Linking scales: simulation and visualisation

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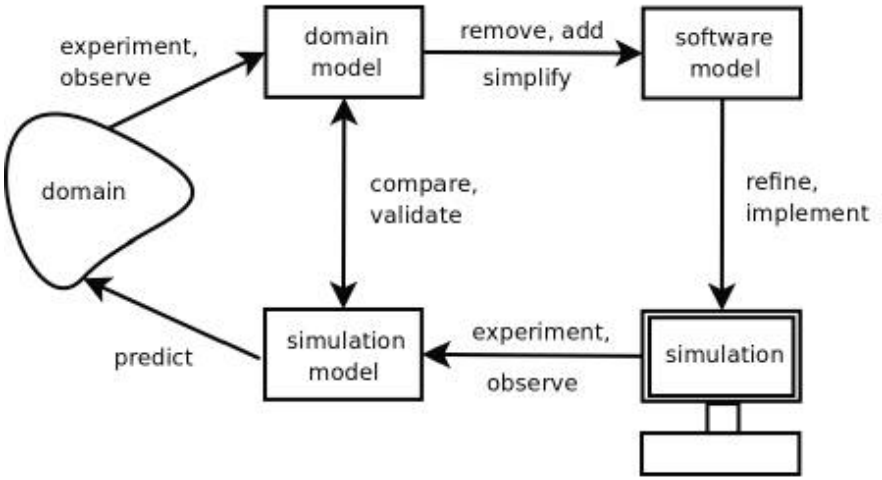
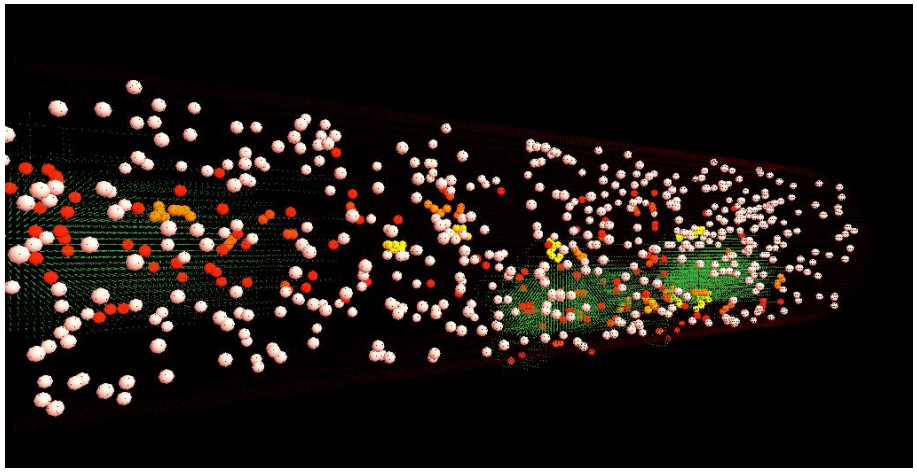
Context

- Simulation as a scientific instrument
- Engineering in-silico experiments
- The problems of multi-scale systems
- Making a simulation useful in practice





Multiple scales

- **Space**
  - physical or state or phenotype or ...
  - different sizes; hierarchies
  - different kinds of spacial connectivity
- **Time**
  - different rates of change
  - different temporal resolutions

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Multiple scales

- **Uncertainty**
  - the things we can't measure accurately
  - the things we can't measure reproducibly
  - the things we can't measure *at all*

CRISP's application: cancer

- Enormously complex biological systems
- Simulation for drug discovery, personalised drugs
  - Justifiable complexity
- **Multiple physical scales:**
  molecule, cell, growth, organ, body
- **Multiple temporal scales:**
  milliseconds, hours, lifetimes
- **Multiple degrees of uncertainty:**
  competing models, individuals differ, wet-lab experimentation difficult and expensive, hard to get many time points

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The scaling-up problem

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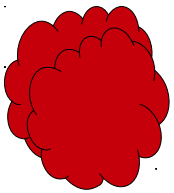

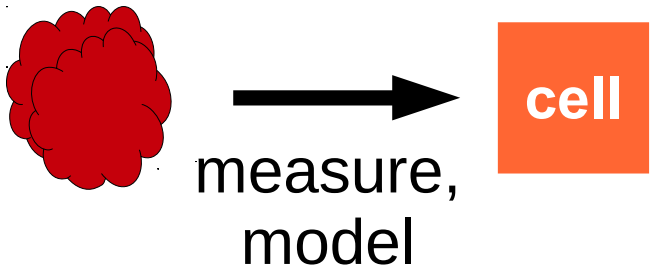
measure,
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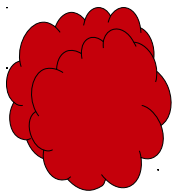

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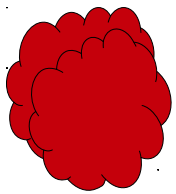

