Erythrocyte shape, metabolism and membrane transport – computations

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Our aim in modelling cellular responses to chemical and physical perturbations is to gain insights into underlying structural, transport, and metabolic mechanisms. Such models can enable predictions of cell behaviour under conditions that are not experimentally accessible; or the models can be added to others thus building up the complexity of the model to describe highly-nonlinear cellular phenomena such as metabolic and structural oscillations. The cellular system under study has been the human erythrocyte. Data on cell shape on the minute-to-hour time scale have been obtained with NMR-diffusion spectroscopy and differential interference contrast (DIC) light microscopy; on the sub-second time scale fast image capture of membrane 'flickering' has been carried out with DIC microscopy. Data processing and modelling of cell shape-changes and membrane flickering have been carried out by using Mathematica. A drive to understand the "link" between the rate of transmembrane pumping of Na^+ *via* the Na,K-ATPase, and the rate of glycolysis has used multinuclear NMR spectroscopy. Again modelling of the system has been set up in Mathematica. The next challenge is fitting multi-parameter models to real experimental data. For this we are using a Monte Carlo Markov chain (MCMC) approach.

Acknowledgements: Ron Clarke, Bob Chapman, Gemma Figtree, Stuart Grieve, Tim Larkin, Christoph Naumann, David Philp, Max Puckeridge, David Szekely, Jamie Vandenberg.