Cime Course Proposal

Title: Multiscale and Adaptivity

Organizers: Giovanni Naldi (Università degli Studi di Milano)
Giovanni Russo (Università degli Studi di Catania)

Location: **Cetraro** (Italy)

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Motivations and description of the course:
Physical, chemical, and biological processes for many problems in computational physics, biology, and materials sciences span length and time scales of many orders of magnitude.
Traditionally, scientists and research groups have typically focused on methods that are particularly applicable in only one regime, and knowledge of the system at one scale has been transferred to another scale only indirectly. Microscopic models, for example, have been often used to find the effective parameters of macroscopic models, but for obvious computational reasons, microscopic and macroscopic scales have been treated separately.
The enormous increase in computational power avaibalbe to various research groups (due to the improvement of computer speed and efficiency of numerical methods) allow in some cases the treatment of systems involving scales of different orders of magnitude, arising, for example, when effective parameters in a macroscopic model depend on a microscopic model, or the presence of a singularity in the solution produces a continuum of lenght scales.
However, the numerical solution of such problems by classical methods often lead to an inefficient use of the computational resources, even up to the point that the problem cannot be solved numerically. The reasons for this are, e.g., that the necessary resolution of a fine scale entails an overresolution of coarser scales, the position of the singularity is not known beforehand, the gap between the scales is too big for a treatment in the same framework. In other cases, the structure of the mathematical models that treat the system at the different scales varies a lot, and therefore new mathematical techniques are required to treat systems described by different mathematical models. Finally, it is very common that one is interested in the accurate treatment of a small portion of a large system, and it is too expensive to treat the whole system at the required accucary.

Techniques that have been developed in order to overcome the aforementioned difficulities are:

* Multiscale modeling. A broad range of scientific and engineering problems involve multiple scales. Traditional monoscale approaches have proven to be inadequate, even with the largest supercomputers, because of the range of scales and the prohibitively large number of variables involved. Thus, it is necessary to develop systematic modeling and simulation approaches for multiscale problems. By its nature, multiscale modeling is highly interdisciplinary, with developments occurring independently across fields.

*Adaptivity. With the help of so-called a posteriori error estimators, the grids are adjusted in an automatic way to properties of the concrete solution such as singularities, layers, regions of different characterstic lengths.

* Wavelets and multiscale bases. They allow good localization both in space and in frequency and can “read” the properties of a function directly on the sequence of its coefficients in a multiscale decomposition.

* Multidimensional systems and multiphysics. Different regions of large systems are treated with a different level of detail, both from the dimensional and physical point of view. For example, if one is interested in a detailed behavior of blood flow in a small portion of a vessel, which is part of a large body then one can treat the small region by detailed 3D Navier-Stokes equationm while the rest of the body is “lumped” into a lower dimensional system, whose aim is to provide reasonable boundary conditions for the region of interest. In semiconductor device simulation, different mathematical models can be used for the treatment of charge carriers. Channels in submicron device, for example, require kinetic, or even quantum treatment, while the behavior of bulk regions is adequately treated by the more treatable drift-diffusion model.

The courses will overview these techniques, addressing both theoretical and practical aspects.

Tentative list of lecturers and breaf description of their course

Bjorn Engquist (ICES, University of Texas at Austin)
Multiscale Modeling
Description of the course
This course will focus on the efficient coupling of microscale and macroscale models in the same simulation. This type of strategy is needed for problems with a very wide range of scales. Two cases will be studied. In one the the domain of the independent variables is decomposed into separate parts for the two models. The challenge is then to develop and analyze the boundary conditions connecting the models. In the other the macroscale model gets data from the microscale model, which is solved in sampled subdomains throughout the computational domain.

Alfio Quarteroni (EPFL Losanna, Politecnico Milano)
Adaptivity in mathematical modeling
Description of the course
For the description and simulation of complex physical phenomena, combination of hierarchical mathematical models can be set up with the aim of reducing the computational complexity.This lecture will mainly focus on models with variable geometrical dimension, reduced basis algorithms, and their application to the simulation, control and optimization of problems arising in life sciences and environmental sciences.

Ricardo H. Nochetto (University of Maryland)

Andreas Veeser (Università degli studi di Milano)
Convergence and Complexity of Adaptive Finite Elements
Description of the course
This course, in two part, will overview a posteriori error estimation and give an introduction to recent results about the convergence and complexity of adaptive finite element methods. The focus will be on methods of the form SOLVE-ESTIMATE-MARK-REFINE and the role of the a posteriori error estimator within adaptivity.

Kunibert G. Siebert (Universität Augsburg)
Implementation of Adaptive Finite Element Methods
Description of the course
This course will give an introduction into the toolbox ALBERTA for the implementation of adaptive finite element methods. The toolbox ALBERTA, which was created by Alfred Schmidt and Kunibert G. Siebert, is freely available. It gives access to algorithms for local mesh modifications, handling of various kinds of ansatz functions (higher order discretizations, e.g.), full administration of all degrees of freedom defined on a mesh, integration and assemblage routines, solvers for the resulting (non)linear (sub)systems, and adaptive methods for stationary problems of the form SOLVE-ESTIMATE-MARK-REFINE, as well as instationary problems. Using these library tools, it is possible to implement a solver for the solution of a specific problem that does not depend on the dimension, i.e. the solver can be implemented in 1d or 2d and works in 3d too. This feature reduces the amount of implementation time tremendously.

Silvia Bertoluzza (IMATI-CNR Pavia)
Adaptive wavelet methods
Description of the course
This course will first deal with the concept of nonlinear sparse wavelet approximation of a given (known) function. Next it will show how the tools just introduced can be applied in order to write down efficient adaptive schemes for the solution of PDEs. We will finally consider the problem of using in a finite element context some of the concepts developed in the wavelet framework.