

# Engineering Concurrent Simulations of Complex Systems

## Designing Useful Simulations

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# *CoSMoS: Complex systems modelling and simulation infrastructure*

- Multi-site complex systems project to:
  - ▶ build capacity in generic modelling tools and simulation techniques
  - ▶ support modelling, analysis and prediction
  - ▶ help design and validate simulations of complex systems
  
- Focus on agent-based systems and concurrent process-oriented programming

CoSMoS partners: Computer Science, University of York; Computing Laboratory, University of Kent

CoSMoS collaborators: Jim Bown, University of Abertay; Alan Winfield, University of the West of England

See also the next two presentations, relating to implementation aspects



# Complex systems simulation

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

- To support scientific investigation
  - ▶ Can we capture enough reality to do experiments *in silico*
- To support a dependability argument
  - ▶ How does a human-scale system behave
- When is a simulation valid?
  - ▶ When it looks ok?
  - ▶ When it produces the right results?
  - ▶ When its internals are like the real system?
- The answer depends on the purpose
- Here, we want to support scientific investigation
  - ▶ Acceptable results from adequately equivalent processes
- Understanding of **assumptions** is vital



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# Our inspiration . . .

## High-integrity and dependable systems engineering

- For example, design, analysis and certification of safety critical systems
  - ▶ Well-researched area, with industrial application
  - ▶ Guiding principle to show that quality goals are met
    - ▶ That risk is *as low as reasonably practicable*
  - ▶ Depends on understanding and controlling emergent behaviours or properties
    - ▶ Risk mitigation
- Safety cases based on the reasoned acceptability of evidence

Also Reactive Animation from the group led by Cohen and Harel:

- Similar approach, using state charts to model agents and interaction, reasoned evidence, etc., but . . .
  - ▶ More sophisticated modelling
  - ▶ Different target implementation
  - ▶ Sophisticated (proprietary) platform and applications



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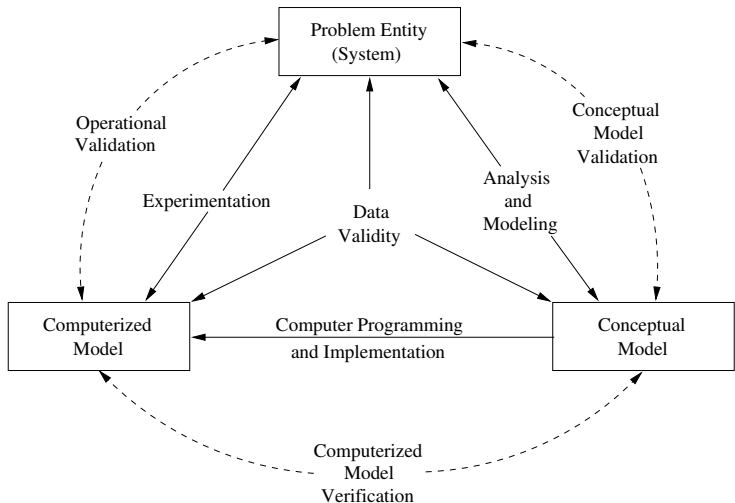
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# Dependable systems and validity

## Sargent's lifecycle model for conventional computer simulation



# Verification and Validation

Verification: traditional software engineering:

- Continuity between models and code
  - ▶ Minimise design decisions, semantic gap
- Consistency across views
- For process-oriented programming, state transition models capture most relevant detail

Validation:

- Traceability from problem entity to concepts to code
- Justification and recording of abstractions, simplifications
- Systematic analysis of justifications
- Presentation of a clearly argued statement of how and to what extent we model the reality

For example, the lymphocyte capture models . . .



