Special Session 79: Numerical Methods Based on Homogenization and on Two-Scale Convergence

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The aim of this Special Session is to take stoke of Numerical Methods for solving Partial Differential Equations that manage Multi-Scale Phenomena, Oscillations and Heterogeneities by incorporating concepts coming from Homogenization Theory and Two-Scale Convergence.

At the present time, there are several research program exploiting this kind of ideas. They concern Hyperbolic, Elliptic and Parabolic PDE. The application fields are Environmental Sciences, Fluid Dynamics, Elasticity, Tokamak Physic, ...

One of the goal of this special session is to gather people working in different teams of different countries and having in mind different applications in order to exhibit and synthesize what is common between the different fields.

Reduced basis finite element heterogeneous multiscale method

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In this talk, we introduce a new multiscale method for elliptic homogenization problems, that combines the finite element heterogeneous multiscale method (FE-HMM) with reduced basis (RB) techniques based on offline-online strategy [A. Abdulle, Y. Bai, submitted to J. Comput. Phys., 2011]. The FE-HMM, relies on a large number of micro problems with increasing degrees of freedom to achieve optimal convergence rates [A. Abdulle, SIAM, Multiscale Model. Simul., 2005]. In contrast the RB-FE-HMM needs only a small number of micro problems selected by a rigorous a posteriori error estimator, computed accurately in an offline stage. Suitable interpolations of the pre-computed microsolutions are used in an online stage to compute the macro solution in a very efficient way, specially for high order macro methods or three dimensional multiscale computations. Adaptive FE-HMM [A. Abdulle, A. Nonnenmacher, Comput. Methods Appl. Mech. Engrg., 2011] is also shown to benefit from the RB approach. A priori error estimates of the RB-FE-HMM and numerical examples illustrating the performance of our approach will be discussed.

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Neutrino transport in core collapse supernovae by the Isotropic Diffusion Source Approximation

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Simulations of core collapse supernovae require models that couple hydrodynamics of the background matter with radiative transfer of neutrinos. Full coupling of hydrodynamic and Boltzmann equations in 3D will probably remain computationally too costly even on supercomputers of the next generation. This is mainly due to regimes described by the Boltzmann equation in which high density of neutrinos, i.e., small mean free paths prevail. Therefore, one seeks approximations of the Boltzmann equation that capture the main processes of neutrino transport, e.g., in these regimes, while being computationally cheaper. A basic physical observation is that trapped neutrinos in high density regimes behave like diffusive particles whereas neutrinos in low density regimes are practically freely streaming particles. In both cases, the Boltzmann equation can be reduced considerably. This observation leads to the idea of considering the distribution function of the neutrinos to be decomposed additively into a trapped and a streaming particle component and to describe the behavior of these components by reduced equations. This is the underlying idea of the Isotropic Diffusion Source Approximation (IDSA) by Liebendörfer et al. The major challenge of this approximation is to find an appropriate coupling of the reduced equations. In this talk, we will give an introduction into the IDSA in spherical symmetry, both from a physical and a mathematical perspective. In particular, we will provide a justification of the IDSA by asymptotic analysis applying Chapman–Enskog and Hilbert expansions. We will also address the discretization and the numerical solution of the IDSA and introduce a solution technique for a full Boltzmann model that involves time splitting and finite volumes. Numerical results that compare the IDSA with the full Boltzmann model in 1D will conclude the talk.

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Location problems by shape and topological optimization

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In this talk, we are going to present works on shape and topological optimzation. This consists on studying location problems in order to optimize a criterion. We point out links between heterogeneity/homogeneity of domains and the achievement of the optimality of the considered criteria. As applications, we quote the crystal photonics and the identification of the interface with two fluids to get optimal design of a material, the placement of obstacle in a material so as to minimize the first eignenvalue of the Laplacian operator.

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Some numerical simulations on sand transport

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We develop a numerical method to simulate sand transport in tidal area. This method is based on two scale convergence method due to G. Allaire and G. Nguetseng and permits to get a new model which approaches the initial model. Using the equation modeling sand transport and its scaling, we get a model of short term dynamics of dunes and its to scale limit. We give some numerical results obtained by the two scale numerical method and we compare the evolution of the solutions of the initial model and its two scale limit at different time .

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Synthetic introduction to homogenization based numerical methods

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This talk is a synthetic introduction to the Special Session. I will introduce basic concepts of Homogenization and Two Scale Convergence, for nonspecialists. Then, I will explain how those concepts are used to set out efficient numerical methods to tackle problems where several scales are present. Among those problems, I will evoke questions in elliptic, parabolic and hyperbolic pde with oscillating coefficients or boundary conditions. I will also talk about the way those concepts are used for analyzing data with heterogeneities or in the context of optimal shape design.

