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Asynchronous coupling of hybrid models for efficient simulation of multiscale systems

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ABSTRACT

We present a new coupling approach for the time advancement of multi-physics models of multiscale systems. This extends the method of E et al. (2009) [5] to deal with an arbitrary number of models. Coupling is performed asynchronously, with each model being assigned its own timestep size. This enables accurate long timescale predictions to be made at the computational cost of the short timescale simulation. We propose a method for selecting appropriate timestep sizes based on the degree of scale separation that exists between models. A number of example applications are used for testing and benchmarking, including a comparison with experimental data of a thermally driven rarefied gas flow in a micro capillary. The multiscale simulation results are in very close agreement with the experimental data, but are produced almost 50,000 times faster than from a conventionally-coupled simulation.

1. Introduction

A multi-physics description of a multiscale system is often referred to as a 'hybrid' model. In fluid dynamics, a typical hybrid combines a molecular treatment (a 'micro' model) with a continuum-fluid one (a 'macro' model), with the aim of obtaining the accuracy of the former with the efficiency of the latter [1–4]. The micro and macro models generally have characteristic timescales that are very different, which means that time-accurate simulations can be extremely challenging: the size of the timestep required to make the micro model stable and accurate is so small that simulations over significant macro-scale time periods are intractable. If the system is 'scale-separated', a physical (as distinct from numerical) approximation can be made that enables the coupled models to advance at different rates (asynchronously) with negligible penalty on macro-scale accuracy. E et al. [5] were the first to introduce and implement this concept in a time-stepping method for coupled systems, referred to in the classification of Lockerby et al. [6] as a continuous asynchronous (CA) scheme ('continuous' since the micro and macro models advance without interruption [5]). In this paper we extend this idea to multiscale systems comprising an arbitrary number of coupled models.

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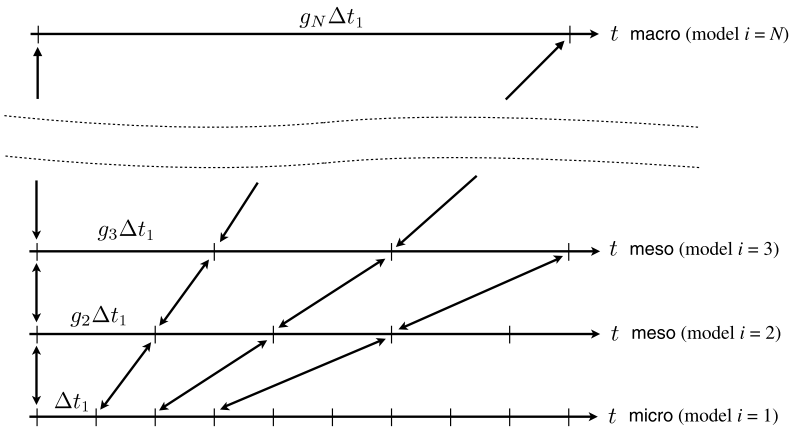

Fig. 1. The continuous asynchronous (CA) coupling scheme extended to multi-model multiscale systems.

2. Extension to multi-model systems

We consider an N-model timescale-separated system, where the ith model has a characteristic timescale T_i, and indexing is ordered such that

$$T_i \leq T_{i+1} \quad \text{for } i = 1, \ldots, N-1. \tag{1}$$

Model $i = 1$ is the micro model and $i = N$ is the macro model; models $i = 2$ to $i = N-1$ are 'meso' models. The degree of scale separation S_i between model i and $i+1$ is

$$S_i = \frac{T_{i+1}}{T_i} \geq S_{\text{tol}}, \tag{2}$$

where the tolerance S_{tol} requires each distinct model of the system to be scale separated from every other to some degree, for example, $S_{\text{tol}} = \mathcal{O}(10)$. If this condition is not met, the two models are treated as one, and coupling is performed conventionally.

In general each model can be considered to have its own time variable (t_i), and be represented by

$$\frac{dX_i}{dt_i} = \mathcal{F}_i\big(X(t_i)\big), \tag{3}$$

where X_i are the set of variables of the ith model, and $\mathcal{F}_i$ is some function of the complete system's variables, $X = \{X_1, X_2, \ldots, X_N\}$. It is important to make clear the distinction between the characteristic timescale of the ith model in isolation (T_i) and the timescale of its variables within the coupled system; they are, potentially, completely different.

To solve this set of models, the independent time variables must be related to each other. If all time variables are equal (i.e. $t = t_{1\ldots N}$) the system is conventionally coupled. However, we can advance models at different rates with the physical modification

$$t_1 = t_2/g_2 = \cdots = t_N/g_N, \tag{4}$$

where g_i is the rate that the ith model advances relative to the micro model. This approximation provides a means to exchange fine timescale resolution for long timescale predictions, and the extent to which it is valid depends on the degree of scale separation between models, i.e. on the magnitude of S_i. For coupled models that are highly scale separated ($S_i > S_{\text{tol}}$), the smaller-scale model will remain quasi-equilibrated to the dynamics of the larger-scale model despite the physical modification, and so behave similarly to as in the unmodified system. The aim is thus to represent the scale-separated system ($> S_{\text{tol}}$) with one that is less, but still significantly, scale separated ($= S_{\text{tol}}$): this is how acceptable values of g_i are determined (see below for the specific procedure). Detailed analyses of the error associated with this physical approximation for a two-model system are given in E et al. [5] and Lockerby et al. [6].

Fig. 1 provides an illustration of a numerical implementation of Eq. (4) using different timestep sizes for each model, while exchanging variables as if the timesteps were equivalent (this is *asynchronous* coupling). The timestep of the ith model is

$$\Delta t_i = g_i \Delta t_1, \tag{5}$$

where Δt_1 is the micro model timestep.

The aim of this asynchronous coupling scheme is to maximise the total simulated period. This is done by maximising the timestep in each model subject to the following constraints: