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A NEW PARALLEL SCIENTIFIC COMPUTING PLATFORM: RIGOROUS ADVANCED PLASMA INTEGRATION TESTBED (RAPIT)

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Summary. In this study, the development of a new C++ object-oriented multi-physics parallel simulation platform, named *Rigorous Advanced Plasma Integration Testbed* (RAPIT) using unstructured meshes, is reported. Because of the design of the data structure, RAPIT can easily accommodate continuum- and/or particle-based solvers with some proper hybridization algorithm in a self-consistent way. For the former, it may include, but not limited to, the Navier-Stoke (NS) equation solver for general gas flow modeling, the plasma fluid modeling code for modeling general low-temperature gas discharges, and the time-dependent Maxwell equation for electromagnetic wave simulation. For the latter, it may include the particle-in-cell Monte Carlo collision (PIC-MCC) and the direct simulation Monte Carlo (DSMC) solvers. Some results of DSMC, PIC-MCC, NS equation and fluid modeling solvers based on RAPIT are presented in this study. More details of the study will be presented in the meeting.

1 INTRODUCTION

Numerous industrial and scientific related technology developments require modeling of complex plasma and flow physics, i.e., multiphsyics and multiscale coupling, which may apply hybridization of different continuum- and/or particle-based solvers. Examples may include gas discharge modeling in plasma enhanced chemical vapor deposition, magnetron sputtering plasma and plasma etching for semiconductor fabrication; atmospheric-pressure plasma jet for surface cleaning, biomedicine, and agriculture; and ion thruster plume analysis, among others. The general wisdom is to employ solvers developed independently and integrate them in a weakly coupled approach, which limits their future application. In addition, these computations generally involve objects with complex geometry and are very time-consuming. Thus, a highly flexible yet efficient simulation platform, which allows easy addition and integration of different solvers with a self-consistent approach while maintaining efficient computations, is strongly required to challenge problems with complex plasma physics and others.

2 RIGOROUS ADVANCED PLASMA TESTBED

2.1 Overview

For efficiently modeling complex plasma/flow problems we have developed the **RAPIT** multi-physics software framework, which allows extreme flexibility for the programmer to add and hybridize different kinds of continuum- and particle-based solvers [1]. Note **RAPIT** applies, but not limited to, the cell-centered collocated finite-volume method using unstructured meshes. Fig. 1 shows the architecture of **RAPIT**, in which each block shows an independent module (or "object") with specific function. The simulation framework is designed to run across different OS platforms, which include Linux, MS-Windows and Macintosh that allows highest flexibility of the software usage under different hardware conditions. The code is written using the C++ object-oriented language, which ensures a highly modular coding structure and easier software maintenance. Since the software framework is inherently parallelized to enable computations of large-scale problems, the message passing interface (MPI) protocol is used to communicate among processors. In addition, the well-known graph partition libraries such as METIS [2] are used to partition the unstructured mesh per the function call in the application code, which makes the dynamic domain decomposition possible.

2.2 Particle data management

Fig. 2 shows the architecture/procedure of parallel particle data management, in which an accompanying "Pointer Tree" is created as a pointer to the Particle Data Pool (bi-direction data pointer) with four management head pointers (Empty, Buffer, Send, Recv) and a species data pointer of number of all species under simulation. Note a new particle is generated by linking from "Empty" to the species data pointer, while a particle is deleted by linking itself to "Empty". "Buffer" is used for temporary particle data storage when new particles are generated due to Monte Carlo reactions, and "Send" and "Recv" are used for particle data communication between processors. These four management heads exchange with the data pointer of number of all species within the "Pointer Tree". For a typical particle data transfer between two processors, the particle links to "Send" within its original processor, then links to the "MPI Tree Transfer" and finally links to "Recv" in the destination processor. With this implementation, the number of particles, which can be simulated, is only limited by the available physical memory of the computers without the need of presetting the array size.

2.3 Developed continuum- and particle-based solvers

Under the current multi-physics **RAPIT** framework, we have completed the preliminary implementation of the DSMC code (**ultraSPARTS**), the PIC-MCC code (**ultraPICA**), the NS equation solver (**ultraNSMod**) and the plasma fluid modeling code (**ultraFluMod**) [3]. Due to the limitation of the space, details of numerical methods and code implementations are not described here and will be presented in the meeting. Simulation results of one typical example of plasma fluid modeling for an axisymmetric argon capacitively coupled plasma applied sinusoidal voltage of 200 V (V_{rf}) and a frequency of 12 MHz are presented in Fig. 3. More results of other standalone solver and hybridization between solvers will presented in the meeting.

