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Comparative Study of LC Scheme with Some Conventional Schemes by Truncation Error Analysis

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선형특성 (LC) 법과 그 외 고전적 방법들과의 절단오차 분석에 의한 비교연구

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Abstract

A recently developed spatial differencing scheme, Linear Characteristic (LC) scheme is compared with some traditionally used schemes such as Step Difference (SD), Diamond Difference (DD), and Step Characteristic (SC) scheme by analyzing the truncation error calculated numerically in slab geometry.

Those four candidate schemes are applied to one simple source sink problem and two criticality problems (one is calculation of multiplication factor and the other is slab critical half thickness). The calculated results are then examined by some equitable measures of error.

It is concluded that the LC scheme is terribly more powerful than any other candidate scheme that has been prevalent up to the present time.

Moreover, the LC scheme estimates integral parameter such as multiplication factor and critical half thickness much more efficiently than SD or SC scheme. This is due to the fact that the fortuitous error cancellation, which occurs when the deviations of cell average flux are summed over the whole gamut of spatial meshes, happens much more favorably to the LC scheme.

요 약

최근 개발된 유한차분법의 하나인 선형특성 (LC) 법을 절단오차의 분석을 통하여 계단형차분 (SD) 법, 다이아몬드형차분 (DD) 법, 그리고 계단형특성 (SC) 법과 비교했다.

제시된 4가지 방법들이 선속 계산문제, 유효증배계수 계산문제, 그리고 임계평판 두께 계산문제에 적용되었으며, 그때 계산된 결과들은 몇몇의 절단오차 측정 기준들에 의해 평가되어졌다.

본 연구의 주요 결론으로, 모든 경우에 있어서 어느정도 기대했던 바와 같이 선형특성법이 가장 우수하다는 것이 밝혀졌으며, 특히, 선형특성법은 유효증배계수와 임계평판두께 같은 적분 인자들을 정확하게 계산하는 데, 이는 선형특성법이 다른 방법들에 비해 오차소거(Error Cancellation) 작용이 효과적으로 일어나기 때문으로 밝혀졌다.

I. Introduction

Increasingly, the discrete ordinates method/codes have been the dominant means for solving radiation transport problems for reactor core and extensive shielding design in nuclear fission power plants, as well as for blanket and shield design of a fusion reactor.

In this situation, the ability to compute positive and accurate numerical solution to the discrete ordinates equations has been a long-standing problem. One is usually faced with the choice of using a relatively accurate nonpositive scheme such as Diamond Difference (DD) scheme or a less accurate noncentered positive scheme such as one of the Weighted Diamond Difference (WD) schemes.[1] To avoid this unpleasant choice or to improve the convergence rate, extensive studies on various spatial difference schemes have been made.

Recently, Gopinath and his co-workers approximated[2] the iterative source distribution in a spatial mesh with some mathematically reasonable linear functions. In their paper, four variants of Linear Characteristic (LC) schemes were derived and investigated, and it was concluded that the one retaining the cell average source and gradient of two cell edge sources provided much better accuracy than any other variant.

In this study, therefore, only the most accurate variant mentioned above is picked up and compared with some traditionally used spatial difference shcemes such as Step difference (SD),[3] Diamond Difference (DD),[4] and Step Characteristic (SC)[5] scheme to determine whether the scheme is more efficient than traditionally used schemes and if more, how much.

Only one group and slab geometry test problems are considered and all calculations are carried out by VAX-8700 computer system at Hanyang University.

II. Candidate Schemes

In slab geometry, the discrete ordinates approximation to the multigroup neutron transport equation can be written as

$$\mu_m \frac{d}{dx}\psi_{gm}(x) + \sigma_{tg}(x)\psi_{gm}(x) = S_{gm}(x) \tag{1}$$

where $S_{gm}(x)$ is the source obtained from the previous iteration using the Legendre moments.[6]

Since we are now discussing the spatial solution of Eq. (1), in which energy and angle do not vary, the indices 'g' and 'm' are henceforth dropped.

$$\mu \frac{d}{dx}\psi(x) + \sigma_t(x)\psi t(x) = S(x) \tag{2}$$

A general method of obtaining a supplementary equation is to integrate Eq. (2) over a spatial cell, say *cell i*, using integrating factor, to yield

$$\psi_{i+1/2} = \psi_{i-1/2}\exp(-\epsilon_i) + \frac{1}{\mu}\int_{x_{i-1/2}}^{x_{i+1/2}} dx\, S(x)\exp\left[\frac{-\sigma_{ti}(x_{i+1/2}-x)}{\mu}\right] \tag{3}$$

where $\epsilon_i = \sigma_{ti}\Delta x_i/\mu$, optical distance in mean free path of the travel across *cell i*.

