Investigation of load imbalance in the hybrid atomistic-continuum simulation based on geometric coupling

Qian Wang[a], Xiaoguang Ren, Chao Li and Wenjing Yang

College of Computer, National University of Defense Technology, Changsha, China,
State key Laboratory of High Performance Computing, National University of Defense Technology, Changsha, China.

Abstract. The hybrid atomistic-continuum (HAC) simulation based on geometric coupling has intrinsic load imbalance under conventional parallel decomposition method. This paper presents qualitative guiding rules for alleviating load imbalance in the HAC simulation. We reveal the intrinsic load imbalance in the HAC parallel simulation, analyze the coupling procedures involved in the coupling exchange and present two qualitative decomposition rules for the atomistic region decomposition. The results of the benchmark case show the decomposition style under the guiding rules instruction performs much better than the default decomposition method which coupling overhead is only 58% of the default and communication time consuming is 75% of the default.

Keywords: qualitative guiding rules, load imbalance, hybrid atomistic-continuum method.

1 Introduction

The hybrid atomistic-continuum method (HAC)[1]based on the geometric coupling is a reliable simulation approach capable of accurately describing the flow characteristics at micro- and nano-scales[2,3]. The HAC method based on geometric domain decomposition splits the simulation domain into the continuum region, the atomistic region and the overlap region, which exchanges the simulation data between the previous two regions to keep the physical properties consistently, i.e., density, velocity and temperature, etc.[4].

In the previous research, the parallel HAC coupling framework based on the geometric domain decomposition consists of the continuum solver (CFD solver), the atomistic solver (MD solver) and relatively coupling operations for data exchanging[5,6]. There are several coupling procedures involved to correctly exchanging data between two simulation solvers. Reasonable parallel coupling operations plays an important role on efficient coupling simulation. There are also different multi-scale coupling methods, i.e., Finite Volume Method and Lattice Boltzmann Method[7], Finite Volume Method and Brownian Configuration Method[8], etc.

Nevertheless, there are much more parallel issues to be investigated about the HAC coupling method. For there are two kinds of simulation scales and methods in one parallel simulation. There are many subtle parallel issues in the HAC simulation. The previous research had scarcely taken consideration on the parallel issues. Although the HAC method has already gained simulation efficiency, these coupling operations will still lead the coupling oriented load imbalance in the

[a] Corresponding author : wangqiannudt@gmail.com

coupling simulation and must be further investigated. In this paper, we present numerical analysis of the parallel load imbalance in the geometric coupling simulation. The main contributions of this paper are as follows:

1. We analyze the coupling oriented load imbalance phenomenon in the geometric coupling simulation method and propose decomposition guiding rules for the atomistic region.
2. We design and implement the Hybrid Atomistic-Continuum framework based on open source code OpenFOAM and LAMMPS. The coupling time probes are implemented in the hybrid framework.
3. We verify our decomposition guiding rules through benchmark experiments on our hybrid framework. The results indicate that the decomposition style under the guiding rules instruction performs coupling overhead only 58% of the default and communication time consuming 75% of the default.

2 Numerical modeling

In this section, we present our hybrid atomistic-continuum coupling framework using LAMMPS and OpenFOAM. OpenFOAM servers as the main framework which is highly modular and elegant extendibility[9] and LAMMPS[10] is built as a library to be called from.

For a 2D simulation domain, the computational domain is split into an atomistic region and a continuum region, using an overlap region to alleviate dramatic density oscillation and couple the results of these two regions. The outer boundary of the continuum region which resides in the atomistic region is called hybrid solution interface (HSI)[1].The overlap region contains a control region (control region), a buff region (buffer region), an atomistic-coupled-to-continuum-region (A→C region) and a continuum- coupled-to-atomistic region (C→A region). In the control region, there is a reflecting wall boundary condition to prevent particles leaving the atomistic region freely and the outer boundary is the MD-continuum interface. The schematic diagram of the domain decomposition based on HAC method is depicted in Figure 1.