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Reduced basis method in the numerical homogenization of a nonlinearly coupled system: Application to nuclear waste storage

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We are interested in the homogenization of a nonlinearly coupled system of PDEs describing radionuclide transport in a periodic porous media modelling a repository of nuclear waste storage. The resulting effective model is a nonlinearly coupled system of PDEs posed in a homogeneous domain with homogenized coefficients evaluated by solving so-called cell problems. Due to the coupling, the homogenized (or effective) coefficients always depend on the slow variable (as a parameter x), even in the simple case when the porosity is taken purely periodic. Therefore, the determination of these coefficients is the most important part of the computational time for the numerical simulation of such problems. We propose a new numerical algorithm based on Reduced Basis techniques, which significantly improves the computational performances. Some features of this work are that the homogenized coefficients are unbounded, the parameter x belong to $\mathbb{R}^d$ which is not a compact set and the dependence of these coefficients upon x is not affine, while the reduced basis method is designed to simply deal with bounded coefficients with affine dependence upon a parameter belonging to a compact set. Eventually, we provide some 3D numerical results in order to show the computational advantages of our method.

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Filtering partially observed multiscale systems with heterogeneous multiscale methods based reduced climate models

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In this talk, I will discuss a fast reduced filtering strategy for assimilating multiscale systems in the presence of observations of only the macroscopic (or large-scale) variables. This reduced filtering strategy introduces model errors in estimating the prior forecast statistics through the Heterogeneous Multiscale Methods (HMM) based reduced climate model as an alternative to the standard expensive direct numerical simulation (DNS) based fully resolved model. More importantly, this approach is not restricted to any analysis (or Bayesian updating) step from various ensemble-based filters. In a regime where there is a distinctive separation of scales, high filtering skill is obtained through applying the HMM alone with any desirable analysis step from ensemble Kalman filters. When separation of scales is not apparent as typically observed in geophysical turbulent systems, an additional procedure is proposed to reinitialize the microscopic variables to statistically reflect pseudo-observations that are constructed based on the unbiased estimates of the macroscopic variables. Specifically, these pseudo-observations are constructed off-line from the conditional distributions of the microscopic forcing to the macroscopic dynamics given the macroscopic variables with the method-of-moments estimator. This HMM based filter is comparable to the more expensive standard DNS based filter on a stringent testbed the two-layer Lorenz' 96 model in various regimes of scale gap, including the not so apparent one. This high filtering skill is robust in the presence of additional model errors through inconsistent pseudo-observations and even when macroscopic observations are spatially incomplete.

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Error control for heterogeneous multiscale approximations of nonlinear monotone problems

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In this talk, we introduce and analyse a heterogeneous multiscale finite element method (HMM) for monotone elliptic operators with rapid oscillations [Henning, Ohlberger, *On the implementation of a heterogeneous multiscale finite element method for nonlinear elliptic problems*, Proceedings of the DUNE-User Meeting 2010, 2012]. We first present a macroscopic limit problem for the oscillating nonlinear equations in a general heterogeneous setting and then show the convergence of the HMM approximations to the solution of the macroscopic limit equation. On the basis of this, we derive an optimal a-posteriori error estimate for the L^2-error between the HMM approximation and the solution of the macroscopic limit equation [Henning, *Heterogeneous multiscale finite element methods for advection-diffusion and nonlinear elliptic multiscale problems*, PhD Thesis, University of Münster, 2011]. The a-posteriori error estimate is obtained in a general heterogeneous setting with scale separation without assuming periodicity or stochastic ergodicity. The applicability of the method and the usage of the a posteriori error estimate for adaptive local mesh refinement is demonstrated in numerical experiments. The experimental results underline the applicability of the a-posteriori error estimate in non-periodic homogenization settings.

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Two-scale asymptotic-preserving particle-in-cell method for a Vlasov-Poisson system

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The aim of this work is to test on a simplified model the Two-Scale Asymptotic-Preserving Schemes. The model is a two dimensional in phase space Vlasov-Poisson equation with a small parameter, which induces high frequency oscillations in the solution. The aim of the model is to be used for a long time simulation of a beam in a focusing channel. This work was already done in the case where the solution is approximated by the two scale limit. The goals are first to improve this approximation, by going further, to the first order one, and secondly, to replace this approximation by an exact decomposition, using the macro-micro framework. This last approach will permit to treat the case of a not necessary small parameter.