Because the exact variation of the source through *cell i* can not be known, as it were, only the pointwise sources of cell average and two cell edges can be known, the iterative source must be approximated using these three pointwise values.

The principal idea of LC scheme is to approximate *S(x)* in *cell i* with a certain linear function,

$$S(x)=a_0+a_1(x-x_{i-1/2}),\ \text{for } x \in (x_{i-1/2}, x_{i+1/2}) \quad (4)$$

The constants a_o and a_1 can be obtained by various selections and the one set regarded as the most reasonable is constructed by conservating/retaining cell average source and gradient of two cell edge sources. Then, LC scheme for $\mu > 0$ can be written as[7]

$$[\text{LC}]\ \psi_{i+1/2}=\psi_{i-1/2}\exp(-\epsilon_i)+\frac{\bar{S}_i}{\sigma_{ti}}[1-\exp(-\epsilon_i)]+\frac{S_{i+1/2}-S_{i-1/2}}{\sigma_{ti}}\{1+(\frac{1}{2}+\frac{1}{\epsilon_i})[1-\exp(-\epsilon_i)]\} \quad (5)$$

This LC shceme proved to be positive one and the calculational effort to solve one cell problem is estimated roughly twice that of DD scheme by simple hand calculation.[8] In the similar way above, the other candidate schemes can be derived as following form.

$$[\text{SD}]\ \psi_{i+1/2}=\frac{1}{1+\epsilon_i}\psi_{i-1/2}+\frac{1}{1+\epsilon_i}\frac{\bar{S}_i}{\sigma_{ti}} \quad (6)$$

$$[\text{DD}]\ \psi_{i+1/2}=\frac{2-\epsilon_i}{2+\epsilon_i}\psi_{i-1/2}+\frac{2\epsilon_i}{2+\epsilon_i}\frac{\bar{S}_i}{\sigma_{ti}} \quad (7)$$

$$[\text{SC}]\ \psi_{i+1/2}=\psi_{i-1/2}\exp(-\epsilon_i)+\frac{\bar{S}_i}{\sigma_{ti}}[1-\exp(-\epsilon_i)] \quad (8)$$

The scheme, DD is not positive shceme, for it is clear that even if $\psi_{i-\frac{1}{2}}$ and $\bar{S}_i$ are positive, Eq. (7) can produce negative value for $\psi_{i+\frac{1}{2}}$ in case $\epsilon_i > 2$. This often happens even for small mesh size when σ_i is sufficiently large and/or μ is sufficiently small. Thus, as pointed by Lathrop, auxiliary negative flux fix-up is needed in conjunction with this DD scheme to guarentee positivity of the flux. Such negative flux fix-up schemes are successful in one space-dimension but become excessively complicated in two dimensions. Futhermore, this kind of fix-up is unable to correct the oscillatory character of DD scheme except when negative fluxes occur. This oscillatory behavior can interact unfavorably with convergence acceleration divices such as synthetic method and coarse mesh rebalance method resulting in unstable and divergent algorithm.

III. Proposed Test Calculation

a) Source sink problem

A simple model of following S_2 one grop test problem is considered with $\sigma_t=2$, $\sigma_s=1$, and $Q(x)=1$.

$$\mu_m\frac{d}{dx}\psi_m(x)+\sigma_t\psi_m(x)=\sigma_s\sum_{m=1}^{2}\omega_m\psi_m(x)+Q(x) \quad (9)$$

with boundary conditions, $\psi_1(-1)=\psi_2(1)=0$.

To evaluate the accuracy of each candidate scheme, some measures of error are introduced. As preliminary definitions, fractional deviation is defined by

$$\| f \| \equiv \frac{f-f^{ex}}{f^{ex}} \quad (10)$$

and deviation is

$$\| f \|^* \equiv \| f \| \times f^{ex}=f-f^{ex} \quad (11)$$

where f^{ex} is the exact/reference value and f is the numerically calculated one. Then, following three measures of error can be defined.

1) Edge error norm: This error norm determines the accuracy of cell edge flux, and is the maximum absolute value of fractional deviations of cell edge fluxes over all spatial cells,

$$\| \phi \|_{edge}^{max} \equiv \max_i |\ \| \phi \|_{edge,i+1/2}|,\quad i=0,1,2,\ldots,I. \quad (12)$$

2) Average error norm: This error norm determines the accuracy of cell average flux, and is the maximum absolute value of the fractional deviations of cell average fluxes,

Table 1. Edge Error Norm for Various Mesh Size when Iteration Rumber is Large to Converge.

