Arguing the Validity of Models and Simulations for Scientific Exploration

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Motivation: Computer Simulation in Science

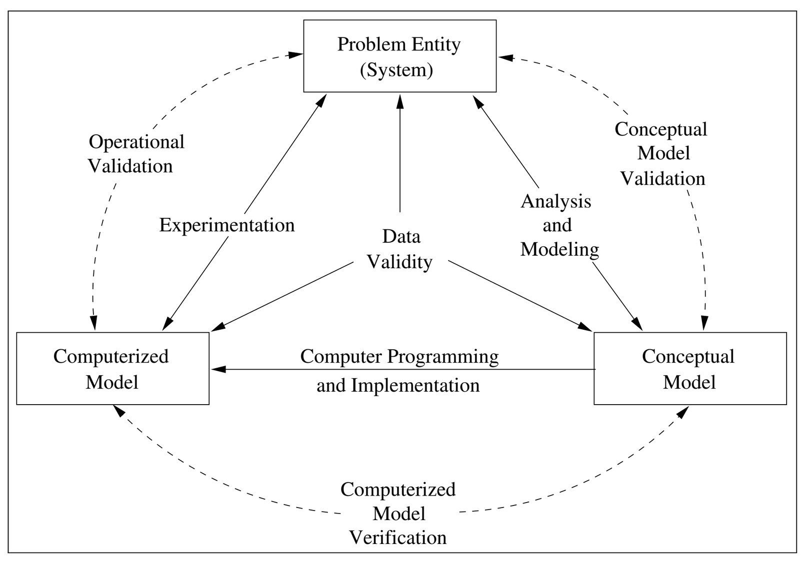
Reductionist approaches and experiments cannot express complex structures and interactions in areas such as systems biology

- Agent-based computer simulation is one potential tool to test hypotheses and understanding of complex systems
  - Simulation can be used for *in silico* experimentation if scientists and modellers are confident of the appropriateness and role of the simulation
  - Confidence requires understanding — demystifying interdisciplinary science; being explicit about each discipline's conventions; stating assumptions and simplifications
- Mutual understanding and confidence in the role of simulations can be improved by rational arguments over evidence
  - identify and present assumptions, simplifications, rationale, and design decisions using argumentation techniques

Traditional Simulation Validation

Simulation of traditional systems such as kernel behaviour has been long studied
e.g. Sargent's simulation lifecycle devised in 1980s:

- Validation of models against problem entity
- Validation between conceptual model and computational model (simulation)
- Validation of data used in simulation



R. G. Sargent, Winter Sim. Confs, 1991–2009

Validation of Complex Systems Simulation

For complex systems

- No absolute assurance of validity, only *is it good enough for our purpose?*
  - Is a model a good enough representation of reality?
  - Do we accept that an implementation is a good representation of its design?
  - Do we accept that any emergent behaviour simulates emergence in the reality?
  - Are the scale and scope sufficient for our purpose?

Developing Simulations for Complex System Exploration (see separate poster)

- Scientists and modellers identify a mutually-acceptable interpretation of the science to simulate and the *in silico* experiments to conduct
  - Scientists contribute their existing understanding; identify sources; describe components and interactions; outline environment; select data . . .
  - Modellers ask questions to clarify their understanding of the systems that can express the science; consult scientists over abstractions, scale and scope; work out algorithms and initialisation
- Modellers apply quality software engineering to produce a simulation, recording design decisions and compromises made
- Scientists work with modellers to run *in silico* experiments and interpret the results — and devise new experiments
- The basis of co-operation needs to be captured, updated, challenged — we use argumentation techniques

Logical Arguments

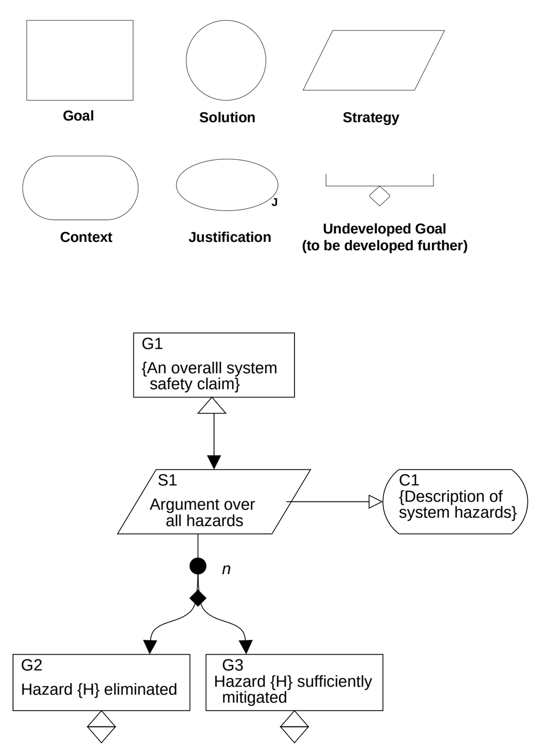
- Reasoning from premises to conclusion using propositions or predicates
  - The premise is a collection of propositions
  - The conclusion is a single proposition
  - A proposition can be either true or false
- An argument is sound if its premises are true
- An argument is consistent if all premises and the conclusion can be true at the same time
- An argument is valid if true premises cannot be associated to a false conclusion

