Computational Methods in Plasma Physics. Lecture II

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Single particle motion in an electromagnetic field

- In the *Particle-in-cell* (PIC) method the Vlasov-Maxwell equation is solved in the *Lagrangian frame* in which the phase-space is represented by *finite-sized* "macro-particles".
- In the Lagrangian frame the distribution function remains constants along *characteristics* in phase-space.
- These characteristics satisfy the ODE of particles moving under Lorentz force law

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$
$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}(\mathbf{E}(\mathbf{x},t) + \mathbf{v} \times \mathbf{B}(\mathbf{x},t))$$

- We will first focus on solving the equations-of-motion for the macro-particles, leaving solution of Maxwell equations and coupling to particles for Lecture 2.

Simple harmonic oscillator

Consider first the simple harmonic oscillator

$$\frac{d^2 z}{dt^2} = -\omega^2 z$$

This has exact solution $z = a\cos(\omega t) + b\sin(\omega t)$, where a and b are arbitrary constants. How to solve this numerically? Write as a system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = -\omega^2 z$$

Note that the coordinates (z, v) label the *phase-space* of the harmonic oscillator. Multiply the second equation by v and use the first equation to get

$$\frac{d}{dt}\left(\frac{1}{2}v^2 + \frac{1}{2}\omega^2 z^2\right) = 0.$$

This is the *energy* and is *conserved*.
Question: how to solve the ODE such that the energy is conserved by the discrete scheme?

Harmonic oscillator: Forward Euler Scheme

First attempt: use the simplest possible scheme, replace derivatives with difference approximations

$$\frac{z^{n+1} - z^n}{\Delta t} = v^n; \quad \frac{v^{n+1} - v^n}{\Delta t} = -\omega^2 z^n$$

or

$$z^{n+1} = z^n + \Delta t v^n; \quad v^{n+1} = v^n - \Delta t \omega^2 z^n$$

This is the *forward Euler* scheme. Lets check if the discrete scheme conserves energy:

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (1 + \omega^2 \Delta t^2)((v^n)^2 + \omega^2 (z^n)^2)$$

The presence of the $\omega^2 \Delta t^2$ in the bracket spoils the conservation. So the forward Euler scheme *does not* conserve energy. Also, note that the energy, in fact, is *increasing*!

Harmonic oscillator: Forward Euler Scheme

Closer look: write as a matrix equation

$$\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \Delta t \\ -\omega^2 \Delta t & 1 \end{bmatrix}}_{\text{Jacobian, } J} \begin{bmatrix} z^n \\ v^n \end{bmatrix}.$$

Observe that the determinant of the Jacobian is $\det(J) = (1 + \omega^2 \Delta t^2)$ which is the same factor as appears in the energy relation. One may reasonably conjecture that when this determinant is one, then perhaps energy is conserved.

Volume Preserving Scheme

We will call say a scheme preserves *phase-space* volume if the determinant of the Jacobian is $\det(J) = 1$.

Harmonic oscillator: Mid-point Scheme

Perhaps a better approximation will be obtained if we use *averaged* values of z, v on the RHS of the discrete equation:

$$\frac{z^{n+1} - z^n}{\Delta t} = \frac{v^n + v^{n+1}}{2}$$
$$\frac{v^{n+1} - v^n}{\Delta t} = -\omega^2 \frac{z^n + z^{n+1}}{2}$$

This is an *implicit* method as the solution at the next time-step depends on the old as well as the next time-step values. In this simple case we can explicitly write the update in a matrix form as

$$\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \frac{1}{1 + \omega^2 \Delta t^2/4} \begin{bmatrix} 1 - \omega^2 \Delta t^2/4 & \Delta t \\ -\omega^2 \Delta t & 1 - \omega^2 \Delta t^2/4 \end{bmatrix} \begin{bmatrix} z^n \\ v^n \end{bmatrix}.$$

For this scheme $\det(J) = 1$. So the mid-point scheme conserves phase-space volume! Some algebra also shows that

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2$$

showing that energy is also conserved by the mid-point scheme.

Harmonic oscillator: Mid-point Scheme is symplectic

A more stringent constraint on a scheme for the simple harmonic oscillator is that it be *symplectic*. To check if a scheme is symplectic one checks to see if

$$J^T \sigma J = \sigma$$

where σ is the *unit symplectic matrix*

$$\sigma = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

Turns out that the mid-point scheme for the harmonic oscillator is also symplectic. Note that if a scheme conserves phase-space volume, it *need not* be symplectic.

