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Volume averaging: Local and nonlocal closures using a Green's function approach

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ABSTRACT

Modeling transport phenomena in discretely hierarchical systems can be carried out using any number of upscaling techniques. In this paper, we revisit the method of volume averaging as a technique to pass from a microscopic level of description to a macroscopic one. Our focus is primarily on developing a more consistent and rigorous foundation for the relation between the microscale and averaged levels of description. We have put a particular focus on (1) carefully establishing statistical representations of the length scales used in volume averaging, (2) developing a time–space nonlocal closure scheme with as few assumptions and constraints as are possible, and (3) carefully identifying a sequence of simplifications (in terms of *scaling postulates*) that explain the conditions for which various upscaled models are valid. Although the approach is general for linear differential equations, we upscale the problem of linear convective diffusion as an example to help keep the discussion from becoming overly abstract.

In our efforts, we have also revisited the concept of a closure variable, and explain how closure variables can be based on an integral formulation in terms of Green's functions. In such a framework, a closure variable then represents the integration (in time and space) of the associated Green's functions that describe the influence of the average sources over the spatial deviations. The approach using Green's functions has utility not only in formalizing the method of volume averaging, but by clearly identifying how the method can be extended to transient and time or space nonlocal formulations.

In addition to formalizing the upscaling process using Green's functions, we also discuss the upscaling process itself in some detail to help foster improved understanding of how the process works. Discussion about the role of *scaling postulates* in the upscaling process is provided, and poised, whenever possible, in terms of measurable properties of (1) the parameter fields (including the indicator fields describing the medium geometry) associated with the transport phenomenon of interest, and (2) measurable properties of the independent variable itself. To highlight the relevance of this interpretation we study the benchmark problem of linear nonlocal diffusion in porous media.

1. Introduction

Transport phenomena modeling in hierarchical, multiscale systems requires the systematic passing of information from one scale to the others. Despite current advances in computational capabilities, it is still generally not feasible to model a complete macroscopic system (such as the discretely hierarchical system depicted in Fig. 1) by performing direct numerical simulations of microscale formulations. Furthermore, even if such a feat were possible, there is the question about how one would usefully apply such information. One method to address this problem is to directly derive models at an intermediate level of resolution between the microscale and the macroscale, using an averaging operator. The averaging operator itself may be viewed as the response of an instrument probing intensive field variables; this interpretation has been discussed by Baveye and Sposito [9] and by Cushman [24]. In this special issue of *Advances in Water Resources* two different (but related) perspectives on averaging are presented. One (known generally as the method of volume averaging with closure, or MVA) is represented by this paper; the second presents an overview of the thermodynamically constrained averaging theory (TCAT), which has been clearly presented in a separate paper by Gray et al. [34].

In this work, we consider the averaging of a linear convection–dispersion-reaction equation starting from the sub-pore scale of resolution. Developing an averaged model consists of applying an averaging operator to the relevant balances as they occur for the microscale level of resolution (Level I in Fig. 1). The averaging process allows one to develop a set of equations and boundary conditions at the macroscale level (Level III in Fig. 1). The result is a systematic reduction in the number of degrees of freedom involved in the microscale model by means of the process of upscaling (*cf.*

