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Velocity Interfacial Conditions for Two-atom Chains

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ABSTRACT

Multiscale computations have become increasingly important in revealing the nature for applications in various disciplines. The development of multiscale algorithms requires a good understanding to the physics, mathematics, as well as computational processes. The key index that identifies a good algorithm is the efficiency, namely the ratio between fully resolved fine scale computing load and the multiscale computing load. The computing load counts not only the CPU time in running a program, but also the efforts needed in programming. For this reason, a simple and clean algorithm is much desirable.

We have proposed the first fully finite difference approach for concurrent multiscale computations of crystalline solids [1]. This approach mainly combines three techniques, a coarse grid scheme derived by matching differential operator method (MDO), a fast averaging technique (FAT), as well as a velocity interfacial condition (VIC). These techniques may be adopted independently with other algorithms. They are simple, and have balanced accuracies. Among these ingredients, the interfacial condition turns out to be most important in improving accuracy. With the VIC technique, we can readily compute for solids with strong nonlinearity and large deformation.

In this talk, we shall present our recent results on velocity interfacial conditions for an atom chain that comprises two types of atoms. With two types of atoms, it is well-known that an optic branch appears, besides the acoustic branch. The way to treat optic branch seems not very well resolved in the literature. Using our understanding on wave operator splitting for incoming and outgoing waves, we are able to identify incoming and outgoing waves, as well as acoustic and optic waves. Treating each type of wave by a specific velocity interfacial condition, we obtain an accurate way to eliminate spurious reflecting waves.

We shall develop the continuous velocity conditions, and the discrete velocity interfacial conditions. Numerical tests will be presented.

REFERENCES

[1] S Tang, "A finite difference approach with velocity interfacial conditions for multiscale computations of crystalline solids", *J. Comput. Phys*., accepted for publication, (2007).