Simulation Governance
An idea whose time has come

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Simulation governance

• The idea is so simple that it is self-evident: Management has to exercise command and control over all aspects of numerical simulation.
  • Closely related to resource allocation.

• Implementation is not at all simple, however.
  • Simulation technology is evolving. Keeping pace is challenging.
  • Limitations in legacy software tools: Meeting the technical requirements of numerical simulation requires a high level of expertise.
  • Mission-dependence.
Example: Design rules for mechanical and structural engineering

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<th>Application</th>
<th>Formulation</th>
<th>Maintenance (CBM)</th>
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<tr>
<td>$F_{\text{max}} \leq F_{\text{all}}$</td>
<td>What is $F_{\text{all}}$?</td>
<td>What is $\Pr(N_f &lt; N)$?</td>
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- Code, data and solution verification
- Expert-designed standard processes
  - Validation
  - Uncertainty quantification
  - Update or revise models
Why important and timely?

Management faces:

– Increasing complexity.
– Increasing costs.
– Changing technology.
– The need to preserve and maintain corporate know-how in the face of changing workforce.
– Confusing marketing claims.
What are mathematical models?

Mathematical models are transformations:

\[
D \overset{\text{(I, p)}}{\rightarrow} F, \quad (D, p) \in \mathbb{C}
\]

where \(D\) data, \(I\) idealization, \(p\) parameters, \(F\) quantities of interest (QoI), \(\mathbb{C}\) the domain of calibration (also known as: domain of application).

In the following we assume that \(|F_{num} - F| \ll |F|\).

**Example**: Crack propagation in an aircraft component driven by cyclic loads. The quantity of interest \(F\) is the probability distribution of crack length.
The main elements of transformation in the applied sciences

The right arrow in $D \xrightarrow{(l, p)} F$ means:

- **Input $D$**
  - Geometry
  - Properties
  - Loading

- **Transformation**
  - Mathematical model
    - Linear Elasticity
    - Predictor
    - Statistical Model

- **Output $F$**
  - Probability of outcome

- **Auxiliary hypotheses** (these are being investigated)
- **Hard core assumptions** (validated component)
Paris and Erdogan

• Proposed an empirical relationship relating crack growth rate to the amplitude of the stress intensity factor:

\[
\frac{da}{dN} = C (K_{max} - K_{min})^m
\]

where \(a\) is the crack length, \(K\) is the stress intensity factor, \(N\) is the cycle count, \(C\) and \(m\) are empirical material-dependent constants (1961, 1963).

• This is known as Paris’ law or the Paris–Erdogan equation.

• The domain of calibration includes the restrictions:

\[
a_1 \leq a \leq a_2, \quad k_1 \leq (K_{max} - K_{min}) \leq k_2
\]

\[
r_1 \leq K_{min}/K_{max} \leq r_2
\]
According the two-dimensional theory of linear elasticity, the stress field at the notch tip is:

\[
\begin{align*}
\sigma_x & = \sum_{i=1}^{\infty} c_i r^{|\lambda_i|} \phi_x^{(i)}(\theta) \\
\sigma_y & = \sum_{i=1}^{\infty} c_i r^{|\lambda_i|} \phi_y^{(i)}(\theta) \\
\tau_{xy} & = \sum_{i=1}^{\infty} c_i r^{|\lambda_i|} \phi_{xy}^{(i)}(\theta)
\end{align*}
\]

In linear elastic fracture mechanics:

\[
\alpha = 0, \quad \lambda_1 = -1/2, \quad \lambda_i \geq 0 \quad \text{for} \quad i \geq 2,
\]

\[
c_1 = K / \sqrt{2\pi}
\]
Example

- Linear solution: Distribution of the von Mises stress in a notched panel subjected to tension.
- Typical $hp$-mesh: The size of the elements is graded in geometric progression toward the singular point.
- The numerical error in the maximum stress is infinity.
- The error in $K$ is much less than 1 percent.
Conceptual issues

- The formulation is strictly 2D – Neither the plane stress nor the plane strain conditions can be reproduced exactly in a physical experiment.

