Recent development of a large-scale parallel PIC code named NEPTUNE3D

Ye Dong*, Wenyuan Yang, Jun Chen, Qiang Zhao, Xiaowen Xu, Hanyu Li,

Zhiwei Dong, Haijing Zhou, Zeyao Mo

Institute of Applied Physics and Computational Mathematics, Beijing, 100094, China

Abstract: A large-scale parallel electromagnetic FDTD and PIC code named NEPTUNE3D is introduced for 3D beam-wave interaction simulations. The code is developed under a parallel adaptive structured mesh infrastructure named JASMIN, which provides novel parallelization techniques for high parallel efficiency and good expansibility. Now, the code has been provided with improved algorithms to represent various structural geometries. Many typical physical function modules are added or improved in the code, for example, kinds of particle emissions, multi-port wave loading, PML absorber, secondary emission, Monte-Carlo Collision, and Finite-Conductivity-Wall. Some typical High Power Microwave (HPM) devices have been simulated by the code successfully, such as backward wave oscillator, vircator, klystron, and gyrotron. Two recent applications are presented. One is a magnetically insulated line oscillator (MILO) together with a plate-inserted mode-transducing antenna. The other is a Folded Waveguide Traveling Wave Tube (FWTWT) which working at THz band.

Keywords: beam-wave interaction; 3D electromagnetic and PIC code; massively parallel

I Introduction

Due to the nonlinear process of beam-wave interaction and time consumption to design the HPM tubes in experiment, numerical simulations have been critical to understanding and design of tubes. The 2.5D PIC codes are not enough to analyze and design HPM tubes, because some devices are unsymmetrical with complex structures or with axially symmetrical in structure, but operating mode are unsymmetrical or mode competitions should be considered. There are kinds of commercial 3D PIC codes, such as MAGIC3D and KARAT3D. However, compared with 2.5D codes, the runtime cost is much increased. With the development of parallelization technique, taking advantage of the latest parallel high-performance computing resources, parallel 3D codes, such as ICEPIC, appear in succession in the HPM field.[1] From 2007, we began to develop a parallel 3D fully electromagnetic PIC code named NEPTUNE3D[2-3] with the support of a parallel adaptive structured mesh applications infrastructure named JASMIN[4]. The code can be used to simulate plasma physics processes, especially beam-wave interactions in HPM tubes. Though the code is still in development now, it has successfully simulated real-world HPM devices, such as MILO, backward wave oscillator, vircator, klystron, and gyrotron.

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II Governing equations and basic algorithms

In NEPTUNE3D, electromagnetic fields are governed by Maxwell equations, as follows

$$\partial \mathbf{B}/\partial t = -\nabla \times \mathbf{E}, \quad \partial \mathbf{D}/\partial t = \nabla \times \mathbf{H} - \mathbf{J} \tag{1}$$

Particle motion abides by the relativistic Newton-Lorentz force equation

$$d(\gamma m \mathbf{v})/dt = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{2}$$

The code adopts Cartesian coordinates. The electromagnetic fields are updated using Yee's FDTD scheme [5]. Particles position and velocity are updated using Buneman-Boris advance scheme [6]. Fields and particles are coupled using linear interpolation of PIC method and the electric field is corrected by Boris correction. [6] The computational flow of the code is shown in Fig.1. The basic functional modules are written in FORTRAN and the interface statements with JASMIN are compiled with C++. In parallel design, the two-level parallel domain decomposition strategy and the parallel time integration algorithm are applied [7], shown in Fig.2. Pre/post-process strategies are also applied for the convenience of adding new physical modules. Thus the code has high parallel efficiency and good expansibility.

