In search of sound ‘in silico’ research – validating a complex system simulation

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1. Validation and Safety Critical Systems

In logic, a *valid* argument connects *true* premises to *true* conclusions. Absolute truth values are, however, hard to obtain in our real, context dependent world.

In domains such as Safety Critical Systems , evidence and arguments are used for claiming *adequacy.*

Structuring arguments through notations such as GSN – the Goal Structuring Notation, brings clarity, support of incremental development and reuse.

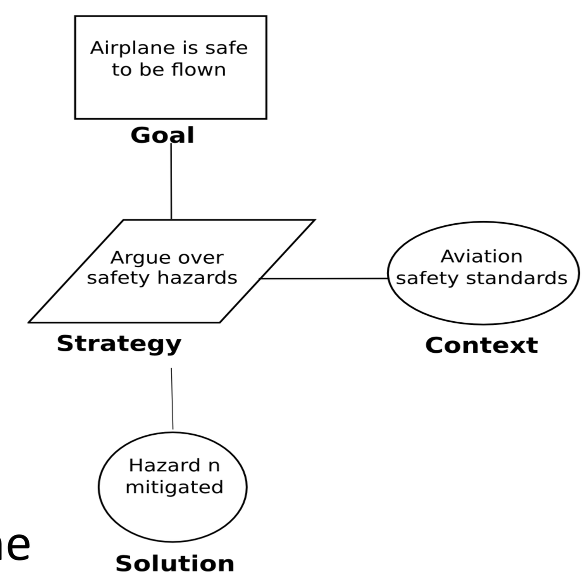

Fig. 1: GSN example

2. ‘In silico’ scientific research

Theories, (software) models and simulations are the foundation of ‘in silico’ research. Each implies making assumptions while filtering away information.

The relevance of results is then… arguable.

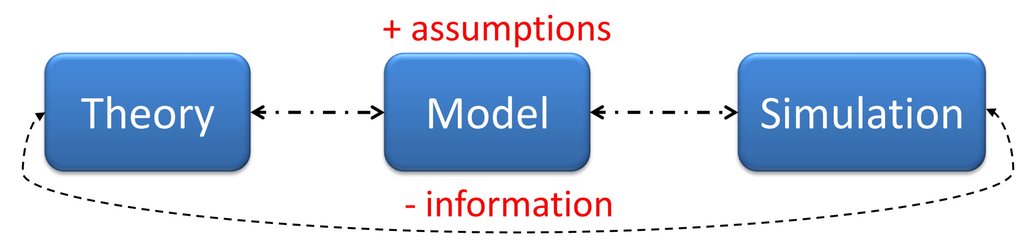

Fig. 2: ‘In silico’ research life-cycle

3. Plant ecology case-study

Bown et al [1] claim their agent-based model generates ecological responses that are *consistent* with field observations and mathematical derivations. Still…

What are the criteria for accepting a claim?

How strong is an argument? Is there guidance for finding weaknesses or improving arguments? Are there argumentation patterns? GSN might have an answer.

In order to replicate results, we obtained the source code of the simulation, ‘cplants’. We constructed also what could have been Bown et al’s GSN argument for the adequacy of their simulation (fig 3-5).

