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Assyr Abdulle

Solving Multi-Scale problems with heterogeneous finite difference methods

Multi-scale differential equations are problems in which the variables can have different length scales. The direct numerical solution of differential equations with multiple scales is often difficult due to the work for resolving the smallest scale. We present here a strategy which allows the use of finite difference methods for the numerical solution of parabolic multi-scale problems, based on a coupling of macroscopic and microscopic models for the original equation.

1. Parabolic Multi-Scale Problems

We consider the following multi-scale parabolic equation:

$$\begin{aligned} \frac{\partial u^\varepsilon}{\partial t} &= \nabla \cdot \left(A(\frac{x}{\varepsilon}) \nabla u^\varepsilon \right) \text{ in } (0,T)\times\Omega && (1)\\ u^\varepsilon &= 0 \quad \text{on } (0,T)\times\partial\Omega && (2)\\ u^\varepsilon(0,x) &= g_\varepsilon(x) \in L^2(\Omega) && (3) \end{aligned}$$

where $u^\varepsilon = u^\varepsilon(t,x)$, $x \in \Omega \subset \mathbb{R}^d$ is a bounded domain, and $A^\varepsilon(x) = A(\frac{x}{\varepsilon}) = (A_{ij}(\cdot))_{i,j=1}^d$ with $A_{ij}(\cdot) \in L^\infty(\mathbb{R}^d)$, is uniformly elliptic, bounded and periodic in each of its spatial direction i.e.,

$$\begin{aligned} &\left(A(\frac{x}{\varepsilon})\xi, \xi \right) \geq \alpha|\xi|^2, \quad |A(\frac{x}{\varepsilon})\xi| \leq \beta|\xi| \quad \text{with } \alpha,\beta > 0, && (4)\\ &A_{ij}(y_1 + l_1, \ldots, y_d + l_d) = A_{ij}(y_1, \ldots, y_d), && (5) \end{aligned}$$

where we set $y_i = x_i/\varepsilon$ and $A(x/\varepsilon) = A(y)$. The functions $A_{ij}(y)$ will be referred as $y-$periodic functions.

Classical homogenization theory tells us that (see [2, chap.1,2])

$$u^\varepsilon \rightharpoonup u^0 \text{ weakly in } \quad L^2\left((0,T); H_0^1\right), \tag{6}$$

where u^0 is the solution of the so-called homogenized problem obtained from the solution of equations (1-3) in which A^ε is replaced by A^0 the *homogenized matrix* which does not contain the $\varepsilon-$scale. The homogenized equations are usually found by asymptotic expansion (see [2, chap.1,2]). However, in general it is not trivial, sometimes even impossible, to obtain the homogenized equations explicitly. Therefore it is of interest to design numerical methods that are based on the original microscale model (1-3).

2. Finite difference HMM

If we apply a standard finite difference scheme to equations (1-3), the discretization should satisfy $\Delta x < \varepsilon$ if we want to resolve the $\varepsilon-$scale. This can be prohibitive if ε is small. To overcome this problem we propose a "heterogeneous" discretization which cares about the fine scale *only on small representative regions of size* ε of the spatial domain. We give an overview of the method and refer to [1] for more details. We also refer to [3] for a general methodology for coupling macroscopic and microscopic models for several class of problems.

Let us consider the domain $\Omega = [0,1]\times[0,1]$ (for simplicity) of $\mathbb{R}^2$, and we discretize it with a coarse equidistant mesh (x_{1i}, x_{2j}), $i,j = 1,\ldots,N$, for which $\Delta x = x_{1i+1} - x_{1i} = x_{2j+1} - x_{2j}$ is much larger than ε. We define also $d_- = (\Delta x - \varepsilon)/2$, $d_+ = (\Delta x + \varepsilon)/2$ and four $\varepsilon-$cells around each point (x_{1i}, x_{2j}):

$$\begin{aligned} &I_1^\varepsilon = [x_{1i} - d_-, x_{1i} - d_+] \times [x_{2j} - \varepsilon/2, x_{2j} + \varepsilon/2], I_2^\varepsilon = [x_{1i} + d_-, x_{1i} + d_+] \times [x_{2j} - \varepsilon/2, x_{2j} + \varepsilon/2], && (7)\\ &I_3^\varepsilon = [x_{1i} - \varepsilon/2, x_{1i} + \varepsilon/2] \times [x_{2j} - d_-, x_{2j} - d_+], I_4^\varepsilon = [x_{1i} - \varepsilon/2, x_{1i} + \varepsilon/2] \times [x_{2j} + d_-, x_{2j} + d_+]. && (8) \end{aligned}$$

The idea is to evolve a macroscopic model for the flux form of the parabolic equation (1-3)

$$\frac{\partial U}{\partial t} = \nabla \cdot P, \tag{9}$$

on a *coarse grid* with *large time steps*, where $P(t, x_{1i}, x_{2j}) = (P_1, P_2)$ is estimated by solving the original equations around (x_{1i}, x_{2j}). Notice that a macroscopic model is known to exist from the homogenization theory. The goal is to estimate it by considering only the microscale equations (1-3).

