Verification and Validation of Agent-based Scientific Simulations

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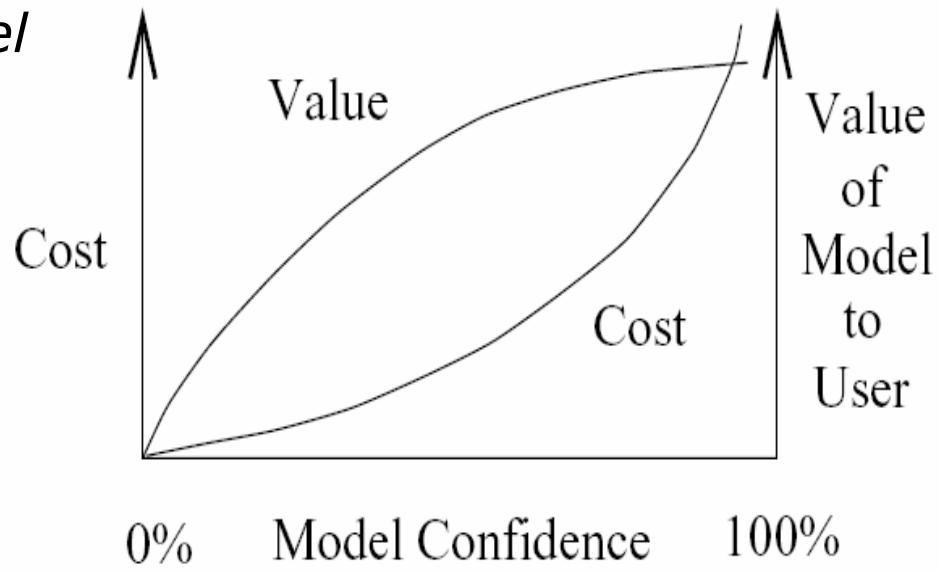
Overview

- Introduction
  - Concepts of Verification and Validation
  - Research Objectives and Methods
- A Case Study
- Apply Verification and Validation Methods to the Case Study
- 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 acceptance level



*Adapted from Sargent: "Verification and Validation of Simulation Models"

V & V for Agent-based Simulation

- Agent-based modeling is a new approach
- Different than Queuing Models
  - Entities: large number of heterogeneous active objects vs. passive objects
  - Space: continuous or discrete grid space vs. network of servers and queues
  - Interactivity: high vs. low
  - Active components: agents vs. queues and servers
  - Goal: discovery vs. design and optimization
- Few literature to date address the formalized methodology for V & V of Agent-based Simulations

What and How

- Research objective
  - Generate guidelines or a formalized methodology for V & V of Agent-based Simulations
- How
  - NOM project as a case study
  - Evaluate and adapt the formalized V & V techniques in industrial and system engineering for DES
  - Identify a subset of these techniques that are more cost-effective for Agent-based Simulations

