Advanced Science and Technology Letters
Vol.120 (CCSC 2015), pp.727-734
http://dx.doi.org/10.14257/astl.2015.120.145

M2P2: the pre-processing software tool for Micro-Macro coupling fluid simulation

Qian Wang[1,2], Wenjing Yang[1,2], Fu Li[1,2], Xiaoguang Ren[1,2], Yuhua Tang[1,2]

[1] College of Computer,
National University of Defense Technology, Changsha, China
[2] State key Laboratory of High Performance Computing
National University of Defense Technology, Changsha, China
{wangqian, wenjing.yang, renxiaoguang}@nudt.edu.cn, {lifunudt, yhtang62}@163.com

Abstract. Fluid simulation is an important application of High Performance Computing. The micro-macro coupling simulation can effectively handle the contradictory of the reduction of the simulation scale and the increase of computation load when try to improve the accuracy. The pre-processing of the coupling simulation is quite important in the whole simulation and requires the support of an efficient, user-friendly interface. Under the demand of efficient coupling simulation, we, based on SALOME, develop a visual pre-processing framework, M2P2, for unified micro-macro and apply into the coupling simulation process. The experimental verification indicates that our M2P2 framework can offer efficient, easy-to-use pre-processing for the micro-macro coupling simulation, and effectively improve the efficiency of the simulation.

Keywords: HPC, Fluid simulation, micro-macrocosmic coupled simulation, pre-processing

1 Introduction

High Performance Computing (HPC) technology has made computing to be the third scientific method, following theory and experiment. Generally, the accuracy of computer simulation is in inverse proportion of the scale of the model abstraction [1]. When the scale of the simulation decreases to nanoscale, the computing load would be getting so heavy that HPC becomes a bottleneck, sometimes even Milky-way 2 cannot meet the computational demand. How to get satisfied results with current computational power becomes a challenge. Fortunately, the so-called Micro-Macro multi-scale simulation method is proposed [2, 3].

The key idea of the Micro-Macro simulation method is the domain decomposition of the simulation area, thus the pre-processing, which generates input data for the solver, turns out to be an important component of the whole simulation framework. In macroscopic computational fluid dynamics, the mesh generation, parallelism partition and boundary definition of simulation domain are done in pre-processing, while in molecular dynamics, the pre-processing finishes the configuration of the physical parameter and simulation box.

ISSN: 2287-1233 ASTL

The pre-processing tool is a necessity in the coupling simulation of Micro-Macro. The absence of a user-friendly pre-processing tool would cause low efficiency, while a visual tool of good availability, low threshold of relevant tech background may contribute to the improvement of the efficiency and the reduce of cost. The currently available pre-processing tools, always in single scale, cannot meet the demand of Micro-Macro coupling simulation.

In this paper we present a Micro-Macro coupling simulation oriented Pre-processing tool based on SALOME. We analyze the basic framework, execution mechanism and development method of SALOME software. Based on the analysis, we design and implement an user-friendly and effective pre-processing tool. The contributions of this paper are as follows:

1. Associated with the demand of Micro-Macro coupling simulation and the analysis of SALOME, we designed the main framework of an user-friendly pre-processing tool – M2P2.
2. We design and implementation of the M2P2 pre-processing tool. We implemented the user interface and core functions, which simplified the operations and improve the efficiency of the pre-processing.
3. We verify M2P2 through the experiment. The result indicates that our pre-processing tool is able to offer efficient and user-friendly pre-processing for users.

2 Background

Micro-Macro coupled simulation process can be divided into three basic stages as pre-processing, simulating and post-processing. Pre-processing is separated from the core simulating and post-processing in the time-domain as shown in Fig. 1.

