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Progress in the Study of Mesh Refinement for Particle-In-Cell Plasma Simulations and its application to Heavy Ion Fusion

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Abstract. The numerical simulation of the driving beams in a heavy ion fusion power plant is a challenging task, and, despite rapid progress in computer power, one must consider the use of the most advanced numerical techniques. One of the difficulties of these simulations resides in the disparity of scales in time and in space which must be resolved. When these disparities are in distinctive zones of the simulation region, a method which has proven to be effective in other areas (e.g. fluid dynamics simulations) is the Adaptive-Mesh-Refinement (AMR) technique. We follow in this article the progress accomplished in the last few months in the merging of the AMR technique with Particle-In-Cell (PIC) method. This includes a detailed modeling of the Lampel-Tiefenback solution for the one-dimensional diode using novel techniques to suppress undesirable numerical oscillations and an AMR patch to follow the head of the particle distribution. We also report new results concerning the modeling of ion sources using the axisymmetric WARPRZ-AMR prototype showing the utility of an AMR patch resolving the emitter vicinity and the beam edge.

1. Introduction

The numerical simulations of the beam ions transport in a Heavy Ion Fusion [1] accelerator and reaction chamber currrently model different stages of the process separately. A completely self-consistent simulation, which is ultimately needed, requires an end-to-end simulation from the ion source to the fusion target. This represents a real challenge even extrapolating near-future computer power from current state and past progress and we must consider the use of the most advanced numerical techniques. One of the difficulties of these simulations resides in the disparity of scales in time and in space which must be resolved. When these disparities are in distinctive zones of the simulation region, a method which has proven to be effective in other areas (e.g. fluid dynamics simulations) is the Adaptive-Mesh-Refinement (AMR) technique. We have begun at LBNL the exploration of introducing this technique into the method that we use the most (i.e. Particle-In-Cell or PIC) and started a collaboration with NERSC researchers to develop an AMR library of subroutines targeted at providing AMR capabilities for existing plasma PIC simulation codes[5]. In [5], we have exposed the main issues associated with the coupling of the AMR and PIC techniques, for both electrostatic and magnetostatic simulations. In this article, we present additional results obtained with a one-dimensional and a two-dimensional axisymmetric prototypes of Particles-In-Cell+Adaptive-Mesh-Refinement code.

2. Time-dependent modeling of transient effects in diode with fast rise-time

The control of the beam head by using appropriate shapes and rise-time of the applied voltage controling the beam extraction and acceleration in the source is of great importance if one needs to avoid ion loss to the wall and its adverse effects. Fig.1 displays snapshots of the beam head in the matching section of the High-Current Experiment (HCX[2]) conducted at LBNL for two different rise-time (using the same waveform obtained from experimental data). Using a rise-time of 800ns, the simulation predicts a significant mismatch of the head resulting with loss of a small fraction of particles at the wall. According to the simulations, shortening the rise-time to 400ns provides a better match of the beam head with outer particle trajectories away from any structure.

Short pulse (200ns flat top) with very short rise-time (¡50ns) are envisioned for the next possible HIF experiment, the Integrated Beam Experiment (IBX[2]). The modeling in this range of parameter is quite challenging and the simulation tools must first be proven to be efficient on similar problems for which the solution is known.

For a one-dimensional diode, Lampel and Tiefenback [4] demonstrated that an analytical solution for a waveform of the applied voltage producing a Heaviside step for the current profile existed and is given by

$$V(t) = \frac{1}{3}\frac{t}{t_{transit}}\left[4 - \left(\frac{t}{t_{transit}}\right)^3\right] V_{max} \tag{1}$$

where V_{max} is the voltage that is applied at steady state and $t_{transit}$ is the transit time of a particle from the emitter to the collector. The latter quantity is given by

$$t_{transit} = 3 \cdot d \cdot \sqrt{\frac{m}{2qV_{max}}} \tag{2}$$

where q and m represent the charge and mass of particles and d is the distance between the emitter and the collector.

In WARP[3], the standard algorithm for injecting particles uses a virtual surface located at distance d_i from the emitting surface. After a field solve, the potential drop V_i computed between the emitter and the virtual surface is used to evaluate a current $I = \chi V_i^{3/2}/d_i^2$ assuming a Child-Langmuir emission between the two surfaces ($\chi = \frac{4}{9}\varepsilon_0\sqrt{2q/m}$). The obtained current is used to launch N new macroparticles using the formula $N = I\delta t/q_m$ where q_m is the charge of a macroparticle and δt is the time step.

Using this algorithm on a uniform grid of 160 cells, a diode length of 0.4 meters, a time step of 1ns and a steady-state current of 30A with the Lampel-Tiefenback waveform as given in (1), we have obtained the current history given in Fig.2,a). We observe that we get large amplitude low-frequency oscillations slowly damping in time. The history of the number of particles injected at each time step that is given in Fig.3 also features high amplitude low-frequency oscillations which may be the cause of the oscillations observed on the current history.

