Verification and Validation of Scientific and Economic Simulations

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Overview

- Introduction
  - Concepts of Verification and Validation
  - Research Objectives and Methods
- Case Studies
  - An Agent-based Scientific Model
  - An Equation-based Economic Model
- Conclusion
- Future Work
Model Verification & Validation (V & V)

- V & V
  - Verification: 
    - *get model right*
  - Validation: 
    - *get right model*

- The cost and value influence confidence of model

- Want to utilize V & V for optimal cost-effectiveness

*Adapted from Sargent: “Verification and Validation of Simulation Models”*
Verification and Validation Process

*Adapted from Sargent: "Verification and Validation of Simulation Models" and Huang: "Agent-Based Scientific Simulation"
Applicable Verification and Validation Methods

*Balci: “Handbook of Simulation: Principles, Methodology, Advances, Applications, and Practice” lists more than 75 Methods
V & V: Subjective Analysis

- Examples of V & V Techniques
  - Face Validity
    - Animation
    - Graphical Representation
  - Turing Test
  - Internal Validity
  - Tracing
  - Black-Box Testing
V & V: Quantitative Analysis

- Examples of V & V Techniques
  - Model-to-Model Comparison (Docking)
  - Historical Data Validation
  - Sensitivity Analysis/Parameter Variability
  - Prediction Validation
What and How

- Research objective
  - Perform V & V on distinct models and identify the more cost-effective techniques

- How
  - Two very different projects as case studies
  - Evaluate and adapt the formalized V & V techniques in industrial and system engineering
Case Study 1: An Agent-based Scientific Model

- NSF funded interdisciplinary project
  - Understanding the evolution and heterogeneous structure of Natural Organic Matter (NOM)
  - E-science example
  - Chemists, biologists, ecologists, and computer scientists
- Agent-based stochastic model
- Web-based simulation model
Case Study 1: NOM

- What is NOM?
  - Heterogeneous mixture of molecules in terrestrial and aquatic ecosystems

- Why study NOM?
  - Plays a crucial role in the evolution of soils, the transport of pollutants, and the global carbon cycle
  - Understanding NOM helps us better understand natural ecosystems
Case Study 1: The Conceptual Model I

- **Agents**
  - A large number of molecules
    - Heterogeneous properties
      - Elemental composition
      - Molecular weight
      - Characteristic functional groups
  
- **Behaviors**
  - Transport through soil pores (spatial mobility)
  - Chemical reactions: first order and second order
  - Sorption
Case Study 1:  
The Conceptual Model II

- **Stochastic Model**
  - Individual behaviors and interactions are stochastically determined by:
    - Internal attributes
      - Molecular structure
      - State (adsorbed, desorbed, reacted, etc.)
    - External conditions
      - Environment (pH, light intensity, etc.)
      - Proximity to other molecules
    - Length of time step, \( \Delta t \)

- **Space**
  - 2D Grid Structure

- **Emergent properties**
  - Distribution of molecular properties over time
Case Study 1: Implementations

Conceptual Model (Agent-based Stochastic model)

- AlphaStep
  - Features: Batch, Closed System, Standalone

- FlowSorption
  - Features: In Porous Media

- No-FlowSorption
  - Features: Surface Water

- FlowReaction
  - Features: Web-based, Standalone

- No-FlowReaction
Case Study 1: Face Validity
Case Study 1: Internal Validity I

![Graph showing the number of molecules at the end step vs. seed numbers. The graph compares 'After' and 'Before' scenarios, with peaks and troughs indicating variability in molecule counts.]
### Case Study 1: Internal Validity II

<table>
<thead>
<tr>
<th>Number of Molecules</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>125.0</td>
<td>60</td>
</tr>
<tr>
<td>1275.0</td>
<td>50</td>
</tr>
<tr>
<td>1325.0</td>
<td>40</td>
</tr>
<tr>
<td>1375.0</td>
<td>30</td>
</tr>
<tr>
<td>1425.0</td>
<td>20</td>
</tr>
<tr>
<td>1475.0</td>
<td>10</td>
</tr>
<tr>
<td>1525.0</td>
<td>0</td>
</tr>
</tbody>
</table>

