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Sequential Multiscale Modeling Using Sparse Representation†

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Abstract. The main obstacle in sequential multiscale modeling is the pre-computation of the constitutive relation which often involves many independent variables. The constitutive relation of a polymeric fluid is a function of six variables, even after making the simplifying assumption that stress depends only on the rate of strain. Precomputing such a function is usually considered too expensive. Consequently the value of sequential multiscale modeling is often limited to "parameter passing". Here we demonstrate that sparse representations can be used to drastically reduce the computational cost for precomputing functions of many variables. This strategy dramatically increases the efficiency of sequential multiscale modeling, making it very competitive in many situations.

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In recent years, multiscale modeling has attracted a great deal of attention across a wide spectrum of disciplines in science and engineering [1–4]. This has opened up the possibility of analyzing the macroscopic behavior of a system based on first principles, by linking together macroscopic and microscopic models, bypassing the necessity of making

†Dedicated to Professor Xiantu He on the occasion of his 70th birthday.

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ad hoc modeling assumptions such as the ones that underly the empirical constitutive relations in continuum mechanics. In broad terms, such multiscale methodologies can be divided into two categories, sequential coupling methods and concurrent coupling methods [1, 4]. In the sequential strategy, the needed model input for the macroscale model is computed from microscale models beforehand. One then has an effectively closed macroscale model which can be used for analytical or computational purposes. Such a strategy has a very long history. It is a standard practice to obtain the transport coefficients of fluids such as viscosity or diffusion coefficients from kinetic theory or molecular dynamics simulations. Other examples of sequential coupling include calibrating empirical atomistic potentials used in molecular dynamics using models from quantum mechanics, determining the rates used in Monte Carlo simulation using molecular dynamics or quantum mechanics models, computing the equation of state for gases using kinetic theory, etc. However, for a long time, this procedure has been limited to the passage of a few parameters, due to the fact that the computational cost associated with computing the full constitutive relation is often too expensive. For example, the constitutive relations for fluids in general depend on at least six variables, and precomputing a function of six variables is simply too expensive. Therefore, one has to make a priori assumption about the functional form of the constitutive relation, and microscale models are then used to determine a few parameters in the functional form. The assumed functional form is often quite ad hoc, and this has been the main drawback for sequential modeling.

The philosophy of concurrent coupling is to access such information "on-the-fly" as the computation proceeds. The advantage of such a concurrent strategy is quite clear: Even though the needed constitutive relation may depend on many variables, in any particular simulation, one does not need to know the constitutive relation within the full range of these variables – only the values that actually occur in the simulation are needed, and these might be a very small subset of the entire range. The best example for illustrating the advantage of such a concurrent approach is the Car-Parrinello molecular dynamics in which the needed constitutive relation is the atomic potential. This function may depend on the coordinates of all the atoms in the system, which can easily be a function of tens of thousands of variables. However, in any particular simulation, one does not need to know this function entirely, but only the values needed for the particular sequence of atomic configurations that occur in the simulation, and this is a tiny subset of the tens of thousands dimensional space [5]. A very informative discussion of the relative merits of sequential and concurrent coupling strategies can be found in [1].

However, whenever possible, it is still advantageous to have the constitutive relations precomputed, since this information can be used for many other purposes, such as analyzing the properties of the system. Knowing the constitutive relations of a fluid helps us to understand the nature of the macroscopic response of the fluid, whether it is shear thinning or shear thickening, for example. The main purpose of the present paper is to demonstrate that the sequential coupling strategy can be made much more powerful through the use of *sparse representation*. For example, instead of representing the functions on tensor-product grids, one can use sparse grids and this drastically decreases