Δx(cm) \ scheme	SD	DD	SC	LC
2^{0}	2.409×10^{-1}	2.438×10^{-1}	6.322×10^{-2}	1.534×10^{-2}
2^{-1}	1.425×10^{-1}	4.656×10^{-2}	2.701×10^{-2}	1.035×10^{-3}
2^{-2}	8.078×10^{-2}	1.093×10^{-2}	8.017×10^{-3}	6.580×10^{-5}
2^{-3}	4.356×10^{-2}	2.675×10^{-3}	2.100×10^{-3}	4.120×10^{-6}
2^{-4}	2.282×10^{-2}	6.683×10^{-4}	5.312×10^{-4}	2.343×10^{-7}

Table 2. Ratio(R_m*) of Error Norm.

m \ scheme	SD	DD	SC	LC
1	1.69	5.24	2.34	14.89
2	2.14	4.26	3.37	15.73
3	1.85	4.09	3.82	15.97
4	1.91	4.00	3.95	17.61

$$*R_m=\frac{\text{Edge Error Norm }(\Delta x=2^{-m+1})}{\text{Edge Error Norm }(\Delta x=2^{-m})}$$

$$\|\phi\|^{max}_{edge}\equiv\max_i\ |\ \|\phi\|_{averge,i}\ |,\quad i=1,2,\ldots,I. \tag{13}$$

3) Sum error norm: This error norm determines the accuracy of integral parameter such as collision densities and eignvalues, defined by

$$\|\phi\|^{max}_{average}\equiv\frac{\|\sum_i\bar{\phi}_i\Delta x_i-\sum_i\bar{\phi}_{iex}\Delta x_i\|}{\|\sum_i\bar{\phi}^{ex}_i\Delta x_i\|} \tag{14}$$

If all mesh sizes are equal, this error norm is directly proportional to the summation of deviations of cell average fluxes over all spatial cells.

b) Criticality Problem

Two criticality problems-one is calculation of multiplication factor and the other is calculation of critical half thickness-are considered with a transport equation as

$$\mu\frac{d}{dx}\psi(x,\mu)+\sigma_t\psi(x,\mu)=\left(\frac{\sigma_s^{iso}+\nu\sigma_f}{2}\right)\int_{-1}^{1}\psi(x,\mu')d\mu'+ \tag{15}$$

$$\sigma_s^{aniso}\sum_{n=0}^{2}b_n P_n(\mu)\int_{-1}^{1}P_n(\mu')\psi(x,\mu')d\mu'$$

subjected to the vacumn boundary conditions on both sides of the slab.

In above transport equation, the anisotropic scatterer is represented by a three term Legendre expansion and the b_n of elastic hydrogen scattering were used as an example.[(9),(10)]

We now solve these equatjions for several values of the secondary ratio $c+c'$ where c is the anisotropic scattering ratio, defined by

$$c=\sigma_s^{aniso}/\sigma_t$$

and c' is the isotropic scattering ratio

$$c'=(\sigma_s^{iso}+\nu\sigma_f)/\sigma_t$$

To evaluate the accuracy, two measures of error are introduced as follows.

1) Absolute fractional deviation(%) of effective multiplication factor:

$$\|K_{eff}\|_{abs}=\left|\frac{K_{eff}-K_{eff}^{ex}}{K_{eff}^{ex}}\right|\times100(\%) \tag{16}$$

2) Absolute fractional deviation(%) of critical

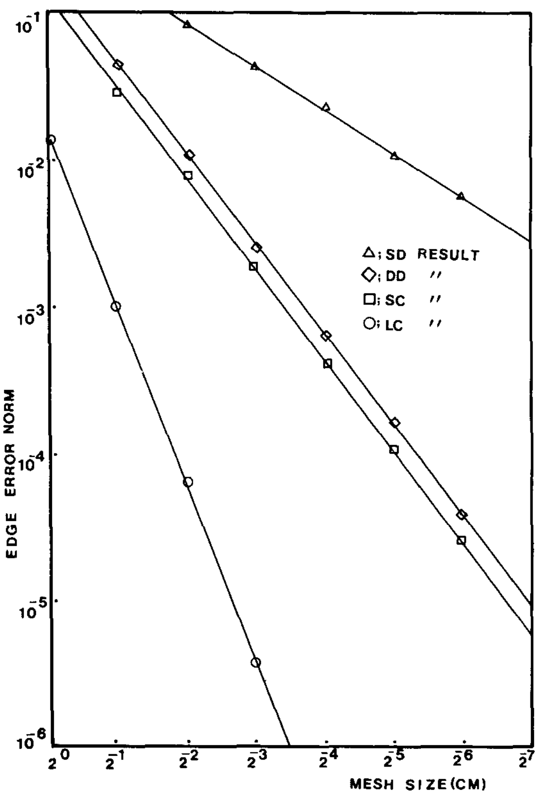

Fig. 1. Calculated Edge Error Norm.

