ON MULTISCALE APPROACHES IN MODELING OF ATOMISTIC TO CONTINUUM COUPLING

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Multiscale (MS) modeling incorporates forming of a material model that spans over several orders of magnitude in the time and/or length scale. Usually MS methods are used to connect fine scale of atoms and more coarse scale of continuum mechanics (CM). By this coupling one is able to, in the same model, study nanostructure in the localized region of special interest where dynamics of individual atom is relevant and use computation less expensive CM in the area, where deformation is more homogenous and smooth.

Concurrent MS methods are applied in cases when two or more different scales are simulated simultaneously in the same model. In these approaches atomistic model, that is studied by using molecular mechanics (MM), is surrounded by finite element (FE) mesh. Depending on the type of transitions between two regions, different computational strategies are developed. Frequently used methods are Quasicontinuum (QC) method developed in late 90's by Tadmor, Ortiz and Phillips [1] and Bridging Domain (BD) developed by Belytschko and Xiao in 2003 [2].

In QC method the coupling of atomistic and continuum model is achieved by refining FE mesh in the area of special interest until one node corresponds to one atom. In the rest of the model one FE incorporates more atoms. Figure 1 shows concept of transition from atomistic to QC model around the crack tip.

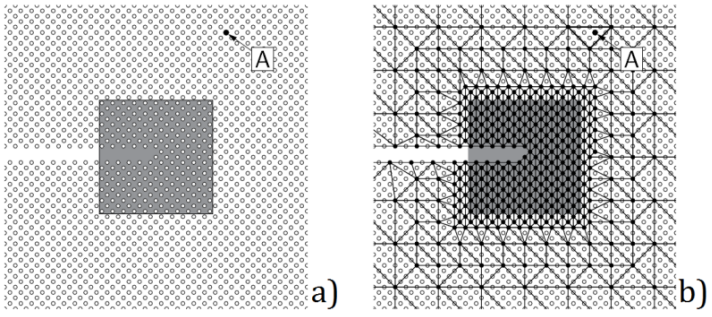

Figure 1 Transition from full atomistic to MS model in the QC method, a) completely atomistic model, b) same model discretized with QC triangular FE (white dots are atoms, black dots are FE nodes, in dark gray shaded area one node corresponds to one atom) [3]

In the atomistic area motion of nodes/atoms are governed by MM. In the continuum area, where one FE represents set of atoms properties of FE, are also done by MM, but it is not necessary to track displacement of every atom. Instead, it is sufficient to analyze just several

atoms coincident with FE nodes, often called representative atoms (RA). Therefore, only RA have independent degrees of freedom, while other atoms have to follow the interpolated motion of RA. The function that governs the motion of atoms can be a standard FE shape function. For calculating energy of the system correctly the Cauchy-Born rule [4] is implemented. QC method has been used to study basic aspects of deformation in the crystalline solid, fracture and grain boundary slip.

To make less sudden transition from atomistic into continuum mechanics in BD method so called handshake region (HR), where atomistic and continuum models are present, is introduced. Figure 2 a) shows basic principle of domain partition. The atomistic domain Ω^a is analyzed by MM, while the discretization of the continuum part Ω^c is done by FEs. Both models are present and are overlapping in the HR Ω^b. Compatibility between atomistic and continuum method is done by imposing interpolated displacement field on the HR atoms. To avoid double energy counting in the HR, the total energy is calculated as a sum of the atomistic and continuum energies. BD method is suitable to be used for studying nano-defects in a bigger model, but the area of interest has to be far enough from the HR.

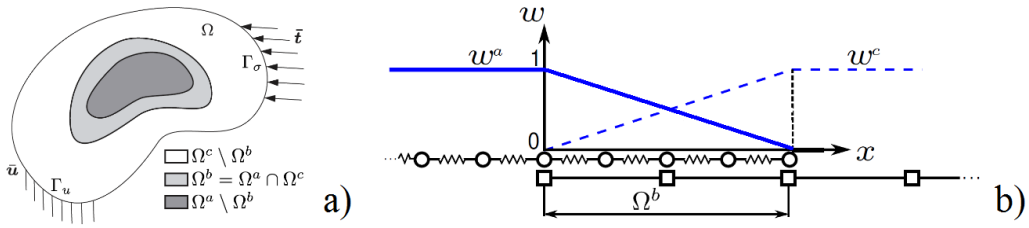

Figure 2 Transition from atomistic to continuum model in the BD method, a) scheme of coupled regions in BD method, b) 1D model of linear energy weighting functions in the bridging zone (w^a is the weighting function of atomistic and w^c weighting function of continuum region) [5]

Both methods are generating undesirable ghost forces in the transition area. The reason for that is the difference between atomistic and CM calculating of forces. Additionally, different mesh density of two scales in the transition area may cause undesired wave phenomena like reflection at atomistic/continuum interface. Those waves might be trapped in the atomistic region and cause unphysical internal energy content rising the temperature. The goal of proper modeling is to avoid these phenomena so they have to be carefully monitored.

Acknowledgments

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