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Flow dynamics of complex fluids using numerical methods

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Abstract
Modelling can be done by means of theory, laboratory prototypes, or numerical methods and various techniques often these theoretical models often use, especially in complicated many-body problems, macroscopic equations to describe the physical phenomenon at hand, thereby neglecting many microscopic details of the system. Numerical methods usually lack this problem, and they are normally inexpensive in comparison with laboratory experiments. Numerical methods also provide efficient benchmarks for theoretical models. They can address details of complex phenomena that can be difficult for theory as well as for experiments.

Keywords: Macroscopic equations, efficient benchmarks and numerical methods

Introduction
We are surrounded by a variety of fluids in our everyday life. Besides water and air, it is common to deal with fluids with peculiar behaviours such as gel, mayonnaise, ketchup and toothpaste, while water, oil and other so-called simple (Newtonian) fluids "regularly" flow when we apply a force, the response is different for complex fluids. In some cases, we need to apply a stress larger than a certain threshold for the material to start flowing, for example, to extract toothpaste from the tube; the same paste would behave as a solid on the toothbrush when exposed only to the gravitational force. In other cases the history of past deformations has a role in the present behaviour [2, 3, 4]. In some applications, complex fluids can be successfully modelled just by considering that their response is related to the memory of the deformation rate history; in other words, they have a time-dependent viscosity if exposed to a constant value of the shear rate [7, 8]. Two main kinds of such fluids can be identified: thixotropic fluids whose effective viscosity decreases with the accumulated strain and rheopectic fluids, whose effective viscosity increases with the accumulated strain [6].
Why computer simulations: Modelling can be done by means of theory, laboratory prototypes, or numerical techniques. The theoretical models often use, especially in complicated many-body problems, macroscopic equations to describe the physical phenomenon at hand, thereby neglecting many microscopic details of the system. Numerical methods usually lack this problem, and they are normally inexpensive in comparison with laboratory experiments. Numerical methods also provide efficient benchmarks for theoretical models [7]. They can address details of complex phenomena that can be difficult for theory as well as for experiments.
Experimental difficulties may arise from complexity, expenses, danger or hazardous condition of the phenomenon. For example, in a dense suspension flow, measuring of the local instantaneous flow quantities such as velocities and stresses, separately for both phases, is not feasible. Such information can however be attained from numerical simulations of the suspension flow. Also, numerical techniques are versatile enough to combine or distinguish different physical phenomena, which have made them popular tools of analysis [8, 9, 10].
The results of numerical techniques are however subject to uncertainties that arise from *e.g.* the flow model and the numerical techniques used. Care must therefore be taken when expressing the results of numerical simulations, and they should be supported by theoretical and/or experimental benchmarks.
In this paper mainly two numerical techniques have been used for simulation of flow problems, especially multiphase phenomena, starting from microscale molecular dynamics of

spherical particles up to mesoscale simulations of capillary rise phenomena, shear or Poiseuille flow of suspension, and clogging of suspension flow in channels. In each case, experimental or theoretical evidence have been used for benchmarking the method. Numerical methods therefore have a wide range of applications in numerous scientific fields. In physics, for instance, these methods are used to obtain approximate solutions of important differential equations such as the diffusion and wave equation and also discussed to understanding the numerical methods and the numerical solutions of widely used equations in physics, such as the wave and heat equation, are known and there are different methods to solve them.

Numerical simulations at different relevant length scales

In colloidal suspensions, for example, there are three important length scales, the microscopic size of the relevant molecules, the mesoscopic scale related to the size of colloidal particles, and the macroscopic scale which is that of the effective fluid motion. In particulate suspensions the size of the suspended particles can be in the macroscopic scale.

As the relevant length scales in suspensions differ by several orders of magnitude, it is not possible to simulate them by including details at all these length scales. All numerical methods are based on one basic length scale. For macroscopic modelling the suspension must be regarded as a continuum medium, and the description is in terms of the variations of the macroscopic velocity, density and pressure (and temperature) with space and time.

The macroscopic scale simulations, which usually go under the general name of computational fluid dynamics [22, 23] (CFD), use macroscopic continuum equations like the Navier-Stokes equation, whose solutions are very sensitive to the boundary conditions. Various CFD methods offer successful simulation tools for different single-phase fluid dynamics problems within many branches of science and engineering [24]. For suspensions however, these methods are difficult to apply due to the moving boundaries of the suspended particles. In recent finite-element simulations it has been possible to analyse only cases with small numbers of particles [25, 26], or simulations were limited to simple and regular particle geometries [27, 28].

