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IEEE Transactions on Nuclear Science, Vol. NS-32, No. 5, October 1985

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# NUMERICAL SIMULATION OF HIGH POWER MICROWAVE SOURCES\*

A.T. Drobot, C-L Chang, K. Ko, A. Mankofsky, A. Mondelli, L. Seftor, and P. Vitello

Science Applications International Corporation 1710 Goodridge Drive McLean, Virginia 22102

### Introduction

Electromagnetic fully relativistic particle-in-cell codes are a powerful tool for modeling and designing components of high power microwave sources and accelerator systems. This paper reviews the principles and properties of numerical simulation codes as applied to problems of microwave generation. The important aspects which can be treated with such codes are, improved representation of microwave circuits in complicated geometries, proper treatment of nonlinear particle wave interaction in the body of a device, inclusion of self-consistent self-field effects, and treatment of surface properties such as emission, secondary particles, and surface breakdown. Examples of application of two- and three-dimensional codes to specific devices such as gyrotrons, magnetrons, and klystrons is presented. The information obtained from large numerical simulation codes provides both detailed insight into source physics as well as the basis for improved design technology.

A numerical simulation is in many respects analogous to a laboratory experiment. For even the simplest of devices there is a large number of parameters that may be varied but the practical number of simulations which can be performed is limited and the original design must in some sense be approximately correct. This is usually accomplished by either extrapolation from existing designs or theoretical analysis. In the exploration of an initial design a numerical simulation has several advantages over an experiment. The diagnostics available are comprehensive, nondestructive, direct, and can provide detailed microscopic view of the physical processes which could at best be inferred experimentally. Additionally, the cost associated with changing parameters in a code, such as the shape of a cavity in a circuit structure, is negligible and can be performed rapidly when contrasted with the same situation in an experiment.

There are of course disadvantages with using simulations as a primary tool in the design process. The most obvious are constraints on numerical techniques and the consequences for accuracy and resolution in approaching "real world" problems. Less obvious, and perhaps more dangerous, is the question of completeness. By this we mean missing physics which precludes successful simulation of a particular problem. This necessitates a choice of architecture for the numerical software which permits addition of new physics packages and allows for ease of code maintenance. Finally, to be successful, the process of code construction should be coupled to systematic code validation against experimental data.

During the last decade a number of two- and three-dimensional codes have been constructed and have proceeded in an evolutionary fashion to improve the quality and sophistication of microwave device simulation. These codes include: CCUBE and IVORY built by Brendan Godfrey of MRC; MAGIC and SOS constructed by Bruce Goplen of MRC; MASK and ARGUS which were built at SAIC. The two dimensional versions (CCUBE, MAGIC, and MASK) have been used extensively and there is a considerable base of experience which includes many successful results. The increase in the speed and availability of large computers for performing numerical simulations now makes it possible to contemplate the use of three-dimensional simulation codes (IVORY, SOS, and ARGUS) on a routine basis. Expected imnprovements in algorithms and multiprocessor systems may bring the costs associated with large simulations down to the point where they are a commonplace design tool.

In writing this paper we have not attempted to review what others have done in the short space allotted but have instead concentrated on the work we have been involved in during the last few years. A description of simulation codes and their underlying basis is presented in the following section and is followed by a number of examples and a brief discussion.

### Numerical Simulation Techniques

The traditional modeling of microwave devices has been done with codes of reduced dimensionality or approximate physics. In many situations this is highly appropriate and effective. For microwave tubes where the electron beam is tenous it is often sufficient to perform particle orbit calculations in electromagnetic fields which are prescribed determined by the geometry of the device. As the beam strength increases the interaction may modify the frequency of the device and a.c. field pattern. This kind of calculation can usually be done with weak perturbation theory. At higher beam strengths self-field effects become important and are included either through the single wave approximation or the introduction of some affected parameter in modeling the circuit response. For high power devices, however, these kind of approximations fail because phenomena in the body of a tube may include strong self field effects, multiple waves, and a multitude of nonlinear processes which are not obviously approximated.

