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INTERPRETATION OF CLOSURE VARIABLES IN UPSCALING

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Summary. In many engineering applications, it is common to find systems that involve transport at several scales. To study these systems it is convenient to derive models at an intermediate level of scale between the microscale and the macroscale; this is the average scale. This can be achieved using the method of volume averaging. The results from this method are averaged transport equations expressed in terms of effective medium coefficients that can be computed from the solutions of associated closure problems. Such solutions are often written as superpositions of the so-called closure variables and the average sources of deviation. In this work, we revisit the concept of a closure variable based on an integral formulation in terms of Green's functions. Our analysis demonstrates that a closure variable represents the integration (in time and space) of the associated Green's functions that describe the influence of the average sources on the deviation fields of a given property at a certain time. In this way, the Green's functions are responsible for capturing the essential information from the microstructure. Extensions to cases involving transport with nonlinear reaction are also discussed.

1 INTRODUCTION

Most engineering applications involve transport across several levels of scale, which are deeply coupled. Despite current computational capabilities, it is still generally not feasible (or desirable) to model a complete macroscopic system (as the one depicted in Fig. 1) by performing direct numerical simulations at the microscale. To overcome this issue, one may derive models at an intermediate level of resolution between the microscale and the macroscale; this is the average scale (Fig. 1). Average models consist of a set of effective medium equations and boundary conditions that result from a systematic reduction in the number of degrees of freedom involved in the microscale model by means of the process of upscaling [1, 2]. In other words, the derivation of models at the average scale can be achieved by *filtering* redundant information from the microscale. This is possible by

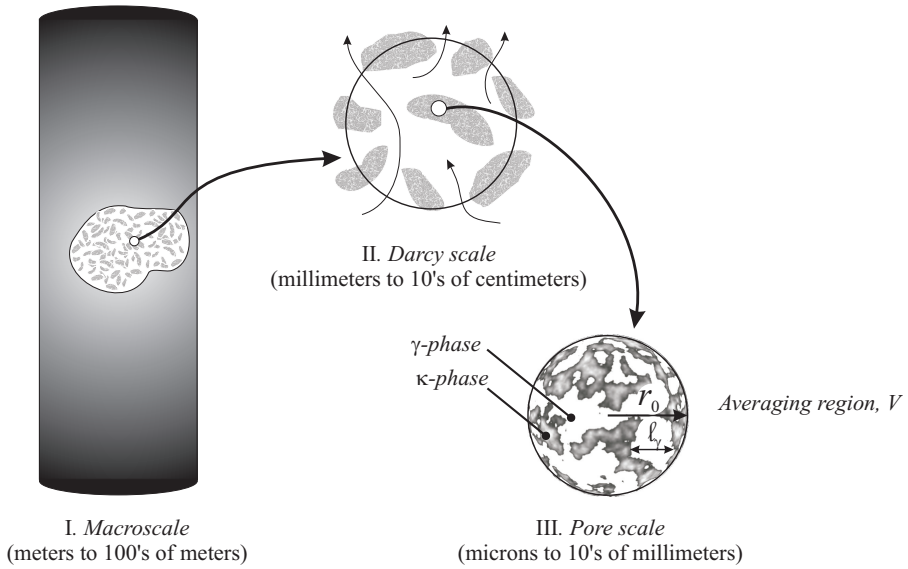

Figure 1: Characteristic lengths of a typical engineering system.

adopting a set of *scaling laws*, in the form of temporal and spatial constraints and assumptions that bound the validity of the model [3]. This approach leads to upscaled models containing effective medium coefficients that are the connection with the microscale.

In the method of volume averaging [2], the effective medium coefficients are often expressed in terms of (volume and/or surface) integrals of the so-called *closure variables*, which result from solving associated boundary-value problems in a representative model of the microstructure (i.e., the unit cell). In this work, we discuss the method of volume averaging as one approach to upscale microscale balance equations for transport in porous media. Our particular focus is to illustrate how the closure problem solutions can be posed in terms of Green's functions to generalize the averaging approach. In this way, the kernel of the microstructure information is given by the Green's functions; while the integration of the product of the deviation sources with the kernel defines the closure variables. Furthermore, the integral formulation derived here can serve as the starting point for the solution of closure problems involving nonlinear terms. These types of problems are relevant in many fields of science and engineering, including reactive transport in porous media, transport in biofilms, chemotaxis in contaminated aquifers, among many others. For the sake of briefness in presentation, in the following paragraphs we will describe our approach in general terms.

