Development of a Particle In Cell code with Structured Adaptive Mesh Refinement for Plasma Focus devices breakdown simulation

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Abstract

The aim at simulating the very early breakdown phase of a Plasma Focus (PF) discharge follows the need to fully understand the dynamics of such device, in order to retrieve useful informations for the design and optimization of the machine itself.

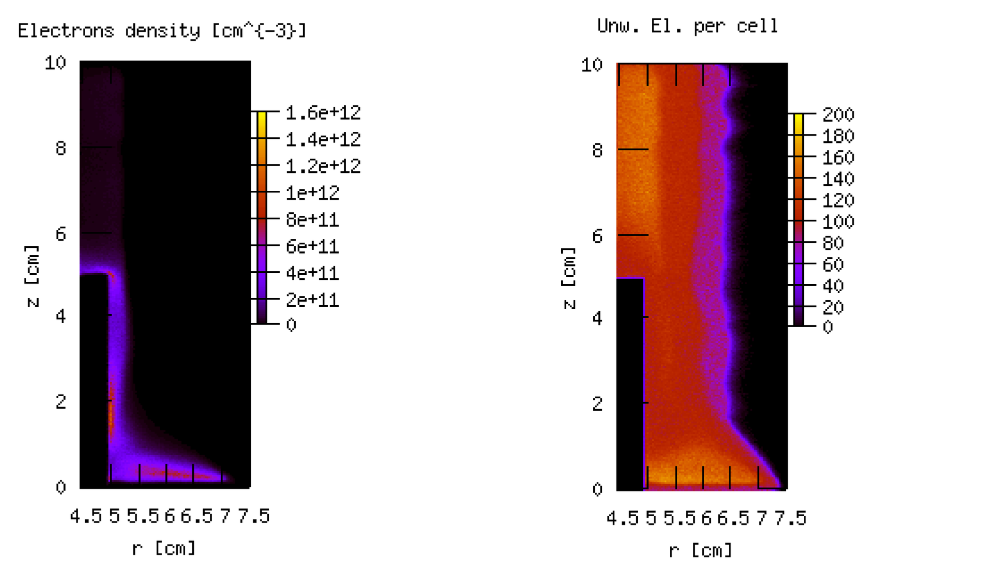
PFs are compact devices able to generate, accelerate, compress and confine a plasma by means of strongly varying electric and magnetic fields. In the final phase of the discharge, the generated plasma collapses in a high density region (the focus) where nuclear reactions occur. The choice of the gases composing the plasma tunes the nuclear reactions in order to characterize the device as a possible neutron free Short Life Radioisotopes (SLRs) generator for PET (f.i. F^{18} and O^{15}), as well as a neutrons or collimated electrons beams source for radio-therapy applications.

An electrostatic-collisional Particle In Cell (PIC) code (***es-c*PIF**) has already been developed to investigate the breakdown phenomenon and the formation of the plasma seed within the device: the exact knowledge of the phase space distribution function (strongly deviating from the Maxwellian equilibrium one) is a fundamental basis indeed for the whole discharge simulation. In order to extend the present simulations towards the complete evolution of the plasma seed into the running plasma sheath, the code is being re-structured for strong parallelization and inclusion of Structured Adaptive Mesh Refinement (SAMR) capabilities. In this poster the development frame as well as the software design architecture are presented together with the features that will be provided by the new **SAMR*es-c*PIF** code.

1 Introduction

The formation of a plasma within a PF device is due to the electric breakdown of the filling gas caused by the closure of a condensers bank over the two electrodes delimiting the reaction chamber of the device itself: as a matter of fact the high-collision condition leads to the avalanche ionization of the gas and the initial formation of a plasma seed.

The further evolution of the breakdown and its sustainment are then due to the action of Secondary Electrons Emission (SEE) phenomena from the boundary walls (both the electrodes and the dielectric insulating those latter), as the latest simulations performed with the existing ***es-c*PIF** code confirm.



The breakdown phase of a PF discharge is therefore an interesting matter of study both on a physical and a numerical point of view: the lack of an exact physical knowledge about the involved phenomena requires to turn to a microscopical analysis of the breakdown. The simulation of such a phenomenon results therefore in a High Performance Computing (HPC) task due to the huge number of microscopical particles to be studied in order to investigate the whole system behavior in the formation of the plasma sheath characterizing the discharge.

2 Development framework

The Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI) is a C++ framework designed to provide a self consistent environment to develop SAMR codes within. The framework architecture, achieved by means of deep patterns design, structures the tool as a general purpose host: a framework is indeed a "set of cooperating classes that make up a reusable design for a specific class of software" (E. Gamma *et al.*. *Design Patterns: elements of reusable Object-Oriented software*).

A pre-defined infrastructure (providing automatic methods for mesh generation, parallel data communication, time integration and problem solution) dictates the architecture of the application. Within the framework, it is possible to design the layout of the resulting code by choosing among the different multigrid generation techniques and integration schemes provided, and characterize then the most suitable architecture chosen with problem specific code.

