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Progress on Developing a Multi-physics Simulation Platform: Rigorous Advanced Plasma Integration Testbed (RAPIT)

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Many space and industrial related technology development require modeling of complex plasma and flow physics applying hybridization of different continuum- and/or particle-based solvers. Examples may include plume analysis of reaction control thrusters on upper-stage rocket and satellite in orbit, rocket plume analysis at high altitude, ion thruster plume analysis, and plasma distribution in an etching chamber, to name a few. These studies often utilize solvers developed independently and integrate them in a non-self-consistent approach, which makes their applications and future extension highly inflexible. Thus, a highly flexible simulation platform, which allows easy addition and integration of different solvers with a self-consistent approach while maintaining efficient computation, is strongly needed to tackle problems with complex physics, such as flow/plasma in space related technology. In this paper, we report the development of a new C++ object-oriented multi-physics simulation platform named *Rigorous Advanced Plasma Integration Testbed* (RAPIT) using unstructured meshes with parallel computing. The proposed 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 and the plasma fluid modeling code for general low-temperature gas discharges. For the latter, it may include the particle-in-cell Monte Carlo collision (PIC-MCC) and the direct simulation Monte Carlo (DSMC) solvers. Some preliminary results of DSMC, PIC-MCC, NS equation and fluid modeling solvers based on RAPIT are presented in this paper. Future direction of the RAPIT is also outlined at the end of the paper.

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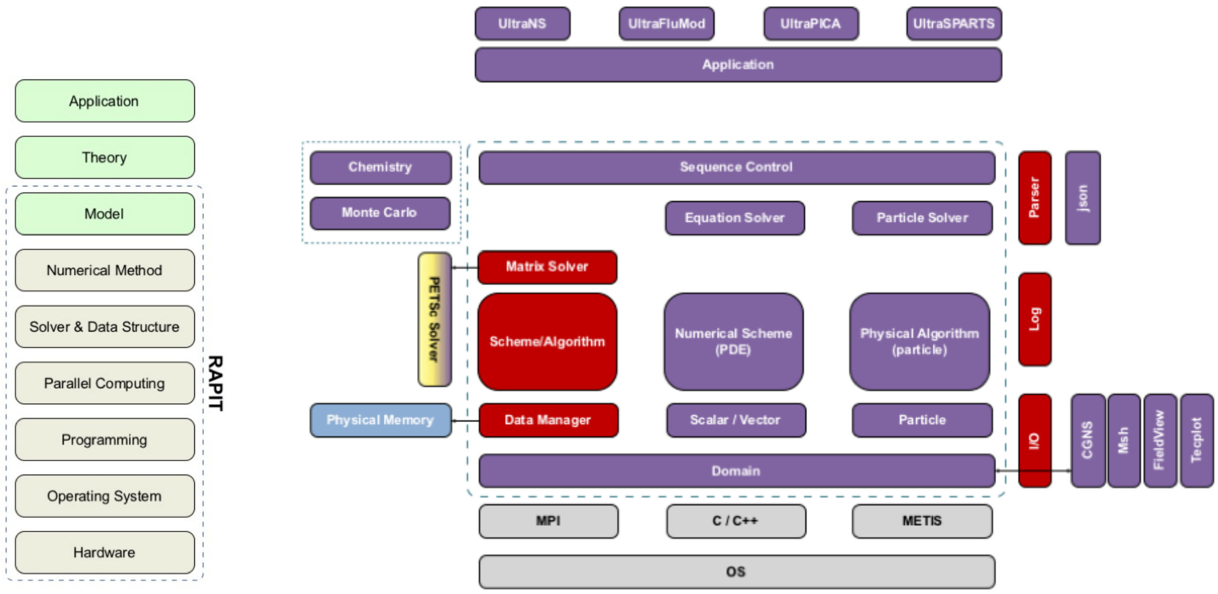
I. Background and Introduction

There are many challenging and important space and industrial technologies related plasma and flow problems, which require modeling with hybridization of different kinds of solvers including both/either continuum- and/or particle-based solvers. For example, hybridization of the direct simulation of Monte Carlo method (DSMC)[1] and the Navier-Stokes (NS) equation solver are needed for proper modeling the plume under highly rarefied condition such as reaction control thrusters of the upper-stage rockets and satellites in orbit and the rockets at high altitude[2-9]. For proper modeling the plume of ion thrusters of a spacecraft, the surface charging of a satellite in low earth orbit (LEO), and ion energy and angular distribution function at the wafer of a DC/RF magnetron sputtering chamber, one needs to couple the particle-in-cell Monte Carlo collision (PIC-MCC) method and the DSMC method.[10-14] For modeling plasma etching chamber, an appropriate approach is to hybridize the PIC-MCC method and the fluid modeling method.[15-18] However, in the aforementioned studies, there seems to be no studies which apply a self-consistent software framework in integrating different solvers. This makes the programming and further extension rather tedious and difficult. Thus, how to hybridize different solvers using a more self-consistent computational approach is very important to further extend the application of these tools and methods to a wider range of physical problems.

Generally, there are two classes of hybridization of numerical solvers. One is on the spatial basis, while the other is on the temporal basis. *The first class* applies to some flow/plasma problems, in which the computational domain consists of regions with different rarefaction/non-equilibrium levels that require different numerical approaches. In this class, the continuum method (e.g., NS equations, plasma fluid modeling equations) is applied to the continuum region, while the particle method (i.e., PIC-MCC, DSMC) is applied to rarefied region. Hybridization is performed through information exchange between continuum- and particle-based solvers based on some breakdown parameters which determine the location of interfacial boundary between continuum and particle solvers. Information exchange may include mass, momentum and energy fluxes by enforcing fluxes continuity. A typical example is the hybrid DSMC-NS scheme[5,6], in which DSMC solves the domain of high rarefaction and non-equilibrium flows, and the NS equation solves the region of continuum flows. *The second class* applies to some physical problems with either continuum- or particle-based modeling method, in which the characteristic time scales are utterly disparate and require much different marching time steps for reducing the computational cost that is otherwise prohibitively high even using the modern supercomputer system. Some efficient and accurate algorithms of information exchange at different times between modeling equations during runtime is needed. A typical example is the hybrid NS equation and plasma fluid modeling (PFM) scheme, named as temporal multiscale algorithm (TMA).[19,20] As mentioned earlier, the solvers were seldom hybridized in a self-consistent way. For example, the grid distribution requirements can be quite different for different solvers because of physical requirements. Interpolations of data from different solvers between different grids are often needed, which becomes very tedious, especially for unstructured meshes. In addition, the numerical solvers of interest were often developed at different times and independently by different groups of researchers. They could use different grid topologies (structured or unstructured) and could be either a serial code or parallel code. Thus, it often takes a long time to integrate different solves to really hybrid for a specific physical problem. There have been nearly no simulation platforms which were developed to efficiently address this problem. In this paper, we propose a new C++ object-oriented software framework, named *Rigorous Advanced Plasma Integration Testbed* (**RAPIT**©), which can easily accommodate different types of continuum- and particle-based solvers. **RAPIT**© applies the cell-center collocated finite volume method using unstructured grid with parallel computing based on MPI protocol throughout this paper, unless otherwise specified.

II. Rigorous Advanced Plasma Integration Testbed

For efficiently modeling complex plasma/flow problems we have developed the **RAPIT**© multi-physics software framework using C++ object-oriented language, which allows extreme flexibility for the programmer to add and hybridize different kinds of continuum- and particle-based solvers. Note **RAPIT**© applies, but not limited to, the cell-centered collocated finite-volume method using unstructured meshes. For 2D and axisymmetric applications, the grid can be either pure triangular or pure quadrilateral mesh, or combination of both. For 3D applications, the mesh can consist of either pure tetrahedral or pure hexahedral elements, or mix of tetrahedral, pyramid and hexahedral cells. Fig. 1 shows both the conceptual and detailed architecture of **RAPIT**© under development. Fig. 1a shows that it consists of hardware, operating system (OS), programming, parallel computing, solver & data structure, numerical method and model, where the application and theory can be easily added based on needs. In Fig. 1b, 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, message passing interface (MPI) protocol is used to communicate among processors. Combination of OpenMP and MPI for both continuum and particle solvers, with Graphic Processor Unit (GPU) computing for particle solvers are also possible to make the most usage of computing resources in the future. In addition, well-known graph partition libraries such as METIS[21] are used to partition the unstructured mesh per the function call in the application code, which makes the dynamic domain decomposition possible. For other important modules of **RAPIT□**, they are described in detail in the following in turn.



(a) (b)

Figure 1. RAPIT□ software framework: (a) conceptual (b) detailed.