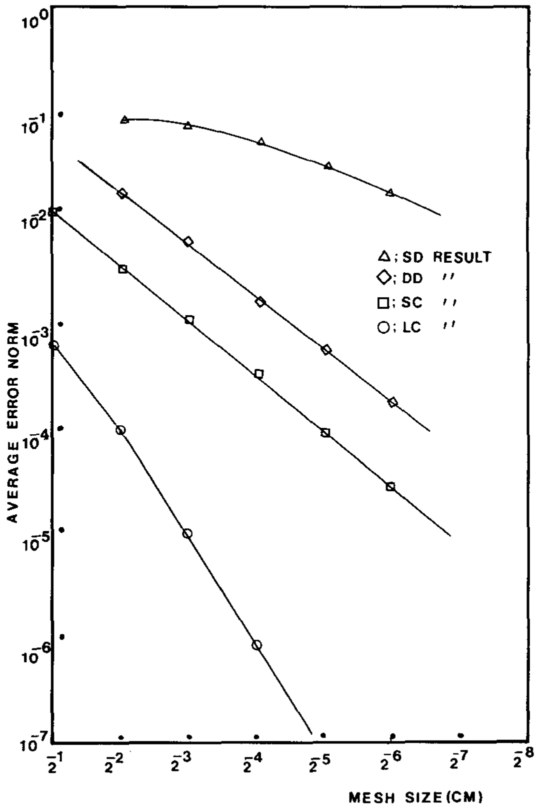

Fig. 2. Calculated Average Error Norm.

half thickness:

$$\| t_{c1/2} \|_{abs} = \left| \frac{t_{c1/2}-t^{ex}_{c1/2}}{t^{ex}_{c1/2}} \right| \times 100(\%) \qquad (17)$$

A computer program using conventional 'Power Iteration Method' is fabricated to solve the test problems. In this program, four candidate schemes are implemented as subprograms. Convergence criterions of 10E-5 are used in criticality problems. In source sink problem, however, iteration is controlled simply by the number of iterations.

IV. Results and Discussion

A sequence of five uniform spatial meshes are considered in Table 1 and 2, and each spatial mesh is succeeded by one twice as fine. As seen in these tables, edge error norms of SD, DD, SC, and LC scheme decrease roughly by the factor of 2, 4, 4, and 16, respectively. Therefore, it can be asserted that these respective schemes are first, second, second, and forth order of spatial truncation error. This numerical result is consistent with a previous work made by S. M. Lee and his co-worker who have studied on the comparison of the orders of approximation in several spatial difference schemes by mathematical approach.[11]

Edge and average error norms are plotted in Fig. 1 and 2 when iteration number(=100 fixed) is sufficiently large to converge. For various mesh size, LC scheme produces smaller error norms than any other candidate schemes, especially than SD scheme. As the mesh refined, this phenomenon becomes more striking, that is to say, LC solution converge more rapidly to the exact solution as mesh size thends to zero. This is due to the fact that LC is the highest order accurate scheme of the four candidate schemes. In addi-

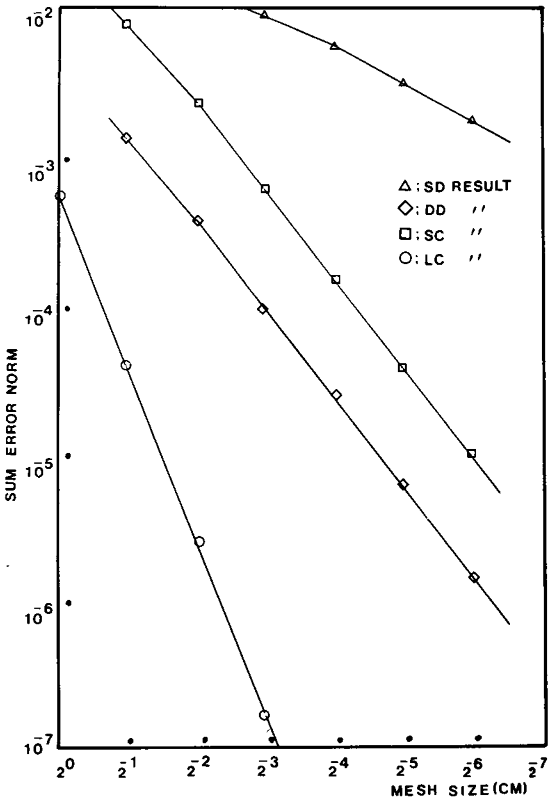

Fig. 3. Calculated Sum Error Norm.

