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http://www.oii.ox.ac.uk/microsites/eresearch08/index.cfm

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Parameters and visions: data flows in computational and mathematical biology

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Computational biology

- Paradigmatic of e-science
- Supercomputing and quantificational science
- Quantification, mathematisation and the history of science, from Galileo to the present
- Biology and other life sciences as the latest conquest of quantificational science

Trading zones

- Computational biology = trading zone for quantificationally minded scientists (mathematics, physics, engineering and computer science) and qualitatively minded biologists?
- Ranges from peaceble and mutually profitable trading, to battle and imperialism
- Pidgins and creoles
- Hybrid visual perception and observation

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Processes of research in computational biology (1)

QuickTime™ and a
decompressor
are needed to see this picture.

[BURTON ET AL.: INDIVIDUALIZED CARDIAC 3D MODELS]

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Processes of computational biology (2)

QuickTime™ and a
decompressor
are needed to see this picture.

[Plotkowiak et al: High Performance Computer Simulations of Cardiac Electrical Function Based on High Resolution MRI datasets]

+ mathematical models

+ numerical analysis

+ algorithmic solution of models

+ computer programming for simulations and visualisations

Computational Biology: current status

- Computational biology is not yet firmly established as a scientific area of research
- It has many enthusiasts, but it also has many detractors
- Funding, doctoral training centres, industry interest
- It is still a programme of research in need of validation
- Varying degrees of uptake in different areas
- PR strategies as important as the science

Rhetorical strategies

'In this paper, we review a number of mathematical models that have been developed to describe some of the above aspects of tumour growth. In so doing, we aim to show how mathematical modeling, computation and analysis can generate useful insight into the mechanisms that underpin this devastating disease' (1564); at the beginning of the conclusion: 'Through the development of well-founded theoretical models of solid tumour growth, such as those reviewed in this article, we believe that mathematics, in conjunction with related experimental work, can be a valuable tool with which to address such questions' (1572); and finally as the last sentence of the paper: 'We hope that in the future, as these benefits become more widely recognized, mathematicians will be routinely involved in the design and analysis of experimental work' (1575). (Byrne et al, 2006)

Heart and cancer modellers

- History of development in both areas
- Existence of interdisciplinary individuals
- Epistemic cultures and practices
  - Experimental physiologists
  - Biologists

Differences on the usefulness of theories ….

‘Traditionally, theoretical models in biology have been associated with the singling out of one particular dynamic, of one particular kind of mechanism, and the message drawn from increasing visual access underscores, once again, how far the range of biological innovation exceeds the range of human imagination. Indeed, for many, merely being able to identify the mechanisms involved suffices as an explanation. For others [conspicuously mathematical biologists], however, the identification of new mechanisms points in just the opposite direction, serving as a spur to new theoretical formulations’ (Keller 2002: 232).

Differences on the usefulness of models

It is futile to conjure up in the imagination a system of differential equations for the purpose of accounting for facts which are not only very complex, but largely unknown (Eric Ponder, quoted by Keller 2002: 100)

Differences in basic processes

'A lot of the time, we're just looking down microscopes' (A biologist).

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‘Biologists often just want to know that something happens, two proteins interact which regulate the expression of some other protein [now, that’s it, they just want to know that that’s the mechanism. We want to know exactly how much of that protein has to be present in order to cause exactly what degree of regulation of this other protein so we can build a model which explains the concentration of the thing that caused the regulation of that other thing [by] a series of graphs [and a] model to reproduce those graph. Biologists don’t and can’t typically do that. They just know that these proteins are present in the system. They just tell you they’re there. No concentrations, rate constants, absolute concentrations in any particular situation. Biologists either can’t do that or they won’t because it’s not what they’re interested in.’ (A mathematician)