First, there is one important basic module, named "Domain" (Fig. 1b), which handles the tasks related to I/O (mesh loader and cell data output), construction of required cell connectivity of unstructured grid(s), domain decomposition, calculation of cell and face related coefficients associated with finite-volume discretization, and some calculation of properties, to name a few. The current I/O capability includes those mesh types in CGNS, msh, FieldView and Tecplot (output only). In addition, chemical reaction (species and channels) and collision cross section data can be easily input through *json* format[22]. A log file is also generated automatically to record the runtime related information.

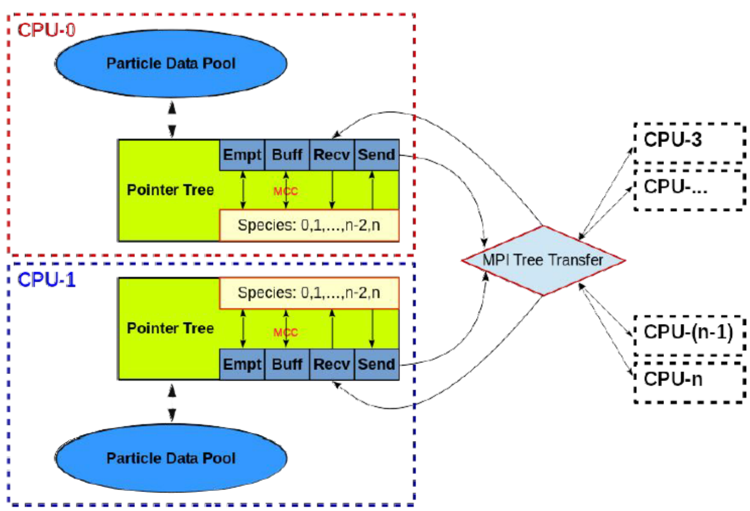


Figure 2. Parallel particle data management in RAPIT□.

Second, "Data Manager" (Fig. 1b) is used to handle memory allocation and de-allocation, and communication among processors. It includes two other modules, "Scalar/Vector" and "Particle". The former deals with inter-processor ghost cells data update, and fast cell mapping and data interpolation between different meshes, which may be for either the same or different or overlapping domain(s). This feature enables the flexibility of performing computations in different meshes with different materials (e.g., dielectric, metal, gas, liquid) and phases (e.g., solid, gas, liquid). The latter is specially designed for the particle method dealing with parallel data management of particles, which uses the concept of "Particle Data Pool" in each processor. 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.

Third, "Scheme/Algorithm" (Fig. 1b) consists of two major modules, which are "Numerical Scheme" for the continuum-based partial differential equations (PDE) approach and "Physical Algorithm" for the particle method. For the former, several well-known numerical schemes are implemented mainly for discretizing the convection term, such as 1st and 2nd order upwind schemes[23], and the HLL scheme[24], to name a few. A finite-volume based central-difference type discretization is used for treating the diffusion term. Also, the initial and boundary conditions are enforced in this module. In the latter, several core modules of the particle method are implemented, which include particle pusher with the Leapfrog/Boris integration algorithm, Monte Carlo collision, particle tracking, charge/force interpolation between particles and grid nodes, particle data sampling, and enforcement of initial as well as boundary conditions. In addition, load balancing among processors based on the distribution of the number of particles is also implemented here, which allows efficient dynamic domain decomposition. Note this is especially important for enhancing the parallel computing efficiency for computation of large-scale particle numbers, such as DSMC and PIC-MCC, since the steady-state or quasi-steady-state distribution of particles are unknown prior to the start of simulation. Note these modules are common for most particle methods, such as DSMC and PIC-MCC.

Fourth, "Equation Solver" (Fig. 1b) is the module, in which the set of discretized equations of interest can be constructed, including unsteady, convection, diffusion and source terms. For some specific PDEs, they can be implemented here by integrating some of the modules (convection and diffusion terms), which were described earlier in "Numerical Scheme". The complete set of discretized equations is then solved using a parallel matrix solver with preconditioning through the use of the PETSc library[25]. Similarly, "Particle Solver" is the module designed for the particle method. For example, for DSMC computation, one can simply call modules such as particle pusher, particle tracking, Monte Carlo collision, and particle data sampling with enforcement of initial and boundary conditions. For computation with the PIC-MCC method, one can simply add two more modules such as charge/force interpolation between particles and grid nodes, and the Poisson equation solver or even the Maxwell equation solver if needed.

Fifth, in the most top layer of **RAPIT**, named "Sequence Control" (Fig. 1b), one can control the sequence of solving different species (PDE or/and particle) for some special application. For example, for the plasma fluid modeling with relatively low pressure environment, one can define "electron" as a particle species, and "ions" and "neutral" as PDE species. Then, conservation equations or particles of these species can be solved one by one following the standard sequence of fluid modeling[26]. Of course, some auxiliary calculations are needed for a complete fluid modeling. For example, velocity moments of EEDF (electron energy distribution function) from the electron species lead to electron density, electron momentum, and electron energy (or electron temperature) without assuming the thermal equilibrium of electrons, which is otherwise not justified under very low-pressure environment, such as those in magnetron sputtering plasma and etching plasma.

Under the current multi-physics **RAPIT** framework, we have completed the preliminary implementation of the DSMC simulator (**ultraSPARTS**), the PIC-MCC simulator (**ultraPICA**), the NS equation solver (**ultraNSMod**) and the the plasma fluid modeling code (**ultraFluMod**). The corresponding numerical schemes/algorithms adopted by these solvers are briefly described next.

III. Numerical Schemes and Algorithms

ultraSPARTS

ultraSPARTS® stands for **ultra**-fast **S**tatistical **PART**icle **S**imulation Package, which is originated from PDSC^{++}[27] (Parallel Direct Simulation Monte Carlo Code), is a particle-based C++ object-oriented simulation code developed on **RAPIT**® for efficiently solving gas flow problems with rarefaction and strong non-equilibrium. This software employs the DSMC method for directly solving the Boltzmann equation statistically. Fig. 3 illustrates the important features of **ultraSPARTS**®, which applies many state-of-the-art schemes/algorithms to greatly reduce the computational time and sophisticated physical models needed for modeling complex flow phenomena. These include, but not limited to, parallel computing with dynamic domain decomposition (DDD)[28], variable time-step scheme (VTS)[29], transient adaptive subcell (TAS)[30], virtual mesh refinement (VMR)[31], automatic steady-state detection (ASSD, to be published), 2D-axisymmetric modeling without particle cloning (to be published), fast unsteady DSMC (DREAM)[32], iterative pressure boundary treatment method[33,34], and total collision energy model for reacting flow[35], to name a few. In addition, PDSC^{++} has been successfully applied to hybridize with a NS equation solver for complex 2D/3D gas flows using breakdown parameters to decide the interfacial region for switching between DSMC and NS equation solvers.[5] In general, it can deal with rarefied gas flows with object(s) having complex geometry using 2D/axisymmetric/3D hybrid unstructured grid. The package has been applied for modeling general rarefied gas dynamics such as hypersonic non-reacting and reacting gas flows, vacuum pumping flows, satellite plume impingement[36], MEMS/NEMS gas flow[34], comet gas/dust plume[37,38], and physical vapor deposition (e.g., organic light emitting diode, copper indium gallium, E-beam metal vapor), to name a few.

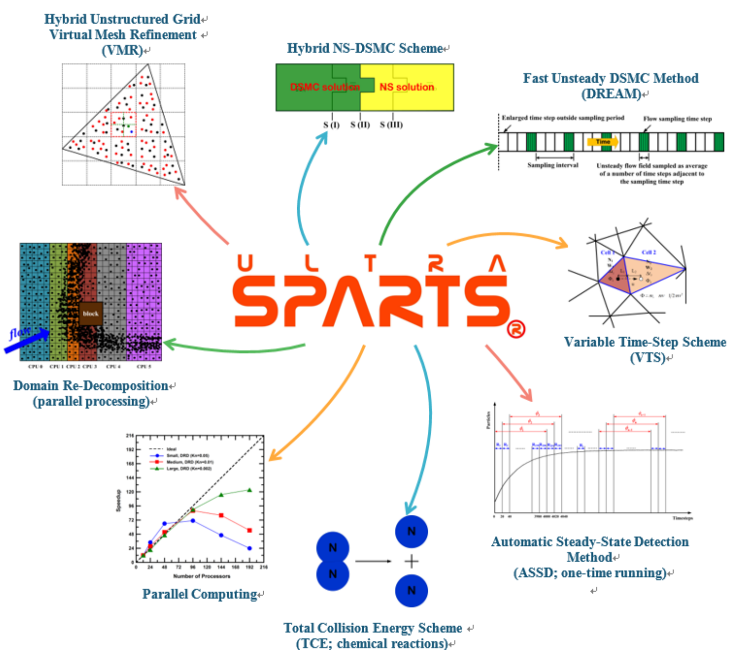


Figure 3. Important features of ultraSPARTS®.