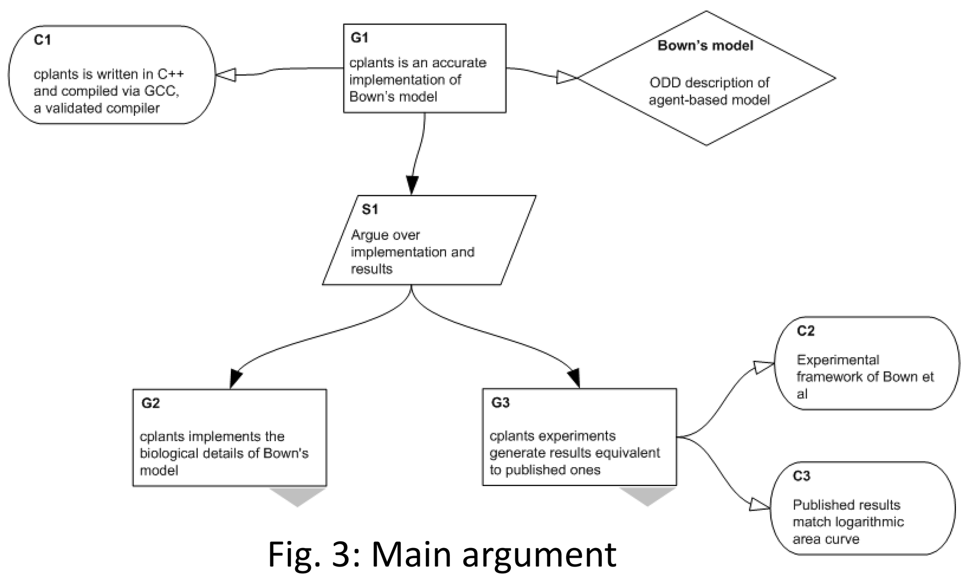

Fig. 3: Main argument

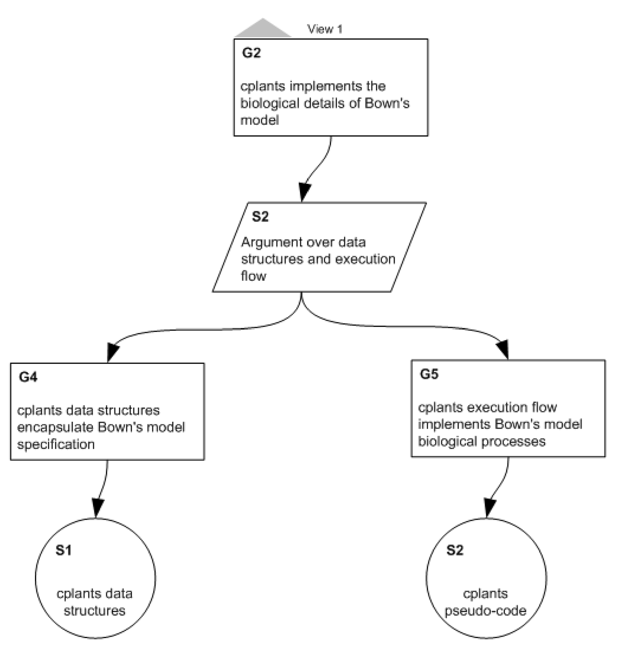

Fig. 4: Argument over implementation

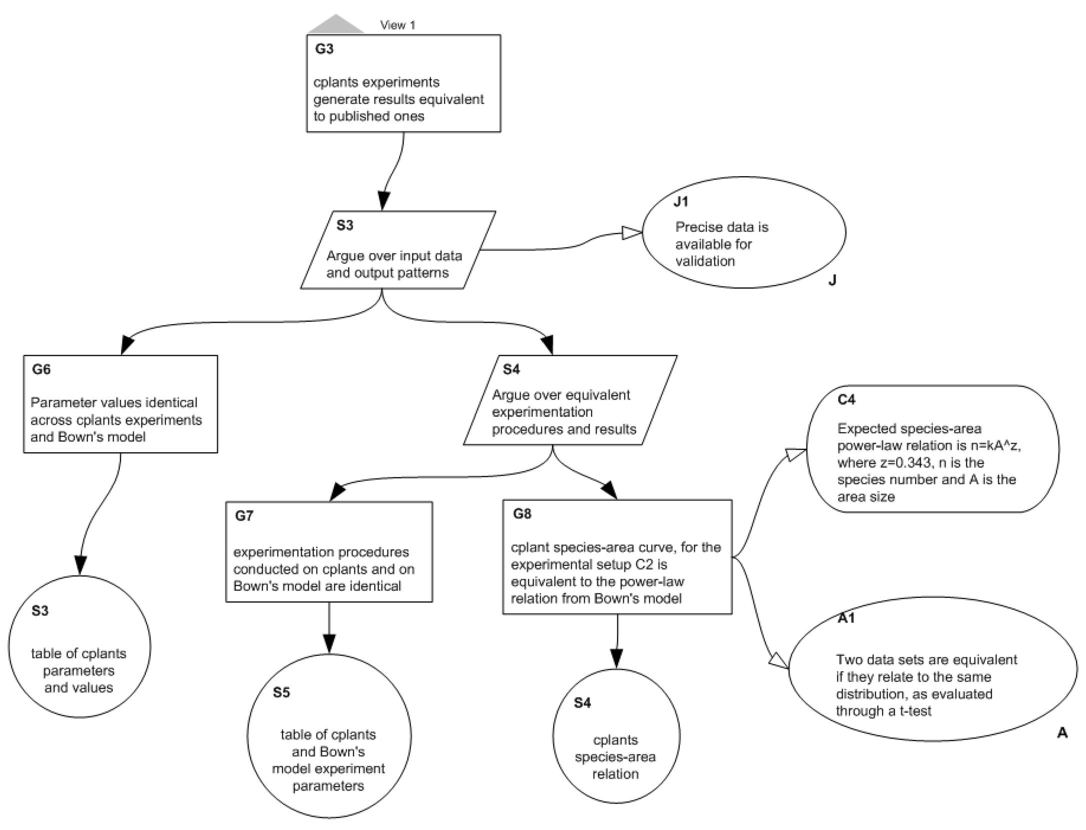

Fig. 5: Argument over results

Each argument element can be challenged. Evaluation of solution S2, for example, showed a discrepancy between the model and the code.

- correcting the code led to unexpected behaviours (fig. 6), although the overall output seemed adequate (fig. 7).
- invalidating Bown et al’s work [1] requires a clear mapping of all their claims. Only then figure 6 can be considered a corner stone.