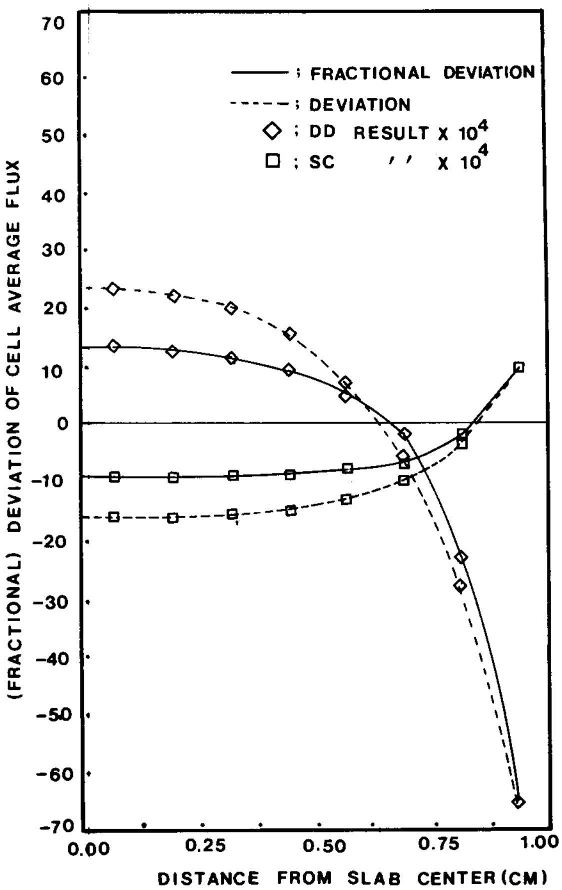

Fig. 4. (Fractional) Deviation of Cell Average Flux as a Function of Distance from Slab Center.

tion, the numerical results of error norms are described as about straight lines, and the slops depend entirely upon the orders of spatial truncation error, as we have expected so. On the other hand, it can also be seen that SC scheme produces somewhat smaller value than DD scheme for edge error norm, and for average error norm by factor of about seven times, but that the gap between the error norms of DD and SC scheme is roughly the same, not increase as mesh size tends to zero, this is due to the fact that both DD and SC are second order accurate schemes.

Sum error norms are plotted in Fig. 3 when iteration number(=100 fixed) is sufficiently large to converge. Again, LC scheme is substantially accurate than any other schemes for various mesh size. But, sum error norm of SC scheme is much larger than that of DD scheme by factor of about six times. At first appearance, this situation is unlikely to be happen and seems unreasonable (remind the fact that average error norm of SC scheme is much smaller than that of DD scheme), but if we introduce following concept of error cancellation, it can be explained clearly.

Spatial distrbution of deviation and fractional deviation of cell average flux are shown in Fig. 4 for our explanation of the error cancellation. As can be seen in this figure, although average error norm (it is the maximum absolute value of fractional deviations of cell average fluxes as defined) of DD scheme is greater than that of SC scheme, sum error norm (it is also directly proportional to the summation of the deviations of cell average fluxes under considering the sign of each value) of DD scheme is smaller; in the case of DD scheme, the amount of the error cancellation in deviations

Table 3. Slab Critical Half Thickness and It's Absolute Fractional Deviation(%) from DTF-code Result (in parentheses).