2.1 Particles management

A first important extension of the framework has been achieved by developing the missing classes for particles management on the dynamically evolving multigrid. SAMRAI integrates indeed only grid-located data classes, which are automatically initialized on multilevel patches and communicated every time the grid hierarchy is redefined. Particles, however, cannot be described as grid-located data, since they may move upon the grid, as well as agglomerate or disperse locally. A new kind of variable has to be defined into the framework in order to represent all the dispersed data just slightly connected to the grid.

It is not possible either to describe particles as a simple array for each patch, since, on the other hand, a back trace to the belonging cell must be granted as it is required by the collisional module, by the charge to node deposition function (the shape function proper of PIC codes) and by optimization techniques already present in the ***es-c*PIF** code. Every grid cell must therefore reference the proper (whatever) set of particles belonging to the cell's domain.

By making use of indexed patch data classes, the new "particle" variable has been defined into the framework: such a kind of data cannot be univocally or regularly defined onto the multigrid hierarchy, nor easily managed for intra-processors communication by means of the existing grid-located data types. All the characterizing classes and communication instances have been therefore completely written from scratch to provide the flexible tool yet missing into the framework.

3 SAMR*es-c*PIF architecture

The development of the **SAMR*es-c*PIF** code within the SAMRAI framework requires the creation of a specific class implementing the application object, a main program summarizing the overall architecture, and all the physical methods modeling the phenomenon provided as external Fortran subroutines.

3.1 Code layout and features

The application class must define all data to be allocated on the grid hierarchy (field, charge density, particles), as well as the concrete implementations of the virtual methods for grid management and the interfaces to the external physical functions. It therefore characterizes the code by tailoring the whole framework to suite the problem of interest.

In particular, the **SAMR*es-c*PIF** application object will implement the methods for the dynamic refinement of the grid based upon the field source gradient detection: the exact knowledge of the self consistent field by means of a fine improvement of the solution is fundamental in order to simulate the local effect of charge separation onto the plasma dynamics.

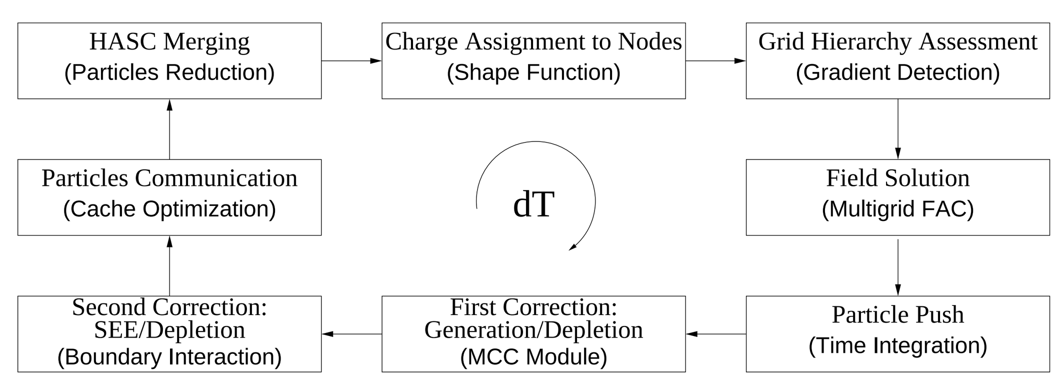
The massive parallelization of the code will allow an increase in simulation particles number, required by PIC methods for the statistical representativeness of the simulating system. The multilevel simulation domain will be decomposed in patches and distributed among the available processors together with the proper simulation particles belonging to. The concurrent solution on each patch and the separate particles management are the key features of the overall scheme: an accurate, efficient load balancing will at least grant the effective speed-up of the code, which will be monitored by means of integrated calls to the Tau profiler.

The numerical features of the present ***es-c*PIF** code, such as the Monte Carlo Collisional (MCC) module, the improved cache management or the simulation particles number control via the Hierarchical Agglomerative Sub-Clustering (HASC) merging, will be kept, extended to the 3D scheme.

The following table summarizes the **SAMR*es-c*PIF** code features.

	***es-c*PIF**	**SAMR*es-c*PIF** (expected)
model	$2\frac{1}{2}$D	3D
grid	static	SAMR
solver	SOR	multigrid FAC
simulation particles	10 M	(several G)
breakdown time simulated	32 ns	(200 ns)
simulation time	12 h	(24 h)
MCC	yes	yes
SEE models	1-2D	3D
HASC merging	$2\frac{1}{2}$D	3D
cache optimization	yes	yes
integrated profiler	no	yes

3.2 General Scheme



4 Conclusions

The **SAMR*es-c*PIF** code under development will represent the most advanced PIC code for electrical breakdown study: by exploiting the SAMR technique for the dynamical refinement of the field solution, a full 3D geometrical description will be possible. The strong parallelization will furthermore grant the capability of simulating billions particles when run on suitable HPC clusters.

Such a powerful tool, applied to the simulation of the PF breakdown, will allow to push the simulation towards the full plasma sheath formation and the closure of the electrical circuit. The 3D model will also allow the authors to investigate the mechanism of regular (modal) filamentation of the plasma sheath, experimentally observed but not yet well understood.