includes all geometrical attributes, material properties, calibration data and loading information.
  
  - Associated with $D$ are various measures of uncertainty. The transformation maps these measures of uncertainty into corresponding measures of uncertainty associated with $F$.

- The transformation $D \rightarrow F$ consists of a set of operations that include the solution of a mathematical problem, statistical models, constitutive relationships and failure criteria.
  
  - Phenomenological approaches cannot be avoided.
  
  - The epistemic and aleatory uncertainties are mixed.

- The goal of simulation governance is to minimize the epistemic uncertainties.
Example: Safe life design problem

- **Perspective**: Formulation of design rules
- **D**: Information concerning the object of design, the material properties and loading conditions
  - Calibration data (for example S-N curves)
- **D → F** is a set of operations that include
  - Generalization of fatigue test data
  - Statistical models
  - Definition of driver(s) of damage accumulation
  - Formulation of one or more mathematical problems
  - Numerical solution
  - Extraction of the driver(s) of damage accumulation
  - Verification
- **F**: The number of cycles to failure N:
  - *We predict with 95 percent confidence that the probability that N < \(10^6\) is (say) 0.08.*
Typical S-N curves for aluminum alloys
Data analysis

Metallic Materials Properties Development and Standardization Handbook (see page 3-449):

\[ \log_{10} N = 9.73 - 3.24 \log_{10}(\sigma_{\text{max}} (1 - R)^{0.63} - 15.5) \]

Standard error of estimate in \( \log_{10} \) life: \( s = 0.490 \). Sample size: 35 including 4 run-outs. Implied bounds (not explicitly stated in the source document):

\[ 15.5/(1 - R)^{0.63} < \sigma_{\text{max}} < \min(68.0, 74.2/(1 - R)^{0.63}). \]

Assumptions:

1. \( \log_{10} N \) is normally distributed.

2. The sample is a close approximation of the population.

3. The number of cycles to failure is a good approximation for the number of cycles to initiation. (We do not have data for initiation).
Drivers of damage accumulation

Generalization of data collected under specific test condition to general conditions is part of the conceptualization process.

Examples:

1. The maximum normal stress $\sigma_{\text{max}}$.

2. The maximum shear stress subject to the conditions:

$$7.75(1 - R)^{-0.63} < \tau_{\text{max}} < \min(34.0, 37.1(1 - R)^{-0.63})$$

and $\sigma_{\text{max}} > \sigma_{\text{th}} > 0$.

3. The octahedral shear stress subject to $I_1 > (I_1)_{\text{th}}$ where $I_1$ is the first stress invariant and $(I_1)_{\text{th}}$ is a threshold value.

Countless other plausible generalizations are possible.
Bolted lap joint

Two models:
2D: neglects bending and the fastener is modeled by nonlinear springs.
3D: accounts for bending and the elastic contact problem is solved.

Cyclic loading: \(-250 < F < 500\) lbs
Estimated maximum and minimum normal, tangential and shearing stresses (ksi) and the corresponding cycle ratios for Model 1 (2D)

<table>
<thead>
<tr>
<th>Location</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(\sigma_n)_{\text{max}}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$(\sigma_n)_{\text{min}}$</td>
<td>-32.46</td>
<td>-26.66</td>
<td>-0.13</td>
<td>-12.68</td>
<td>-17.45</td>
</tr>
<tr>
<td>$R_n$</td>
<td>undefined</td>
<td>undefined</td>
<td>undefined</td>
<td>undefined</td>
<td>undefined</td>
</tr>
<tr>
<td>$(\sigma_t)_{\text{max}}$</td>
<td>12.85</td>
<td>15.14</td>
<td><strong>30.13</strong></td>
<td>8.57</td>
<td>6.64</td>
</tr>
<tr>
<td>$(\sigma_t)_{\text{min}}$</td>
<td>0</td>
<td>2.08</td>
<td>8.62</td>
<td>6.09</td>
<td>-2.75</td>
</tr>
<tr>
<td>$R_t$</td>
<td>0</td>
<td>0.137</td>
<td>0.286</td>
<td>0.711</td>
<td>-0.414</td>
</tr>
<tr>
<td>$\tau_{\text{max}}$</td>
<td>22.66</td>
<td><strong>20.90</strong></td>
<td>15.07</td>
<td>9.39</td>
<td>12.05</td>
</tr>
<tr>
<td>$\tau_{\text{min}}$</td>
<td>0</td>
<td>1.04</td>
<td>4.38</td>
<td>4.29</td>
<td>-1.37</td>
</tr>
<tr>
<td>$R_\tau$</td>
<td>0</td>
<td>0.050</td>
<td>0.290</td>
<td>0.457</td>
<td>-0.114</td>
</tr>
</tbody>
</table>
Results for Model 2 (3D)

<table>
<thead>
<tr>
<th></th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>((\sigma_n)_{\text{max}})</td>
<td>0</td>
</tr>
<tr>
<td>((\sigma_n)_{\text{min}})</td>
<td>-41.80</td>
</tr>
<tr>
<td>(R_n)</td>
<td>undef</td>
</tr>
<tr>
<td>((\tau_{nt})_{\text{max}})</td>
<td>21.30</td>
</tr>
<tr>
<td>((\tau_{nt})_{\text{min}})</td>
<td>1.66</td>
</tr>
<tr>
<td>((R_T)_{nt})</td>
<td>0.078</td>
</tr>
<tr>
<td>((\tau_{zt})_{\text{max}})</td>
<td>21.16</td>
</tr>
<tr>
<td>((\tau_{zt})_{\text{min}})</td>
<td>3.01</td>
</tr>
<tr>
<td>((R_T)_{zt})</td>
<td>0.142</td>
</tr>
</tbody>
</table>
Cumulative distribution functions

Predictor 1: Applicable to Location 3 only where it is the same as Predictor 2
Predictor 2: Applicable to Locations 1, 2, 3
Predictions and outcomes

The predicted number of cycles (millions) to failure at 90 percent probability

<table>
<thead>
<tr>
<th>Predictor</th>
<th>Model 1 (2D)</th>
<th>Model 2 (3D)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Location 2</td>
<td>Location 3</td>
</tr>
<tr>
<td>Predictor 1</td>
<td>—</td>
<td>0.733 to 23.0</td>
</tr>
<tr>
<td>Predictor 2</td>
<td>0.025 to 1.02</td>
<td>0.713 to 29.2</td>
</tr>
</tbody>
</table>

Outcome 1

Initiation occurs in the vicinity of Location 2 at 0.5 M cycles. In this case Predictor 1 is rejected and either the 3D or 2D model may be used.

Outcome 2

Initiation occurs in the vicinity of Location 3 at 2 M cycles. In this case Predictor 2 is rejected and either the 3D or the 2D model may be used.

Outcome 3

Initiation occurs in the vicinity of Location 3 at 40 M cycles. In this case Predictor 2 is rejected and only the 3D model may be used.
Technical requirements for FEA software

Verification
Determine the approximate value of a set of system response quantities \( \Phi_i(u_{FE}) \) \((i = 1, 2, \ldots, n)\) and show that

\[
|\Phi_i(u_{EX}) - \Phi_i(u_{FE})| \leq \tau_i |\Phi_i(u_{EX})|
\]

where \( \tau_i \) are prescribed error tolerances. It is necessary to show that the realized relative error \( \tau_i^{(R)} \) satisfies \( \tau_i^{(R)} \leq \tau_i \).

Conceptualization
Show that \( \Phi_i(u_{EX}) \) are not significantly affected by restrictive assumptions incorporated in the mathematical model conceived to represent some physical reality.

The conventional FEA software products were not designed to meet these technical requirements.
The problem with conventional FEA

In the early years of FEA the expression for strain was written as:

\[
\{\varepsilon\} = [D]\{u\} = [D][N]\{a\} \equiv [B]\{a\}
\]

where \([D]\) is a differential operator, \(\{u\}\) is the displacement vector, \([N]\) is the matrix of element-level basis functions and \(\{a\}\) is the set of coefficients.

The element level stiffness matrix was written as:

\[
[K_e] = \int_{\Omega_e} [B]^T[E][B] \, dV.
\]

The model definition represented by \([D]\) and the discretization represented by \([N]\) were mixed. This led to the development of large element libraries and the confused notion of “finite element modeling”.

“C3D20RHT: 20-node triquadratic displacement, trilinear temperature, hybrid, linear pressure, reduced integration.”
From the perspective of application of design rules an important element of simulation governance is standardization.

Applications that involve complex nonlinear problems with several parameters are designed by expert analysts for safe use by designers.
Conclusions

- The economic benefits derived from overcoming the prediction challenge in engineering practice are very substantial
  - Reduce reliance on physical testing
  - Increase reliance on simulation
- The prediction challenge can be met only through simulation governance
  - Progressive reduction of aleatory uncertainties
- Simulation governance has different meanings for the
  - Formulation of design rules
  - Application of design rules
- Conventional FEA software tools used in current engineering practice were not designed to meet the technical requirements of simulation governance.
  - A thorough re-thinking and redesign of FEA software tools will be necessary.