c	SD	DD	SC	LC	DTF code
			c+c'=1.1		
0.1	2.2285	2.1651	2.1696	2.1641	2.1631
	(3.0×10^{0})	(9.2×10^{-2})	(3.0×10^{-1})	(4.6×10^{-2})	
0.5	2.4588	2.4126	2.4169	2.4116	2.4103
	(2.0×10^{0})	(9.5×10^{-2})	(2.7×10^{-1})	(5.4×10^{-2})	
0.9	2.8112	2.7920	2.7959	2.7910	2.7892
	(7.9×10^{-1})	(1.0×10^{-1})	(2.4×10^{-1})	$6.5\times10^{-2})$	
			c+c'=1.2		
0.1	1.3272	1.3145	1.3155	1.3140	1.3130
	(1.1×10^{0})	(1.1×10^{-1})	(1.9×10^{-1})	(7.6×10^{-2})	
0.5	1.4310	1.4266	1.4275	1.4262	1.4249
	(4.3×10^{-1})	(1.2×10^{-1})	(1.8×10^{-1})	(9.1×10^{-2})	
0.9	1.5740	1.5815	1.5821	1.5811	1.5793
	(3.5×10^{-1})	(1.4×10^{-1})	(1.8×10^{-1})	(1.1×10^{-1})	
			c+c'=1.3		
0.1	0.9540	0.9529	0.9532	0.9526	0.9514
	(2.7×10^{-1})	(1.6×10^{-1})	(2.0×10^{-1})	(1.3×10^{-1})	
0.2	1.0119	1.0157	1.0159	1.0154	1.0140
	(2.5×10^{-1})	(1.7×10^{-1})	(1.9×10^{-1})	(1.4×10^{-1})	
0.9	1.0857	1.0958	1.0960	1.0956	1.0938
	(7.4×10^{-1})	(1.8×10^{-1})	(2.0×10^{-1})	(1.6×10^{-1})	

of cell average fluxes is greater than that of SC scheme. The accuracy of integral parameter is determined by sum error norm, not by edge or average error norm, the result mentioned above is thus very important. This result will have an absolute effect on the following criticality problems. Pleasantly, as can be seen in Fig. 5, LC scheme also has this advantage of error cancellation roughly as much as DD scheme, but SD scheme has not so much.

Before the criticality problems are prosecuted, some benchmark calculations are have been carried out to verify the usefulness or exactness of our program. In Table 3, critical half thickness calculated by our program with four candidate schemes are compared with those of DTF code, a dicrete ordinates code which uses DD scheme, for various c and c', and absolute values of fractional devitions(%) are also given in parentheses. In DTF calculation, seventy-five spatial intervals were used on the interval [0,t/2] with the first 73 equal intervals and the last two spaced by $x_{74}=4.95$, $x_{75}=4.99$, and $x_{76}=5.00$ (with $t/2=5.00$). Also convergence criterions on the multiplication factor and on the spatial flux of 10E-6, and DP_7 quadrature were used. There are some slight differences between the results of our program and DTF code, which is probably due to the fact that we use somewhat coarser mesh system(16 uniform spatial meshes) and larger convergence criterion(10E-5) than those of DTF code.

Since the calculational effort/time to solve one cell problem by LC scheme was proved to be roughly twice that of DD scheme, the result from DD scheme is compared with that from LC scheme on a spatial grid which has 50% more

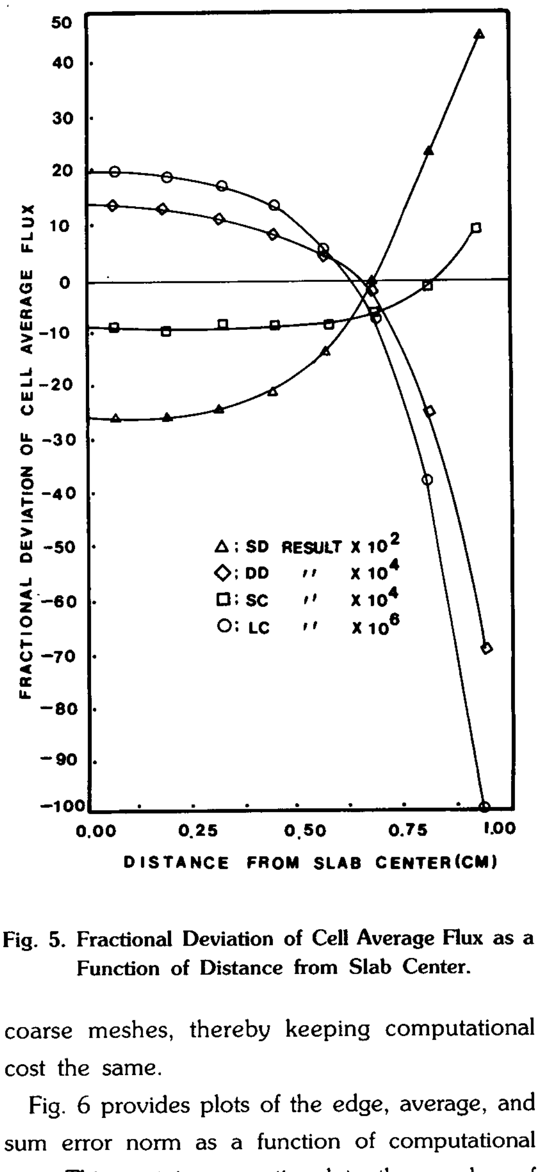

Fig. 5. Fractional Deviation of Cell Average Flux as a Function of Distance from Slab Center.

