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Analysis of a Variational Method Coupling Discrete and Continuum Machanics

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The description and computation of fine scale localized phenomena arising in a material (during nanoindentation, for instance) is a challenging problem that has given birth to some multiscale methods. In this work, we propose an analysis of a simple one dimensional method that couples two scales, the atomistic one and the continuum mechanics one. The method includes an adaptative criterion in order to split the computational domain into two subdomains, that are described at different scales. We study both the general case of a convex energy and a specific example of non convex energy, the Lennard-Jones case. In this latter situation, we show that in some sense the most natural approach might be inappropriate, and we propose a way around this difficulty. We also provide a numerical analysis of the corresponding numerical schemes.

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