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not practical:
insufficient
computational
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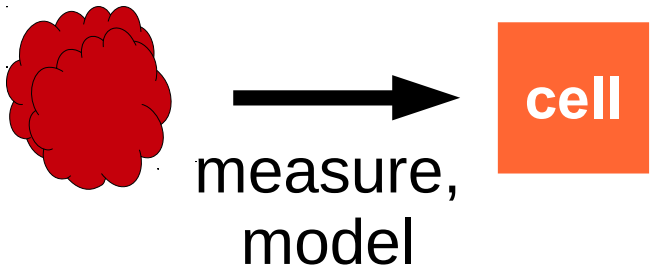
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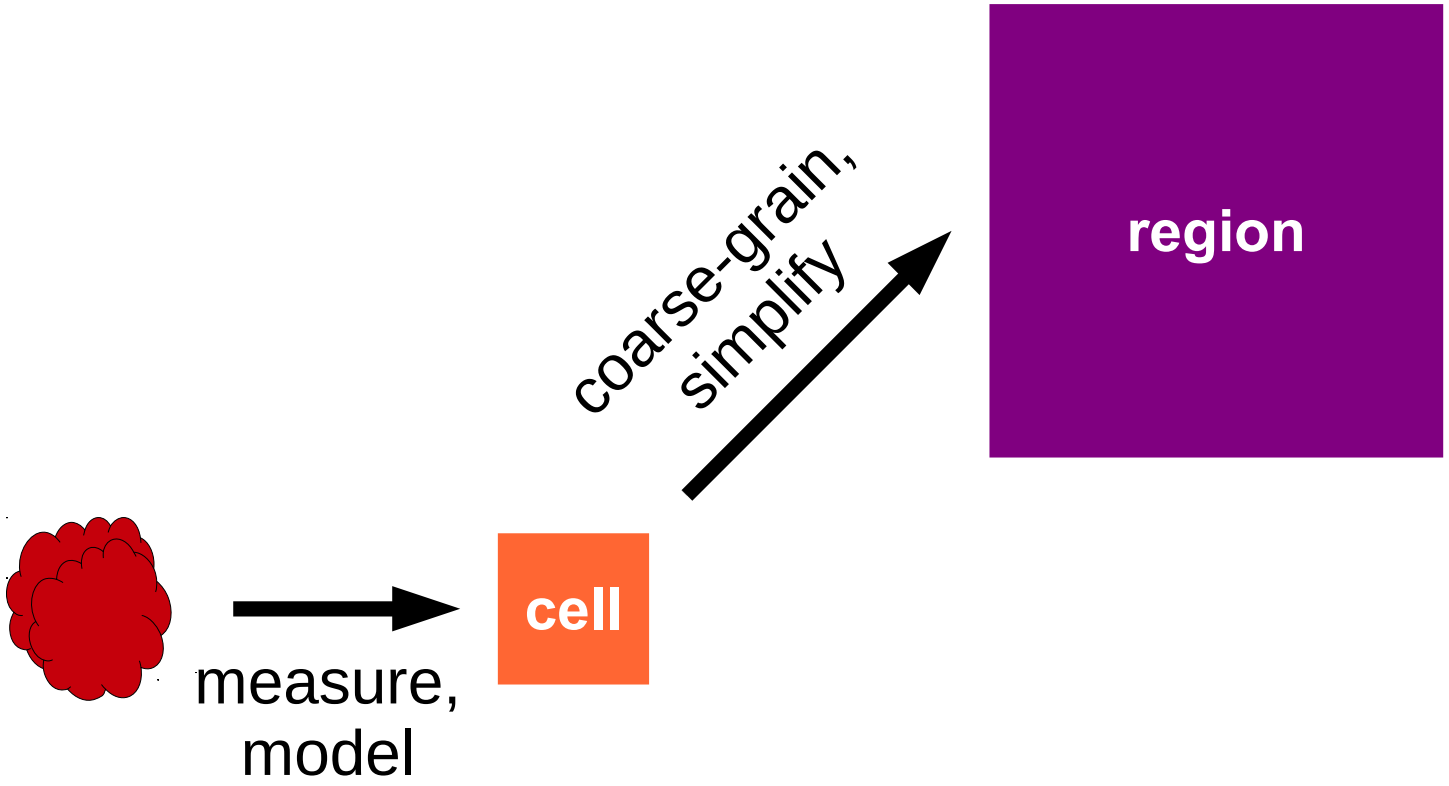