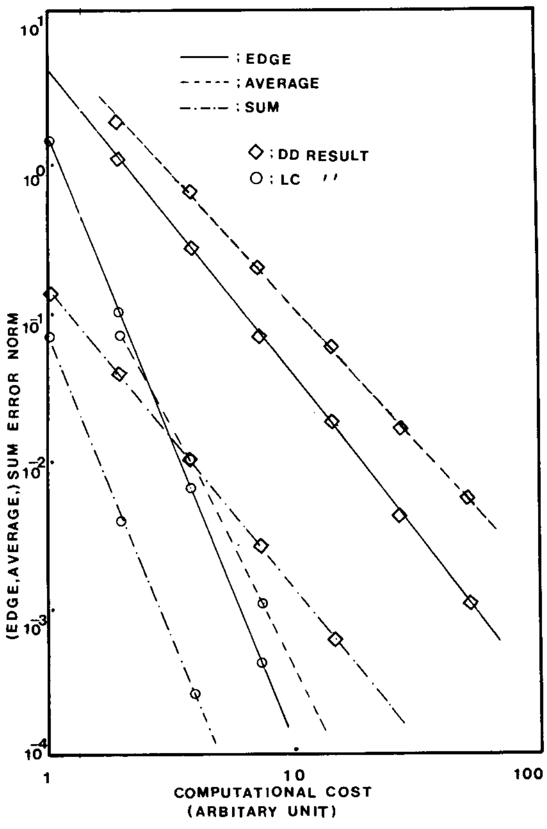

Fig. 6. Edge, Average, and Sum Error Norm vs. Computational Cost.

coarse meshes, thereby keeping computational cost the same.

Fig. 6 provides plots of the edge, average, and sum error norm as a function of computational cost. This cost is proportional to the number of clock cycles required to complete one inner iteration, and cost scale corresponds to mesh size of from 2^{-1} to 2^{-8}[cm] when DD scheme is used, or from 2° to 2^{-7}[cm] when LC scheme used. In this figure, LC scheme produces much smaller error norms than DD scheme in a given cost, therefore, it can be pronounced that LC scheme is more computationally efficient in this simple source sink problem, even assuming double the computational cost per cell.

Absolute fractional deviations(%) of effective multiplication factor and critical half thickness are plotted in Fig. 7 and 8. Exact/reference values are required to perform our error analysis, and they are obtained by using a extremely fine mesh system; (16×200) mesh system has been used for both criticality problems. Figure 7 shows that LC scheme is substantially accurate than any other candidate schemes and this advantage becomes greater if mesh is more refined, and that SC scheme is much less accurate than DD scheme but this disadvantage is the same-it does not increase as the mesh size tends to zero. This situation can be explained well with the previous analysis of sum error norms. Approximately the same situation comes out in Fig. 8, which indicates that if a scheme estimates more accurately the value of multiplication factor, this scheme also estimates more accuratley the value of critical half thickness-

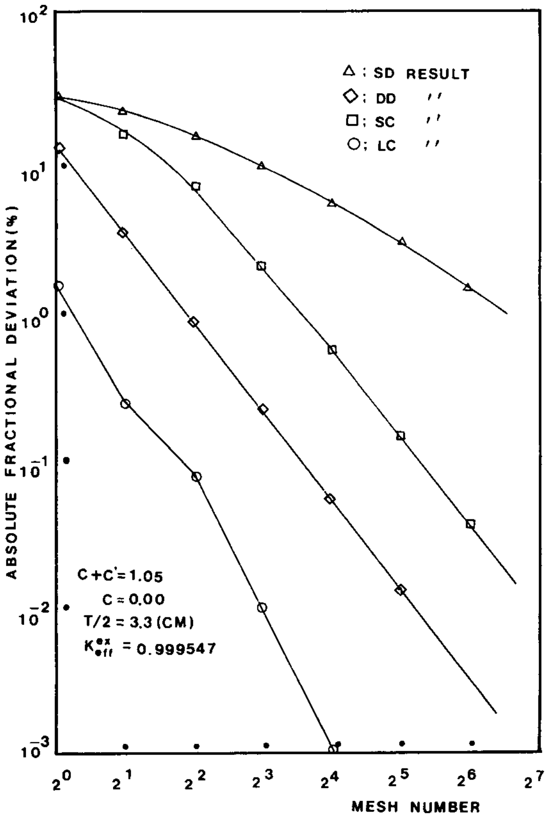

Fig. 7. Calculated Absolute Fractional Deviation (%) of Multiplication Factor.