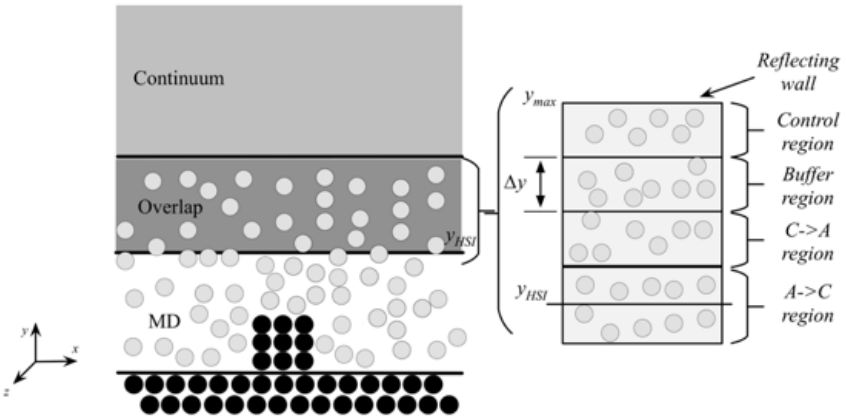

Figure 1. Decomposition of computational domain and the configuration of the overlap region.

We use an incompressible, Newtonian solver as our continuum solver and the truncated and shifted Lennard-Jones (LJ) potential to model the interactions between particles. we choose liquid Argon as the model liquid flow with LJ parameters $\sigma = 0.34$nm, $\varepsilon = 1.67 \times 10^{-21} J$and $m = 6.63 \times 10^{-26} kg$, where m is the particle mass and a well defined liquid phase of Argon with $T k_B \varepsilon^{-1} = 1.1$, $\rho\sigma^3 = 0.81$ and the dynamic viscosity$\mu = 2.14\varepsilon\tau\sigma^{-3}$ where $k_B$is the Boltzmann constant.

In the overlap region, we use constraint dynamic method[1] to exchange CFD data to MD (C->A) and data averaging method to exchange MD data to CFD (A->C).In the *control region*, we use an non-periodic boundary force to remedy the pressure of the atomistic region. Finally, due to the

existing of mass flux through HSI, we use our parallel particle insertion algorithm to handle this exchange. The detailed implementation of these operations can be referenced in our previous work[11,12].

3 Analyze and optimize of load imbalance

In this section, we analyze the coupling procedures in the hybrid atomistic-continuum simulation in detail, formalize the source of the load imbalance and present the guiding rules for the parallel decomposition of the atomistic region.

In the previous section, we give the coupling framework of our HAC method. The certain coupling procedures affects the coupling simulation efficiency as depict in Figure 2.As we all know, the major simulation time of the HAC method sis on the MD part, even though the HAC method narrowing the atomistic region. We can see that the coupling procedures control the particles located in the overlap region and manipulate the physical data exchanging. These coupling procedures, i.e., *C->A, A->C, mass flow and non-periodic boundary force*, append extra particle operations to the original MD operations.

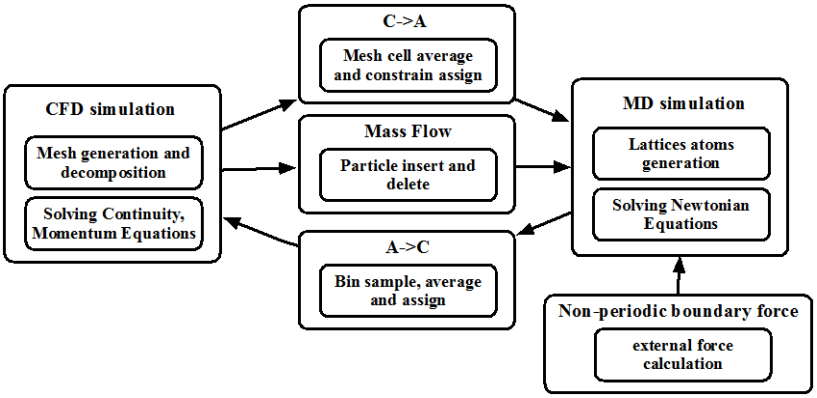

Figure 2. Coupling framework of the HAC method and Detail coupling operations.