An attempt to circumvent the problems with moving or otherwise complex boundaries is provided by lattice-based methods which are based on a mesoscopic basic unit of the system, typically of the order of a micrometer, but depending of course on the details of the system. There are a few popular methods, which use this approach, and they include the lattice-gas automata (LGA), its alteration the lattice- Boltzmann method (LBM) and the method of dissipative particle dynamics (DPD). Each of these methods has its advantages and limitations. Use of mesoscale simulation techniques can allow the exact treatment of small-scale macroscopic systems, and can be used to effectively study *e.g.* the rheology of colloidal suspensions and the dynamics of interfaces. Simulations at the microscopic level have also been attempted in order to understand the truly microscopic behaviour of liquids.

As Monte Carlo simulations are not suitable to describe the dynamic properties [29], the prevalent microscopic simulation method is that of molecular dynamics (MD) [3]. MD methods that apply different numerical techniques have thus been developed to study the dynamical behaviour of a large number of applications, see *e.g.* [29, 30, 31, 32, 33]. MD simulations are computationally very demanding, and obtaining bulk properties of, for example, suspensions, would mean using billions of particles [34].

We review below in more detail the MD method and the LB method used in this work.

Molecular Dynamics Method

Molecular dynamics (MD) provides a reasonable physical description of granular materials including their macroscopic averaged properties, hydrodynamics, and all fluctuations, using only linear dynamics.

A (granular) system of spheres is initialised by first randomly placing the spheres in a box. Then overlapping spheres are randomly moved until no overlaps remain. Thereafter the system evolves in time according to Newton's equations of motion under chosen initial and boundary conditions, and applied forces and fields.

Four major steps are needed to enrol a hard-sphere molecular dynamics simulation: motion control, determination of collision times, collision dynamics, and calculation of the particle properties.

Motion control

The motion of a rigid body of mass m and acceleration a = F / *m*, due to an external force F, follows Newton's Second Law. The total kinetic energy and momentum of the system must be conserved, as well as its total angular momentum where r*i* is the position, v*i* the velocity and ω*i* the angular velocity of particle *i*. *I* is moment of inertia of the particles, which is 2*mR*2 / 5 for a sphere and *mR*2 /2 for disk, with *R* the respective radius of the particle.

Verlet algorithm

For the positions **r** the most popular time integration algorithm is the so-called Verlet algorithm. Forward and backward Taylor expansions of the position as a function of time can be written in the forms.

Adding the above two expressions gives the new position after time δt,

$$\mathbf{r}(t+\delta t)=\mathbf{r}(t)+\delta t\mathbf{v}(t)+(1/2)\delta t^2\mathbf{a}(t)+O(\delta t^3), \quad (1)$$

$$\mathbf{r}(t-\delta t)=\mathbf{r}(t)-\delta t\mathbf{v}(t)+(1/2)\delta t^2\mathbf{a}(t)+O(\delta t^3).$$

$$\mathbf{r}(t+\delta t)=2\mathbf{r}(t)-\mathbf{r}(t-\delta t)+\delta t^2\mathbf{a}(t)+O(\delta t^3). \quad (2)$$

There are several methods to make Eq. (2.3) explicit, the most common of these being the so-called half-step 'leap-frog' scheme [31],

So the velocity of the mid-step may be written as

$$\mathbf{r}\left(t+\delta t\right)=\mathbf{r}\left(t\right)+\delta t\mathbf{v}\left(t+\delta t/2\right). \quad (3)$$

$$\mathbf{v}\left(t+\delta t/2\right)=\mathbf{v}\left(t-\delta t/2\right)+\frac{\mathbf{F}\left(t\right)}{m}\delta t. \quad (4)$$

Similarly for the angle (orientation) of a particle (in the case of non- spherical particles) and for its angular velocity

Later during the step, the current velocities are determined from and similarly for the angular velocities.

