

## FAST COMMUNICATION

### HETEROGENEOUS MULTISCALE METHOD FOR LOCALLY SELF-SIMILAR PROBLEMS\*

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**Abstract.** We present a multiscale method for a class of problems that are locally self-similar in scales and hence do not have scale separation. Our method is based on the framework of the heterogeneous multiscale method (HMM). At each point where macroscale data is needed, we perform several small scale simulations using the microscale model, then using the results and local self-similarity to predict the needed data at the scale of interest. We illustrate this idea by computing the effective macroscale transport of a percolation network at the percolation threshold.

#### 1. Introduction and HMM Upscaling

In the last several years, there has been a tremendous growth of activity on developing multiscale methods in a number of application areas. For some reviews and perspectives, we refer to [4, 5, 8]. The primary goal is to develop computational techniques that can extract accurately the macroscale behavior of the system under consideration, at a cost that is substantially less than the cost of solving the microscale problem. Obviously this can only be done if the problem under consideration has some special features that can be taken advantage of. Up to now, with the exception of renormalization group methods [1], all other existing multiscale techniques assume that there is scale separation in the problem, and this property is used in an essential way in order to design efficient multiscale methods [5, 8].

While many problems, particularly problems with multi-physics, do have scale separation, there are other important problems with multiscales that do not have this property. The most well-known example is the fully developed turbulent flow whose active scales typically span continuously from the large energy pumping scale to the small energy dissipation scale, the ratio of these two scales was estimated by Kolomogorov to be of  $O(Re^{3/4})$  [2, 6]. Here  $Re$  is the Reynolds number of the flow which can easily reach  $10^9$  for atmospheric turbulence.

In the absence of scale separation, we must seek other special features of these problems in order to develop efficient computational methods. The special feature that we will focus on in this paper is (statistical) self-similarity in scales, namely that the averaged properties of the system at different scales are related to each other by simple scaling factors. This feature is approximately satisfied by many important problems such as turbulent flows and sub-surface transport in the inertial range of scales. We will call these type D problems (for the definition of type A, type B and type C problems, see [3]).

To develop an efficient computational technique, it is most convenient to use the framework of the heterogeneous multiscale method (HMM) [3]. HMM has two main components:

- Selecting the macroscale solver;

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- Estimating the needed data for implementing the selected macroscale solver using the microscale model.

For clarity, we will present the proposed method for a specific problem, namely transport over a two-dimensional bond percolation network at the percolation threshold.

In the standard two dimensional bond percolation model with parameter  $p, 0 \leq p \leq 1$ , we consider a square lattice, each bond of the lattice is either kept with probability  $p$  or deleted with probability  $1 - p$ . Of particular interest is the size of the percolation clusters formed by the remaining bonds in the network (see Figure 1.1 for a sample of bond percolation). The critical value for this model is at  $p = p^* = 0.5$ .

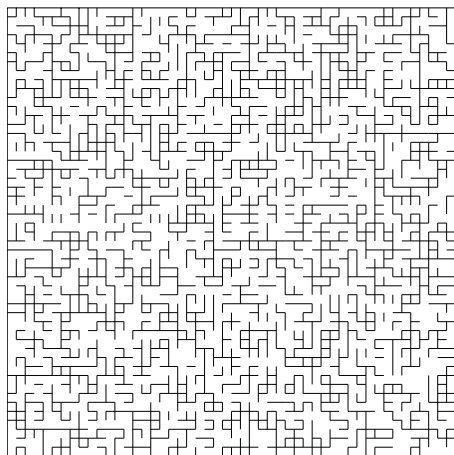


FIG. 1.1. *Bond percolation network on a square lattice at  $p = 0.5$*

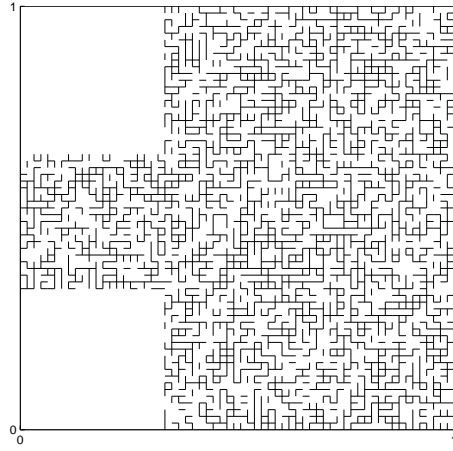
For an infinite lattice, if  $p < p^*$ , the probability of having infinite size clusters is zero. For  $p > p^*$ , the probability of having infinite size clusters is 1. Given the parameter value  $p$ , the network has a characteristic length scale – the correlation length, denoted by  $\xi_p$ . As  $p \rightarrow p^*$ ,  $\xi_p$  diverges as

$$\xi_p \sim |p - p^*|^\alpha, \quad (1.1)$$

where  $\alpha = -4/3$  (see [9]). At  $p = p^*$ ,  $\xi_p = \infty$ . In this case, the system has a continuum distribution of scales, i.e. it has clusters of all sizes. In the following we will consider the case when  $p = p^*$ .