after Kelly 1999, Govier 1992, Toulmin 1958

Certification Argumentation

- Traditional use in certification of safety, and for other critical systems certification
- An argument is valid if it is accepted by certifiers
  - The premises are not obviously false or inconsistent
  - Premises do not admit an obviously false conclusion
  - Agreement that the argument establishes the required quality of the product within stated bounds

GSN: A Notation for Arguments



- The safety claim or *goal* is argued in a *context* , and with appropriate *justifications*, according to a *strategy*
- Subgoals are argued similarly, until evidence is reached, a *solution*

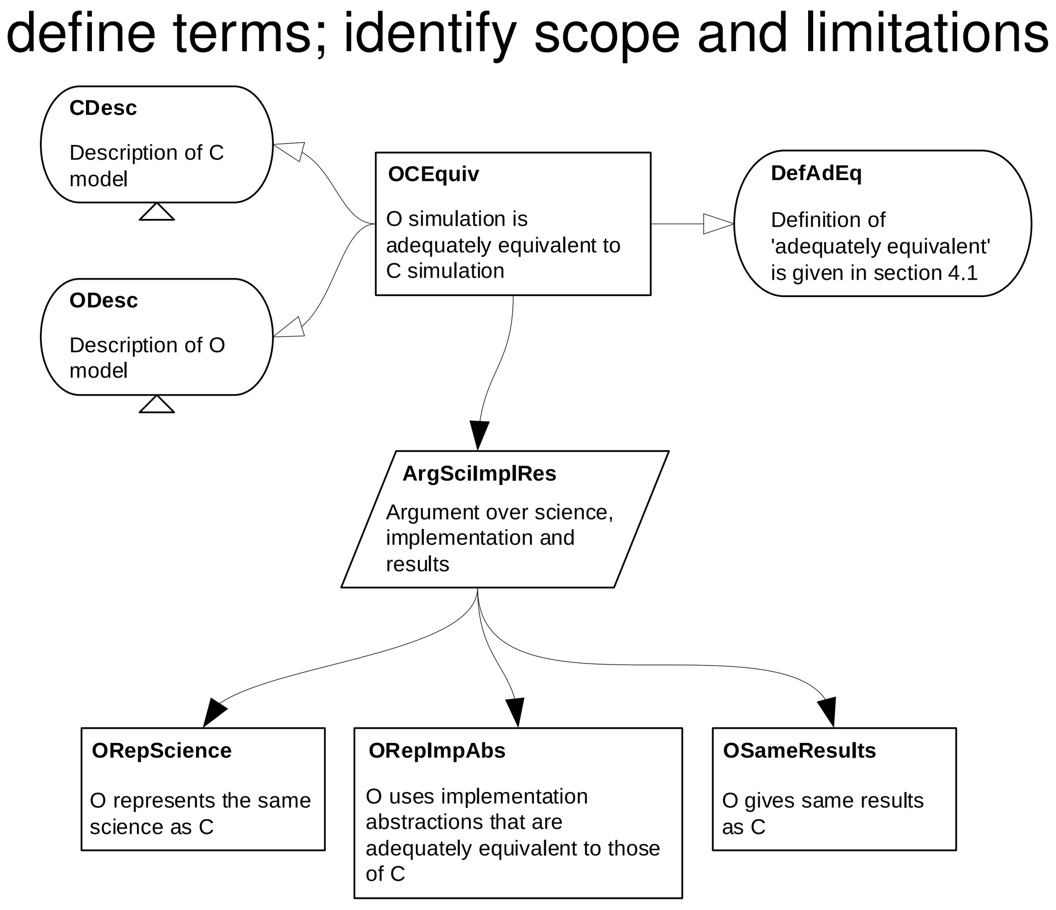
Illustration: An Argument that Two Simulations are *Adequately Equivalent*

An agent model of plant physiology and interactions based on physiological traits needs to be re-engineered to support extension of existing experimental work. The new simulation must be demonstrably similar to the original.