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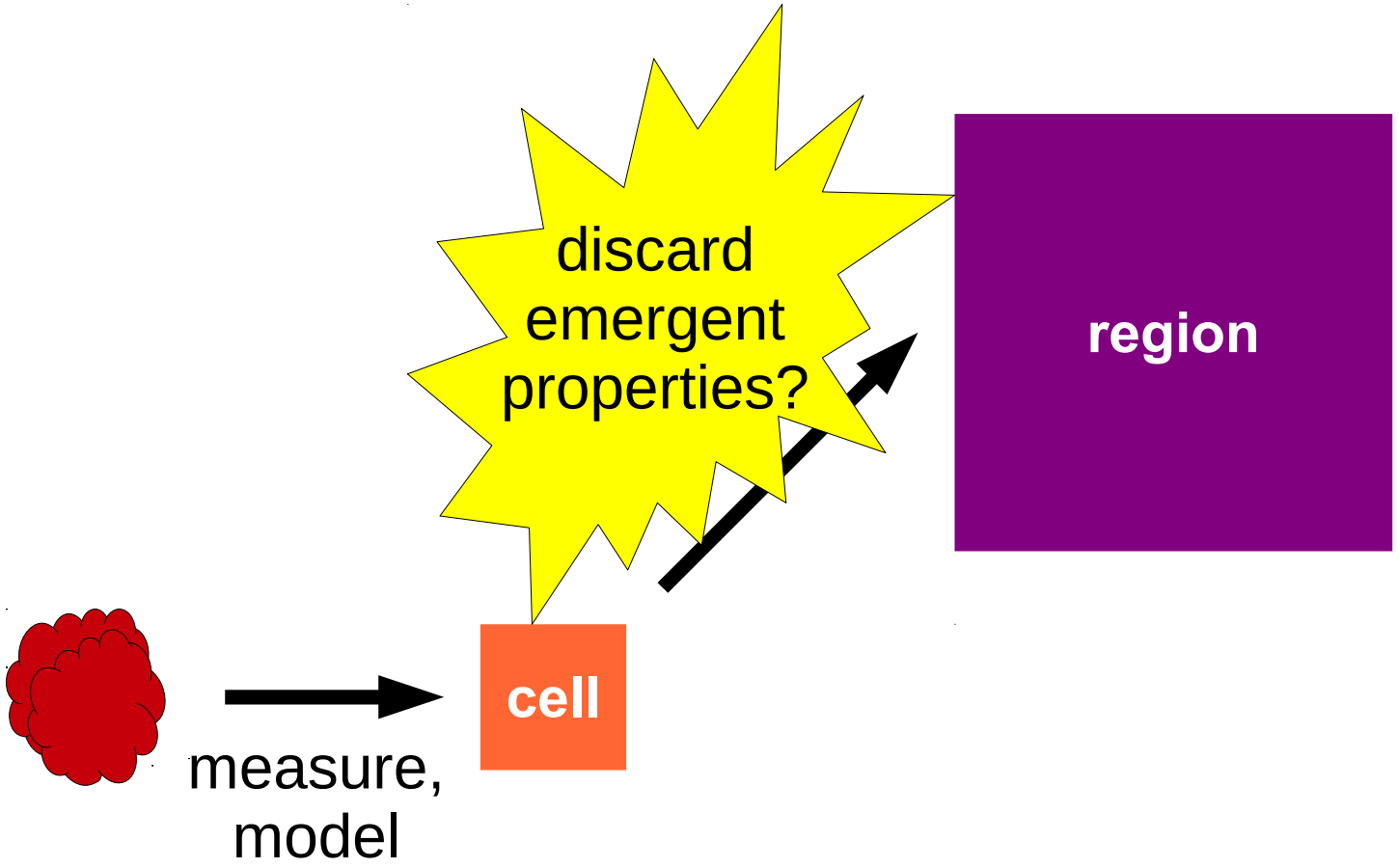
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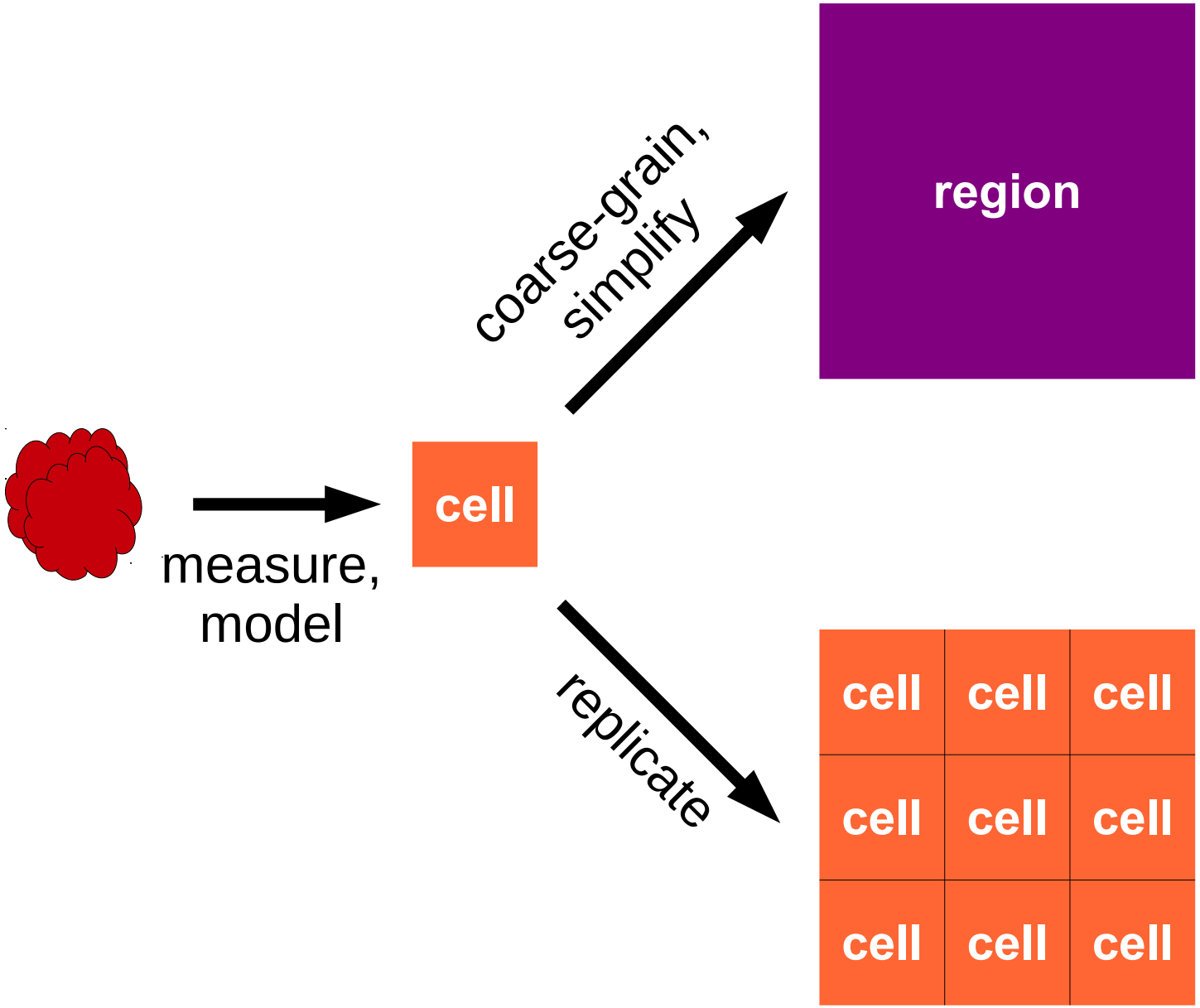
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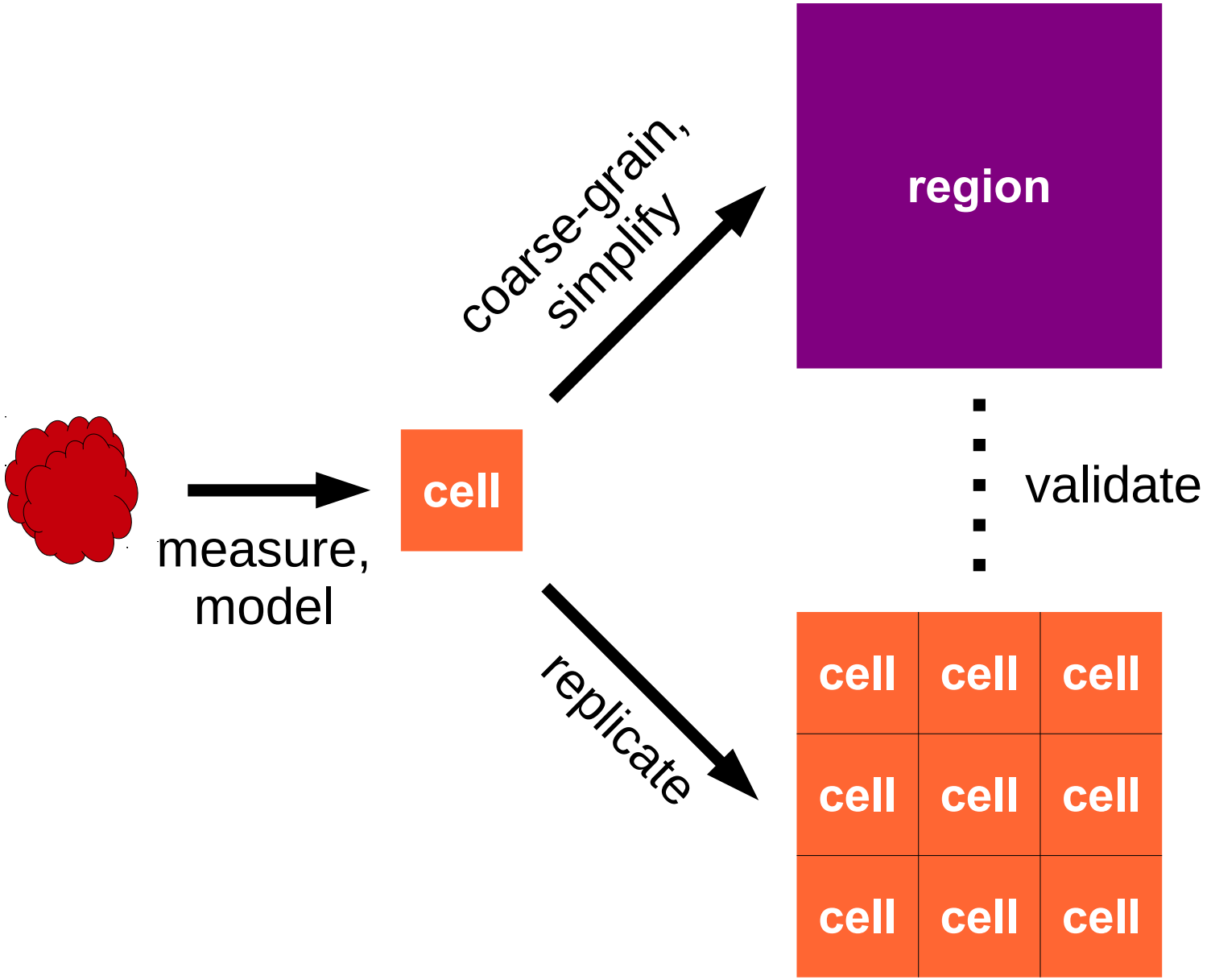
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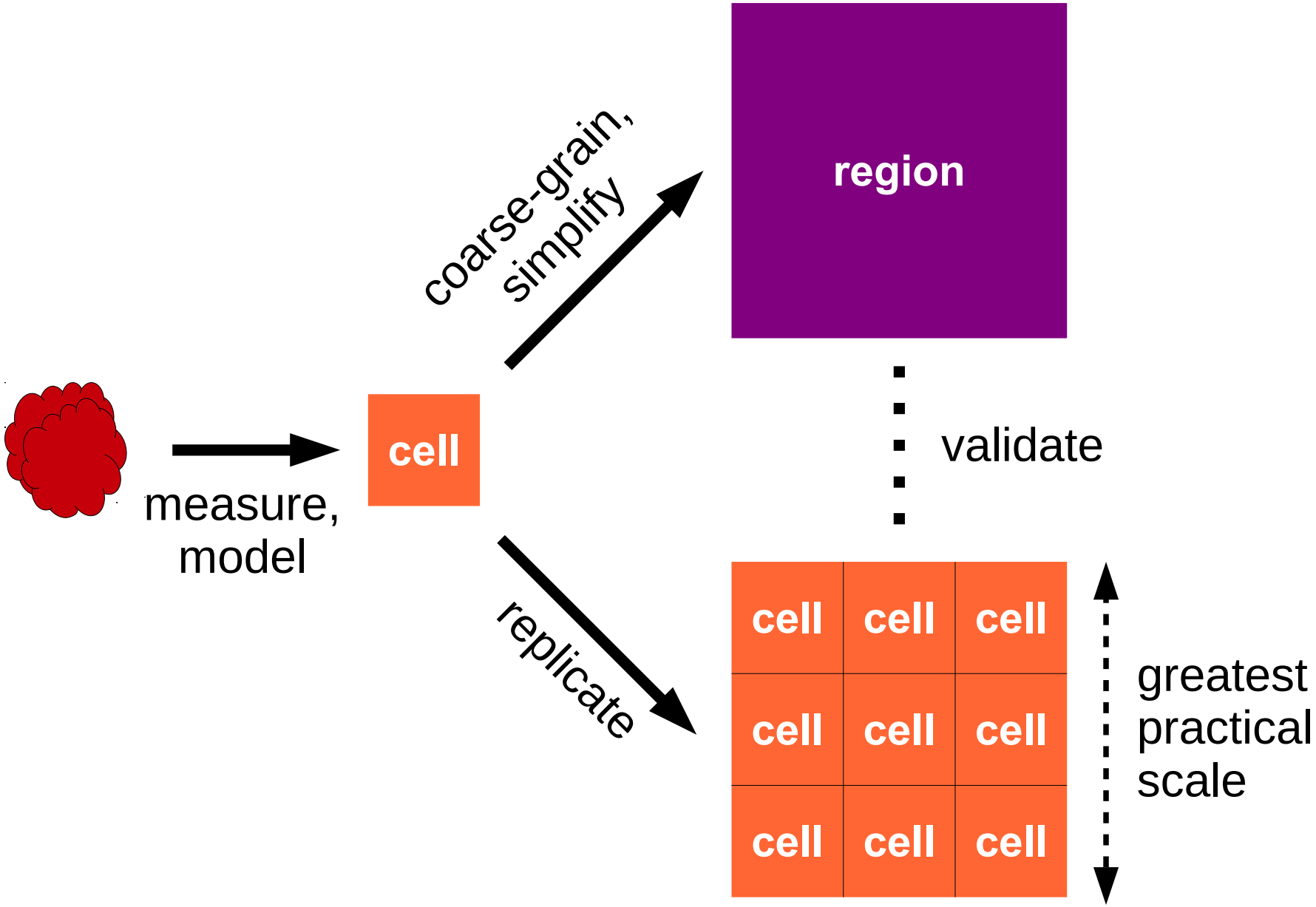
