## **Multi-Scale Modelling of Saliva Secretion**

James Sneyd, Department of Mathematics, University of Auckland David Yule, School of Medicine and Dentistry, University of Rochester John Rugis, NeSI, University of Auckland

This interdisciplinary project encompasses a range of activities targeting anatomical data based structural modelling of individual salivary cell clusters, solution of cellular calcium dynamics function in full 3D simulations, interactive visualisation of resultant calcium waves and validation of results by comparison to experimental data. The model will be used to test duct cell function and for the testing of pathological conditions. The overall project is funded by the National Institutes of Health, USA (Sneyd, Yule).

## **Current activity and results**

Real biological samples where digitized using fluorescent markers and confocal microscopy. A sample image slice in which individual cell outlines can be seen is shown in Figure 1. The cell membranes are colour coded red and the interconnecting lumen is colour coded green. Note that, in living beings, the saliva secreted from the cells is transported through the assumed tube-like lumen structure.

Figure 1: Colour coded digitised image slice.

The full set of images slices was used as the basis for a full 3D graphics model reconstruction of one cluster of cells as shown in Figure 2. The tube-like structure of the lumen can now be clearly seen. This anatomically correct model was used in turn as the basis for the creation of a 3D tetrahedral mesh suitable for finite element simulations.

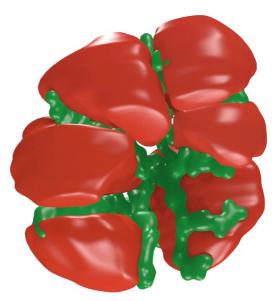


Figure 2: Full 3D mesh model of a cluster of cells.

The same underlying 3D graphics mesh was used in the animated visualisation of the calcium concentration simulation time series results. One time series frame is shown in Figure 3.



Centre for eResearch

University of Auckland Private Bag 92019 Auckland 1142 New Zealand

Physical address: Room G021, Building 409 24 Symonds Street Auckland 1010, New Zealand www.eresearch.auckland.ac.nz

Contact:
Professor Mark Gahegan,
Director
m.gahegan@auckland.ac.nz
DDI +64 9 9231891

Marcus Gustafsson, Manager <u>m.gustafsson@auckland.ac.nz</u> DDI +64 9 923 2231



Through NeSI, the University of Auckland Pan cluster was used for both graphics model rendering and running the finite element simulations. Thanks to NeSI, we were able to render higher quality images and run many more simulation variants than would have been possible on a desktop computer. This facility will also enable us to scale up our model to include many more cells.

## What's next

As expected, simulation results for each of the cells differ somewhat. Further work will include a detailed analysis of how cell geometry effects the generation and propagation of calcium waves within each cell. We also plan to construct a larger model based on new digitisations using refined microscopy techniques.

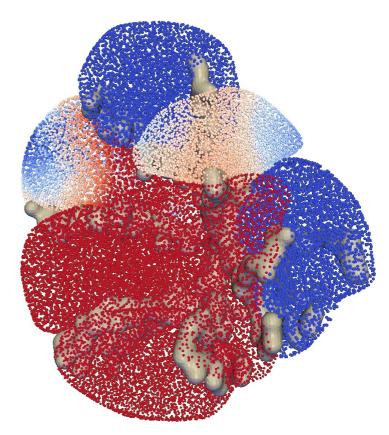


Figure 3: Simulation output snapshot

## **Contact**

James Sneyd, Department of Mathematics, University of Auckland Email: j.sneyd@auckland.ac.nz