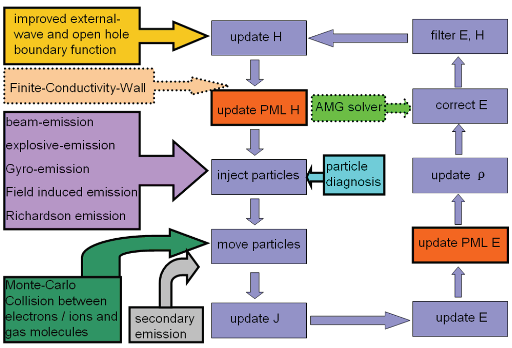


Fig.1 NEPTUNE3D flow diagram

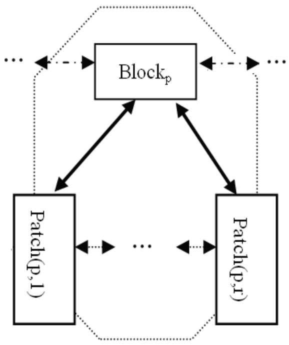


Fig.2 Two-level domain decomposition

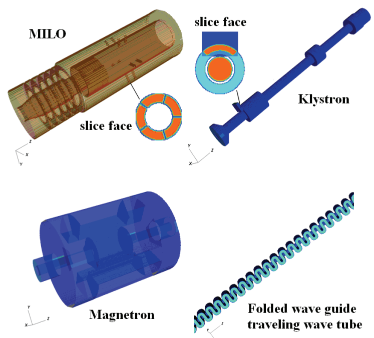
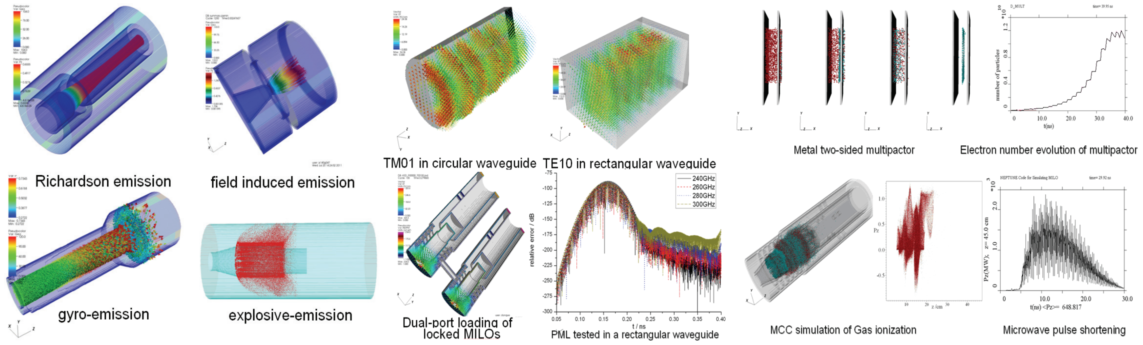


Fig.3 Some HPM tubes structures

III Geometric modeling and physical functions

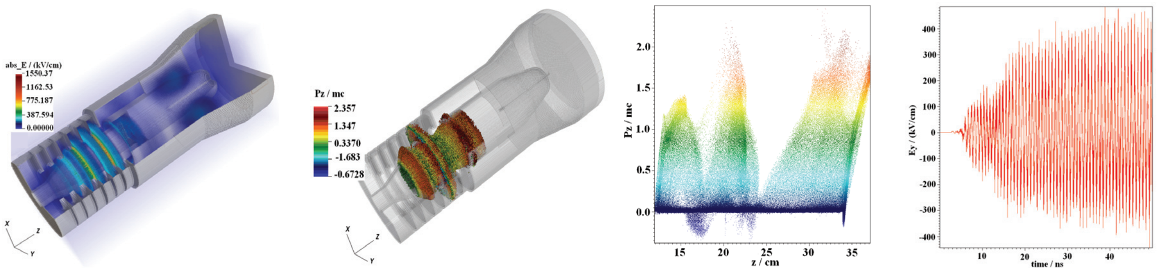
NEPTUNE3D can construct arbitrary axial symmetric or orthogonal projection structures, coupling holes, slow-wave-structures, metal foils, linear and corkscrew metal rods et al. Some complex geometric structures of HPM tubes constructed by the code are shown in Fig.3. The physical function of the code is relatively abundant, shown in Fig.4. For example, particle emission[8] include beam, space-charge-limited, gyro, Richardson, and field induced emission. The code provides various external magnetic field loading ways, such as coils, permanent magnet, distribution expressions, et al[9]. The boundary conditions supported currently are perfectly conducting metal, plane-wave and PML absorber. It is worthy to mention that external waves (TE, TM or TEM modes) can be input into the simulation area from both the axial and radial direction, whether the port is cylindrical, rectangular or coaxial structure [8]. Recently, the secondary emission and Monte Carlo Collision modules are added for studying the mutipactor discharge and gas ionization courses which cause the pulse shortening in HPM tubes [10]. Simulation results could be plotted by a parallel visualization system Javis.