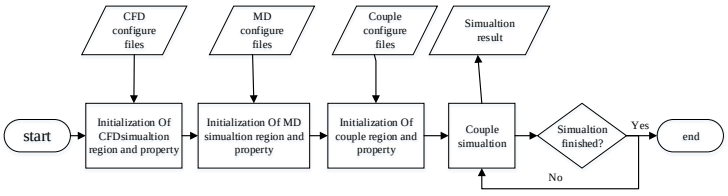

Fig. 1. Flowchart of Micro-Macro coupled solver

We present a brief introduction to the pre-processing process taking the simulation of Couette flow as an example. Couette flow refers to the viscous fluid flow between two mutually moving plates in parallel, see Fig. 2. Which includes the following steps: Firstly, the users define the geometric region, namely to determine the CFD region and the MD region. We can simply partition the whole space into two sub regions, as shown in Fig. 3. Secondly, considering using OpenFOAM as the CFD computing platform, the CFD region must be organized into an OpenFOAM-supported format and the corresponding boundary conditions specified. The mesh can be generated with either the self-designed tool of OpenFOAM or others. Thirdly, considering using LAMMPS to conduct the MD simulation, since there are no

suitable configuration tools for MD simulation until now, users have to extract the complex situation of the MD region into a simple configuration profile.

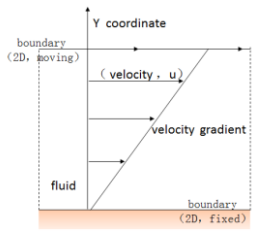

Fig. 2. Illustration of Couette flow field

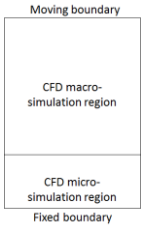

Fig. 3. Partitions of the overall space into CFD and MD regions

So far, there are many sophisticated pre-processing software, but most of them are of single-scale rather than multi-scale [4]. For CFD pre-processing, ICEM CFD, PointWise and Gridpro are commonly used for mesh generation [7], either for solid or liquid simulation region. Some software, like Gridpro, can only generate structured mesh, while TGrid is professionally for unstructured mesh generation[12], which is independent of the geometry complexity and size constraints. For MD, there are few pre-processing software [5].

3 Framework of M2P2 pre-processing software

According to the requirements analysis above, the SALOME [13] software is used as the Pre-Processing development platform. SALOME is an open-source software that provides a generic Pre-Processing platform for numerical simulation [8]. SALOME applies CORBA technology and modeling methods of distributed system in software architecture.

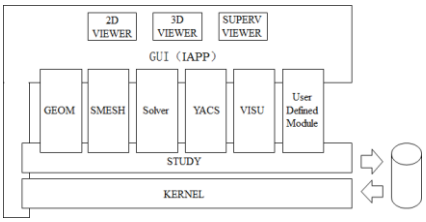

Fig.4. The software framework of SALOME

As shown in Fig. 4, SALOME integrates lots of Pre-Processing modules of CFD. KERNEL module provides an available interface for integration of other modules. GUI module offers a visible interface for data operation for users. Geometric models are produced in GEOM module. SMESH module generates meshes for geometric objects with various meshing algorithms. Visual operation of data is performed in

VISU module [6]. Modules perform information communication and data exchange with each other through core module using protocol of CORBA.

The architecture of M2P2 (Micro-Macro Pre-Processing) tool based on SALOME platform is proposed in this section. It consists of GEOM module, SMESH module integrated in SOLOME. M2P2 tool utilizes the modules in SALOME without any changes and adds some new Pro-Processing modules. M2P2 separates tasks reasonably and coordinates those existing modules to perform Micro-Macro coupling simulation in Pre-Processing. Fig. 5 shows the architecture of Micro-Macro Pre-Processing platform. Which mainly includes the procedures in the following:

Firstly, definition of the geometry region with the GEOM module. GEOM performs 2D/3D modeling and supports import of geometry models even derived from other advanced geometric modeling tools.

Secondly, designation of the computation region with the GEOM module. The MD region must be rectangle in this work and is generated using simple graphics generation tools.

Thirdly, generation of configuration files for the MD region with the Pre-Processing module. Deal with the imported configuration information and geometric information from the GEOM module, the Pre-Processing module exports the MD computational configuration files.

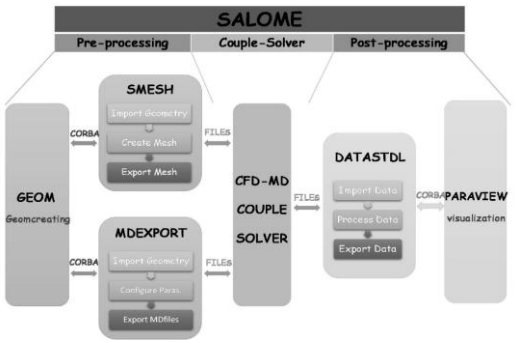

Fig.5. Framework of M2P2 pre-processing tool

Fourthly, mesh generation of the CFD domain with SMESH module. Getting the geometrical model from the GEOM module, particular mesh generation algorithm is applied to the geometrical model with the help of SMESH module and the SMESH module exports the mesh information into standard format.