Accuracy and Stability

To study the stability, accuracy and convergence of a scheme one usually looks at the first order ODE

$$\frac{dz}{dt} = -\gamma z$$

where $\gamma = \lambda + i\omega$ is the complex frequency. The exact solution to this equation is $z(t) = z_0 e^{-\gamma t}$. The solution has damped/growing modes ($\lambda > 0$ or $\lambda < 0$) as well as oscillating modes.

- The forward Euler scheme for this equation is

$$z^{n+1} = z^n - \Delta t \gamma z^n = (1 - \Delta t \gamma) z^n.$$

- The mid-point scheme for this equation is

$$z^{n+1} = \left(\frac{1 - \gamma \Delta t/2}{1 + \gamma \Delta t/2} \right) z^n$$

Accuracy and Stability

We can determine how *accurate* the scheme is by looking at how many terms the scheme matches the Taylor series expansion of the exact solution:

$$z(t^{n+1}) = z(t^n)\left(1 - \gamma\Delta t + \frac{1}{2}\gamma^2\Delta t^2 - \frac{1}{6}\gamma^3\Delta t^3 + \dots\right)$$

- The forward Euler scheme matches the *first two terms*

$$z^{n+1} = z^n(1 - \Delta t\gamma)$$

- The mid-point scheme matches the *first three terms*

$$z^{n+1} = z^n\left(1 - \Delta t\gamma - \frac{1}{2}\gamma^2\Delta t^2 - \frac{1}{4}\gamma^3\Delta t^3 + \dots\right)$$

Accuracy and Stability

We can determine if the scheme is *stable* by looking at the amplification factor $|z^{n+1}/z^n|$. Note that for damped modes ($\lambda > 0$) this quantity *decays* in time, while for purely oscillating modes ($\lambda = 0$) this quantity remains *constant*.

- The amplification factor for the forward Euler scheme in the absence of damping is $1 + \omega^2 \Delta t^2 > 1$, hence this scheme is *unconditionally unstable*.
- The amplification factor for the mid-point scheme in the absence of damping is exactly 1, showing that the mid-point scheme is *unconditionally stable*, that is, one can take as large time-step one wants without the scheme "blowing up". Of course, the errors will increase with larger Δt.

Runge-Kutta schemes

- Even though the forward Euler scheme is unconditionally unstable, we can use it to construct other schemes that *are* stable and are also more accurate (than first order).
- For example, a class of Runge-Kutta schemes can be written as a combination of forward Euler updates. In particular, the *strong stability preserving* schemes are important when solving hyperbolic equations. Note that these RK schemes will *not* conserve energy for the harmonic oscillator, but *decay* it.
- Other multi-stage Runge-Kutta schemes can be constructed that allow very large time-steps for diffusive processes, for example, that come about when time-stepping diffusion equations.

Simple harmonic oscillator

We looked at

$$\frac{d^2z}{dt^2} = -\omega^2 z$$

and wrote it as system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = -\omega^2 z$$

Now introduce energy-angle coordinates

$$\omega z = E\sin\theta; \quad v = E\cos\theta$$

then $E^2 = \omega^2 z^2 + v^2 \equiv E_0^2$ is a constant as we showed before. Using these expressions we get the very simple ODE $\dot{\theta} = \omega$. This shows that in phase-space $(v, \omega z)$ the motion is with uniform angular speed along a circle.

Simple harmonic oscillator: Phase-errors

The mid-point scheme had

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2 = E_0^2$$

which means that the mid-point scheme gets the energy coordinate *exactly* correct. However, we have

$$\tan \theta^{n+1} = \frac{\omega z^{n+1}}{v^{n+1}}.$$

Using the expressions for the scheme and Taylor expanding in Δt we get

$$\tan \theta^{n+1} = \tan \theta^n + \frac{\omega E_0^2}{(v^n)^2} \Delta t + \frac{\omega^3 z^n E_0^2}{(v^n)^3} \Delta t^2 + O(\Delta t^3)$$

The first three terms match the Taylor expansion of the exact solution $\tan(\theta^n + \omega \Delta t)$ and the last term is the *phase-error*.

Single particle motion in an electromagnetic field

- In PIC method the Vlasov-Maxwell equation is solved in the *Lagrangian frame*: the phase-space is represented by *finite-sized* "macro-particles".
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- These characteristics satisfy the ODE of particles moving under Lorentz force law

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$
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- In the absence of an electric field, the kinetic energy must be conserved

$$\frac{1}{2}|\mathbf{v}|^2 = \text{constant}.$$

  This is independent of the spatial or time dependence of the magnetic field. Geometrically this means that in the absence of an electric field the velocity vector rotates and its tip always lies on a sphere.

