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A multiscale computational framework for modelling biological systems: Chaste

The Chaste framework (http://web.comlab.ox.ac.uk/chaste) in an Open Source numerical library which enables multicellular and multiscale simulations of biological processes. In this, the first talk of the mini-symposium, we introduce the multiscale framework on which Chaste is based on, discuss the development of the framework, and provide a demonstration of how to set up a simulation.

The mathematical framework is based upon the observation that the natural structural unit of biology is the cell, and it consists of three main scales: the tissue level (macro-scale); the cell level (meso-scale); and the sub-cellular level (micro-scale), with interactions occurring between all scales. The cell level is central to the framework and cells are modelled as discrete interacting entities using one of a number of possible modelling paradigms, including lattice based models (cellular automata and cellular Potts) and off-lattice models (cell centre and vertex based representations). The sub-cellular level concerns numerous metabolic and biochemical processes represented by interaction networks rendered stochastically or into ODEs. The outputs from such systems influence the behaviour of the cell level affecting properties such as adhesion and also influencing cell mitosis and apoptosis. Tissue level behaviour is represented by field equations for nutrient or messenger concentration, with cells functioning as sinks and sources. This modular approach enables multiple models to be simulated and is easily extensible allowing more realistic behaviour to be considered at each scale.

Chaste is comprised of libraries of object orientated C++, developed using an agile development approach. All software is tested, robust, reliable and extensible. The library enables general simulations to be undertaken and includes tools to automatically curate and store simulation results expediting model development. One key aspect of such a framework is the ability to model specific biological systems using multiple modelling paradigms, as a case study we present a simple model of the colorectal crypt using four different cell level models and illustrate the similarities and differences.