2.1. Application of the Lampel-Tiefenback method at the discrete level

The only parameter controling the number of particles injected at each time step is the voltage drop V_i computed between the emitter and the virtual surface. Getting a Heaviside current profile implies to emit a fix number of particles per time step from time zero, implying to start with a non-zero applied voltage, in contradiction with the Lampel-Tiefenback profile. In order to circumvent this contradiction which was due to the application of a solution obtained using infinitesimal calculus to discretized simulations, we decided to apply the method that Lampel and Tiefenback used to derive their solution at the discretized level directly. Knowing the current I and the distance d_i, the quantity V_i is uniquely determined by $V_i = \left(Id_i^2/\chi\right)^{2/3}$and must be a constant to ensure a constant number of particles emitted per time step. Using the linearity of the Poisson equation, we can separate the overall solution into one component V_0 resulting from the emitter-collector system with applied voltage but no charge between the electrodes and another component V_g resulting from the system with charge but grounded electrodes. We name V_{0i} and V_{gi} the potentials corresponding to these two components at the virtual surface location. At any given step, we want $V_i = V_{0i} + V_{gi} = Constant$. The charge density profile is known from the particle distribution at all time steps. Thus V_{gi} is always defined and we can compute $V_{0i} = V_i - V_{gi}$. Remarking that V_0 is a scaling of the solution at maximum voltage without charge, we get that the voltage that is to be applied between the electrodes at a given time step is given by $V_{applied} = V_{max} \cdot V_{0i}/V_{imax} = V_{max}\left(V_i - V_{gi}\right)/V_{imax}$ where V_{imax} is the voltage on the virtual surface at maximum voltage with no charge. The history of the voltage thus obtained is displayed in Fig.4,a) and compared to the infinitesimal Lampel-Tiefenback solution. As expected, the voltage does not start at zero but at almost a quarter of the maximum voltage. It is quite remarkable to notice that for times greater from the transit time of particles from the emitter to the virtual surface, the computed voltage history catch-up with the infinitesimal profile and become indistinguishable from it. As can be seen on Fig.2,b), starting at a non-zero value for the voltage in order to get a constant number of particles emitted at each time step provides a current history profile which is closer to a Heaviside step, except for a peak at the front.

2.2. Subgridding of the emitter to virtual surface region

As informative and useful the application of the Lampel-Tiefenback technique at the discrete level to obtain an ideal current profile is, it is of little help for modeling the beam response to profiles that differ from the ideal profile, as may be imposed by experimental constraints. However, if we can get to lower the initial voltage value as obtained by this technique to a negligible value, then applying this technique or applying the infinitesimal voltage solution will be equivalent.

If we set the maximum voltage to start the simulation with to be one per-cent of V_{max}, then we get from the previous relations and a little algebra that we would have to augment the resolution by a factor of 10000, meaning a grid of 1.6 million meshes for a 1-D simulation. It is clear that the use of an irregular mesh imposes itself at this point. For easy extension to 2-D and 3-D (which description is differed to another article), we have opted for a subgrid patch which extends from the emitter to the virtual surface. In order to be able to get to a very fine resolution close to the emitter, we set the mesh spacing so as to obtain a uniform charge density in the patch at steady-state (assuming Child-Langmuir flow). At each time step, the potential is first obtained on the main regular grid and the boundary values of the patch are interpolated from the main grid solution. The field is then solved inside the patch (note that charge density deposition is performed inside both the main grid and the patch). Using 200 cells in the patch allows for an initial applied voltage to be less than one per-cent of V_{max} and we can check on Fig.4,b) that the voltage history profile obtained from the simulation is now undistinguishable from the infinitesimal Lampel-Tiefenback solution from the start. This has been obtained without deterioring the current profile, as can been checked in Fig.2,c), which is almost identical to the one of Fig.2,b). The peak, however, that we may have assumed to be caused by the voltage starting at a non-zero value is still present. Our assumption was at this point that the peak is due to an underresolved front of the particle distribution.

2.3. Application of an Adaptive-Mesh-Refinement patch following the particle distribution front

In order to check this assumption, we have added an Adaptative-Mesh-Refinement patch following the front of the particle distribution. The patch had a resolution sixteen times higher than the main grid and its position was reset at each time step according to the front position, computed by locating the maximum absolute value of the current profile space derivative. The result is displayed in Fig.2,d) and shows that the peak has now disappeared, giving a result remarkably close to the infinitesimal solution. Another calculation was made at four times the resolution used so far (mesh size x4, nb particles x4, time step/4) and snapshots of the results are displayed in Fig.5. It shows that all the computed quantities are very close to the infinitesimal solution.