The Plasma Physics community has produced a number of what are called particle-in-cell codes which model electron and ion dynamics using relativistic equations of motion coupled to self consistent description of static or electromagnetic fields (1-5). The remarkable feature of these codes is that they have permitted the users to model problems which are intractable analytically, highly nonlinear, and for which it is difficult to determine the importance of physical processes experimentally. To begin with the codes modeled simple geometries and simple processes. Over time the sophistication and numerical fidelity of the codes has improved considerably so that complicated geometries, chemistry, particle interaction with surrounding structures and emission processes can be modeled. We have been involved in the construction of two codes MASK (6) and ARGUS (7) and will describe the components of these codes and the philosophy behind them. The first of these MASK, is a two-dimensional model designed for initial value problems. The second is a three-dimensional model that is really a collection of codes with a common architecture and is intended as a general purposes package.

The first ingredient of both MASK and ARGUS is particle integration which in a discrete form treats particle orbits. The equations are

$$\frac{d\underline{U}}{dt} = \frac{q}{m} \left( \underline{E} + \underline{V} \times \underline{B} \right) - \left( \nu \, \underline{U} + \underline{\Theta} \times \underline{V} \right) \tag{1}$$

$$\frac{dx}{dt} = \underline{V}$$
(2)

where <u>x</u> is the particle position,  $\underline{U} = \gamma \underline{V}$ .  $\gamma$  is the relativistic factor. v is a stopping factor for interaction with materials, and  $\theta$  corresponds to elastic scattering. The terms for the field quantities are interpolated from a mesh to particle positions to get an accurate representation of forces affecting the particle dynamics. A typical mesh is shown in Figure 1 for the two-dimensional case. The interparticle forces in this kind of model are determined from a global solution of the field equations using averaged particle quantities such as currents or charge density as sources. The particle contributions to the source terms are in turn determined by the location of particles relative to nearby mesh points through an inverse interpolation scheme. The set of equations for the fields can consist of the static solution of Poisson's Equation

## **Field Mesh**



Fig. 1 Typical nonuniform field mesh used in two-dimensional simulation code.

$$\nabla \cdot \mathbf{E} = \rho/\epsilon \tag{3}$$

$$\nabla \mathbf{x} \mathbf{B} = \mu \mathbf{J} \tag{4}$$

on the discrete grid. For the electromagnetic case the full set of Maxwell's equations is solved in discrete form

$$\frac{\partial \underline{B}}{\partial t} = - \underline{\nabla} \times \underline{E}$$
 (5)

$$\frac{\partial \mathbf{D}}{\partial \mathbf{t}} = \nabla \mathbf{x} \mathbf{H} - \mathbf{J} - \sigma \mathbf{E} \qquad (6)$$

where  $\underline{B} = \mu \underline{H}$ ,  $\underline{D} = \epsilon E$ , and  $\sigma$  is the background conductivity.

The simulation codes can operate in two distinct modes as depicted in Figures 2 and 3. For the static case particles (electrons or ions) are launched into a known geometric configuration with an approximate field solution. While the orbits are integrated for test particles their contribution to the current and charge density is calculated, this contribution is used as a source in the field calculation which now contains self-fields. This process is repeated until a convergence criteria is met. The assumption here is that a steady state exists. This method has been successfully used for gun design, beam transport, and electrostatic acceleration. The major new improvement has been the ability to efficiently handle three-dimensional situations as with the ARGUS code.



Fig. 2 Flow of calculation for a static simulation assuming steady state flow.

For the dynamic case self consistency is imposed by the choice of a sufficiently small time step. For a typical large problem tens of thousands of particle orbits are advanced forward in time by a step using the interpolated fields from the previous step. The new source terms are found, the field equations are also advanced by a timestep and the cycle is repeated again leading to a self-consistent dynamical evolution of the system as depicted in Fig. 3.



Fig. 3 Flow of calculation for dynamic simulation of an initial value problem.

The particle "pusher" and field solvers in these two codes really account for a small fraction of code written, probably less than 10%. The bulk of the coding is actually concerned with:

- o input of problem definition
- diagnostics of various kinds
- o graphics
- system calls
- o data handling
- auxiliary physics packages.

