

Recent advances in large-signal beam-wave interaction solvers for klystrons

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A klystron is a microwave vacuum electronic device that converts the kinetic energy of an electron beam into microwave signal energy based on the principle of velocity modulation. Owing to its high peak power, high efficiency, and high gain, the klystron has been widely used in scientific research, national defense, and industrial applications. The interaction between the electron beam and the radio-frequency (rf) field within the resonant cavities, known as the beam-wave interaction, is the core physical process governing klystron operation. A detailed understanding of this process, together with accurate numerical simulation using computational solvers, is essential for optimizing device performance and shortening the development cycle. This paper reviews the large-signal beam-wave interaction solvers commonly used in klystron design and development in mainland China, along with several internationally recognized simulation codes. The discussed solvers cover a range of computational dimensions from one-dimensional (1D) to three-dimensional (3D). Finally, the challenges and future prospects for the development of klystron beam-wave interaction solvers are discussed.

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I. INTRODUCTION

The klystron is a microwave vacuum electronic device that converts the kinetic energy of an electron beam into microwave signal energy based on the principle of velocity modulation. It features high power, high gain, and high efficiency, along with stable and reliable operation and a long lifetime, which makes it widely used in scientific research, national defense, and industrial applications [1]. During the development of klystrons, the theory of beam-wave interaction and the associated numerical solvers have played a crucial role. These tools enable designers to gain a deeper understanding of the device's operating mechanisms, provide guidance for the design of new klystrons, and help identify pathways for performance enhancement. Compared with experimental approaches, computer simulation offers a more economical and efficient means to investigate the device comprehensively and nondestructively, providing detailed insight into its internal physical processes. However, achieving numerical algorithms that

ensure stability, accuracy, and completeness of the modeled problem remains a major challenge. Attaining “first pass design success” [2] has therefore been one of the ultimate goals in klystron research and development.

To gain a deeper understanding of the physical mechanism of beam-wave interaction in klystrons, researchers developed the small-signal theory in the late 1930s to analyze the motion of electrons in the presence of microwave fields. Two representative theoretical frameworks were established: the kinematic theory [3–5] and the space-charge wave theory [6–10]. The kinematic theory can describe certain nonlinear phenomena; however, it neglects the influence of the space-charge field on electron bunching, making it unreliable when the electron beam has a high space-charge density. In contrast, the space-charge wave theory treats the electron beam as a continuous fluid and takes into account the effect of the space-charge force. It describes the bunching process of electrons under small-signal and small-amplitude conditions and can be used to calculate the gain-frequency characteristics of klystrons in the linear regime. Nevertheless, because it is based on the linear approximation, this theory cannot adequately describe nonlinear physical processes.

The kinematic theory and the space-charge wave theory are the two primary theoretical frameworks for analyzing klystron operation under small-signal conditions, and they have been widely applied in the research and development

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of klystrons. In addition to these classical approaches, several extended small-signal theories have been proposed to provide a more comprehensive description of the beam-wave interaction process. Examples include the debunching theory [5], which introduces the effect of the space-charge field into the kinematic framework; the electron-stream oscillation theory [11], which emphasizes the oscillatory behavior of electrons based on the debunching concept; the dynamic power theorem [12], derived from the principle of energy conservation of the electron beam; and the coupled-mode theory [13,14], which represents the high-frequency interaction circuit or electron beam as a linear combination of orthogonal modes and describes the beam-wave interaction through intermode coupling. Other theoretical approaches include the belt-coordinate method for analyzing orbit distortion [15], the polarization-based approach grounded in elasticity theory for studying electron displacement [16,17], the multivelocuity theory that considers the statistical distribution of electron velocities [18–22], and the quantum-mechanical approach proposed by Smith [23]. Although each of these theories offers unique physical insights and mathematical perspectives, most have not been widely adopted due to their analytical complexity and limited applicability.

In practical klystron operation, the electron beam exhibits a high charge density, and pronounced particle overtaking occurs, making the motion of electrons and the amplification of microwave signals a highly complex and nonlinear process. Under such conditions, the small-signal theory becomes invalid, and analysis must rely on the large-signal theory together with the corresponding beam-wave interaction solvers. The large-signal theory simultaneously accounts for the following three aspects: (1) the alternating modulation voltage is no longer much smaller than the dc voltage, and higher-order terms of the modulation coefficient cannot be neglected; (2) the alternating current is comparable in magnitude to the dc current, corresponding to the large-amplitude regime; and (3) severe particle overtaking occurs during the bunching process of the electron beam.

In 1955, Tien *et al.* proposed the one-dimensional electron disk model [24–26], which served as the theoretical basis for establishing the large-signal theory of traveling-wave tubes. Building upon this work, Webber applied the model to investigate the large-signal bunching processes in two-cavity and multicavity klystrons [27,28], thereby promoting the development and application of large-signal theory in klystron analysis. On this foundation, many researchers subsequently developed large-signal computational codes based on the one-dimensional electron disk model [29–31]. However, this model considers only the axial motion of electrons, and therefore fails to account for the effects of external magnetic fields on beam oscillations or the influence of the radial distribution of the cavity-gap electric field on device efficiency.

To overcome the limitations of one-dimensional computational codes, Kosmahl and Albers introduced the electron ring model to account for the transverse motion of electrons [32]. Simulation codes that include both the radial and axial components of the electromagnetic fields while allowing charged particles to possess three-dimensional velocity components are generally referred to as 2.5-dimensional (2.5D) solvers. With the continuous advancement of computational technology, fully three-dimensional time-domain particle-in-cell (PIC) simulation solvers have been applied to the study of beam-wave interaction in klystrons. These 3D solvers enable the simulation of non-axisymmetric klystron structures and the investigation of the interactions between multiple modes and the electron beam, thereby providing valuable design guidance for suppressing oscillations and reducing spurious and higher-harmonic components.

PIC simulations require tracking large numbers of charged particles, imposing high computational demands and relatively slow execution. Consequently, low-dimensional beam-wave interaction solvers, which are computationally efficient, are typically used in early device design for analysis and optimization, while particle-based simulations are reserved for final-stage verification and detailed modeling. To meet this practical need, klystron beam-wave interaction solvers ranging from one-dimensional to fully three-dimensional—including several 1.5-dimensional (1.5D) codes—have been continuously developed.

Over the past decades, numerous large-signal beam-wave interaction solvers for klystrons have been developed by academic institutions and national laboratories worldwide. Most, however, remain proprietary or restricted to internal use, with limited publicly available details. Given the diversity of existing solvers, a comprehensive review of all is impractical. This paper therefore focuses on solvers commonly employed in klystron design and manufacturing in China, alongside several internationally recognized codes, while acknowledging other theoretical and computational efforts developed elsewhere. Table I summarizes the main solvers examined in this study.

Among klystron beam-wave interaction solvers, only fully three-dimensional particle-based codes are broadly applicable to diverse device geometries. Low-dimensional solvers, by contrast, are generally limited to single-beam, single-gap cavities typical of high-power klystrons, such as AJDISK. Few specialized codes can model unconventional configurations: KLY and TESLA handle multibeam klystrons, while KLYC (i.e., KlyC) accommodates extended-interaction and sheet-beam designs. Consequently, in early design stages where a dedicated solver is unavailable, designers often approximate the target klystron as a conventional high-power single-beam device and employ low-dimensional solvers like AJDISK for simulations.

The remainder of this paper is organized as follows. Section II introduces the 1D and 1.5D large-signal

TABLE I. Large-signal beam-wave interaction solvers for klystrons applied in mainland China, as well as some internationally recognized solvers.

Code	Dimension	Institution
JPNDISK/AJDISK [31–33]	1	Stanford Linear Accelerator Center, United States; Toshiba Corporation, Japan
KLY/KLY6 [34,35]	1	Institute of Electronics, Chinese Academy of Sciences (IECAS)
KLYC [36–44]	1/1.5	CERN (European Organization for Nuclear Research), University of Electronic Science and Technology of China
LSP [45,46]	2.5	Institute of Electronics, Chinese Academy of Sciences (IECAS)
KLY2D [47,48]	2.5	Institute of Electronics, Chinese Academy of Sciences (IECAS)
MASK [49–51]	2.5	Stanford Linear Accelerator Center, United States
CONDOR [52–58]	2.5	Lawrence Livermore National Laboratory, Stanford Linear Accelerator Center, United States
KLSC [59]	2.5	Los Alamos National Laboratory, United States
FCI [60]	2.5	High Energy Accelerator Research Organization, KEK, Japan
KLYSTRON-MSU [61]/ARSENAL-MSU [62,63]/PARS [64,65]	1.5/2.5	Moscow State University, Russia
TESLA [66–71]	1.5/2.5	United States Naval Research Laboratory, United States
MTSS [72]	1/2.5	University of Electronic Science and Technology of China
CHIPIC [73–76]	3	University of Electronic Science and Technology of China
UNIPIC [77–85]	2.5/3	Northwest Institute of Nuclear Technology, China
BUMBLEBEE [86–90]	3	University of Electronic Science and Technology of China
NEPTUNE [91–93]	3	United States Naval Research Laboratory, United States
CST PIC/MAFIA [94–103]	3	Computer Simulation Technology, Dassault Systemes
MAGIC [104–118]	2/3	Mission Research Corporation, United States
KARAT [119,120]	3	JIHT RAS, Moscow, Russia
ICEPIC [121,122]	3	Air Force Office of Scientific Research, United States
EMPIRE [123,124]	3	Sandia National Laboratories, United States
VSim/VORPAL [125–141]	3	Tech-X Corporation, United States

beam-wave interaction solvers, including AJDISK, KLY6, and KLYC. Section III presents the 2D and 2.5D large-signal solvers, such as LSP, KLY2D, MTSS, TESLA, and PARS. Section IV discusses the 3D particle simulation codes, including UNIPIC, CHIPIC, BUMBLEBEE, NEPTUNE, and CST-PIC. Finally, Sec. V summarizes the current progress in large-signal klystron beam-wave interaction solvers and outlines possible directions for future development.

II. 1D/1.5D LARGE-SIGNAL BEAM-WAVE INTERACTION SOLVERS

A. AJDISK

AJDISK [31–33] is a one-dimensional large-signal beam-wave interaction simulation code developed at the Stanford Linear Accelerator Center (SLAC). Although uncertainties may arise in relativistic regimes and it cannot accurately describe the effects of external magnetic fields on electron beam oscillations or the influence of the transverse electric field distribution in cavity gaps on efficiency, AJDISK remains widely used in klystron design and manufacturing in mainland China, playing a critical role.

The main features of AJDISK include: numerical integration of electron motion equations with relativistic corrections; simulation of the cavity-gap electric field distribution using Gaussian functions; the ability to simulate sheet

beams; and the capability to model higher-harmonic cavities. Additionally, AJDISK accounts for space-charge effects and incorporates relativistic corrections.

