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MATHEMATICAL RELATIONSHIP BETWEEN GRID AND LOW PECLET NUMBERS FOR THE SOLUTION OF CONVECTION-DIFFUSION EQUATION

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ABSTRACT

The problems of grid structure for the numerical calculations are heavily discussed in computational fluid dynamics. In this research, the importance of the relationships between the grid structure and the flow parameters in convection-diffusion problems is emphasized. In particular, we propose a systematic technique in setting the grid number based on its relationship with low Peclet number. Such linear mathematical connection between the two non-dimensional parameters serves as a guideline for a more structured decision-making and improves the heuristic process in the determination of the computational domain grid for the numerical solution of convection-diffusion equations especially in the prediction of the concentration of the scalar. The results confirm the effectiveness of the new approach.

Keywords: convection-diffusion equations, finite difference method, uniform grid, grid number, tridiagonal matrix algorithm.

1. INTRODUCTION

In Cartesian coordinates and tensor notation following the Einstein convention, the generic conservation equation in the partial differential form is

$$\partial_t(\rho\varphi) + \partial_{x_j}(\rho u_j \varphi) - \partial_{x_j}\left(\epsilon \partial_{x_j}\varphi\right) - s_\varphi = 0, \qquad (1)$$

where ρ is the density, φ is the conserved property, u_j are velocity components of the fluid in the axes directions at the point (x_1, x_2, x_3) at time t, ϵ is the diffusivity of φ, and s_φ is the source or sink of φ. Navier-Stokes equations, which have special features of mass and momentum conservations, are extensions of this equation.

The convection-diffusion equation (CDE) takes the simplified form of (1)

$$D_t(\rho\varphi) - \partial_{x_j}\left(\epsilon \partial_{x_j}\varphi\right) = 0, \qquad (2)$$

where zero source/sink is assumed. The first term in (2) is called the substantial derivative

$$D_t(\rho\varphi) = \partial_t(\rho\varphi) + \partial_{x_j}(\rho u_j \varphi). \qquad (3)$$

The substantial derivative $D_t(\rho\varphi)$ is physically interpreted as the time rate of change in $(\rho\varphi)$ following a moving fluid element. The first and second terms on the RHS of (3) are called the local derivative $\partial_t(\rho\varphi)$ (i.e. the physical change in $(\rho\varphi)$ with time at a fixed position), and the convective derivative $\partial_{x_j}(\rho u_j \varphi)$ (i.e. the physical change in $(\rho\varphi)$ with time due to the mass transfer and change in its properties from one spatial position to another), respectively. Substituting (3) into (2) we have

$$\partial_t(\rho\varphi) + \partial_{x_j}(\rho u_j \varphi) - \partial_{x_j}\left(\epsilon \partial_{x_j}\varphi\right) = 0. \qquad (4)$$

In the case of the fluids at rest, or of small velocity ($u_j \approx 0$), or large diffusivity ϵ, as well as solids, (4) is further simplified into

$$\partial_t(\rho\varphi) - \partial_{x_j}\left(\epsilon \partial_{x_j}\varphi\right) = 0,$$

representing the pure diffusion process where the local derivative $\partial_t(\rho\varphi)$ is balanced by the diffusive derivative $\partial_{x_j}\left(\epsilon \partial_{x_j}\varphi\right)$.

In this paper, we consider the steady one-dimensional convection-diffusion problem where (4) reduces to

$$\partial_x(\rho u\varphi) - \partial_x(\epsilon \partial_x \varphi) = 0, \qquad (5)$$

involving the scalar whose concentration is denoted by φ. Such scalar is carried along with the moving fluid element (convection) and spreads due to diffusion. Given appropriate boundary conditions, it can be shown that at relatively high velocity u, or low diffusivity ϵ, the scalar concentration φ initially grows slowly in space and then suddenly rises over a defined distance. The sudden growth of φ not only provides a severe test of the discretization method, but also in the selection of compatible grid structure over the computation domain. Note that the solution of (5) is linear in space when u is negligible.

We investigate the relationship between the flow parameter of interest (i.e. the Peclet number Pe) in CDE and the uniform grid structure with grid number N in finite difference numerical scheme, and formulate the mathematical relationship between N and Pe which is necessary in achieving physically realistic solution of the equation, thus unify the deduction of heuristic selections of minimum grid number for solving the contaminated fluids problem that leads to less pre-computation time.

Note that too much reduction of the grid number may result in the solutions being nonphysical.

2. GRID ISSUES

The issues on grid types and their selection for the numerical solution of a governing equation are important in computational fluid dynamics (CFD), and have been considerably discussed for decades. One of the primary concerns is the influence of a grid structure on numerical accuracy, and its effectiveness in reducing computation time [1]–[10]. Grid concepts of interest may involve two-grid schemes [11], [12], grid refinement or un-refinement [13], minimization of grid number [14], multigrid methods [15]–[20], and numerical oscillation [21].

