NUMERICAL INSTABILITY OF NEUTRON DIFFUSION FINITE-DIFFERENCE EQUATIONS

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Keywords: Numerical stability; Finite-difference equations; Neutron diffusion equation

ABSTRACT

The neutron diffusion kinetic equations including numerical errors introduced by explicit and implicit time-integration methods are derived. The impulse response functions based on these equations are demonstrated to investigate the numerical stability of the discretized systems. These demonstrations indicate unconditional stability for the implicit method but present the possibility of numerical instability for the explicit method. An upper limit of time-mesh spacing for the stability is formulated. This formula suggests that finer time-mesh should be specified with a decrease in space-mesh spacing. In a neutron non-multiplicative medium, further finer time-mesh is required than that in a multiplicative one.

1 . INTRODUCTION

In the choice of numerical time-integration scheme for initial value problem, not only the accuracy but the numerical stability should be considered. When a numerical scheme is applied to an initial value problem, a pseudo oscillation may appear in the solution. This oscillation originates from the numerical instability of the discretized differential equations and is physically of no significance. For the avoidance of the instability, numerical stability of applied scheme must be known, in advance. In the field of computational fluid dynamics, the numerical stability of finite-difference equations obtained by various time- and space-integration schemes has been investigated (*e.g.* Roache, 1976). In the field of reactor physics, however, the numerical stabilities of discretized neutron equations are still not completely clarified. Usually, on the basis of experience or a trial-and-error approach, a numerical scheme and a set of mesh spacings are chosen to obtain a stable solution. Recently, an investigation on the numerical stability of one-point kinetic difference equations was reported (Hashimoto, et al., 2000). In this investigation, the stability of various schemes was estimated and the stability limit of time-mesh spacing was determined. No report on the stability of space-dependent neutron equations could be seen.

We have attempted to estimate theoretically the numerical stability of neutron diffusion kinetic equations discretized by various time- and space-integration schemes. In this paper, the stabilities of diffusion kinetic equations discretized by explicit and implicit time-integration methods are estimated. Time-integration methods employed are described in section 2, and the diffusion equations including the errors introduced by these methods are derived in section 3. The impulse response functions based on these equations are demonstrated in section 4. The stability limit of time-mesh spacing for the explicit method is given in section 5. This stability limit is available not only for solving explicit difference equations, but also for doing implicit difference equations by predictor-corrector method. The predictor, as which explicit solution is employed, should be numerically stable.

2 . TIME INTEGRATION METHOD

In this study, we consider a discretization in temporal and spatial domains for the following diffusion kinetic equations:

$$\frac{1}{\mathrm{v}}\frac{\partial \Phi(t,x)}{\partial t} = D\frac{\partial^2 \Phi(t,x)}{\partial x^2} - \Sigma_a\Phi(t,x) + (1-\beta)\nu\Sigma_f\Phi(t,x) + \lambda C(t,x), \tag{1-1}$$

$$\frac{\partial C(t,x)}{\partial t} = \beta\nu\Sigma_f\Phi(t,x) - \lambda C(t,x), \tag{1-2}$$

where notations of above equations are conventional. To simplify the following formulation, the above kinetic equations are described under one-energy, one delayed-group and one-dimensional theory. The explicit (Euler) time-integration of Eqs.(1-1) and (1-2) results in the following difference equations:

$$\frac{1}{\mathrm{v}}\frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta t} = D\,\frac{\Phi_{i+1}^n - 2\Phi_i^n + \Phi_{i-1}^n}{\Delta x^2} - \Sigma_a\Phi_i^n + (1-\beta)\nu\Sigma_f\,\Phi_i^n + \lambda C_i^n, \tag{2-1}$$