2 METHODOLOGY

2.1 Microscale model

Consider the balance equation for a given property (ψ_γ) in a two-phase (fluid-solid) system, such as the porous medium sketched in Fig. 1. The fluid phase is identified as the

γ-phase, while the rigid solid is represented by the κ-phase. For the developments that follow we assume that the problem is linear (or can be linearized) and let the governing differential equation for the transport of ψ_γ at the microscale be expressed as

$$\lambda\{\psi_\gamma\} = f, \text{ in the } \gamma\text{-phase}, \tag{1}$$

where f denotes a source term, which for the sake of simplicity is assumed to be known and independent of ψ_γ. In Eq. 1 $\lambda\{\cdot\}$ denotes a given linear differential operator, which may contain space and time derivatives and given transport coefficients.

The boundary condition at the solid-fluid interface can be written, in general, as a jump condition [4]

$$\varphi\{\psi_\gamma\} = g, \text{ at the } \gamma\text{-}\kappa \text{ interface}, \tag{2}$$

in which, $\varphi\{\cdot\}$ is a linear differential operator and g is an interfacial source term. The microscale description is completed with the corresponding boundary conditions at the entrances and exits of the macroscopic system and the initial condition, which are not provided here for the sake of briefness in presentation.

2.2 Upscaling

To spatially smooth the microscale governing equations let us introduce a support averaging region V (REV) of volume $\mathscr{V}$ (Fig. 1) [2]. In this way, the averaging region can be decomposed according to, $\mathscr{V} = \mathscr{V}_\kappa + \mathscr{V}_\gamma$, with $\mathscr{V}_\kappa$ and $\mathscr{V}_\gamma$ being the volumes of the κ- and γ-phases within the REV, respectively. The radius of the averaging region (r_0) should be sufficiently large with respect to the characteristic length of the microscale (ℓ_γ) but, at the same time, sufficiently smaller than the characteristic length of the macroscale (L); that is, $\ell_\gamma \ll r_0 \ll L$.

In terms of the averaging region V, let us introduce the intrinsic averaging operator as

$$\langle\psi_\gamma\rangle^\gamma = \frac{1}{\mathscr{V}_\gamma}\int_{V_\gamma} \psi_\gamma dV, \tag{3}$$

which is related to the superficial averaging operator, $\langle\psi_\gamma\rangle$, by $\langle\psi_\gamma\rangle^\gamma = \varepsilon_\gamma^{-1}\langle\psi_\gamma\rangle$, with ε_γ being the volume fraction of the γ-phase within the averaging region.

Our next step in the analysis is to apply the intrinsic averaging operator (Eq. 3) to the microscale governing equation (Eq. 1), in order to obtain

$$\langle\lambda\{\psi_\gamma\}\rangle^\gamma = \langle f\rangle^\gamma. \tag{4}$$

Upon properly interchanging differentiation and integration, this expression can be written as

$$\Lambda\{\langle\psi_\gamma\rangle^\gamma\} + \mathscr{M}\{\psi_\gamma\} = \langle f\rangle^\gamma, \tag{5}$$

where the differential operator $\Lambda\{\langle\psi_\gamma\rangle^\gamma\}$ contains spatial and temporal derivatives of $\langle\psi_\gamma\rangle^\gamma$. The integro-differential operator $\mathscr{M}\{\cdot\}$ contains the *filters of information* from the

microscale [2]. In order to avoid expressing Eq. 5 in terms of the point variable ψ_γ, we use the spatial decomposition [5]

$$\psi_\gamma = \langle \psi_\gamma \rangle^\gamma + \widetilde{\psi}_\gamma, \tag{6}$$

so that Eq 5 can be rewritten as

$$\mathscr{L}\{\langle \psi_\gamma \rangle^\gamma\} + \mathscr{M}\{\widetilde{\psi}_\gamma\} = \langle f \rangle^\gamma, \tag{7}$$

where $\mathscr{L}\{\langle \psi_\gamma \rangle^\gamma\} = \Lambda\{\langle \psi_\gamma \rangle^\gamma\} + \mathscr{M}\{\langle \psi_\gamma \rangle^\gamma\}$. Note that, in general, $\mathscr{L}\{\cdot\} \neq \lambda\{\cdot\}$. Our next step in the analysis is to express the deviation fields, $\widetilde{\psi}_\gamma$, in terms of $\langle \psi_\gamma \rangle^\gamma$; this process is usually termed *closure*.