Single particle motion in an electromagnetic field

- A mid-point scheme for this equation system would look like

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \frac{\mathbf{v}^{n+1} + \mathbf{v}^n}{2}$$
$$\frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \frac{q}{m}\left(\overline{\mathbf{E}}(\mathbf{x}, t) + \frac{\mathbf{v}^{n+1} + \mathbf{v}^n}{2} \times \overline{\mathbf{B}}(\mathbf{x}, t)\right)$$

  The overbars indicate some averaged electric and magnetic fields evaluated from the new and old positions. In general, this would make the scheme nonlinear!

- Instead, we will use a *staggered* scheme in which the position and velocity are staggered by half a time-step.

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \mathbf{v}^{n+1/2}$$
$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}^n, t^n) + \frac{\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}^n, t^n)\right)$$

The Boris algorithm for the staggered scheme

The velocity update formula is

$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}^n, t^n) + \frac{\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}^n, t^n)\right)$$

This appears like an implicit method: most obvious is to construct a linear 3×3 system of equations and invert them to determine $\mathbf{v}^{n+1}$. Puzzle to test your vector-identity foo: find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$.
The Boris algorithm updates this equation in three steps:

$$\begin{aligned}
\mathbf{v}^- &= \mathbf{v}^{n-1/2} + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2} \\
\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} &= \frac{q}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}^n \\
\mathbf{v}^{n+1/2} &= \mathbf{v}^+ + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2}
\end{aligned}$$

Convince yourself that this is indeed equivalent to the staggered expression above. So we have two electric field updates with half time-steps and a rotation due to the magnetic field. Once the updated velocity is computed, we can trivially compute the updated positions.

The Boris algorithm for the staggered scheme

How to do the rotation? The Boris algorithm does this in several steps:

- Compute the $\mathbf{t}$ and $\mathbf{s}$ vectors as follows

$$\mathbf{t} = \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}$$
$$\mathbf{s} = \frac{2\mathbf{t}}{1 + |\mathbf{t}|^2}$$

- Compute $\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$ and finally $\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$.

See Birdsall and Langdon text book Section 4-3 and 4-4 and figure 4-4a. Easily extended to relativistic case.

Note that in the absence of an electric field the Boris algorithm conserves kinetic energy.

Why is the Boris algorithm so good? Can one do better?

See paper by Qin at. al. Phys. Plasmas, **20**, 084503 (2013) in which it is shown that the Boris algorithm *conserves phase-space volume*. However, they also show that the Boris algorithm is *not* symplectic.

- The relativistic Boris algorithm does not properly compute the $\mathbf{E} \times \mathbf{B}$ velocity. This can be corrected. For example Vay, Phys. Plasmas, **15**, 056701 (2008). The Vay algorithm however, breaks the phase-space volume preserving property of the Boris algorithm.
- Higuera and Cary, Phys. Plasmas, **24**, 052104 (2017) showed how to compute the correct $\mathbf{E} \times \mathbf{B}$ drift velocity and restore volume preserving property. Seems this is probably the current-best algorithm for updating Lorentz equations.
- The saga for better particle push algorithms is not over! For example, an active area of research is to discover good algorithms for *asymptotic* systems, for example, when gyroradius is much smaller than gradient length-scales or gyrofrequency is much higher than other time-scales in the system. Common in most magnetized plasmas.

Solving Maxwell equations

Besides pushing particles in electromagnetic fields, we need to compute these fields self-consistently from currents and charges by solving Maxwell equations. First consider Maxwell equations in vacuum:

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$
$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = 0$$

For these we have the conservation laws

$$\frac{d}{dt} \int_\Omega \mathbf{E} \times \mathbf{B} \, d^3\mathbf{x} = 0$$
$$\frac{d}{dt} \int_\Omega \left(\frac{\epsilon_0}{2} |\mathbf{E}|^2 + \frac{1}{2\mu_0} |\mathbf{B}|^2 \right) d^3\mathbf{x} = 0.$$

Note these are *global* conservation laws and one can instead also write *local* conservation laws that include momentum and energy flux terms. How to solve these equations efficiently and maintain (some) conservation and geometric properties?