3. Progress on the simulation of ion source using WARP axisymmetric AMR prototype

We have also pursued the simulation of the configuration of the source using the axisymmetric PIC-AMR model prototype implemented in WARP, as described in [5]. We have showed in [5] that setting a mesh refinement patch around the emitter region was helpful in getting result almost as accurate as a run at higher resolution, at a fourth of the computational cost. The edge of the beam, however, did not seem to be as well modeled as the core and we have done the same simulation using this time an Adaptive-Mesh-Refinement patch which covers the vicinity of the emitter but also follows the beam edge (see Fig.6, top). Fig.6,bottom) displays a comparison of the emittance profiles obtained once the beam has reached steady-state for three different resolutions without using AMR (ngf: factor of number of grid meshes for each dimension, npf: factor number of particles) and one case using AMR. The phase-space projection in the space R-R' and the charge density profiles taken at the exit of the source are also given in Fig.7. Using four times less particles, the run using AMR uses a fourth of the memory and a fourth of the run time necessary to achieve essentially the same result as obtained from a run on a unique regular grid at the highest resolution used in this test.

4. Conclusion

We have extended the work presented in [5] by performing a 1-D time-dependent and a 2-D axisymmetric converged to steady-state tests using both the AMR method coupled to the Particle-In-Cell technique. For time-dependent simulation, the use of the AMR patch as proved to be, together with the use of an irregular gridded patch, indispensable for reaching an accurate modeling of the beam front. For steady-state simulations, AMR is essential for modeling the beam edge with accuracy while maintaining a good level of statistic in the core of the beam. The obtained results demonstrate that the Adaptive-Mesh-Refinement technique can be successfully used with the Particle-In-Cell technique and open the way to simulations that would otherwise be out of reach on current and near-future hardwares.

[1] http://hif.lbl.gov
[2] http://hif.lbl.gov/VNLresearch
[3] D. P. Grote, A. Friedman, I. Haber, "Three-Dimensional Simulations of High Current Beams in Induction Accelerators with WARP3d". Fus. Eng. & Des. **32-33**, 193 (1996)
[4] M. Lampel and M. Tiefenback, "An Applied Voltage to Eliminate Current Transients in a One-dimensional Diode", *Appl. Phys. Lett.* **43**, No. 1, 1 (1983)
[5] J.-L. Vay et al, "Mesh Refinement for Particle-In-Cell Plasmas Simulation: application - and benefits for - Heavy Ion Fusion", *Laser and Particle Beams*, to be published

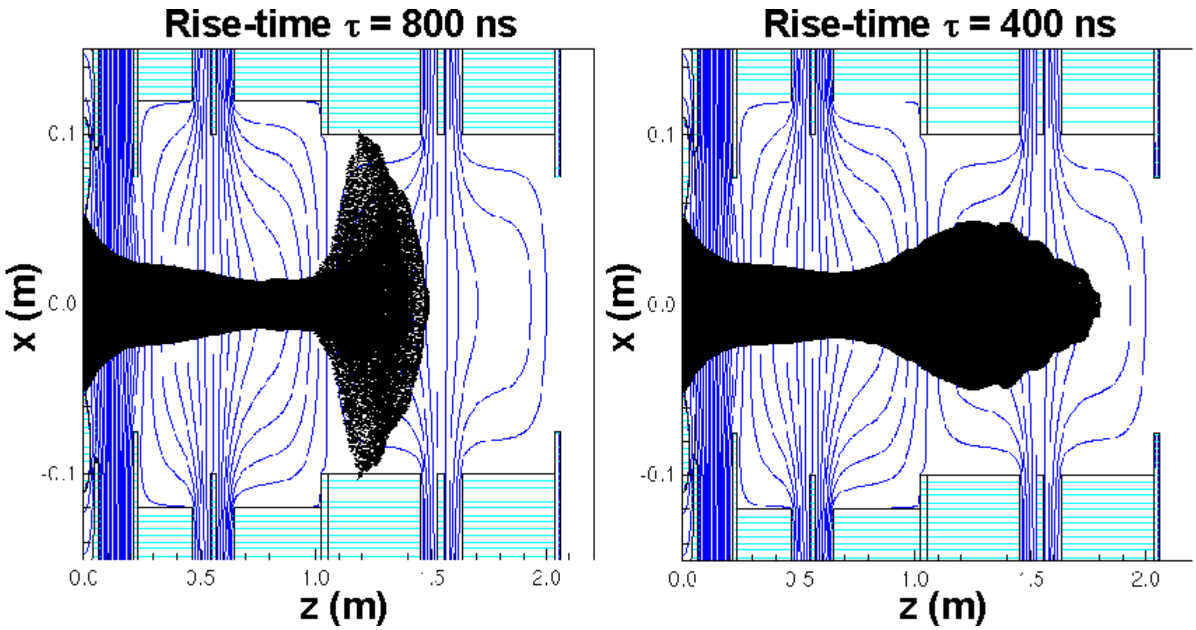

Figure 1. Snapshot of the beam head for simulations of the HCX experiment for two different rise-time of the applied voltage. On the left, the rise-time was of 800 ns (wavefrom and rise-time were given from actual experimental data) and the simulation predicts an explosion of the beam head, leading to loss of particles at the wall and raising concerns for potential breakdowns and electron effects. The same simulation using a shorter rise-time (400ns) predicts better control of the beam head.