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Nomenclature

a	radius of the cylindrical-shaped obstacle in Chang's unit cell, m
$\mathbf{A}_\gamma$	a closure variable that maps $\nabla\nabla\langle\psi_\gamma\rangle^\gamma$ onto $\tilde{\psi}_\gamma$, m^2
$\mathcal{A}_{\gamma\kappa,M}$	surface domain of the fluid–solid interface within the entire macroscopic volume $\mathcal{V}_M$
$\mathcal{A}_{\gamma e,M}$	surface domain associated with the external boundary of the macroscopic volume $\mathcal{V}_M$ and intersecting the γ-phase
$\mathcal{A}_{\kappa e,M}$	surface domain associated with the external boundary of the macroscopic volume $\mathcal{V}_M$ and intersecting the κ-phase
$\mathcal{A}_{e,M}$	surface domain associated with the external boundary of the macroscopic volume $\mathcal{V}_M$ ($\mathcal{A}_{e,M} = \mathcal{A}_{\gamma e,M} \cup \mathcal{A}_{\kappa e,M}$)
$\mathcal{A}_{\gamma\kappa}(\mathbf{x})$	surface domain of the fluid–solid interface within the averaging region
$\mathcal{A}_{\gamma e}(\mathbf{x})$	domain of the entrance/exit boundaries on the surface of the averaging domain $\mathcal{V}(\mathbf{x})$
$A_{\gamma\kappa}(\mathbf{x})$	area of the γ–κ interface within the averaging domain $\mathcal{V}(\mathbf{x})$, m^2
$\mathbf{b}_\gamma$	closure variable that maps $\nabla\langle\psi_\gamma\rangle^\gamma$ onto $\tilde{\psi}_\gamma$, m
$c_{A\gamma}$	microscale concentration of species A in the γ-phase, mol/m^3
$\tilde{c}_{A\gamma}$	concentration deviations of species A, mol/m^3
$\langle c_{A\gamma}\rangle^\gamma$	intrinsic averaged concentration, mol/m^3
$\mathbb{C}_\gamma$	intrinsic averaged concentration, used in Section 7 to simplify notation, mol/m^3
$\mathcal{D}_\gamma$	molecular diffusion coefficient, m^2/s
$\mathbf{D}_\gamma$	diffusion tensor in the γ-phase, m^2/s
$\mathbf{D}_{0,eff}$	effective diffusivity tensor, m^2/s
$\mathbf{D}_{2,eff}$	second-order correction tensor, m^4/s
$\mathbf{e}_i$	unit vectors defining Cartesian coordinate system, $i = \zeta, \eta, \xi$
f	microscale volumetric source term
$\langle f\rangle^\gamma$	intrinsic average of f
$\mathcal{F}\{\cdot\}$	Fourier transform
$\mathcal{F}^{-1}\{\cdot\}$	inverse Fourier transform
g	microscale surface source term
$G(\mathbf{x}, t; \mathbf{y}, \tau)$	a Green's function
$\mathcal{G}$	source term in the closure problem, as defined by Eq. (5.3b)
I	initial distribution of ψ_γ
$\mathcal{I}$	initial distribution of $\tilde{\psi}_\gamma$, as defined by Eq. (5.3d)
$\mathbf{I}$	the identity tensor
k_1	homogeneous first-order reaction rate parameter in the γ-phase
k_s	heterogeneous first-order surface reaction rate parameter at the γ–κ interface
$\mathbf{K}_0, \mathbf{K}_1, K_2, K_3$	kernel functions
$\mathbf{l}_i$	unit cell lattice vectors, $i = x, y, z$, m
ℓ_γ	the characteristic length (integral scale) for the indicator function Φ_γ, m
ℓ_{p_γ}	integral scale for the parameter field $p_\gamma(\mathbf{x})$, where $p_\gamma(\mathbf{x})$ may be any of the parameter fields that appear in the microscale differential balance for ψ_γ
ℓ_{ch}	diameter of Chang's unit cell, m
ℓ_K	characteristic length associated with a kernel function, m
$\ell_{\tilde{\psi}_\gamma}$	characteristic length associated with the dependent variable deviation field, m
L	characteristic length associated with the macroscale, m
$L_{\mathbb{P}_\gamma}$	characteristic length (integral length scale) associated with the average of a parameter or source field $\mathbb{P}_\gamma$, m
