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COMMENT

Non-negativity condition for cellular automata and other massively parallel computer algorithms

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Abstract. The importance of satisfying the non-negativity condition given in the original paper (1993 *J. Phys. A: Math. Gen.* **26** L209) in derivations and computer algorithms is noted. When the non-negativity condition is ignored, as was done by Gómez-Vilar and Solé, non-physical results may be obtained. In contrast, when the step sizes go to zero in a manner consistent with the non-negativity condition, it can be shown that the difference equations are pointwise consistent with the continuum equations of quantum theory.

A numerical method which used local rules of updating that required only the values of nearest-neighbouring grid points or sites at the previous time was recently presented for solving quantum equations [1]. The method also conserves probability and mass, and when properly used cannot produce results that grow without bound. In contrast with other local methods which can produce answers that grow without bound especially in regions where the potential is large, the new method may be suitable for use with massively parallel computers. The method is based on equations (1)–(12) of [1] and the paragraph of text following equation (12) of [1], which gives the procedure for determining the direction of transfer of mass between subsites and which explicitly states the essential non-negativity condition:

'We add the condition that the mass at any subsite cannot be less than zero.' [1]

This non-negativity condition was easily incorporated into the computer program. There are many ways in which this can be done. When the transfer rules (1)–(12) of [1] indicated a transfer of mass from a subsite which was larger than the mass at that subsite, the simplest way was to transfer no more mass than was available at the subsite. In that way the mass or probability never became negative. It was found that the resulting error could be made arbitrarily small by appropriately reducing the step sizes (the time step size was reduced more rapidly than the space step size). In this way excellent agreement was found with the exact solutions of the Schrödinger equation.

The non-negativity condition of [1] is an essential part of this method. Of course, in derivations the range of use of any equations employing equations (1)–(12) of [1] must be consistent with the non-negativity condition. Thus, equation (13) and (18) of [1] should not be used when the non-negativity condition is not satisfied. In their perturbation analysis, Gómez-Vilar and Solé [2] do use equations (13) and (18) of [1] when the non-negativity

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condition is not satisfied and thus it is not surprising that they derive physically meaningless results such as that probability can go to minus infinity.

The correct method of using equation (13) of [1] in derivations requires that the non-negativity condition be satisfied. For example, the pointwise consistency of this equation with non-relativistic quantum theory for vanishingly small step sizes can be demonstrated by requiring that as the time step size Δt approaches zero, the spatial step size Δx should approach zero by an equation such as

$$\Delta x = A(\Delta t)^{1/3}$$

where A is a positive constant. This condition guarantees that in the limit $\Delta t \to 0$ the non-negativity condition will be satisfied and thus equation (13) of [1] can be used in this limit. In contrast Gómez-Vilar and Solé [2] imposed no such conditions on their time and space step sizes as the step sizes approach zero and thus they violated the non-negativity condition explicitly stated in [1]. By violating the non-negativity condition they have used equation (13) of [1] outside its range of validity and have obtained invalid results.

To prove pointwise consistency, we note that the truncation error at subsite j at time t for equation (13) of [1] is

$$\epsilon_j = \frac{1}{\Delta t}\left[M_j - m_j + \frac{\overline{h}\Delta t}{\mu(\Delta x)^2}[(m_j n_{j-1})^{1/2} + (m_j n_{j+1})^{1/2} - 2(m_j n_j)^{1/2}] - 2V_j\frac{\Delta t}{\overline{h}}(m_j n_j)^{1/2}\right]$$
$$= \frac{1}{\Delta t}\left[M_j - m_j + \frac{\overline{h}}{\mu}\frac{\Delta t}{(\Delta x)^2}[a_j b_{j-1} + a_j b_{j+1} - 2a_j b_j] - 2V_j\frac{\Delta t}{\overline{h}}a_j b_j\right]$$

where V_j is the potential at site j and the amplitudes a_j and b_j are the real and imaginary parts of the wavefunction at site j as defined in [1]. In the limit of small time and spatial steps we have the Taylor series expansions

$$M_j = [a_j(t + \Delta t)]^2 = \left[a_j(t) + \Delta t\frac{\partial a_j}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2 a_j}{\partial t^2} + \cdots\right]^2$$

$$b_{j-1} + b_{j+1} - 2b_j = (\Delta x)^2\frac{\partial^2 b}{\partial x^2}(x,t) + \frac{(\Delta x)^4}{12}\frac{\partial^4 b}{\partial x^4} + \cdots$$

which, when combined with the expression for the truncation error gives us

$$\epsilon_j = \left[2a\frac{\partial a}{\partial t} + \frac{\overline{h}}{\mu}a\frac{\partial^2 b}{\partial x^2} - 2\frac{V}{\overline{h}}ab\right] + \Delta t\left[a\frac{\partial^2 a}{\partial t^2} + \frac{\partial a}{\partial t}\frac{\partial a}{\partial t}\right] + \frac{\overline{h}}{\mu}\frac{(\Delta x)^2}{12}a\frac{\partial^4 b}{\partial x^4} + \cdots.$$

As discussed in [1], the term in the first bracket is zero since it is the expression for the real and imaginary amplitudes of the Schrödinger equation. Thus the truncation error of the finite difference equation (13) of [1] is

$$\epsilon_j = \mathrm{O}(\Delta t) + \mathrm{O}((\Delta x)^2).$$

Thus, as the step sizes go to zero, the truncation error goes to zero. This derivation shows that the finite difference equation (13) of [1] is pointwise consistent with the continuum equations of non-relativistic quantum theory.

Gómez-Vilar and Solé also incorrectly claim without foundation that κ going to zero makes the method impracticable, where

$$\kappa = \frac{\overline{h}}{\mu}\frac{\Delta t}{\Delta x^2}.$$

That this type of claim is incorrect can easily be seem by referring to the very practical and widely used finite difference explicit method for solving the diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}.$$

In the finite difference equation for the explicit method the parameter

$$\beta = D\frac{\Delta t}{(\Delta x)^2}$$

occurs. Both β and κ have the same dependence on $\Delta t/(\Delta x)^2$. If we set

$$\Delta x = B(\Delta t)^{1/4}$$

where B is a positive constant and let the time step Δt go to zero, then β goes to zero and it is well known and easily proven that the explicit finite difference equation becomes pointwise consistent with the diffusion equation.

In summary, in both derivations and computer algorithms it is essential that the non-negativity condition given in the original paper [1] be satisfied. This was not done by Gómez-Vilar and Solé [2], and they obtained results that are non-physical. In contrast, when care is taken to satisfy the non-negativity condition, it can be shown that the difference equations are pointwise consistent with the continuum equations of quantum theory.

References

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