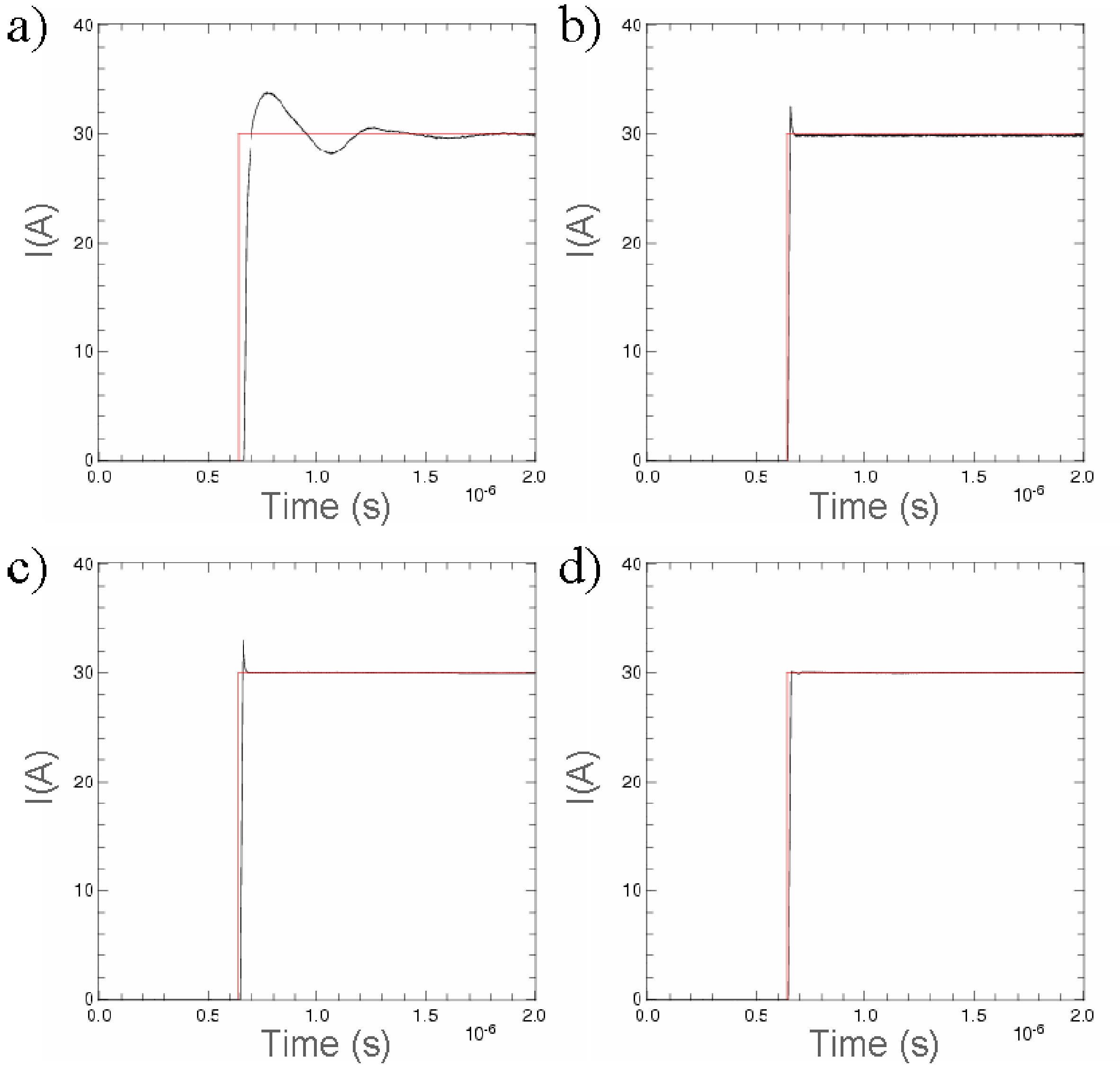

Figure 2. The current history is plotted versus time for four simulations using different numerical techniques. The black curve represents the history profile obtained from the simulation (averaged over ten time steps to damp high-frequency statistical noise). The red curve is the analytic solution. Details of algorithms are given in the text.