ultraPICA®

ultraPICA® stands for **ultra**-fast **P**article-**I**n-**C**ell Monte Carlo **A**nalysis, which is the software programmed on **RAPIT**® based on the PIC-MCC method for solving the Boltzmann equation with charged species statistically. Important features of this tool include a particle pusher with the Leapfrog and Boris integration scheme, an optimized particle tracking on unstructured grid (the same as **ultraSPARTS**®), a Monte Carlo collision module, and a Poisson equation solver. Note a time-dependent Maxwell equation solver is currently under development to enrich the future application if high-frequency EM wave is involved. Thanks to the "particle" module in **RAPIT**®, it also features parallel computing with DDD similar to **ultraSPARTS**®, which is very important in optimally utilizing the computing resources. It is the tool designed to numerically investigate plasmas under highly rarefied conditions. It can generate important non-equilibrium plasma properties such as IEDF (ion energy distribution function) and IADF (ion angle distribution function) at the wall (or electrode), which are very important for film deposition, etching and sputtering, in addition to electron and ion densities as well as temperatures. In general, it can simulate complex low-pressure plasma flows using 2D/axisymmetric/3D unstructured meshes. Potentially it can be applied to simulate plasmas like very low-pressure PECVD (plasma enhanced chemical vapor deposition) process, ICP (inductively coupled plasma) process, DC/RF magnetron sputtering process[39], surface charging of spacecraft in low earth orbit, and hall effect thruster (HET) and ion thruster of spacecraft, to name a few.

ultraNSMod□

ultraNSMod□, which stands for **ultra**-fast **N**avier-**S**tokes Equation **Mod**eling Package, is a continuum neutral gas flow solver for modeling flow and heat transfer at all speeds using 2D/axisymmetric/3D unstructured meshes. The modeling equations include conservation of mass, conservation of momentum and conservation of energy (total enthalpy) with an ideal-gas equation of state. Some special effects, such as conjugate heat transfer between solid and gas, and automatic slip boundary conditions of velocities and temperature under rarefied condition, are also considered. It employs an extended SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm similar to Hu *et al*.[40] with a pressure smoothing technique. In addition, source terms in the momentum and energy equations are numerically treated in such a way that this solver can efficiently exchange the data with other software package such as **ultraFluMod□** if needed. This package is mainly designed to hybridize easily with either **ultraSPARTS□** or **ultraFluMod□** for different types of plasma/flow problems. Moreover, considering some practical application, an Euler equation solver is also developed on **RAPIT□**.

ultraFluMod□

ultraFluMod□ (**ultra**-fast Plasma **Flu**id **Mod**eling Package) is a continuum-based simulation code developed on **RAPIT□** for solving the velocity moments of the Boltzmann equation considering charged particles. It solves a set of fluid modeling equations including the continuity equations, the momentum equations, the energy equation for electrons and ions, and the Poisson equation for electrostatic potential similar to our previous studies[40-44]. The Scharfetter-Gummel scheme[45] is used for discretizing the convection-diffusion type equation related to electrons, while the HLL Approximate Riemann Solver is used for discretizing the convection term of ion momentum equations with consistent numerical and physical acoustic speed[46]. In general, it can deal with gas discharges of low-temperature plasma with complex geometry using 2D/axisymmetric/3D hybrid unstructured mesh with parallel computing. The package can be used to model general low-temperature plasma or gas discharges with complex chemistry and complex geometry such as PECVD, ICP, and APP (atmospheric-pressure plasma), to name a few.

IV. Demonstration Numerical Results

In this section, we report our progress on developing the application packages based on the proposed **RAPIT□**. These include **ultraSPARTS□**, **ultraPICA□**, and **ultraNSMod□** and **ultraFluMod□**, which are described next.

A. ultraSPARTS□

Two test cases, including non-reacting and reacting hypersonic rarefied gas flows, are presented in this section for **ultraSPARTS□** demonstration. The first case is the hypersonic flow of nitrogen passing an axisymmetric 25°-55° double cone with free-stream conditions: $M_{\square} = 15.6$, $n_{\square} = 3.779\times10^{21}$ m^{-3}, $T_{\square} = 42.6$ K[47]. Fig. 4a shows the detailed dimensions of the double cone. We have applied the diffusive boundary condition at all solid walls with a temperature of 297.2 K and a rotational relaxation number of 5. This test case consists of 348,043 cells with ~13 million particles during steady state, and took 7.2 hours of runtime on a PC cluster (ALPS of NCHC, Taiwan) with 96 processors. No particle cloning is employed during the runtime through the proper combination of VTS, TAS, and radial weighting. Note particle cloning in such a Monte Carlo simulation often leads to undesired random walk phenomenon, which is often inevitable in most DSMC simulations[1]. Fig. 4b shows the variations of particle number and relative residues of particle number, velocities and temperature using the ASSD scheme. It appears that the flow reaches a steady state essentially, as the residues are all smaller than 5×10^{-6}, after which the DSMC code automatically starts to sample the data. Note this value is purely empirical, but relatively consistent based on our numerical experience. Fig. 5 shows the computed temperature distribution, and the comparison of axial surface pressure and temperature against previous experiment and simulations. It is obvious that **ultraSPARTS□** can reproduce the experiments with much fewer particles due to the use of VTS, TAS, and radial weighting as compared to other studies.

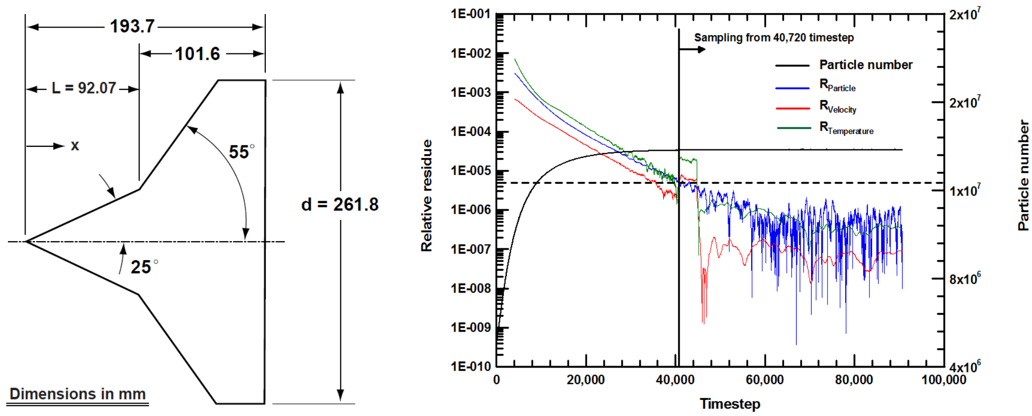


Figure 4. Nitrogen hypersonic flow past a 25°-55° double cone. (a) Configuration; (b) Time variation of ASSD parameters.

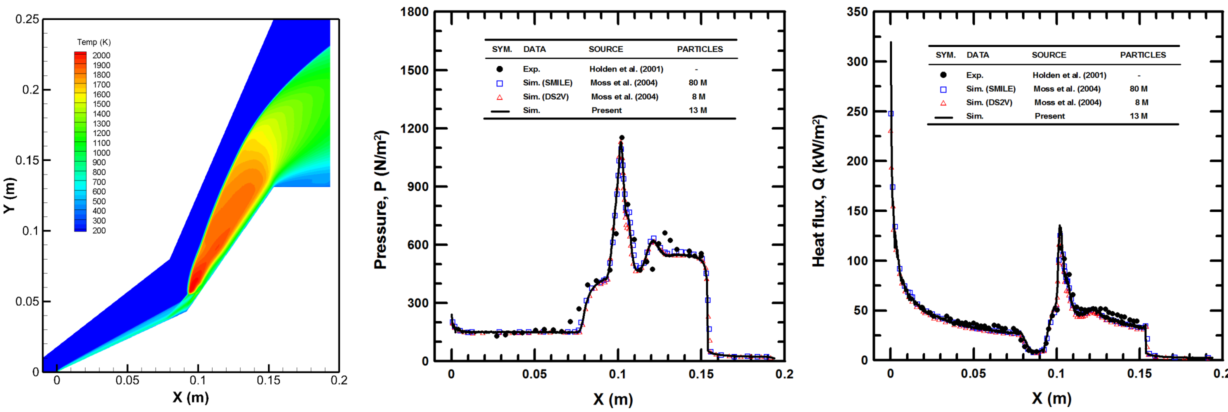


Figure 5. Simulation results of nitrogen hypersonic flow past a 25°-55° double cone. (a) Temperature distribution; (b) Axial surface pressure distribution; (c) Axial heat flux distribution.

The second case is the Apollo reentry reacting flow at 95 km with an angle of attack of 25°. The detailed simulation conditions are described in Moss *et al.*.[48] The numerical results are plotted in Fig. 6. The distribution of merit of collision (MOC = mean collision distance / mean free path) near the surface shows that MOCs are still slightly larger than unity, which indicate that the computation is very demanding even though we have used up to 200 million particles. However, the corresponding aerodynamic coefficients are in good agreement with Moss *et al.*, even though no detailed simulation conditions were provided therein.