NOM Agent-based Simulation 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

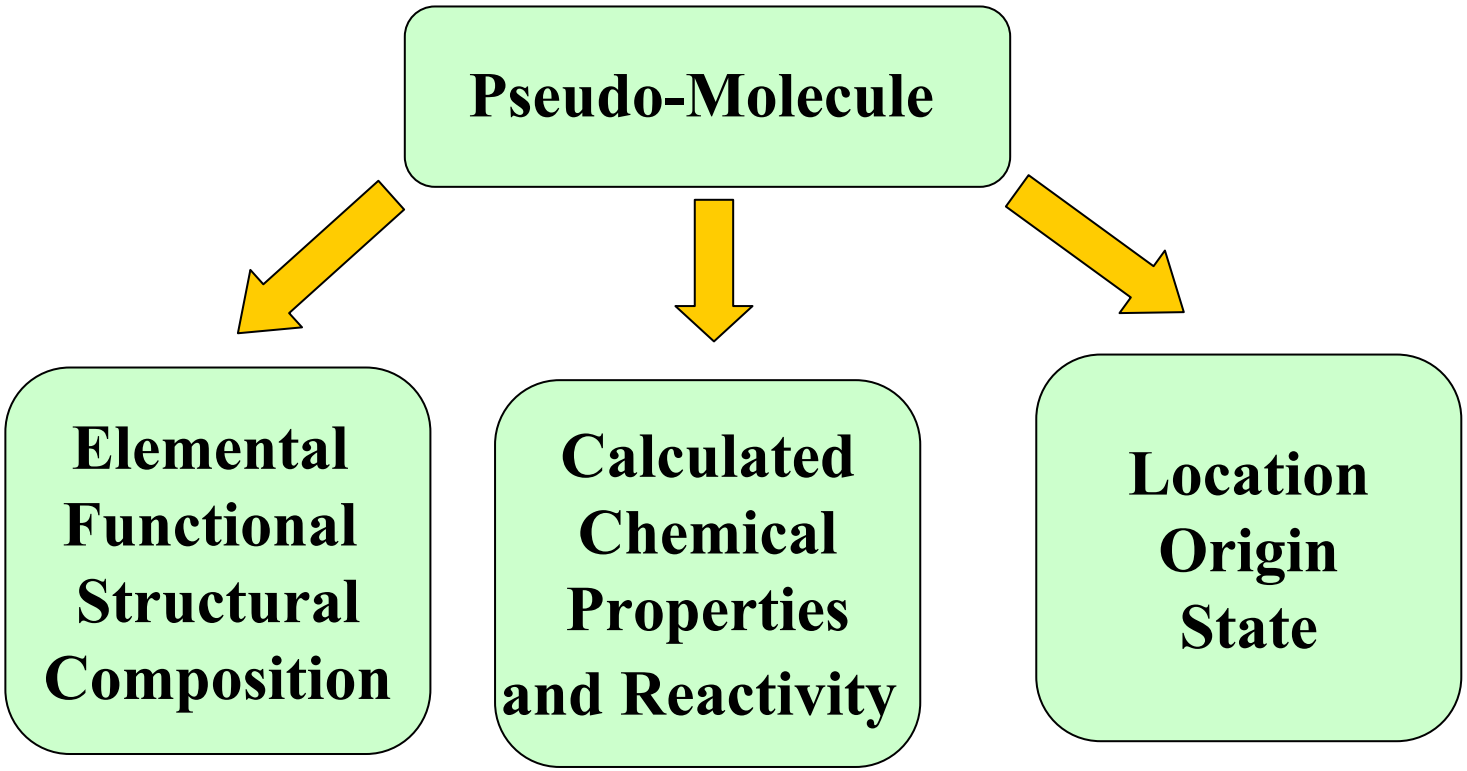
NOM

- 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

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

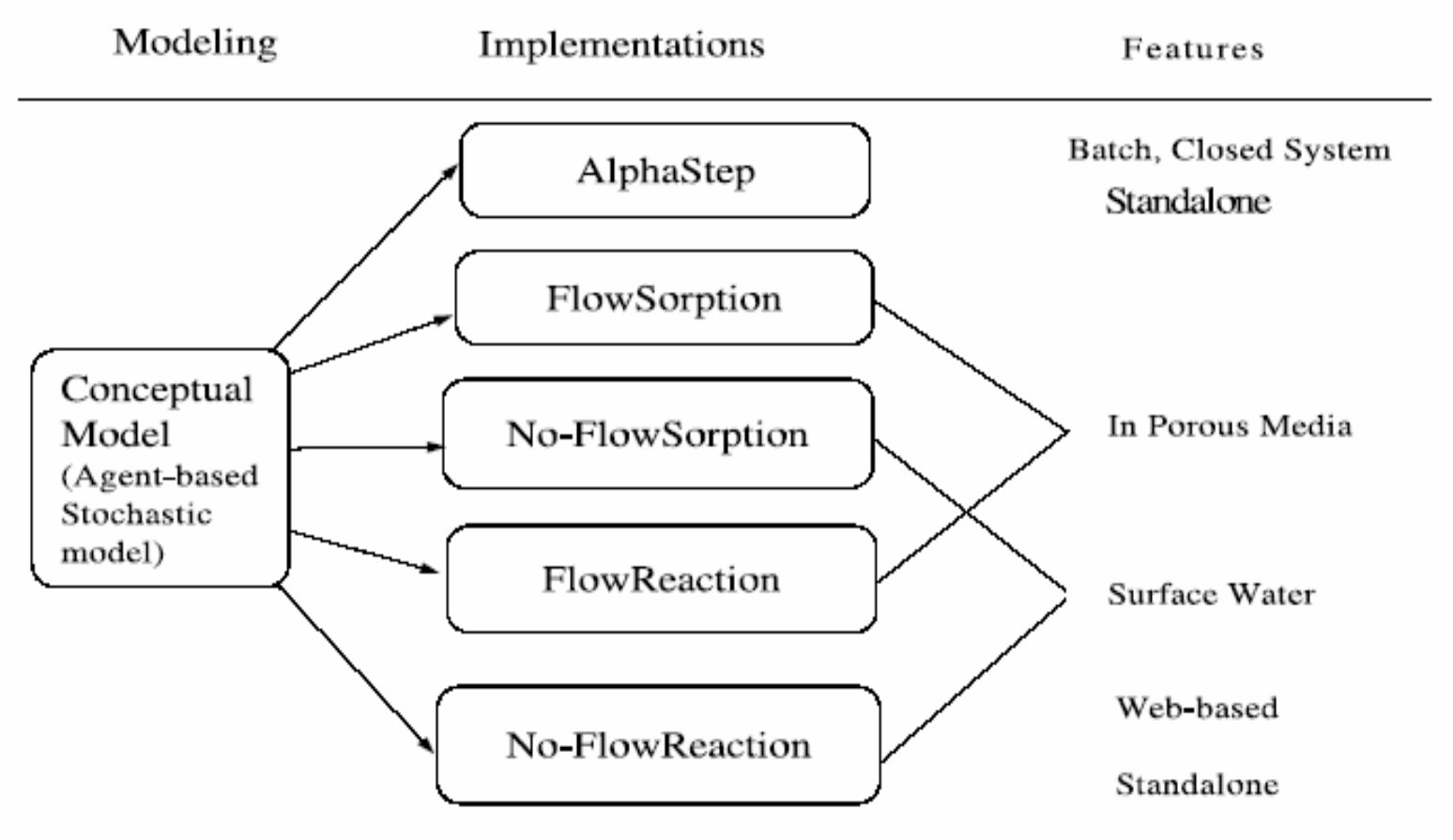
Stochastic Synthesis: Data Model



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, Δt
- Space
  - 2D Grid Structure
- Emergent properties