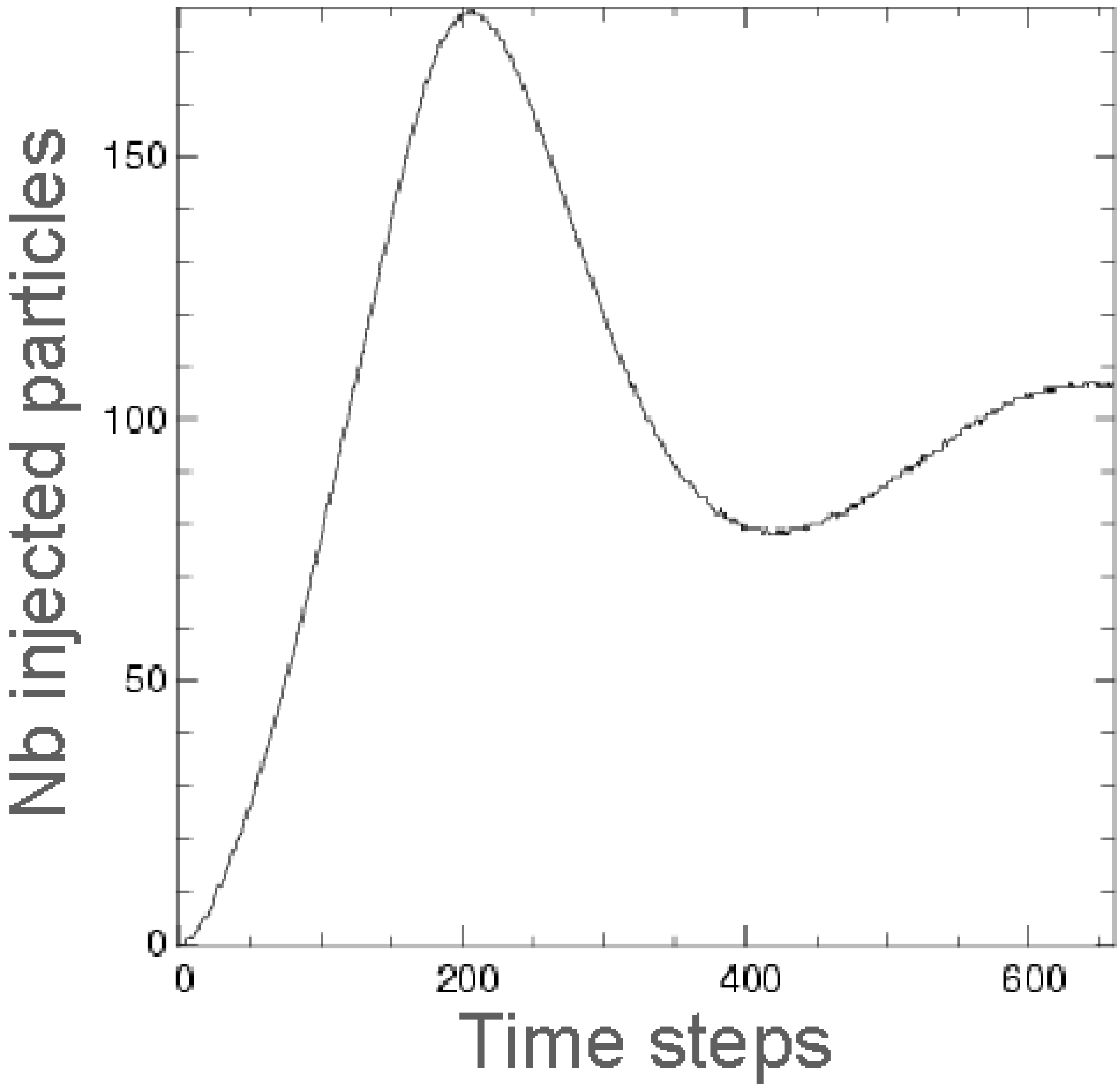

Figure 3. History of the number of particles injected per time step for the first 660 time steps corresponding to the case of Fig.2,a.