In order to clearly depict the intrinsic load imbalance in the HAC simulation, we categorize processes involved in the HAC simulation as follows:

- *Pure CFD process*, P_{CFD}: only contain sub mesh on it;
- *Pure MD process*, P_{MD}: only contain sub domain on it;
- *Couple process*, P_{Couple}: contain both sub mesh and sub domain on it ;

The schematic diagram of parallel decomposition for both the overlap region and the atomistic region is depicted in Figure 3 with 12 degree of parallelism. As the Figure 3 shows, the process *P2*, *P5*, *P8* and *P11* are the *Couple process*, while others are the *Pure MD process*.

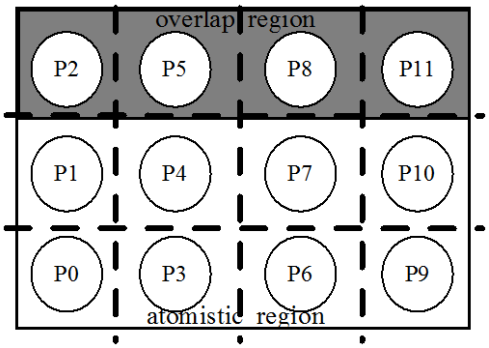

Figure 3. Default parallel decomposition of the atomistic region and the overlap region.

The particles in the overlap region are named as *couple particle*, while others particles are named as *normal particle*. The simulation time distribute on theT_{pcfd}, $T_{pmd}$and $T_{cp}$are defined as follows:

$$T_{pcfd} = T_s + T_{comm}$$

$$T_{pmd} = T_s + T_{comm}$$

$$T_{cp} = T_s + T_{comm} + \mathrm{T}_{couple}$$

where$\mathrm{T_s}$ represents the serial computation time of solving one linear system and one sub lattice domain, $\mathrm{T_{comm}}$ is the corresponding communication overhead.$\mathrm{T_{couple}}$is the corresponding overhead for coupling procedures. In order to fully use the simulation power, in one HAC simulation, there are usually only PMD and PCouple. For each process in the HAC simulation, we can define the balance ratio among them as follows:

$$\mathrm{r_{balance}} = \mathrm{P^i_{MD}}/\mathrm{P^j_{Couple}}$$

In the HAC simulation, the processes need several barriers to correctly exchange data and coupling simulation. The diagram of the barrier timing is depicted in Figure 4. Less barrierbetween all processes will lead less communication time between processes.

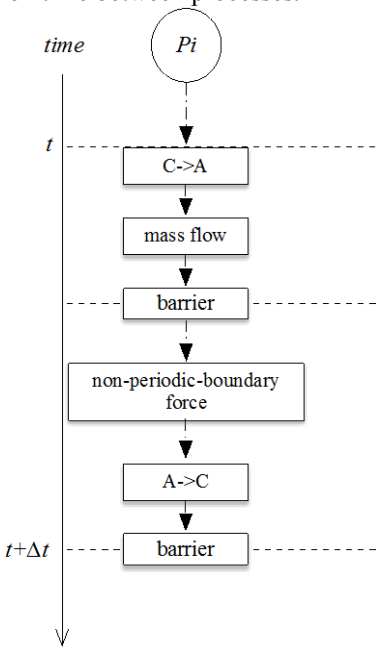

Figure 4. Time line of coupling operations.

The key of decomposition of the atomistic region is to balance the coupling overhead for each process. The closer $\mathrm{r_{balance}}$ to 1, the more balance among the whole simulation. The qualitative guiding rules of the parallel decomposition are to make the process to be the Couple process and allocate the overhead of coupling procedures to the highest number of processes.