The software reads input data from predefined files and initializes the cavity-gap voltage with a small value. It then integrates the equations of motion for each electron disk, from the entrance to the exit of the interaction region, to calculate the induced currents in each cavity. Through Fourier expansion of the induced current and combining it with the cavity impedance, the fundamental and harmonic components of the gap voltage are computed. The process is iterated, considering space-charge forces, until the voltage converges. Since cavities near the input section converge faster, AJDISK monitors only the convergence of these cavities and, once convergence is achieved, uses the converged data to proceed with the remaining cavities.

Figure 1 shows the large-signal beam-wave interaction of a 3.5 GHz two-cavity klystron simulated with AJDISK. This project serves as a built-in benchmark example included in the AJDISK software package. The evolution of the electron phase trajectories and harmonic beam currents demonstrates increasing modulation depth and enhanced fundamental and second harmonic components. The axial velocity distribution indicates progressive beam bunching, and in the output section most electrons decelerate, converting kinetic energy into microwave power.

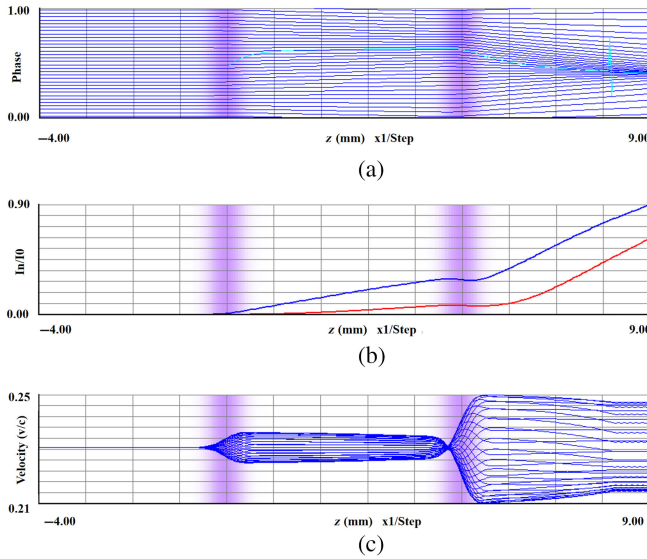


FIG. 1. (a) Electron phase trajectories. (b) Variation of the normalized beam current harmonic components along the axial direction. (c) Variation of the electron velocity normalized to the speed of light along the axial direction [31].

B. KLY6

KLY6 [34,35] is a one-dimensional large-signal beam-wave interaction simulation code developed by the Institute of Electronics, Chinese Academy of Sciences (IECAS). It features the capability to model broadband and multibeam klystrons, supports various broadband output circuit configurations such as filter-loaded and double-gap cavity structures, and includes functionality for tracking slow or returning electrons in the output section.

In the traditional one-dimensional electron disk model, significant overshoot between adjacent disks can lead to noticeable errors in calculating the axial space-charge force. To address this issue, KLY6 incorporates a dynamic tracking algorithm. While maintaining a constant tracking period length, the algorithm dynamically adjusts the number of particles tracked within each period. The fundamental assumption is that particle motion is time-periodic—that is, two particles launched one period apart follow identical trajectories. The leading edge of the dynamic wavelength is defined by the particle located at the maximum axial position, whereas the trailing edge corresponds to the position reached one period earlier. The dynamic wavelength continuously absorbs new particles at the leading edge and releases old ones at the trailing edge, ensuring particle-number consistency within each period.

During computation, KLY6 sequentially identifies particles leaving the trailing edge and verifies the positional stability of previously exited particles, ensuring their variations remain within a predefined tolerance. A relaxation method is employed to accelerate convergence and suppress numerical oscillations.

C. KLYC

KLYC [36–44] is a 1/1.5D large-signal beam-wave interaction simulation code developed at the European Organization for Nuclear Research (CERN). The software is capable of simulating beam-wave interactions from premodulated electron beams and can model both hollow-beam and multibeam klystrons. It allows for the specification of mismatched rf loads to simulate reflected oscillations and can also simulate cavity self-excitation in klystrons. Higher-harmonic cavities can be included in the beam-wave interaction, and the software supports batch processing for parameter scans and sensitivity analyses.

KLYC contains built-in optimization modules for both global and local optimization, as well as a semianalytical parameter-scaling program, which allows existing klystron designs to be scaled to different operating frequencies, beam powers, and perveances while preserving electron bunching and deceleration processes. Under small-signal conditions, KLYC can simulate the effects of collector-reflected electrons on the beam-wave interaction. The following section introduces the physical model implemented in KLYC.

1. Electron beam model and particle emission

KLYC 1D employs a one-dimensional electron disk model, while KLYC 1.5D uses a two-dimensional electron ring model. The software is based on a metallic surface emission model, enabling simulation of the space-charge depression on the emission surface and its evolution. To ensure convergence in the presence of reflected electrons, KLYC incorporates a specialized absorbing boundary.

2. Cavity rf fields

KLYC incorporates an eigenmode solver capable of computing both one-dimensional Gaussian and two-dimensional electromagnetic (EM) cavity modes. The Gaussian mode approximates the normalized axial electric field using a Gaussian profile, while the EM mode solver calculates two-dimensional field distributions for axisymmetric cavity geometries. Figure 2 shows examples of the E_z component simulated by the EM module for three typical rf cavity configurations. KLYC also allows importing eigenmode

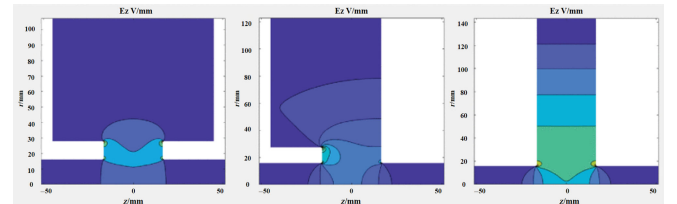


FIG. 2. An example of the 2D diagram of the E_z component simulated by the KLYC EM solver for three common rf cavity topological structures [36].

field data from external electromagnetic solvers such as CST MWS and Ansys HFSS.

3. Space-charge field and electron motion

In an axisymmetric system, the space-charge field can be derived by integrating the Green's function corresponding to the field distribution generated by point charges [36]. For 1.5D simulations, both the space-charge field and the charge density depend on the radial position. Given the known rf field in the cavity and the space-charge field, the electron motion can be described under the influence of relativistic effects by applying the Lorentz equation.

4. Field excitation

KLYC employs an infinite longitudinal magnetic field to constrain the circular electron beam, which allows for the consideration of only the longitudinal electric field. The cavity excitation equations are constructed using waveguide modes. Additionally, KLYC provides internal calibration for generating rf power based on electron beam power loss. For multigap output cavities, KLYC uses weak coupling theory by adding excitation terms from adjacent cells, modifying the excitation equations for output cavity modes in the mathematical model, and representing the electromagnetic coupling between cavity cells using a coupling coefficient matrix. Furthermore, KLYC approximates electromagnetic coupling by using the overlap of eigenfields of individual cells. Under the 1.5D assumption, KLYC also efficiently handles beam-wave interaction for ribbon-shaped beams, simplifying the radiation layer-wise for a specific transverse direction and averaging in the other direction.

5. Optimization

KLYC incorporates two types of optimizers: the global optimization genetic algorithm and the local optimization pattern search algorithm [38]. The genetic algorithm offers two optimization approaches: one optimizes the entire klystron, while the other applies a grouped optimization strategy for the difference between the bunching and output sections of the klystron, optimizing the first N cavities differently from the remaining cavities. The pattern search algorithm avoids gradient computation, preventing the optimizer from converging to numerical poles. For large-loop iterations, the algorithm considers neighboring points to determine the direction for the next optimization step.

6. Self-excited oscillation

KLYC introduces both small-signal and large-signal analysis functionalities for specific resonant modes. In the presence of space charge and relativistic effects, KLYC can simulate self-excitation oscillations of cavities quickly, but this can only be done for steady-state parameters where no radial motion occurs in the particles. Under

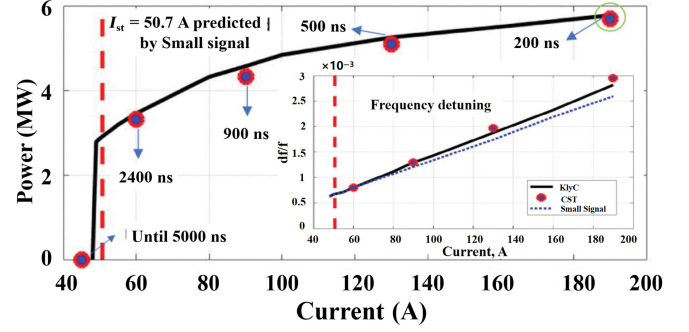


FIG. 3. Comparison between KLYC large- and small-signal simulations (solid and dashed lines) and CST/3D PIC simulations (circles) for a beam voltage of 400 kV. The time labels on the plot correspond to the onset time of the monotron oscillation in the PIC simulations [39].

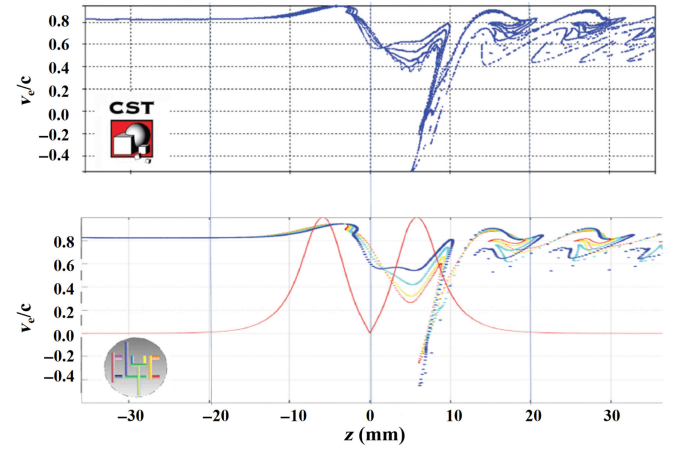


FIG. 4. Photographs of the particle phase space calculated in CST/3D (top) and KLYC (bottom) for the operating point with $V = 400$ kV and $I = 190$ A [39].

small-signal conditions, the system is dominated by the dc state, while for large-signal conditions, only the output cavity of the klystron is analyzed.

Figure 3 shows the beam-wave interaction results from KLYC 1.5D and CST 3D at a voltage of 400 kV with different electron beam currents. Both codes exhibit good agreement in the calculated output power and oscillation frequency. Figure 4 presents the particle phase space diagrams obtained from KLYC 1.5D and CST 3D simulations, where the oscillation time of the device increases as the electron beam current approaches the threshold current.

III. 2D/2.5D LARGE-SIGNAL BEAM-WAVE INTERACTION SOLVERS

A. LSP

LSP [45,46] is a 2.5D large-signal nonlinear beam-wave interaction solver for the klystron, developed by the Institute of Electronics, Chinese Academy of Sciences.