The reduction of simulation time by means of lattice Boltzmann scheme (LBS) was discussed by [1] and [6], where the performance of LBS was found to be similar to that of one-step second-order Lax–Wendroff scheme, and greater than that of finite difference scheme based on projection method. In [5], [9], and [10], high-order-accuracy schemes were introduced for solving the convection-diffusion equation. In particular, [9] proposed a comprehensive numerical procedure including the employment of a fourth-order compact difference scheme, usage of the Richardson extrapolation technique, and application of an operator interpolation scheme to achieve the sixth-order accurate solution on the fine grid.

The component-wise splitting method was given in [3] as an absolutely stable finite difference scheme where the irregular mesh size seemed to greatly reduce the grid number of the analysis system. It is worth to note that the reduction of grid number should be done with careful since it may lead to numerical oscillation. Such problem was clearly illustrated by [21] while suggesting that the penalized version of upwind hybrid difference method for the convection dominated diffusion equation is capable to reduce severe numerical oscillations. A more general term called 'unphysical solution' was coined by [8] in which three second-order discretization schemes, namely SMART, MINMOD, and Superbee, have proven to produce physically realistic results of calculation.

In this paper, the steady one-dimensional CDE is discretized by finite difference techniques on uniform grids, where the expansion factor $r_e = 1$. The nominal minimum grid number below which the φ profile is nonphysical is then formulated. The formulation is an alternative to that of low Peclet number based grid expansion factor that was discussed in [22].

3. DISCRETIZATION AND SOLUTION OF THE GOVERNING EQUATION

The starting point is the CDE in differential form as given by (5);

$$\partial_x(\rho u\varphi) - \partial_x(\epsilon\partial_x\varphi) = 0.$$

Defining the boundary conditions as

$$\varphi(0) = 0, \quad \varphi(1) = 1. \tag{6}$$

Here we define the Peclet number Pe as

$$Pe = \frac{\rho u L}{\epsilon}.$$

The influence of the Peclet number Pe on the diffusivity coefficient ϵ can be found in [23].

The φ profiles for different ranges of Pe are illustrated in Figure-1.

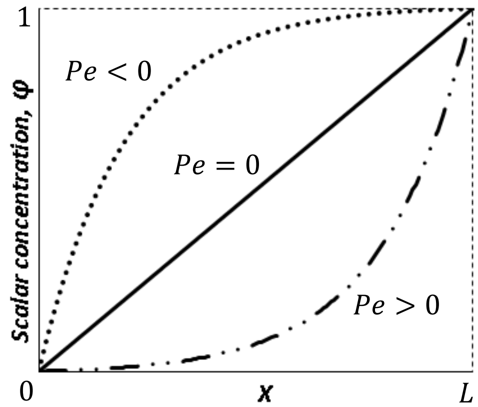

Figure-1. Boundary conditions and solution profiles as a function of the Peclet number.

The corresponding solution domain is covered by a grid. We define the independent variables x whose domain is discretized. The interval $x = [0, (N-1)]$ is subdivided into $(N-1)/h$ subintervals where N and h are odd and even integers, respectively. The nodes are defined by

$$x_{i+1} = x_i + r_e\Delta x_i,$$

where $1 \le i \le (N-1)$, $i \in \mathbb{Z}$, and r_e is the grid expansion factor. Clearly $\sum \Delta x_{i+1} = (N-1)$. The grid is shown in Figure-2.

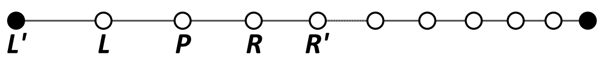

Figure-2. Computational molecules.

At each node, the governing equation is approximated by replacing the partial derivatives with nodal values. The result is an algebraic CDE per node, in which the variables at that and immediate nodes appear as unknowns. The system of equations is expressed by

$$C_P\varphi_P + \textstyle\sum_m C_m\varphi_m = Q_p \tag{7}$$

where P signifies the nodes at which the equations are assigned and m index runs over the immediate nodes. The corresponding matrix C in (7) has non-zero terms only on its main diagonal (represented by C_{ii}) and the diagonals immediately above and below it (represented by C_R and C_L, respectively). The matrix elements are stored as three $n \times n$ array. Using the three-point computational molecules, (7) becomes

$$C_P\varphi_P + C_R\varphi_{i+1} + C_L\varphi_{i-1} = Q_P \tag{8}$$

Since the convection-diffusion differential equation is linear, then the approximation contains only linear terms, and the numerical solution will not require linearization.