Rule 1: allocate the overlap region to the highest number of processes for the load balance sake;

Rule 2: the minimum length of the atomistic sub domain should larger than the cutoff radius of the pair potential.

Using the above guiding rules, we can further improve the simulation efficiency of the HAC simulation.

4 Experiments and results

In this section, we use the benchmark case, i.e., the channel flow past the rough wall to verify our guiding rules of the parallel decomposition.

The test case is the channel flow past the rough wall as shown in Figure 5. The simulation domain is $x \times y = 384 \times 384\sigma^2$, while the z direction of the MD domain is 10σ. We use a large simulation domain to present the load imbalance problem and the degree of parallelism is 192 processors. The moving and still wall are no slip boundary condition. The length of cell and bin are the same with 2σ. The rough bottom wall consists two layers of FCC (111) solid particles and the height of it is about 8σ. The cutoff radius is chosen 2.2σ for time sake. The velocity of the top wall is$U_w = 3.0\,\sigma/\tau$. The time step of MD is 0.005τ .

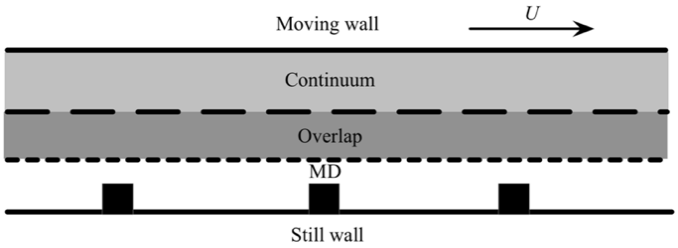

Figure 5. The simulation domain of the benchmark case.

In such configuration of the simulation domain, the default decomposition of the atomistic region is 24×8. We choose another five kinds of decomposition style to compare with the default one and check the effective of the guiding rule.

Table 1. Parameters of decomposition styles for the atomistic regions.

Style	Length of subdomain (x direction)	Number of bins (x direction)
192×1	2σ	1
96×2	4σ	2
64×3	6σ	3
48×4	8σ	4
32×6	12σ	6
24×8	16σ	8

The surface-to-volume ratio of these six styles are calculated in the following Table 2. We can see that the default decomposition method has the minimum surface-to-volume ratio.

Table 2. Surface-to-volume ratio of six styles.

Style	Surface area of all sub domains	Surface-to-volume ratio
192×1	2728.00	2.60
96×2	1648.00	1.57
64×3	1314.67	1.25
48×4	1168.00	1.11
32×6	1061.33	1.01
24×8	1048.00	1.00

We compare the following time consuming to show our guiding method superiority over the default method, i.e., the ratio of couple simulation time $T_{cp}$and communication time T_{comm}over the total simulation time. The pure CFD calculation and pure MD calculation are almost the same for these six styles.

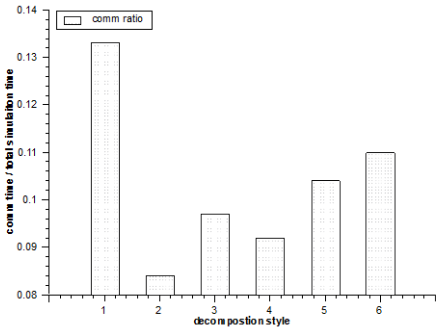

Figure 6. The ratio of the communication time to the total simulation time among six decomposition styles.

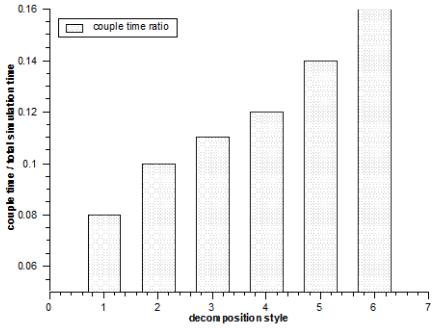

Figure 7. The ratio of the couple operation time to the total simulation time among six decomposition styles.