The auxiliary packages contain information on particle creating, by emission, injection, production of secondaries and ionization. They also deal with superposition and interaction with external fields due to coils, charged surfaces, and cavities not in Treatment of particle the simulation region. backscattering from walls, finite conductivity of surrounding materials, and resistivity of background gas is included. Problems involving ionization or chemistry, as in gas switches for example, are considered.

In transitioning from two to three-dimensional codes the emphasis on understanding of computer science becomes much more important. The volume of data increases dramatically and it is difficult to fit problems in the main memory of even large computers such as a CRAY with 2-4 million words available. A large part of ARGUS, accordingly, is devoted to efficient I/O transfer of data on and off the disc. Problem size then becomes limited by budget and disc space available. Because one cannot expect every user to become computer scientists, great care has been taken to make this activity transparent to the user who interfaces with the code through simple input procedures.

# Examples

The MASK and ARGUS codes have been tried on over 50 different problems. These have included microwave devices, diodes, beam-plasma interaction, wave propagation, and simulation of nonlinear diagnostic instruments. We have selected a number of applications to illustrate the utility of these codes for microwave device design. The first set of problems considered is just the calculation of circuit parameter in a given geometry. The understanding of electromagnetic wave properties for complicated circuits usually consumes a tremendous amount of time theoretically, numerically, and experimentally because the first two approaches are considered inaccurate and unreliable. Without particle dynamics the electromagnetic codes described in this paper can perform circuit parameter calculations exceedingly well and cost effectively. The geometry and boundary conditions for a given circuit are defined. A point disturbance is initiated in one of the field components and allowed to propagate through the circuit. By saving data at other test locations and fourier analyzing it in time the eigenfrequencies of a circuit can be found. This is true because the initial disturbance is formally a δ function in space and time and consists of all the eigenfunctions in the structure. By examining the spectrum and then driving antennas at the resonant frequency the mode patterns can be determined. An example of this is shown in Fig. 4. The figure shows the frequency spectrum from a numerical cold test of a folded waveguide with a beam hole. The calculation was performed with ARGUS and compared well to experimental data for the same structure. The figure also shows the mode pattern for the magnetic field projected on the midsection of the structure. This is a fully three dimensional case for which there is no comparable method for determining its properties in



Fig. 4 Spectral analysis of cold testing and driver mode pattern for a folded waveguide with a driftspace.

In a similar study we examined the such detail. elimination of competing modes in a gyrotron cavity by the introduction of lateral slits. The MASK code was used to determine the shifts in the frequency spectrum as a function of slit size and the Q's of the unwanted modes. The desired pattern for the TE<sub>11</sub> mode are shown in Fig. 5. The mode patterns were found by excitation at the resonant frequency.





Fig. 5 The electric field pattern and contours of magnetic field for a  $TE_{11}$  mode in a slit cavity.

A second example is the application of the MASK code to the modeling of the SLAC klystrons with the goal of developing designs at 2.85 GHz with powers as high as 150 MW. This study resulted in many modifications to the code. The appropriate timescale for running the simulations is determined by transit times through a structure at the speed of light. This is a transient timescale when compared to the 1-5  $\mu sec$ pulse length in a klystron. To obtain steady state operating conditions it was necessary to find an iteration scheme for the phase and amplitude of the voltages at the cavity entrances (8). This allowed the simulation of a steady state. An example from simulation is shown in Fig. 6 which shows the phase space and particle map from a successful run. The code has produced results comprable to those found experimentally showing efficiencies of ~50% and correct gain characteristics.



Fig. 6 The phase space of axial velocity vs. axial position in five cavity klystron and the projection of selected particles on the (R,Z) at a given point in time. (courtesy K. Epply SLAC)

High power gyroklystrons are currently being considered as possible sources for higher frequency accelerators. In modeling these it usually suffices to deal with TE modes only. At the higher powers however self-space charge effects become important and the selection of mode and beam parameters is restricted by limiting current considerations. We are currently investigating these effects in a study to design a 300MW gyroklystron with efficiency exceeding 50%. The contours in Fig. 7 show the self fields from a 200 Amp, 500 V beam which will be used in a preliminary 30MW experiment at the University of Maryland. We have found that in this case the self space charge effects have negligible effect on device operation. The figure also shows the eigenmode pattern of the azimuthal electric field projected on the (R,Z) plane. The mode is quite strongly altered by the presence of the beam drift tube. This effect is important for calculation of start oscillation conditions.