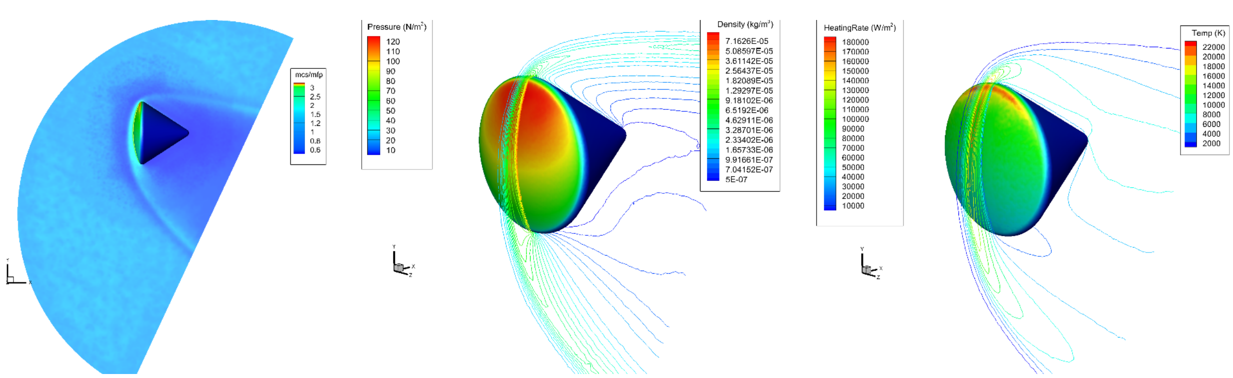


Figure 6. Numerical results of Apollo reentry flow at 95 km with an AOA of 25°. (a) Merit of collision distribution; (b) Surface pressure and spatial density distributions; (c) Surface heat flux and spatial temperature distributions.

B. ultraPICA

B.1 Parametric Study of Numerical Heating, Slowing and Deflection Times

We have performed a detailed study of the numerical heating time, slowing time and deflection time of **ultraPICA** due to cell size, number of pseudo particles per cell and background temperature. Note the former are three important parameters, which stands for the accuracy/quality of the PIC modeling under all kinds of simulation conditions. The definition of these terminologies can be found in Ref. 49.

Figure 7 shows the numerical heating, slowing time and deflection time as a function of cell size relative to the Debye length with the test conditions of $n_i=n_e=10^{16}$ m^{-3} and $T_i=T_e=1$ eV. The results show that both the heating time and slowing time increase with decreasing cell size, while the deflection time remain approximately the same. This means that the increasing the spatial resolution of the grid improves the accuracy of the PIC modeling as expected. Figure 8 shows the effect of number of pseudo particles per cells on the numerical heating time, slowing time and deflection time at two different temperatures ($T_i=T_e=1$ and 2 eV). The results show that all three numerical times are nearly proportional to the number of pseudo particles per cell. It also demonstrates that the higher the temperature the longer the numerical times. Note these results presented in Figure 7 and Figure 8 are similar to those in the Ref. 49. The above validate the implementation of the current PIC-MCC code on **RAPIT**.

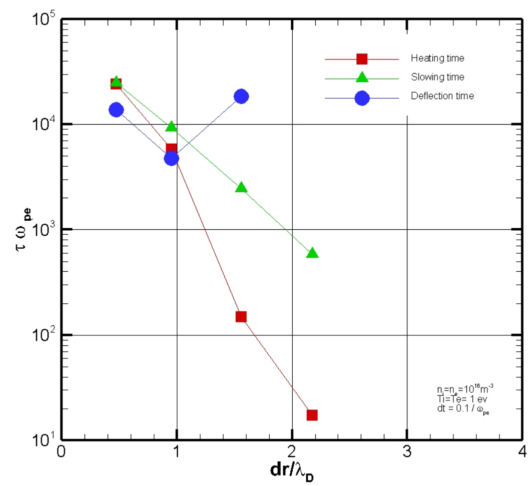


Figure 7. Numerical heating time, slowing time and deflection time as a function of dimensionless cell size of ultraPICA.

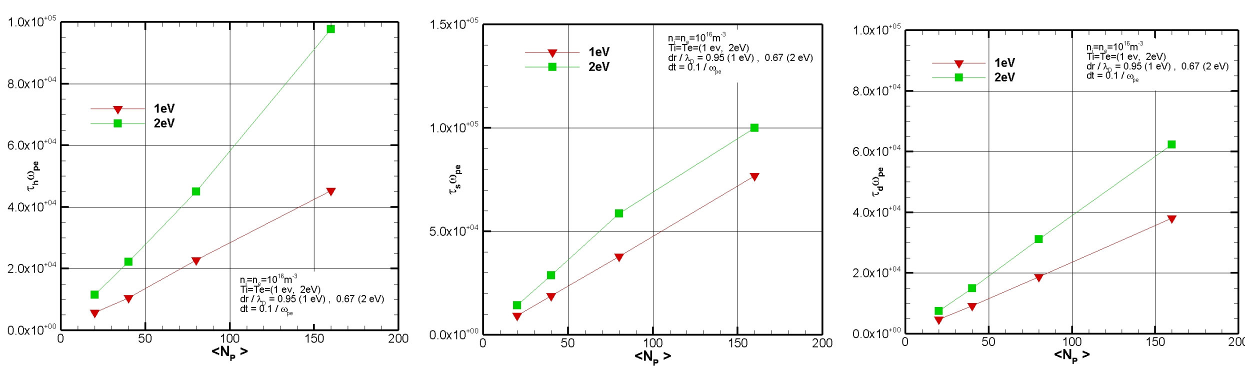
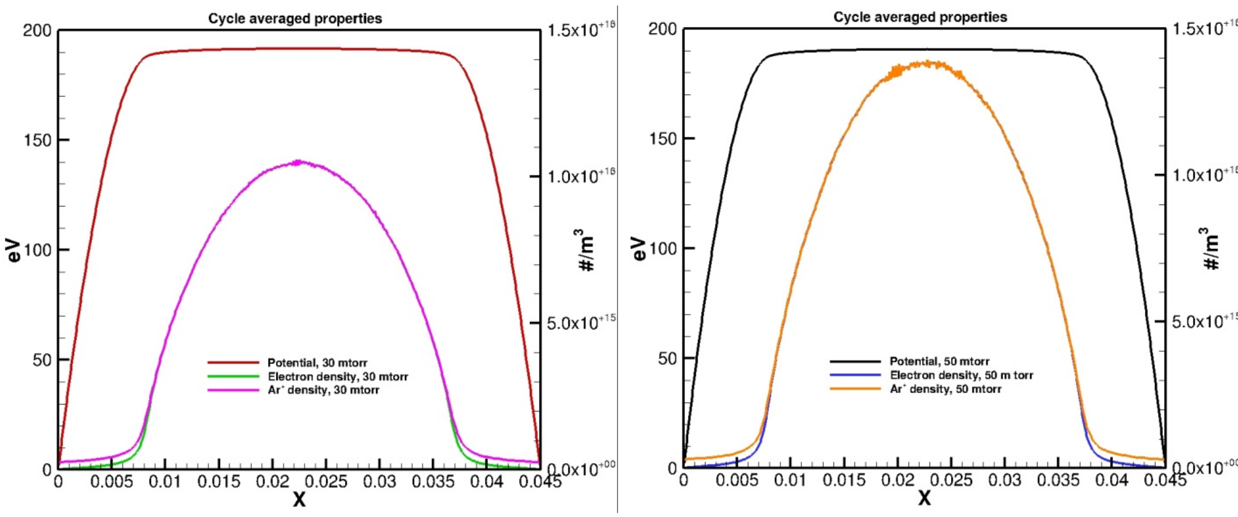


Figure 8. Effect of number of pseudo particles per cell on numerical heating time, slowing time and deflection time of ultraPICA at two different background electron and ion temperatures.

B.2 Quasi-1D Argon Capacitively Coupled Plasma (CCP)

Two test cases of quasi-1D argon plasma in two infinite parallel electrodes under different low pressures (30 mTorr and 50 mTorr) are presented here. The gap size between the two parallel electrodes is 45 mm, in which one electrode is grounded and another plate is connected to a RF power source. The radio frequency and voltage amplitude of power source is 13.56MHz and 220V, respectively. A uniform structured mesh with a grid size of 0.1 mm was used in this simulation. Both triangular and quadrilateral meshes were also tested, which produces essentially the same results. Figure 9 shows the cycle averaged plasma properties in the 1000th RF period. The results show the potential distribution is approximately the same for both cases; however, the plasma density of the 50 mTorr case is higher that of 30 mTorr because of higher density of the former. Figures 10 and 11 show the EEDF and IEDF near the sheath edge. The electrons of 30 mTorr appear to be more energetic than those of the 50 mTorr case, which is reasonable since less electron-neutral collision for the former. IEDFs are highly non-equilibrium in this region for both cases. More realistic 2D planar, 2D axisymmetric and 3D test cases will be presented in the meeting.