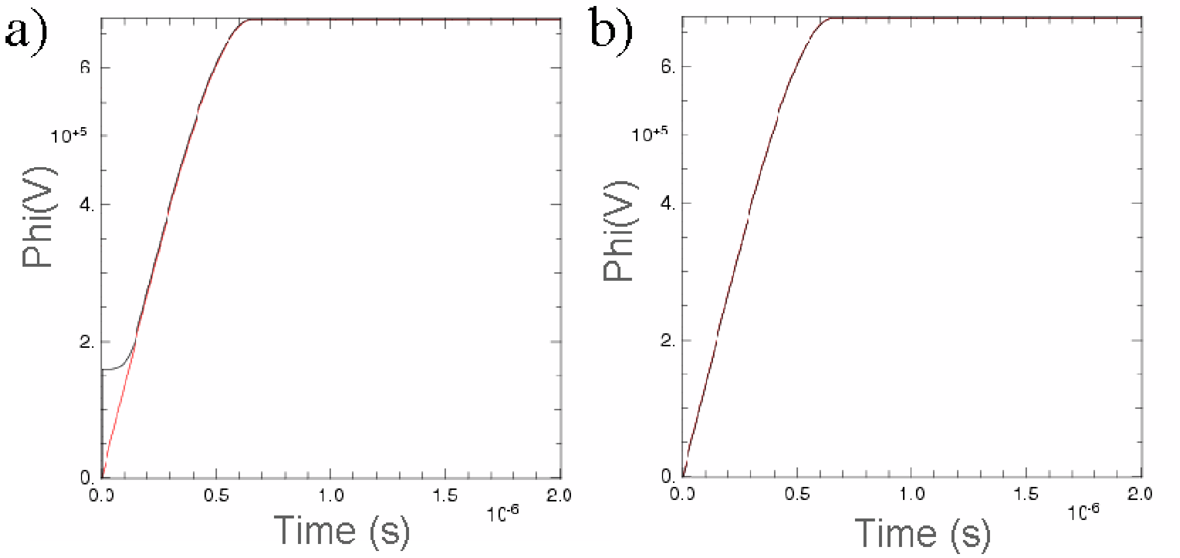

Figure 4. Voltage history used in results displayed in Fig.2,b) and Fig.2,c) respectively (black curves). The red curves is the infinitesimal Lampel-Tiefenback solution.

