**Concurrent Multiscale Methods of Modeling and Simulation**

1. ***Direct Coupling (DC) and non-DC Methods:*** Approaches that relate atoms andFE nodes in a one-to-one manner will be referring to direct coupling (DC) methods. Most existing multiscale methods belong to DC, but GP and ESCM are non-DC methods in which a statistical averaging of atoms or particles within their neighbor link cells (NLC) of a particle or FE node are used.

**QC[ ]** Short for quasi-continuum method. It uses Cauchy-Born rule for the first time to calculate the strain energy density W in the FE region, thus both atomistic and continuum region can be treated with atomic potential function. It was proposed in 1996 with a lot of applications.

**GP[ ]**  Short for generalized particle methods. It consists of different scales of particle domains to keep material structure and numerical algorithm the same as atomic scale. Both bottom-up and top-down scale transition are through atoms/particles in NLC. FE mesh only appears for large-size models in the far remote field from atomistic scale to avoid ghost force.

**CAC[ ]** Short for “concurrent atomic to continuum” which is proposed to improve the simulation of material defects. Within each element, lattice defects are not allowed. However, between elements, neither displacement continuity nor strain compatibility is required. In mathematical community, the same CAC terminology is used which investigates convergence theory of domain truncation, etc. [ ]

**CADD[  ]** Short for couples atomistic analysis with the discrete dislocation (DD) method. Based on the need to create the force boundary by a superposition process, the method is force-based multiscale analysis. The focus on dislocation of the CADD method necessitates the use of linear elasticity.

**ESCM[ ]** Short for embedded statistical coupling method which uses statistically averaging over selected time interval and volume in atomistic subdomains at the MD/FE interface to determine nodal displacement for the continuum FE domain.

1. **Existing codes for multiscale modeling**

Given the limitation of the resources, in the following we recommend one source code in the public domain that is the QC code. The important thing is how the users can use some executable code for applications such as NAMD for biomaterials. Here, we will introduce the usage of the code of PMAP which is developed by the IIMMM in the past 10 years based on the GP method.

**QC code:** can be downloaded here with <http://qcmethod.org/qc/download>; More informationcan be obtained from the above website.

**PMAP of the GP code:** Short for The Particle-Based Multiscale Analysis Program. In this website, the user manual and its tutorial will be offered for model development and simulation. For some potential users who hope collaboration to use PMAP and other codes that IIMMM has or will have we will offer more materials including detail examples for applications to help the users.

Other Code sources:

<http://www.octa.jp/> Developed in Japan for multiscale analysis of soft materials

<http://libmultiscale.gforge.inria.fr/> Developed in France for solid mechanics and materials

<http://www.sandia.gov/~sasilli/> Developed by Sandia Nat. Laboratory for peridynamics.