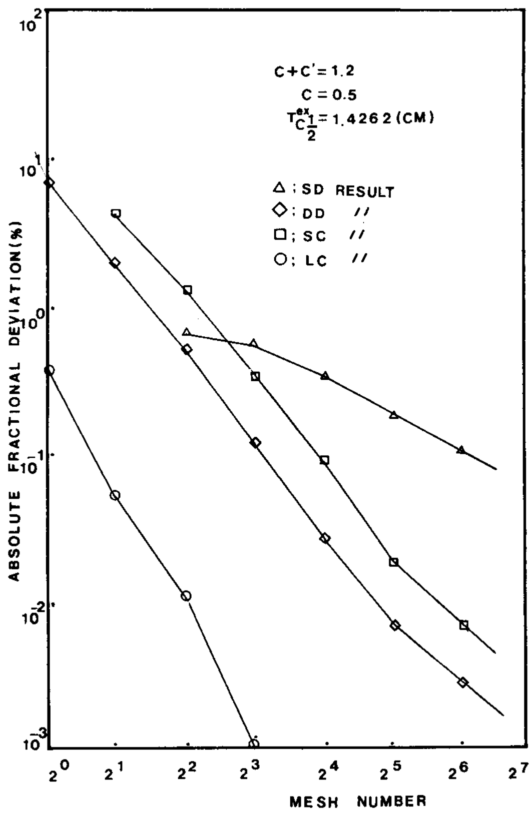

Fig. 8. Calculated Absolute Fractional Deviation of Slab Critical Half Thickness.

-it is not clear to us why the situation is not true of SD scheme when the number of spatial meshes is less than about 8.

Figure 9 shows absolute fractional deviation of effective multiplication factor and critical half thickness as a function of computational cost. The cost scale corresponds to the spatial mesh number of from 2^1 to 2^8 when DD scheme is used, or 2^0 to 2^7 when LC scheme is used. In this figure, it can be seen that LC scheme produce much smaller error at a given cost, therefore, it can be also asserted that LC scheme is more computationally efficient than DD scheme in this criticality problem, even assuming double the computational cost per cell.

V. Conclusions

This study shows that LC scheme significantly outperforms DD scheme which has been traditionally used in most discrete ordinate codes even assuming double the computational cost per cell and the error cancellation happens much more favorably to LC scheme.

Additionaly, SC scheme is substantially more accurate than DD scheme in calculation of pointwise fluxes such as cell edge flux and cell average flux, but much less accurate in calculation of integral parameter such as multiplication factor and stab critical half thickness.

This study is limited to only slab geometry case and the result from LC scheme is considerably satisfactory, therefore, it must be worthwhile to

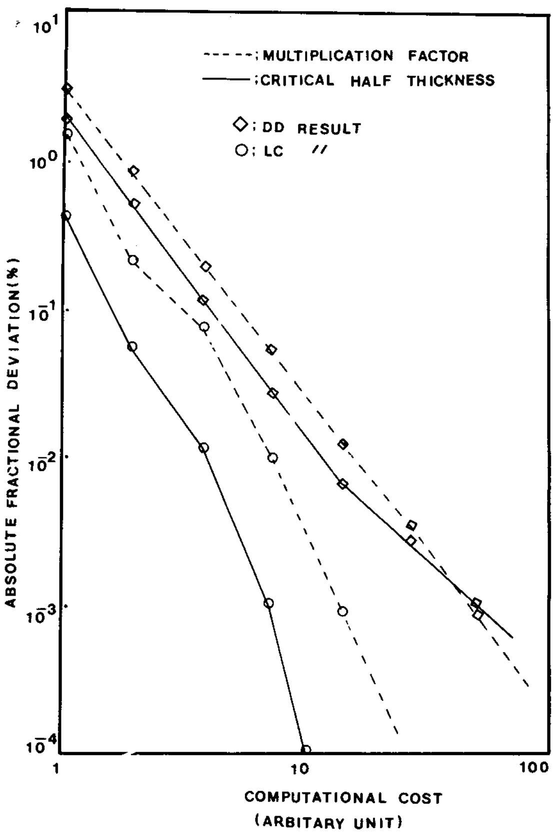

Fig. 9. Absolute Fractional Deviation of Multiplication Factor and Slab Critical Half Thickness vs. Computational Cost.

study on application of LC scheme to other geometries.

Study on oscillatory behavior is another important subject to guarantee superiority of LC scheme to DD scheme. This oscillatory behavior can interact unfavorably with convergence acceleration devices, resulting in an unstable and divergent algorithm; as a matter of fact, DD scheme seriously suffers from this oscillatory behavior.

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