Predictive numerical simulation of microwave generation and plasma interactions requires resolution of multiple length and time scales in complex 3-dimensional geometries. The Particle-in-Cell (PIC) method for the numerical formulation of the basic governing equations is a well-understood and reliable approach if we are able to assume that short-range collisional effects are on average small. Particle collisions can be included in the PIC formulation through the use of Monte Carlo Collision models, and non-linear materials for which the permittivity depends on the strength of applied fields can be incorporated into the PIC formulation if proper attention is paid to issues of numerical stability of the expanded set of governing equations. Accurate modeling of time-dependent physics in complex geometries requires careful formulation of the numerical equations and the dynamic ability to evolve the image of a decomposed domain across thousands of computational cores.

Over the past two decades, the Directed Energy Directorate of the US Air Force Research Laboratory has developed the ICEPIC code\textsuperscript{1,2} to capture all necessary physics to enable predictive numerical simulation while taking advantage of high performance computing architectures to enable complex simulations to be performed in reasonably finite time. As it is our goal to perform virtual prototyping of compact, efficient microwave sources, we optimize complex designs by employing the Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) toolkit from Sandia National Laboratories. In this talk, we present the mathematical formulation of the design problem, and illustrate its strengths by showing recent designs for high-efficiency microwave sources. We will show parallel computing performance and optimized designs for both high peak power and high average power magnetrons.


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