  - Distribution of molecular properties over time

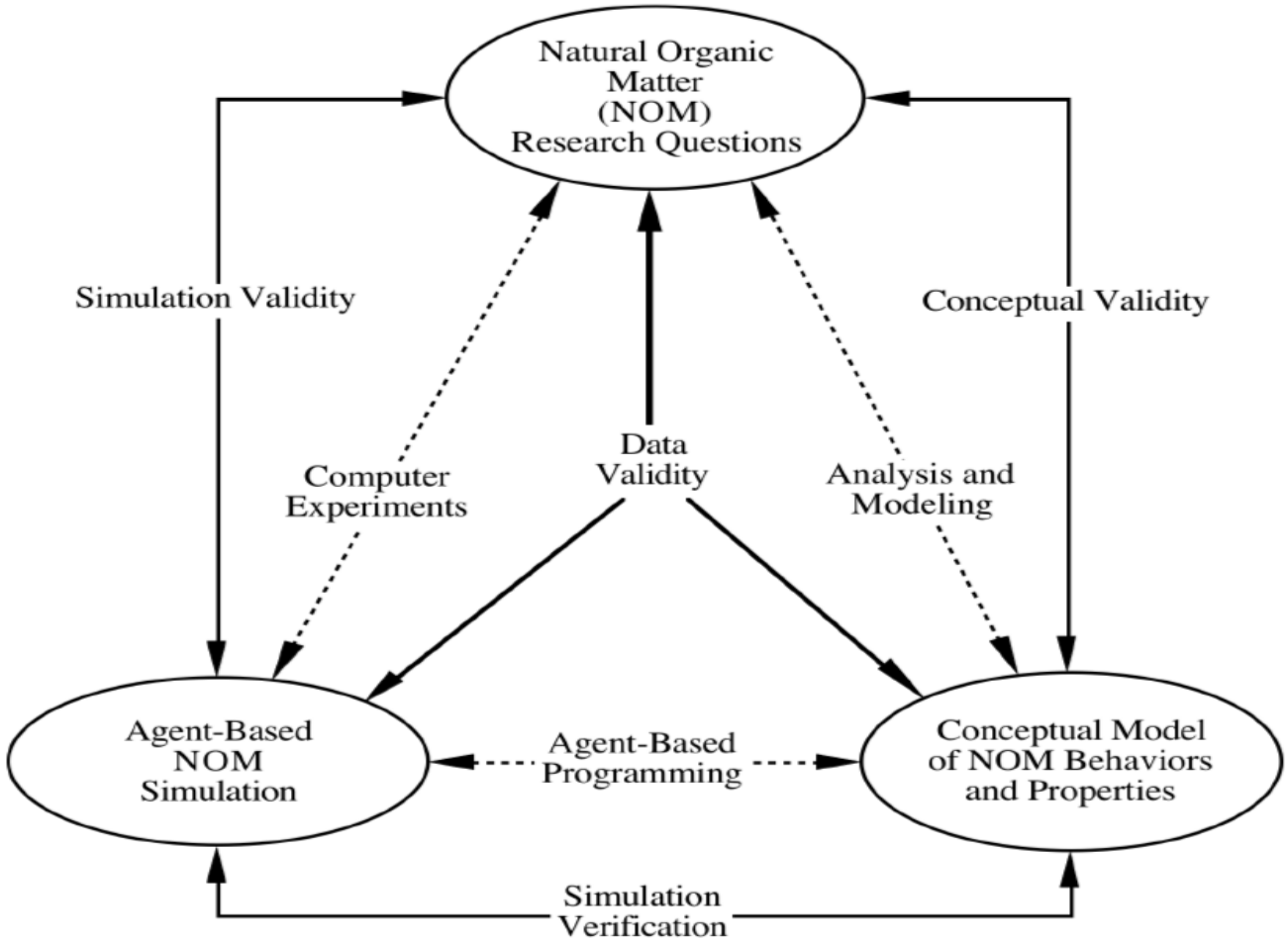
Implementations



V & V of the NOM Model

- Examples of V & V techniques
  - Face validity
    - Animation
    - Graphical representation
  - Tracing
  - Internal validity
  - Historical data validation (calibration sets and test sets)
  - Sensitivity analysis
  - Prediction validation
  - Comparison with other models
  - Turing test

