Engineering Simulations as Scientific Instruments: A Pattern Language

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With Kieran Alden, Paul S. Andrews, James L. Bown, Alastair Droop, Richard B. Greaves, Mark Read, Adam T. Sampson, Jon Timmis, Alan F.T. Winfield

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Preface

Computer-based simulation is a key tool in many fields of scientific research. *In silico* experiments can be used to explore and understand complex processes, to guide and complement *in vitro* and *in vivo* experiments, to suggest new hypotheses to investigate, and to predict results where experiments are infeasible. Simulation is an attractive, accessible tool: producing new simulations of simple systems is relatively easy. But it is also a dangerous one: simulations (and their underlying models) are often complex, buggy, and difficult to relate to the real world system.

A recent UK Government report on computational modelling ([95], condensed as [44]) makes several recommendations, including

> Decision-makers need to be intelligent customers for models, and those that supply models should provide appropriate guidance to model users to support proper use and interpretation. This includes providing suitable model documentation detailing model purpose, assumptions, sensitivities, and limitations, and evidence of appropriate quality assurance.

In this book we describe the CoSMoS (Complex Systems Modelling and Simulation) approach, a pattern-based approach to engineering trustworthy simulations: simulations that are both scientifically useful to the researcher, and scientifically credible to third parties. The CoSMoS approach emphasises three key aspects to this development of a *simulation as a scientific instrument*: the use of *models* to capture the scientific domain and the simulation platform; the use of *arguments* to provide evidence that the scientific instrument is fit for purpose; and the *close co-working* of domain scientists and simulation software engineers.

The CoSMoS approach is generic: it does not mandate a particular modelling technique, a particular implementation language, or a particular real world application domain. What it does mandate is the careful and struc-

tured use of models and arguments, to ensure that the simulation is both well-engineered, and seen to be well-engineered.

The book is useful for domain scientists who wish to see what is needed to build and use scientifically credible simulations, and for software engineers who wish to build scientific simulations that are useful and usable. The examples in the book focus mainly on biological simulations, to exploit the specific experience of the authors, but the CoSMoS approach is not restricted to this domain. The approach we describe is also useful for building simulations as part of the process of building engineered systems. There are some differences between scientific simulation (crudely, simulating the world as it is) and engineering design simulation (simulating the world as we wish it to be), but much of the approach is common. These differences are noted when they occur.

What this book is not

This is not a book about software engineering. Where we advocate particular software engineering approaches and good practices for building simulations, we mention them in the endnotes[1] and refer to standard literature discussing them.

Neither is this a book about specific modelling approaches or notations[2], whether mathematical, computational, or otherwise. Again, there is much excellent literature available on specific modelling techniques, to which we refer.

Nor is it a book about experimental methods, although the simulations are used to perform (numerical, virtual) experiments in a way analogous to real world experiments.

Nor is it a book about developing bio-inspired algorithms (which are abstractions of biology, but not simulations of biology).

What this book is

This is a book about how to combine well-established approaches in a manner that leads to a robust and argued-trustworthy simulation: how to combine modelling to build an appropriate scientific instrument, software engineering to build the instrument appropriately, and experimental techniques to use the instrument appropriately for scientific investigation.

Part I provides a managerial overview: the rationale for and benefits of using the CoSMoS approach, and a small worked example to demonstrate the approach in action.

Part II is a catalogue of the core CoSMoS patterns. Start your project at the CoSMoS Simulation Project (92) pattern, and follow the guidance, using the other referenced patterns as your specific context demands. The development and use of a simulation as a scientific instrument will probably include most of these core patterns.

Part III is a catalogue of "helper" patterns. These are more specific patterns of use only in certain domains, for certain purposes, or with certain modelling and implementation approaches. Use of these is not required to develop a CoSMoS simulation, but they provide possible routes for doing so.

Part IV documents CellBranch, a substantial case study developed using the CoSMoS approach.

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A list of CoSMoS publications and associated tools is available in the endnotes[3].

The York Computational Immunology Lab (YCIL) is using CoSMoS for many of its projects. It has made extensive material available, including simulations, simulation analysis tools, and fitness-for-purpose argumentation tools, available at www.york.ac.uk/computational-immunology/software/.

The author team have made substantial and various contributions to the CoSMoS project, to the CellBranch project, to YCIL projects, and during all stages of the development of this book. In addition to their overall work on the structure, writing, and editing of this book, they have had the following specific roles on the projects, and, as far as can be determined from such a joint effort, have made the following specific contributions to the book:

- Susan Stepney (Principal Investigator of CoSMoS and CellBranch): developer of the detailed pattern language structure

- Fiona Polack (Co-Investigator of CoSMoS): developer of the detailed argumentation pattern suite
- Kieran Alden (Research Associate applying CoSMoS in YCIL): contributor to Calibration and Sensitivity Analysis patterns
- Paul Andrews (Research Associate on CoSMoS): developer of the initial CoSMoS philosophy, process, phases, and high-level models: contributor to Chapter 1
- James Bown (advisory member of CoSMoS): contributor to Chapter 2
- Alastair Droop (owner of the AlKan worked example in Chapter 3): contributor to Chapter 3
- Richard Greaves (Research Associate on CellBranch): developer of Part IV
- Mark Read (then PhD student applying CoSMoS in YCIL): contributor to Calibration and Sensitivity Analysis patterns
- Adam Sampson (Research Associate on CoSMoS): contributor to documentation and real world patterns
- Jon Timmis (Co-Investigator of CoSMoS; applying CoSMoS in YCIL): contributor to Chapter 1
- Alan Winfield (advisory member of CoSMoS): contributor to Chapter 2, embodied simulation pattern, and several antipatterns

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