PARAMETERIZATION FOR SOME MULTISCALE PROBLEMS IN BIOLOGY AND TURBULENCE

By

Adnan Ahmed Khan

An Abstract of a Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the Degree of

DOCTOR OF PHILOSOPHY

Major Subject: Mathematics

Examining Committee:

Peter R. Kramer, Thesis Adviser
Shekhar Garde, Member
Gregor Kovacic, Member
Victor Roytburd, Member

Rensselaer Polytechnic Institute
Troy, New York

January 2007
(For Graduation May 2007)

ABSTRACT

We consider mathematical techniques for studing some multiscale problems in this thesis. The problems we consider are assumed to have a wide separation of scales, this assumption which is true for some systems also makes the problems mathematically more tractable. We want to obtain coarse grained models at the largest scale in the problem.

In the first chapter we study the dynamics of water molecules around a solute. Instead of resolving the dynamics explicitly we want to capture their dynamical behaviour using a suitable "parameterization". To this end we consider two drift-diffusion parameterizations. The drift and diffusion coefficients in our models are obtained using data from an MD simulation. The first model we consider, which we call the "DD-I" model has a drift proportional to the gradient of the potential of the mean force due to the solute (which as mentioned is obtained from an MD simulation). The diffusion coefficient in this model is simply the bulk diffusivity of water. In the next model, which we call the "DD-II" model, both the drift and diffusion coefficients are calculated from the MD data. We then compare the two models using a suitable metric. Our study indicates that the DD-II model does a better job at capturing the dynamics of the water molecules.

The second chapter is a study of the advection diffusion equation, where the advective velocity field is assumed to have two widely separated scales. We consider a velocity field with a large scale "mean flow" and small scale periodic "fluctuations". This is a simplifed model developed to understand the turbulent transport of passive scalars. We consider the case where the mean flow is stronger than the fluctuations. We want to obtain a "homogenized" equation at the large scale where the effects of the fluctuations have been coarse grained and are captured using a suitable parameterization. It turns out that the effects can be captured in an "enhanced diffusivity". We show that standard homogenization theory, which is applicable to the cases where either the mean flow is weak or of equal strength to the fluctuations, seems to break down in this case. We then use stochastic differential equations for trajectories of tracer particles to obtain the enhancement in diffusivity. We also compute the enhanced diffusivity by extrapolating the homogenization code for the equal strength case. Comparing the two we note that homogenization theory in-fact does work in this case as well. Next we develop a mathematical framework of "Non Standard" homogenization theory to explain the numerical result. The crucial factor turns out to be whether the mean scale flow components are in low or high order rational ratio. Finally we develop homogenized equations for both these cases.

The third and final chapter of the thesis involves a rigorous development of the Method of Multiple Scales. Specifically we develop the method for the case where three scales are present in the system. We propose a solvability condition to be used in supressing secularities in the asymptotic hierarchy. We apply the method to two simple systems, the Duffing oscillator and the cubically damped oscillator. We compare our asymptotic results to numerical solutions of the full equations and observe a good match. We also show that our method does better than other asymptotic methods like averaging.