$$\boldsymbol{\theta}\left(t+\delta t\right)=\boldsymbol{\theta}\left(t\right)+\delta t\boldsymbol{\omega}\left(t+\delta t/2\right), \quad (5)$$

$$\boldsymbol{\omega}(t+\delta t\,2)=\boldsymbol{\omega}(t-\delta t\,2)+\frac{\mathbf{T}(t)}{I}\,\delta t. \quad (6)$$

$$\mathbf{v}(t)=\frac{1}{2}(\mathbf{v}(t+\delta t\,2)+\mathbf{v}(t-\delta t\,2)), \quad (7)$$

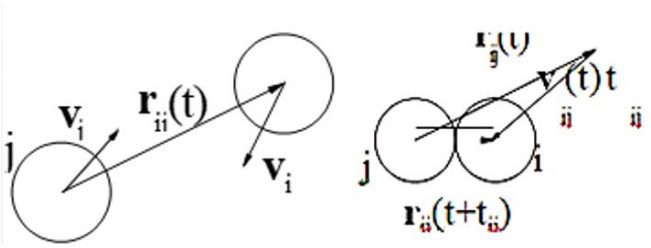

Fig 1: Smooth hard-sphere collision: situation before and at the collision moment.

Numerical analysis and discretization

Finite difference methods (FDMs) are frequently used in numerical analysis to solve partial differential equations. In these methods a PDE is solved on a grid of discrete points with, for instance, $x_n = n\Delta x$ and $t_j = j\Delta t$, where n and j are integers [1, 2, 3]. Continuous derivatives are then replaced by finite difference approximations. The solution of complex differential equations can be obtained by dividing space-time into a discrete set of points in this manner. The finite difference equation, for example, can be a forward, backward or centered difference. Each choice needs to be tested in various ways such as its stability, accuracy and speed.

A numerical method is stable if the errors in the method do not increase as the solution moves forward in time. There can be several sources of errors in a numerical method. These include, for example, the truncation and round-off errors. The round-off error results from finite precision representation of real numbers on a computer. Truncation errors arise from representing continuous derivatives with finite differences which involves truncating termsfrom the Taylor series. The leading terms in the truncation error determines the accuracy of a FDM.

What makes a particular numerical method feasible is its consistency, i.e., whether the finite difference equation (FDE) approaches the PDE as the interval size vanishes. In other words, a numerical scheme is consistent if the truncation error goes to zero as Δx, Δt 0. Similarly, convergence is also important and requires the solution of the FDE to converge to the exact solution in the limit Δx, Δt 0 According to the Lax equivalence theorem, if a finite difference method is consistent (FDE approaches the PDE as grid interval size approaches zero) and stable (errors do not grow) than convergence (discrete solution converges to the actual solution as grid interval size approaches zero) is guaranteed. In short, consistency and stability imply convergence.

The most convenient way to test the stability of a finite difference method is by employing the Von Neumann stability analysis. In this method we test how a Fourier mode behaves on the grid. Compared to other methods, such as the matrix method, this analysis is a convenient way to test the stability of a method. One short coming of this method is that it ignores the boundary conditions. This is why the limits obtained are necessary but not sufficient to guarantee stability. But this short coming, in a way, is useful in our case since the limits we get would be independent of the boundary conditions of the problem. In FDMs, a first order derivative in space and time can be approximated by a forward time and space difference as follows

$$\frac{\partial u}{\partial x} \approx \frac{u_{j+1}-u_j}{\Delta x}, \quad (8)$$

$$\frac{\partial u}{\partial t} \approx \frac{u^{n+1}-u^n}{\Delta t}, \quad (9)$$

Where, i = 0, 1, 2... M and n = 0, 1, 2... N. Amongst several methods used, two

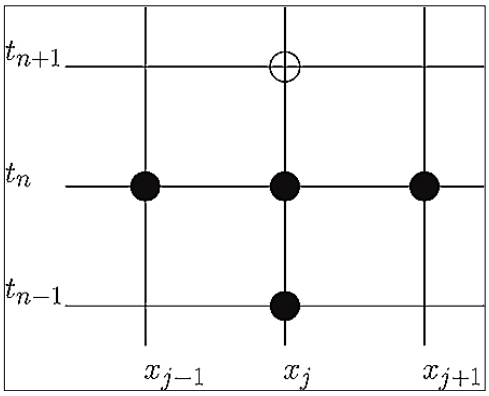

Fig 2: Stencil for the FDM of the 1-D wave equation.