To study transport, say of some pollutants whose concentration density will be denoted by  $c$ , we embed this percolation model into a domain  $\Omega \in R^2$ . We denote by  $\varepsilon$  the bond length of the percolation model, and  $L$  the length scale for the domain  $\Omega$ . We will consider the case when  $\varepsilon/L$  is very small. In our numerical example, we set  $\Omega = [0, 1]^2$ . In order to introduce interesting macroscale behavior, we assume that the lower- and upper-left corners of the domain are impermeable (see Figure 1.2). We will consider the following boundary condition: No-flow at the upper boundary ( $y = 1$ ) and lower boundary ( $y = 0$ ),  $c = 1$  at the left boundary ( $x = 0$ ),  $c = 0$  at right boundary ( $x = 1$ ).

Denote by  $S_{i,j}, i, j = 1, \dots, N$  the  $(i, j)$ -th site of the percolation network, and

FIG. 1.2. *Microstructure and the macro domain*

$c_{i,j}$  the concentration at that site. Define the fluxes

$$\begin{aligned}
 \text{the flux from right} & f_{i,j}^r = B_{i,j}^x (c_{i+1,j} - c_{i,j}), \\
 \text{the flux from left} & f_{i,j}^l = B_{i-1,j}^x (c_{i-1,j} - c_{i,j}), \\
 \text{the flux from top} & f_{i,j}^t = B_{i,j}^y (c_{i,j+1} - c_{i,j}), \\
 \text{the flux from bottom} & f_{i,j}^b = B_{i,j-1}^y (c_{i,j-1} - c_{i,j}).
 \end{aligned}$$

Here the various  $B$ 's are bond conductivity for the bond specified by the difference in the parenthesis. The bond conductivity  $B$  is zero if the corresponding bond is deleted, and 1 if the bond is retained. At each site  $S_{i,j}$ , from mass conservation, we have

$$f_{i,j}^t + f_{i,j}^b + f_{i,j}^r + f_{i,j}^l = 0, \quad (1.2)$$

i.e. the total flux to this site is zero. This will be our microscale model.

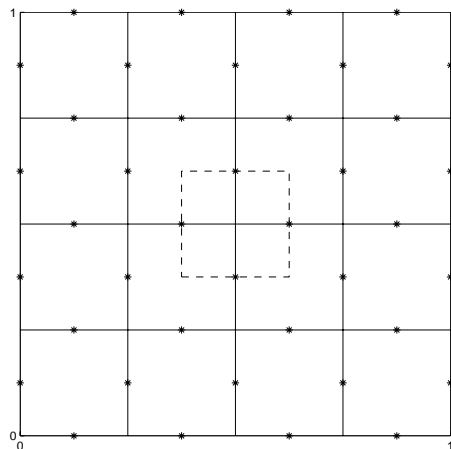
For the macroscale solver, we will choose a finite volume scheme over a macroscale grid  $\Omega_H$  where  $H$  is the size of the finite volume cell (see Fig 1.3). The data that we need to estimate from the microscale model, here the percolation model, are the fluxes at the mid-points of cell boundary. Since the present problem is linear, we only need to estimate the effective conductivity for a network of size  $H$ . We note that since  $p = p^*$ , the effective conductivity is strongly size-dependent. In fact there are strong evidences that the following relation holds [7]:

$$\kappa_L = C_0 L^\beta \quad (1.3)$$

where  $\kappa_L$  is the mean effective conductivity at size  $L$ .

Our basic strategy is to make use of such relations in estimating the effective fluxes in the case when  $\varepsilon \ll H$ .

For this purpose, we perform a series of microscopic simulations on systems of size  $L_1$  and  $L_2$  where  $\varepsilon \ll L_1 < L_2 \ll H$ . From the results we estimate  $\kappa_{L_1}$  and  $\kappa_{L_2}$ . We next use these results to estimate the parameter values  $C_0, \beta$  in (1.3). Once we have these parameters, we can use (1.3) to predict  $\kappa_H$ .

