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Implementation of high order spline interpolations for tracking charged particles in discretized fields

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Introduction

We consider the problem of tracking nonrelativistic charged particles in turbulent electromagnetic fields:

$$\begin{cases} \partial_t \mathbf{r} = \mathbf{v} \\ \partial_t \mathbf{v} = \dfrac{q}{m}(\mathbf{e}(\mathbf{r}) + \mathbf{v} \times \mathbf{b}(\mathbf{r})) \end{cases} \tag{1}$$

In numerical approaches, two main issues have to be addressed. First, an accurate solution for the **time evolution** of the particle position and velocity has to be computed. Second, an accurate **interpolation** of the fields $\mathbf{e}(\mathbf{r})$ and $\mathbf{b}(\mathbf{r})$, generally available only on a discrete grid, is needed.

Although most of the information presented here is valid for a wide range of systems, the discussion is restricted to the simple case of particles submitted to electric and magnetic fields obtained from the magneto-hydrodynamic (MHD) equations:

$$\begin{aligned} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= (\mathbf{b} \cdot \nabla)\mathbf{b} + \nu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f} \\ \partial_t \mathbf{b} + (\mathbf{u} \cdot \nabla)\mathbf{b} &= (\mathbf{b} \cdot \nabla)\mathbf{u} + \eta \nabla^2 \mathbf{b} \end{aligned} \tag{2}$$

In this case, the self-consistent electric field is:

$$\mathbf{e} = -\mathbf{u} \times \mathbf{b} + \eta \nabla \times \mathbf{b}. \tag{3}$$

We obtain solutions of the MHD equations with a spectral solver, so that they are periodic in the three spatial directions. The vector potential $\mathbf{a}$ ($\mathbf{b} = \nabla \times \mathbf{a}$) can then easily be derived from the magnetic field and the electric field can easily be decomposed into its scalar potential and vector potential parts:

$$\mathbf{e} = -\nabla \Phi - \partial_t \mathbf{a}. \tag{4}$$

Time evolution: In this work, composition methods (CM) based on the splitting from ref. [1] will be used. These time integration schemes are not symplectic (except for the simple case $\mathbf{b} = 0$), but they have the advantage of being very efficient as they are explicit. Any numerical integration scheme will give an error in the position of the order of τ^ℓ, where τ is the timestep being used. The tests presented here have been performed using the fourth order Blanes & Moan schemes CM4 ($\ell = 4$) and the sixth order Kahan & Li scheme CM6 ($\ell = 6$), as described in [4].

Interpolation

Concerning the interpolation of the fields, the literature mostly mentions the uses of the multilinear or cubic spline interpolation [2, 3]. We present a hierarchy of spline interpolations well suited for dynamic fields represented on regular, rectangular spatial grids. Used in conjunction with the interpolation through potentials method presented in [5], they allow for a systematic approach to the study of particle transport in turbulent fields. Consider a function f. The polynomial

$$s^{(n)}(x) = \sum_{k=0}^{n} a_k^{(n)} x^k \tag{5}$$

is an Hermite spline interpolation of f for $x \in [0,1]$ if the following conditions are satisfied:

$$\begin{cases} \frac{d^l s^{(n)}}{dx^l}(0) = \frac{d^l f}{dx^l}(0) \\ \frac{d^l s^{(n)}}{dx^l}(1) = \frac{d^l f}{dx^l}(1) \end{cases}, \ l = \overline{0,m} \tag{6}$$

where $m = (n-1)/2$ is the highest derivative that is kept continuous for the interpolation s. In many situations, the field f is not known analytically and the derivatives must be estimated from grid values. Here, we approximate the derivatives by their centered difference approximations using $2g+1$ grid points:

$$\frac{d^l f}{dx^l}(j) \approx f^{\langle l,q \rangle}(j) = \sum_{i=j-g}^{j+g} c_i^{(l,q)} f(i), \tag{7}$$

the solution of (6) can be rewritten as

$$s^{(n,q)}(x) = \sum_{i=0-g}^{1+g} f(i) \beta_i^{(n,q)}(x). \tag{8}$$

where $q = 2g+2$ is the number of grid nodes contributing to the approximation. The splines are controled by two parameters then: their order n (or their **smoothness** m) and q (directly related to their computation time, and the **accuracy** of the centered differences). Tensor product splines can be used for 3D fields:

$$s^{(n,q)}(\mathbf{r}) = \sum_{0-g}^{1+g} \left(f(\mathbf{i}) \prod_{j=1}^{3} \beta_{i_j}^{(n,q)}(x_j) \right) \equiv S^{(n,q)}(\mathbf{r}) f \tag{9}$$

