Validation and simulation: engineering simulations for science

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EPSRC grants EP/E053505/1 and EP/E049419/1
www.cosmos-research.org

EmergeNET April 2010

Complex systems simulation for science

Simulation: A model executed on a computer to reveal time-dependent behaviour

- e.g. Agent-based models to support scientific research
  - Modelling at individual level
  - Inherent modelling in time and space
- Problem: “opaque thought experiments” [Bullock et al]
  - Throw-away simulations that only address one question
  - Naive simulations that scientists cannot use effectively
  - Simulations that are not validated w.r.t. science

Focus on validation

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Validating simulations

- Validation seeks to show that the right system has been built
- Validity is determined with respect to that purpose [Sargent 2005]
- Validation guidance exists for conventional simulations
  - but does not adapt directly to complex systems

Conventional simulation validation 1

Animation, Face validity, Turing test	Evaluation of observables: outputs and parameters
Comparison, historical or predictive validation	Against *valid* analytical models or other simulations
Degenerate and extreme tests, parameter variability, sensitivity analysis	Domain-style testing under normal and extreme conditions
Event validity	Compare events in real and simulated systems
Internal validity	Consistency of results across runs

[after Sargent 2005]

Conventional simulation validation 2

Combination of "traditional methods":	Validate assumptions, compare to sound theory, and do empirical validity checks

[after Sargent 2005]

Traditional approaches:

- Rationalism: Assumptions are rationally justifiable; valid models arise from valid assumptions
- Empiricism: Assumptions and outcomes are empirically validated
- Positive economics: The model can predict the future, so causal relationships and mechanisms are of no concern

Complex simulation validation: summary of problems

- No existing validated models to compare with
- Existing understanding of event, behaviours is limited
- Very different systems give similar observables
  - ... and the same systems has different observables in different situations

So, use multiple validation approaches
Validation becomes relative not absolute

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Arguing validity

- Establish the basis for believing that a simulation is an adequate model
  - relative to its purpose, criticality and impact
- Summarise evidence to support the argument
- Expose the argument to critical review

Techniques from critical systems engineering can help:

- Deviational analysis, flaw hypothesis
- Argumentation development and representation

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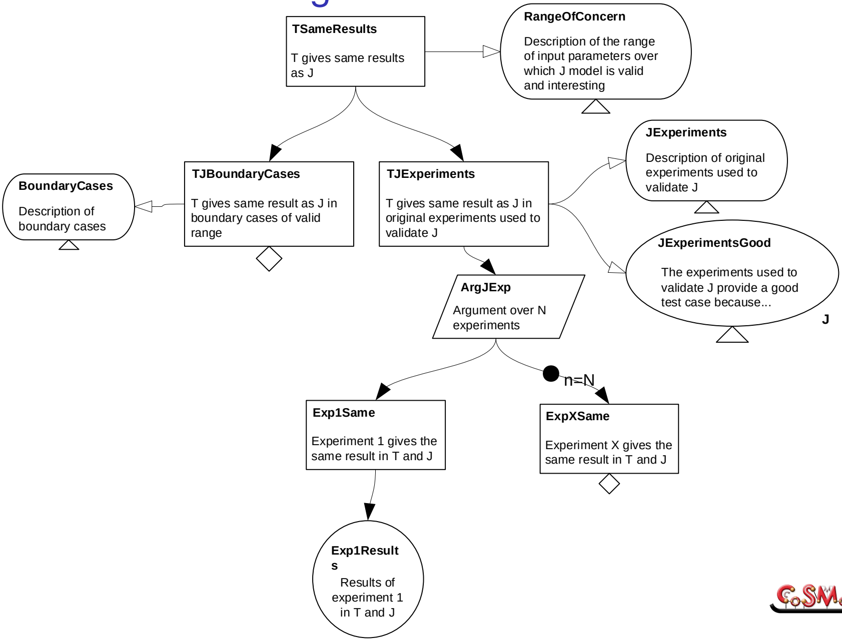
Part of a validation argument



Divide and conquer: three aspects of validity

- *Engineering validation*: conventional development and verification activities on the simulation product
  - exposes design decisions, implementation compromises
- *Calibration*: tuning parameters, behaviours, scales of operation
  - exposes assumptions, abstractions, simplifications and mappings
- *Scientific validation*: demonstrate the scientific use of the simulation, for instance by simulating real experiments and comparing results

Argument of validity over these

- Sufficient to convince those who need to be convinced!

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Purpose revisited: criticality and impact

Careful definition of purpose (domain, domain model)

- Scientific purpose identifies domain of interest
- Engineering purpose expressed in a domain model
- domain and domain model determine criticality and impact of simulation

Criticality and impact

- *Criticality* relates to the role of the simulation in context.
  - A speculative exploration of possible factors has low criticality
  - A simulation that aims to contribute scientific understanding has high criticality.
- *Impact* is relative importance of simulation findings to research area
  - where few research tools exist or the area is new, impact is usually high
  - if simulation findings are subsequently backed by traditional research, impact is low

If impact or criticality is high, then explicit validation of the engineering and the science must be planned

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Summary

- Complex systems simulation need to be validated, but traditional methods are not directly applicable
- Instead, construct an argument over evidence of why the simulation is believed to be valid for the purpose
- Focus on issues relating to engineering, calibration and sensitivity, as well as assumptions and design decisions
- Do what is merited by the purpose, criticality and impact of the simulation
  - Aim to convince those using the simulation and its results
  - And expose the basis for belief in validity to review and critique