V & V of NOM Simulation Model



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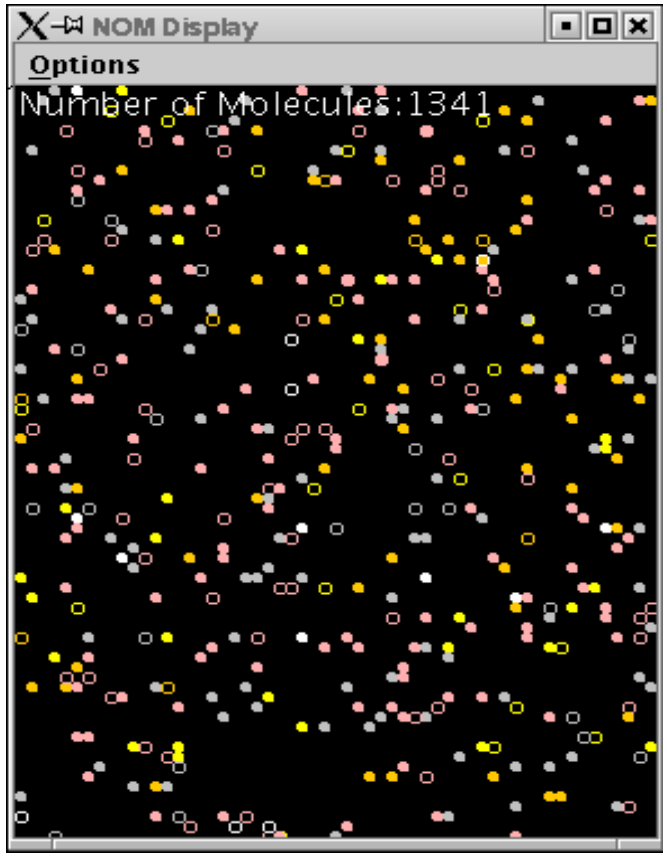