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greatest
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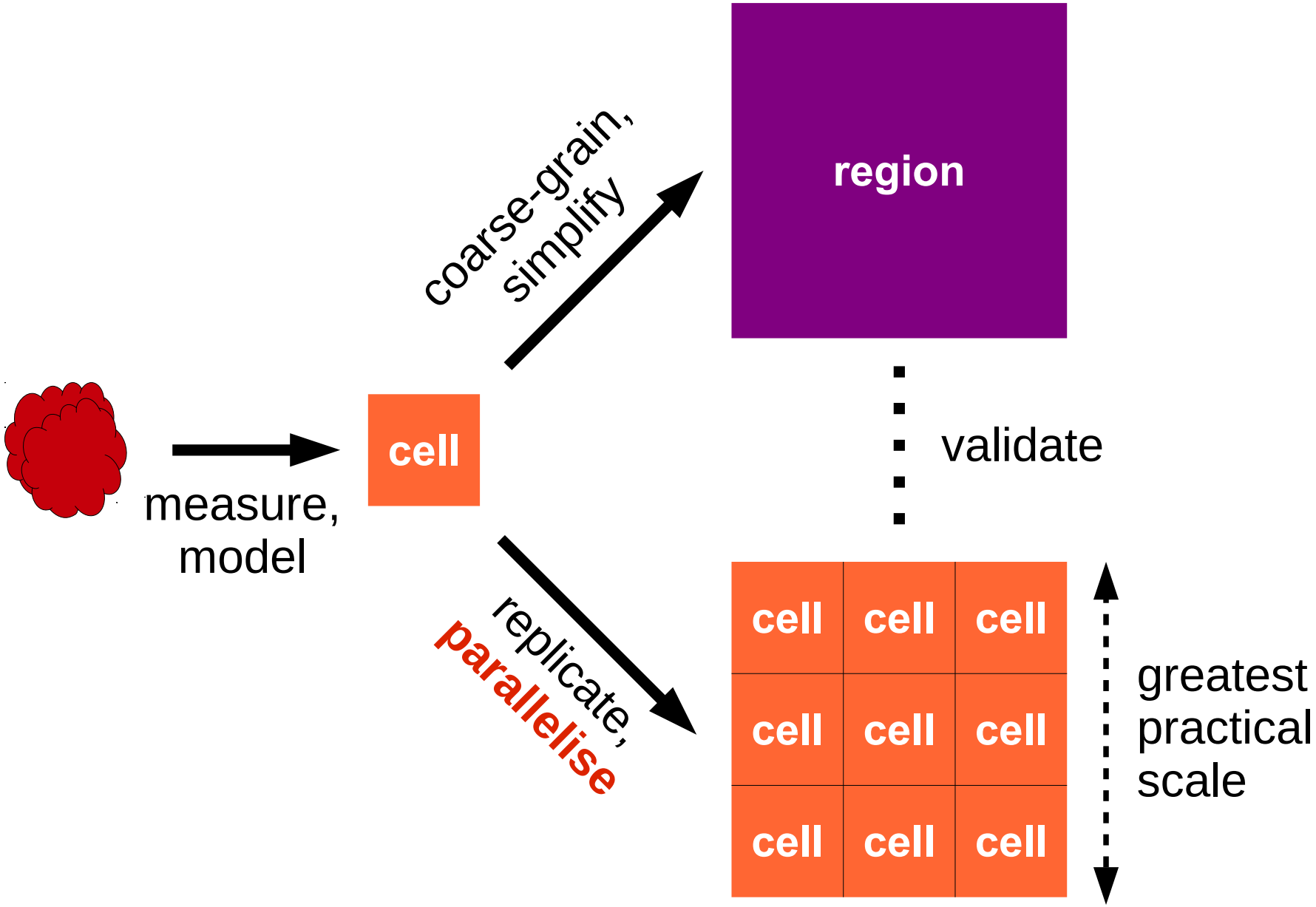
scale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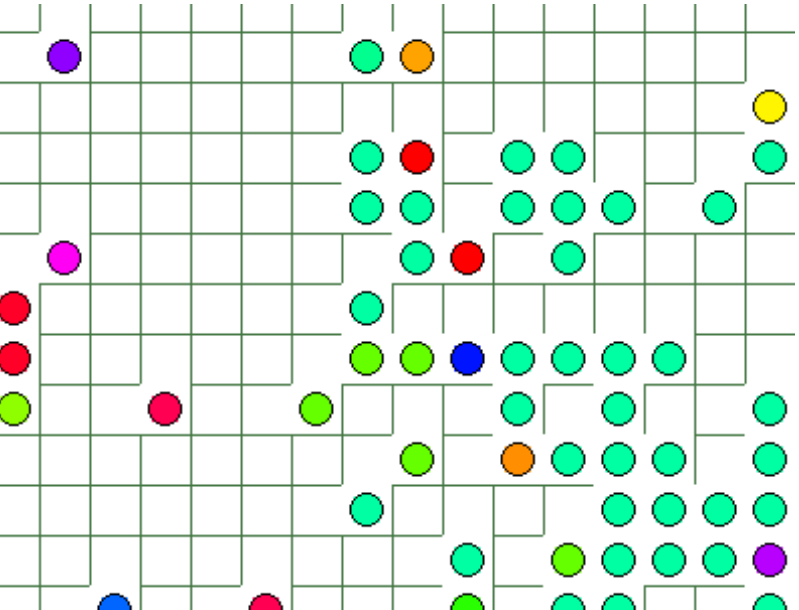
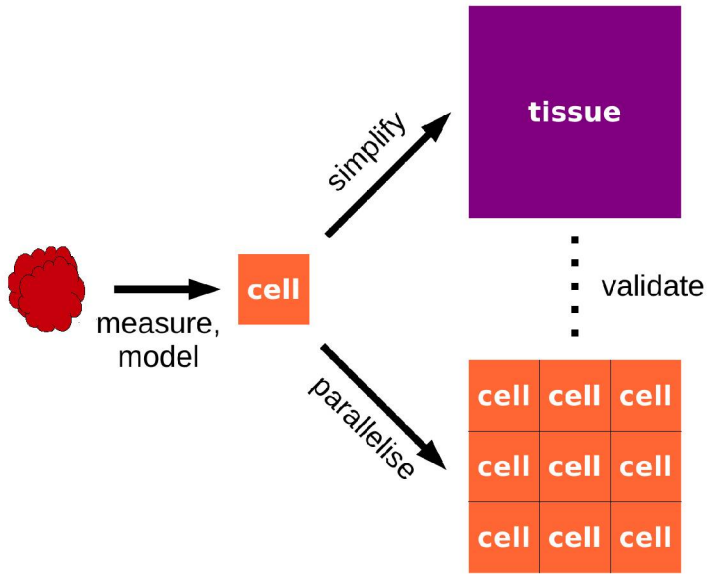
scale