CONTOURS OF  $\phi$  SELF POTENTIAL



CONTOURS OF E ELECTRIC FIELD

Fig. 7 Contour of self potential and of the dominant  $TE_{o1}$  mode from a four cavity gyroklystron simulation.

Finally, we have included the results from a cross field FEL simulation (9). In this case a large orbit beam circulates around the core of a coaxial cavity due to the presence of an axial magnetic field. A transverse wiggler field is used to induce an interaction. The results in Fig. 8 show that two wiggler periods in a  $120^{\circ}$  sector interact with the circulating beam yielding upshifted radiation at shorter wavelengths as in a FEL. The figure shows both the phase space and mode patterns when the instability that leads to radiation is in its linear phase.



Fig. 8 The phase space (theta momentum vs. angle) and field patterns from a cross-field free electron laser simulation. (courtesy Ruth Shefer MIT)

The examples shown in this section while not explored fully we hope convey the large variety of problems which are amenable to simulation techniques. Doubtlessly further improvements will need to be made to codes of this type but even at the present time they have the ability to effectively simulate what are extremely difficult interaction problems. Unlike previous models the simulations are self-consistent and include, complete wave dynamics, self electric and magnetic fields, dynamic nonharmonic wave generation, proper geometry, and effects of externally applied fields.

# Acknowledgments

We would like to thank Drs. Hannerfeld, Herrmansfeld, and Epply of SLAC, Drs. Yu and Nielsen of LLNL, and Dr. R. Shefer of MIT. Interaction with them has made much of the progress reported here possible. \*This work was partially supported by the Stanford Linear Accelerator Center under Contract 515-PS-167, Department of Energy under Contract Number DE-AS05-78ERO 5940 and Office of Naval Research under Contract Number N00014-82-C-0746.

# References

- [1] R.W. Hockney and J.W. Eastwood, in <u>Computer</u> <u>Simulation Using Particles</u>, McGraw-Hill, 1981.
- [2] A.B. Langdon and B.F. Lasinski, <u>Methods of</u> <u>Computational Physics</u>, Vol. 16, pp. d327-366, (John Killeen, ed.) Academic Press, 1976.
- [3] B. Adler and S. Fernbach, ed., <u>Methods in</u> <u>Computational Physics</u>, Vol. 9, Academic Press. 1970: articles by R.W. Hockney, pp. 136-212: R.L. Morse, pp. 213-240; and C.K. Birdsall, A.B. Langdon and H. Okuda, pp. 241-258.
- [4] J.P. Boris and R.A. Shanny, eds., "Proceedings 4th Conference on Numerical Simulation of Plasmas", Naval Research Laboratory, Washington, D.C., Nov. 2-3, 1970.
- [5] John M. Dawson, "Particle Simulations of Plasmas", Rev. Mod. Phys. <u>55</u>(2), 1983.
- [6] A. Palevsky and A.T. Drobot, "Application of Electromagnetic P.I.C. Codes to Microwave Devices", Proc. 9th Conf. on Numerical Simulation of Plasmas, Northwestern University, Evanston, IL June 30-July 2, 1980.
- [7] A. Mankofsky, L. Seftor, C.L. Chang, A. Mondelli, and A.T. Drobot, "ARGUS A General Three-Dimensional Plasma Simulation Model", Bull. Am. Phys. Soc. <u>28</u>(8). p. 1124, 1983.
- [8] Simon Yu, "Particle Simulation of High Power Klystrons", SLAC, AP Note 34, 1984.
- [9] F. Harteman, G. Bekefi, R. Shefer, "The Rippled-Field Magnetron (Cross-Field FEL)" MIT Rpt. PFC/JA-85-13, March 1985.