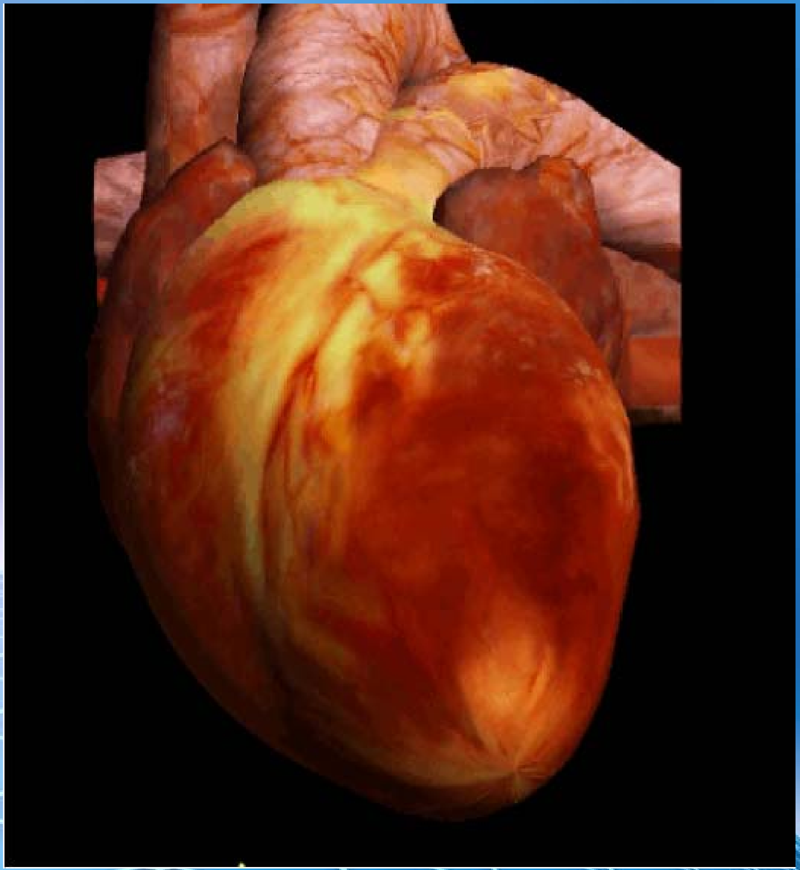
Parameter values and why they're hard to get

- Computational and mathematical biologists need to obtain parameter values from experiments, obstacles to obtaining them include:
    - Difficulty or impossibility of experimentally acquiring the data required for specific questions posed by computational or mathematical biologists;
    - Time-consuming nature of the experiments
    - Research questions extraneous to biologists' interests
    - Tediousness or low-level nature of the experiments