It represents the expression given in equation (9). Important ones are the explicit and implicit methods. Each of these has its own benefits in terms of stability, speed and accuracy of the solution. The explicit method, which is a forward difference method, is fast but less stable since it usually requires limits on the space and time step sizes. In the explicit method the state of the system at a time t_{n+1} is evaluated from the state at time t_n or a prior time (t_{n-1},..), namely

$$u_{n+1} = f(u_n, t_n). \quad (10)$$

The implicit method, which is a backward difference method, is slow and more numerically stable. In this method the state of the system at a later time is not an explicit function of the state at earlier times. For this case, therefore, the state of the system at a later time would typically be given by

$$u_{n+1} = f(u_n, u_{n+1}, t_{n+1}). \quad (11)$$

The factor that makes this method more stable is that the time step is usually not constrained by a stability condition. A larger time step Δt can therefore be used to solve the system. However the above equation is usually a non-linear system of equations and needs additional time to solve. Therefore this method is slower than the explicit method. We will focus on the explicit method in the following sections.

Wave equation: Speed Limit

In this section, we show that employing the explicit finite difference method in solving the wave equation can lead to a limit on the propagation speed of waves. The wave equation is a hyperbolic PDE and describes the propagation of waves. Hyper- bolic PDEs describe systems with a finite speed of propagation. Consider the one dimensional wave equation:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}. \tag{12}$$

We can solve the wave equation using the explicit method by replacing the derivatives by centered differences in space and time (leapfrog method) as follows

$$\frac{\partial^2 u}{\partial x^2} = \frac{u^n_{j+1} - 2u^n_j + u^n_{j-1} + O(\Delta x^2),}{\Delta x^2} \tag{13}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{u^{n+1}_j - 2u^n_j + u^{n-1}_j + O(\Delta t^2),}{\Delta t^2} \tag{14}$$

Where, $u^n_j \equiv u(x_j, t_n)$. The truncation error in this case is $O(\Delta x^2)$ and $O(\Delta t^2)$ and arises from truncating terms from the Taylor expansion. The leading terms in the truncation error of this method are given by

$$T^n_j = \frac{1}{12} v^2 (\Delta x)^2 u_{xxxx} - \frac{1}{12} (\Delta t)^2 u \tag{15}$$

Dropping the truncation error we get the following approximation

$$u^{n+1}_j = r^2(u^n_{j+1} - u^n_{j-1}) + 2(1 - r^2)u^n_j - u^{n-1}_j, \tag{16}$$

Where, $r = v\Delta t/\Delta x$. To study the stability of this method we use the Von Neumann or Fourier analysis. We look for solutions of the form

$$u^n_j = e^{ik(j\Delta x)} G^n(\Delta t, \Delta x, k), \tag{17}$$

and get the following equation for the growth factor

$$G^2 - 2[1 - 2r^2 \sin^2(k\Delta x)]G + 1 = 0. \tag{18}$$

The requirement that $|G| \leq 1$ leads to the following CFL condition for stability

$$v \leq \frac{\Delta x}{\Delta t} \tag{19}$$

In 3 dimensions, the CFL condition for stability is given by [2]

$$\Sigma v \frac{1}{\Delta t} \leq \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}^{\Sigma - 1/2} \equiv \Delta v_{grid}, \tag{20}$$

Which for a cubic grid ($\Delta x = \Delta y = \Delta z$) will be

$$v \leq \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t} \equiv \Delta v_{grid}. \tag{21}$$

Here Δv_{grid} is the average grid velocity and can be viewed as the speed with which information moves across the grid [4]. We can view equation (12) as a limit on the velocity of the wave. It requires the domain of dependence of the wave equation to be within the numerical domain of dependence. The question of making Δx and Δt smaller is an important one in numerical analysis. As Δt is made smaller the time for the computation increases rapidly. So, practicality also dictates Δt not to be too small.