Finally, solving with Micro-Macro-coupled solver. The solver will generate CFD and MD simulation results separately. As this part beyond the scope of this work, the usages or operations with the simulation results will not be discussed.

4 Implementation of the pre-process software platform M2P2

4.1 CORBA engine in the M2P2

The definition of the CORBA engine of the M2P2 is implemented in M2P2.idl [9]. M2P2.idl just defines but not implements the interface. The Property structure of the definition contains the configuration information, such as the fluid density, the solid density, the width of the coupling, etc.

The MDobject structure of the definition constitutes the core data structure of the M2P2 pre-processing module, which contains the geometric object GEOM::GEOM_Object defined by Property and GEOM modules. The main function of MDobject is to store the MD region geometric object transmitted by GEOM module and the configuration information of the object.

M2P2_Gen inherits from Engines::EngineComponent that defined by KERNEL, and it is the engine definition of the M2P2 module. The functions defined in M2P2_Gen constitutes the core service and interface of the M2P2 module. In other part of the M2P2 module, such as GUI, the core data structure can be operated by instantiating this engine. M2P2_Gen defines three interface functions: the setData() interface writes data to the data index, the getData() interface get data from the data index and the processData() interface process these data.

4.2 Specific classes in the M2P2

The core functions of the M2P2 pre-processing platform are implemented in the related function of M2P2GUI class [11]. The graphical module includes the initialization function Initialize(), the module activation function activateModule(), the module deactivation function DeactivateModule(), the data transmitting function OnRetrieveData() and the data processing function OnProcessData().

When the M2P2 is activated, the compiled link libraries of module are loaded to main memory; The createModule() function is executed to active the object related to GUI on the first step; the GUI object takes control of the program and creates menu, object browser, visualization window, etc.; The module loading process completes and waits for user operation [10].

Data can be organized in different forms, we use index and queue to organization data. DataModel uses tree structure to organize data, and we can get the root data through the root() function with returned Object, Data Object. The function of Data Object is to provide a common interface that can be accessed by other objects but shield the difference of data operations. This shield enhances the independence between objects and increases the scalability and robustness of modules.

5 Experimental Verification

This section is mainly about the result of the M2P2 pre-processing module through snaps of the software. The example we took was the computation Couette benchmark flow mentioned above.

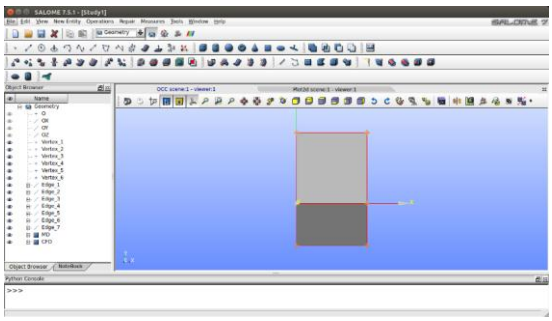

Fig. 6 Modeling with GEOM module

Fig. 6 illustrates the modeling of the computing domain with the GEOM module of SALOME. We applied CFD on the upper half of the area while MD was used on the bottom half.

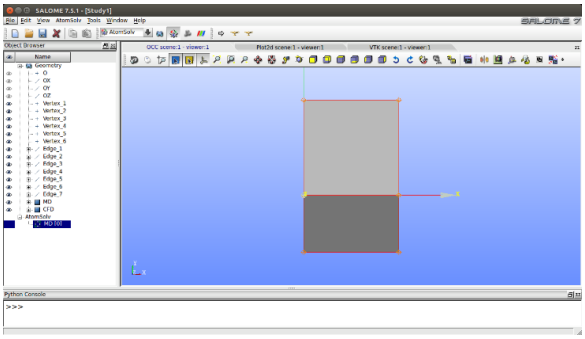

Fig. 7. Transferring data from GEOM module

Fig. 7is the process that transferring the data of MD field generated in the GEOM module within the M2P2 module, saving it in the form of its own data structure, and printing it in the data browser.