The problems of simulation

- **Scalability**: we must be able to handle realistically large simulation volumes
  - Use **concurrent** software engineering techniques to exploit parallel and distributed hardware
  - Use **cross-scale validation** to build simplified higher-level models that capture the necessary characteristics from the lower level





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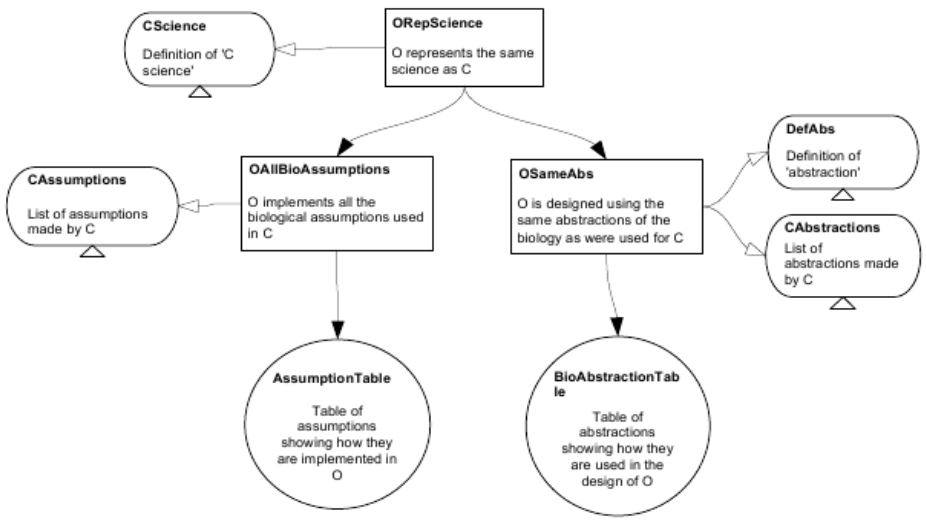
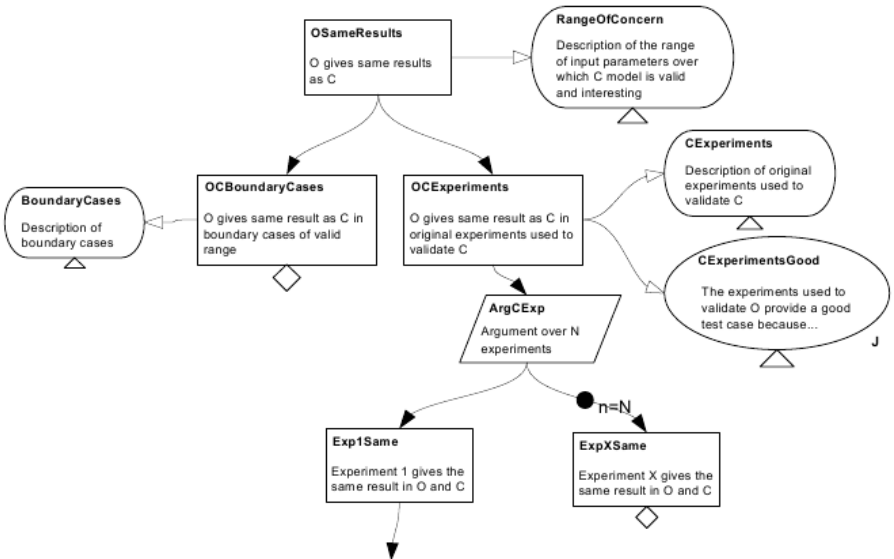
The problems of simulation