Std. Dev = 100.79  
Mean = 1473.9  
N = 450.00
Case Study 1: Model-to-Model Comparison I

- Compare the model with validated one
- Compare the model with non-validated one
- Different implementations
  - Different programming languages
  - Different packages
- Different modeling approaches
  - Agent-based approach vs. Equation-based approach
- Powerful method for ABS
# Case Study 1: Model-to-Model Comparison II

<table>
<thead>
<tr>
<th>Features</th>
<th>Alpha Step</th>
<th>No-flow Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Developing Group</td>
<td>University of New Mexico, Department of Chemistry</td>
<td>University of Notre Dame, Computer Science and Engineering</td>
</tr>
<tr>
<td>Programming language</td>
<td>Pascal</td>
<td>Java (Sun JDK 1.4.2)</td>
</tr>
<tr>
<td>Platforms</td>
<td>Delphi 6, Windows</td>
<td>Red hat Linux cluster</td>
</tr>
<tr>
<td>Running mode</td>
<td>Standalone</td>
<td>Web based, standalone</td>
</tr>
<tr>
<td>Simulation package</td>
<td>None</td>
<td>Swarm, Repast libraries</td>
</tr>
<tr>
<td>Animation</td>
<td>None</td>
<td>Yes</td>
</tr>
<tr>
<td>Spatial representation</td>
<td>None</td>
<td>2D grid</td>
</tr>
<tr>
<td>Second order reaction</td>
<td>Random pick one from list</td>
<td>Choose the nearest neighbor</td>
</tr>
<tr>
<td>First order with split</td>
<td>Add to list</td>
<td>Find empty cell nearby</td>
</tr>
</tbody>
</table>
Case Study 1: Model-to-Model Comparison III

Total Number of Molecules in the System

Z Average
The Average Charge on Each Molecule at pH=7
Case Study 1: Model-to-Model Comparison IV
Case Study 1: Model-to-Model Comparison V

- Total Mass of Carbon
- The Weight Percentage of Carbon
Case Study 2: An Economic Model

- Interdisciplinary project
  - Initially written in Matlab within Department of Finance
  - Converted to C++ by Computer Scientists
  - Equation-based system
  - Concerned with identifying ideal economic variables, such as debt, money growth, and tax rate
Case Study 2: The Conceptual Model

- Equation-based system
- Nonlinear projection methods used to solve Ramsey problems in a stochastic money economy
- Goal is to generate the best social welfare for a given economy
- Motivation

\[
\hat{\mu}_{t+1}(\theta_t, g_t, b) = \sum_{i=1}^{n_g} \sum_{j=1}^{n_g} b_{ij} \psi_{ij}(\theta_t, g_t),
\]

\[
\hat{\tau}_t(\theta_t, g_t, d) = \sum_{i=1}^{n_g} \sum_{j=1}^{n_g} d_{ij} \Omega_{ij}(\theta_t, g_t),
\]

\[
\hat{H}_t(\theta_t, g_t, q) = \sum_{i=1}^{n_g} \sum_{j=1}^{n_g} q_{ij} \Phi_{ij}(\theta_t, g_t),
\]

\[
\hat{\lambda}_{gt}(\theta_t, g_t, v) = \sum_{i=1}^{n_g} \sum_{j=1}^{n_g} v_{ij} \Gamma_{ij}(\theta_t, g_t).
\]
## Case Study 2: Face Verification

<table>
<thead>
<tr>
<th></th>
<th>LaGrange Multiplier</th>
<th>Labor</th>
<th>Money Growth</th>
<th>Tax Rate</th>
<th>Cash Good</th>
<th>Credit Good</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matlab</td>
<td>0.138</td>
<td>0.309</td>
<td>-0.009</td>
<td>0.188</td>
<td>0.486</td>
<td>0.621</td>
</tr>
<tr>
<td>C++</td>
<td>0.138</td>
<td>0.309</td>
<td>-0.009</td>
<td>0.188</td>
<td>0.486</td>
<td>0.621</td>
</tr>
<tr>
<td>Steady State</td>
<td>0.138</td>
<td>0.309</td>
<td>-0.009</td>
<td>0.188</td>
<td>0.485</td>
<td>0.620</td>
</tr>
</tbody>
</table>
Case Study 2: Tracing

