Mathematical Modelling of Chemical Diffusion through Skin

C. E. Goodyer[1], J. D. Wood[2], and M. Berzins[3]

Abstract: The skin forms the interface between the body and the external environment. It has several functions including thermal regulation, sensory perception, excretion, and as a barrier to protect against infection, dehydration and chemical assault. Its role as a water barrier is critical to our ability to survive on land, and any significant departure from normal barrier function leads to serious health effects and in extreme cases, death. Even healthy skin is an imperfect barrier, and for some chemicals skin permeation may be the most important, or even sole, route of human exposure. Besides the interest in delivering drugs to or through the skin, there is a pressing need to estimate the potential health risk arising from skin exposure to the many different chemicals we encounter in our jobs, homes and in the environment.

The barrier to permeability comes mainly from the heterogeneous structure of the outer layer of the skin. This is made up of planes of impermeable blocks (called corneocytes) which are surrounded a thin lipid bi-layer through which the chemical must diffuse.

Numerical modelling of chemical diffusion through membranes such as skin has been previously restricted to, at most, 2-d in work by several authors (Heisig *et al.*, Frasch *et al.*, Cussler *et al.*). In our work we are tackling the full three dimensional structure of the skin, hence are able to generate results for a much wider range of cases.

In this talk we describe the application of unstructured 3-d finite elements to our model. It will be explained how Grid Computing techniques are used to control multiple simulations on remote distributed Grid resources from a Problem Solving Environment on the user's desktop. This will provide steering of the simulation and result visualisation in real time. The effectiveness of this Grid-based approach in improving the quality of the simulation is assessed.

Discussion will be made about future extensions to the necessary multiscale modelling required for even more accurate representations.

[1,2] School of Computing
University of Leeds, Leeds, UK
ceg@comp.leeds.ac.uk, jason@comp.leeds.ac.uk

[3] School of Computing, University of Utah, Salt Lake City, USA
mb@sci.utah.edu