This solver is capable of accurately describing the main physical processes inside the device while maintaining high computational efficiency, enabling designers to test more initial parameters within a limited time frame. The key features of LSP include: moderate computational load, stable and reliable program execution, and the use of time as the independent variable. The solver employs an efficient and accurate table lookup method to calculate the space-charge force between particles, and a self-consistent method to trace the particle motion. The cavity-gap voltage is determined self-consistently through an iterative process, including in cases of dual-gap output cavities. Additionally, LSP can handle the issue of drift tube wall interception of moving particles. The following section provides a detailed description of the physical model of LSP.

1. Electron beam model

LSP uses a 2D electron ring model and assumes that the axial thickness of the ring remains constant and does not distort. The electron beam maintains laminar flow during motion, with the beam concentrated near the axis. The space-charge field and the focusing magnetic field across the beam cross section are approximately uniform, and the ring as a whole has the same angular velocity.

2. Cavity rf field

LSP models the rf field distribution between the drift tube ends of the cavity using a hyperbolic cosine function [142]. Starting from the wave equation, the two-dimensional electric field distribution in the gap is derived using a contour integral method, though it only supports the calculation of reentrant cavity rf field distributions.

3. Space-charge field and electron motion

The space-charge forces between charged rings are computed using the Green's function method. To simplify the formulation, the gaps between cavities are neglected, and all charged rings are assumed to reside within an infinitely long, perfectly conducting cylindrical surface, which provides analytically tractable boundary conditions. Within this framework, each ring is assumed to carry a uniformly distributed charge, enabling accurate evaluation of the resulting electric potential and field. The particle dynamics are advanced by solving the relativistic Lorentz force and Newton's equations of motion using the Runge-Kutta integration method, which ensures numerical stability and convergence of particle trajectories.

The computation of the space-charge force between two charged rings involves summing an infinite series containing modified Bessel functions, which is computationally expensive. To improve efficiency, the LSP code adopts an interpolation-based force lookup strategy: interring forces

are first calculated at selected spatial positions and stored in a "force table." During simulation, the code retrieves and interpolates these precomputed values to determine the required forces, significantly reducing computational cost without compromising accuracy. Moreover, to ensure beam stability and maintain a physically consistent electron flow, users can manually define the initial positions and velocity components of each charged ring according to the conditions of a balanced electron beam, thereby providing greater control over the initial configuration and enhancing the reproducibility of the simulation.

4. Electron capture processing

Whether the charge carried by the electron ring is lost due to drift tube wall interception depends on its radial position and radial velocity. The basic judgment criterion is: if the particle's radial position $r > 0.95a$ and radial velocity $v_r > 0$, the particle is considered to be fully intercepted by the tube wall. If $r > 0.95a$ and $v_r \leq 0$, the particle will lose the portion of charge outside the drift tube. If the remaining charge of a particle is less than 10% of its initial charge, it is considered fully lost.

5. Self-consistent iteration of cavity gap voltage

LSP first provides an initial guess for the cavity-gap voltage and then uses numerical methods to compute the electron beam motion corresponding to that guess. The induced current is then calculated, and the new gap voltage is obtained. This process is repeated until convergence. A relaxation factor can be introduced to accelerate convergence. For dual-gap output cavities, the induced voltages of the two working gaps are related to the induced current generated by the electron beam excitation using a complex impedance matrix. The elements of this matrix are determined experimentally.

Figure 5 shows the results of the simulation for the S-band 50 MW peak power klystron KS-4119 computed by LSP. Figure 5(a) illustrates that electron trajectories exhibit minimal radial fluctuations in the bunching cavity, whereas larger fluctuations occur in the output cavity. Figure 5(b) shows pronounced velocity dispersion of electrons within the output cavity, with the majority contributing to microwave amplification. Figure 5(c) indicates that, as the excitation power increases, the maximum output power predicted by KLY6 surpasses that of LSP. This overestimation arises because the 1D klystron large-signal solver KLY6 concentrates electron momentum along the longitudinal axis, thereby exaggerating the beam-wave interaction efficiency. Figure 5(d) demonstrates good agreement between LSP simulations and experimental measurements: at a 309 kV electron beam acceleration voltage, the strong magnetic field effectively suppresses radial fluctuations, maintaining good beam laminarity and resulting in consistent outcomes between experiment and simulation.

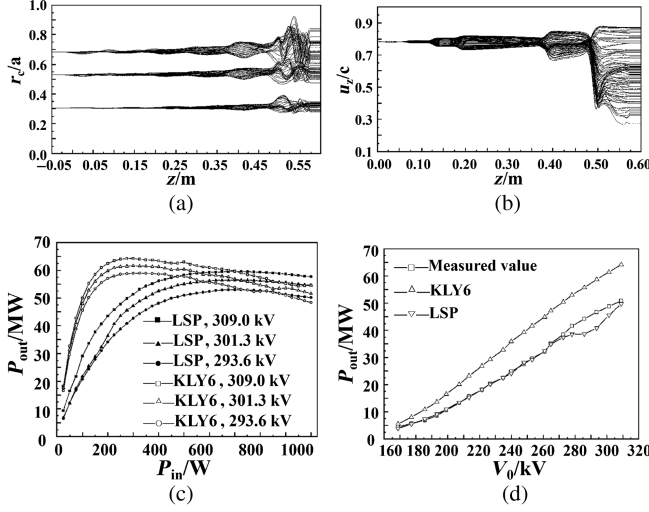


FIG. 5. (a) Motion trajectories of charged particles in the $r-z$ plane. (b) Variation of the axial velocity component of charged particles along the longitudinal distance. (c) Transmission characteristic curves at different operating voltages calculated by LSP and KLY6. (d) Output power as a function of dc voltage: comparison among LSP calculations, KLY6 calculations, and experimental measurements [45].

B. KLY2D

KLY2D [47,48] is a 2.5D large-signal klystron beam-wave interaction solver developed by the Institute of Electronics, Chinese Academy of Sciences. Its main features include the particle-in-cell method for assigning particle charge and beam current to the computational grid while solving Maxwell equations with the finite-difference time-domain (FDTD) algorithm; modeling two-dimensional rf field distributions in reentrant cavities using a hyperbolic cosine function, with the option to import numerical field distributions from other electromagnetic solvers; updating particle velocities and positions through the Boris rotation scheme to solve the Lorentz force equation, with cylindrical coordinate adjustments to avoid singularities near the beam axis; and handling various boundary conditions, including metallic walls, symmetry axes, and absorbing boundaries at the drift tube exit. The following section describes the physical model and implementation in detail.

1. Space-charge field and electron motion

As shown in Fig. 6, KLY2D assigns particle charges to grid cells using an area-weighting scheme and computes cell currents via the continuity equation. The electric and magnetic fields are then obtained from the full Maxwell equations using the FDTD method. This approach supports various boundary conditions, including perfect conductors, dielectrics, absorbing layers, and particle emission surfaces.

At each time step, KLY2D interpolates the Lorentz force on each particle from both the space-charge and rf cavity fields. Particle velocities and positions are updated by

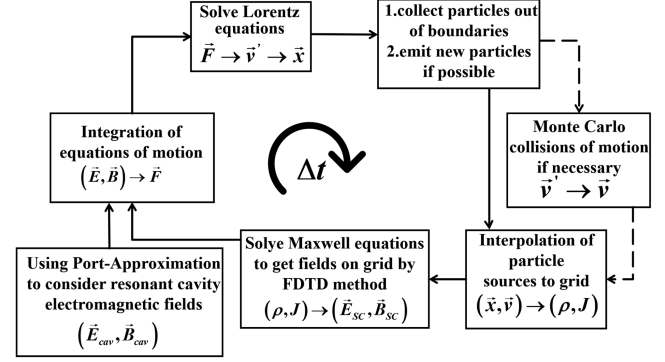


FIG. 6. Program flux of code KLY2D [47].

integrating the relativistic Lorentz equation using the Boris rotation algorithm. To prevent numerical divergence at $r = 0$, positions and velocities are advanced in Cartesian coordinates and then mapped back to the cylindrical system. A Monte Carlo Collision (MCC) model is also employed to simulate electron-ion interactions within the klystron.

Simple Dirichlet or Neumann boundary conditions can lead to electron reflections near the collector, potentially destabilizing the beam-wave interaction. To mitigate this, KLY2D implements convolutional perfectly matched layer boundaries, which efficiently absorb outgoing waves and suppress reflections. The FDTD algorithm strictly satisfies the Courant stability criterion, ensuring both numerical stability and accuracy.

2. Particle charge assignment and current deposition

At each time step, the charge on the computational mesh is computed using an area-weighting algorithm. KLY2D adopts a charge-conserving current deposition scheme that keeps Gauss's law satisfied if it is initially fulfilled. When a particle crosses several cells in one step, its displacement is segmented at cell boundaries, and each segment contributes current independently to ensure charge conservation and numerical accuracy.

Figure 7 shows the beam-wave interaction simulation results of the S-band 50 MW klystron KS4119, developed by the Institute of Electronics, Chinese Academy of Sciences, obtained using KLY2D.

Figure 7(a) shows the axial momentum distribution of electrons along the z direction at the final simulation time. Most electrons experience rapid deceleration in the output cavity region, where their kinetic energy is efficiently converted into microwave power. Figure 7(b) presents the corresponding radial momentum distribution. As electrons travel toward the output section, the dispersion of radial momentum increases, reflecting more complex transverse dynamics. Figure 7(c) compares output power versus input power characteristics obtained from KLY2D, LSP, and KLY6 under identical beam acceleration voltages. The

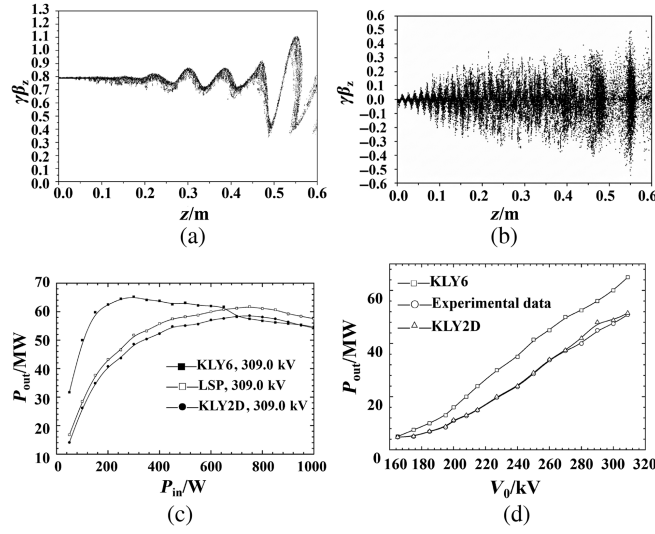


FIG. 7. (a) Axial momentum distribution of electrons along the z direction at the final time step of the simulation. (b) Radial momentum distribution of electrons along the z direction at the final time step of the simulation. (c) Output power of the beam-wave interaction as a function of input power, calculated by KLY2D, LSP, and KLY6 under the same electron beam acceleration voltage. (d) Comparison of output power obtained from KLY2D and KLY6 simulations with experimental measurements, where the variable is the electron beam acceleration voltage [47].

one-dimensional solver KLY6 ignores the radial momentum component of electrons, leading to an overestimation of beam-wave interaction efficiency. The output power predicted by KLY2D is slightly lower than that of LSP because strong electron overtaking and trajectory crossing in the output cavity reduce beam laminarity, violating the ring-beam assumption used in LSP. Figure 7(d) compares the calculated output powers of KLY2D and KLY6 with experimental measurements at different beam acceleration voltages. The results show that KLY2D provides better agreement with experimental data, confirming its higher accuracy in modeling klystron performance under strong beam-wave interaction conditions.