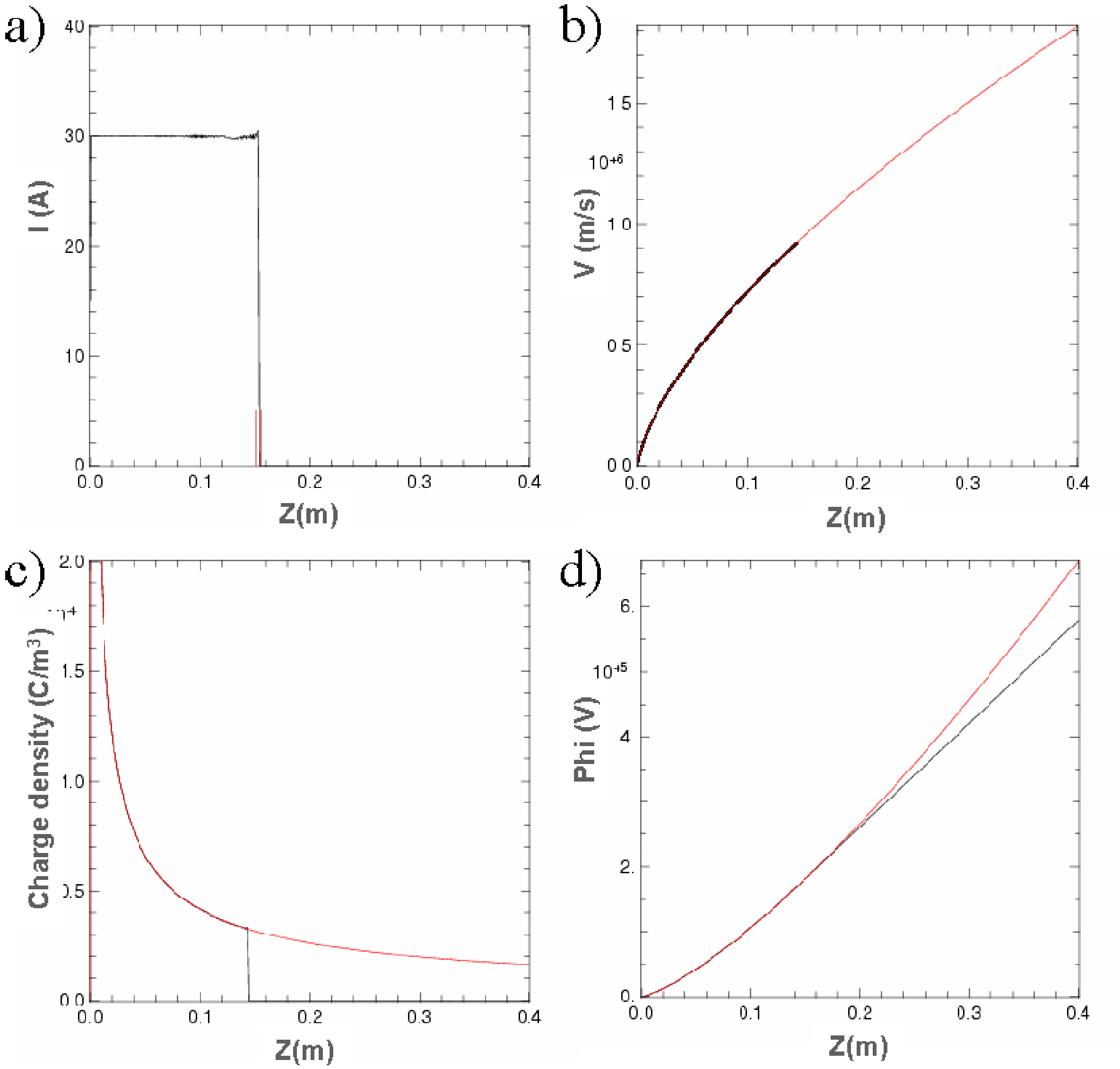

Figure 5. Snapshots of a) current profile, b) z-Vz phase-space, c) charge density, d) applied voltage versus z (black curves). The red curves represent the infinitesimal steady-state solutions except on a) where the steady-state current solution is not displayed and the two red marks show the limits of the AMR patch as located at the time step of measurement (the snapshots are from a calculation at four times the resolution of results displayed on previous figures).

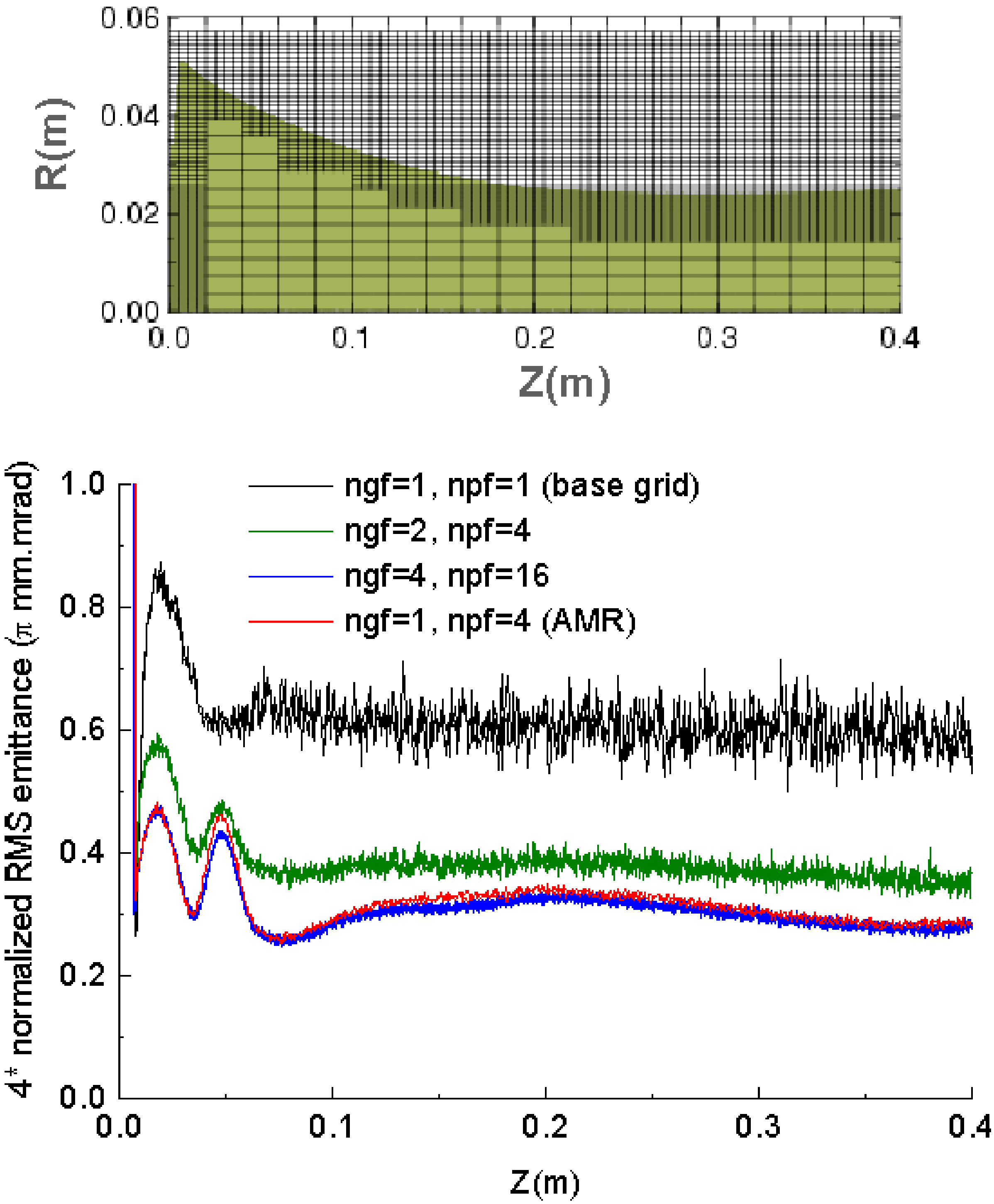

Figure 6. Top: prototype of AMR meshing used to follow the beam edge. The fine gridded area is remapped at each time step to cover the emitter region and the edge of the beam. Bottom: comparison of emittance results for three different resolutions without AMR and for one run using AMR.