- **Matlab:**
  - it 44, af 3.7496e-08, rc 0, timer 11.1, l 0.1382704496, m -0.0092286139, t 0.1881024991, h 0.3093668925
  - cc1 0.4861695543, cc2 0.6212795130, rl 1.0092221442
  - it 45, af 2.64653e-08, rc 0, timer 11.0, l 0.1382704643, m -0.0092286175, t 0.1881024947, h 0.3093668931
  - cc1 0.4861695553, cc2 0.6212795120, rl 1.0092221442

- **C++:**
  - it: 44 af: 0.00144839 rc: 0 l: 0.138359 m: -0.00936025 t: 0.188252 h: 0.309338
  - cc1: 0.486205 cc2: 0.621244 rl: -0.65888
  - it: 45 af: 0.00144784 rc: 0 l: 0.138401 m: -0.00937062 t: 0.188239 h: 0.30934
  - cc1: 0.486208 cc2: 0.621241 rl: -0.665511
Case Study 2: Implementation Characteristics

<table>
<thead>
<tr>
<th>Features</th>
<th>Matlab</th>
<th>C++</th>
</tr>
</thead>
<tbody>
<tr>
<td>Developing Group</td>
<td>University of Notre Dame, Department of Finance</td>
<td>University of Notre Dame, Computer Science and Engineering</td>
</tr>
<tr>
<td>Language</td>
<td>High-Level</td>
<td>Lower-Level</td>
</tr>
<tr>
<td>Compiler</td>
<td>Interpreted</td>
<td>GNU Compiler</td>
</tr>
<tr>
<td>Good For</td>
<td>Prototyping</td>
<td>Speed</td>
</tr>
<tr>
<td>Platforms</td>
<td>Linux, Windows</td>
<td>Linux</td>
</tr>
<tr>
<td>Running mode</td>
<td>Standalone</td>
<td>Standalone</td>
</tr>
<tr>
<td>Packages</td>
<td>LAPACK, etc...</td>
<td>STL</td>
</tr>
<tr>
<td>Variables</td>
<td>Implicit</td>
<td>Declared</td>
</tr>
</tbody>
</table>
Case Study 2: Performance

<table>
<thead>
<tr>
<th></th>
<th>5 Iterations</th>
<th>50 Iterations</th>
<th>500 Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matlab</td>
<td>58 s</td>
<td>568 s</td>
<td>8872 s</td>
</tr>
<tr>
<td>C++</td>
<td>2 s</td>
<td>17 s</td>
<td>176 s</td>
</tr>
</tbody>
</table>
Summary & Conclusion

- Applied V & V to distinct case studies to increase model confidence
- Some techniques are more cost-effective

<table>
<thead>
<tr>
<th>For our models:</th>
<th>Agent-based</th>
<th>Equation-based</th>
</tr>
</thead>
<tbody>
<tr>
<td>Face Validation/Verification</td>
<td>Very Good</td>
<td>Very Good</td>
</tr>
<tr>
<td>Turing Test</td>
<td>Very Good</td>
<td>Good</td>
</tr>
<tr>
<td>Internal Validity</td>
<td>Very Good</td>
<td>n/a</td>
</tr>
<tr>
<td>Tracing</td>
<td>Fair</td>
<td>Excellent</td>
</tr>
<tr>
<td>Black-Box Testing</td>
<td>Good</td>
<td>Good</td>
</tr>
<tr>
<td>Model-to-Model Comparison</td>
<td>Very Good</td>
<td>Very Good</td>
</tr>
<tr>
<td>Historical Data Verification</td>
<td>Very Good</td>
<td>Very Good</td>
</tr>
<tr>
<td>Sensitivity Analysis</td>
<td>Good</td>
<td>Good</td>
</tr>
<tr>
<td>Prediction Validation</td>
<td>Good</td>
<td>Fair</td>
</tr>
</tbody>
</table>
Future Work

- Collect and evaluate more statistical data
- Compare simulation results against empirical data
- More stringent and formalized V & V
- Perform more statistical tests
Questions or Comments?