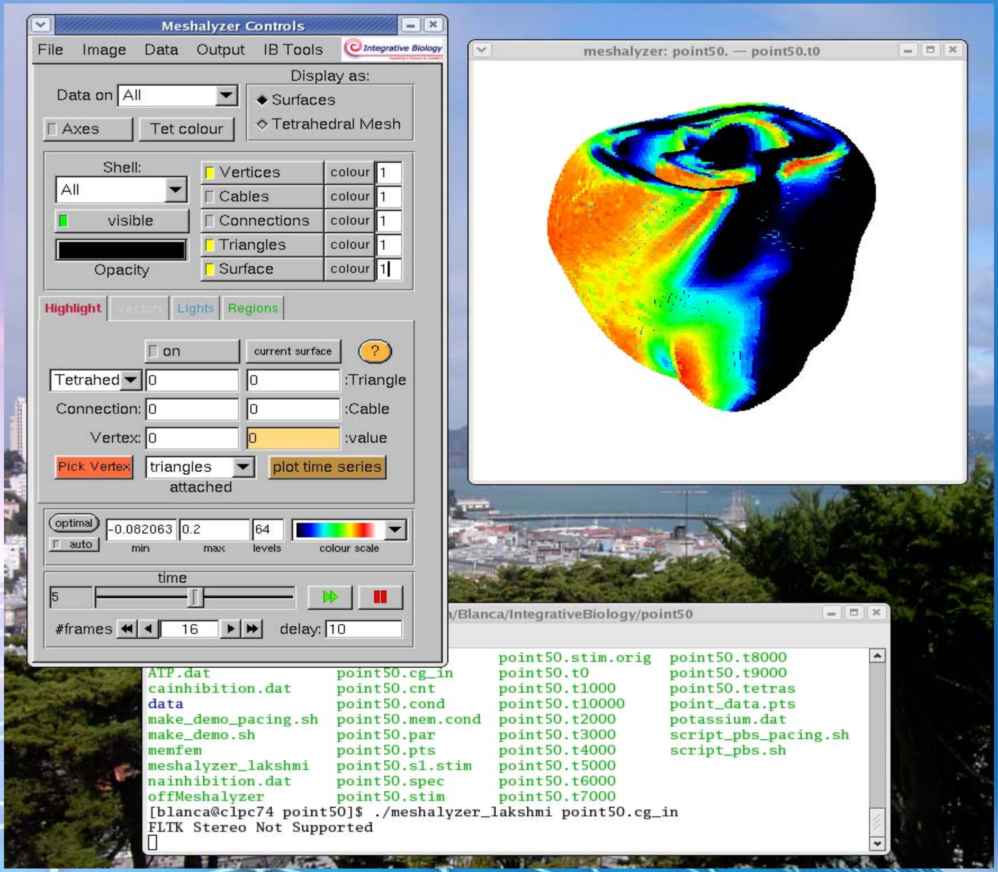
Visualisations as mediators

- The role of visualisations
- Visually render the outputs of simulations
- Used in a number of different contexts: papers, presentations, workshops, as ‘trademarks’ and icons
- ‘Compelling’, ‘beautiful’, very strong aesthetic qualities
- Visualisations have epistemic, cognitive, social, stylistic and aesthetic aspects: not separately but inextricably intertwined

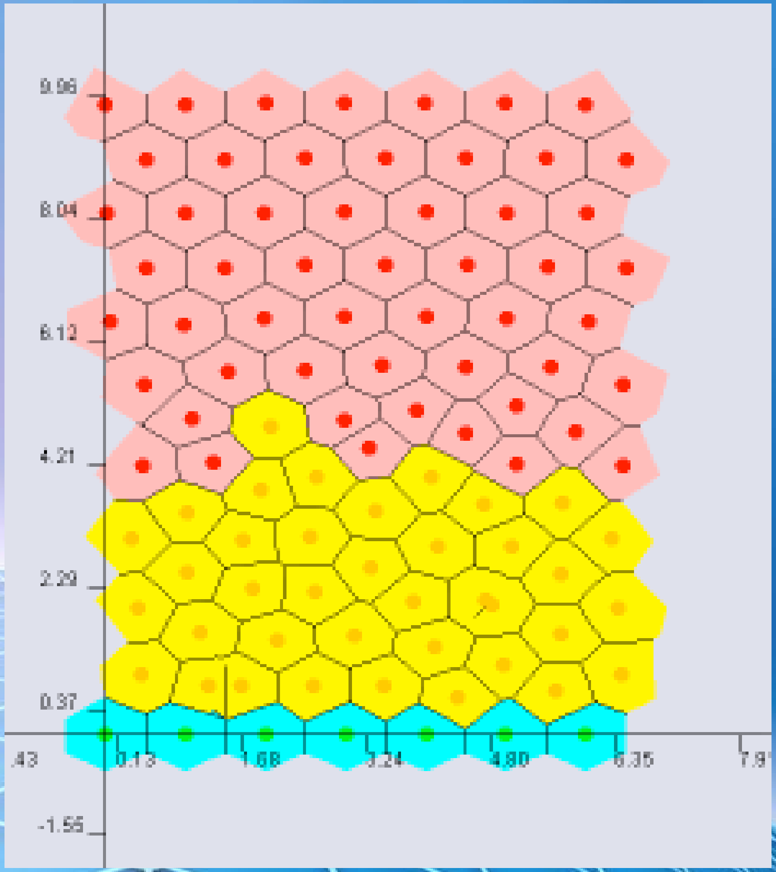
Naturalistic heart simulation



Visualising results: heart modelling



Visualising results: colorectal cancer



Parameters and visions

- Visualisations are a fusion of quantitative and qualitative epistemic processes
- Render mathematics to visual perception
- Visual concretisation of the process and point of obtaining parameter values
- Emblematic of the compromises, trades, battles and conquests of e-science