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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. Despite the increasing computational capabilities, it is still not feasible to model a complete macroscopic system by direct numerical simulations at the microscale. Actually, it is more convenient to derive models at an intermediate level of scale between the microscale and the macroscale; this is the average scale. The derivation of models at this scale can be carried out by means of 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. While the physical interpretation of the effective coefficients is usually well-understood, the same is not true for the closure variables, which are probably the most obscure part of the upscaling process. In this work, we revisit the concept of a closure variable based on an integral formulation in terms of Green's functions. Our analysis evidences 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. This integral formulation is applied to unsteady dispersion of a solute in a capillary tube and to dispersion in porous media. In both cases, the profiles of the closure variables involved negative and positive values that are determined by time, the flow field and the microstructure of the system.