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Generalized bridging domain method for coupling finite elements with discrete elements

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Abstract

The concurrent coupling of finite elements and discrete elements is an effective DOF reduction methodology for reproducing the granular flow phenomenon as discrete element method does. In this paper, we present a novel coupling strategy named the generalized bridging domain method. This method introduces independent functions to weight the material properties of the continuum and those of the discrete element model, and then the equilibrium of each new model is guaranteed by imposing compensation forces. The compensation force of continuum is determined by force and displacement compatibility requirements of continuum with respect to discrete elements, and vice versa. Utilizing different weighting functions, four typical coupling methods, the bridging domain method, edge-to-edge coupling, separate domain coupling, and separate edge coupling, are obtained. Additionally, a new integration algorithm with multiple time steps is developed for the separate edge coupling. The numerical performance of the separate domain coupling, where displacement compatibility condition of continuum and that of discrete elements are individually enforced by the Lagrange multiplier method, has been investigated in detail. Results of several numerical examples show that the separate domain coupling outperforms other methods in avoiding spurious reflection and the separate edge coupling is effective enough for coupling finite elements with discrete elements. Due to the truncation of high frequency waves, there exists energy loss but at an acceptable level if the waves can be resolved by the macroscopic finite element model.

Keywords: Discrete element method; Finite element method; Multiscale method; Spurious wave reflection; Granular flow phenomenon

1. Introduction

The fracture and failure of geotechnical structures such as slope sliding and fault propagation are often accompanied by highly localized granular flow phenomenon between fracture planes within which massive

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grain detaching, sliding and rolling can occur [1]. Conventional macroscale methods, which are typically based on the Cauchy–Born rule and discretized by a mesh, fail to reproduce such processes because of the phenomenological descriptions of the constitutive models and the mesh sensitivity induced by strain localization [2,3]. On the other hand, although the discrete element method [4,5], which focuses on modeling particle motion and interaction, is able to capture the main physics of such phenomena, direct application of this method for large scale engineering problems remains impractical because of the prohibitive computational costs [6,7]. Therefore, the concurrent multiscale method [8], in which microscale and macroscale models are coupled and run concurrently, has been developed in an effort to analyze the local failure domain of interest at the microscale level and the remaining domain at the macroscale level. In the concurrent multiscale methods, a crucial component is the coupling scheme that is designed to transfer the key information across the coupling domain. However, due to the disparate nature between the microscale model and the macroscale model, it is very challenging to formulate a coupling scheme that does not suffer from spurious reflection and energy loss, especially in dynamic analyses [9–11].

Broadly categorizing, there are two major types of coupling schemes in the literature. The energy-based methods postulate that dissimilar models share a common energy functional with explicit consideration of compatibility, from which the equilibrium of each model can be derived. In the pioneering work of Abraham et al. [12,13], the Hamiltonians were averaged for constructing a common energy functional and the finite element mesh was refined to the atomistic scale for strong compatibility in the coupling domain. The energy-based quasicontinuum method [14–16] used atomistic model in the domain of interest and finite element mesh to interpolate the atomistic displacements in the remaining domain. The bridging scale method [17,18], proposed firstly by Wagner and Liu, decomposed the molecular displacements into fine and coarse scales and computed the internal forces of a finite element by averaging the inter-atomistic forces within it. To eliminate the fine scale degrees of freedom in the macroscale domain without spurious reflection, a special boundary condition, which is similar to the generalized Langevin equation, has to be imposed on the micro model at the interface. To achieve a gradual transition from one model to another, Dhia et al. presented the Arlequin method [19,20]. This is a general framework that employs energy partition for constructing a common energy functional, and a weak compatibility condition between different models is introduced into the functional by the penalty method. Based on this framework, the bridging domain method has been proposed [21,22]. This method constructs a weak compatibility condition in the physical subspace of the molecule and has been shown to be able to filter high frequency waves as the width of the bridging domain increases. When the scales of the atom and the finite element are the same, Aubertin et al. [9,10] improved the time integration algorithm for the bridging domain method to keep energy conservation and to avoid spurious reflection. Note that in all the above methods, the compatibility condition between different models is inter-dependent, which may lead to the generation of ghost forces that produce spurious reflections [11].

The other category of the coupling schemes is the force-based methods, in which the compatibility conditions of different models are directly enforced as boundary conditions to obtain the equilibrium of each model. Although this kind of coupling scheme seems much simpler than the energy-based method, this method can lead to serious energy loss. For example, Fischmeister et al. [23] proposed a two-layer transition zone to individually enforce the strong compatibility condition on the atomistic surface and that on the continuum surface. It was shown that the finite-sized transition zone can overcome some of the problems associated with the non-local characteristics of the inter-atomic forces. To avoid ghost force, Dobson and Luskin [24,25] proposed a force-based quasicontinuum method, where strong compatibility conditions are directly applied as boundary conditions to different models at the interface. Based on quasicontinuum method, Li et al. [26] blended atomistic and continuum forces in the coupling domain to achieve the equilibrium. It was shown that the transition is much smoother when handling the coupling in a finite-sized domain instead of a sharp interface. Parks et al. [27] presented an overlapping domain method, where artificial boundary of the continuum model and that of the atomistic model were misaligned. Strong compatibility conditions were imposed independently on these boundaries. This method requires only local energy functionals for the atomistic and continuum domains, and a global energy functional is never needed. Currently, the domain coupling method using independent compatibility conditions appears to be the state-of-the-art method in the area of multiscale coupling.