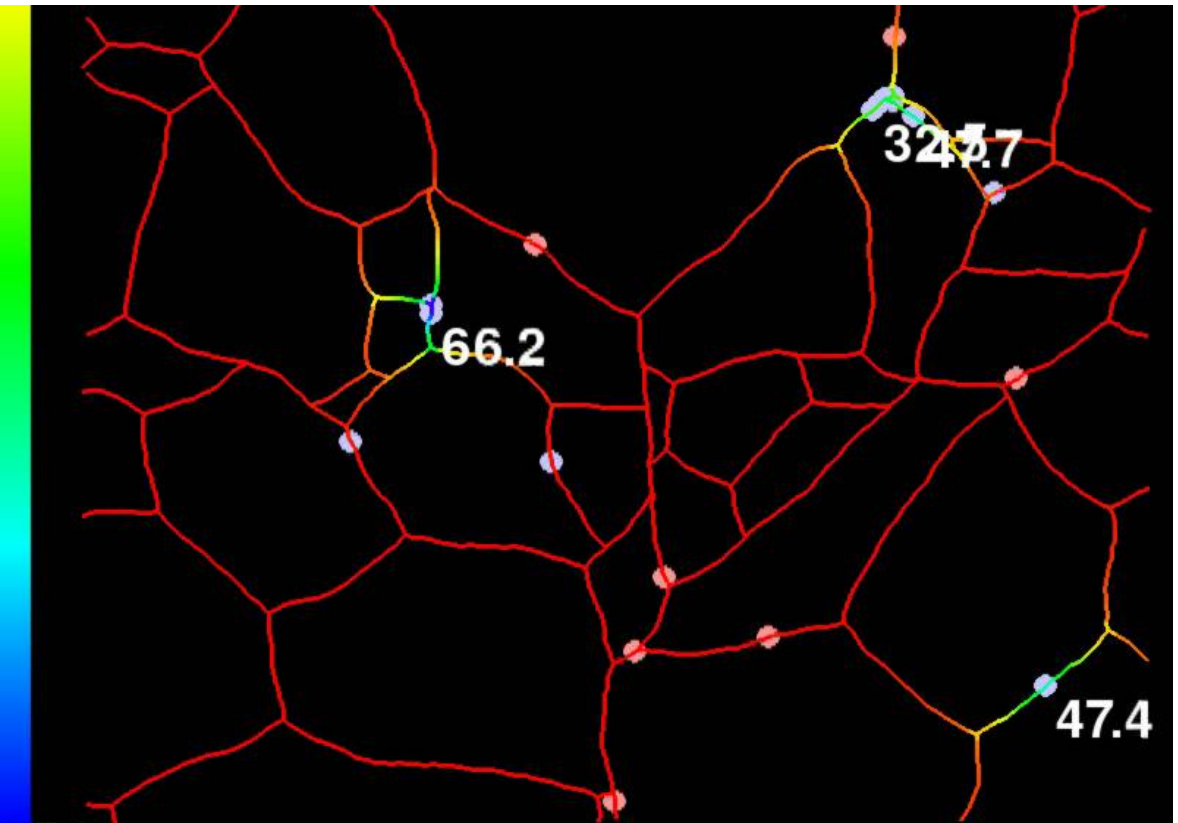
- **Trust**: need confidence that we've designed and implemented our simulation correctly
  - Standard software engineering: configuration management, code reuse, design patterns, testing, output validation – and **argumentation** to tie it all together into a convincing argument

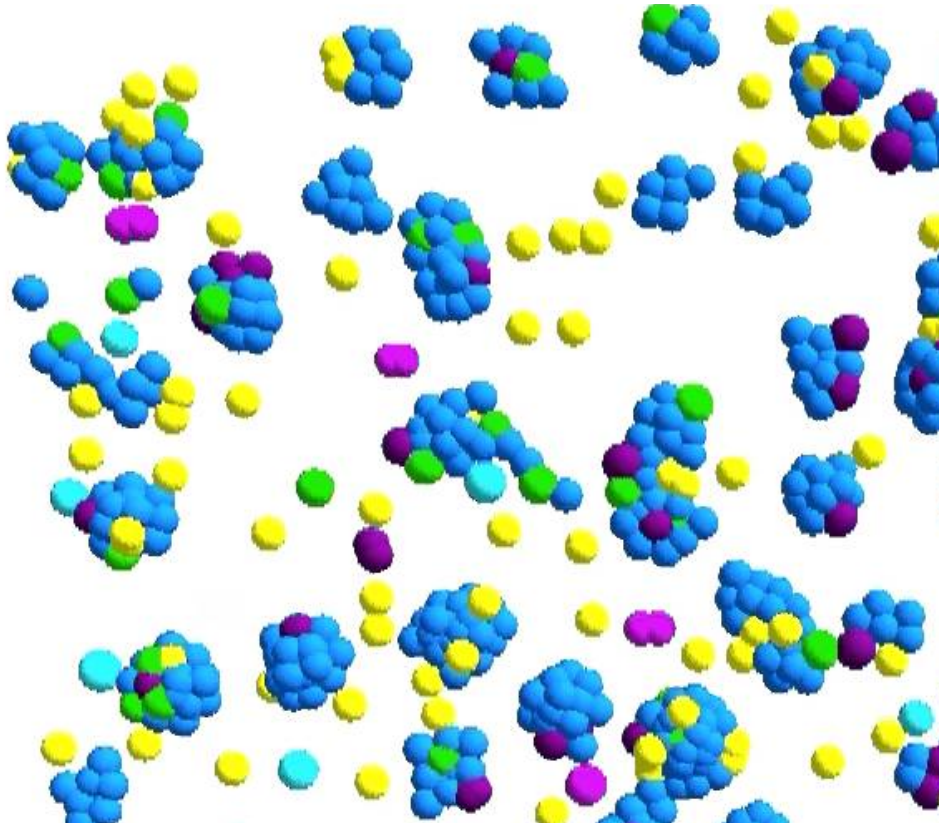




The problems of simulation

- **Comprehensibility**: experimenters must be able to set up experiments – and understand what the simulation is telling them
  - For this, you need effective **visualisation**





Visual analytics

- Need to understand the **biology** and the **psychology** of how we interpret information
- Design patterns – an **engineering** approach
- Use existing visual languages – but don't mislead
- Can quantify the effectiveness of visualisation and interaction designs
  - eye-tracking, stress measurement, biofeedback...