C. MTSS

MTSS [72] is a microwave tube simulator suite developed by the Laboratory of Computer Simulation Technology at the University of Electronic Science and Technology of China. Its built-in module, BWISKLY, is a 2.5D large-signal steady-state frequency-domain beam-wave interaction solver for klystrons. The program features the capability to simulate high-power klystrons with circular electron beams, extended-interaction klystrons, and 1D sheet-beam klystrons. The steady-state frequency-domain model employs a spatial step iterative algorithm that enables rapid convergence. BWISKLY can also handle cases where moving

particles are intercepted by the drift-tube wall. The physical model of MTSS is introduced below.

1. Field excitation described by telegraph equations

MTSS formulates generalized telegraph equations for the beam tunnel and resonant cavities based on waveguide and cavity modes, where the equations include line integrals along the waveguide cross-sectional boundary. When the boundary is an ideal conductor, the boundary term vanishes. However, if the boundary has finite impedance or if coupling apertures exist between the beam tunnel and the outer cavity, the boundary term becomes nonzero. By enforcing the continuity of the transverse field at the common boundary between the cavity and the beam tunnel, MTSS defines a coupling matrix linking them. For the input and output waveguides, the transverse fields are expressed as superpositions of forward and backward propagating modes, and the corresponding telegraph equations for the input and output cavities are updated accordingly.

2. Space-charge field and electron motion

MTSS employs a simplified two-dimensional spatial model to compute the axial and radial space-charge forces on particles. At each axial step, a reduced one-dimensional radial Poisson equation is solved and integrated to obtain the potential, from which the axial space-charge force is derived based on the potential difference between adjacent grid points. During trajectory updates, only a single computation of the dc space-charge field is required, avoiding the complexity of iteratively solving the full two-dimensional Poisson equations in both radial and axial directions. The electron beam is represented as a sector of charged macro-particles capable of three-dimensional motion, allowing simulation of azimuthal field nonuniformity caused by higher-order spatial harmonics and azimuthal particle motion induced by axial magnetic fields, while accounting for relativistic effects. This 3D particle motion model provides accurate incident energy distributions for collector analysis.

3. Steady-state solution

At steady state, the time derivatives of modal voltage and current within the cavity are zero. The input cavity accounts for the input waveguide and input power, while the output cavity includes the output waveguide and output power. By simultaneously solving the steady-state equations governing modal voltages and currents in all cavities, the steady-state parameters of the system can be obtained.

D. TESLA

TESLA [66–71] (the Telegraphist Equations Solution for Linear Amplifiers), developed by the U.S. Naval Research Laboratory (NRL), is a 2.5D large-signal beam-wave interaction solver for klystrons. Its main capabilities

include simulating extended-interaction klystron (EIK) and multibeam klystron, coupling the electron beam with the rf fields of high-frequency structures through an impedance matrix, and modeling the effects of slow and reflected electrons on device performance. The code can characterize the impedance matrices of composite structures and employs the Nyquist method to evaluate device stability. It also uses the adjoint equation technique to determine the sensitivity of device parameters to various quality factors. TESLA supports end-to-end simulations from the electron gun through the beam-wave interaction region to the collector, and it incorporates a reduced 1.5D algorithm that accelerates particle integration by restricting particle motion to the z direction. The physical model of TESLA is described in detail below.

1. Cavity rf field

In the original TESLA solver, each cavity is modeled as an RLC circuit, with its parameters such as resonant frequency and quality factor specified by the user. The field is represented as a superposition of local fundamental modes with amplitudes that vary along the axial direction and in time. The updated solver, TESLA-Z, employs computational electromagnetics (CEM) codes to obtain the eigenmode field distributions and determine the corresponding eigenparameters. CEM tools such as Ansys HFSS and Analyst can compute rf fields for high-frequency circuits with arbitrary geometries.

2. Separate beam-wave interaction computation

In TESLA, the fields inside and outside the beam tunnel couple at the cavity gap boundaries via an impedance matrix. This matrix, obtained from CEM codes, enforces continuity of the tangential electric and magnetic fields. Fields inside the beam tunnel are computed with and without the electron beam. Boundary conditions for both cases are set by the tangential electric field voltage at the drift-tube gap. These calculations determine the surface current distribution and drift-tube mode voltage. Voltages and currents at the input and output ports relate to those at the cavity gaps through an extended impedance matrix.

3. Particle model and self-field

TESLA represents each macroparticle as a charged ring with coordinates $[r(z), t(z)]$ capable of full three-dimensional motion. The azimuthal momentum component is driven by the Lorentz force in the presence of an external magnetic field and is retained even under azimuthally symmetric fields. A radial grid assigns fields and accumulates current. Current densities along the radial and axial directions are projected onto the basis functions used for the fields, removing the need to assume a fixed axial wavenumber.

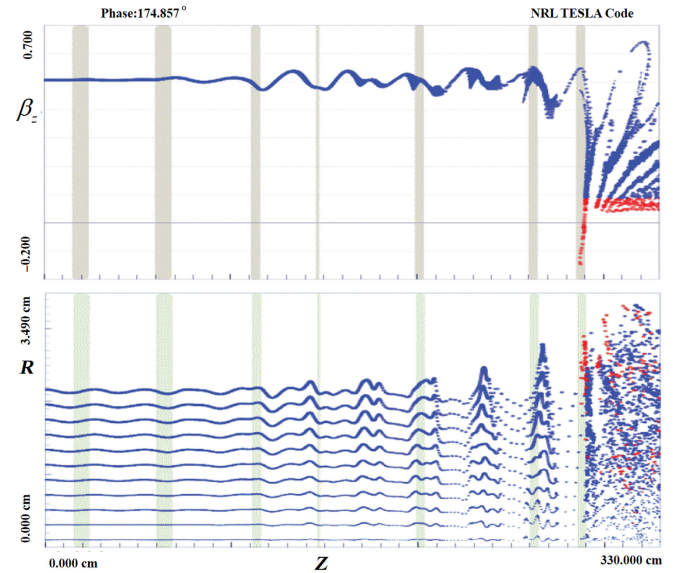


FIG. 8. Distributions of particle axial momentum (top) and radial motion (bottom) along the z coordinate calculated using the TESLA code for the seven-cavity SLAC klystron [2].

4. Treatment of special particles

During beam transport through the interaction region, TESLA continuously monitors the axial velocity of each particle. When the normalized axial velocity of a particle falls below a user-defined threshold, the particle is transferred from the group tracked as a function of position $t(z)$ to a special group tracked as a function of time $z(t)$. These special particles are followed until their velocity exceeds the threshold, at which point they are returned to the $t(z)$ tracked group. Particles that strike the drift tube wall or exit the simulation domain are permanently removed from the particle population. Figure 8 presents the TESLA simulation results for the SLAC seven-cavity klystron, where special particles with normalized axial velocities below the threshold are indicated in red.

5. Combination of impedance matrices

For large and complex rf structures, direct computation of the classical impedance matrix using three-dimensional finite-element electromagnetic codes is often limited by computational memory and runtime, which can lead to slow convergence or insufficient accuracy. TESLA addresses this issue by applying Kirchhoff's laws to decompose the overall structure into several independent subcomponents. The impedance matrices of these subcomponents are then combined to construct the equivalent impedance matrix of the complete structure. This approach ensures high computational efficiency while maintaining numerical accuracy.

6. Device stability analysis

TESLA-Z provides a general frequency-domain framework for stability analysis. To assess device stability, a

frequency-dependent gain function is first computed, and the Nyquist criterion is used to determine the existence of unstable modes. The procedure begins with the definition of an admittance matrix that characterizes the properties of the beam-loaded interaction circuit. After obtaining the impedance and admittance matrices, they are combined to form a gain matrix. This gain matrix fully describes the closed feedback loops within the device and accounts for the effects of reflections on system stability, making it suitable for self-oscillation analysis. The growth rate of unstable solutions corresponds to complex frequencies, which require evaluation of the impedance and admittance matrices in the complex frequency domain. Since these matrices are generally computed at real frequencies, the Nyquist method can be employed to determine whether any complex frequencies in the upper half-plane satisfy the instability condition.

7. Parallel computing and multibeam device simulation

TESLA-MB incorporates parallel processing using the Message Passing Interface. This capability enables fast and accurate predictions of the performance of the MBK-2 device developed at the U.S. NRL, including the intercepted current in each beam channel. The code also allows investigation of higher-order mode instabilities that may occur in the dual-gap input cavity of the 18-beam MBK-3. Figure 9 presents the bandwidth calculation results for the 18-beam MBK-3 obtained with TESLA-Z. In addition, the impedance-matrix formulation adopted in the code can account for the effects of filter loads and dual-gap cavity configurations on the overall system response.

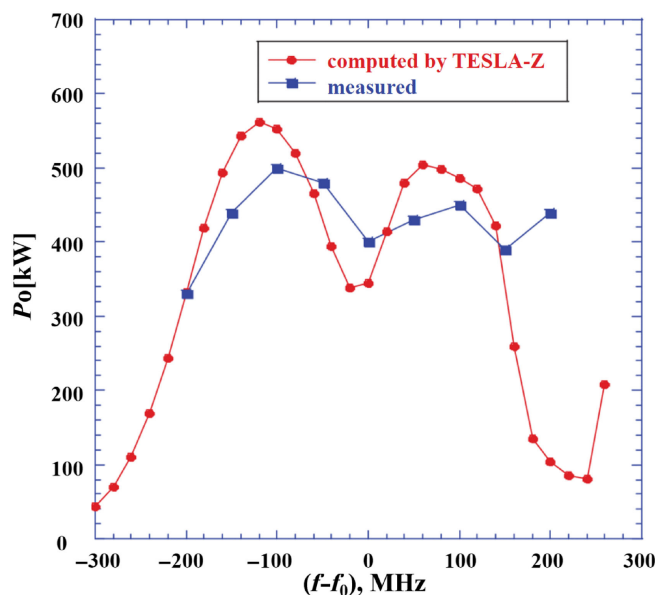


FIG. 9. Comparison between the bandwidth computed by TESLA-Z and the measured bandwidth of MBK-3 [143].

8. End-to-end coupling of electron gun and large-signal codes

The TESLA large-signal simulation suite includes several simplified internal beam models, such as immersed, rigid-rotor, and partially or fully shielded cathode models. TESLA also supports importing initial beam distributions from electron gun simulation codes such as MICHELLE, which provide detailed information on emission processes, gun geometry, and focusing fields. After the beam-wave interaction simulation is completed, TESLA can export the depleted beam data for collector modeling and design, enabling a comprehensive end-to-end analysis from the electron gun to the collector.

