# A Maximum Likelihood Method for Linking of Particle-in-Cell and Monte Carlo Simulations

Kevin J. Bowers, Barbara G. DeVolder, Thomas J. T. Kwan, and Lin Yin
*Applied Physics Division*
*Los Alamos National Laboratory*
*Los Alamos, NM 87545*

To support the design and analysis of x-ray radiographic facilities and experiments at Los Alamos, we have developed an integrated chain model, which is a set of linked physics simulation codes to generate self-consistent synthetic radiographs of experiments [1]. The expectation-maximization (EM) algorithm [2] has recently been used to great advantage to link particle-in-cell (PIC) methods, which model electron propagation to a converter target, and Monte Carlo transport methods, which model bremsstrahlung photon generation and transport through the radiographic object onto a detector. The EM algorithm is a maximum-likelihood technique to estimate the probability density function (PDF) of a set of measurements. A high performance implementation of the EM algorithm to characterize multidimensional data sets using a PDF parameterized as a Gaussian mixture has been developed (GMIX). The resulting PDFs compare favorably to histograms / tallies---no binning artifacts and less noisy (especially in the tails). GMIX is being used extensively in the radiographic chain model to quantify bremsstrahlung x-ray emission from rod-pinch diodes and other devices. In particular, the PIC simulation code MERLIN is used to model the dynamics of the rod-pinch diode in the Los Alamos radiographic machine Cygnus for the linked calculations. The rod-pinch diode used in Cygnus consists of a 9-mm diameter aperture cathode and a 0.75-mm diameter needle anode. A TEM pulse launched at one simulation boundary sets up the voltage required for the electron emission. The electron trajectories are followed self-consistently in the electromagnetic fields as the electron beam pinches at the anode tip with energies up to 2.25 MeV. The Monte Carlo transport code MCNP is used to track the bremsstrahlung photons generated by electrons incident on the anode tip. GMIX is used to "up-sample" the PIC electrons to provide a suitably large population for the Monte Carlo calculation ($10^7$ or greater) that would have been computationally expensive to generate directly.

The motivation, the mathematical properties, and the implementation details, and applications of GMIX to plasma and Monte Carlo simulations will be discussed, including: improved coupling of PIC to Monte Carlo simulations, adaptive PIC simulations, and characterization of the Cygnus radiographic parameters such as energy and angular spectra, spot size, and dose.

[1] T.J.T. Kwan, A.R. Mathews, P.J. Christenson, C.M. Snell, "Integrated System Simulation in X-ray Radiography," Computer Physics Communications, 142, 263-269 (2001).
[2] Dempster, Laird, and Rubin, "Maximum Likelihood from Incomplete Data via the EM Algorithm," J. R. Stat. Soc. B, 39, 1-38 (1977).