Solving Maxwell equations

- Maxwell equations have a very special geometric structure. The electric field $\mathbf{E}$ is a *vector* while the magnetic field $\mathbf{B}$ is a *bivector* (this is disguised in the usual formulations of Maxwell equations).
- (In spacetime formulations the complete electromagnetic field is represented as a single bivector in 4D space-time).
- The fact that we are dealing with two objects of *different* geometric types indicates that the discrete Maxwell equations should also inherit this somehow.
- The Yee algorithm, often called the *finite-difference time-domain* algorithm is the most successful (and simple) algorithm that accounts of this geometric structure. It is implemented in most PIC codes, though recent research has focused on structure preserving finite-element and other methods.

Solving Maxwell equations: The Yee-cell

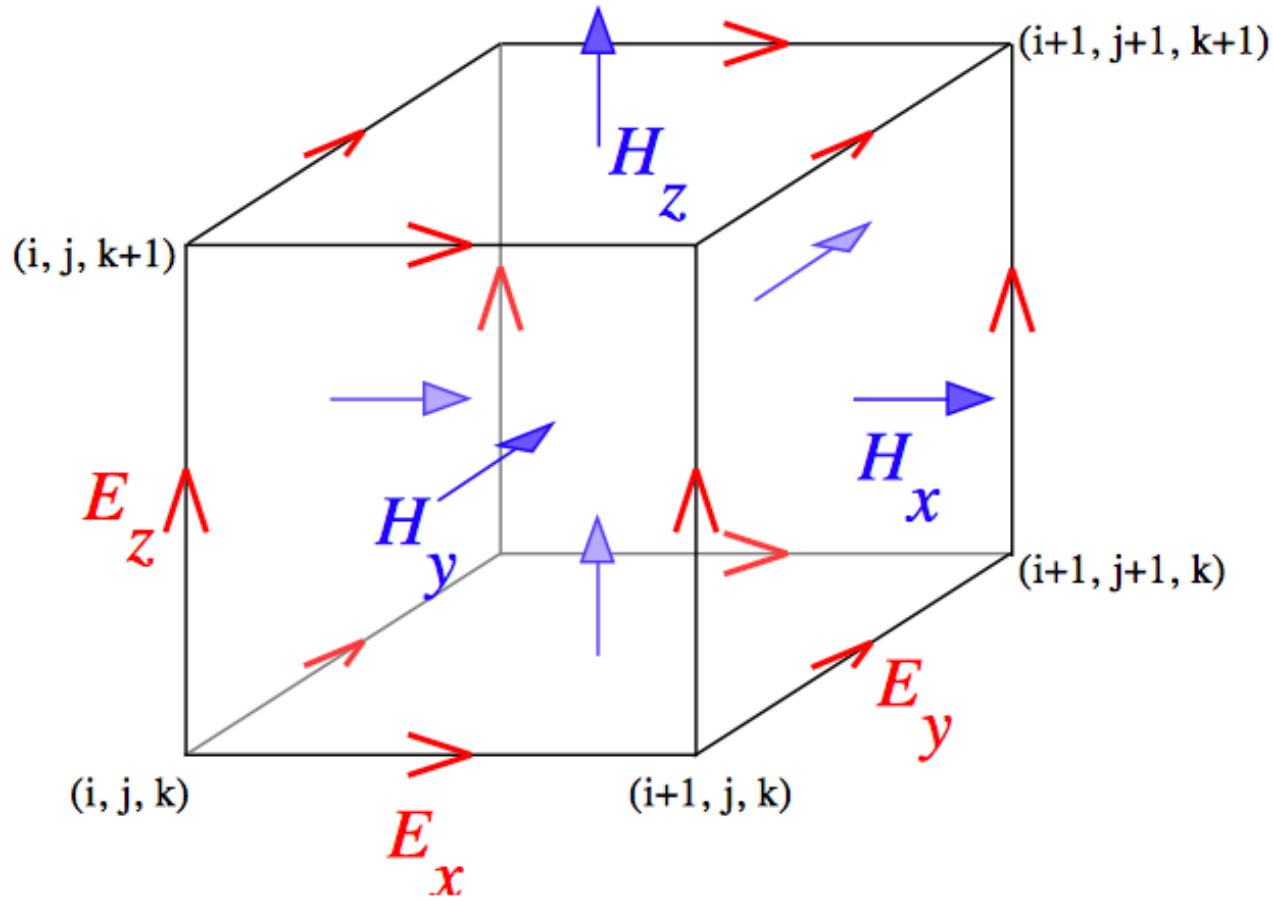

Figure: Standard Yee-cell. Electric field components (vectors) are located on edges while magnetic field components (bivectors) are located on faces.

