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Predictor-Corrector Methods for Dynamically Coupling Multiscale Simulation Codes

Yuan He, Joshua Gray, Richard C. Alkire, and Richard D. Braatz
Department of Chemical & Biomolecular Engineering
University of Illinois at Urbana-Champaign

Applications in materials, medicine, and computers are being discovered where the control of events at the molecular and nanoscopic scales is critical to product quality, while the primary manipulation of these events during processing occurs at macroscopic length scales.[1] In such applications, one of the most significant engineering challenges is to achieve control over phenomena that occur simultaneously at different length and time scales that can span in excess of ten orders of magnitude. With the limitation of the dynamic and local information that can be collected experimentally, multiscale computation is needed to provide predictions at all scales.

There are numerous examples where the simulation of multiple length scales are coupled in a serial fashion, where the results from a simulation code is used in another simulation code.[2] For example, continuum Stokes equations were combined with the direct simulation Monte Carlo (DSMC) method[3] by an overlapped Schwarz alternating method with Dirichlet–Dirichlet type boundary conditions. Alternatively, the quasi-continuum method[4] couples the atomistic and continuum scales by using a system-wide finite element mesh that is refined to the atomic dimensions where needed. Unlike conventional finite elements, the energy of each cell is computed from the underlying atomistic Hamiltonian. As a further variation, the FE/MD/TB hybrid approach[5] spatially divides the system into continuum, atomistic, and handshake regions where different numerical models are appropriate, and Hamiltonian-based boundary conditions are shared among the various regions to obtain a self-consistent solution.

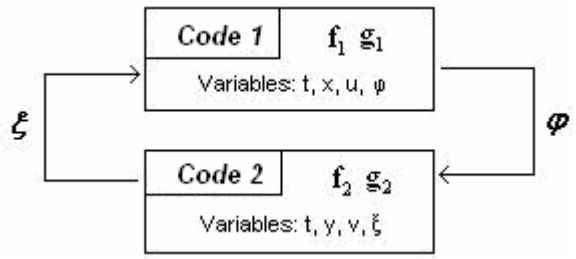
In recent years many researchers have dynamically coupled simulation codes at each length scale to run simultaneously, with each code continually passing updated boundary conditions to the other codes.[6] Many papers have proposed iterative algorithms to converge coupled codes at multiple length scales to a steady-state or quasi-steady-state solution.[7] A modification of this approach uses internal iterations to force convergence of the information passed between simulation codes.[8] While this approach can provide physical and numerical consistency between coupled codes, a large perturbation in external variables (e.g., as may occur at the beginning of a simulation or during a sharp transition) can result in numerical stability problems in one of the individual codes, resulting in an internal iteration that cannot converge. In this presentation, we propose numerical coupling algorithms to suppress numerical instabilities and improve the numerical accuracy of simulation codes dynamically coupled at physical boundaries. With the existence of physical boundaries, the model and time and length scales in each individual simulation code can be vastly different, which can result in significant external perturbations to the individual codes. Note that such coupled problems are different from so-called sub-domain problems,[9] in which there only exist virtual boundaries between the simulation sub-domains.

Code 1 solves

$$\frac{dx}{dt} = f_1(t,x,u,\varphi), \qquad 0 = g_1(t,x,u,\varphi)$$

Code 2 solves

$$\frac{dy}{dt} = f_2(t,y,v,\xi), \qquad 0 = g_2(t,y,v,\xi)$$



t: independent variable; *x, y*: vectors of differential variables; *u, v*: vectors of algebraic variables
φ, ζ: vectors of linked or external (differential and algebraic) variables

Figure 1. A semi-explicit DAE problem simulated by dynamically coupling two codes.

Although the proposed algorithms can be applied to dynamically couple continuum-continuum or continuum-noncontinuum simulation codes, the analysis was applied to the situation where both codes simulate DAEs (see Figure 1), to facilitate the numerical analysis. Numerical algorithms are proposed that guarantee unconditional absolute stability and second-order accuracy in the solution of coupled semi-explicit stiff DAE problems with index up to 2. We started with the analysis of the numerical accuracy and stability properties of multiscale predictor-corrector methods with the presence of external perturbations at the interface between the individual simulation codes. It was demonstrated that to ensure second-order accuracy and absolute stability of the predictor-corrector (PC) methods in solving stiff DAEs, the external perturbations ε in the state variables (i.e., the errors caused by the dynamically updating the value of the external variables) should be controlled at $||\varepsilon|| < a(h^2)$, $a \in (h, 1/h)$, where h is the integration step size. We analyzed the advantages and disadvantages of the PC algorithm and an implicit variation on PC algorithm. The PC algorithm requires lower computational cost and is easier for load-balancing on parallel computers. Using the most recently calculated value of the external variables (the Gauss-Seidel approach) in the PC algorithm is shown to lower the numerical accuracy of the coupled simulations to first order, regardless of the numerical accuracy of the individual simulation codes.

This numerical analysis motivated an error-control climbing mechanism, which limits the perturbation in the external variables via partial integration steps to satisfy the absolute stability requirement. The algorithm starts off with adding a fraction of the change in each external variable at each partial integration step. This fractional addition is selected to be small enough that a condition for the unconditional stability of the PC method is satisfied. This fractional addition is relaxed dynamically depending on convergence along the progress of the solution, and the number of partial integrations at each solution step changes accordingly. The climbing algorithm was motivated by the need to gain unconditional stability in solving coupled stiff ODE/DAE problems with the presence of external perturbations, while the existing multirate[10] or multistage algorithms (e.g., Runga-Kutta) are targeted for accuracy control and are not sufficient for stability control.