As described in section 2, in order for the explicit method to be feasible it should also be convergent. The truncation error for this method given in equation (8) is $O(\Delta x^2, \Delta t^2)$ and vanishes in the limit $\Delta x, \Delta t \to 0$. However, as the grid interval size approaches zero we need to specify the relationship between Δx and Δt. We approach $\Delta x, \Delta t \to 0$ such that the ratio $\Delta x/\Delta t$ is kept constant. This is referred to as the *refinement path* [3]. Furthermore, the speed with which numerical information for the explicit method flows on the grid is different from the physical speed of information transfer. Herein we will assume that the numerical speed of information becomes equal to the physical speed of information as the grid approaches the continuum limit. In other words, numerical causality merges with physical causality in the continuum limit. Therefore, taking the limit $\Delta x, \Delta t \to 0$ while keeping the instantaneous velocity v_{grid} constant we get

$$v \leq v_{grid} = c,$$

$$v \leq c, \tag{22}$$

Where, the constant c is the speed of light. It is the limiting speed with which information travels in the continuum limit. Therefore, by assuming the numerical speed to be the same as the physical speed limit as $\Delta x, \Delta t \to 0$, we get a limit on the speed of waves which obeys causality. This limit also ensures the stability of the explicit method.

Note that the numerical solution of Maxwell's equation is obtained using the Finite Domain Time Difference (FDTD) method and results in a conditional stability limit similar toequation (13) (see, for example, chapter 4 of ref. [5]). For the case of

Maxwell's equation the condition (13) becomes equality in the continuum limit.

The domain of dependence (DoD) and range of influence (RoI) of a hyperbolic PDE is shown in Fig. 3. The DoD of a point in the solution domain is the set of points on which the solution at a particular point depends. Similarly, the RoI is the solution domain which is affected by the solution at a particular point. The

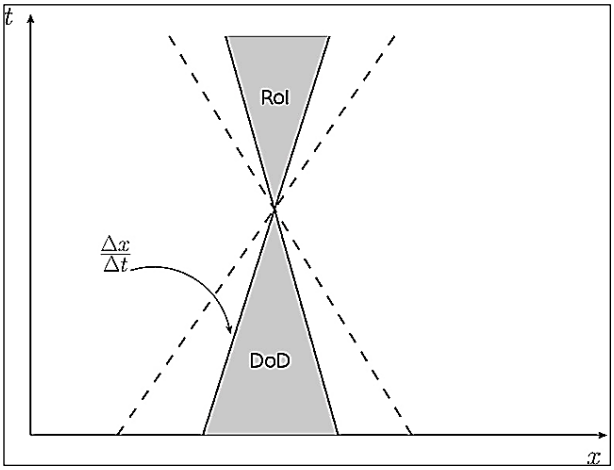

Fig 3: Figure shows the domain of dependence and range of influence for the 1-D wave equation.

The gray region bounded by the solid line represents the continuous PDE whereas the dashed line shows the boundary of the numerical solution. The CFL condition in equation (12) requires the DoD of the PDE to be contained within the DoD of the numerical solution. As the grid interval size approaches zero the slope of the dashed boundary representing the numerical PDE should approach the limiting speed with which information can be transferred across the grid.

CFL condition in equation (12) also ensures that the PDE domain of dependence stays within the numerical domain of dependence as shown in Fig.3. The gray region is the DoD of the PDE which is contained in the DoD of the numerical solution. The numerical value of the solution at a node (x_i, t_n) depends on the values at the nodes lying within the numerical domain of dependence. The wave equation therefore obeys causality and, particularly, in the continuum limit, equation (15) guarantees that physical causality is always satisfied.

The above equation implies that in order for the numerical solution of the Schrodinger equation be stable the grid interval must satisfy the above limit. The above limit is valid for any grid size but for the method to be viable this should particularly be true for the limit Δx, Δt 0. As mentioned earlier, convergence is an important condition for a FDM to be viable. Therefore, in the limit Δx, Δt 0 we approach the quantum realm and in addition make sure that our difference method is convergent.

Refinement path: As we approach the limit Δx, $\Delta t \rightarrow 0$ we should also specify the relationship between Δx and Δt. As we approach the limit Δx, $\Delta t \rightarrow 0$, the truncation error approaches zero, and the grid velocity v_{grid} remains constant. Here v_{grid} is the speed with which numerical information flows on the grid. As the mesh interval size approaches zero this is the limiting speed with which information can be transmitted on the grid. Therefore, Δx and $\Delta t \rightarrow 0$ such that $v_{grid} = c$ and the limits on the length and time intervals are

$$\Delta t \geq \frac{2\mathrm{k},}{mc^2} \tag{23}$$

Or

$$\Delta x \geq 2\sqrt{3\lambda_c}, \tag{24}$$

Where, $\lambda_c = \mathrm{k}/mc$ is the reduced Compton wavelength. Another implication of these limits is that the truncation error in the FDE is $O((\Delta x)^2)$ " $O(\lambda^2)$. Note that we have assumed a cubic grid to derive this limit and similar limits would be true for Δy and Δz.

