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On the CFL limit for stability of the Hamilton–Jacobi–Bellman equation

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On the CFL limit for stability of the Hamilton–Jacobi–Bellman equation

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Contents

The objective of this technical report is to describe the Courant–Friedrichs–Levy (CFL) limit for stability, as it applies to the solution of the Hamilton–Jacobi–Bellman equation with explicit finite difference methods. Recently Schneider et al. [2022] demonstrated that the Hamilton–Jacobi–Bellman equation for optimal control can be recast in the form of a Schrödinger equation.[1] Finite difference methods for solving Schrödinger-type equations are often either of the Crank-Nicolson type (implicit second order) or the Euler type (explicit first order) [Wu, 1996]. Another consideration is that conservative numerical methods – methods that preserve mass or energy – are frequently desirable for solving the nonlinear Schrödinger equation. The Crank–Nicolson method is a commonly used example of a method that preserves conservation laws [Antoine et al., 2013, Bao and Cai, 2013, Gong et al., 2017, Wang and Wang, 2018, Henning and Wärnegård, 2021]. As an implicit method, the Crank–Nicolson method is also unconditionally stable; in contrast, most of the conventional explicit schemes, including Euler-type schemes, are unconditionally unstable for Schrödinger-type equations [Chan et al., 1986]

This work is pedagogical in nature. We survey the literature on numerically solving Schrödinger-type equations, and explore stability limits of unstable. We begin with a description of an Euler-type explicit integration scheme where the stability of the numerical scheme is limited.

1 | Introduction to explicit time integration of the Schrödinger equation

Let us consider the solution of the one-dimensional Schrödinger equation, namely

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi(t,x)\ . \tag{1.1}$$

A first-order Euler method can be used to discretize the time derivative in this equation, in the following way

$$\frac{\partial}{\partial t}\psi(t,x) = \frac{\Delta\psi}{\Delta t} = \frac{\psi_{i+1,j}-\psi_{i,j}}{t_{i+1}-t_i} + \mathcal{O}\left((t_{i+1}-t_i)\frac{\partial^2}{\partial t^2}\psi(t,x)\right)\ . \tag{1.2}$$

Here $i = 0, 1, 2, 3, ...N$ is a discretization of time. This is described as a first-order method because the error is proportional to the time-step $\Delta t = t_{i+1} - t_i$ to the power of one.
A second-order central scheme is often used to discretize the second order spatial derivative. We derive that by beginning with a first-order Euler step

$$\frac{\partial}{\partial x}\psi(t,x) = \frac{\psi_{i,j+1}-\psi_{i,j}}{x_{j+1}-x_j}\ . \tag{1.3}$$

Here $j = 0, 1, 2, 3, ...M$ is a discretization of the spatial coordinate. We then apply this to obtain the second derivative

$$\frac{\partial^2}{\partial x^2}\psi(t,x) \quad = \quad \left(\frac{\psi_{i,j+1}-\psi_{i,j}}{x_{j+1}-x_j} - \frac{\psi_{i,j}-\psi_{i,j-1}}{x_j-x_{j-1}}\right)\frac{1}{x_{j+1}-x_j}\ . \tag{1.4}$$

[1] A large body of literature has been devoted to the well-posedness of the Schrödinger equation in various formulations. Here we assert that the simple one-dimensional example problem we examine is well-posed without further examination.

If the spacing in x is regular, *i.e.* $x_{j+1} - x_j = x_j - x_{j-1} = \Delta x$, we can combine these neatly so that

$$\frac{\partial^2}{\partial x^2}\psi(t,x) = \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{\Delta x^2} + \mathcal{O}\left(\Delta x^2 \frac{\partial^4}{\partial x^4}\psi(t,x)\right) . \tag{1.5}$$

This is described as a second-order method because the error is proportional to the grid size $\Delta x = x_{j+1} - x_j$ to the power of two. This numerical scheme involves values of ψ at three spacial points and two time points, which is displayed on a plot in Figure 1.1. This is typically described as the *stencil*. The usual way to confirm the order of a method is to run several simulations with different Δx and Δt, then compare the solutions using a function Err$= |\psi_{\text{smallest}} - \psi_n|$. Here ψ_{smallest} represents the solution with the smallest grid spacing, and thus smallest error, and ψ_n represents another grid. Plots can then be made of Err vs. Δx and vs. Δt.

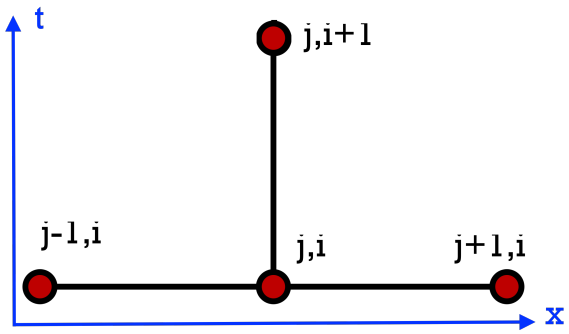

Figure 1.1: Stencil for this 4-point discretization scheme.