The second-order error-control climbing algorithm was applied to the simulation of a semi-explicit index-2 stiff DAE system that models an electrochemical process (see Figure 2). The mathematical model of pit initiation at single sulfide inclusions in stainless steel was developed by Webb and Alkire[11,12] for predicting the pitting potential, based on the local

chemical environment produced by dissolution of a sulfide inclusion on stainless steel (see references for details on the physical problem, computational domain, and simulation parameters). The results were compared to the results of previous simulations that used a monolithic code that solves a single DAE system consisting of the diffusion-migration equations, equilibrium expressions for the bulk species, and chemical and electrochemical reactions at the surface.

In this study, the corrosion process was simulated as two coupled codes (see Figure 1) using the error-control climbing algorithm. The coupling of the simulation codes showing the boundary information passed between codes is shown in Figure 2. This application of finite differences in the spatial dimensions to the algebraically constrained 2D PDE model results in large-scale highly stiff DAEs for 21 chemical species with multiple chemical and electrochemical reactions with vastly different rates. The transient codes simulate the local concentration and potential values in the coupled micro-crevice and bulk regions, which can not be measured experimentally but are essential to the understanding of the role of sulfide inclusions in the initiation mechanism of localized corrosion of stainless steel.

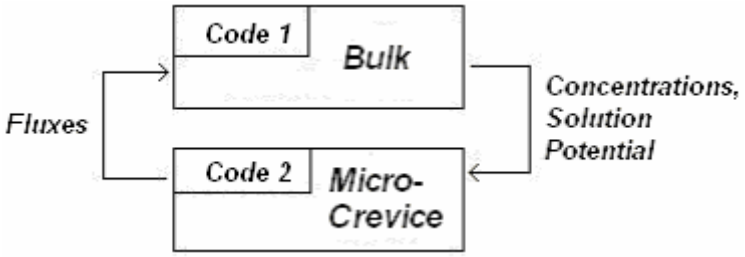


Figure 2. Coupled simulation of the pit initialization in stainless steel.

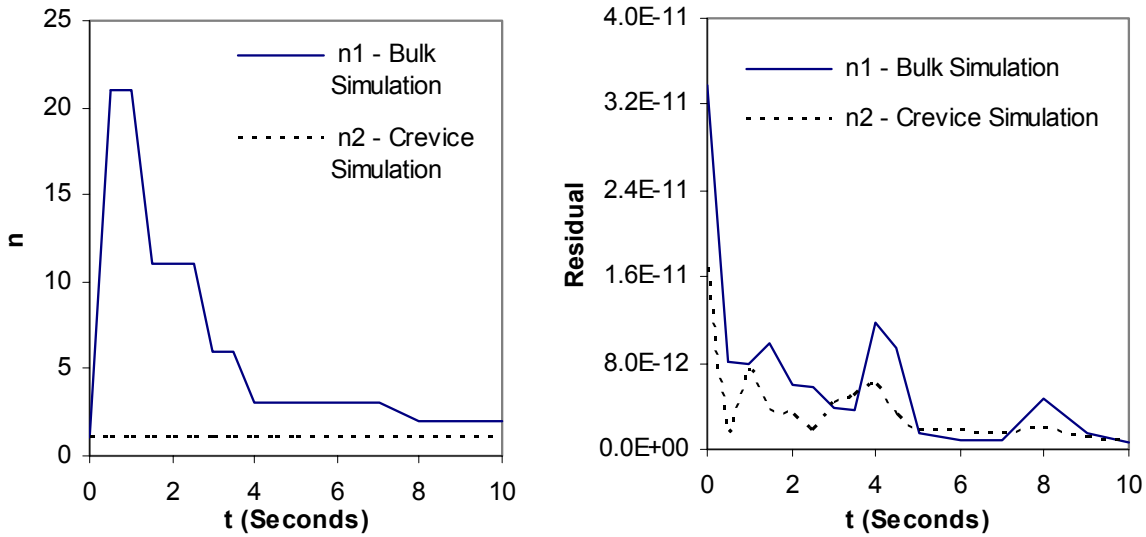


Figure 3. The number of internal iterations n and the function residuals for the individual codes in the dynamically coupled simulation.

The number of partial integration steps and residuals in each code is shown in Figure 3, in which the linking time step was 0.5 s. It is evident from the residuals in Figure 3b and by

comparison of the simulated results to those of the monolithic code that the climbing predictor-corrector algorithm numerically stabilized the simulation with a high level of numerical accuracy. No partial integration steps were needed by the crevice simulation to converge at each iteration, whereas the bulk simulation needed as many as 21 partial integration steps before passing boundary information to the crevice simulation (see Figure 3a). The number of partial integration steps needed by the bulk simulation to satisfy the absolute stability convergence criterion reduced to 2 after 8 s, and remained at 2 for the remainder of the simulation. Hence the overall computational cost of the second-order-accurate numerical algorithm for time after the initial period of 8 s is within a factor of 2 of using direct coupling of the two codes, which was shown by numerical analysis to only be first-order.

The initial large and varying number of partial integration steps in Figure 3a prevents efficient load-balancing on parallel computers, and is computational expensive for short simulation times. We are currently investigating modifications of the initialization of the dynamically coupled codes to reduce the initial number of partial integration steps. The goal is to retain second-order accuracy while requiring the minimum number of extra iterations.

Acknowledgments

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