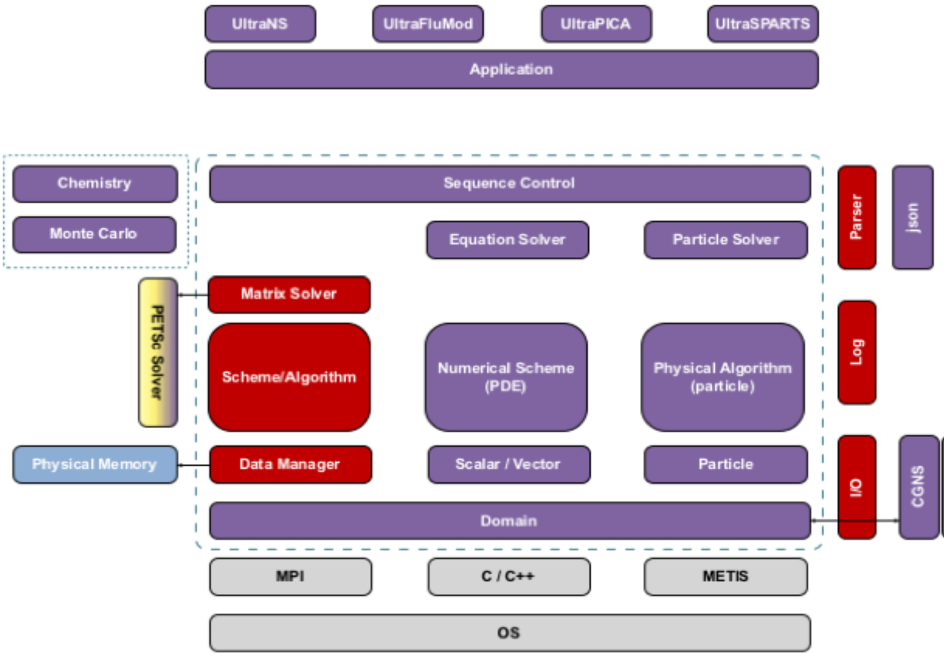

Figure 1: Software architecture of RAPIT.

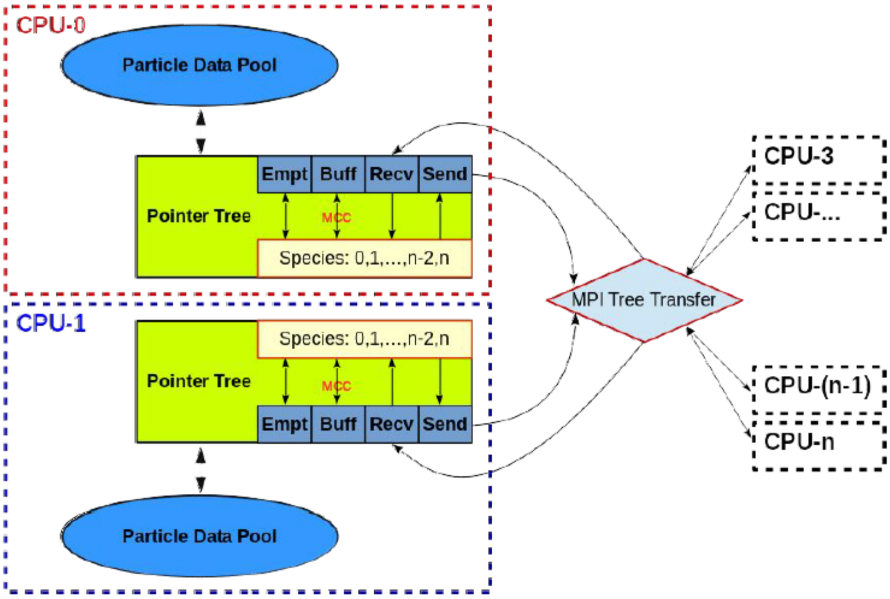

Figure 2: Parallel data management of RAPIT.

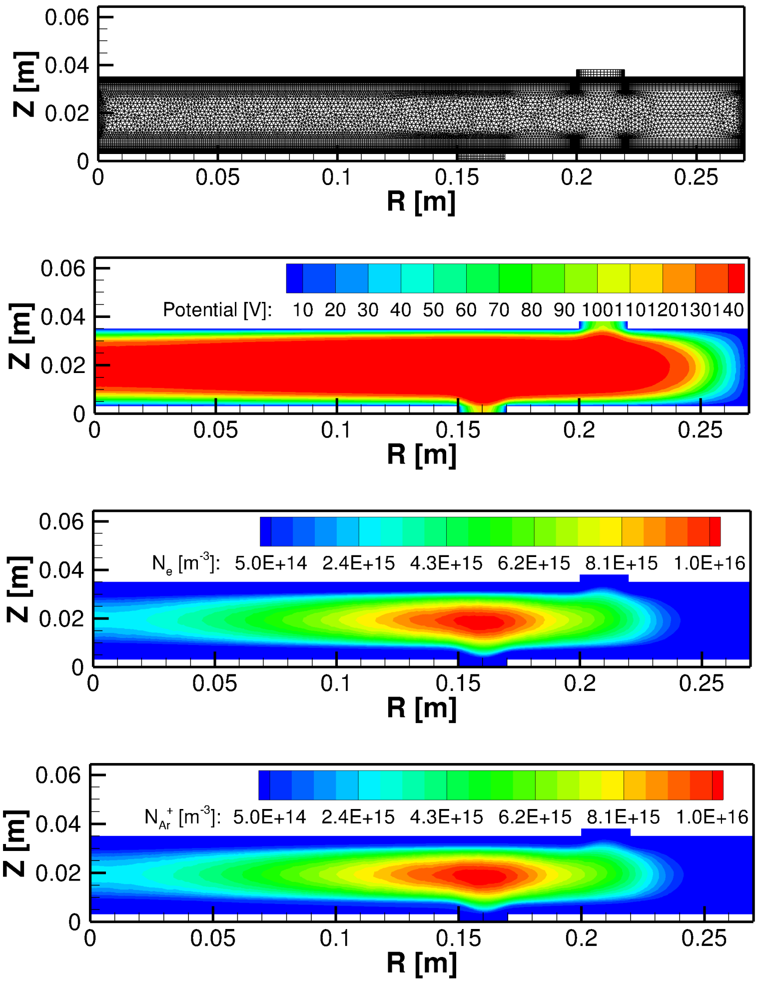

Figure 1: Averaged simulated plasma properties of an argon capacitively coupled plasma with a background pressure of 100 mtorr at 10,000th cycle.

CONCLUSIONS

In this study, we have successfully developed a new parallel (distributed-memory) computing platform, named RAPIT (Rigorous Advanced Plasma Integration Testbed), which can used for simulating ggeneral plasma related problems through continuum- and particle-based numerical methods. Many challenging examples will be presented in the conference.

REFERENCES

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