The result of the first style, i.e., 192×1 which has a length of 2σ in x direction perform a worse communication time. Because the side length of the sub domain is smaller than the cutoff radius and disobey Rule 2 with worse communication time. In Figure 6 and Figure 7, we can see that the second style with obeys Rule 1and Rule 2 performs the best result than the other decomposition. The 96×2 style performs the best communication time even though the surface-to-volume ratio is larger than the default one and $r_{balance}$ is more closer to 1. Furthermore, the 96×2 style balances the coupling overhead to the highest number of processes so to further improve the efficiency.

From Figure 6 and Figure 7 we can find that reasonable decomposition for the HAC simulation can further reduce unnecessary overhead and improve simulation efficiency.

5 Conclusions

This paper gives qualitative guiding rules for alleviate the load imbalance phenomenon in the hybrid atomistic-continuum simulation based on geometric coupling. The results of the benchmark case show the decomposition style of the guiding rules perform much better than the default decomposition method which coupling overhead is only 58% of the default and communication time consuming is 75% of the default. The decomposition guiding rules could have quantitative description. We aim to propose the quantitative rules for the parallel decomposition of the atomistic region in the future.

Acknowledgments

The authors declare that there is no conflict of interest regarding the publication of this paper. The authors would like to thank the National Natural Science Foundation of China (Grant no. 61303071 and 61120106005) and the Open fund from State Key Laboratory of High Performance Computing (no. 201303-01, 201503-01 and 201503-02) for funding.

References

1. S. T. O'Connell, and P. A. Thompson. 1995. *Molecular dynamics-continuum hybrid computations: A tool for studying complex fluid flows, Phys Rev E Stat Phys Plasmas Fluids Relat Interdiscip Topics, 52: R5792-R95.*
2. T. M. Squires, and S. R. Quake. 2005. *Microfluidics: Fluid physics at the nanoliter scale, Rev Mod Phys, 77: 977-1026.*
3. G. M. Whitesides. 2006. *The origins and the future of microfluidics, Nature, 442: 368-73.*
4. T. Werder, J. H. Walther, and P. Koumoutsakos. 2005. *Hybrid atomistic-continuum method for the simulation of dense fluid flows, Journal of Computational Physics, 205: 373-90.*
5. P. Neumann, H. Flohr, R. Arora, P. Jarmatz, N. Tchipev, and H. J. Bungartz. 2016. *MaMiCo: Software design for parallel molecular-continuum flow simulations, Computer Physics Communications, 200: 324-35.*
6. M. K. Borg, D. A. Lockerby, and J. M. Reese. 2013. *A hybrid molecular-continuum simulation method for incompressible flows in micro/nanofluidic networks, Microfluid Nanofluid, 15: 541-57.*
7. S. Zou, X. F. Yuan, X. J. Yang, W. Yi, and X. H. Xu. 2014. *An integrated lattice Boltzmann and finite volume method for the simulation of viscoelastic fluid flows, Journal of Non-Newtonian Fluid Mechanics, 211: 99-113.*
8. X.-W. Guo, X.-H. Xu, Q. Wang, H. Li, X.-G. Ren, and X. Yang. 2016. *A hybrid decomposition parallel algorithm for multi-scale simulation of viscoelastic fluids. In IPDPS2016.*
9. OpenFOAM. 2016. *http://www.openfoam.org/.*
10. S. Plimpton. 1995. *Fast Parallel Algorithms for Short-Range Molecular Dynamics, Journal of Computational Physics, 117: 1-19.*
11. Q. Wang, X.-H. Xu, C. Li, H.-Y. Ji, X.-G. Ren, and X.-J. Yang. 2016. *Coupling Strategies Investigation of Hybrid Atomistic-Continuum Method Based on State Variable Coupling.*
12. W.-J. Yang, W. Yi, X.-G. Ren, L.-Y. Xu, X.-H. Xu, and X.-F. Yuan. 2015. *Toward large scale parallel computer simulation of viscoelastic fluid flow: A study of benchmark flow problems, Journal of Non-Newtonian Fluid Mechanics, 222: 82-95.*