- The calibration data are polluted by the effects of the vertex singularities.

- The dimension of the stress intensity factor is $ksi \sqrt{in}$. At the vertices it is something else, and there is a transition zone.

- The predictor can be validated for long cracks in plates only (crack length $>>$ thickness).
Calibration

- D. A. Virkler tested 68 centrally cracked aluminum panels under cyclic loading.
  - There are 11,162 data points.
- The assignment of a pdf for $Pr(N|\alpha)$ is straightforward, however we need $Pr(\alpha|N)$. 
Reporting

• **Good practice:** Virkler reported the applied load, the crack length and $N$, as it should be done.
  
  • The load level was controlled to within 0.2%.
  
  • The crack length measurements were accurate to within 0.00141 mm.

• **Bad practice:** Often $da/dN$ is reported as a function of $(K_{\text{max}} - K_{\text{min}})$.
  
  • This precludes the investigation of alternative predictors: The recorded data implies the assumption of the predictor: The reported data are theory laden.
  
  • Uncertainty about how accurate the calculation of $K$ was.
The domain of calibration

In the Virkler dataset the smallest crack length-to-thickness ratio is 3.5. The 2D approximation is reasonable.

In the case of a small crack the 2D approximation would not be reasonable.

Common mistake: Using data that are far outside of the domain of calibration.
Example: Aloha flight 243 (Boeing 737-200)
April 28, 1988
General Dynamics F-111 Aardvark

• The production of this swing-wing supersonic bomber began in 1964.
• In December 1969, a catastrophic wing failure occurred during a pull-up from a simulated bombing run at Nellis Air Force Base (Nevada).
• That aircraft had only about 100 hrs of flight time. The failure originated from a fatigue crack that emanated from a forging defect in the wing-pivot fitting.

Origin of the F-111 Wing Defect [Rudd, et al., 1979]
**Damage tolerance**

- Damage tolerant design was formally adopted by the US Air Force as part of the Airplane Structural Integrity Program (ASIP) [MIL-STD-1530, 1972].
- It is assumed that flaws can exist in any part of the structure and such flaws propagate with usage.
- A structure is damage tolerant if a maintenance program has been implemented that will result in the detection and repair of accidental damage, corrosion and fatigue cracking before such damage reduces the residual strength of the structure below an acceptable limit.
Tools

• Damage Tolerance Analysis (DTA) tools in professional use designed to calculate stress intensity factors, crack growth life and critical crack size:
  • AFGROW (Air Force Grow), was developed by The Air Force Research Laboratory. It is now being further developed and maintained by LexTech, Inc.
  • NASGRO was jointly developed by Southwest Research Institute (SWRI) and NASA. Maintained by SWRI.
  • OEM’s proprietary manuals.
Thomas Kuhn (1922-1996)

- Challenged the notion that science is a rational, objective and cumulative enterprise.
- Scientific truth is determined by a consensus of the scientific community which tends to have dogmatic adherence to a paradigm.

www.thwink.org/sustain/glossary/KuhnCycle.htm
The Kuhn Cycle in linear elastic fracture mechanics

• Normal science (1921 to about 1980)

• Model drift (from about 1980)
  • Dogmatic adherence to the idea that the predictor of crack propagation is the stress intensity factor.

• Model crisis (now)
  • Inability to extend the domain of calibration. Use of correction factors.
Model crisis

The model development program (MDP), known as linear elastic fracture mechanics, has been stagnating for decades. It is now in crisis.