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \beta\nu\Sigma_f\,\Phi_i^n - C_i^n, \tag{2-2}$$

$$\Delta t \equiv t_{n+1} - t_n,\ \Delta x \equiv x_{i+1} - x_i,\ \Phi_i^n \equiv \Phi(t_n, x_i),\ C_i^n \equiv C(t_n, x_i),$$

where the central-difference method is employed as space-integration scheme. On the other hand, the implicit time-integration of Eqs.(1-1) and (1-2) leads to the following difference equations:

$$\frac{1}{\mathrm{v}}\frac{\Phi_i^{n+1}-\Phi_i^n}{\Delta t}=D\,\frac{\Phi_{i+1}^{n+1}-2\,\Phi_i^{n+1}+\Phi_{i-1}^{n+1}}{\Delta x^2}-\Sigma_a\Phi_i^{n+1}+(1-\beta)\nu\Sigma_f\,\Phi_i^{n+1}+\lambda C_i^{n+1}, \quad (3\text{-}1)$$

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=\beta\nu\Sigma_f\,\Phi_i^{n+1}-C_i^{n+1}. \quad (3\text{-}2)$$

3 . KINETIC EQUATIONS WITH DISCRETIZING ERROR

In this section, we derive an expression for the diffusion equation with discretizing error (*i.e.* truncation error) according to an approach of Hirt (1968). First, we derive the expression including the numerical error introduced by explicit time-integration method. The Taylor-series expansions of unknowns around a time- and space-mesh point can be described as

$$\Phi_i^{n+1}=\Phi_i^n+\Delta t\;\partial\,\Phi(t_n,x_i)/\partial t+\Delta t^2/2\;\partial^2\Phi(t_n,x_i)/\partial t^2+\Delta t^3/6\;\partial^3\Phi(t_n,x_i)/\partial t^3+\cdots, \quad (4\text{-}1)$$

$$C_i^{n+1}=C_i^n+\Delta t\;\partial\,C(t_n,x_i)/\partial t+\Delta t^2/2\;\partial^2 C(t_n,x_i)/\partial t^2+\Delta t^3/6\;\partial^3 C(t_n,x_i)/\partial t^3+\cdots, \quad (4\text{-}2)$$

$$\Phi_{i\pm1}^n=\Phi_i^n\pm\Delta x\;\partial\,\Phi(t_n,x_i)/\partial x+\Delta x^2/2\;\partial^2\Phi(t_n,x_i)/\partial t^2\pm\Delta x^3/6\;\partial^3\Phi(t_n,x_i)/\partial t^3+\Delta x^4/24\;\partial^4\Phi(t_n,x_i)/\partial t^4+\cdots. \quad (4\text{-}3)$$

The substitution of the above equations into Eqs.(2-1) and (2-2) gives the following expression.

$$\frac{1}{\mathrm{v}}\left(\frac{\partial\Phi(t,x)}{\partial t}+\frac{\Delta t}{2}\frac{\partial^2\Phi(t,x)}{\partial t^2}+\frac{\Delta t^2}{6}\frac{\partial^3\Phi(t,x)}{\partial t^3}+\cdots\right)$$

$$=D\left(\frac{\partial^2\Phi(t,x)}{\partial x^2}+\frac{\Delta x^2}{12}\frac{\partial^4\Phi(t,x)}{\partial x^4}+\cdots\right)-\Sigma_a\Phi(t,x)+(1-\beta)\nu\Sigma_f\Phi(t,x)+\lambda C(t,x), \quad (5\text{-}1)$$

$$\frac{\partial C(t,x)}{\partial t}+\frac{\Delta t}{2}\frac{\partial^2 C(t,x)}{\partial t^2}+\frac{\Delta t^2}{6}\frac{\partial^3 C(t,x)}{\partial t^3}+\cdots=\beta\nu\Sigma_f\Phi(t,x)-\lambda C(t,x). \quad (5\text{-}2)$$

where an arbitrarily assigned time- and space-point is replaced by universal notation as follows.

$$(t_n, x_i) \rightarrow (t, x).$$

Equations (5-1) and (5-2) include the numerical error terms introduced by explicit integration method, and can be reduced to Eqs.(1-1) and (1-2) in infinitely fine mesh.