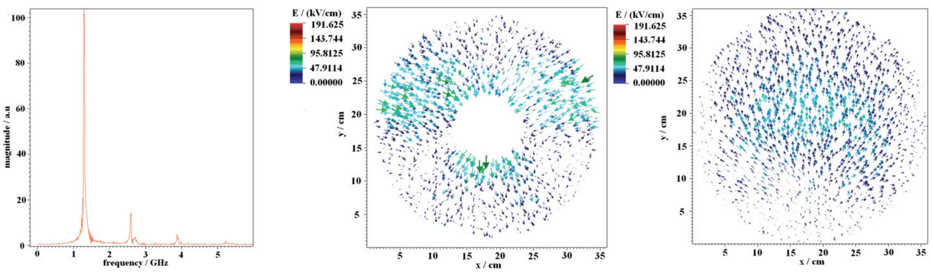
(a) some typical emission models (b) External-wave and PML modules (c) Multipacting and gas ionization

Fig.4 Simulation results of some physical function modules

IV Numerical examples and results



(a) electric field intensity (b) electron distributions (c) Pz-z phase distributions (d) Waveform of E_y at output end



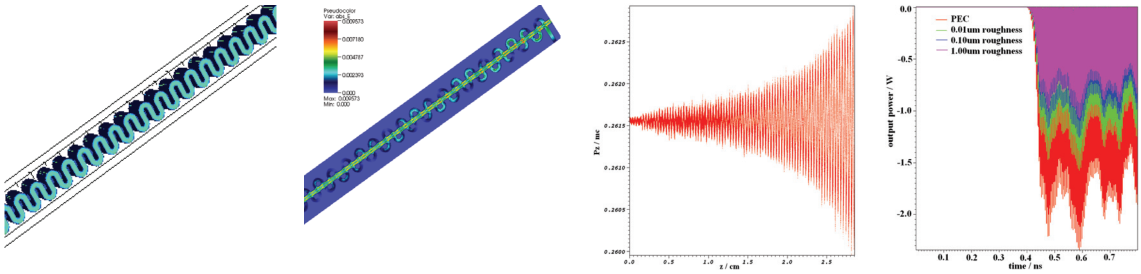
(e) spectrum of E_y at output end (f) electric field at the mode transaction position and the output end

Fig.5 Typical simulation results of an L-band MILO including a plate-inserted mode-transducer antenna

As an example, an L-band MILO including a plate-inserted mode-transducing antenna is simulated by NEPTUNE3D. Four plates are inserted in the output coaxial region. Both the inner and outer conductor is assumed as perfectly conducting metal. The PML absorber is used at the right port. A trapezoidal voltage pulse is applied to the left port. Space-charge-limited emission is adopted. The averaged voltage and current are about 460 kV and 40 kA respectively. The computing scale is about 27 million cells and 3 million particles. Only 3 hours are used on 1024 CPUs for 50ns physical duration. The parallel efficiency reaches 50%. Typical simulation results are shown in Fig.5. From (a), it can be seen the tube operates in near π-mode as expected. The choke vanes work well and there is almost no RF leakage. In (b) and (c), electron spokes can be seen clearly. This indicates that electrons are modulated relatively well and effective beam-wave interaction occurs. (d) shows the time plot of the electric field E_y at the output end. The working frequency is about 1.3GHz (seeing (e)).

It can be seen from (f) that the TEM mode from the coaxial-line near the extractor gap is converted into a circular TE_{11} mode at the output window after mode transaction region.

The other example is a 0.22THz FWTWT. The size is only about sub-millimeter to millimeter. The computing scale is about 5 million cells and 2 million particles, 1.5 hours are used on 128 CPUs. Simulation results are shown in Fig.6. From (b), it can be seen the electromagnetic field is amplified along axial direction. In (c), electron-bunching is clear, effective beam-wave interaction occurs. Output power can be seen in (d), which considers electromagnetic loss on metal boundaries by using latest Finite-Conductivity-Wall [11] module.



(a) geometric structure (b) electric-field distribution (c) Pz-z phase distributions (d) output power

Fig.6 Typical simulation results of a 0.22 THz FWTWT

V Conclusions

In order to meet the need of 3D simulation, a massively parallel 3D fully electromagnetic PIC code named NEPTUNE3D is developed by us with the support of a parallel adaptive structured mesh applications infrastructure JASMIN. The code has successfully simulated beam-wave interactions of many real-world HPM devices. Many physical functions are added or improved for different applications. Two recent simulation examples are presented, one is an L-band MILO together with a plate-inserted mode-transducing antenna, and the other is a THz-FWTWT. Depending on high parallel efficiency and good expansibility, it is suitable to simulate large scale models with complex geometry on high performance computers.

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