9. Geometry-driven framework, computational accuracy, and performance optimization

The original version of TESLA was written in Fortran 66/77, whose outdated structure and static memory model imposed severe limitations on memory efficiency and algorithmic scalability. The code has since been completely rewritten in Fortran 2003, adopting dynamic memory allocation and a highly modular programming architecture. Memory resources are now assigned dynamically at runtime according to user-defined input parameters, ensuring full adaptability. This modernization has significantly improved computational efficiency and facilitated the extension of existing algorithms, providing a robust foundation for future feature development and high-precision modeling.

E. PARS

PARS [64,65], developed at Lomonosov Moscow State University, is a 2.5D large-signal klystron simulation code derived from ARSENAL-MSU. The main features of PARS include the capability to model broadband klystrons, simulate beam-wave interactions in broadband output circuits loaded with filters, and analyze dual-gap coupled cavities with filter loads. The frequency dependence of the circuit impedance matrix can be provided as an external input file. The code also supports multibeam klystrons, taking into account the effect of variations in the characteristic impedance R/Q at different radial beam positions on the beam-wave interaction. In addition, PARS can model relativistic and extended-interaction klystrons and incorporates an automatic optimization module [61,63,144].

PARS employs a macroparticle representation of the electron beam, providing a self-consistent analysis of beam-field interactions under relativistic conditions. The code consists of three primary modules: an electron optics module, a resonant cavity rf field solver, and a beam-wave interaction solver. The cavity module is a two-dimensional electromagnetic field solver capable of computing the resonant frequencies and field distributions of cavities with realistic geometries. The electron optics module calculates the electrostatic field and electron

trajectories in axisymmetric systems. PARS also integrates a two-dimensional magnetic field solver developed by the Institute of Electronics, Chinese Academy of Sciences, which determines the axial magnetic field distribution produced by electromagnetic coils and permanent magnets.

At the entrance of the interaction region, the macro-particle data can be specified analytically or obtained from the output of the PARSTATIC electron optics module within PARS. The code accounts for radial beam dynamics in focusing magnetic fields, as well as layer formation, dynamic defocusing, conversion of beam kinetic energy into bunching potential energy, effects of radius variation in drift regions, and power losses caused by beam current deposition on the walls of the interaction structure. For space-charge field computation, PARS uses a local Galerkin method to solve the driven Maxwell equations, where the electric and magnetic field components are expanded in local Galerkin series. The relativistic equations of motion are integrated using a fourth-order Runge-Kutta method, ensuring high numerical accuracy in beam trajectory and field evolution calculations.

The automatic optimization module in PARS employs a composite local optimization algorithm. The parameters involved in the optimization include the input power, drift tube length, frequency tuning, and cavity Q -factor. Cavity parameters such as wave impedance and eigenfield distribution are treated as predefined constants and remain unchanged during the optimization process. The objective function of the algorithm is the electronic efficiency of the device. Optimization can be performed at a single input signal frequency or over a frequency band. In the latter case, the objective function is defined as the average electronic efficiency within the specified frequency range. A penalty function system is incorporated into the algorithm. It is activated when the current deposition on the walls of the interaction structure or the voltage amplitude in intermediate cavities exceeds preset limits. Each parameter to be optimized must have its own specified variation range. The number of iterations required to reach the maximum of the objective function depends on the number of parameters and the width of their variation ranges, and the resulting local maximum, representing the optimal combination of klystron parameters, is also influenced by these factors.

The optimization process begins with two or three cavity klystrons. Additional cavities are then introduced sequentially while keeping the parameters of the preceding cavities and drift tubes fixed, and the optimal design is determined at each stage. To improve computational efficiency, a 1.5D optimization is performed prior to the 2.5D optimization. The results of the 1.5D optimization define the parameter variation ranges for the 2.5D case, thereby reducing the time required to locate the global maximum of the objective function. Figure 10 presents the 2.5D PARS optimization results for a high-power klystron developed by the University

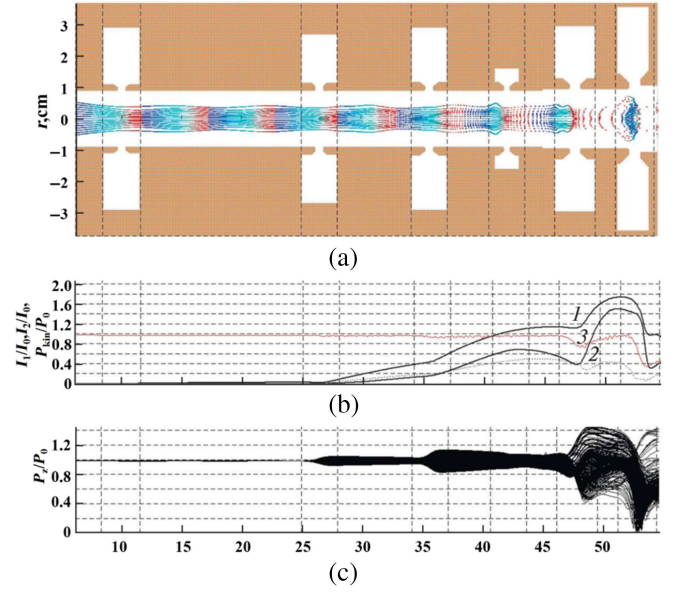


FIG. 10. (a) Design of the upgraded UESTC klystron with a second harmonic cavity and the calculated snapshot of large particles. (b) Calculated longitudinal dependences of the first (curve 1) and second (curve 2) harmonics of convection current and of the electron power carried in the form of kinetic energy (curve 3); and (c) distributions of the longitudinal electron momentum component [65].

of Electronic Science and Technology of China (UESTC) for accelerator applications [65].

IV. 3D PARTICLE-IN-CELL SOLVERS

A. UNIPIC

UNIPIC [77–85], developed by the Northwest Institute of Nuclear Technology in China, is a three-dimensional particle simulation solver. Its main features include 2.5-dimensional fully electromagnetic particle simulation capabilities, as well as three-dimensional parallel full electromagnetic simulation. The code incorporates a parallel genetic algorithm for vacuum electronic device optimization and employs conformal meshing to accurately model complex three-dimensional vacuum electronic structures, achieving large-scale parallel computation efficiency. UNIPIC implements a fully electromagnetic particle simulation algorithm based on the discontinuous Galerkin time-domain (DGTD) method, which significantly enhances its ability to model complex geometries. In addition, a potential correction equation is introduced into the time-domain electromagnetic field solver to reduce errors caused by charge nonconservation in DGTD-based full electromagnetic simulations. The physical model of UNIPIC is described in detail below.

1. 2.5D full electromagnetic particle simulation

The UNIPIC-2.5D code is primarily designed to simulate beam-wave interaction processes in vacuum electronic

devices, covering both nonrelativistic and relativistic regimes. It supports three types of two-dimensional coordinate systems: $x - y$, $z - r$, and $r - \phi$. The code allows for various electromagnetic boundary conditions, including perfect conductors, lossy conductors, incident-wave excitation, and wave absorption. Multiple emission mechanisms are implemented, such as thermionic emission, field emission, secondary emission, explosive emission, and photoemission. UNIPIC-2.5D can also simulate various collision processes between charged particles and neutral gases, including elastic scattering, ionization, excitation, charge exchange, and recombination. In addition, the code can be coupled with a parallel genetic algorithm to perform multiparameter optimization of vacuum electronic devices.

2. 3D full electromagnetic particle simulation

The UNIPIC-3D code is developed to study nonlinear beam-wave interactions in fully three-dimensional vacuum electronic devices. It enables the construction of complex 3D geometries and supports conformal mesh generation along the x , y , and z directions. The core computational module employs a domain decomposition algorithm to achieve efficient parallel computation. Various electromagnetic boundary conditions are available, including perfect and lossy conductors, port-mode excitation, and perfectly matched layer (PML) absorbing boundaries. Charged particles can be generated through field emission, beam emission, or explosive emission, enabling flexible modeling of diverse device configurations.

As shown in Fig. 11(a), the global mesh is divided into four subdomains by decomposition1 and decomposition2, thereby partitioning the global physical region into four corresponding subregions, denoted as PhysRgn1, PhysRgn2, PhysRgn3, and PhysRgn4. These subregions are assigned to processes 1 through 4, respectively. To ensure accurate boundary information exchange during parallel computation, an additional guard-cell layer is added by extending the upper and lower boundaries of each physical region by one mesh layer. Figure 11(b) illustrates the extended local mesh region, ExtendedRgn1, which is

obtained by expanding the physical region PhysRgn1 assigned to process 1. Each process then computes the intersection between its extended mesh region and the physical regions of other processes. If a nonzero intersection is found, electromagnetic field data exchange is performed between the corresponding processes to maintain consistency and continuity of the global field solution.

3. Discontinuous Galerkin time domain

UNIPIC incorporates a 2.5-dimensional full electromagnetic particle simulation code based on DGTD framework. By introducing an auxiliary correction potential, the code effectively suppresses numerical errors caused by charge nonconservation. The computational domain is discretized using an unstructured triangular mesh, and both scalar and vector basis functions are employed in the DGTD formulation for electromagnetic fields. Voltage-wave loading boundary conditions are implemented using the total-field/scattered-field approach, while truncated port boundaries are treated with the complex-frequency shifted perfectly matched layer technique. The code also supports axisymmetric and metallic-wall electromagnetic boundary conditions. For the interaction between charged particles and electromagnetic fields on unstructured meshes, efficient algorithms for particle localization as well as charge and current deposition are implemented.

To obtain the electromagnetic field components at particle positions, the element index and local coordinates of each particle within its host element must be determined. UNIPIC adopts a spatial grouping strategy to organize unstructured mesh elements within the computational domain. The entire domain is uniformly divided into a virtual structured mesh composed of $N_x * N_y$ rectangular cells. All unstructured triangular elements that spatially overlap with a given virtual cell are grouped together. Owing to the regular arrangement of the virtual grid, the index of the virtual cell containing a particle can be rapidly computed from its physical coordinates, thereby identifying the associated group of triangular elements. This strategy significantly enhances the efficiency of particle localization on unstructured meshes.