FIG. 1.3. *Finite volume mesh with size of  $H$* 

## 2. Numerical Results

In the following, we present some numerical results. In order to test the accuracy of such a procedure, we compare the  $\kappa_H$  values predicted in this way, and the  $\kappa_H$  values that are computed directly on a system of size  $H$ . We then present one example in which we perform the full HMM computation.

**Validation of self similarity.** We consider bond percolation on the domain  $\Omega = [0, 1]^2$  with bond length  $\varepsilon = 1/1024$  (see Figure 1.1 for a sample). In Figure 2.1 we show a log-log plot of the effective conductivity as a function of scale. One sees clearly that the power law behavior is validated.

To see how much statistical fluctuation there is, we compare the actual and predicted (using self-similarity) values of the conductivity for a number of realizations of the percolation network. The results are shown in Figure 5. In this figure  $L = 128$  and the predicted values are computed using simulated values from lattices with  $L = 16$  and  $L = 32$ .

**Validation of the HMM upscaling procedure.** Next we test the HMM procedure for a problem shown in Figure 2. To establish the microstructure, a bond percolation network on the domain  $\Omega = [0, 1]^2$  with bond length  $\varepsilon = 1/2048$  and  $p = 0.5$  was first generated, then the bonds in the squares of size  $1/3$  at the lower- and upper-left corners were all removed (see Figure 1.2 for a sample).

At the macroscale, the finite volume method was used on a uniform grid with grid size  $H = 1/16 = 128\varepsilon$  (see Figure 1.3). The “exact” solution for this problem is shown in Figure 2.3 which was obtained by using the actual computed effective conductivity  $\kappa_H$ . Results using the method presented in this paper are shown in Figures 2.4 and 2.5. These are obtained by the following procedure. For each macro cell boundary, instead of the actual effective conductivity, we use the value predicted by (1.3) from the averaged values of  $\kappa_{L_1}$  and  $\kappa_{L_2}$  with  $L_1 = 16\varepsilon$  and  $L_2 = 32\varepsilon$ . The difference between Figure 2.4 and Figure 2.5 is in how the ensemble averages are taken to compute the effective conductivity. In Figure 2.4,  $\kappa_{L_1}$  and  $\kappa_{L_2}$  were obtained by averaging the effective conductivities on 16 different nearby  $L_1 \times L_1$  and  $L_2 \times L_2$  blocks respectively. In Figure 2.5, only 4 different blocks were used to compute the average values. We see that the results in Figure 2.4 is smoother.

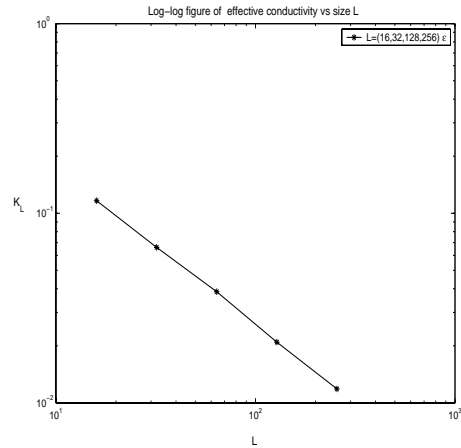


FIG. 2.1. *Effective conductivity at different scale  $L = (16, 32, 64, 128, 256)\epsilon$  for a realization of the percolation network with  $p = p^* = 0.5$ .*