The central difference scheme (CDS) is used to discretize the diffusion term, both for the outer derivative

$$-[\partial_x(\epsilon\partial_x\varphi)]_i \approx \frac{(\epsilon\partial_x\varphi)_{i+\frac{1}{2}} - (\epsilon\partial_x\varphi)_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i-1} - x_{i+1})} \tag{9}$$

and the inner derivative

$$\left.\begin{aligned} (\epsilon\partial_x\varphi)_{i+\frac{1}{2}} &\approx \epsilon\frac{\varphi_{i+1} - \varphi_i}{x_{i+1} - x_i} \\ -(\epsilon\partial_x\varphi)_{i-\frac{1}{2}} &\approx \epsilon\frac{\varphi_i - \varphi_{i-1}}{x_{i-1} - x_i} \end{aligned}\right\}, \tag{10}$$

as well as the convection term

$$-[\partial_x(\rho u\varphi)]_i \approx \rho u\frac{\varphi_{i+1} - \varphi_{i-1}}{x_{i-1} - x_{i+1}}. \tag{11}$$

The contributions of the diffusion and convection terms to the coefficients of the algebraic equation (8) are therefore;

$$\begin{aligned} C_R &= C_R^{conv} + C_R^{diff} \\ &= \frac{\rho u}{x_{i+1} - x_{i-1}} - \frac{2\epsilon}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}; \\ C_L &= C_L^{conv} + C_L^{diff} \\ &= -\frac{\rho u}{x_{i+1} - x_{i-1}} - \frac{2\epsilon}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})}; \\ C_P &= C_P^{conv} + C_P^{diff} \\ &= -\left(C_R^{diff} + C_L^{diff}\right). \end{aligned}$$

Tridiagonal matrix algorithm is applied for solving linear system of the algebraic equation (8). We set

$$\rho = 1.0, u = 1.0, r_e = 1. \tag{12}$$

Note that the minimization of grid number might lead to numerical oscillation, where the solution is nonphysical as depicted in Figure-3.

4. SEQUENCES OF THE PECLET NUMBERS AND THE GRID NUMBERS

The range of low Peclet numbers Pe of interests is $[0,100]$. The mathematical relationship between Pe and grid numbers N is represented by a set of ordered pairs $(Pe_i, N_i), i = 1,2, \ldots, \mathrm{n}$.

We define a sequence of Pe by

$$\begin{aligned} &Pe_i, \\ &Pe_{i+1} = Pe_i/p, \\ &Pe_{i+2} = Pe_{i+1}/p, \end{aligned}$$

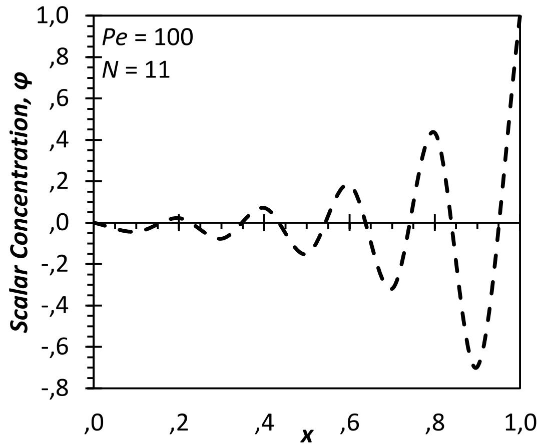

Figure-3. Nonphysical behaviour of scalar concentration profileφdue to the insufficient grid number in computational domain.

$$\begin{aligned} &Pe_{i+3} = Pe_{i+2}/p, \\ &\cdot \\ &\cdot \\ &\cdot \\ &Pe_n = Pe_{n-1}/p, \end{aligned} \tag{13}$$

where the constants $i, p \in \mathbb{Z}^+$.
Next, defining a sequence of N by

$$\begin{aligned} &N_i, \\ &N_{i+1} = floor\left(\frac{N_i + 1}{q}\right), \\ &N_{i+2} = floor\left(\frac{N_{i+1} + 1}{q}\right), \\ &N_{i+3} = floor\left(\frac{N_{i+2} + 1}{q}\right), \\ &\cdot \\ &\cdot \\ &\cdot \\ &N_n = floor\left(\frac{N_{n-1} + 1}{q}\right), \end{aligned} \tag{14}$$

where the constants $i, q \in \mathbb{Z}^+$.

Let W and X be the domain and the target of g, respectively, where the function$g$ from W to X is a collection of ordered pairs of the form (Pe, N). Note that Pe and N are in W and X, respectively. The following conditions need to be satisfied by the collection;

Condition a For each Pe in W, there is an element N in X such that (Pe, N) is one of the ordered pairs. In other words, each element Pe in the domain of g has a value $g(Pe)$ under g.