The stability condition for the Schrodinger equation is derived using the FDTD method. The limit in equation (28) for that case is k/m instead of $2\mathrm{k}/m$. Similarly, other higher order methods [12] also lead to stability condition similar to equation (28). Therefore the stability requirements on the limit on grid interval size for various schemes can be written as

$$\Delta x \geq a_0 \lambda_c, \tag{25}$$

Where, a_0 is a constant of order unity and varies from one explicit scheme to another. Hence, in addition to viewing Compton wavelength as a limitation on measuring the position of a particle it can also be viewed as the minimum grid length that can be resolved in order to ensure causality in the stability analysis of the Schrodinger equation. Furthermore, assuming a minimum length in this manner renders the theory the same causal structure as the wave equation.

The explicit method and its implications

We have seen in previous sections that the explicit method can shed light on some important ideas in physics. It is important to note the difference between the explicit and implicit method. The explicit method is fast but less stable and requires small time steps for more accuracy. The implicit method is slower, more stable and allows a larger time-step. In addition to these factors, the explicit method has some important features that make it different from implicit methods. Following can be the two reasons as to why the explicit method yields these important relationships in contrast to the implicit methods:

1. The solutions at present time are explicit functions of solutions of past.
2. The solutions at a grid location do not instantaneously effects the solutions at the entire grid [4]. This implies a finite speed of information transfer which is called the grid speed.

We can better understand these points by considering the example of the heat equation which does not limit the speed of heat transmission. However, when using the explicit finite difference method in seeking the numerical solution of a differential equation this might not necessarily hold. The heat equation, for instance, has the instant messaging property but it does not hold when we employ the explicit method to solve it [4]. The speed with which information travels through the grid is $\Delta x/\Delta t$ and not infinite. This, of course, implies that the explicit method is not the perfect method to solve the heat equation but at the same time it does render the system a causal structure. The implicit method, however, does have the instant messaging property and this is apparently the reason it is unconditionally stable. Therefore, the numerical propagation speed of information for explicit methods is finite whereas that of implicit method is infinite.

The Schrodinger's equation is similar to the heat equation but with an imaginary diffusion coefficient. In other words although it satisfies the mathematical test of a parabolic equation which describes diffusive processes it allows plane wave solutions. In both cases, however, the explicit finite difference method when employed allows only a finite speed of propagation.

Conclusion

We discussed how the techniques used in numerical analysis might be more than tools to obtain solutions of partial differential equations. Finite difference methods and, in particular, explicit methods might help us further understand some fundamental ideas in physics. Explicit methods used in solving finite difference equations are often conditionally stable. The explicit finite difference method for the wave equation can lead to a limit on the speed of waves to be less than the grid speed. As the grid approaches the continuum limit, we assumed that the idea of numerical causality merges with physical causality and the speed of numerical information transfer be- comes equal to the physical speed limit, i.e., the speed of light. This leads to a limit on the speed of waves that ensures stability of the explicit method. Similarly, the explicit method of the Schrodinger equation yields a limit on the minimum length and time interval. To ensure convergence of the explicit method, we approach zero interval size along the refinement path $v_{grid} = c$. This can be understood as follows. In the continuum limit, the grid interval, being a measure of the position of the particle, suffers from similar limitations as those obtained in quantum mechanics. These limits result from the Von Neumann stability analysis. Therefore, the explicit method endows a causal structure to the Schrodinger equation which is similar to that of the wave equation and as a result implies the minimum grid interval size to be of the order of Compton's wavelength to guarantee stability.

Finally, we also discussed the importance of the explicit finite difference method in numerical analysis. The Von Neumann stability analysis used to test the stability of explicit methods implies that our conclusions are essentially independent of boundary conditions. The fact that this method preserves the finite speed of information transfer can be two important reasons it yields important limits on the spatial and temporal grid interval sizes.

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