Next, we derive the expression including the numerical error introduced by implicit time-integration method. In this case, the Taylor-series expansions around an advanced time-mesh point are made as

$$\Phi_i^n = \Phi_i^{n+1} - \Delta t \ \partial \Phi(t_{n+1}, x_i)/\partial t + \Delta t^2/2 \ \partial^2 \Phi(t_{n+1}, x_i)/\partial t^2 - \Delta t^3/6 \ \partial^3 \Phi(t_{n+1}, x_i)/\partial t^3 + \cdots, \tag{6-1}$$

$$C_i^n = C_i^{n+1} - \Delta t \ \partial C(t_{n+1}, x_i)/\partial t + \Delta t^2/2 \ \partial^2 C(t_{n+1}, x_i)/\partial t^2 - \Delta t^3/6 \ \partial^3 C(t_{n+1}, x_i)/\partial t^3 + \cdots, \tag{6-2}$$

$$\Phi_{i\pm1}^{n+1} = \Phi_i^{n+1} \pm \Delta x \ \partial \Phi(t_{n+1}, x_i)/\partial x + \Delta x^2/2 \ \partial^2 \Phi(t_{n+1}, x_i)/\partial t^2 \pm \Delta x^3/6 \ \partial^3 \Phi(t_{n+1}, x_i)/\partial t^3 + \Delta x^4/24 \ \partial^4 \Phi(t_{n+1}, x_i)/\partial t^4 + \cdots. \tag{6-3}$$

Substituting the above equations into Eqs.(3-1) and (3-2), and making the following replacement of notation:

$$(t_{n+1}, x_i) \rightarrow (t, x),$$

we obtain

$$\frac{1}{v}\left(\frac{\partial \Phi(t,x)}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 \Phi(t,x)}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 \Phi(t,x)}{\partial t^3} - \cdots\right)$$

$$= D\left(\frac{\partial^2 \Phi(t,x)}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 \Phi(t,x)}{\partial x^4} + \cdots\right) - \Sigma_a \Phi(t,x) + (1-\beta)\nu\Sigma_f \Phi(t,x) + \lambda C(t,x), \tag{7-1}$$

$$\frac{\partial C(t,x)}{\partial t} - \frac{\Delta t}{2}\frac{\partial^2 C(t,x)}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 C(t,x)}{\partial t^3} - \cdots = \beta\nu\Sigma_f \Phi(t,x) - \lambda C(t,x). \tag{7-2}$$

The numerical error introduced by implicit integration is formulated in the above equations. Compared with Eqs.(5-1) and (5-2), these equations have only the difference in sign of odd-order error terms.

4 . IMPULSE RESPONSE FUNCTION WITH DISCRETIZING ERROR

In this section, the impulse response functions with discretizing errors are derived and the numerical stabilities of the discretized equation systems are investigated from Bode diagrams of the response functions. First, we derive the impulse response functions for the explicit method. Attaching the following disturbance term to the right-hand side of Eq.(5-1),

$$+ S_0\, \delta(t)\, \delta(t),$$

and Laplace-transforming the result and Eq.(5-2), the implulse response function for the explicit method can be obtained as

$$G(s_t, s_x) \equiv \beta \nu \Sigma_f \tilde{\Phi}(s_t, s_x) / S_0 = \beta / Y(s_t, s_x), \tag{8}$$

where

$$\begin{aligned} Y(s_t, s_x) &= \frac{1/\mathrm{v}}{\nu \Sigma_f \Delta t}\left(e^{\Delta t s_t} - 1\right) - \frac{D}{\nu \Sigma_f \Delta x^2}\left(e^{\Delta x s_x} + e^{-\Delta x s_x} - 2\right) \\ &\quad + \frac{\Sigma_a}{\nu \Sigma_f} - 1 + \beta \frac{\frac{1}{\Delta t}\left(e^{\Delta t s_t} - 1\right)}{\lambda + \frac{1}{\Delta t}\left(e^{\Delta t s_t} - 1\right)}, \end{aligned} \tag{9}$$

and

$$\tilde{\Phi}(s_t, s_x) = \int_0^{\infty} dt \int_0^{\infty} dx\, \Phi(t, x)\, e^{-s_t t} e^{-s_x x}. \tag{10}$$

