Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0171

Vol. **24**, No. 3, pp. 672-694
September 2018

Comparison of Preconditioning Strategies in Energy Conserving Implicit Particle in Cell Methods

Lorenzo Siddi[1], Emanuele Cazzola[2] and Giovanni Lapenta[1,*]

[1] *Department of Mathematics, KULeuven, University of Leuven, Belgium (EU).*
[2] *Department of Mathematics, University of Surrey, Guildford, Surrey, UK.*

Received 10 August 2017; Accepted 15 September 2017

Abstract. This work presents a set of preconditioning strategies able to significantly accelerate the performance of fully implicit energy-conserving Particle-in-Cell methods to a level that becomes competitive with semi-implicit methods. We compare three different preconditioners. We consider three methods and compare them with a straight unpreconditioned Jacobian Free Newton Krylov (JFNK) implementation. The first two focus, respectively, on improving the handling of particles (particle hiding) or fields (field hiding) within the JFNK iteration. The third uses the field hiding preconditioner within a direct Newton iteration where a Schwarz-decomposed Jacobian is computed analytically. Clearly, field hiding used with JFNK or with the direct Newton-Schwarz (DNS) method outperforms all method. We compare these implementations with a recent semi-implicit energy conserving scheme. Fully implicit methods are still lag behind in cost per cycle but not by a large margin when proper preconditioning is used. However, for exact energy conservation, preconditioned fully implicit methods are significantly easier to implement compared with semi-implicit methods and can be extended to fully relativistic physics.

AMS subject classifications: 65Z05, 65F08, 65M75

Key words: Preconditioners in Particle-in-Cell, energy conserving Particle-in-Cell, plasma numerics.

1 Introduction

Particle in cell plasma simulations [1, 13] are amongst the most successful in obtaining new physics and in running at top performance on supercomputers [2]. Recently, this success has attracted several new developments. Among them, we focus the attention here on implicit and semi-implicit PIC methods. Given their simplicity and flexibility, these PIC formulations have gained wide use as effective computational tools for the

*Corresponding author. *Email addresses:* `lorenzo.siddi@kuleuven.be` (L. Siddi), `e.cazzola@surrey.ac.uk` (E. Cazzola), `giovanni.lapenta@kuleuven.be` (G. Lapenta)

simulation of multiscale plasma phenomena in a variety of fields from space [19], astrophysics [30], laser-plasma interaction [29], magnetic fusion [6] and space propulsion [7]. The interest on (semi-)implicit PIC has been intensified by the presentation of exactly energy conserving schemes [10,27]. Semi-implicit methods had been previously developed along two lines of research (e.g. [3, 20] for a review): *moment implicit* [4] and *direct implicit* [17]. In these methods, the coupling between particles and fields is represented via a linear response: the direct implicit method uses a sensitivity matrix while the implicit moment method uses a Taylor expansion similar to the Sonine polynomial expansion of the Chapman-Enskog moment method [8]. Both methods found very successful applications either in commercial codes (`www.orbitalatk.com/lsp/`) or in research codes used by the plasma physics community: Venus [4], Celeste [18, 33], Parsek2D [25] and iPic3D [26].

Very recently, a new variant of semi-implicit method, ECsim [21] has been proposed. The new method is based on constructing a so-called mass matrix that represents how the particles in the system produce a plasma current in response to the presence of magnetic and electric fields. This response is linear and the ECsim method belongs to the class of semi-implicit methods. However, its key difference compared with the previously mentioned semi-implicit methods is that its mass matrix formation leads to exact energy conservation. A theorem proves the energy conservation to be valid at any finite time step [21], a conclusion confirmed to machine precision in practical multidimensional implementations [22].

Fully implicit methods had been deemed impractical in the past decades, but recent developments in handling non linear coupled systems made them practical. The original particle mover and field solver of the implicit moment method were already exactly energy conserving [27]. This property is however broken by the Taylor expansion. If instead the discretised field and particle equations are solved directly as a coupled non-linear system, energy is conserved exactly [27]. Several variants can include charge conservation besides energy conservation [10], for electromagnetic relativistic systems [23] and for the so-called Darwin pre-Maxwell approximation [9].

Even in our times, non-linear systems still are a formidable numerical task, especially for a large number of unknowns. For an efficient implementation, the numerical method used for solving the system needs to be carefully designed. So far, the research has focused on the Jacobian-Free Newton Krylov method (JFNK) [14] and on Picard iterations [32]. The performance of the non linear solver can be improved dramatically if good preconditioners are designed [16]. Preconditioners are operators that invert part of the problem, increasing the speed of convergence of the solution of the Jacobian problem needed for each Newton iteration.

In the context of implicit PIC, the attention has focused on the so-called particle hiding (or particle enslavement) approach [15, 27], especially suitable to hybrid architectures [11], and the use of fluid preconditioning for the fields [12].

In the present paper we revisit the particle hiding preconditioning and compare it with a number of new preconditioning methods able to significantly accelerate the itera-