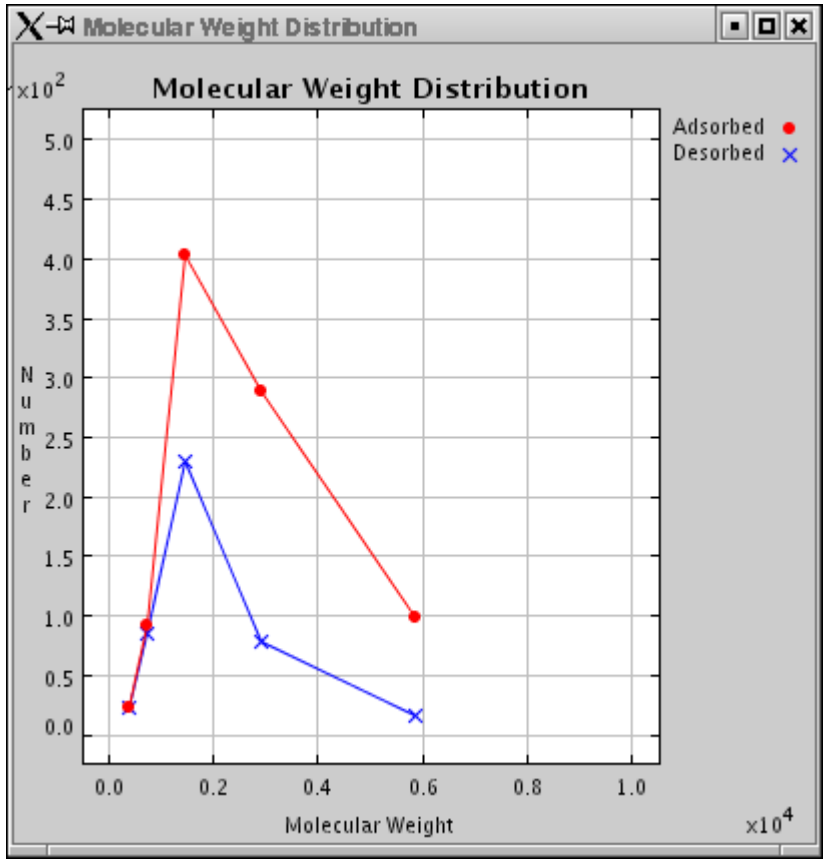
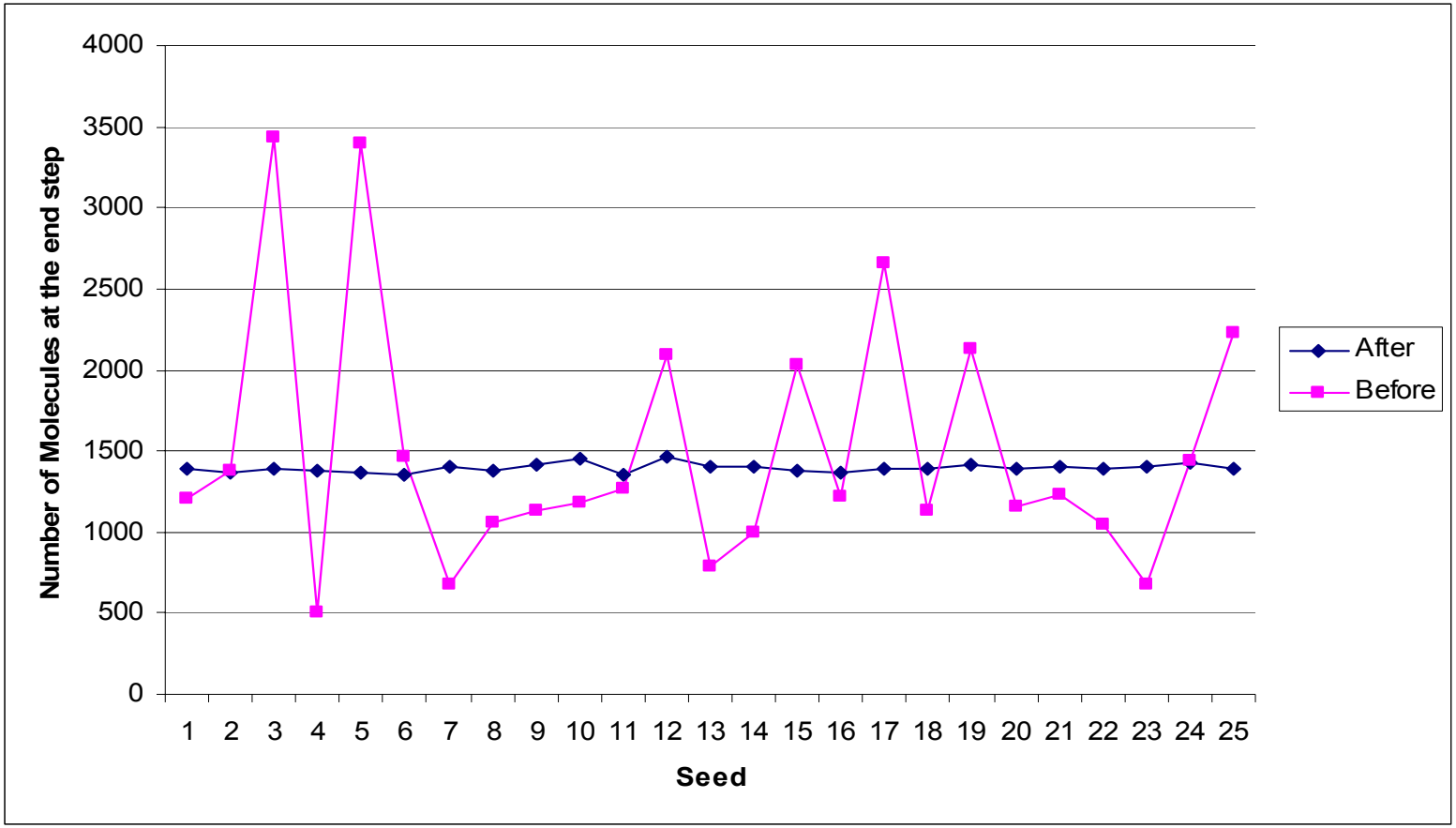
Face Validity