Solving Maxwell equations: The Yee-cell

On the Yee-cell the difference approximation to Maxwell equations "falls out", almost like magic. The updates are staggered in time and use two *different* discrete curl operators:

$$\mathbf{B}^{n+1/2} = \mathbf{B}^{n-1/2} - \Delta t \, \nabla_E \times \mathbf{E}^n$$
$$\mathbf{E}^{n+1} = \mathbf{E}^n + \Delta t / c^2 \, \nabla_F \times \mathbf{B}^{n+1/2}$$

Here the symbols $\nabla_F \times$ and $\nabla_E \times$ are the discrete curl operators:

- The first takes *face-centered* magnetic field and computes it curl. This operator *puts the result on cell edges*.
- The second takes *edge-centered* electric field and computes it curl. This operator *puts the result on cell faces*.
- The structure of Yell-cell also indicates that *currents* must be co-located with the electric field and computed at half time-steps.

This duality neatly reflects the underlying geometry of Maxwell equations. The staggering in time reflects the fact that in 4D the electromagnetic field is a bivector in spacetime.

Divergence relations are exactly maintained

We can show that the discrete Maxwell equations on a Yee-cell maintain the divergence relations exactly:

$$\nabla_F \cdot \mathbf{B}^{n+1/2} = 0$$
$$\nabla_E \cdot \mathbf{E}^{n} = 0.$$

There is an additional constraint of Maxwell equations in a plasma, that is, the current conservation:

$$\frac{\partial \varrho_c}{\partial t} + \nabla \cdot \mathbf{J} = 0.$$

where ϱ_c is the charge density and $\mathbf{J}$ is the current density. On the Yell-cell this becomes

$$\frac{\varrho_c^{n+1} - \varrho_v^{n}}{\Delta t} + \nabla_E \cdot \mathbf{J}^{n+1/2} = 0.$$

One must ensure that current from particles is computed carefully to ensure that this expression is satified. See Esirkepov, Comp. Phys. Communications, **135** 144-153 (2001).

Other schemes: Finite-Volume method for Maxwell equations

Consider the 1D source-free Maxwell equations

$$\frac{\partial}{\partial t}\begin{bmatrix} E_y \\ B_z \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} c^2 B_z \\ E_y \end{bmatrix} = 0.$$

Basic idea is to transform the equation into uncoupled advection equations for the *Riemann variables*. This is always possible in 1D for *linear hyperbolic* systems. For the above system, multiply the second equation by c and add and subtract from the first equation to get

$$\frac{\partial}{\partial t}\left(E_y + cB_z\right) + c\frac{\partial}{\partial x}\left(E_y + cB_z\right) = 0$$
$$\frac{\partial}{\partial t}\left(E_y - cB_z\right) - c\frac{\partial}{\partial x}\left(E_y - cB_z\right) = 0.$$

Note that these are two uncoupled passive advection equations for the variables $w^{\pm} = E_y \pm cB_z$ with advection speeds $\pm c$.

Finite-Volume method for Maxwell equations

- Instead of using the Yee-cell one can solve Maxwell equations using finite-volume methods developed in aerospace and fluid mechanics.
- In these schemes one uses the local characterstic direction to "upwind" values at cell faces, adding stability to the scheme when simulating small-scale features.
- Finite-volume schemes are as cheap (or expensive) as Yell-cell based FDTD schemes and are also easy to implement for Maxwell equations. However, they suffer from some disadvantages.
- First, it is very hard to ensure divergence relations are maintained. One needs to correct the divergence errors somehow, by adding some additional equations to the system.
- Energy is not conserved by finite-volume schemes that use upwinding. Special choices of basis-functions can be used to construct energy conserving schemes, but these have other issues (also shared by FDTD schemes).
- However, in some situations, FV based Maxwell solvers are useful and have been successfully applied in many large-scale problems.

Choice of numerical fluxes for Maxwell equations impacts energy conservation

The electromagnetic energy is given by

$$\mathcal{E} = \frac{\epsilon_0}{2} E_y^2 + \frac{1}{2\mu_0} B_z^2$$

Notice that this is the L_2 norm of the electromagnetic field.

- Hence, as we will show tomorrow, if we use upwinding to compute numerical fluxes, the *electromagnetic energy will decay*.
- If we use central fluxes (average left/right values) then the EM energy will remain conserved by the *time-continuous* scheme. However, the Runge-Kutta time-stepping will add small diffusion that will decay the total energy a little.
- However, the energy decay rate will be *independent* of the spatial resolution and will reduce with smaller time-steps.