B. EMPIRE

ElectroMagnetic Plasma In Realistic Environments [123,124] (EMPIRE) is an electromagnetic plasma simulation software developed by Sandia National Laboratories (SNL) for next-generation high-performance computing platforms. Its key features include the capability to perform high-confidence simulations of the full process of high-power pulse generation, propagation, and interaction with matter; portability across different computing platforms; support for multiple parallel backends through the Kokkos abstraction layer; scalable exascale (10^{18} operations) parallel computing via asynchronous multithreading, effectively enhancing the utilization of heterogeneous compute

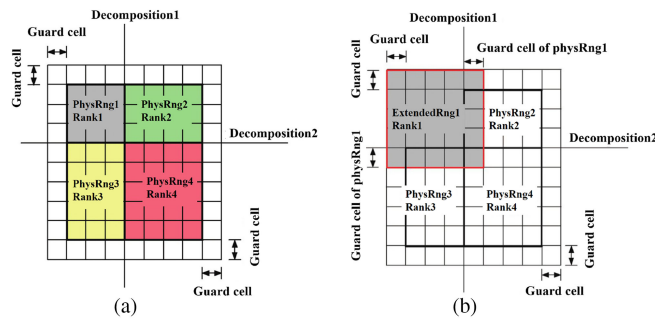


FIG. 11. Domain decomposition and extended grid layer by parallel computation. (a) Computational domain decomposition. (b) Extended grid layer of physical domain [82].

nodes; incorporation of advanced time-integration schemes, both implicit and explicit, with performance exceeding traditional forward simulations, along with embedded sensitivity and adjoint analysis capabilities; uncertainty quantification facilitated by the Sacado automatic differentiation tool; integration of state-of-the-art plasma physics simulation techniques; and implementation of advanced verification and validation procedures, together with workflow services for continuous improvement and upgrades. The following sections describe the software architecture and its physical models.

1. EMPIRE software architecture

The core modules of EMPIRE can operate independently or in a modular, combined fashion, and primarily include the electromagnetic solver EMPIRE-EM, the particle simulation solver EMPIRE-PIC, the fluid solver EMPIRE-Fluid, and the fluid-particle hybrid solver EMPIRE-Hybrid, as illustrated in Fig. 12.

EMPIRE-EM rigorously solves the source-free Maxwell equations within complex geometries, including closed-space electrostatic, magnetostatic, and electromagnetic problems under electromagnetic, electrostatic, ideal electrostatic, ideal magnetostatic, and mixed boundary conditions. EMPIRE-PIC, applied to complex geometries under vacuum or near-vacuum conditions, uses the PIC method to simultaneously solve the source-free Boltzmann equation, the MCC equation, and Maxwell equations. Coupled with the direct simulation Monte Carlo (DSMC) method, it forms the EMPIRE-DSMC/PIC module, enabling accurate simulation of rarefied gas and plasma dynamics in vacuum electronic devices. It can also simultaneously solve the Boltzmann equation under nonelectromagnetic external forces and Maxwell equations, resulting in the EMPIRE-DSMC/PIC module. EMPIRE-Fluid applies various physical assumptions and fluid dynamic methods to address specific physical problems in complex geometries, enabling the study of plasmas under high-density or high-pressure conditions. EMPIRE-Hybrid focuses on problems involving moderate-density plasmas by organically coupling the electromagnetic solver, particle simulation solver, and fluid solver. It simultaneously solves different partial differential equations and relies on a multi-algorithm framework, including the discontinuous Galerkin finite-element method, compatible with the finite-element

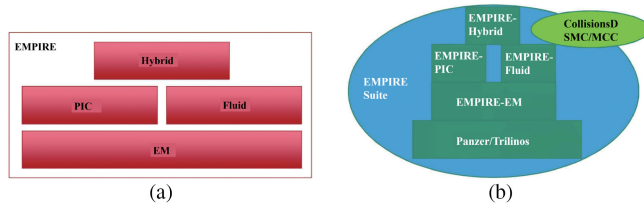


FIG. 12. Basic architecture of the EMPIRE. (a) Physical model composition. (b) Algorithm module composition [123].

method (FEM), macroparticle or fluid collision and merging algorithms, as well as a combination of explicit and implicit time-integration schemes [123].

2. Core mathematical and physical models in the EMPIRE-PIC module

The EMPIRE-PIC module is primarily used to model beam-wave interactions in vacuum electron devices. It is based on the finite-element method with an unstructured mesh and employs the Klimontovich and Maxwell equations as its fundamental physical models. Particle motion is advanced using the Boris push algorithm. The computational workflow of the EMPIRE-PIC module is illustrated in Fig. 13.

EMPIRE-PIC is an unstructured mesh particle simulation module based on FEM and implemented in C++. It supports multiple mesh topologies, including quadrilateral, hexagonal, triangular, and tetrahedral elements. Compared with conventional PIC programs using the Yee-grid FDTD method, EMPIRE-PIC can more accurately and efficiently solve complex systems containing fine structures. The software also supports a dual-mesh approach: the electromagnetic field is solved on a tetrahedral FEM mesh that allows local refinement to enhance resolution where needed, while particles are advanced on a regular mesh. EMPIRE-PIC extensively utilizes the Trilinos library and leverages Kokkos to achieve large-scale efficient parallelism, cross-platform portability, and user-friendly control. Particle collisions and chemical reactions are modeled using SNL SPIN particle reaction and cross-section libraries.

Within the FEM framework, particle pushing follows the same methodology as in FDTD; however, the field update differs. Maxwell's equations are solved in a weak form: starting from Ampère's law, the equations are multiplied by test functions and integrated over the domain, the solution is expanded in the test function space, and the curl terms are integrated by parts to form the resulting matrix system. The magnetic field equations are treated similarly, producing corresponding matrices.

In the EMPIRE software ecosystem, the underlying Kokkos library supports cross-platform heterogeneous

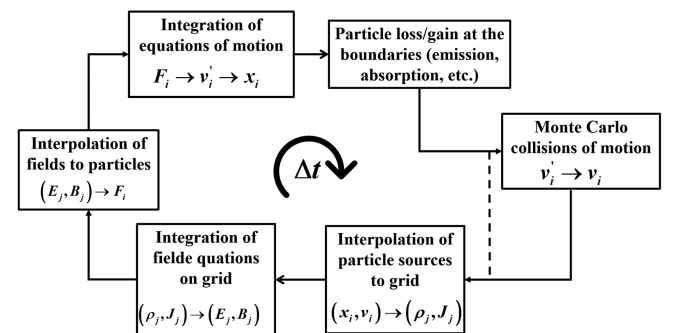


FIG. 13. Flowchart of the EMPIRE-PIC module calculation process [123].

computing. Trilinos serves as a general-purpose solver library for the numerical computation modules. SPIN provides collision cross-section data for probabilistic modeling in MCC and DSMC processes. The PIC, Fluid, and EM modules constitute the three core physics modules and are responsible for the discrete solution of partial differential equations that govern complex physical processes.

C. vSim

vSim [125–141], developed by Tech-X Corporation in the United States, is a three-dimensional multiphysics simulation software, with its earlier version known as VORPAL. The software is widely applied in the analysis of physical processes such as plasma acceleration and plasma discharges. It is also employed to solve electromagnetic and electrostatic problems in complex dielectric and metallic structures, to compute the radiation characteristics and eigenmodes of rf components and microwave vacuum devices, and to evaluate multipacting effects over a range of input powers. The following sections provide a more detailed overview of its capabilities.

1. Visual setup

vSim provides a hierarchical graphical modeling interface, Visual Setup [126], supporting Boolean geometry construction and interactive entity selection. It imports CAD models in STEP, STL, POLY, and VTK formats, and employs a no-time-counter approach for efficient, time-independent modeling. Material properties, including user-defined parameters, can be assigned to individual geometries. The grid resolution and absorber thickness are adjustable according to the material wavelength, and electromagnetic sources can be configured in both space and time to analyze specific modes or frequency bands. During model assembly, the geometry, particle sources, and current sources are rendered in real time, enabling intuitive inspection and verification of the simulation configuration.

For curved regions of devices, vSim approximates surfaces using trapezoidal or triangular elements to improve geometric accuracy. The electromagnetic and particle emission models employ the Dey-Mitra cutting-cell technique to support field computations on complex boundaries, enhancing the precision of electromagnetic simulations in curved or intricate configurations. Both metallic and dielectric structures can incorporate complex shapes, and in particle emission models, the cutting-cell method improves the accuracy of particle velocity and flux. These capabilities enable full-3D, full-physics simulations of practical engineering structures.

2. Numerical algorithms and parallel computing

vSim integrates several numerical approaches, including the FDTD, PIC, finite-volume, and DSMC methods. Interactions among plasma particles and with their

surroundings are governed by the Maxwell equations or the electrostatic Poisson equation, while macroparticle dynamics are tracked through relativistic equations of motion. The collision framework incorporates both the conventional null-collision model and alternative unbiased and empty-selection schemes that efficiently sample all simulated particles. Supported processes include elastic scattering, excitation, ionization, and recombination, as well as multiple ionization in electron-ion collisions, field-induced ionization, and the decay of unstable species. With the Tech-X cut-cell algorithm, high numerical precision is achieved without additional computational cost. Operating as a time-domain solver, vSim performs full-wave analysis, extracting broadband frequency responses and transient behavior within a single simulation run.

vSim provides scalable parallel computing, allowing large-scale problems to be solved efficiently on computing clusters and supercomputers. Optimized algorithms for high-performance systems enable rapid execution, supporting the design and analysis of devices with volumes reaching several million cubic wavelengths.

3. Electromagnetic field models

vSim is built upon the MultiField framework, which serves as the foundation for field modeling and allows selection among various electromagnetic field representations. Standard options include electromagnetic modeling on a Yee grid and electrostatic modeling based on the Poisson equation. The integrated Maxwell and Poisson solvers support simulations of laser, microwave, rf, and dc devices, capturing complex dielectric, magnetic, and conductive behavior. Within the framework, users can modify and extend field models by defining custom finite-difference schemes and time-stepping methods, incorporating dispersion models, and, in multiphysics simulations, coupling additional fields such as thermal or flow fields to the electromagnetic fields. A flexible combination of solvers is available, with linear equation solvers that permit low-level reconstruction of solver operations and customization of boundary conditions, field distributions, and particle densities.

4. Data analysis and postprocessing

vSim provides a comprehensive suite of postprocessing and data analysis tools that enable detailed examination of simulation outcomes, including extraction of frequencies and modes, S-parameter evaluation, data binning, particle density assessment, and far-field computations. Preconfigured analysis modules allow users to extend the software with custom routines and visualize new results. The platform also supports advanced parallel three-dimensional visualization, where field distributions, particle trajectories, and surface meshes can be displayed together, with full control over rotation, scaling, translation, and slicing. Temporal evolution of quantities such as particle counts, currents, far-field

components, and voltage can be monitored dynamically throughout the simulation.

5. Software architecture

VSim consists of three principal software packages—VSimEM, VSimVE, and VSimPlasma—and incorporates four primary modules: VSimEM, VSimMD, VSimPA, and VSimPD [125]. The platform accommodates one-, two-, and three-dimensional simulations, allowing researchers to combine packages to create customized simulation environments. For instance, VSimEM can compute the rf field distribution and resonant frequencies within a klystron cavity, while VSimMD can simulate beam-wave interactions in the device. Figure 14 presents the overall software architecture and illustrates the functions of each module.

6. Module functions of VSim

VSimEM module. VSimEM [127] is an optimized FDTD solver for electromagnetic and electrostatic simulations in complex dielectric and metallic environments. Curved geometries are represented with second-order accurate algorithms, and advanced graphical features allow detailed visualization of field distributions. The solver supports large-scale devices with billions of grid cells and provides precise far-field computations. Applications include phased array antenna systems, radar devices, photonics, propagation modeling of high-power antennas in plasma environments, photonic crystals, and other optical components, as well as analysis of field distributions, dispersion properties, and resonant modes in rf circuits of vacuum electronic devices.