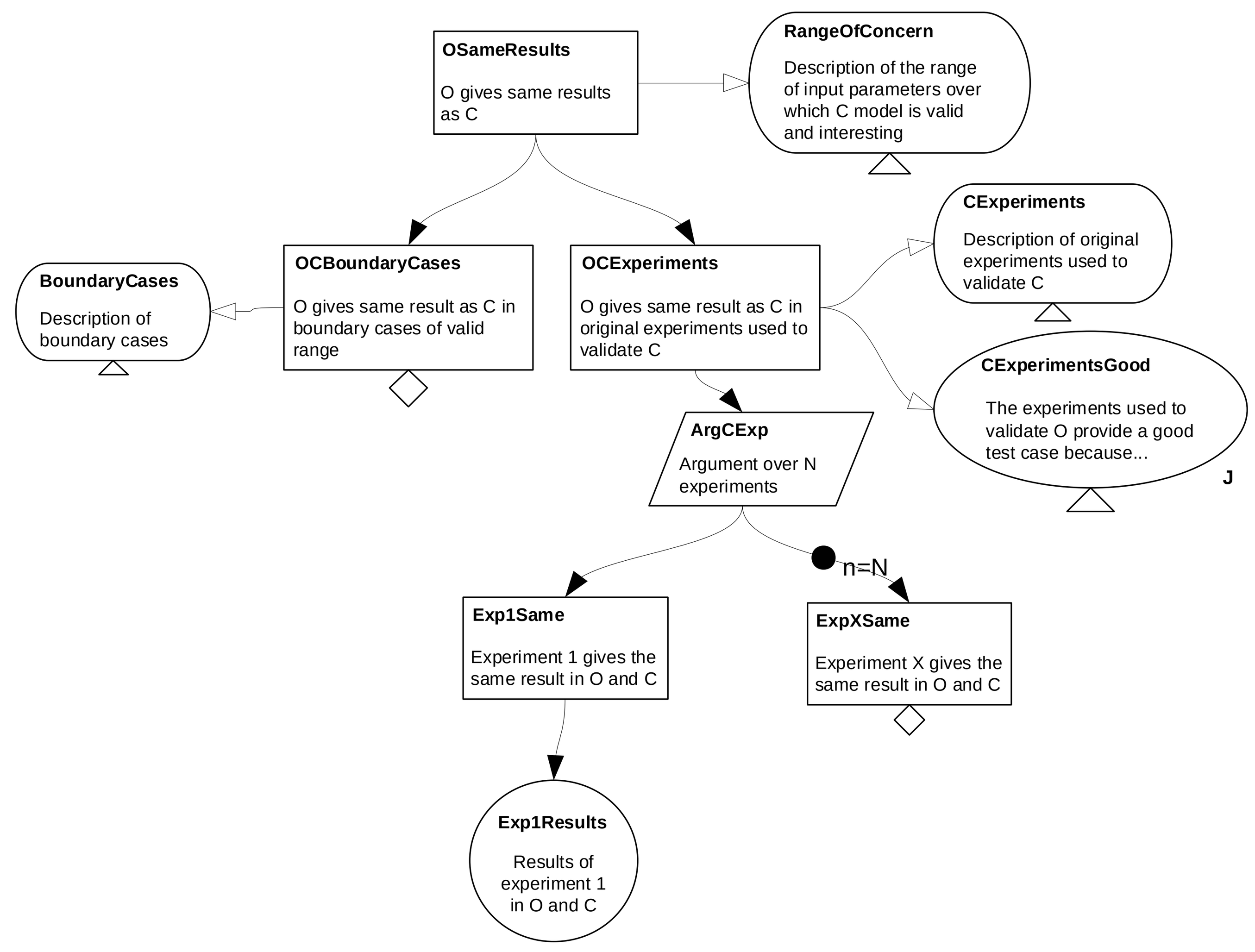
- Create an argument with the purpose of demonstrating equivalence
- Argument needs to be acceptable to the scientist responsible for original simulation

After T. Ghetiu, R. D. Alexander, P. S. Andrews, F. A. C. Polack, and J. Bown, Equivalence Arguments for Complex Systems Simulations, 2nd CoSMoS Workshop, August 2009.

First, agree a possible basis for comparison; define terms; identify scope and limitations:



Work through an argument for each subgoal, recording evidence, rationale . . . e.g. *Results*:



Until scientists and modellers are confident in the new simulation

http://www.cosmos-research.org/ info@cosmos-research.org