Here the electromagnetic fields are obtained from direct simulations of the MHD equations. In order to test energy conservation, the instantaneous fields **b** and **e** are frozen, so that the time derivative of the vector potential can be removed from the electric field which then derives from a scalar potential.

The operator $S^{(n,q)}$ can be used in two ways [5] for the magnetic field $\mathbf{b}$:

$$\hat{\mathbf{b}}^{(n,q)} = S^{(n,q)}\mathbf{b} \quad \text{or} \quad \tilde{\mathbf{b}}^{(n,q)} = \nabla \times (S^{(n,q)}\mathbf{a}) \tag{10}$$

Similarly we consider $\hat{\mathbf{e}}^{(n,q)}$ or $\tilde{\mathbf{e}}^{(n,q)} = -\nabla(S^{(n,q)}\Phi)$. Note that $\tilde{\mathbf{b}}$ is exactly divergence free by construction, and $\tilde{\mathbf{e}}$ is exactly curl free. But $\tilde{\mathbf{b}}$ is slower to compute.

So we obtain two hierarchies of Lorentz forces: $\hat{\mathbf{F}}^{(n,q)}$ and $\tilde{\mathbf{F}}^{(n,q)}$. Our purpose here is to study the differences, if any, between these two hierarchies and between their individual elements. One can in principle improve the interpolation (with higher q-s and n-s) until the results converge.

Results and discussion

We consider a set of particles with random initial conditions (but fixed initial kinetic energy). We then evolve this same set of particles in a fixed discretized electromagnetic field, using several approximations $\hat{\mathbf{F}}^{(n,q)}$ and $\tilde{\mathbf{F}}^{(n,q)}$ and different time evolution schemes.

