Accelerated Particle in Cell with Monte Carlo Collisions (PIC/MCC) simulation for gas discharge modeling in realistic geometries.

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In plasma physics Particle in Cell methods are among the few popular numerical schemes that are currently used to compute the properties of charged particle systems on the particle level. The adaptation of these algorithms to HPC infrastructure is of key importance in cases when realistic geometries are needed to be included, as those cannot be described by the most simple, numerically very efficient one-dimensional models. Massively parallel PIC simulations are already available for collision-less plasmas, where the particles interact only with the force fields. In most technological and laboratory gas discharges, however the collisions of the charged particles with the background gas molecules are of crucial importance both for sustainment of the discharge and the desired plasma applications. The stochastic Monte Carlo type description of these elementary collision events heavily builds on random choices and features a high degree of code branching, thus is difficult to implement efficiently on SIMD architecture. Recently we have developed a CUDA implementation of our 2D3V (2D in real-space and 3D in velocity-space) simulations for argon and neon gases in cylindrical and Cartesian coordinates for direct current and radio frequency excited low pressure gas discharges. The simulation includes our own implementation of the parallel random number generator, which is significantly faster than CURAND, scaled physical quantities to fit the single precision floating point data type, and a black-red successive over-relaxation iterative solver for the electric field. This new implementation on Pascal architecture does reach a speedup factor of 100 compared to our earlier MPI implementation executed on 24 cores of a Xeon SMP node. Besides the implementation details we present physical results for the PK-4 dusty plasma experiment that is currently in operation onboard the International Space Station (ISS).