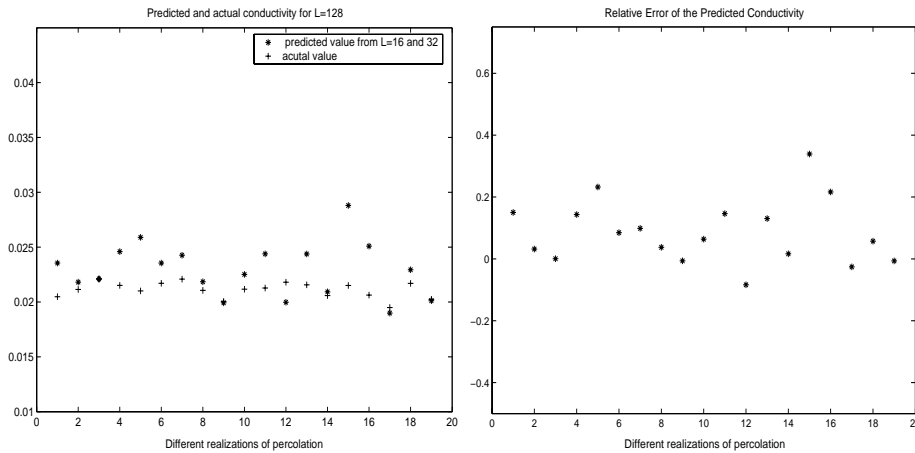


FIG. 2.2. *Effects of fluctuaton: Effective conductivity at scale  $L = 128\epsilon$  for different realizations of the percolation network with  $p = 0.5$ . Left: the actual values and values predicted from  $L = 16\epsilon$  and  $32\epsilon$ ; Right: relative error between predicted and computed values.*

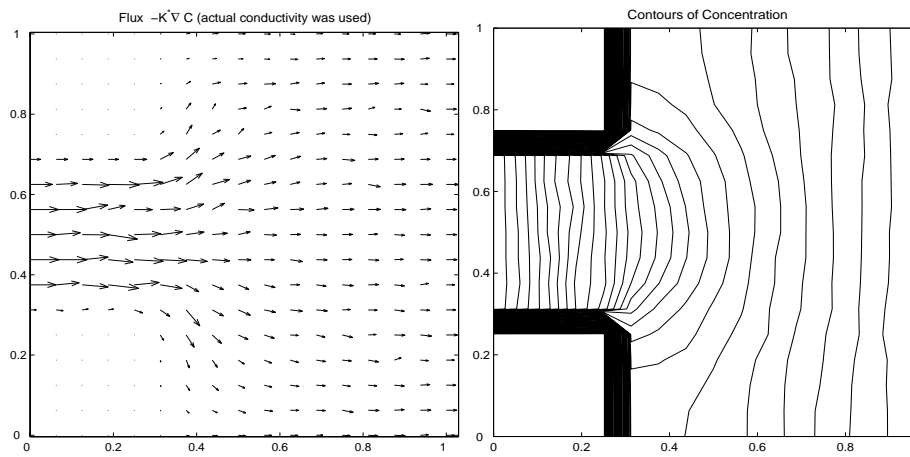


FIG. 2.3. Results of flux and concentration distribution at the macro scale. Actual values of the effective conductivity were used.

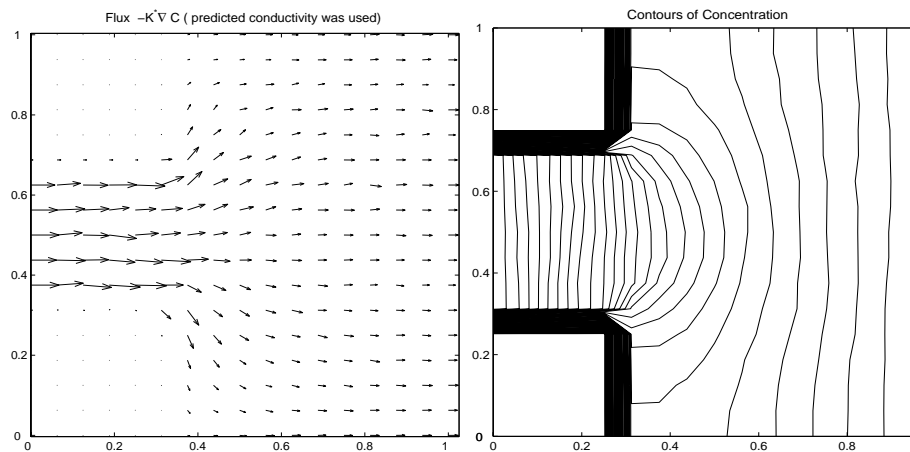


FIG. 2.4. Results of flux and concentration distribution at the macro scale. Effective conductivity  $\kappa_H$  was predicted by ensemble averaged values of  $\kappa_{L_1}$  and  $\kappa_{L_2}$  with  $L_1 = 16\varepsilon$  and  $L_2 = 32\varepsilon$  over 16 blocks at each macro cell boundary.

As far as efficiency is concerned, for the present example there is not much savings in the HMM procedure compared with direct computation. This is because the fine scale problem is not that large. Imagine a case where the fine scale problem is 100 times larger in each direction (i.e. the bond length is 100 times smaller), then direct computation with the microscale model becomes impossible, but the HMM procedure will have the same cost as the present example, since the macro domain has not changed.