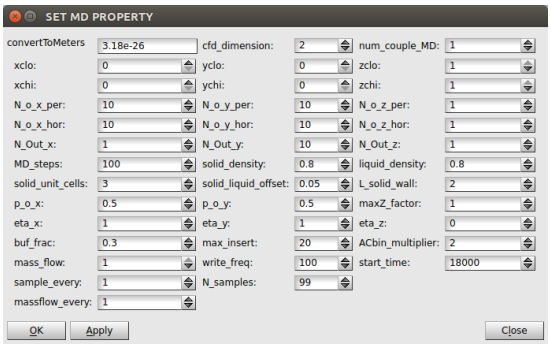

Fig. 8. Dialog for configuring the MD field information

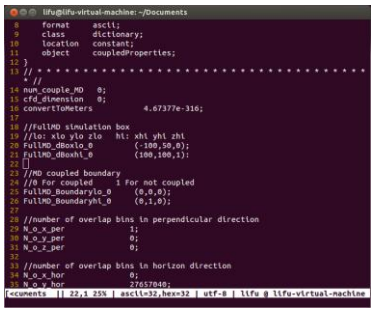

Fig. 9. CoupleProperties file

Fig. 8 is the dialog that configured the key word of MD field information in M2P2 module, including CFD_dimension, solid_density, etc. This dialog was popped up when clicking on the button of "information configuration and output of the MD field". The default values were the values of the field configuration information in this example.

After closing the dialog, M2P2 module would combine the field information from the GEOM module and the MD field information configured by users, and generate the coupleProperties file, which has the content showed in Fig. 9

6 Conclusion

This paper design the structure of the efficient pre-processing tool that based on SALOME for the coupling simulation of macroscopic and microscopic scale simulation. Associated with the pre-processing of the coupling simulation, we design and implement the M2P2 tool based on SALOME. The experimental verification indicates our M2P2 tool is able to significantly improve the efficiency of pre-processing of the coupling simulation of the fluid in both macroscopic and microscopic scale.

Reference

1. Guangxian Xu. The hierarchy and scale of the material structure [J]. Science & Technology Review, 2002, 20(1):3-6. DOI:10.3321/j.issn:1000-7857.2002.01.001.
2. Bo Zhan. CFD simualtion of flow and mass transfer in nanofluids[D]. Tianjing University, 2012.
3. Hadjiconstantinou N G, Garcia A L, Bazant M Z, et al. Statistical error in particle simulations of hydrodynamic phenomena[J]. Journal of Computational Physics, 2003, 187(1):274–297.
4. HM S, W T. QM/MM Methods for Biomolecular Systems[J]. Angewandte Chemie International Edition, 2009, 48(7):1198–1229.
5. Valiev M, Bylaska E J, Govind N, et al. NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations.[J]. Computer Physics Communications, 2010, 181(9):1477-1489.
6. CG. B. A Simple Method of Resolution of a Distribution into Gaussian Components[J]. Biometrics, 1967, 23(1):115-35.
7. Yuxin Dong, Zheng He. CAD/CAM and mesh generation [J]. Applied Science and Technology, 2007, 34(6):43-45. DOI:10.3969/j.issn.1009-671X.2007.06.012.
8. Hao Zhang. the design of finite element analysis process automation software framework based on Salome platform [D]. Wuhan University of Technology, 2013.
9. Henning M, Vinoski S. Advanced CORBAr Programming with C[C]. //ISBN 9-780201379273, Addison-Wesley A.7 INTERNET 83 A.7 Internet [39] The World Wide Web Consortium http://www.w3.org/ Publications of many standards and drafts related the the Internet and World Wide Web. 1999.
10. Hébert A. Integration of the DRAGON5/DONJON5 codes in the SALOME platform for performing multi-physics calculations in nuclear engineering[J]. Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo, 2014.
11. Ribes A, Bruneton A. Visualizing results in the SALOME platform for large numerical simulations: an integration of ParaView[J]. IEEE Symposium on Large Data Analysis & Visualization, 2014:119 - 120.
12. Nunio F, Manil P. SALOME as a Platform for Magneto-Mechanical Simulation[J]. IEEE Transactions on Applied Superconductivity, 2012, 22(3):108-110.
13. Salome : The Open Source Integration Platform for Numerical Simulation. http://www.salome-platform.org.