Making the similar operations as above, the impulse response function for the implicit method can be derived from Eqs.(7-1) and (7-2). The response function is described by replacing Eq.(9) by the following function:

$$\begin{aligned} Y(s_t, s_x) &= -\frac{1/\mathrm{v}}{\nu \Sigma_f \Delta t}\left(e^{-\Delta t s_t} - 1\right) - \frac{D}{\nu \Sigma_f \Delta x^2}\left(e^{\Delta x s_x} + e^{-\Delta x s_x} - 2\right) \\ &\quad + \frac{\Sigma_a}{\nu \Sigma_f} - 1 - \beta \frac{\frac{1}{\Delta t}\left(e^{-\Delta t s_t} - 1\right)}{\lambda - \frac{1}{\Delta t}\left(e^{-\Delta t s_t} - 1\right)}. \end{aligned} \tag{11}$$

Here the above response functions are demonstrated to investigate numerical stability of the difference equation system, where a set of macroscopic constants are given as follows.

$$\Sigma_\mathrm{a}/(\nu\Sigma_\mathrm{f}) = 0.98,\ D/(\nu\Sigma_\mathrm{f}) = 5.0,\ 1/\mathrm{v}/(\nu\Sigma_\mathrm{f}) = 4\times10^{-5},\ \lambda = 0.08,\ \beta = 0.0056$$

The response function can be numerically determined by making the following replacement:

$$s_t \to j\omega,\ s_x \to jk_x,$$

where

$$\omega:\ frequency\ (/s),\ k_x:\ wave\ number\ (1/cm),\ j \equiv \sqrt{-1}.$$

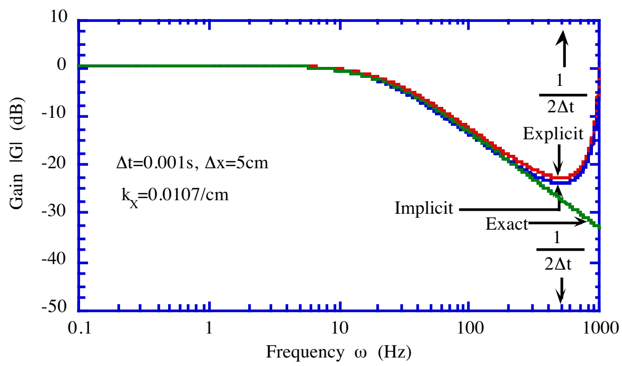
The discussion on the response function should be confined to the lower frequency range than the Nyquist frequency. The frequency is defined as

$$\omega_N = 1\,/\,(\,2\,\Delta t\,) \tag{12}$$

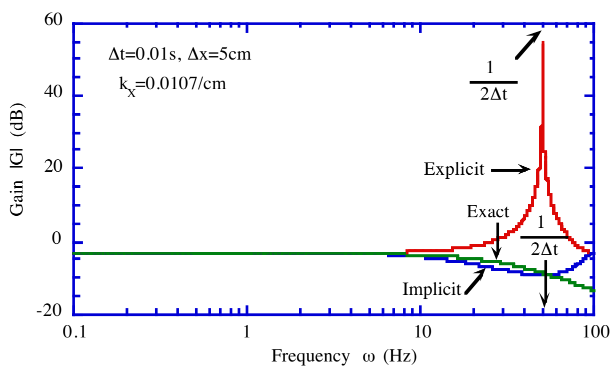
which specifies resolving frequency of a numerical calculation. Similarly this discussion should be confined to the lower wave number than the following resolving number:

$$k_{xN} = 1\,/\,(\,2\,\Delta x\,) \tag{13}$$

Figure 1 shows the gain of the response functions based on explicit and implicit time-integration methods, where two time-mesh spacings of 0.001s(a) and 0.01s(b) are specified. The space-mesh spacing is 5cm and the number is set to 0.0107. Included in this figure for comparison is the exact curve, to which the response functions can be reduced in infinitely fine mesh. Compared with the exact curve, the gain of the response function for the explicit method is enhanced in the higher frequency range. In the time-mesh spacing of 0.001s, the enhancement is nevertheless not so significant as to unstabilize a discretized system. In the



(a) Δt=0.001s



(b) Δt=0.01s

Fig.1 Gain of impulse response function with discretizing error (Δx=5cm) spacing of 0.01s, however, we can observe a sharp peak in the gain curve for the explicit method. This peak suggests that numerical instability must force all unknowns to oscillate at the the Nyquist frequency and hence no solution can be obtained. In the explicit method, such a coarse time-mesh should never be employed. In contrast the implicit method never makes oscillation peak and has no limitation of time spacings for numerical stability.

