"Development of a Wavelet-based Multiphysics/Multiscale Framework and its Application to Diffusion Problems with Chemically Reactive Boundary"

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Summary

Coupled processes involving various multi-component interactions are prevalent in many science applications, manufacturing and industrial processes. These interactions typically exhibit an unusual degree of complexity across a large range of spatial and temporal scales. Not only one has to deal with orders of magnitudes in differences in time- and length-scales, one has to also deal with different governing equations and/or constitutive relationships for the same process at different scales. We have developed and implemented a novel multiscale/multiphysics computational framework that can consistently transfer relevant information across scales efficiently (both upscaling and downscaling) to simulate coupled process dynamics efficiently. Specifically this framework has been successfully applied to problems with chemically reactive boundary coupled with diffusion process as these constitute building blocks in a wide variety of chemical processes.

The current computational tools used in various scientific endeavors or for design of industrial and manufacturing are often *ad hoc* and empirical when it comes to modeling long spatial- or time-scale phenomena. This is due to the fact that the current available models at the macro-scale can not resolve the physics at the micro-scale or the atomistic-scale which often control the processes at the macro-scale. At the same time the computational expense prohibits simulating the macro-scale processes using the models available at the micro-scale or the atomistic-scale. The accurate simulation of macro-scale processes only needs relevant information from the micro-scale or the atomistic-scale and we have developed and implemented a wavelet based compound matrix method (Fig. 1) which enables efficient exchange of the relevant information between various scales. This research is being carried out under the project titled "Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMM-HCRF) Over Catalytic/Solid Surfaces" and is a joint collaboration between Oak Ridge National Laboratory, University of Arizona, Ames Laboratory and National Energy Technology Laboratory.

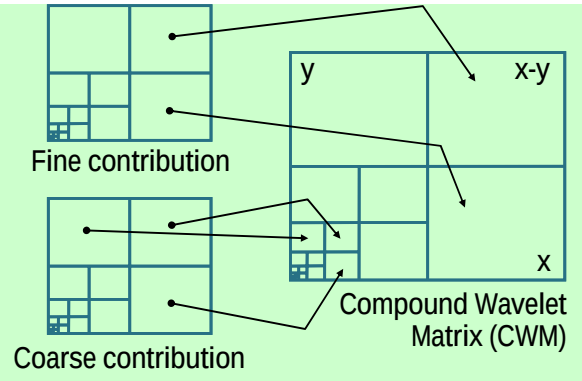

Fig. 1: Compound Wavelet Matrix: An effective way to couple multiphysics/multiscale simulation components.

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Chemically reacting flows over catalytic and non-catalytic surfaces are one of the elementary operations in chemical processing plants and represent a model problem with rich multiscale phenomena. To demonstrate the seamless coupling achieved by CWM framework, we have considered coupling of two prototype methods for the problem of species generated on a chemically reactive boundary and diffusing through the bulk (see Ref. 1 for more details). The two methods consider different time and length scales. The first method in this coupling, termed "fine," models the chemical reactions on the reactive boundary stochastically by the kinetic Monte Carlo method (KMC) and the diffusion in the medium deterministically using relatively small time increments and small spatial discretization mesh size. The second method, termed "coarse," models both the reaction and the diffusion deterministically and uses drastically larger time increments and spatial discretization size than the fine model. The two methods are coupled by forming a spatiotemporal Compound Wavelet Matrix (CWM) that combines information about the time and spatial scales contained in them (Fig. 1) and the results show that the true solution is recovered through the multiscaling approach. We have also extended this approach to two-dimensions (see Ref. 2 for more details) and detailed analysis of the computational accuracy and efficiency has been performed. We have observed an order of magnitude savings using the current multiscale approach as compared to a brute force solution using the fine model.

Recently we have extended the computational approach to handle non-stationary processes so that the method is applicable to a broad set of applications involving mutliscale or multiphysics processes. This has been demonstrated using a 1-D reaction-diffusion process modeled by two methods at differing levels of accuracy. Information from both methods is then combined seamlessly in a concurrent fashion to provide a multiscale representation of the non-stationary evolving system and more details will be reported in Ref. 3. Currently work is underway to generalize and extend this framework to handle other multiphysics models (like Lattice Boltzmann Model for flow). In addition, the framework is being ported to scalable architectures.

References:

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