Evidence: Given a centrally cracked panel and a load spectrum, predict the crack length as a function of the number of cycles.
Advice to management: Break the Kuhn cycle

- **Recognize** that simulation governance is your responsibility, no one else’s.
- **Understand** the technical requirements of simulation governance.
- **Reject** improper models.
- **Coordinate** experimental and analytical work. Testing without model development and model development without testing make no sense.
- **Maintain** detailed documentation.
- **Insist** on VVUQ evidence for all model-generated information.
- **Create** conditions favorable to the evolutionary development of mathematical models.
- **Resist** the temptation to believe that there are easy solutions for complicated problems.
Imre Lakatos (1922-1974)

• The descriptive unit of scientific activities is a research program (or model development program).
• The constituent parts of a research program are:
  • A set of **hard core assumptions**.
  • A sequence of **auxiliary hypotheses**.
  • A problem **solving machinery**.
• Lakatos missed the essential role of the domain of calibration.
Demarcation

• According to Lakatos, a research programme is
  • progressive if theory leads to the discovery of novel facts (example: theory of relativity),
  • degenerating if theories are fabricated to accommodate known facts (example: Marxism).

• We propose the following adaptation for the applied sciences:
  A model development program is
  • progressive if the size of the domain of calibration is increasing;
  • stagnant if the size of the domain of calibration is not increasing;
  • improper if it does not conform with the hard core theory.
The causes of stagnation

• The major stakeholders have not demanded the application of VVUQ processes. Simulation governance has not been exercised.

• The Paris law (1963) was not seen as the first step in an evolutionary process of model development: It was allowed to ossify into a dogma.

• The predictor is routinely used outside of its domain of calibration.

• Discrepancies between predicted and observed crack propagation events have been handled through correction factors.
  
  • “A research programme is degenerating if theories are fabricated to accommodate known facts” (Lakatos).
  
  • “Blind commitment to a theory is not an intellectual virtue: it is an intellectual crime”. (Lakatos).
Example: An alternative predictor of crack propagation

Let us define on 3-dimensional stress fields:

\[ P_{\alpha\lambda\varrho} = \frac{1}{\varrho^\alpha V_c} \int_{\Omega_c} |x|^{\alpha} \sigma_1^\lambda \bar{\sigma}^{1-\lambda} dx dy dz, \quad a \geq 0, \quad 0 \leq \lambda \leq 1, \quad \varrho > 0 \]

where \( \alpha, \lambda, \varrho \) are adjustable parameters and:

\[ \Omega_c = \{ x | \sigma_1(x) > 0, \quad |x| < \varrho \}, \quad V_c = \int_{\Omega_c} dx dy dz \]

In the case of a 2D stress \( \lambda = 1, \quad \alpha = \frac{1}{2} \) and we have:

\[ K = \frac{\pi \sqrt{2\pi}}{3} \lim_{\varrho \to 0} (\sqrt{\varrho} P_{\alpha\lambda\varrho}) \]
Calibration

The goal is to find $p$ in $D \xrightarrow{(I, p)} F$:
The goal is to find the predicted value of $F$ in $D \rightarrow F$: 

![Diagram showing the process of prediction]

1. **Mathematical model**
   - Linear Elasticity
   - Predictor
   - Statistical Model

2. **Formulation**
   - Calibration
     - a-N data
   - da/dN data

3. **Calibration**
   - Prediction
   - Test conditions
Validation
The entire process
Summary of the main points

• A key goal of simulation governance is to foster the evolutionary development of mathematical models.

• Model development projects are progressive, stagnant or improper.
  • Progressive model development projects are applications of the concepts and procedures of VVUQ.
  • On a sufficiently small domain of calibration any model, even improper models, can be validated.

• Model development projects are open-ended. No one has the right to claim the last word.

• There is a very substantial unrealized potential in numerical simulation technology.
Outlook

• Artificial intelligence (AI) will bring radical changes to numerical simulation technology.

• Progress will first occur in the standardization of engineering workflows through expert-designed engineering simulation applications (Sim Apps) equipped with autonomous error control procedures.

• AI will change the technical requirements for model development projects
  • Track the evolutionary stages, the relevant data and documentation.

• AI will help navigate numerical simulation projects.
  • Prevent the use of intuitively plausible but conceptually wrong input data.
  • Shorten training time for the operators of simulation software tools.

• AI will make it possible to create smart discretizations that will take into account the goals of computation and the input data.
References