$L_{\langle\psi_\gamma\rangle^\gamma}$	characteristic length (integral length scale) associated with $\langle\psi_\gamma\rangle^\gamma$, m
$\mathcal{L}\{\cdot\}$	linear second-order differential balance operator, m/s
$\mathcal{L}_0\{\cdot\}$	portion of $\mathcal{L}\{\cdot\}$ containing averaged parameter fields, m/s
$\tilde{\mathcal{L}}\{\cdot\}$	portion of $\mathcal{L}\{\cdot\}$ containing deviations of the parameter fields, m/s
M_p	p-th moment of distribution
$\mathbf{n}_{\gamma\kappa}$	unit normal vector directed from the γ-phase toward the κ-phase
N	nonlocal contribution associated with $\langle\psi_\gamma\rangle^\gamma$, and defined in Eq. (4.14b)
$\mathcal{N}$	nonlocal contribution associated with $\tilde{\psi}_\gamma$, and defined in Eq. (4.14c)
$\mathbf{O}$	order of magnitude symbol
p_γ	a generic parameter or source field for the microscale balance; p–γ may be a scalar, vector, or tensor field
$\mathbb{P}_\gamma$	intrinsic average of p_γ
$\tilde{p}_\gamma$	spatial deviations of p_γ
$\mathcal{P}$	a closure variable
$\mathcal{Q}$	contribution of the initial condition to the fields of $\tilde{\psi}_\gamma$, as defined by Eq. (5.3c)
r	the radial component of a cylindrical coordinate system, m
$\mathbf{r}$	position vector, m
r_0	radius of the averaging region, m
R_{K_2}	microscale correlation function associated to the kernel function K_2, m^{-2}
$R_{\langle\psi_\gamma\rangle^\gamma}$	macroscale correlation function associated to $\langle\psi_\gamma\rangle^\gamma$, m^{-2}
s_γ	closure variable that maps $\langle\psi_\gamma\rangle^\gamma$ onto $\tilde{\psi}_\gamma$
$\mathcal{S}$	source term in the closure problem, as defined by Eq. (5.3a)
$\mathbb{S}_\gamma$	second spatial moment (normalized) of a kernel function, m^2
t	time, s
t^*	characteristic time measure associated with the microscale, s
t^*_K	characteristic time measure associated with a kernel function in the closure problem, s
T^*	characteristic time (the integral time scale) associated with the macroscale, s
$T^*_{\langle\psi_\gamma\rangle^\gamma}$	characteristic time (the integral time scale) associated with the changes in $\langle\psi_\gamma\rangle^\gamma$, s
$\mathbf{v}_\gamma$	convective fluid velocity in the γ-phase, m/s
$\langle\mathbf{v}_\gamma\rangle^\gamma$	superficial average fluid velocity in the γ-phase, m/s
$\tilde{\mathbf{v}}_\gamma$	deviation for the fluid velocity in the γ-phase from the spatial average velocty, m/s
$\mathcal{V}_M$	domain of the entire macroscopic volume under consideration (Fig. 1)
$\mathcal{V}_{\gamma,M}$	domain of the fluid phase within the entire macroscopic volume $\mathcal{V}_M$
$\mathcal{V}_{\kappa,M}$	domain of the solid phase within the entire macroscopic volume $\mathcal{V}_M$
$\mathcal{V}(\mathbf{x})$	$= \mathcal{V}_\gamma(\mathbf{x}) \cup \mathcal{V}_\kappa(\mathbf{x})$, domain of an averaging volume
$\mathcal{V}_\gamma(\mathbf{x})$	domain occupied by the γ-phase within the averaging volume $\mathcal{V}(\mathbf{x})$
$\mathcal{V}_\kappa(\mathbf{x})$	domain occupied by the κ-phase within the averaging volume $\mathcal{V}(\mathbf{x})$
$V(\mathbf{x})$	volume of the averaging domain $\mathcal{V}(\mathbf{x})$, m^3
$V_\gamma(\mathbf{x})$	volume of the γ-phase contained within the averaging domain $\mathcal{V}(\mathbf{x})$, m^3
$\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$	position vectors, m

Greek symbols

α_1, α_2	measures of the magnitude of a Green's function as specified by Eqs. (5.12a) and (5.12b)
ε_γ	volume fraction (porosity) of the fluid phase
δ	Dirac's delta function