A Separate Quasi-Particle Multiscale Method

Zhenqing Wang[a], Zengjie Yang, Qinghua Meng,
College of Aeropace and Civil Engineering, Harbin Engineering University,Harbin, 150001, China

INTRODUCTION

In the present work, the multi-scale analysis of quasi-particle system was separated into the calculation of quasi-particle displacement and the calculation of quasi-particle interaction so that a new multi-scale method referred to as separate quasi-particle dynamics method was proposed. Further, the quasi-particle crystalline structures of FCC crystal lattice were designed. Based on the theoretical analysis on the quasi-particle dynamics method, the stress-strain cures of three-dimensional model of copper bar were discussed. Results showed that this separate method could correct the error of other multi-scale methods.

GEOMETRIC MODEL

The multi-scale geometric model of separate quasi-particle dynamics method is divided into different scales according to the model emphasis region and the deformation gradient. Specifically, in the core area or the inhomogeneous area (e.g. the crack-tip area, the materials surface and the interface between different materials) the molecular dynamics method is employed to calculate the model. In other area or the homogeneous area the separate quasi-particle dynamics method is proposed for the different quasi-particle scales.

The material model contains several quasi-particle domains β_n of different scales n, in an especial order with n=1 denoting the atomistic scale. The quasi-particle domain β_n is a one-to-one correspondence to material domain α_n with atomic structure. In Fig. 1 the cyan balls denote the atoms, with the distance a_0, which will be replaced by quasi-particles of different scales. The upper and lower in Fig. 1 are respectively the 2-time and 3-time quasi-particle regions with the $2a_0$ and $3a_0$ quasi-particle distances in the second scale situation. In practical multi-scale simulation, the 2-time, 3-time or even 4-time quasi-particle regions are employed to substitute for the corresponding atomic region according to the complexity and size of simulation model.

In a general situation, the quasi-particle model consists of three essential components: atom region, second scale quasi-particle region and third scale quasi-particle region (as shown in Fig. 2). The first component is not new to this work, and is simply taken from the well-developed methods (e.g. molecular dynamics method). The second component and third component are similar to the first component except the different potential functions which would be presented in the latter parts.

The two imaginary domains and their overlapping with the real model domains shown in Fig. 3 are exemplified for the boundary between left domain, the atomic scale (n=1), and right domain, second-scale quasi-particle domain (n=2). Right imaginary area with the width W_a is located to the right of the boundary by overlapping with the second scale quasi-particle domain. This imaginary domain consists of image atoms that connect and interact with the real atoms on the other side of the boundary. The other imaginary area with width W_{II} is located to the left of the boundary by overlapping with the real atomic domain. The imaginary domain consists of image quasi-particles of the second scale that connect and interact with the quasi-particles on the other side of the boundary.

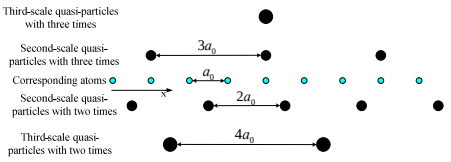


Fig. 1 Schematic diagram of quasi-particle model in one-dimensional condition domain

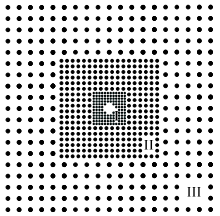


Fig. 2. Three scales quasi-particle model of a plate

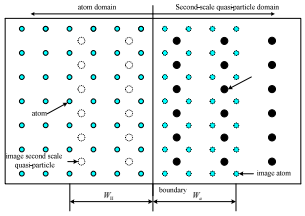


Fig. 3 Natural boundary between the atomic domain and the second scale quasi-particle

DYNAMICS EQUATIONS

Let $V_{ij}^{a}(r_{ij})$ denotes the potential function of atom system. Its derivative is expressed as $G_{ij}^{a}(r_{ij})$. $V_{IJ}^{A}(R_{IJ})$ denotes the potential function of quasi-particle system. Its derivative is expressed as $G_{IJ}^{A}(R_{IJ})$. Here r_{ij} denotes the vector between atom i and atom j. R_{IJ} denotes the vector between quasi-particle I and quasi-particle J. If following does not specify, lowercase indicates the atom and uppercase indicates the quasi-particle. The subscripts appeared in formulas do not follow the dummy index summation convention. The acceleration of atom i can be expressed as

$$\boldsymbol{a}_i = \frac{\boldsymbol{f}_i}{m_i} = \frac{1}{m_i}\sum_{j(j\neq i)} \boldsymbol{f}_{ij}(\boldsymbol{r}_{ij}) \tag{1}$$

[a] Corresponding author. Email: wangzhenqing@hrbeu.edu.cn.

where $\boldsymbol{f}_i$ is the total force applied on atom i. m_i denotes the mass of atom i. j is summed over all atom within the scope of cutoff radius r_{cut}, excepting atom i. The force $\boldsymbol{f}_{ij}(\boldsymbol{r}_{ij})$, applied on atom i by atom j along the direction from atom i to j can be obtained by

$$\boldsymbol{f}_{ij}(\boldsymbol{r}_{ij}) = -\frac{dV_{ij}^{a}(\boldsymbol{r}_{ij})}{d\boldsymbol{r}_{ij}} = -\boldsymbol{G}_{ij}^{a}(\boldsymbol{r}_{ij}) \tag{2}$$