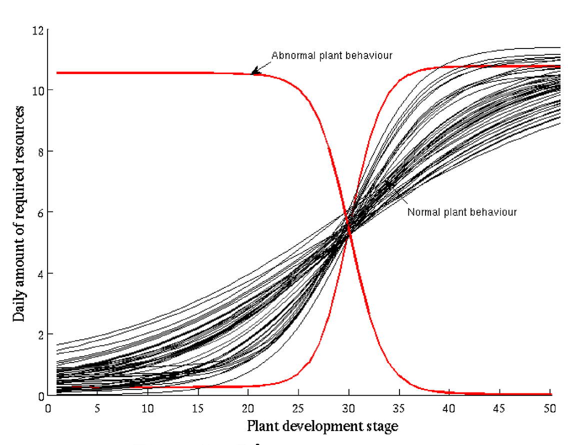

Fig. 6: Plant requirements

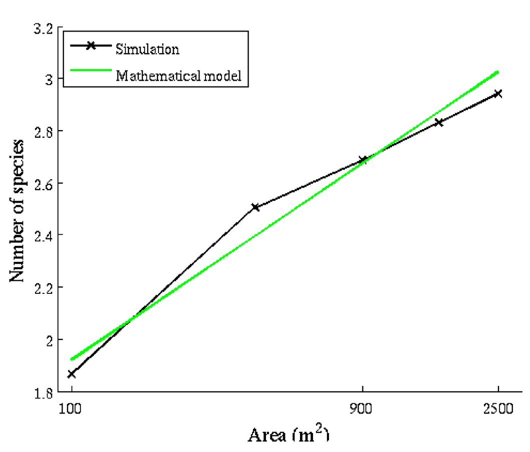

Fig. 7: Simulation outcome

4. The bigger picture

Similar to software testing, scientific validation should be a comprehensive, strategic effort assuring the quality of each phase of research.

Scientific claims are built usually on explicit or implicit sub-claims, addressing different domains. Plurality widens the scope of research, but may also affect its *adequacy.*

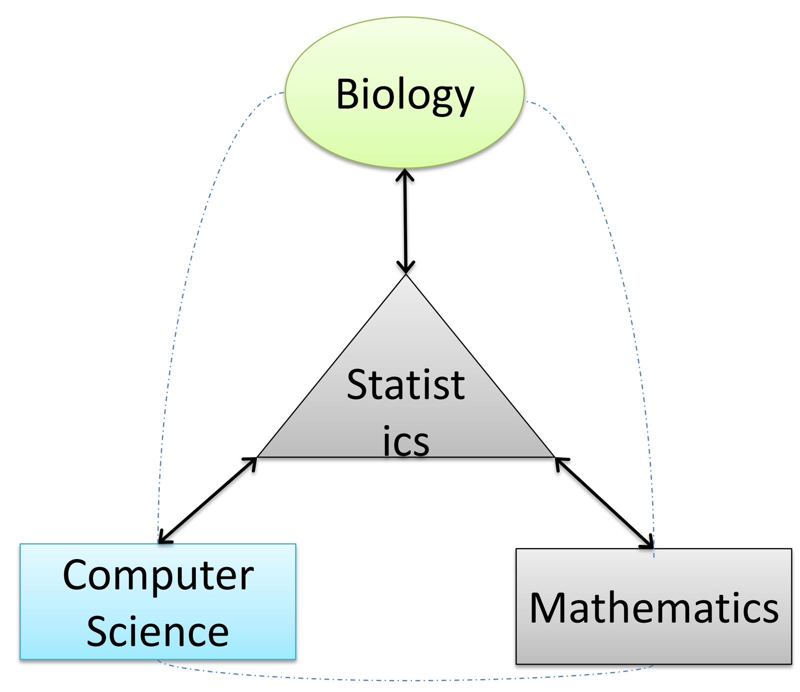

Fig. 8: Scientific loop

In the plant ecology case-study, simulation results are validated against the biology, via statistical methods.

- the validation process should be itself sufficient and `valid’
- if one side of the argument is invalidated, the whole argument may collapse

Observing patterns in the myriad of argument structures could facilitate the creation of a “library of patterns and anti-patterns” for scientific research.

5. Conclusions

- **Safety Critical Systems, ‘in silico’ research and Software Engineering can obtain significant benefits from cooperating**
- **Scientific validation requires competences from all the domains included in the research.**
- **Vague claims are hard to invalidate. Structured arguments facilitate the identification of such weaknesses.**
- **Further efforts need to be invested in validity arguments [2] and their scientific applicability.**

References

[1] J. L. Bown, E. Pachepsky, A. Eberst, U. Bausenwein, P. Millard, G. R.Squire, and J. W. Crawford, “Consequences of intraspecific variationfor the structure and function of ecological communities: Part 1. modeldevelopment and predicted patterns of diversity,” Ecological Modelling,vol. 207, no. 2-4, pp. 264–276, 2007

[2] Ghetiu T. and Alexander, R. and Andrews, P. and Polack, F. and Bown, J., “Equivalence Arguments for Complex Systems Simulations - A Case-Study” in CoSMoS Workshop '09, Luniver Press

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