The solver accommodates diverse material properties, including lossless and lossy media, nonlinear and anisotropic materials, second-order dispersion, and frequency-dependent behavior. Field excitations can be specified through mode calculations, discrete elements, surface ports, plane waves with elliptical polarization, scattering inputs, or waveguide ports. Supported boundary conditions encompass embedded boundaries, port boundaries, periodic and

phase-shift constraints, the Dey-Mitra cut-cell method, and PML or MAL absorbing layers.

VSimEM offers advanced data analysis for far-field computations using the Kirchhoff method, evaluation of radiation fields, S-parameters, and frequency-based mode extraction. Additional capabilities include specific absorption rate assessment, modeling of linear plasma media, and parameterized geometric optimization.

VSimVE module. VSimVE [128] corresponds to the VSimMD module, an optimized particle dynamics solver integrating comprehensive electromagnetic field and particle modeling capabilities. It enables simulations of rf and microwave devices as well as vacuum electronic devices, including electron guns and collectors in electron-optical systems, and beam-wave interactions in amplifiers such as klystrons, magnetrons, and traveling-wave tubes.

Primary particle emission includes Child-Langmuir space-charge-limited emission, Fowler-Nordheim and Richardson-Dushman mechanisms, and user-defined models, while secondary emission can be treated with preconfigured SEY models or custom implementations. High-performance computing-optimized algorithms and field-scaled particles permit simulation of multipacting effects at multiple power levels within a single run. VSimMD provides diagnostic parameters such as quality factors, geometric factors, operating modes, power, electron trajectories, voltage, phase space, and current, supported by advanced postprocessing and visualization for detailed analysis of particle distributions and cross-sectional data.

Three-dimensional modeling allows partially transparent absorbers, and particle properties include surface emission, electron-induced emission, controlled emission, field scaling, space-charge limitation, thermionic emission, secondary emission, dynamic particle weights, and particle consumption. Signal excitations are implemented through total-field/scattered-field sources, current sources, circuit equations, and Cherenkov noise filtering, while boundary conditions include absorbing and reflecting boundaries, resistive wall losses, and PML or MAL layers. Field and radiation functionalities include field emission, Fowler-Nordheim emission, laser-induced emission, specified emission, static magnetic field analysis and import, and feedback control.

Integration with VSimEM adds far-field diagnostics and second-order accurate material models, whereas coupling with VSimPD extends capabilities to additional plasma reactions and beam-material interactions. Figure 15 illustrates the simulated spectrum of a THz miniature klystron amplifier, with successful cavity excitation at the fundamental mode of 354 GHz and the third harmonic at 657 GHz. VORPAL, the predecessor of VSim, functioned as the simulation engine for modeling vacuum electronic devices.

VSimPlasma module. VSimPlasma is a powerful PIC software that incorporates the VSimPA and VSimPD modules and

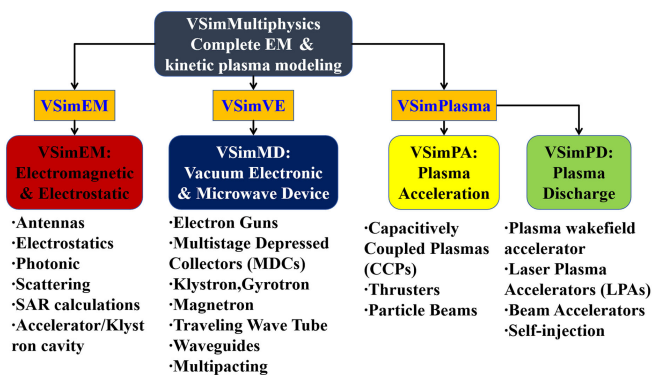


FIG. 14. Software architecture and module functionality of VSim.

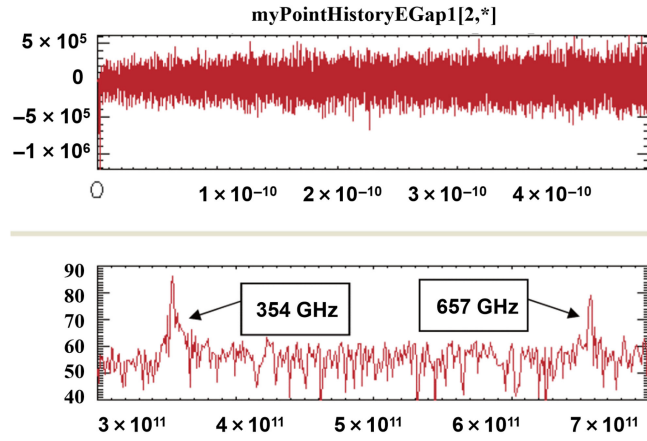


FIG. 15. Spectrum of the proposed THz klystron cavity obtained from VORPAL simulations. The cavity is successfully excited at the fundamental mode of 354 GHz and the third mode of 657 GHz [139]. VORPAL, the predecessor of VSim, functioned as the simulation engine for modeling vacuum electronic devices.

allows import of CAD and GDSII files. It features a comprehensive set of plasma chemical reactions, including DSMC and MCC techniques, and is specifically tailored for plasma simulations. The software accurately resolves the dynamics of electrons, ions, and neutral particles in gases across a wide range of pressures, capturing elastic, excitation, and ionization collisions. The combination of the cut-cell algorithm with the integrated FDTD-PIC framework enables efficient and high-precision modeling of complex, multidimensional plasma discharges. An extensive set of particle reactions is available within the module, as summarized in Table II. In Table II, *A*, *B*, *C*, and *D* generally represent atoms, ions, or neutral molecules, while

TABLE II. Particle reactions available in VSimPlasma packages.

Particle reaction	Expression
Binary (in)elastic	$A + B \rightarrow A + B$
Electron scatter	$e + A \rightarrow e + A$
Binary excitation	$A + B \rightarrow A^* + B$
Charge exchange	$A^+ + B \rightarrow A + B^+$
Binary reaction	$A + B \rightarrow C + D$
Electron attachment	$e + A \rightarrow A^-$
Negative ion detachment	$A^- + B \rightarrow A + B + e$
Impact ionization	$A + B \rightarrow A + B^+ + e$
Electron ionization	$A + e \rightarrow A^+ + 2e$
Dissociative ionization	$AB + e \rightarrow A^+ + B + 2e$ $AB + e \rightarrow A^+ + B^+ + 3e$
Field ionization	$A + E \rightarrow A^+ + e$
Decay	$A \rightarrow B + \gamma$ $A \rightarrow B$
Binary recombination	$A^+ + e \rightarrow A$
Three body recombination	$A^+ + e \rightarrow A + 2e$
Dissociative recombination	$AB^+ + e \rightarrow A + B$
Electron impact dissociation	$AB + e \rightarrow A + B + e$

AB denotes a molecule or a composite particle. Symbols with an asterisk, such as A^* or B^* , indicate excited-state particles. The symbol e refers to an electron. γ denotes a photon or radiative particle, and E represents an externally applied electric field. The arrow “ $\rightarrow$ ” indicates the reaction direction, describing the transformation from reactants to products.

VSimPA [129] is an integrated software solution developed for plasma acceleration simulations. It models interactions between laser pulses, relativistic electron beams, and complex plasma environments, including field ionization processes, and supports advanced acceleration studies such as ionization injection, colliding pulse injection, and down-ramp injection through numerical experiments. The software enables laser wakefield acceleration simulations using simplified approaches, including envelope approximations with optional phase tracking, avoiding full resolution of the laser wavelength while controlled dispersion algorithms minimize numerical artifacts.

Particle features in VSimPA include charged and neutral particles, variable weights, relativistic and higher-order particles, surface charges, and secondary emission. Boundary conditions cover absorption, collisions, field ionization, matched absorbing layers, and noise filtering, whereas field and fluid properties include cold and relativistic fluids, Eulerian fluids, and static background gases.

VSimPD [130] is a specialized module for plasma discharge simulations, capable of accurately tracking particle dynamics in gases at arbitrary pressures. Particle boundary conditions include absorption, reflection, periodic constraints, surface charge accumulation, and partial transparency, with particle properties largely consistent with those in VSimMD. Field and fluid features encompass conductive and dielectric boundaries, charge and current deposition, Eulerian fluids, and static background gases. The module supports advanced meshing and visualization, including the Dey-Mitra cut-cell method, spatially varying grids, and multidimensional configurations.

D. NEPTUNE

NEPTUNE [91–93] is a particle simulation software developed at the U.S. NRL. It adopts a time-domain simulation approach based on spatial discretization over a Cartesian structured mesh. User simulations are defined and executed through the high-level scripting language Lua, which is also deeply integrated into NEPTUNE’s internal architecture to handle simulation setup, parameter management, and core time-domain loop control. The core numerical algorithms and data structures are implemented in C++, with multicore parallelism supported by Intel’s Threading Building Blocks library and many-core acceleration enabled via NVIDIA’s CUDA framework. This hybrid parallel architecture ensures high computational efficiency and scalability across heterogeneous computing platforms.

1. Electromagnetic time-domain solver

NEPTUNE solves Maxwell's equations on nonuniform Cartesian meshes using the Finite Integration Technique (FIT). Its key EM solver features include: efficient computation of the discrete "curl" operator on GPUs via kernel functions; integration of material distribution and local geometric properties into material matrices, allowing conformal modeling of metal-dielectric interfaces and user-defined frequency-dependent material responses through simple modifications of matrix elements; implicit geometric modeling using combinations of basic primitives to represent complex structures; and spatial discretization of geometry and fields on a three-dimensional nonuniform Cartesian mesh.

EM model. The FIT method achieves second-order convergence within the simulation domain but requires conformal treatments at material interfaces not aligned with the grid. NEPTUNE employs Zagorodnov's Simplified Conformal method with modified edge-field correction constraints to improve accuracy while maintaining the diagonal structure of the material matrix, ensuring computational efficiency on GPUs. Additionally, NEPTUNE implements a Conformal Surface Impedance Boundary Condition to model frequency-dependent surface losses and introduces a dedicated digital filter to approximate the $f^{0.5}$ behavior over wide bandwidths.

Boundary conditions. Within a finite simulation domain, the outer boundaries can be assigned specific local or global boundary conditions to enhance the physical fidelity of the model. The natural boundary conditions at the grid edges are typically implemented as perfect electric conductor or perfect magnetic conductor boundaries, which can also serve to define symmetry planes in the geometry. By exploiting these field symmetries, it is often sufficient to simulate only a portion of the computational domain in the time domain, while the full field distribution can be accurately reconstructed through symmetric extension, thereby reducing computational cost without compromising accuracy.

NEPTUNE implements three principal types of boundary condition models. The fixed-impedance boundary condition is applied to coaxial waveguide ports. Since the characteristic impedance of the transverse electromagnetic (TEM) mode is frequency-independent, enforcing a matched discrete surface impedance at the boundary allows nearly perfect absorption of outward-propagating TEM waves. Furthermore, by prescribing appropriately matched time-varying surface current distributions, this boundary condition can also be used to inject external dc or rf excitations into the simulation, providing a versatile framework for both wave absorption and excitation.

