NUMERICAL SIMULATION OF CELLULAR TRANSPORT AND REACTION SYSTEMS WITH GENERALISED FINITE ELEMENT DISCRETISATIONS

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Key Words: *GFEM, Interface Problems, Multi-Scale Analysis, Cell Biology.*

ABSTRACT

Based on the development of new experimental techniques, mainly imaging techniques like FRAP and FRET, cellular transport and reaction processes can be better understood than ever before. Cell biology in general offers a whole range of such important applications (in the end all life depends on this complex machinery) which are challenging for mathematical modeling and the performance of existing discretisations and numerical algorithms. A specific property of cellular structures are their compli-cated geometry, here just called "Complex Domains". In this talk we consider complex compartmental structures, i.e. the computational domain has many sub-domains to which molecules are delivered according to different interface or transmission conditions. The respective equations also occur for example in porous media, but here in addition many reactions between the molecules in the reaction volume and along interfaces (membranes) have to be incorporated. We also look at limits where these sub-structures become smaller, leading to new effective equations (homogenization). The complexity of such cellular domains can now be measured much more accurately with the help of modern imaging and image analysis techniques. It is tempting to combine methods from image analysis and numerical simulations in order to get a better understanding how simulations correspond to measured data. Special emphasis is given how the meshfree approach is performing for this type of interface problems as described above. Especially patch generation and the resolution of micro-structures pose severe problems which will be addressed. Finally we discuss the derivation of interface conditions from a multi-scale analysis where transporter molecules (membrane proteins) are described as Markov Chains.

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