2 | Explicit schemes and the concept of numerical stability

The one-dimensional Schrödinger equation in eq. (1.1) can be expressed

$$\frac{\psi_{i+1,j} - \psi_{i,j}}{\Delta t} = F(\psi)_i . \tag{2.1}$$

This allows for the convenient re-arranging of terms

$$\psi_{i+1,j} = \psi_{i,j} + \Delta t F(\psi)_i . \tag{2.2}$$

The right hand side of this equation is entirely at time point i; thus eq. (2.2) is a formula that provides the value of ψ at the future step $i+1$ based only on data available at the current step i. Such schemes are known as explicit numerical schemes, as opposed to an implicit numerical scheme. Explicit integration methods can become unstable when the grid resolution (smaller Δx) cannot "keep up" to resolve the movement of the resolved quantity ψ; the grid spacing then needs to be made finer as ψ moves more rapidly. The movement of ψ through a grid characterized by Δx thus sets an upper limit on the time steps Δt

$$\Delta t_{\text{max}} = C_{\text{CFL}} \frac{\Delta x}{u_{\text{effective}}} . \tag{2.3}$$

This is typically referred to as the CFL condition, and the non-dimensional constant C_{CFL} is called the CFL number or the Courant number [e.g. Moura and Kubrusly, 2012]. When the CFL condition is violated, the numerical integration will typically yield NaNs. In practice Δt is often chosen to be 5–10 times less than Δt_{max} because this provides a lower error, with a comfortable margin for the stability of the solution. This formula contains a term $u_{\text{effective}}$, an effective velocity that tracks the movement of ψ through the grid. This is the most intuitive way to think of the CFL number: as a ratio between the physical velocity and the velocity that can be resolved by the grid. Re-arranging terms, the effective velocity is expressed

$$u_{\text{effective}} = C_{\text{CFL}} \frac{\Delta x}{\Delta t} . \tag{2.4}$$

For the Schrödinger equation [Shen et al., 2013, Bambusi et al., 2013, Huang et al., 2015, Rydin et al., 2021, Ryu et al., 2016, Tan and Heh, 2024], two different possibilities for the Schrödinger CFL number have been published

$$C_{\mathsf{CFL},1} = \frac{\hbar}{m}\frac{\Delta t}{\Delta x^2} \quad \text{and} \quad C_{\mathsf{CFL},2} = \sqrt{\frac{\hbar}{m}\frac{\Delta t}{\Delta x^2}} \; . \tag{2.5}$$

These differ by the use of the square-root; formally what matters is the point where $C_{\mathsf{CFL}} = 1 = \sqrt{1}$, so it may be that this difference was not seen as important. However, comparing these to our typical expression of the CFL number above, these two formulations imply two different effective velocities

$$u_{\mathsf{effective},1} = \frac{\hbar}{m}\frac{\Delta t}{\Delta x^2}\frac{\Delta x}{\Delta t} = \frac{\hbar}{m}\frac{1}{\Delta x} \; . \tag{2.6}$$

or

$$u_{\mathsf{effective},2} = \sqrt{\frac{\hbar}{m}\frac{\Delta t}{\Delta x^2}}\frac{\Delta x}{\Delta t} = \sqrt{\frac{\hbar}{m}\frac{1}{\Delta t}} \; . \tag{2.7}$$

The question of which effective velocity is correct will dictate how close to the CFL number one wishes to run. This could be determined in an experimental fashion, by examining the error of solutions for a range of time steps and grid spacings.

3 | The influence of the magnitude of the potential

In a situation where the potential V in the Schrödinger eq. (1.1) is much larger than the Laplacian term, it will dominate the effective velocity and the limit of numerical stability. Consider the CFL number definition

$$C_{\mathsf{CFL},1} = \frac{\hbar}{m}\frac{\Delta t}{\Delta x^2} \leq 1 \; . \tag{3.1}$$

The formulation of this corresponds to a balance between the time derivative and Laplacian terms in eq. (1.1), namely

$$\frac{\hbar}{\Delta t} \geq \frac{\hbar^2}{m}\frac{1}{\Delta x^2} \; . \tag{3.2}$$

