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Exactly energy conserving semi-implicit particle in cell formulation

Giovanni Lapenta

Department of Mathematics, KU Leuven, University of Leuven, Belgium

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ABSTRACT

We report a new particle in cell (PIC) method based on the semi-implicit approach. The novelty of the new method is that unlike any of its semi-implicit predecessors at the same time it retains the explicit computational cycle and conserves energy exactly. Recent research has presented fully implicit methods where energy conservation is obtained as part of a non-linear iteration procedure. The new method (referred to as Energy Conserving Semi-Implicit Method, ECSIM), instead, does not require any non-linear iteration and its computational cycle is similar to that of explicit PIC.

The properties of the new method are: i) it conserves energy exactly to round-off for any time step or grid spacing; ii) it is unconditionally stable in time, freeing the user from the need to resolve the electron plasma frequency and allowing the user to select any desired time step; iii) it eliminates the constraint of the finite grid instability, allowing the user to select any desired resolution without being forced to resolve the Debye length; iv) the particle mover has a computational complexity identical to that of the explicit PIC, only the field solver has an increased computational cost.

The new ECSIM is tested in a number of benchmarks where accuracy and computational performance are tested.

1. Introduction

The particle in cell (PIC) method has affirmed itself as one of the most widely used numerical methods to model plasmas at the kinetic level [1–3]. The method is often selected for its simplicity that makes any new user or developer readily understand the spirit and implementation. The simplicity is also a great advantage when considering computer science issues relative to the implementation of PIC. Widely different approaches can be quickly implemented to test new software practices and new computer architectures [4–7].

While the PIC method has proven over the last several decades its ability of giving the right answers in many scientific and engineering problems, a number of further improvements are being studied. Prominent among them is the conservation of energy.

The most common implementation of the PIC method is the classic explicit PIC presented in every textbook. The idea is to break the link between particles and fields for the duration of one time step. In each time step, the particles are advanced in the old fields and afterwards the fields are advanced with the particle information just updated. This approach is tremendously simple and successful but at one cost: it does not conserve energy. In fact energy tends to grow in time.

E-mail address: giovanni.lapenta@kuleuven.be.

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This limitation is overcome in practice by judiciously choosing the time step. With sufficiently small, sometimes really very small [8], time steps, energy can be conserved to an acceptable degree.

Recent research has focused on developing a new approach to PIC where energy is exactly conserved [9–11] (we refer to this approach ECPIC in the following). This important result is obtained at the cost of making the PIC scheme fully implicit, meaning that the particle equations and the field equations have to be solved together, coupled via a non-linear Newton or Picard iteration. Energy conservation is in principle exact and its accuracy in practice is controlled by the tolerance of the iterative Newton–Krylov solver used.

The question we ask here is: can energy conservation be achieved in a scheme that retains the feel of explicit PIC avoiding the non-linear iteration? We ask then if one can retain the marching order of explicit PIC: advancing for one time step the particles first and then the fields, then the particles again, without any iteration.

The answer we find is yes. We can, to our knowledge for the first time, design a method that retains that very desirable simplicity of explicit schemes and yet conserves energy exactly. A way to reach this goal is to use the new implementation of the semi-implicit PIC method presented here, called energy conserving semi-implicit method (ECSIM).

Semi-implicit methods retain some of the particle coupling in the field equations through extra terms in the Maxwell's equations that provide a linear approximation to the particle response. The method still advances in its computational cycle as an explicit method but each step in the cycle is somewhat more complex than in the explicit PIC method. Two types of semi-implicit methods have been reported in the literature: the direct implicit method (DIM), developed at Lawrence Livermore National Laboratory and implemented in codes such as AVANTI [12,13] and LSP [14] and the implicit moment method (IMM) developed at Los Alamos National Laboratory [15,16] and used in a family of codes originating with Venus [15], followed by Celeste3D [17,18], Parsek2D [19] and now used in Parsek2D-MLMD [20,21] and iPic3D [22].

Compared with these previous semi-implicit methods, we modify significantly the particle mover and the mathematical procedure used to derive the field equations. The mover is replaced with a new mover that does not require any inner iteration and is in its practical implementation of the same level of complexity as the mover of explicit PIC. The field solver on the other hand is significantly more advanced than in the standard explicit methods requiring a significant amount of extra CPU effort. But it remains formally simple, similar to previous semi-implicit methods. Recalling that the cost of the PIC method is primarily coming from the particle mover, the new method has much potential in terms of computing performance.

The previous semi-implicit methods had many good properties of stability and ability to handle multiple time scale problems [16,15,13]. But they did not conserve energy [23,24]. The new method reported here, instead conserves energy exactly.

The practical implication of full energy conservation will be fully assessed in real world applications that we hope future research using the new method will attempt. We report here results based on a simple but complete MATLAB implementation. Using it we show the following points:

1. The method indeed conserves energy exactly as the mathematical proof we provide promises. We use a direct solver so the conservation is exact to round-off. When iterative linear solvers are used, the accuracy of energy conservation would be controlled by the tolerance of the linear solver.
2. The so-called finite grid instability that in explicit PIC forces users to resolve the Debye length can be completely overcome. We show examples where the grid spacing is 16 orders of magnitude larger than the Debye length and the new method continues to remain stable and well behaved. 16 orders is not a limit, we just stopped out of fatigue. There is no reason to believe the system size could not be increased further while still retaining stability.
3. The anisotropic heating and cooling of standard PIC or even of semi-implicit PIC is completely avoided, just as in fully implicit PIC.
4. The complexity (in terms of number of CPU operations) of the new method is of the same order as in previous semi-implicit PIC.

Below, Section 2 is the central section of the present manuscript and derives the new method, the ECSIM. Section 3 reports the formal proof of energy conservation, exact and to round off. Section 4 provides several benchmarks that confirm the ability of the new method to conserve energy exactly. Section 5 focuses on some additional properties relative to the ability of ECSIM to eradicate completely the grid spacing limitation of the finite grid instability and the unphysical and anisotropic heating/cooling of species. Section 6 draws the conclusions and suggest further needed research.

The appendices report the details of the stability analysis of the new method (Appendix A), the details of the spatial discretization used in the tests reported in Section 4 and 5 (Appendix B) and the order of accuracy in space and time of the specific implementation used here (Appendix C). Appendix D summarizes all the equations comprising the computational cycle of the new method, providing a concise summary to the interested code developer.

2. Energy conserving moment implicit method

Our goal is to derive a variant of the semi-implicit method that conserves energy exactly, borrowing this important property from fully implicit ECPIC, but avoiding the need for a non-linear iteration between particles and fields. Like previous