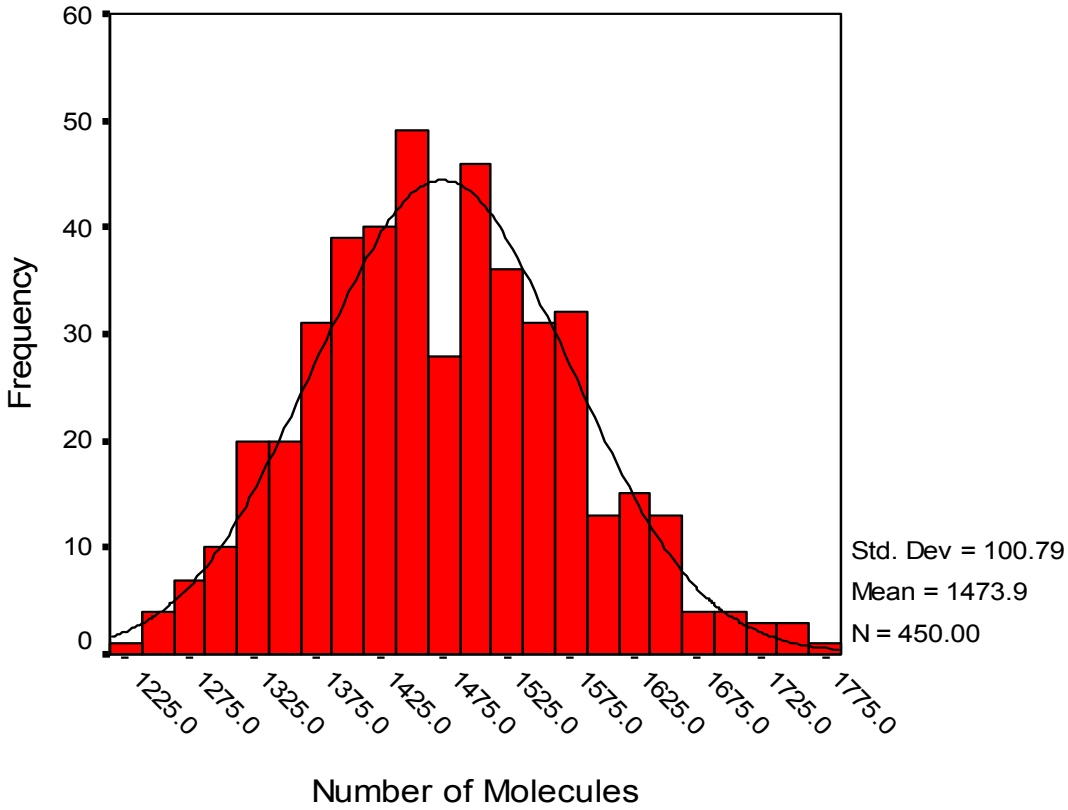




Internal Validity I



Internal Validity II



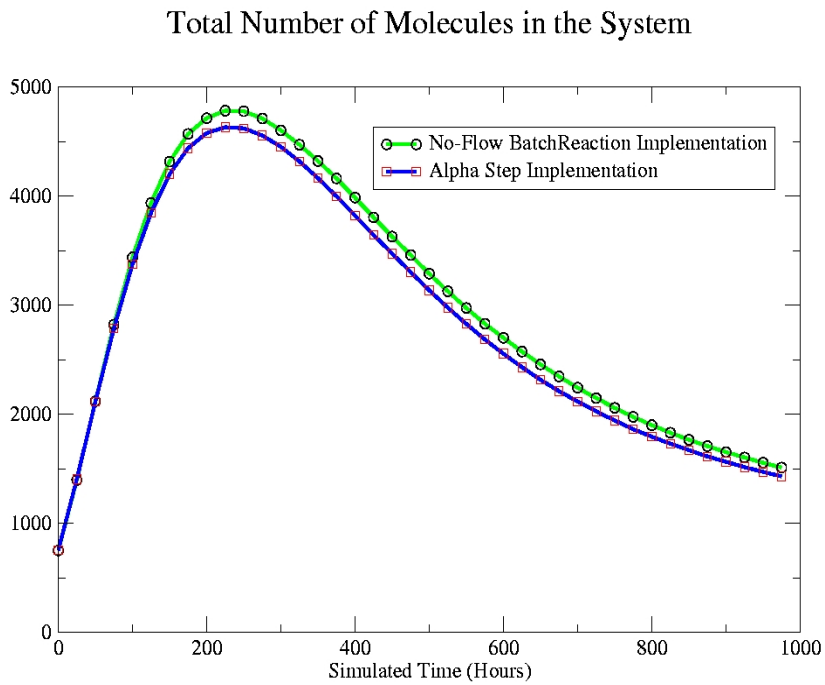
Model-to-Model Comparison I

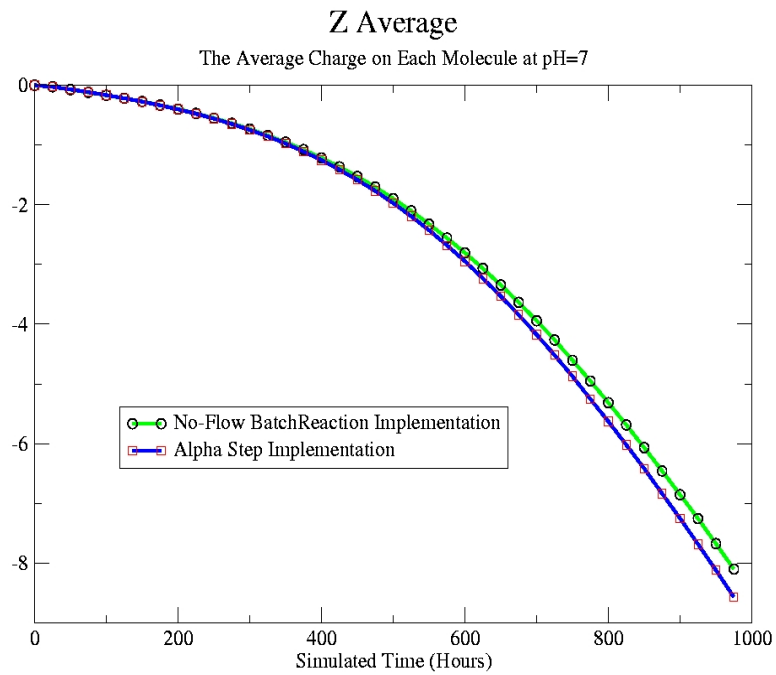
- Compare the model with validated one
- Compare the model with non-validated one
- Different implementations
  - Different programming languages
  - Different packages
- Different modeling approaches
  - Predator-Prey model
    - Agent-based approach vs. System Dynamics approach
- Powerful method for ABS

Model-to-Model Comparison II