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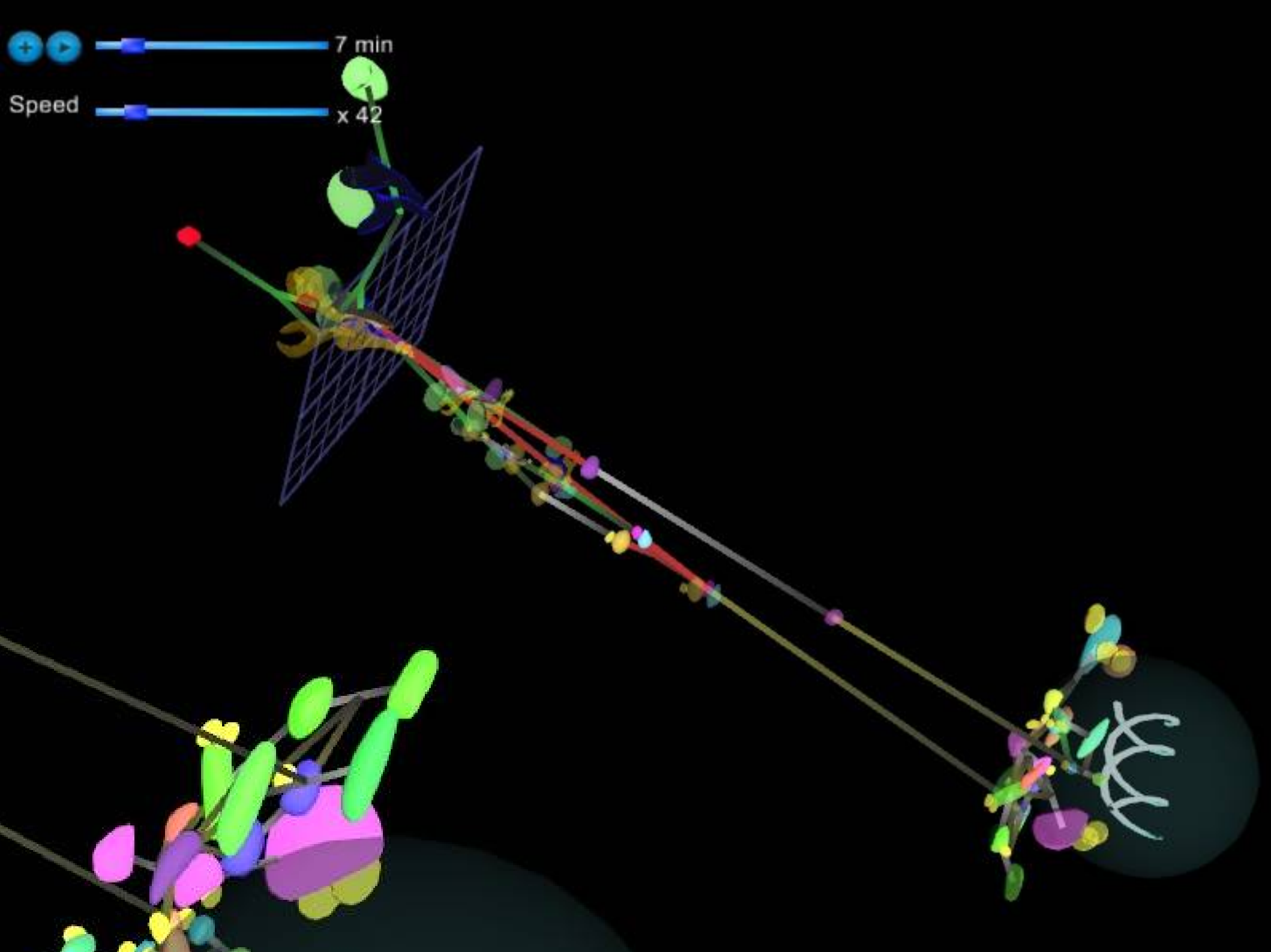
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The visualisation process

- Determine visualisation techniques for the interesting facets of the model
- Convey multiple data dimensions
  - 3D, immersive 3D, audio, haptic feedback...
  - Subtle effects, e.g. motion blur, cueing
- Unconventional views can be effective
  - e.g. Andy's Napoleon diagrams
- How do you convey uncertainty?

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Interaction

- “What happens if I...”
  - “... look at it this way?”
  - “... change this?”
  - “... **do** this?” (participatory simulation)
- Specialised interaction design
  - Lots of work on this for medical data
- Managing interaction latency
  - Not batch simulation any more
  - Harder in the cloud – but this is changing
- Managing (limited) reproducibility

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Visualisation for the modeller

- Adds complexity to the (platform) model
- May require more or different data for effective visualisation
  - or different views/queries on the existing data – change your data model?
- May introduce more scales
  - bird's-eye view, time-lapse
- May change the nature of reality
  - time travel: rewind, try again

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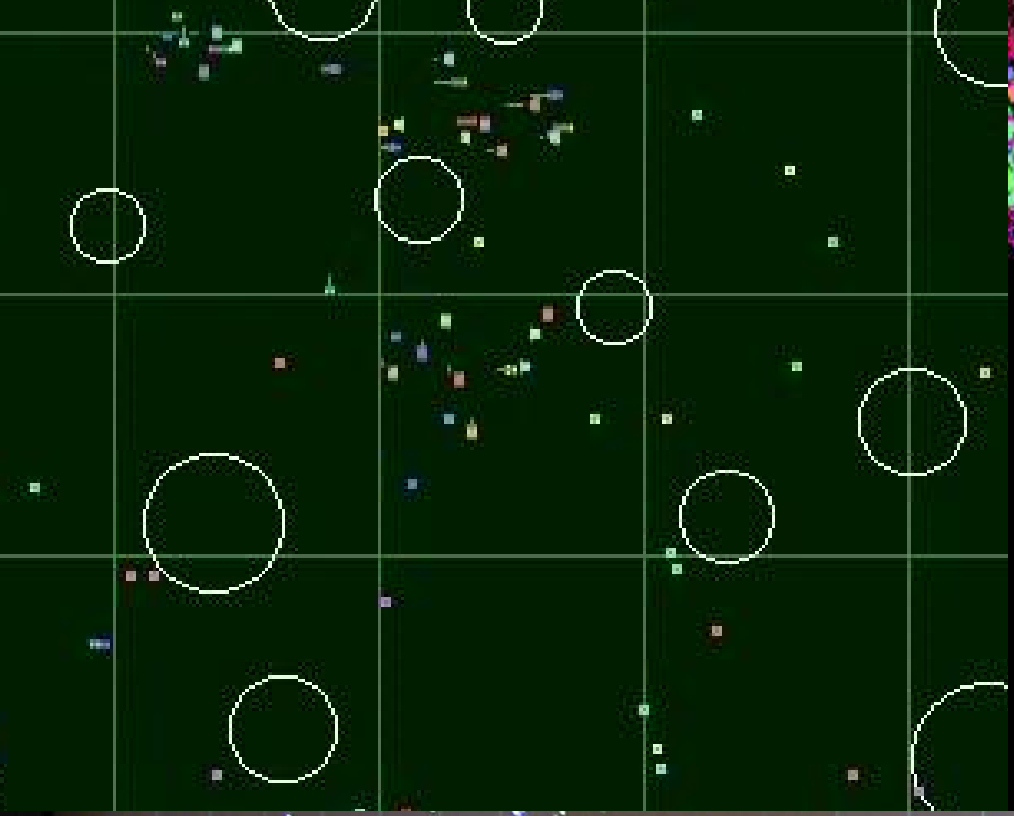
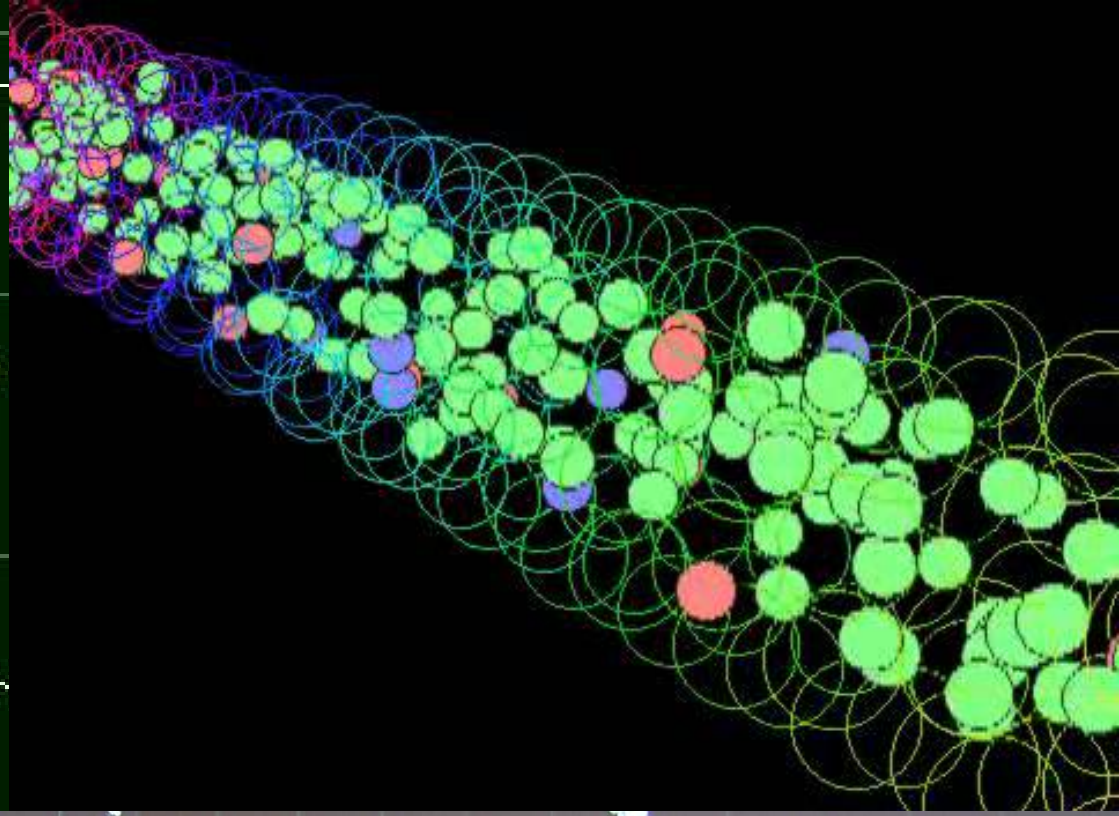
Building interactive simulations