The second-order absorbing boundary condition is applied to transverse electric waveguide modes, whose characteristic impedance varies with the effective propagation angle inside the guide. Structurally similar to a fixed-impedance boundary, this method incorporates a digital

filtering scheme into the normal magnetic field response to achieve improved impedance matching over a wider angular spectrum. As a result, it significantly enhances the absorption efficiency of outgoing waves and reduces numerical reflections within the computational domain.

Finally, the PML technique is commonly used for waveguide port implementation. It provides nearly complete numerical absorption of incident waves with arbitrary characteristic impedances and is considered the standard approach for open-boundary electromagnetic simulations.

2. Electromagnetic particle-in-cell (EM-PIC) solver

The EM-PIC module in NEPTUNE builds upon the broadband, linear EM response captured by FIT-based time-domain modeling. In the PIC algorithm, electron motion is represented by weighted macroparticles, whose relativistic equations of motion are integrated using the Boris pusher. The Lorentz force is evaluated from the discretized EM fields to generate source currents that drive Maxwell's equations. Particle positions, momenta, and weights are stored in separate arrays, and both momentum updates and particle pushes are parallelized within a single GPU kernel. A charge-conserving current deposition scheme ensures strict compliance with Gauss's law throughout the simulation.

High-current electron beams. For simulations involving high-current beams in vacuum electronic devices, numerical dispersion and spurious numerical Cherenkov radiation may occur, leading to high-frequency oscillations. NEPTUNE mitigates this effect using the Friedman filter, which is enabled by default in particle simulations.

Particle injection. NEPTUNE offers multiple particle injection schemes. The simplest involves planar emission with user-defined beam profiles and temporal variations in voltage and current specified via Lua functions. Beam data can also be imported from MICHELLE, supporting both steady-state and time-domain formats. For space-charge-limited emission from conformal metallic cathodes, NEPTUNE provides an embedded emission model enabling self-consistent, end-to-end simulations of devices including the electron gun and collector.

Diagnostics and data interfaces. The EM-PIC module provides a suite of diagnostics for extracting relevant quantities such as voltage, power flow, energy, and intercepted current from raw data. Time-dependent diagnostics are buffered and streamed from GPU to CPU for processing without significantly affecting runtime. NEPTUNE and MICHELLE share common file formats for external magnetic field import and particle data I/O. Magnetic field data from static solvers (e.g., ANSYS/Maxwell or Analyst-MP) can be imported onto uniform Cartesian grids or mapped directly to beam mesh nodes. Particle data may be volumetric or surface-based, and can represent steady-state, cycle-averaged, or time-domain quantities.

E. CST

CST Studio Suite [94–103] is a high-performance three-dimensional electromagnetic simulation platform for the modeling, analysis, and optimization of EM components and systems. Its flagship solver, CST Microwave Studio, was originally developed by Computer Simulation Technology (CST) in Germany, and the company was later acquired by the French corporation Dassault Systèmes. The software is widely used in China’s vacuum electronics community, particularly for klystron design and related applications. It provides a unified environment that integrates a broad portfolio of EM field solvers spanning the full electromagnetic spectrum; these solvers can be coupled to support hybrid and multiphysics simulations.

Within CST Studio Suite, the particle dynamics simulator constitutes a complete computational module. Its time-domain electromagnetic PIC solver is capable of modeling beam-wave interactions in microwave vacuum electronic devices such as klystrons. This solver implements a versatile, self-consistent particle-tracking approach that simultaneously computes particle trajectories and electromagnetic fields in the time domain, while accurately accounting for space-charge effects and the mutual coupling between particles and fields. The key features of this solver are summarized below.

1. General and geometric modeling

CST provides advanced geometric modeling and meshing capabilities tailored to specific solvers. For example, the perfect boundary approximation technique is available for hexahedral meshes, while curved and higher-order elements are supported for tetrahedral meshes to improve geometric accuracy. The ACIS-based parametric solid modeling front end offers excellent visualization, and the feature-based hybrid modeler allows rapid modification of complex geometries. The software supports CAD data import and export in multiple formats, provides a comprehensive material database, and offers geometry templates to simplify model setup.

2. Particle-in-cell solver

Particle data. The PIC simulator supports arbitrary-shaped particle emission surfaces, circular particle sources with spatially nonuniform current distributions, and particle injection under open boundary conditions. It also supports volumetric particle sources with Maxwellian velocity distributions, as well as Gaussian, dc, field, and explosive emission models. Oblique emission is supported, and particle-tracking solvers can be coupled with the PIC solver via an interface. Emission data in ASCII format can be imported, active particle sources can be selectively enabled, and secondary electron emission induced by ions or electrons is supported.

Field data and thermal coupling. Static fields, eigenmode fields, and multiple external field distributions can be applied as additional source fields. Tetrahedral-format source field import is supported. The simulator includes automated breakdown detection for multipulse effects and provides thermal coupling capabilities, enabling the extraction of heat-loss distributions from collisional particle data.

Boundary conditions and pre-/post-processing. The PIC solver supports periodic boundary conditions for particles and is compatible with multi-GPU acceleration, single-node parallelization, and Linux batch processing. Physical quantities can be visualized in real time during simulation, and both time-domain and steady-state field distributions at selected frequencies can be computed. Diagnostic tools are available to monitor quantities such as particle position, momentum, output power, current density, and phase-space evolution. Solid and boundary particle monitors are provided to evaluate emission rates and particle transport.

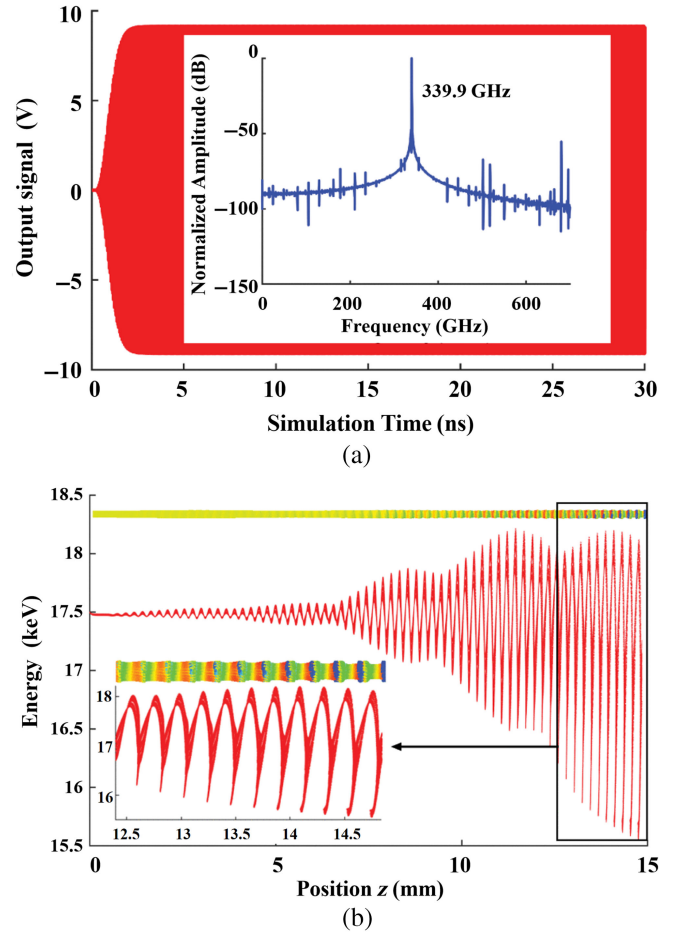


FIG. 16. Calculation results for the 0.34 THz klystron: (a) output signal and frequency spectrum. (b) Beam trajectories (top) and particle kinetic energy distribution (bottom) of the entire circuit. Inset: beam trajectories and particle kinetic energy distribution of the output cavity [101].

A built-in MCC module enables volumetric ionization modeling. Thin-film transparency to particles can be defined, and both isotropic and anisotropic material properties are supported. The software allows arbitrary-order frequency-dependent permittivity and permeability with parameter-fitting capability. Additional supported models include field-dependent microwave plasma, anisotropic gyrotropic media, nonlinear materials, surface impedance boundaries, frequency-dependent multilayer panels, and time-varying conductive materials. In the frequency domain, two-dimensional eigenmode solvers enable efficient port-mode computation, including higher-order modes at specified target frequencies. Automatic waveguide-port mesh adaptation and a customizable excitation-signal database further enhance simulation flexibility.

CST's PIC simulator also provides multiple boundary condition options, including charge-absorbing open boundaries, high-performance radiation/absorption boundaries, and conducting-wall boundaries. Electromagnetic quantities such as electric and magnetic fields, surface currents, and power flow can be computed in both time and frequency domains. Time-averaged power-loss and surface-loss monitors are available. The built-in optimizer enables automatic structure optimization for arbitrary objectives. The simulator supports transient co-simulation with CST Design Studio and thermal coupling with the CST Studio Suite thermal solver.

Figure 16 illustrates CST simulation results for a 0.34 THz extended-interaction klystron (EIK), showing the time-domain and frequency-domain output power, phase-space distribution, and particle bunching behavior.

V. CONCLUSIONS

This review summarizes the large-signal beam-wave interaction solvers widely employed in klystron design and development in mainland China, along with several internationally recognized simulation codes, spanning solver dimensions from one-dimensional to fully three-dimensional. In contemporary solvers, the eigenmode rf fields of klystron cavities are typically obtained from numerical distributions computed via EM solvers, enabling accurate modeling across diverse structural and operational scenarios. Parameterized beam-wave interaction codes, while maintaining computational efficiency, place a strong emphasis on the physical completeness of the models to improve large-signal simulation fidelity. Such capabilities support the study of axial space-charge fluctuations induced by slow or reflected electrons, the generation and suppression of self-oscillations in output cavities, and end-to-end simulation from the electron gun through the interaction circuit to the collector.

Fully three-dimensional PIC solvers inherently support full-field electrodynamic simulations of asymmetric structures without relying on extensive physical assumptions. Research efforts for these solvers are primarily focused on parallel acceleration, particle collision modeling, boundary-

condition implementation, and grid-generation strategies. Emphasis is placed on enhancing computational efficiency, ensuring code portability, and assessing the influence of mesh and boundary conditions on numerical accuracy. As computing advances toward exascale capability, the high-performance deployment of 3D PIC solvers will inevitably rely on heterogeneous computing architectures.

Verification and validation remain essential throughout the software development process. The integration of predictive maturity models, analytical benchmarks, third-party code comparisons, and experimental design ensures software reliability and confidence. Looking forward, the ultimate goal in klystron beam-wave interaction simulation remains the achievement of “single-run success.” Both parameterized beam-wave interaction codes and full 3D PIC solvers offer significant opportunities for further research in model completeness, algorithmic optimization, and engineering validation.

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DATA AVAILABILITY

The data are not publicly available. The data are available from the authors upon reasonable request.

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