In Fig.2, the gain of the response function based on the explicit method is plotted for several choices of wave number, where time- and space-mesh spacings are 0.001s and 5cm, respectively. At wave number of 0.0107, this finite-difference equation is numerically stable as shown in Fig.1. At wave number of 0.0223, however, a sharp peak can be observed. This peak suggests that the equation system is numerically unstable at the Nyquist frequency. At higher wave number, this peak vanishes. These features indicate that the wave number of numerical oscillation observed must be dependent on time-mesh spacing. The oscillation frequency is the Nyquist one, regardless of its time-mesh spacing.

In Fig.3, the gain of impulse response function for the explicit method is plotted on wave number domain, where the frequency is set to the Nyquist one. The wave number of observed peak increses with a decrease in time-mesh spacing and reaches to the resolving number in a fine time mesh. Further decrease in time-mesh spacing extinguishes oscillation peak. This figure suggests that a stability limit condition may be attained under the resolving wave number $1/(2\Delta x)$.

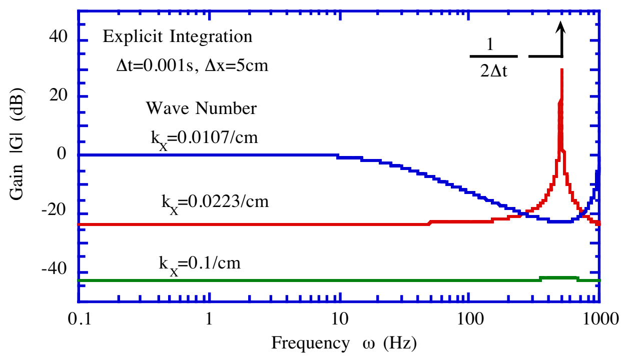


Fig.2 Wave-number dependence of gain of impulse response function (Δt=0.001s)

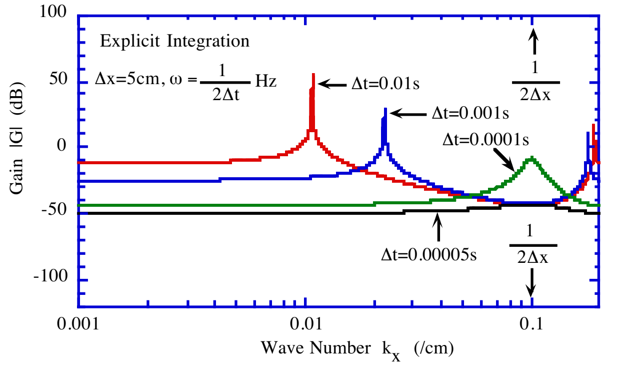


Fig.3 Gain of impulse response function on wave number domain ($\omega=1/(2\Delta t)$)

5 . MESH-SPACING LIMIT FOR NUMERICAL STABILITY

As confirmed in the above section, the application of the explicit method to a coarse mesh system may cause numerical instability. In this section, the mesh-spacing limit for the stability is formulated. For solving implicit difference equations by predictor-corrector method, also, this stability limit is available. The predictor, as which Euler (explicit) solution is employed, should be numerically stable.

Neglecting delay neutron contribution in Eq.(5-1), the following equation for prompt neutron can be obtained.

$$\frac{1}{\mathrm{v}}\left(\frac{\partial \Phi(t,x)}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \Phi(t,x)}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 \Phi(t,x)}{\partial t^3} + \cdots\right)$$

$$= D\left(\frac{\partial^2 \Phi(t,x)}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 \Phi(t,x)}{\partial x^4} + \cdots\right) - \Sigma_a \Phi(t,x) + (1-\beta)\nu\Sigma_f \Phi(t,x). \tag{14}$$