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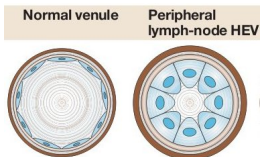
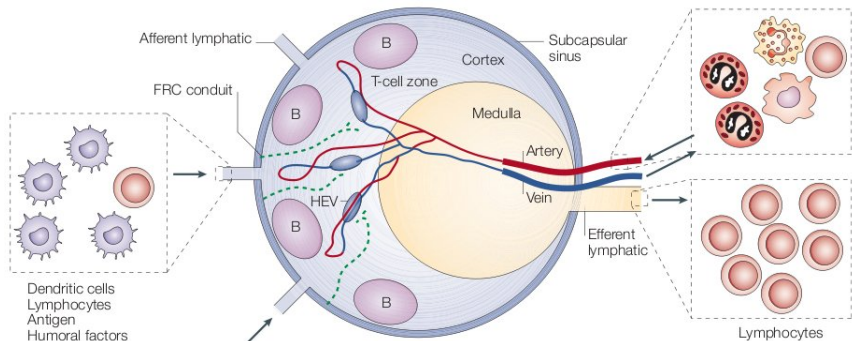
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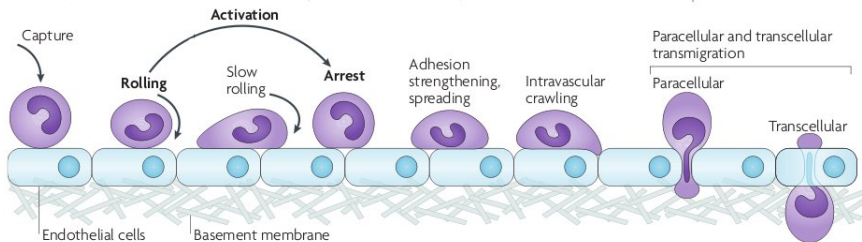
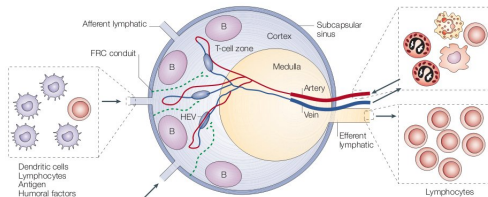
# Biological understanding and abstraction

York Centre for Immunology and Infection



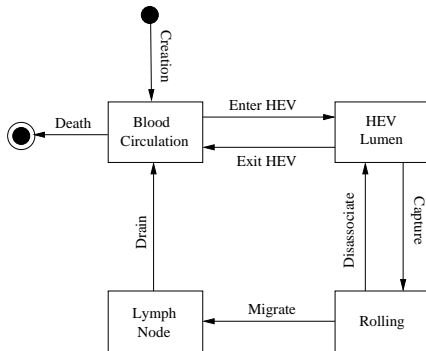
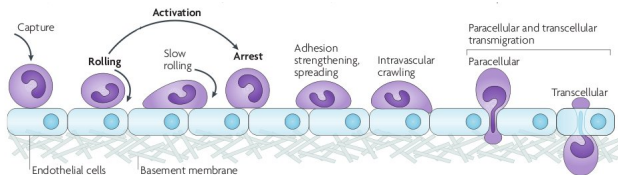
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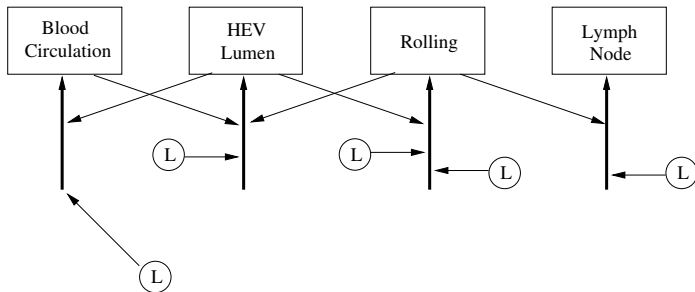
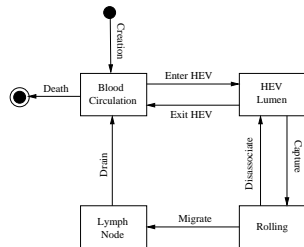


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# Abstracting from biological to a process model