- All of this means that we need to engineer our **model**, **simulation** and **visualisation** together
- Some CoSMoS work on this already
  - Tromsø Display Wall: distributed visualisation; using this to inform distribution of simulation too
  - CoSMoS driver: middleware for connecting simulations and visualisations
- Effective visualisation is useful when developing a model – validate design, spot faults





High-performance interactive simulations

- … also known as **computer games**
- Obvious technology to use: graphics
  - Use realistic games engines to visualise real-world effects – e.g. city planning, police training...
  - Emotional involvement (quantifiable)
- Less obvious: interaction technologies
  - Lots of interesting new motion/position-tracking kit
- Less obvious: simulation technologies
  - Efficient spacial interaction, low-latency distributed simulation...

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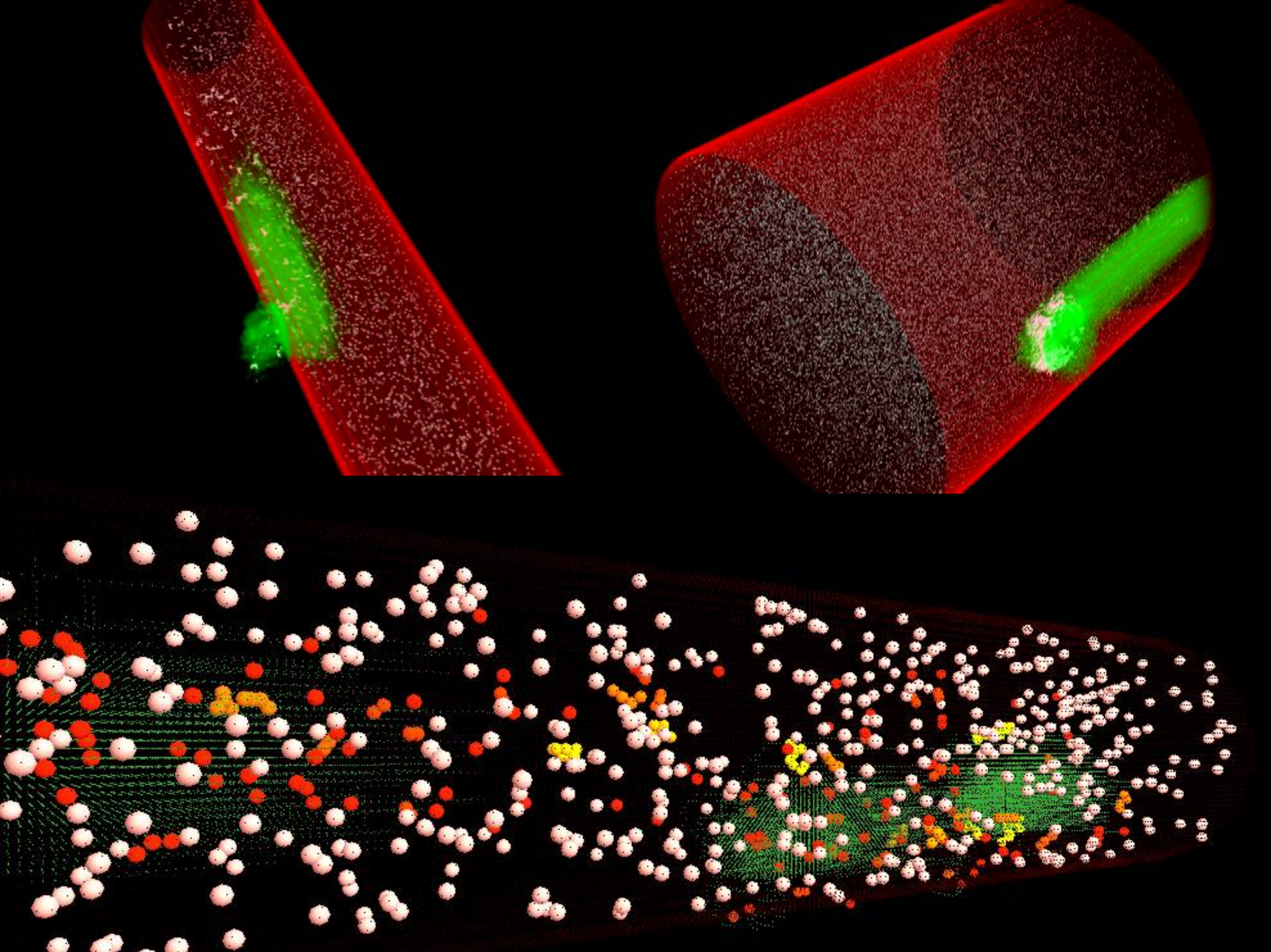

Any questions?

- Thanks to (among others):
  - YCCSA/CoSMoS: Paul Andrews, John Markus Bjørndalen, Teodor Ghetiu, Tim Hoverd, Fiona Polack, Carl Ritson, Elva Robinson, Susan Stepney...
  - WhSpR/CRISP: Jim Bown, Alexey Goltsov, Andy Guest, Mark Shovman, Andrea Szymkowiak, Jiujiang Zhu...

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