(a) (b)

Figure 9 Cycle-averaged distributions of potential and number density of charged particles. (a) 30 mTorr (b) 50 mTorr.

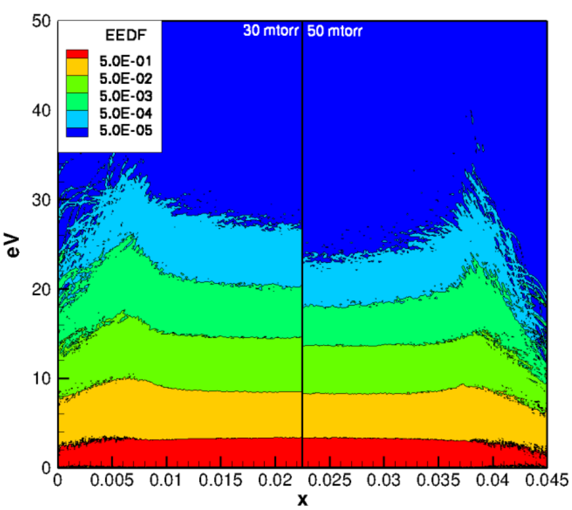


Figure 10 Comparison of electron energy density functions near sheath edge for 30 mTorr and 50 mTorr.

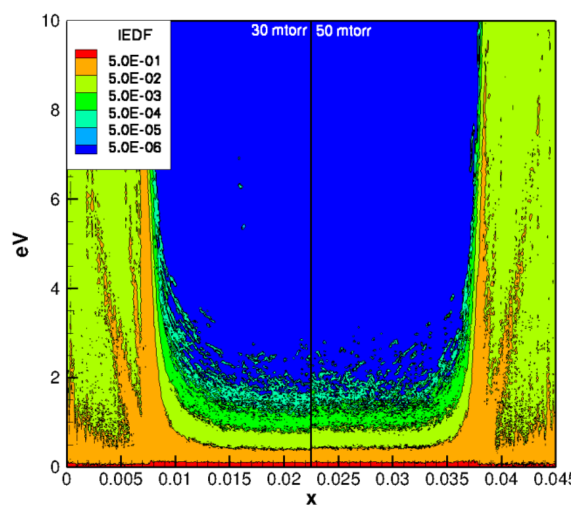
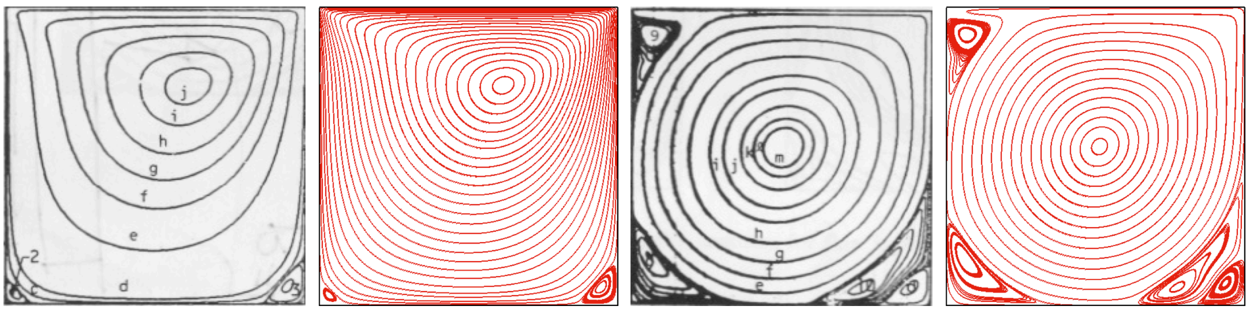


Figure 11 Comparison of ion energy density functions near sheath edge for 30 mTorr and 50 mTorr.

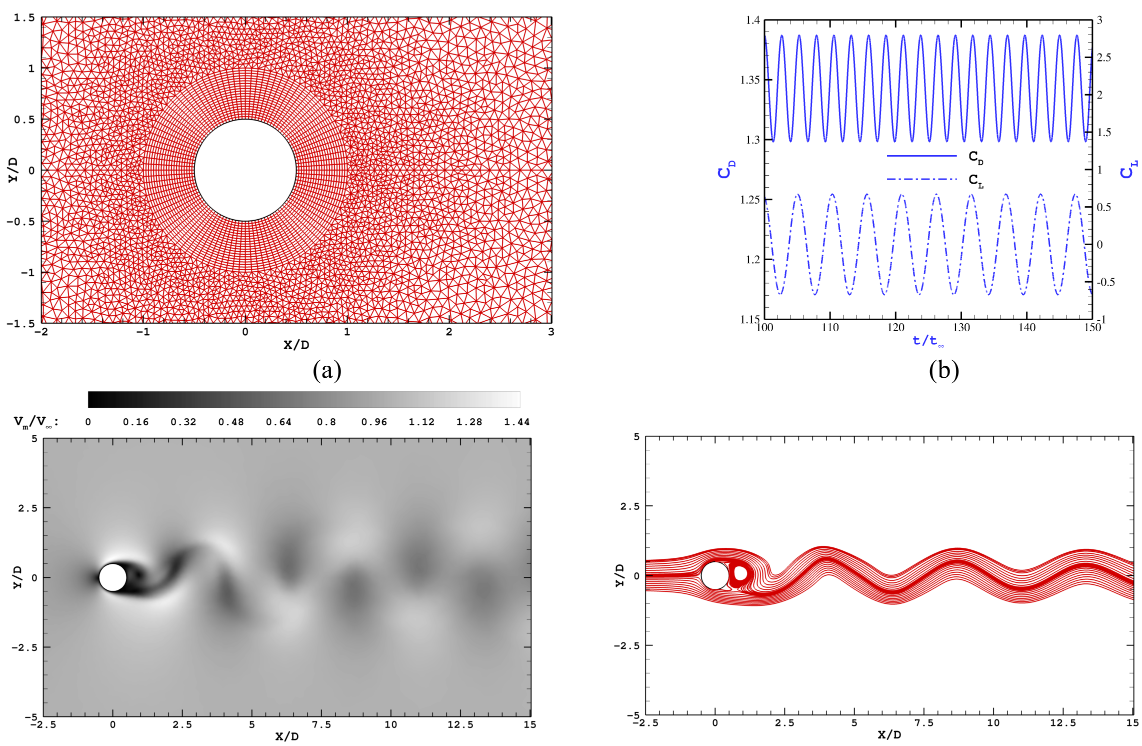
C. ultraNSMod

Three benchmarking test cases from low subsonic to supersonic flows are presented here. The first test case is the classical incompressible lid-driven square cavity flow with Re=100 and Re=10,000. The flow is computed for Re=100 using 128x128 structured cells, and for Re=10,000 using 256x256 structured cells. Fig. 12 shows the comparison of present results with previous numerical study[50]. It can be seen that the numerical results obtained from **ultraNSMod** are qualitatively in excellent agreement with Ghia *et al.*, which demonstrates the solver can faithfully simulate very low subsonic flows such as near-incompressible using the extended SIMPLE algorithm with the pressure smoothing technique. The second test case is the flow past a circular cylinder with Re=200 (M_{∞}=0.03), which is designed to test the code capability in capturing the unsteady (oscillating) phenomenon in the wake. Computations have been performed using an unstructured hybrid quadrilateral-triangular mesh with 76,588 cells. Fig. 13 shows the close-up view of local grid distribution near the cylinder, time-varying drag and lift coefficients, and some instantaneous flow properties. The TVD-MINMOD flux scheme is used for this near-incompressible flow simulation. The result of the current simulation is shown to agree very well with the those of previous numerical studies[51-61], which is summarized in Table 1. The third test case is the slightly rarefied supersonic flow past a square cylinder in a channel with moving top and bottom walls (M_{wall}=2.4261) with free-stream conditions of M_{∞}=2.4261 and Kn_{∞}=0.05. A computational mesh of 2,000x400 uniform cells was used in this study. This test case is designed to test the code capability in simulating high-speed flow, and the function of automatic slip boundary conditions. Fig. 14 shows the distribution of steady-state flow properties. In general, the results agree very well with the result of a previous numerical study[62]. In addition, a by-product of the **RAPIT™** is the explicit Euler equation solver for large scale problem. For example, Fig. 15 shows the surface mesh of a Boeing 787 cruising at Ma_{∞}=0.8 (P_{∞}= 46040 Pa) with 6M tetrahedral cells (CFL#=0.25) and sliced simulated distribution of Mach number.