Such a balance neglects the impact of the potential V on the stability. As a pedagogical aid, in the case where V dominates, we argue dimensionally that one would need to find some constant c related to the potential V, such that

$$\frac{\hbar}{\Delta t} \geq \frac{c}{\Delta x^2} \; . \tag{3.3}$$

The constant $\hbar$ has units of Joules-seconds. The constant c should have units of Joules-times-meters-squared. One possible way to treat this would be to use a global length scale of the system L so that

$$c = V_{\mathsf{max}} L^2 \; . \tag{3.4}$$

For a two-dimensional square grid, for example, L^2 could be $L_x L_y$. This would result in a CFL stability requirement of

$$C_{\mathsf{CFL},3a} = \frac{c}{\hbar}\frac{\Delta t}{\Delta x^2} = \frac{V_{\mathsf{max}} L_x L_y}{\hbar}\frac{\Delta t}{\Delta x^2} \tag{3.5}$$

$$= \frac{V_{\mathsf{max}}\Delta t}{\hbar}\frac{L_x L_y}{\Delta x^2} \leq 1 \; . \tag{3.6}$$

Another alternative would be to use a local length scale like the grid spacing as the important length scale

$$c = V_{\mathsf{max}} \Delta x^2 \; , \tag{3.7}$$

which would reduce more cleanly to

$$C_{\mathsf{CFL},3b} = \frac{V_{\mathsf{max}}\Delta t}{\hbar} \leq 1 \ . \tag{3.8}$$

Recently Tan and Heh [2024] has addressed the question of how to deal with the CFL number in the presence of additional potentials, both vector and scalar. They perform the Von Neumann stability analysis of the problem, which is a rigorous mathematical approach. Their result for the CFL number in eq. (51) of their work, recast in our notation, is

$$C_{\mathsf{CFL},4} = \frac{\Delta t}{2\hbar}\mathsf{max}\left(|H_{k,\mathsf{max}}|, |H_{k,\mathsf{min}}|\right) \ . \tag{3.9}$$

Here the absolute values deal with the case where a potential function is large in magnitude but negative. Neglecting the additional vector potential that Tan and Heh [2024] also treat and expressing their electric potential in terms of the Schrödinger potential, these additional functions are defined in their eqs. (39) and (40)

$$H_{k,\mathsf{max}} = \frac{\hbar^2}{m}\frac{2}{\Delta x^2} + V_{\mathsf{max}} \ , \tag{3.10}$$

$$H_{k,\mathsf{min}} = V_{\mathsf{min}} \ . \tag{3.11}$$

Here we note that, in the case of vanishing potential V, $C_{\mathsf{CFL},1}$ from eq. (2.5) is recovered.
The case that we encounter often in our work is one where $V_{\mathsf{min}} = 0$ but $V_{\mathsf{max}} \gg \frac{\hbar^2}{m}\frac{2}{\Delta x^2}$. In this case, the result of Tan and Heh [2024] implies that

$$C_{\mathsf{CFL},4} \to \frac{\Delta t}{\hbar}V_{\mathsf{max}} \ . \tag{3.12}$$

This result is identical to our second dimensional guess in eq. (3.8), which used the grid spacing to obtain the correct dimensions of the CFL number. An effective velocity in the case where $V_{\mathsf{min}} = 0$ would then be

$$u_{\mathsf{effective},4} = \frac{\Delta t}{2\hbar}\left(\frac{\hbar^2}{m}\frac{2}{\Delta x^2} + V_{\mathsf{max}}\right)\frac{\Delta x}{\Delta t} \ , \tag{3.13}$$

$$= \frac{\Delta t}{\hbar}\frac{\hbar^2}{m}\frac{1}{\Delta x^2}\frac{\Delta x}{\Delta t} + \frac{\Delta t}{2\hbar}V_{\mathsf{max}}\frac{\Delta x}{\Delta t} \ , \tag{3.14}$$

$$= \frac{\hbar}{m}\frac{1}{\Delta x} + V_{\mathsf{max}}\frac{\Delta x}{2\hbar} \ . \tag{3.15}$$

The form of this effective velocity nicely clarifies that for larger V_{max}, a smaller Δx is needed to maintain a given resolution of $u_{\mathsf{effective},4}$. It also demonstrates that, for a fixed Δx, the effective velocity becomes larger as V_{max} is increased. In that case the time step of the calculation will need to be reduced to maintain the CFL number.

4 | Summary

While Euler type finite difference methods and explicit Runge-Kutta schemes can be and sometimes are applied to for the solution of the Schrödinger equation [e.g. Caplan and Carretero-González, 2013], those methods can have undesirable outcomes as far as stability and conservation of mass or energy. Some works have taken care to reformulate those methods to improve their solution of the Schrödinger equation [Cui et al., 2021]. Implicit methods, including the standard workhorse methods of Crank-Nicholson, Leapfrog schemes, or the use of staggered grids are also commonly used to mitigate these problems.

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