# Conceptual model to program design (occam- $\pi$ )



# Realisation

- Two implementations constructed from the same design diagram
  - ▶ parallel, process-oriented programs in *occam- $\pi$*
  - ▶ Processes represent lymphocytes and states
  - ▶ Channel structure allows lymphocytes to move their association between states
  - ▶ Transitions based on rate distributions from biological experiments
- First simulation just runs processes over time, to produce transfer rates
- Second simulation introduces visualisation and thus space
  - ▶ HEV represented as a tube
  - ▶ Lymphocyte can be captured if in contact with tube
  - ▶ Rolling and migration transitions use experimental rates



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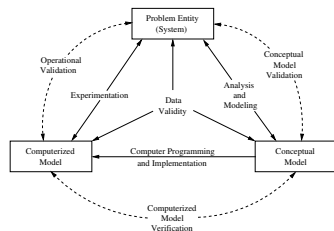
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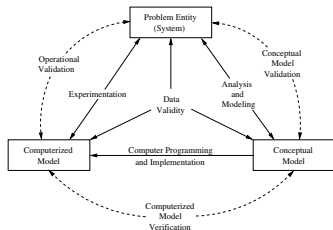


# Conceptual model validation: experts check our model



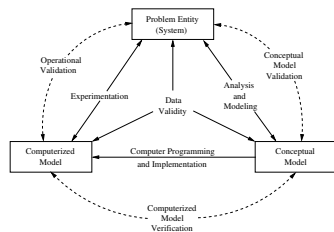
- Conceptual model must address purpose
- Systematically record design decisions and assumptions:
  - ▶ Abstractions are acceptable to CII, eg:
    - ▶ We do not need to look at biochemistry
    - ▶ All lymphocytes are functionally equivalent, etc.
  - ▶ Assumptions are acceptable to CII, eg:
    - ▶ CII probabilities are constant over time, etc

# Validate computer model: First simulation



- Non-visual implementation
  - ▶ Given input rates, do output rates correspond to experimental evidence?
- CII accepted abstractions and assumptions
  - ▶ and we are happy with the model as engineers . . .
- Results meet CII expectations
  - ▶ Basis for further experimentation

# Validate computer model: Second, visual, simulation



- Implementation using spatial representation of HEV and membrane, with moving lymphocytes
  - ▶ Still implements the conceptual model
- Lymphocyte that touches membrane can be captured
  - ▶ CII accepted abstractions and assumptions
  - ▶ And they really like the pictures . . .
- BUT . . .

# Validation issues arising from the visual simulation

- Transition rates are from experimental data
  - ▶ Experimental rates are point observations of populations
  - ▶ Cannot observe or quantify capture at the level of individual lymphocytes
- Rates may not be appropriate to the visual simulation
  - ▶ By introducing spatial location of individual lymphocytes, the simulation has diverged from the scientific basis of the data
- Is the simulation still a valid model?
  - ▶ Needs careful analysis and discussion of assumptions with CII experts
  - ▶ Recorded design decisions and assumptions are the starting point for analysis



# Comments on validation

- Validation does not give an absolute guarantee
  - ▶ Arguing validity exposes misinterpretation, omission . . .
  - ▶ Reviewing validity argument with experts helps simulators and experts to gain confidence
    - ▶ Even if both sides sometimes overlook “errors”
  - ▶ Even a flawed simulation can help if the scientists understand how it is flawed
- Argument construction depends on evidence
  - ▶ Challenging assumptions and decisions
    - ▶ Systematic approaches such as flaw hypothesis, deviational analysis, exist in dependable systems practice and research
  - ▶ Recording sources, justifications, rationale
    - ▶ Use argumentation techniques and visualisations

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# Where next?

- CoSMoS is working on more case studies
  - ▶ Plant modelling, swarm robotics, several other aspects of immunology
  - ▶ Other complex systems studies at York are using the early outputs of CoSMoS
- Working on modelling, validation arguments, evidence
  - ▶ See CoSMoS workshops, September 08 and August 09
- Platform improvement is needed
  - ▶ Patterns, tools, guidance
  - ▶ Systematic, repeatable approaches
- There is more discussion of these in the paper ...



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