ANALYSIS OF MULTI-SCALE MODELS FOR PHYSICAL AND CHEMICAL PROCESSES IN POROUS MEDIA AND APPLICATIONS IN BIOSCIENCES

Willi Jäger

Interdisciplinary Center for Scientific Computing (IWR), Mathematics Center Heidelberg (MATCH), University of Heidelberg
[jaeger@iwr.uni-heidelberg.de]

2000 Mathematics Subject Classification. 35K57, 35B27, 80M35

Keywords and phrases. Multi-scale problems, porous media, membranes, nonlinear differential equations, transmission conditions.

Mathematics is developing theory and tools to improve the understanding and control of physical and chemical processes on all scales, to transfer information obtained for atomic and molecular, for the nano- and micro-scale, into better understanding and quantitative description of structures and function on higher scales. This lecture discusses systems of nonlinear differential equations modelling flow, transport and reactions in porous media on a micro scale and transition to scale limits, to efficient macroscopic systems approximating the micro model systems. Computability is an important aspect of the analysis. Typical cases are chromatographic processes, processes in soil, membranes and tissues in technology as well as in biosciences. The resulting effective equations are including macroscopic and microscopic variables and show a structure, which has to be observed in numerical algorithms. The multi-scale systems are posing new challenges to Nonlinear Analysis and to Numerics. In many cases, mathematical modelling of the micro-processes is a problem by itself, very often leading to non-standard systems of nonlinear differential

equations in complex media. The crucial scales have to be determined depending on the system parameters. In order to reduce the difficulties, the underlying geometry is assumed to generated by translations of a basic cell. The following cases will be considered and the corresponding scale limits will be discussed: Chromatographic columns (flow, diffusion, transport, reactions in the fluid phase; diffusion, transport, reaction in the solid phase (or on its surface); (nonlinear) transmission conditions on the interface); membranes (diffusion, reaction).

In case of the membranes, transmission conditions at the interface can be derived, linking in each point the macro-scale to the micro-scale and taking into account the processes in the microstructure of the membrane. It is natural to keep the structure of the system also in the computational scheme. This is achieved by choosing in a Galerkin Method basis functions adjusted to the transmission conditions properly.

REFERENCES

[1] U. Hornung, W. Jäger, A. Mikelic, *Reactive Transport through an Array of Cells with Semi-Permeable Membranes*, Mathematical Modelling and Numerical Analysis, 28 (1994), 59-94.

[2] M. Neuss-Radu, *Some extensions of two-scale convergence*, C. R. Acad. Sci. Paris, 323 (1996), 899-904.

[3] W. Jäger, L. Simon, *On Transmission Problems for Nonlinear Parabolic Differential Equations*, Annales Univ. Sci. Budapest, 44 (2004), 143-158.

[4] M. Neuss-Radu, W. Jäger, *Effective transmission conditions for reaction-diffusion processes in domains separated by an interface*, SIAM J. Math. Anal., 39 (2007), 687-720.

[5] M. Neuss-Radu, S. Ludwig, W. Jäger, *Multiscale analysis and simulation of a reaction- diffusion problem with transmission conditions*, Nonlinear Analysis-RWA (2008).