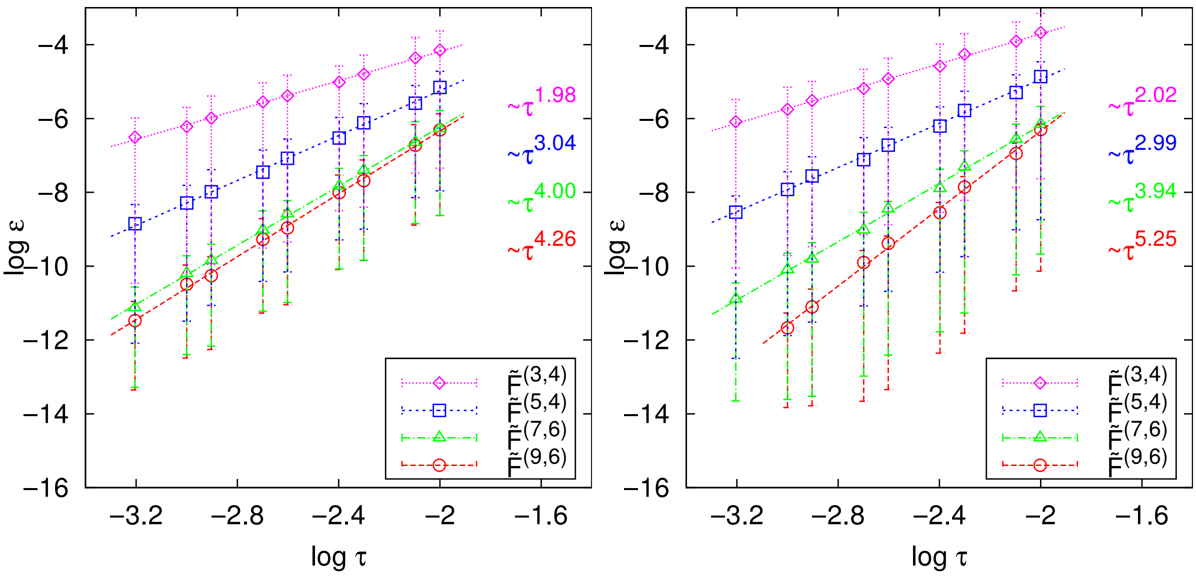

Figure 1: **Effective order of time integration schemes**

The effective order of the integration schemes is measured by evaluating the error ε in the trajectories as a function of the time step τ. Figure 1 shows that this effective order is directly affected by the smoothness of the interpolation scheme $\tilde{\mathbf{F}}$. The exponent n_{eff} in the power $\varepsilon(\tau) \propto \tau^{-n_{\text{eff}}}$ shows the effective order of the scheme. Left and right plots are respectively obtained with the CM4 and CM6 schemes.

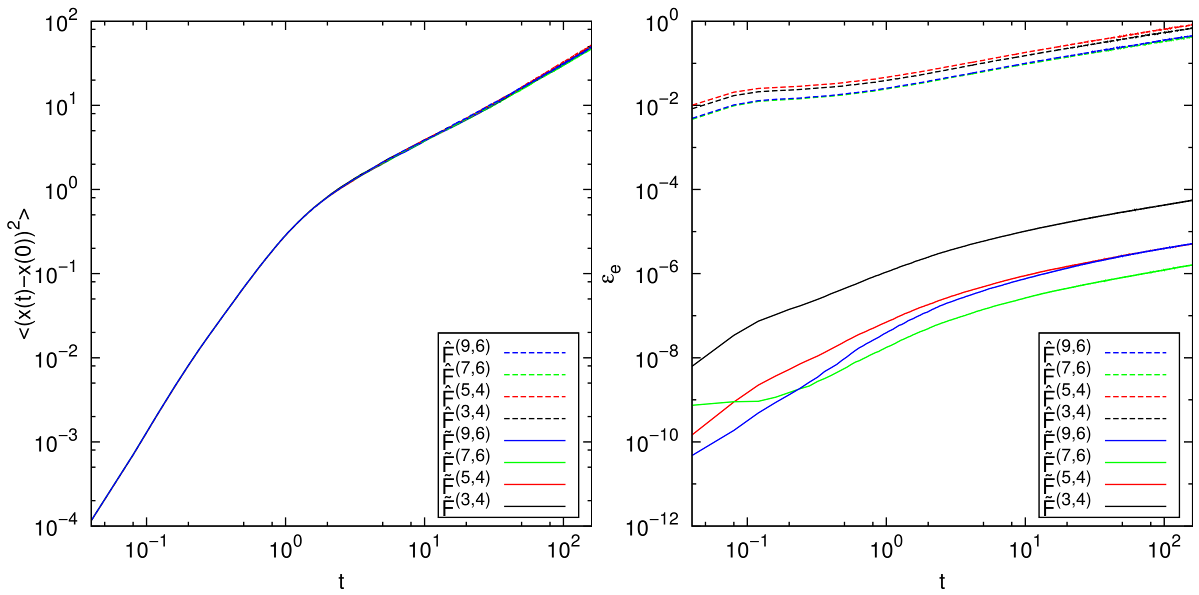

Figure 2: **Transport properties.**

Another test is a simple investigation of charged particle transport. The mean squared displacement along the x axis and the mean energy error are presented in figure 2. For this test we fix the local error ε, and we choose the most efficient method out of CM4 or CM6. This way, we observe that higher order splines allow for smaller computation times, even though the $q = 6$ point interpolation is slower than the $q = 4$ point one. It is obvious that using $\tilde{\mathbf{F}}$ leads to much smaller energy errors.

Note that in regards to transport, many results depend on the specific particle ensemble (fixed initial position, fixed initial kinetic energy, fixed initial total energy, ...). With this work we provide a method for checking if and in what way the errors introduced by the interpolation are relevant.

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