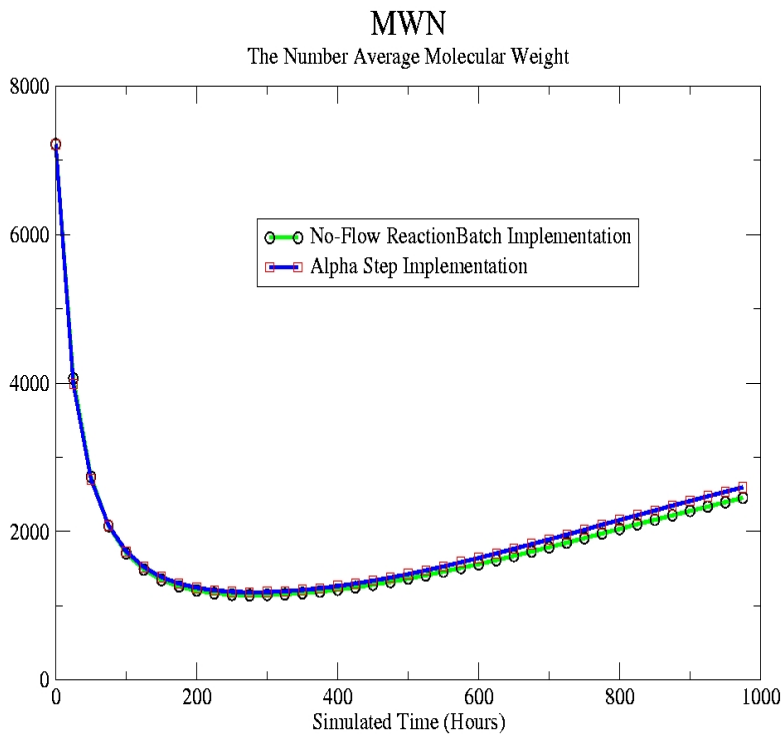
Features	Alpha Step	No-flow Reaction
Developing Group	University of New Mexico, chemists	University of Notre Dame, computer scientists
Programming language	Pascal	Java (Sun JDK 1.4.2)
Platforms	Delphi 6, Windows	Red hat Linux cluster
Running mode	Standalone	Web based, standalone
Simulation package	None	Swarm, Repast libraries
Animation	None	Yes
Spatial representation	None	2D grid
Second order reaction	Random pick one from list	Choose the nearest neighbor
First order with split	Add to list	Find empty cell nearby