By considering the average acceleration method the acceleration of quasi-particle I is suggested as follows

$$\boldsymbol{a}_I = \frac{1}{n}\sum_{i\in I}\boldsymbol{a}_i \tag{3}$$

where the index i represents the *n* atoms which are subordinate to quasi-particle I. Substituting Equation (1) and Equation (2) into Equation (3), the acceleration of quasi-particle I is obtained

$$\boldsymbol{a}_I = -\sum_{i\in I}\sum_{j(j\neq i)}\frac{\boldsymbol{G}_{ij}^{a}(\boldsymbol{r}_{ij})}{m_i} \tag{4}$$

Then according to the quasi-particle position calculated from Equation (4), the force applied on quasi-particle I is obtained as follows

$$\boldsymbol{F}_I = -\sum_{J(J\neq I)}\frac{dV_{IJ}^{A}(\boldsymbol{R}_{IJ})}{d\boldsymbol{R}_{IJ}} = -\sum_{J(J\neq I)}\boldsymbol{G}_{IJ}^{A}(\boldsymbol{R}_{IJ}) \tag{5}$$

Finally, the Equation (4) and Equation (5) are the important formulas of separate quasi-particle dynamics method.

NUMERICAL TEST

In this section, a three-dimensional model of copper nano-wire (as shown in Fig. 4 and Fig. 5) are calculated to validate the separate quasi-particle method. The specimen is then relaxed so that all atoms or particles can reach their equilibrium position. By adjusting the relaxation time for each 0.5% strain, the different average strain rates are obtained in the relaxation process. The comparisons of the stress-strain curves obtained by molecular dynamics method, GP method, average acceleration method, energy conservation method and separate quasi-particle method with different strain rates are shown in Fig. 6. From this comparison, it seems the agreement is satisfactory.

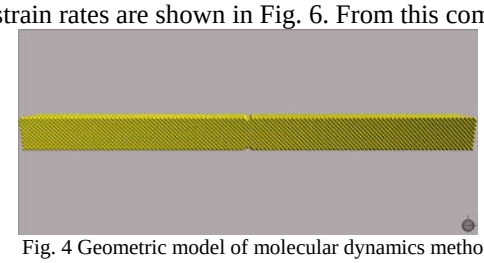


Fig. 4 Geometric model of molecular dynamics method for copper nano-wire

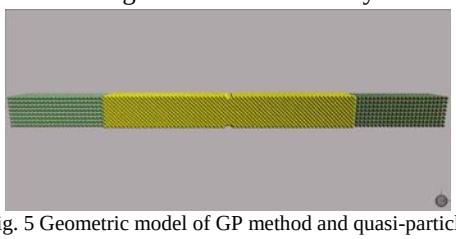
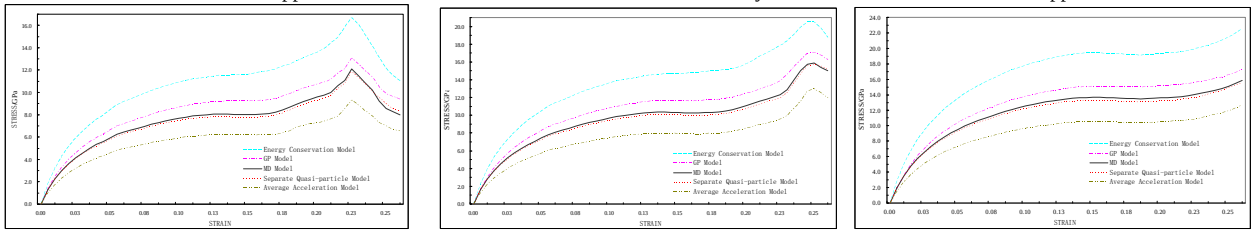


Fig. 5 Geometric model of GP method and quasi-particle dynamics multi-scale method for copper nano-wire



(a) strain rate 1.0×10^{8} (b) strain rate 2.0×10^{8} (c) strain rate 5.0×10^{8}

Fig. 6 Stress-strain cures of five models

CONCLUSIONS

A separate quasi-particle dynamics method was proposed for investigating the connections and transitions between atomistic scale and quasi-particle scale or continuum scale. By introducing the natural boundary conditions, this model separated the multi-scale analysis of quasi-particle system into the calculation of quasi-particle displacement and the calculation of quasi-particle interaction. Comparing to the GP method, the stress-strain curves obtained by separate quasi-particle dynamics method are more conforming to molecular dynamics method in whatever strain rates.

References

[1] H. SU, M. BRIAN, W. K. LIU, G. B. OLSON, J. Comput.-Aided Mat. Des, 10 (2003),pp. 99-142.

[2] H. SU, W. K. LIU, M. BRIAN, V. FRANCK, G. B. OLSON, Comput. Methods Appl. Mech. Eng, 193 (2004),pp. 1865-1908.

[3] J. FAN, Science Press, Bei Jing, China, 2008.

[4] J. FAN, SIAM J, Multiscale Model. Simul, 8 (2009),pp. 228-253