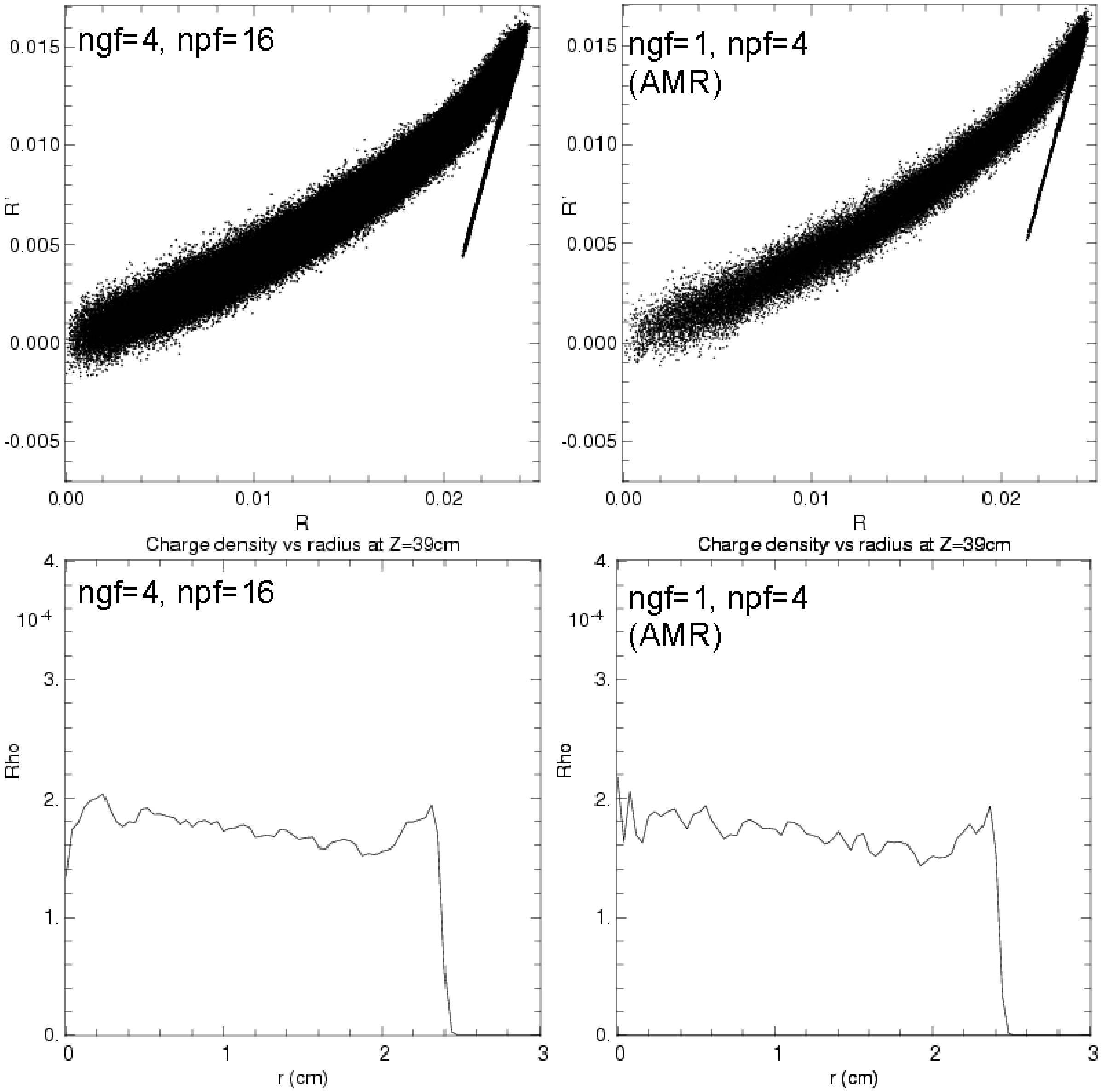

Figure 7. Left: phase-space projection and charge density at grid exit for run on one grid at highest resolution. Right: same data for run at coarser resolution using AMR patch to compensate. The run using AMR takes about a fourth of the run at highest resolution both in computer memory and run time, for an almost equivalent result.