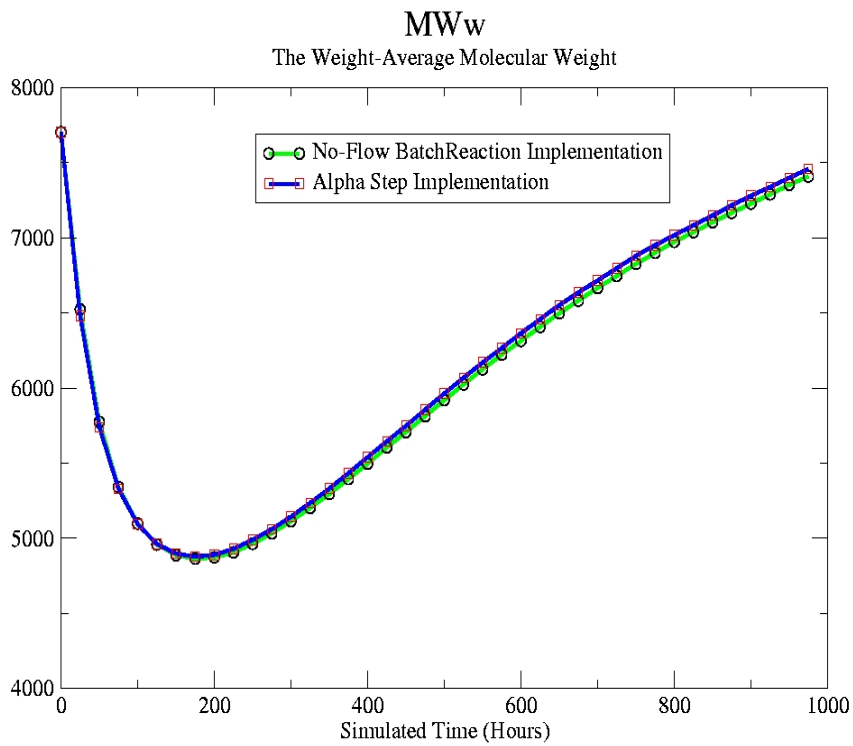
Model-to-Model Comparison III



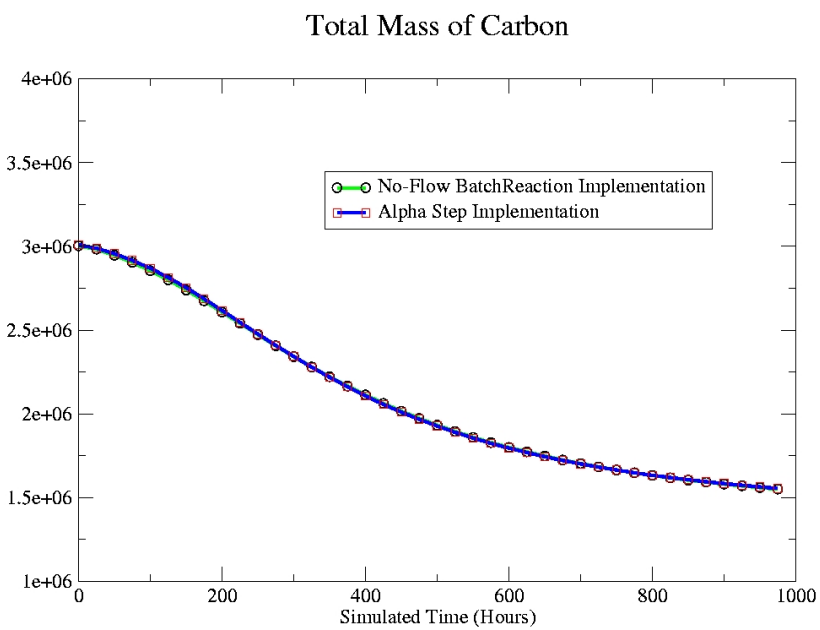


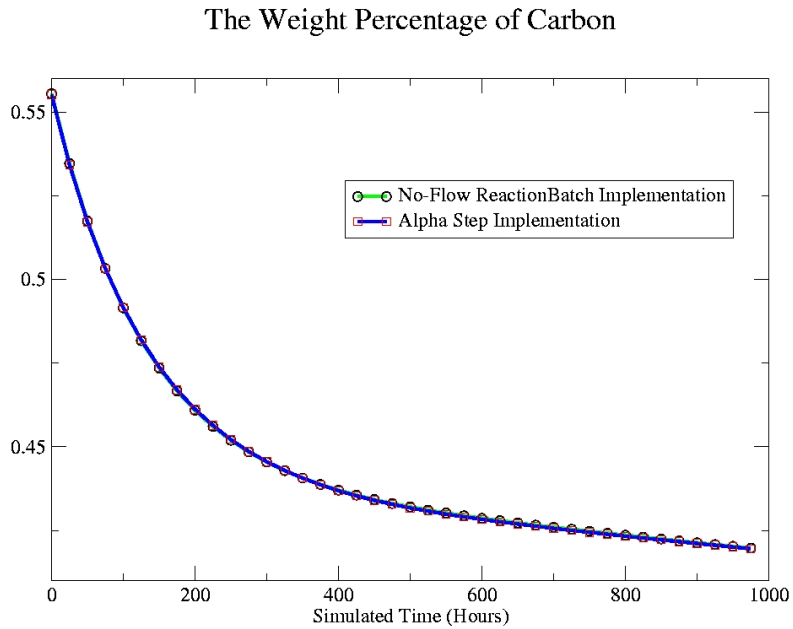
Model-to-Model Comparison IV





Model-to-Model Comparison V





Conclusion and Future Work

- V & V Case Study
- Model-to-Model Comparison is Powerful

- Collect and evaluate more statistical data
- Compare simulation results against empirical data
- Tweak V & V methods
- Generate guidelines and methodology for V & V of agent-based simulation models

Questions or Comments?