Enhanced Nonlinear Krylov Accelerator for Stable Bi-Directional Multiscale Coupling: Application to Pulmonary Airflow

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The multiscale paradigm, wherein three-dimensional (3D) distributed finite-element or finite volume models, are coupled with lower-dimensional ODE or PDE systems of equations, has attracted considerable attention in the biomedical computing community. At its most basic level, this attraction is due to the recognition that lower-dimensional models can 1) address specific biophysics that are not easily modeled as a 3D continuum, and 2) that lower dimensional models can deliver computational efficiency in applications where smaller or larger scales determine dynamic physiological boundary conditions to the 3D model, but are too vast to be accounted for directly.

While the multiscale paradigm is well motivated from a modeling point of view, true bi-directional coupling between scales is numerically challenging. The current state of the art is a class of monolithic methods, wherein the degrees of freedom of lower-dimensional model are directly added to the solution method. The main limitations of this approach are that 1) it is inflexible since it requires the modeler, who may lack numerical sophistication, to consistently discretize the lower-dimensional model and to add the terms of that discretized model to the solution matrix; and 2) not all lower-dimensional models can be easily added to the solution matrix, and some not at all.

In contrast, we present a novel partitioned method for multiscale coupling, utilizing an enhanced nonlinear Krylov accelerator that allows for less frequent evaluation of the Jacobian and thus reduced computational cost. In fact, applied to the problem of coupling multiple lower-dimensional models of distal lung mechanics to imaging-based models of rodent respiration, we show that our partitioned method like the monolithic method requires zero additional cost with respect to an uncoupled model. Moreover, because the CFD and lower-dimensional models are totally separate, 1) this framework does not require consistent discretization that may be beyond the ken of the biomedical practitioner, or worse may not be possible; and 2) this framework affords great flexibility in terms of the type and breadth of the adopted lower-dimensional model, allowing the biomedical researcher to appropriately focus on model design.

In our current application of the method, we focus on linking multiple lower-dimensional models describing the distal lung mechanics to imaging-based 3D CFD models of the upper pulmonary airways in order to incorporate physiologically appropriate outlet boundary conditions. Yet, the passive tissue mechanics of the distal lung is but one part of the process of respiration. In addition, the composition of inspired gases, smooth muscle tone, tissue and blood metabolism, the nervous system, and cardiovascular mechanics all play a part. The relative importance of these features of respiration is a function of the biomedical question one wishes to investigate. We emphasize that our method is not only efficient and robust, but also affords researcher the flexibility to explore the impact and importance of these features in health and disease.

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