The above assumption is valid at the Nyquist frequency where numerical instability can be observed as done in previous section. First, neutron flux is described as

$$\Phi(t,x) = \Phi_0 e^{(\alpha + j\omega_N)t + jk_x x}, \tag{15}$$

where frequency is confined to the Nyquist frequency. An amplitude factor α of the above oscillation mode is examined to judge numerical stability of the mode. When the amplitude factor is negative, the mode is judged stable. The substitution of Eq.(15) into Eqs.(14) gives

$$e^{\alpha \Delta t} = D\mathrm{v}\frac{\Delta t}{\Delta x^2}\left(2 - e^{jk_x \Delta x} - e^{-jk_x \Delta x}\right) + \mathrm{v}\Delta t\left(\Sigma_a - (1-\beta)\nu\Sigma_f\right) - 1. \tag{16}$$

The stability requirement for amplitude factor gives

$$e^{\alpha \Delta t} < 1. \tag{17}$$

Substituting Eq.(16) into Eq.(17), we obtain

$$\Delta t < \frac{2}{\frac{D\mathrm{v}}{\Delta x^2}\left(2 - e^{jk_x \Delta x} - e^{-jk_x \Delta x}\right) + \mathrm{v}\left(\Sigma_a - (1-\beta)\nu\Sigma_f\right)}. \tag{18}$$

This is time-mesh spacing limit for a certain wave number. Furthermore, using the following relation:

$$0 \le 2 - e^{jk_x \Delta x} - e^{-jk_x \Delta x} \le 4, \tag{19}$$

Eq.(18) is reduced to

$$\Delta t < \frac{2}{\dfrac{4D\mathrm{v}}{\Delta x^2} + \mathrm{v}\left(\Sigma_a - (1-\beta)\nu\Sigma_f\right)} . \tag{20}$$

The above equation is final form of time-mesh spacing limit. When time- and space-mesh spacings are specified according to the above criterion, not only a mode at the resolving wave number 1/(2Δx) but also other modes at lower wave number are numerically stabilized. Here, introducing the following assumption:

$$\Sigma_a - (1-\beta)\nu\Sigma_f = 0, \tag{21}$$

Eq.(20) is furhter reduced to

$$\Delta t < \frac{\Delta x^2}{2\mu}\ , \quad \mu = D\mathrm{v}. \tag{22}$$

The above criterion is identical with that available in fluid dynamics (*e.g.* Roache, 1976).

Figure 4 shows neutral boundary for numerical stability. As space-mesh is finer, further finer time-mesh should be specified to obtain a stable solution. In neutron non-multiplicative medium, finer time-mesh is required than that in multiplicative one. These features suggest that a nuclear reactor system containing neutron absorbers may require very fine time-mesh. In coarse spatial mesh, significant difference in stability boundary between Eqs.(20) and (22) can be observed.

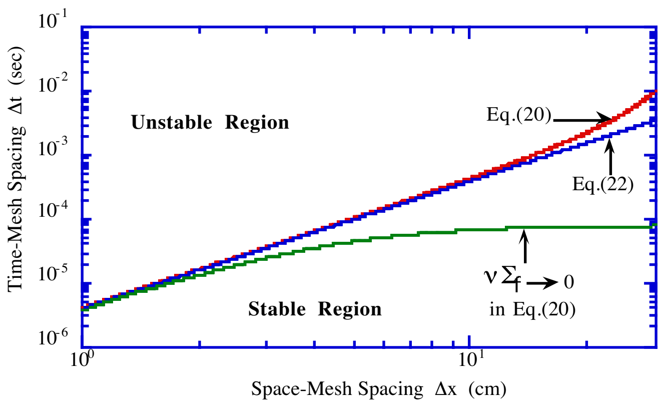


Fig. 4 Numerical stability boundary

6 . CONCLUSIONS

We derived the diffusion kinetic equations considering the numerical errors introduced by explicit and implicit time-integration methods. The impulse response functions based on the present equations were demonstrated to study the numerical stability of the discretized systems. The applications of the implicit method give an undertaking to make numerically stable, while the explicit method makes the numerical system unstable in the time-mesh spacing broader or space-mesh spacing smaller than those determined by a criterion. The criterion could be also formulated.

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