The present example can be treated by a sequential coupling procedure, namely that the effective conductivity at the scale  $H$  can be computed beforehand from the microscale model using the procedure we described since it is just a fixed number.

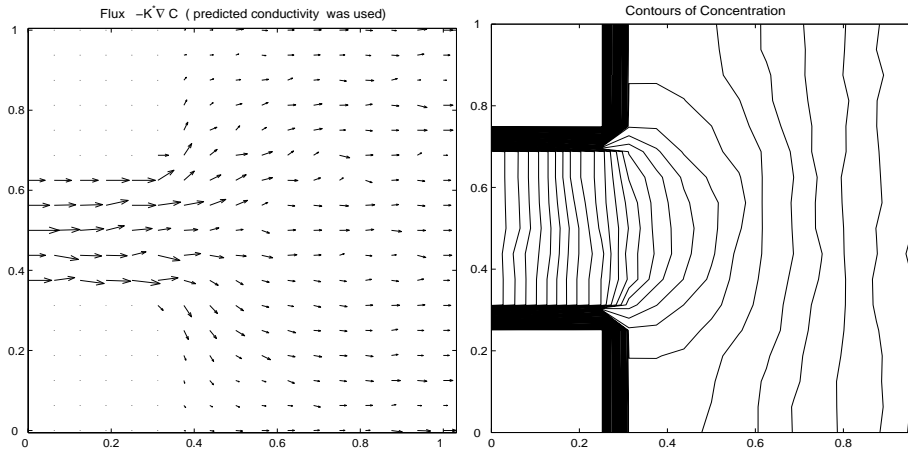


FIG. 2.5. Results of flux and concentration distribution at macro scale. Effective conductivity  $\kappa_H$  was predicted by ensemble averaged values  $\kappa_{L_1}$  and  $\kappa_{L_2}$  with  $L_1 = 16\epsilon$  and  $L_2 = 32\epsilon$  over 4 blocks at each macro cell boundary.

But one can easily imagine other problems for which the needed data depend on more parameters. In these cases, a “on the fly” coupling procedure might be more efficient.

### 3. General Strategy

These examples illustrate very well the overall strategy for data estimation. As was discussed in [3], the general strategy is to extract the information at the scale of interest by performing constrained microscopic simulations on systems of much smaller sizes. If there is scale separation in the system, then the needed quantities should be quite independent of the size of the microscopic system, e.g.

$$\kappa_L = \text{Const}$$

as long as the size of that system is much larger than some characteristic scale of the microscopic model, which might just be the correlation length. But this is certainly not the only situation for which the general philosophy outlined in [3] works. As long as the size dependence is of a simple form, e.g.

$$\kappa_L = f(L) \tag{3.1}$$

where  $f$  depends on few parameters, we can make use of this simple relationship by performing a few (not just one as was done for problems with scale separation) small scale simulations and use the results to predict the needed quantities at a much larger scale. One example of such a situation is when the system exhibits local self-similarity. In this case the dependence in (3.1) is of the form  $f(L) = C_0 L^\beta$  and we can use results of microscopic simulations at two different scales to predict the result at a much larger scale, namely  $H$ , as was done earlier.

The efficiency and accuracy of this procedure depends crucially on how accurate and complex (3.1) is. For many problems, (3.1) only holds in statistical sense, i.e. the data in the left hand side are ensemble averaged quantities. In this case, a crucial point is the size of the fluctuations which will depend on how we sample the microscopic problems. We have done some preliminary study of this problem but it certainly should be investigated more thoroughly in future work.

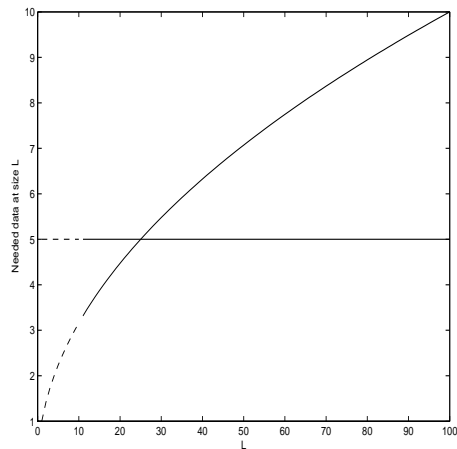


FIG. 3.1. Data estimation for systems with scale separation (straight line) and systems with self-similarity in scales (curved line).

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