2.3 Closure problem

According to Eq. 6, the governing equation for $\widetilde{\psi}_\gamma$ can be obtained by subtracting Eq. 7 from Eq. 1; the result is given by

$$\underbrace{\lambda\{\widetilde{\psi}_\gamma\}}_{local\ transport} - \underbrace{\mathscr{M}\{\widetilde{\psi}_\gamma\}}_{non-local\ transport} = \underbrace{\mathscr{L}^*\{\langle \psi_\gamma \rangle^\gamma\}}_{volume\ sources}, \text{ in the } \gamma\text{-phase}, \tag{8}$$

where $\mathscr{L}^*\{\langle \psi_\gamma \rangle^\gamma\} = \mathscr{L}\{\langle \psi_\gamma \rangle^\gamma\} - \lambda\{\langle \psi_\gamma \rangle^\gamma\} + f - \langle f \rangle^\gamma$. In many application examples, the non-local term can be assumed negligible with respect to its local counterpart on the basis of the length-scale constraint $\ell_\gamma \ll L$. Furthermore, in situations where it is not possible to apply these simplifications, some algebraic re-arrangements can be performed that lead to a local closure problem. For the sake of simplicity, we assume that any of these alternatives are applicable, so that the non-local transport term is neglected in Eq. 8.

The interfacial boundary condition arises from using the spatial decomposition (Eq. 6) in Eq. 2,

$$\varphi\{\widetilde{\psi}_\gamma\} = \underbrace{\mathscr{J}^*\{\langle \psi_\gamma \rangle^\gamma\}}_{surface\ sources}, \text{ at the } \gamma\text{-}\kappa \text{ interface}, \tag{9}$$

where $\mathscr{J}^*\{\langle \psi_\gamma \rangle^\gamma\} = g - \varphi\{\langle \psi_\gamma \rangle^\gamma\}$. In Eqs. 8 and 9, we have identified the volume and surface sources of deviations, which are usually linear combinations of $\langle \psi_\gamma \rangle^\gamma$ and its derivatives. Furthermore, on the basis of the length scale constraint $\ell_\gamma \ll L$, it is reasonable to assume that the boundary conditions at the entrances and exits of the macroscopic region have a limited range of influence. This allows solving the closure problem only in a representative unit cell of the microstructure of the system. Under this assumption, we impose the following boundary condition at the entrances and exits of the unit cell ($A_{\gamma e}$):

$$\widetilde{\psi}_\gamma(\mathbf{r} + \mathbf{l}_i) = \widetilde{\psi}_\gamma(\mathbf{r}) \text{ at } A_{\gamma e},\ i = 1, 2, 3. \tag{10}$$

Finally, we impose the following constraint

$$\left\langle \widetilde{\psi}_\gamma \right\rangle^\gamma = 0, \forall t, \tag{11}$$

which allows setting the levels of the deviation fields.

2.4 Formal solution of the closure problem

In order to formally solve the closure problem given by Eqs. 8-11, in terms of the associated Green's functions, $G(\mathbf{r},t;\mathbf{y},\tau)$, it is necessary to derive the corresponding initial and boundary-value problem for $G(\mathbf{r},t;\mathbf{y},\tau)$. This problem consists of the differential equation

$$\lambda\{G(\mathbf{r},t;\mathbf{y},\tau)\} = \delta(\mathbf{r}-\mathbf{y})\delta(t-\tau), \text{ in the } \gamma\text{-phase}, \tag{12}$$

where δ denotes the Dirac's delta function. Eq. 12 is subject to the homogeneous versions of Eqs. 9-11. In addition, the Green's functions must satisfy the causality principle

$$G(\mathbf{r},t;\mathbf{y},\tau) = 0, \text{ for } t < \tau. \tag{13}$$

which expresses that the Green's function is the response (at position $\mathbf{r}$ and time t) to a source located at $\mathbf{r}=\mathbf{y}$ at time $t=\tau$ and not to any nonzero earlier condition.