Suppose that at time t^k we have a numerical solution of equation (9) on the coarse grid $(x_{1i}, x_{2j}) = x_{ij}$, denoted by U^k_{ij}. To find the coarse solution U^{k+1}_{ij} at time t^{k+1} we proceed in three steps:

1. For each x_{ij}, solve equations (1-3) on the four $\varepsilon-$cells $I^\varepsilon_l,\ l = 1, \ldots, 4$ with corresponding solutions $u^\varepsilon_l,\ l = 1, \ldots 4$ obtained by a finite difference method on a fine spacial grid (which resolves the ε scale) for a small time step δ. The boundary conditions are such that $u^\varepsilon_l(t, x) - U^k(x)$ is $\varepsilon-$periodic and the initial conditions are given by $U^k(x)$, a linear reconstruction of the coarse solution U^k (on each cell I^ε_l).
2. Compute $\nabla P_{ij} = \frac{P^k_{i+\frac{1}{2},j} - P^k_{i-\frac{1}{2},j} + P^k_{i,j+\frac{1}{2}} - P^k_{i,j-\frac{1}{2}}}{\Delta x} = F^k_{ij}(U^k)$, where $P^k_{i+\frac{1}{2},j}$ and $P^k_{i-\frac{1}{2},j}$ are averages of the micro-scale flux computed with the numerical solutions u^ε_l given by step 1 over I^ε_l for $l = 1, 2$. Similarly, $P^k_{i,j+\frac{1}{2}}$ and $P^k_{i,j-\frac{1}{2}}$ are the average of the micro-scale flux computed with the numerical solutions u^ε_l over I^ε_l for $l = 3, 4$.
3. Evolve the equation $\frac{\partial U^k}{\partial t} = F(U^k)$ on the coarse mesh $(x_{1i}, x_{2j}),\ i, j = 1, \ldots, N$, with a large time step Δt.

Be briefly comment on the micro solver. Let u^ε_l be the solution at time $t^k + \delta$ with initial conditions and boundary conditions as explained. The micro time δt should be chosen so that u^ε_l reaches a quasi-equilibrium. It is discussed in [3] that (for one dimensional problems) the "relaxation time" should be of order $\mathcal{O}(\varepsilon^2)$. This is illustrated by numerical computations in [1]. The average fluxes are then (for $l = 1, \ldots, 4$) a discrete version of

$$\frac{1}{|I^\varepsilon_l|} \int_{I^\varepsilon_l} A(x/\varepsilon) \nabla u^\varepsilon_l(t^k + \delta, x) dx. \tag{10}$$

Standard finite difference methods would consist in discretizing the whole domain with the microscopic model and produce a large number of equations (if ε is small compared to Ω). In the proposed finite difference heterogeneous multi-scale method (FD-HMM), based on the aforementioned coupling, the fine discretization is done only on small sub-domains of the original domain, of total measure $(N+1)^2 \cdot \varepsilon^2$, where N^2 is the number of coarse interior points. Notice that for each cell I^ε_l, the number of equations for solving the cell problem is independent of ε. It is shown in [1] that under the hypothesis that u^ε_l reaches a quasi-equilibrium on I^ε, we have

$$|U^n_{ij} - \bar{U}^n_{ij}| \leq \frac{C}{\Delta x} T \varepsilon, \tag{11}$$

where $T = n\Delta t$ and $\bar{U}^k_{ij}$ is the solution of a macroscopic scheme

$$\bar{U}^k_{ij} = \bar{U}^{k-1}_{ij} + \Delta t \cdot \bar{F}^{k-1}_{ij}, \tag{12}$$

chosen such that the micro-scale solver in the algorithm on I^ε_l, is replaced by the solution of the homogenized equations, on the same $\varepsilon-$cell I^ε_l, with the same boundary conditions. This result shows that the FD-HMM is consistent with the macro-scale scheme obtained by using the homogenized solution for the micro solver.

It is sometimes of interest to recover information about the micro-structural scale. This can be done by extending periodically the micro scale functions u^ε_l obtained on I^ε_l, between the coarse points (x_{1i}, x_{2j}). By periodic extension we mean that $u^\varepsilon_l - U^k$ is $\varepsilon-$periodic. We also explained in [1] how to extend the above algorithm for time dependent or rough non-periodic (random) coefficients, and indicate how the above algorithm can be applied to non-conservative problems. It can also be generalized for coefficients of the form $A(x, \frac{x}{\varepsilon})$.

3. References

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Dr.-Math. Assyr Abdulle, CoLab, Computational Laboratory, ETH Zürich, HRS F31, Hirschengraben 84, 8092 Zurich, e-mail abdulle@inf.ethz.ch