(a) (b) (c) (d)

Figure 12. Simulation results of incompressible lid-driven square cavity flow. (a) Re=100[50]; (b) Re=100; (c) Re=10,000[50]; (d) Re=10,000.

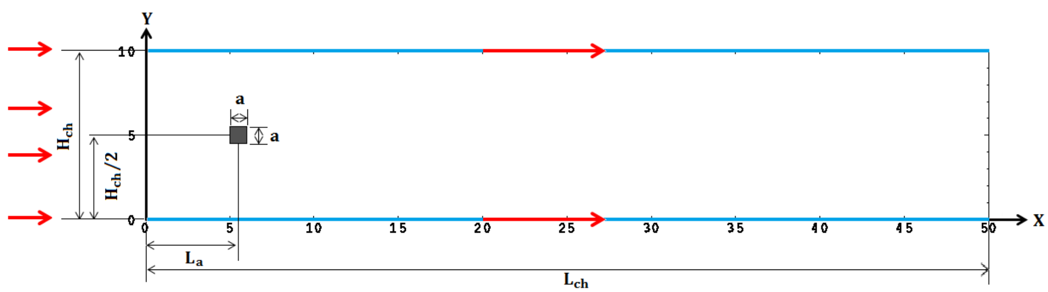


(c) (d)

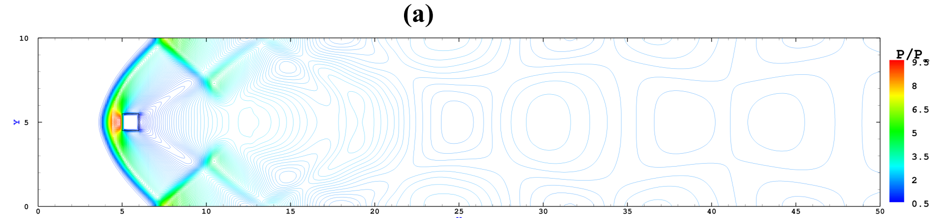
Figure 13. Flow past a circular cylinder with Re=100. (a) Close-up view of the grid near the cylinder; (b) Temporal drag and lift coefficient; (c) Instantaneous mean speed distribution; (d) Instantaneous streamline.

Table 1 Comparison of the present simulation data of drag and lift coefficients with previous studies.

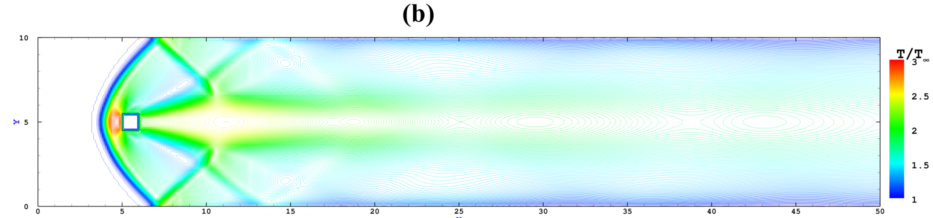
		St	C_L	C_D
Present		0.194	± 0.67	1.343 ± 0.044
Dewey & Smits	[51]	0.196	± 0.68	1.34 ± 0.045
Belov, et al.	[52]	0.193	± 0.64	1.19 ± 0.042
Braza, et al.	[53]	0.2	± 0.75	1.4 ± 0.05
Ding et al.	[54]	0.196	± 0.659	1.348 ± 0.05
Henderson	[55]	0.197	–	–
Kovàsznay	[56]	0.193	–	–
Lecointe & Piquet	[57]	0.194	± 0.5	1.58 ± 0.004
Liu, et al.	[58]	0.192	± 0.69	1.31 ± 0.049
Miller & Williamson	[59, 60]	0.197	–	–
Mittal & Kumar	[61]	0.193	± 0.66	1.316 ± 0.049



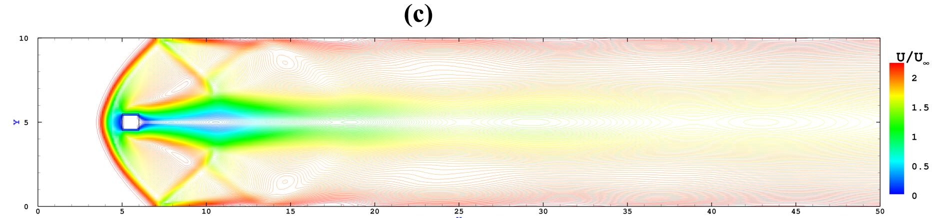
(a)



(b)



(c)



(d)

Figure 14. Flow past a square cylinder in a channel with moving walls with M_{∞}=2.4261 and Kn_{∞}=0.05. (a) Computational domain; (b) Pressure distribution; (c) Temperature distribution; (d) Streamwise velocity.

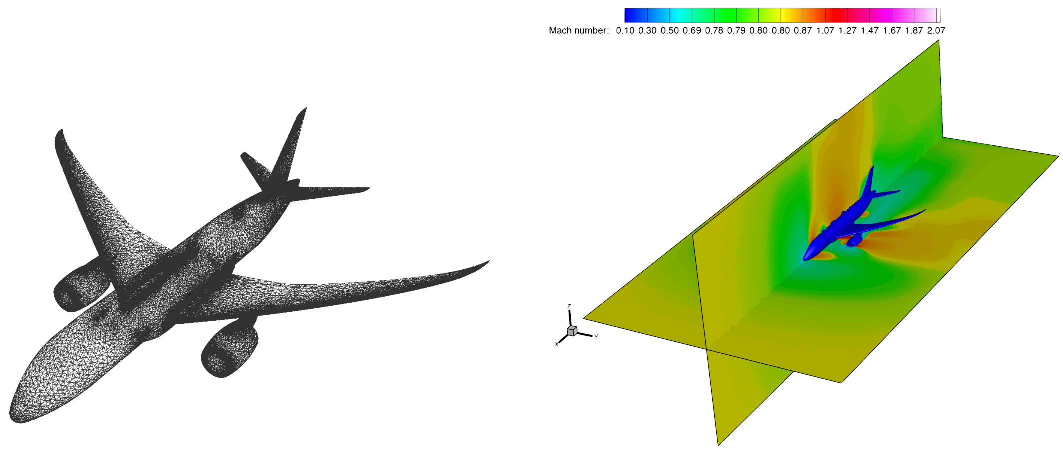


Figure 15. Inviscid flow simulation: (a) surface mesh of a Boeing 787, (2) sliced simulated Mach number distributions. Test conditions: Ma_{∞}=0.8, P_{∞}= 46040 Pa, 6M tetrahedral cells, CFL#=0.25.

D. ultraFluMod

A 2D-axisymmetric capacitively coupled plasma (CCP) is used for testing the implementation of **ultraFluMod**. Fig. 16 shows the schematic diagram of the CCP for the fluid modeling, in which two ring-type die with a peak-to-peak voltage of 400 V lectric materials are used to separate the electrode from the chamber walls. Test conditions include a chamber pressure of 100 mtorr, a gas temperature of 400 K and a driving frequency of power source of 12 MHz. Only a set of simple argon ionization is used for demonstration purpose. 400 time steps per cycle is used for 29,044 quadrilateral cells. Fig. 17 shows a series of cycle-averaged plasma properties at the 1,000th cycle. The results show that the plasma is quasi-neutral in the bulk with a peak plasma density of 1.0E16 m^{-3} and a peak potential of 150 V. Note with the use of unstructured grid there is no need to have mesh in the electrode, which can save a lot of memory and thus computational time.

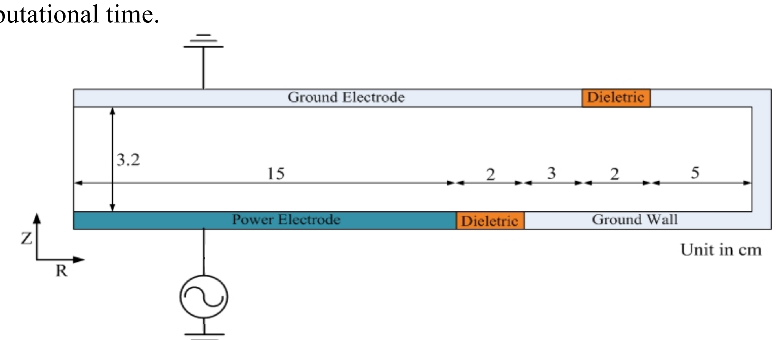
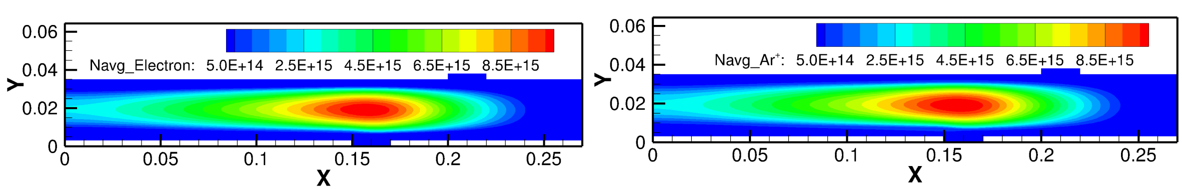


Figure 16. Schematic diagram of a capacitively couple plasma chamber.