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Variance reduction methods in stochastic homogenization

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The simulation of random heterogeneous materials is often very expensive. For instance, in a homogenization setting, the homogenized matrix is defined from the so-called corrector function, that solves a partial differential equation set on the entire space. This is in contrast with the periodic case, where the corrector function solves an equation set on a single periodic cell. As a consequence, in the stochastic setting, the numerical approximation of the corrector function is a challenging computational task. In practice, the corrector problem is solved on a truncated domain, and the exact homogenized matrix is recovered only in the limit of an infinitely large domain. As a consequence of this truncation, the approximated homogenized matrix turns out to be stochastic, whereas the exact homogenized matrix is deterministic. One then has to resort to Monte-Carlo methods, in order to compute the expectation of the (approximated) homogenized matrix within a good accuracy. Variance reduction questions thus naturally come into play, in order to increase the accuracy (e.g. reduce the size of the confidence interval) for a fixed computational cost. In this work, we show that we can apply the classical technique of antithetic variables and get an approximation of the homogenized matrix with a smaller variance, for an equal computational cost. We will demonstrate, both theoretically and numerically, the efficiency of the approach.

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An efficient higher-order heterogeneous multiscale method for elliptic problems and related issues

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In this talk, I will propose an efficient heterogeneous multiscale finite element method based on a local least-squares reconstruction of the effective matrix using the data retrieved from the solution of cell problems posed on the vertices of the triangulation. The method achieves high order accuracy for high order macroscopic solver with essentially the same cost as the linear macroscopic solver. Optimal error bounds are proved for the elliptic problem. Numerical results demonstrate that the new method significantly reduces the cost without loss of accuracy.

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Numerical simulations of confinement for paralic ecosystems

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In this work we present a modelling procedure in order to compute the confinement field of a lagoon. We improve existing models in order to account for tide oscillations in any kind of geometry such as non-rectangular lagoons with a non-flat bottom. The confinement can be defined at various scales (ocean, interior see, large bay, lagoons) and we shall introduce a suitable multi-scale numerical method for the computation of confinement.

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Multiscale geometric integration of deterministic and stochastic systems

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In order to accelerate computations, improve long time accuracy of numerical simulations, and sample statistics distribution by dynamics, we develop multiscale geometric integrators. The talk will be focused on the description of FLow AVeraging integratORs (FLAVORs), which apply to general multiscale stiff ODEs, SDEs, and PDEs. These integrators employ coarse integration steps that do not resolve the fast timescale in the dynamics; nevertheless, they capture the correct effective contribution of the fast dynamics — in fact, we show that FLAVORs converge in a sense called two-scale flow convergence (F-convergence). Distinct from existing approaches, an identification of the underlying slow variables (or process) is not required, and intrinsic geometric structures (e.g., symplecticity, conservation laws, and invariant distribution) can be preserved by the multiscale simulation. These new properties are due to that FLAVORs average flow maps instead of vector fields.

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Design of a Schwarz coupling method for a dimensionally heterogeneous problem

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When dealing with simulation of complex physical phenomena and in order to avoid heavy numerical simulations, one can reduce a complex model in some locations and replace it by simplest ones - usually obtained after simplifications. Such simplifications in the model may involve a change in the geometry and the dimension of the physical domain. In that case, one deals with dimensionally heterogeneous coupling. We will present in this talk the case of 2-D Laplace equation with non symmetric boundary conditions coupled with a corresponding 1-D Laplace equation. We will first show how to obtain the 1-D model from the 2-D one by integration along one direction and after asymptotic analysis, by analogy with the link between shallow water equations and the Navier-Stokes system. Then, we will present an efficient Schwarz-like iterative coupling method. We will discuss the choice of boundary conditions at coupling interfaces. We will prove the convergence of such algorithms and give some theoretical results related to the choice of the location of the coupling interface, and the control of the error between a global 2-D reference solution and the 2-D coupled one. These theoretical results will be illustrated numerically.

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Numerical homogenization with non-separable scales

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Consider homogenization of divergence form operators with L^∞ coefficients which allows non-separable scales, in the sense of approximating the solution space with a finite dimensional space. Our method does not rely on concepts of ergodicity or scale-separation, buton the property that the solution space of these operators is compactly embedded in

H^1 if source terms are in the unit ball of L^2 instead ofthe unit ball of H^{-1}. Approximation spaces are generated by solving elliptic PDEs on localized sub-domains with source terms corresponding to approximation bases for H^2. The H^1-error estimates show that $\mathcal{O}(h^{-d})$-dimensional spaces with basis elements localized to sub-domains of diameter $\mathcal{O}(h^\alpha \ln \frac{1}{h})$ (with $\alpha \in [1/2, 1)$) result in an $\mathcal{O}(h^{2-2\alpha})$ accuracy for elliptic, parabolic and hyperbolic problems. The proposed method can be naturally generalized to vectorial equations (such as elasto-dynamics).

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