ARTIFICIAL BOUNDARY CONDITIONS FOR ATOMISTIC STRAIN MODELS

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ABSTRACT

In this talk we solve continuum and discrete elasticity problems in infinite domains by introducing exact artificial boundary conditions (ABCs) that can be applied at a planar interface below which there are no forces. The problem domain is assumed to be composed of a large regular domain, which can be handled analytically, and a small irregular region, which must be treated by numerically. One example is the atomistic strain model problem with a film deposited on a semi-infinite substrate which occurs during the total elastic energy minimization of a solid composed of two materials. Solution of the elasticity equations can then be performed using this interface as an artificial boundary, often with greatly reduced computational effort. The derivation includes an expression for the total energy in the system (including the region below the artificial boundary) and an energy formula that is a variational principle for the elasticity equations with the artificial boundary condition. Numerical examples illustrate the accuracy and effectiveness of the results. Discrete strain is modeled using lattice statics for application to epitaxial thin films.

INTRODUCTION

Numerical simulation of the strain field in a half-infinite body (e.g., $z < h(x, y)$) requires boundary conditions at a finite depth in the body. If there is no displacement at infinite depth and body forces are not present below a certain depth, then the strain goes to zero as the depth increases. Use of a physical boundary condition, such as zero displacement, requires a large computational domain, because of the long range of elastic interactions. On the other hand, an exact artificial boundary condition (ABC) can be formulated for a half-space problem, which can allow use of a thin computational domain with no loss of accuracy. The method suggested here can be described as follows: First an artificial boundary is introduced, thus dividing a whole domain into a small computational domain and a semi-infinite domain. This boundary is chosen to be a line in 2D and a plane in 3D. Next, on this artificial boundary we find a relation between unknown variables and their derivatives. For example, for the linear elasticity problem, the relations between the displacements and the normal stress tensor are obtained. Results are consistent with the energy minimization problem. Lastly, we use this ABC as a boundary condition on the artificial boundary, and solve the problem in the small computational domain. Numerical results are presented for continuum and discrete elasticity in two and three dimensions in order to confirm the validity of these results and to illustrate their effectiveness.

For the intended application to epitaxial thin films [5],[6], numerical results for an idealized strain computation are also presented.

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