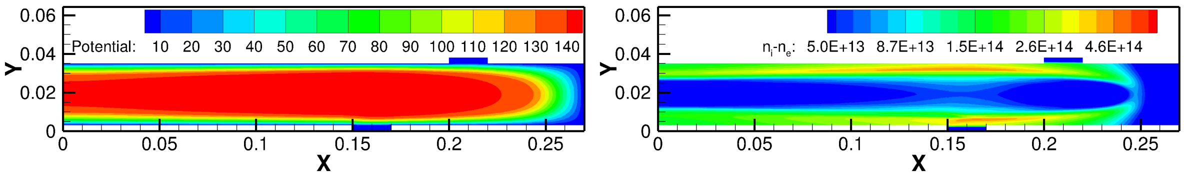


Figure 17. Distribution of plasma properties of a capacitively coupled plasma chamber.

V. Summary and Pending Work (to be reported in the full manuscript)

A multi-physics simulation platform, named as **RAPIT**™ (Rigorous Advanced Plasma Integration Testbed), is proposed in this paper. It utilizes the C++ object-oriented programming language, which makes the platform highly flexible in incorporating either continuum- or particle-based solver, or hybridization of both solvers. PDEs involved in the solver are discretized using the cell-centered finite-volume method with unstructured mesh and parallel computing using the MPI library. Target application solvers on RAPIT include **ultraSPARTS**™ for DSMC simulations, **ultraPICA**™ for PIC-MCC computations, **ultraNSMod**™ for gas flow simulations, and **ultraFluMod**™ for solving plasma fluid modeling. Many verifications and preliminary applications of these solvers are presented. More benchmarking tests and hybridization between different solvers for some challenging problems will be addressed in the near future.

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References

[1] Bird, G.A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford, 1994.

[2] Gatsonis, N. A., Nanson, A. R., and LeBeau, G. J., “Navier-Stokes/DSMC Simulations of Cold-Gas Nozzle/Plume Flows and Flight Data Comparisons,” AIAA Paper 1999-3456, 1999.

[3] Glass, C. E., and Gnoffo, P. A., “3-D Coupled CFD–DSMC Solution Method with Application to the Mars Sample Return Orbiter,” NASA Rept. TM-2000-210322, 2000.

[4] Wang, W. L., Sun, Q. H., and Boyd, I. D., “Towards Development of a Hybrid DSMC–CFD Method for Simulating Hypersonic Interacting Flows,” Eighth AIAA/ASME Joint Thermophysics and Heat Transfer Conference, AIAA Paper 2002-3099, 2002.

[5] Wu, J. S., Lian, Y. Y., Cheng, G., Koomullil, R. P., and Tseng, K. C., “Development and Verification of a Coupled DSMC–NS Scheme Using Unstructured Mesh,” *Journal of Computational Physics*, Vol. 219, No. 2, pp. 579-607, 2006.

[6] Burt, J. M., and Boyd, I. D., “Hybrid Particle Approach for Continuum and Rarefied Flow Simulation,” *Journal of Computational Physics*, Vol. 228, No. 2, pp. 460-475, 2009.

[7] Gu, K., and Watkins, C. B., “Atomistic Hybrid DSMC/NEMD Method for Nonequilibrium Multiscale Simulations,” *Journal of Computational Physics*, Vol. 229, No. 5, pp. 1381-1400, 2010.

[8] Papp, J. L., Wilmoth, R. G., Chartrand, C. C., and Dash, S. M., “Simulation of High-Altitude Plume Flow Fields Using a Hybrid Continuum CFD/DSMC Approach,” 42nd AIAA/ASME Joint Propulsion Conference and Exhibit, AIAA Paper 2006-4412, 2006.

[9] Li, Z. H., Li, Z. H., Wu, J. L., and Peng, A. P., “Coupled Navier–Stokes/direct simulation Monte Carlo simulation of multicomponent mixture plume flows,” *Journal of Propulsion and Power*, Vol. 30, No. 3, pp. 672-689, 2014.

[10] Serikov, V. V., Kawamoto, S., and Nanbu, K., “Particle-in-Cell Plus Direct Simulation Monte Carlo (PIC-DSMC) Approach for Self-Consistent Plasma-Gas Simulations,” *IEEE Transactions on Plasma Science*, Vol. 27, No. 5, pp. 1389-1398, 1999.

[11] Nanbu, K., Morimoto, T., and Suetani, Masaharu., “Direct Simulation Monte Carlo Analysis of Flows and Etch Rate in an Inductively Coupled Plasma Reactor,” *IEEE Transactions on Plasma Science*, Vol. 27, No. 5, pp. 1379-1388, 1999.

[12] Petkow, D., Fertig, M., Herdrich, G., and Auweter-Kurtz, M., “Ionization Model within a 3D PIC-DSMC-FP Code," 39th AIAA Thermophysics Conference, Miami, FL, USA, AIAA-2007-4261, 2007.

[13] Cheng, S., Santi, M., Celik, M., Martinez-Sanchez, M., Peraire, J., “Hybrid PIC–DSMC simulation of a hall thruster plume on unstructured grids,” Proceedings of 18th International Conference on the Numerical Simulation of Plasmas, Computer Physics Communications, Vol. 164, pp. 73–79, 2004.