Given the linear nature of this problem, it is possible to find a unique solution for the fields of $G(\mathbf{r},t;\mathbf{y},\tau)$. Therefore, using standard Green's function analysis, the formal solution of the closure problem can be expressed as follows:

$$\begin{aligned}\widetilde{\psi}_\gamma(\mathbf{r},t) \;=\; & \underbrace{\int_{\mathbf{y}\in V_\gamma} G(\mathbf{r},t;\mathbf{y},0)\widetilde{H}(\mathbf{y})d\mathbf{y}}_{influence\ of\ the\ initial\ condition} \;+\; \underbrace{\int_{\tau=0}^{\tau=t}\int_{\mathbf{y}\in V_\gamma} G(\mathbf{r},t;\mathbf{y},\tau)\mathscr{L}^*\{\langle\psi_\gamma\rangle^\gamma\}(\mathbf{y},\tau)d\mathbf{y}d\tau}_{influence\ of\ the\ volume\ sources} \\ & + \underbrace{\int_{\tau=0}^{\tau=t}\int_{\mathbf{y}\in A_{\gamma\kappa}} \mathscr{H}\left[G(\mathbf{r},t;\mathbf{y},\tau);\, \mathscr{J}^*\{\langle\psi_\gamma\rangle^\gamma\}(\mathbf{y},\tau)\right] d\mathbf{y}d\tau}_{influence\ of\ the\ surface\ sources}\end{aligned} \tag{14}$$

Despite this substantial simplification, we note that the average fields are contained in spatial and time integrals. This means that if $\widetilde{\psi}_\gamma$ is substituted in its present form into the upscaled model (Eq. 7), the result is a non-local macroscale equation. Non-local equations are the least used in practice since they require the solution of a complete space matrix at each time step. However, the length and time scale constraints

$$\frac{r_0}{L} \ll 1;\; \frac{t^*}{T^*} \ll 1, \tag{15}$$

justify taking out the average terms from the integrals in the solution of $\widetilde{\psi}_\gamma$. Under these assumptions, the solution of the closure problem can be written in terms of the n (volume and surface) sources as follows

$$\widetilde{\psi}_\gamma = \sum_{i=0}^{i=n} b_i \mathscr{H}_i^*\{\langle\psi_\gamma\rangle^\gamma\}, \tag{16}$$

where $\mathscr{H}_0^*\{\langle\psi_\gamma\rangle^\gamma\} = 1$, so that b_0 accounts for the non-average sources (e.g., the influence of the initial condition). Since the particular mathematical structure of each source is known, the operators $\mathscr{H}_i^*\{\langle\psi_\gamma\rangle^\gamma\}$ $(i \geq 1)$ can be regarded as known algebraic and/or differential operators. Finally, the variables b_i $(i \geq 0)$ are the so-called closure variables that map the influence of the average sources on the fields of $\widetilde{\psi}_\gamma$ [2] and they can be scalar, vectorial or tensorial fields. From the derivations provided above we note that b_i are kernels resulting from integrations involving the associated Green's function. In Eq. 16 we have made an effort to provide a compact and general expression for the deviation fields, the specific dimensionality of the closure variables are determined by each source term. Indeed, due to the linear nature of Eqs. 8-11, it is possible to obtain Eq. 16 on the basis of the principle of superposition. In fact, this is the approach commonly followed in the volume averaging literature [2], which leads to the solution of $n+1$ independent problems for the computation of all the closure variables that determine the deviation fields.

At this point, it is opportune to stress that if the closure problem involves nonlinear terms, it is not possible, in general, to obtain explicit formal solutions, as the one given in Eq. 16. To overcome this issue, many alternatives are possible, for example one may expand the nonlinear term using Taylor series and conserve only the linear parts of the expansion (i.e., linearization) or use the effectiveness factor concept for nonlinear kinetics as explored by Wood et al.[6]. Another approach is to rely on the integral formulation relating the linear parts of the problem to the associated Green's function and treating the nonlinear terms as special sources. In this form, the nonlinearities are not approximated by linear or semi-linear models, however the price to be paid is that the formal solution is now an implicit expression. To have a clear idea of this approach, consider the case in which the governing differential equation for $\widetilde{\psi}_\gamma$ is given by

$$\lambda\{\widetilde{\psi}_\gamma\} = \mathscr{L}^*\{\langle\psi_\gamma\rangle^\gamma\} + \mathscr{N}\{\widetilde{\psi}_\gamma\}, \text{ in the } \gamma\text{-phase}, \tag{17}$$

