Abstracts

Fully Discrete Heterogeneous Multiscale Methods and Application to Transport Problems in Microarrays

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Physical systems encompassing a variety of strongly coupled scales pose major computational challenges in terms of analysis modeling and simulation. In this report we first discuss a multiscale modeling approach for the transport of particles such as DNA in heterogeneous devices (microarrays). The model involves a multiscale elliptic equation coupled with a multiscale advection-diffusion equation. We introduce a numerical method for the solution of the coupled system of equations. We first discuss a new multiscale finite element method for the solution of the elliptic problem. We then explain how it is possible to use an explicit stabilized method (ROCK) for the numerical solution of the stiff system of ordinary differential equations of large dimension, originating from the method of lines discretization of the advection-diffusion equation.

DNA separation in microarrays. We consider a (square) device with periodic asymmetric obstacles and model the transport of injected mixture with concentration $c(t,x)$ as an advection-diffusion equation given by

$$\frac{\partial c^\varepsilon}{\partial t} + \nabla \cdot (v^\varepsilon c^\varepsilon) = D\Delta c^\varepsilon, \tag{1}$$

where $v^\varepsilon = -\rho k^\varepsilon \nabla u^\varepsilon$ is the velocity field, u^ε is the electrical potential, k^ε is the electrical conductivity and ρ is the charge density of the electrical device. We assume for simplicity that ρ is constant and set it to one. The obstacles of the microdevice introduce a typical self-similar structure (which will also be called a "periodic cell"), and we denote by ε the length of these cells. The equation for the potential u^ε is given by

$$-\nabla \cdot (k^\varepsilon \nabla u^\varepsilon) = 0, \tag{2}$$

with Neumann boundary conditions at the corner of the device and Dirichlet conditions at the charged sites of the boundary. The homogenization problem corresponding to equations (1) and (2), where the heterogeneous fine scale structure is transferred into a homogeneous large scale model, shows that the heterogeneities of the device have no impact on the large scale drift [6]. Thus, the large scale drift does not depend on the diffusion constant or the molecular weight of the particles. The heterogeneous microarrays have an impact only on the large scale diffusion. This gives a quantitative explanation of the model proposed in [11],[12] and explain the experimental results of [10]. In [9] transport problems with compressible flows are studied and it is shown that for such flows, the large scale drift can depend on the small scale diffusion coefficient. In the sequel we explain how to solve numerically the coupled equations (1) and (2).

Fully discrete finite element heterogeneous multiscale methods. Applying a standard finite element method to the variational form of (2) requires usually a meshsize $h < \varepsilon$ for convergence, i.e., to resolve the small scale of the problem. This lead to a complexity of $\mathcal{O}(\varepsilon^{-d})$, where d is the spatial dimension, which makes the direct numerical simulation impossible if ε is small. When the data of the problem are oscillatory with small period, classical two-scale approaches are well established, and the analytical treatment lead to homogenized equations. However, the fine scale behavior, i.e. the oscillations of the solution, are lost in the homogenization process. It can be recovered through the solution of additional "corrector" problems. But these corrector problems again exhibit rapidly oscillating coefficients so that their accurate numerical solution is as expensive as solving the original problem.

In the sequel, we present a new multiscale finite element method for the numerical computation of problems with multiple scales. Define a quasi-uniform macro triangulation $\mathcal{T}_H$ of the domain Ω, assumed to be a convex polygon. The finite element heterogeneous multiscale method (FE-HMM) is based on the following ideas [13],[3],[14],[4].

(1) Associated to the macro triangulation, we define a macro finite element space and a modified bilinear form with unknown input data.
(2) Within each macro triangle we define a sampling domain K_ε of length scale comparable to ε, a micro finite element space and a micro bilinear form based, upon the original multiscale tensor k^ε, which provides input data for the macro problem.

The FE-HMM gives a procedure to obtain an approximation u^H of the homogenized solution u^0, without computing explicitly the homogenized equations. By a post-processing calculation, it is possible to compute an approximation $u^{\varepsilon,h}$ of the fine scale solution u^ε of (2) at a much lower cost than solving the original fine scale problem. Indeed, we solve the fine scales only in sampling domains of size ε^d in the periodic case, within a macro mesh of Ω. Furthermore, the micro problems are independent and can be solved in parallel. In the non-periodic case, K_ε should be chosen as to sample enough information of the local variation of k^ε. Semi-discrete analysis of the method has been given in [3],[14]. In these works, the fine-scale problem involving the micro solver was assumed to be computed exactly. In [4], the first fully discrete analysis of the FE-HMM has been given. This analysis show that the macro and the micro meshes have to be refined *simultaneously*. This has been generalized for elasticity problems in [8].

Solving an advection diffusion problem with ROCK methods. Discretizing the advection-diffusion equation by the method of lines leads to a stiff system of ordinary differential equation of large dimension. Such ODEs, originating from the space discretization of (1) are called *stiff* in the literature [15]. It is also known that implicit solver have better stability properties, but at the expense of solving linear systems of large dimension if the spatial discretization mesh is small.

Chebyshev methods are a class of explicit one step methods with extended stability domains along the negative real axis. With such methods, large time steps can be used. This contrasts with the severe time step restriction given by the CFL condition for standard explicit methods.

Recently, a new strategy to construct higher order Chebyshev methods with "quasi" optimal stability polynomials has been proposed [1],[2]. These methods, called ROCK, together with the FE-HMM have been combined to solve transport problems described by equations (1) and (2) [5]. The numerical simulation of the DNA transport problem has been addressed in [7].

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Solving Partial Differential Equations in Complicated Domains

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(joint work with Christian Engwer)

1. Introduction

Many practical applications require the solution of partial differential equations (PDEs) in complicated domains. We are especially interested in computing the flow around root networks of plants or in the pore space of porous media.