[14] Moore, C. H., et al., "1D PIC–DSMC simulations of breakdown in microscale gaps," Proceedings of the 28th International Symposium on Rarefied Gas Dynamics, pp.629–636, 2012.
[15] Bogaerts, A., Yan, M., Gijbels, R., and Goedheer, W., "Modeling of ionization of argon in an analytical capacitively coupled radio-frequency glow discharge," *Journal of Applied Physics*, Vol. 86, pp.2990-3001, 1999.
[16] Donkó, Z., Hartmann, P., and Kutasi, K., "On the reliability of low-pressure dc glow discharge modelling," *Plasma Sources Science and Technology*, Vol. 15 pp. 178–86, 2006.
[17] Li, C., Ebert, U., Brok, W. J. M., and Hundsdorfer, W., "Spatial coupling of particle and fluid models for streamers: where nonlocality matters," *Journal of Physics D: Applied Physics*, Vol. 41, 032005, 2008.
[18] Eremin, D., Hemke, T., and Mussenbrock, T., "A new hybrid scheme for simulations of highly collisional RF-driven plasmas," *Plasma Sources Science and Technology*, Vol. 25, 015009, 2016.
[19] Gu, B. R., Lin, K. M., Hu, M. H., Hung, C. T., Wu, J. S., and Chen, Y. S., "A temporal multi-scale algorithm for efficient fluid modeling of a one-dimensional gas discharge," *Plasma Sources Science and Technology*, Vol. 23, 065021, 2014.
[20] Gu, B. R., Chen, K. L., Chiou, C. C., Hu, M. H., Hung. C. T., and Wu, J.-S., "Two-Dimensional Axisymmetric Fluid Modeling of Low-Pressure Capacitively Coupled Plasma Using an Extended Temporal Multi-Scale Algorithm," *IEEE Transactions on Plasma Science* (submitted).
[21] Karypis, G., and Kumar, V., *METIS: A Software Package for Partitioning Unstructured Graphs, Partitioning Meshes, and Computing Fill-Reducing Orderings of Sparse Matrices*, 1998.
[22] *https://github.com/nlohmann/json*
[23] Majumdar P., *Computational Methods for Heat and Mass Transfer*, Taylor and Francis: Great Britain, 2005.
[24] Harten, A., Lax, P. D., and van Leer, B., "On upstream differencing and Godunov-type schemes for hyperbolic conservation laws," *SIAM Rev*., Vol. 25, pp. 35-61, 1983.
[25] S. Balay, K. Buschelman, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, B.F. Smith, H. Zhang, PETSc library, http://www.mcs.anl.gov/petsc, 2011.
[26] Zhanga, Y., and Kushner, M. J., "Control of ion energy and angular distributions in dual-frequency capacitively coupled plasmas through power ratios and phase: Consequences on etch profiles," *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, Vol. 33. 031302, 2015.
[27] Su, C. C., "Parallel Direct Simulation Monte Carlo (DSMC) Methods for Modeling Rarefied Gas Dynamics," Ph.D. Thesis, Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, Taiwan, 2013.
[28] Wu, J. S., and Tseng, K. C., "Parallel DSMC Method Using Dynamic Domain Decomposition," *International Journal for Numerical Methods in Engineering*, Vol. 63, pp. 37-76, 2005.
[29] Wu, J. S., Tseng, K. C., and Wu, F. Y., "Three Dimensional Direct Simulation Monte Carlo Method Using Unstructured Adaptive Mesh and Variable Time Step scheme," *Computer Physics Communications*, Vol. 162, pp. 166-187, 2004.
[30] Su, C.-C., Tseng, K. C., Cave, H. M., Lian, Y. Y., Kuo, T. C., Jermy, M. C., and Wu, J.-S., "Implementation of a Transient Adaptive Sub-Cell Module for the Parallel DSMC Code Using Unstructured Grids," *Computers & Fluids*, Vol. 39, Issue 7, pp. 1136-1145, 2010.
[31] Su, C.-C., Tseng, K. C., Wu, J. S., Cave, H. M., Jermy, M. C., and Lian, Y.-Y., "Two-level Virtual Mesh Refinement Algorithm in a Parallelized DSMC Code Using Unstructured Grids," *Computers & Fluids*, Vol. 48, Issue 1, pp. 113-124, 2011.
[32] Cave, H. M., Jermy, M. C., Tseng, K. C., and Wu, J.S., "DREAM: An Efficient Methodology for DSMC Simulation of Unsteady Processes," 26th International Symposium on Rarefied Gas Dynamics, July 21-25, 2008., Kyoto University, Kyoto, Japan.
[33] Wu, J. S., Lee, F., and Wong, S. C., "Pressure Boundary Treatment In Micromechanical Devices Using The Direct Simulation Monte Carlo Method," *JSME International Journal Series B-Fluid and Thermal Engineering*, Vol. 44, No. 3, pp. 439-450, 2001.
[34] Wu, J. S., and Tseng, K.-C., "Analysis of Micro-scale Gas Flows with Pressure Boundaries Using the Direct Simulation Monte Carlo Method," *Computers & Fluids*, Vol. 30, pp. 711-725, 2001.
[35] Lo, M. C., Su, C. C., Wu, J. S., and Tseng, K. C., "Modelling Rarefied Hypersonic Reactive Flows Using the Direct Simulation Monte Carlo Method," *Communications in Computational Physics*, Vol. 18, pp. 1095-1121, 2015
[36] Wu, J. S., Lee, Y. M., Tseng, K. C., Lian Y. Y., Kuo, T. C., and Hsiao, C.-D., "Analysis of Plume Impingement on Spacecraft Using Parallel DSMC Method,"6th Asian CFD Conference, TAIWAN, October 24-27, 2005.
[37] Lin, Z.-Y. *et al*., "Observations and Analysis of A Curved Jet in the Coma of Comet 67P/Churyumov-Gerasimenko," *Astronomy & Astrophysics*, 588, L3, 2016.
[38] Marschall, R. *et al*., "Modelling of the inner gas and dust coma of comet 67P/Churyumov-Gerasimenko using ROSINA/COPS and OSIRIS data - First results," *Astronomy & Astrophysics*, 589, A90, 2016.
[39] Wu, J.-S., Hsu, K.-H., Li, F.-L., Hung, C.-T., and Jou, S.-Y., "Development of a parallelized 3D electrostatic PIC-FEM code and its applications," *Computer Physics Communications*, Vol. 177, pp. 98-101, 2007.
[40] Hu, M.-H., Wu, J.-S., and Chen, Y.-S., "Development of a Parallelized 2D/2D-Axisymmetric Navier-Stokes Equation Solver for All-Speed Gas Flows," *Computers & Fluids*, Vol. 45, pp. 241–248, 2011.
[41] Smith, M. R., Hung, C. T., Lin, K. Mo., Wu, J. S., and Yu, J. P., "Development of a semi-implicit fluid modeling code using finite-volume method based on Cartesian grids," *Computer Physics Communications*, Vol. 182, Issue 1, pp. 170-172, 2011.
[42] Lin, K. M., Hung, C. T., Hwang, F. N., Smith, M. R., Yang, Y. W., and Wu, J. S., "Development of a Parallel Semi-Implicit Two-Dimensional Plasma Fluid Modeling Code Using Finite-Volume Method," *Computer Physics Communications*, Vol. 183, No. 6, pp 1225-1236, 2012.

[43] Lin, K. M., Hu, M. H., Hung, C. T., Wu, J. S., Hwang, F. N., Chen, Y. S., and Cheng, G., "A Parallel Hybrid Numerical Algorithm for Simulating Gas Flow and Gas Discharge of an Atmospheric-Pressure Plasma Jet," *Computer Physics Communications*, Vol. 183, Issue 12, pp. 2550-2560, 2012.

[44] Chen, K. L., Tseng, M. F., Gu, B. R., Hung, C. T., and Wu, J. S., "Numerical Investigation on Ion Inertia Force in Low-Temperature Plasma Using Fluid Model Considering Ion Momentum Equation," *IEEE Transactions on Plasma Science*, Vol. 44, Issue 12, pp. 3127-3134, 2016.

[45] Scharfetter, D. L., and Gummel, H. K., "Large-signal analysis of a silicon read diode oscillator," *IEEE Trans. Electron. Devices*, Vol. 16, pp. 64-77, 1969.

[46] Chen, K.-L., Tseng, M. F., Sharma, S., and Wu, J. S., "Effect of Reconstruction Scheme on the Plasma Fluid Modeling with Original and Reformulated Ion Related Modeling Equations Using HLL Flux Scheme," *IEEE Transactions on Plasma Science* (submitted).

[47] Moss, J. N., "DSMC Simulations of Hypersonic Flows with Shock Interactions and Validation With Experiments," AIAA Paper 2004-2585, 2004.

[48] Moss, J. N., Glass, C. E., and Greene, F. A., "DSMC Simulations of Apollo Capsule Aerodynamics for Hypersonic Rarefied Conditions," AIAA Paper 2006-3577, 2006.

[49] Averkin, Sergey N. and Gatsonis, Nikolaos A., "A parallel electrostatic Particle-in-Cell method on unstructured tetrahedral grids for large-scale bounded collisionless plasma simulations", *Journal of Computational Physics*, Vol. 363, pp. 178–199, 2018.

[50] Ghia, U., Ghia, K. N., and Shin, T. C., "High resolutions for incompressible flow using the Navier–Stokes equations and a multigrid method," *Journal of Computational Physics*, Vol. 48, pp 387-411, 1982.

[51] Chan, S., Dewey, P.A., Jameson, A., Liang, C. and Smits, A.J., "Vortex suppression and drag reduction in the wake of counter-rotating cylinders," *Journal of Fluid Mechanics*, Vol. 679, pp. 343–382, 2011.

[52] Belov, A., Martinelli, L. and Jameson, A., "A new implicit algorithm with multigrid for unsteady incompressible flow calculations," AIAA paper 1995-0049, 33rd Aerospace Sciences Meeting and Exhibit, Reno, NV, January 1995.

[53] Braza, M., Chassaing, P. and Minh, H.H., "Numerical study and physical analysis of the pressure and velocity fields in the near wake of a circular cylinder," *Journal of Fluid Mechanics*, Vol. 165, pp. 79–130, 1986.

[54] Ding, H., Shu, C., Yeo, K.S. and Xu, D., "Numerical simulation of flows around two circular cylinders by mesh-free least square-based finite difference methods," *International Journal for Numerical Methods in Fluids*, Vol. 53, pp. 305–332, 2007.

[55] Henderson, R.D., Unstructured spectral element methods: Parallel algorithms and simulations, PhD thesis, Princeton University, 1994.

[56] Kov´asznay, L. S. G., "Hot-wire investigation of the wake behind cylinders at low Reynolds numbers," *Proceedings of the Royal Society of London, Series A*, *Mathematical and Physical Sciences*, Vol. 198, pp. 174–190, 1949.

[57] Lecointe, Y. and Piquet, J., "On the use of several compact methods for the study of unsteady incompressible viscous flow round a circular cylinder," *Computers & Fluids*, Vol. 12, pp. 255–280, 1984.

[58] Liu, C., Zheng, X. and Sung, C.H., "Preconditioned multigrid methods for unsteady incompressible flows," *Journal of Computational Physics,* Vol. 139, pp. 35–57, 1998.

[59] Miller, G.D. and Williamson, C.H.K., "Control of three-dimensional phase dynamics in a cylinder wake," *Experiments in Fluids*, Vol. 18, pp. 26–35, 1994.

[60] Williamson, C.H.K., "Vortex dynamics in the cylinder wake," *Annual Review of Fluid Mechanics*, Vol. 28, pp. 477–539, 1996.

[61] Mittal, S. and Kumar, B., "Flow past a rotating cylinder," *Journal of Fluid Mechanics*, Vol. 476, pp. 303–334, 2003.

[62] Shterev, K. S., and Stefanov, S. K., "Pressure based finite volume method for calculation of compressible viscous gas flows," *Journal of Computational Physics*, Vol. 229, pp. 461-80, 2010.