where $\mathscr{N}\{\cdot\}$ is a nonlinear (algebraic and/or differential) operator. If one regards this term as a source in the differential equation, one may follow the derivations provided above to obtain a solution of the form

$$\widetilde{\psi}_\gamma = \sum_{i=0}^{i=n} b_i \mathscr{H}_i^*\{\langle\psi_\gamma\rangle^\gamma\} + \int_{\tau=0}^{\tau=t} \int_{\mathbf{y}\in V_\gamma} G(\mathbf{r},t;\mathbf{y},\tau)\mathscr{N}\{\widetilde{\psi}_\gamma\}(\mathbf{y},\tau)d\mathbf{y}d\tau, \tag{18}$$

which is clearly not explicit. The fields of $\widetilde{\psi}_\gamma$ may be obtained through appropriate iterative schemes. Fortunately, the smoothing properties of the integral operators (where the terms to be iterated are contained), allow achieving faster numerical convergence than with traditional schemes which rely on the discretization (and thus propagation) of errors. Notice that, in this case, the operator $\mathscr{L}^*\{\cdot\}$ in Eq. 17 may be nonlinear, and thus the operators $\mathscr{H}_i^*\{\cdot\}$ related to volume sources will also be nonlinear. If the numerical scheme is convergent, one may use Eq. 18 to obtain a closed form of the macroscale model. This constitutes an advantage over the superposition method, which is constrained to linear closure problems.

3 CLOSED UPSCALED MODEL

As a final step in the analysis, let us close the upscaled model by substituting Eq. 16 into Eq. 7; the result can be expressed as follows

$$\mathscr{F}\{\langle\psi_\gamma\rangle^\gamma\} = \langle f\rangle^\gamma, \tag{19}$$

where $\mathscr{F}\{\langle\psi_\gamma\rangle^\gamma\} = \mathscr{L}\{\langle\psi_\gamma\rangle^\gamma\} + \mathscr{M}\left\{\sum_{i=0}^{i=n} b_i \mathscr{H}_i^*\{\langle\psi_\gamma\rangle^\gamma\}\right\}$. Fortunately, in many situations only a subset of the $n+1$ closure variables (say $0 < m < n+1$) passes through the filters in the operator $\mathscr{M}\{\cdot\}$. Analytical solutions of the Green's functions can be obtained in the simple geometries involved in Chang's unit cell as reported by Ochoa-Tapia et al. [7]. Furthermore, for spatially periodic unit cells Wood [3] used a combination of Laplace and finite Fourier transforms in order to obtain an expression for the Green's functions related to dispersion in porous media. Despite these advances, it is certainly worth pursuing the numerical computation of Green's functions in complicated domains for a practical and efficient prediction of the closure variables. We are currently working on these computations and preliminary results are not presented here for the sake of briefness.

4 CONCLUSIONS

In this work we have revisited the concept of a closure variable involved in the upscaling of microscale models using the method of volume averaging. According to our analysis, a closure variable is, in general, the result of integrating (in time and space) the influence function (i.e., the Green's function) that captures the essential information of the transport and geometry in the microscale. This allows expressing the deviation fields as the sum of all the influences of the sources involved in the closure problem. In this form, the closure variables account, in general, for the influence of the initial condition, the volume and surface sources. The boundary conditions at the entrances and exits of the macroscale system are not usually taken into account by the closure variables since their influence is assumed to be of short range when there is a separation of characteristic lengths between the microscale and the macroscale (i.e., $\ell_\gamma \ll L$).

An attractive feature of the integral formulation is the fact that for closure problems containing n source terms, it is only necessary to solve one problem in order to compute the associated Green's function and from it obtain each of the $n+1$ closure variables by performing the corresponding integration steps. This is an improvement from the typical approach used in the volume averaging literature where the governing problem for the spatial deviations is decomposed into $n+1$ independent closure problems. Furthermore, the associated Green's functions arise from solving initial and boundary-value problems that only depend of the local information of the system captured in the representative unit cells and are independent of the average sources. It should be emphasized that this is possible due to the separation of length ($r_0 \ll L$) and time ($t^* \ll T^*$) scales between the microscale and the macroscale. The arguments presented in this work demonstrate that the Green's functions are the kernel of the closure variables, and hence they play a significant role on the computation of the effective transport coefficients involved in upscaled models.

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