Condition b If (Pe, N) and (Pe, N') are both among the ordered pairs that make up the function, then $N = N'$. This means that every element of the domain has at most one value under g. The function g is therefore a

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mechanism that assigns to each element Pe of the domain a unique element $g(Pe)$of the target.
We write

$$N = g(Pe),$$

indicating that the ordered pair (Pe, N) is in the collection of ordered pairs which define the function g. Thus the set $\{g(Pe): Pe$ is a real number in W$\}$ of values of g is the image of g.
Let

$i = 1, n = 6, Pe_1 = 100, N_1 = 81$, and

$$p = q = 2, \tag{15}$$

such that the sequence in (13) and (14)become

$$100, 50, 25, 12.5, 6.25, 3.125$$

and

$$81, 41, 21, 11, 6, 3$$

respectively.

Proposition a The sequences' elements in (13) and (14), whose boundary values and independent variables are given in (15), form the ordered pairs (Pe, N) which satisfy Condition a and b such that;

$$\{(Pe_1, N_1), (Pe_2, N_2), \ldots\ldots, (Pe_6, N_6)\} = \{(100, 81), (50, 41), (25, 21), (12.5, 11), (6.25, 6), (3.125, 3)\}$$

Proposition b If $0 \leq Pe \leq 3.125$, then the ordered pair $(Pe, N) = (Pe, 3)$.

5. RESULTS OF CALCULATIONS

The boundary conditions and other parameter settings for CDE (i.e. equation in (5)) are given in (6), and (12)-(15). The concentration φ profiles which are numerically calculated for $Pe$of interests are plotted in Figure-4, and show correct physical behaviours. This proves *Proposition a*. The results vary exponentially in *x*-direction, and the area under the curve represented by the integral

$$\int_0^1 \varphi(x)dx$$

is inversely proportional toPe.

Note that since $N = 3$ matches $Pe = 3.125$,then $N = 3$ is appropriate for $0 \leq Pe \leq 3.125$ where φ profile is close to linearity with respect to *x*. The grid number $N =$ 3is therefore sufficient for the φprofile to behave physically correctly inthe prediction of Pe within the range. Proposition b is thus proven.

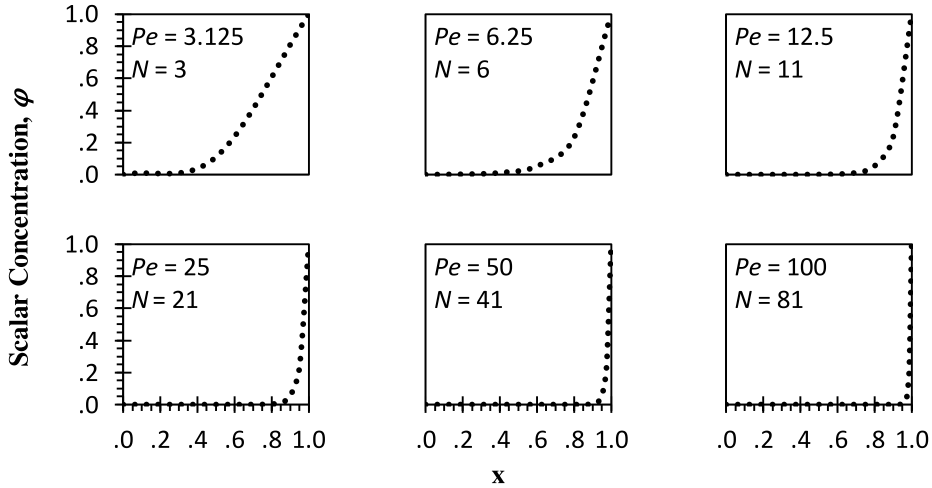

Figure-4. Concentration profile at low Pe, numerically calculated.

In this numerical calculation of a low Peclet number convection-diffusion flow, it is found that the nominal minimum grid number N_{min}which is sufficient for the φ profile to behave physically correctly, is linearly proportional to the Pe as shown in Figure-5.

TheoremLet $0 \leq Pe \leq 100$, the minimum grid number $N_{min}$for solving the convection-diffusion equation in (5), with the flow conditions in (6) and (12), is expressed as a linear function of Pe;

$$\boldsymbol{N_{min} = m\,Pe + b},$$

for $3.125 \leq Pe \leq 100$, and as a constant;

$$\boldsymbol{N_{min} = 3},$$

for $0 \leq Pe \leq 3.125$, where m and b are curve slope and a constant, respectively.

6. FINAL REMARKS

A new technique in the determination of grid number N which represents a quantitative guideline for the numerical solution of the convection-diffusion equations is proposed. The understanding on the influence of the Peclet number Pe on the grid number N formes a basis for a more effective approach in the selection of grid type for the computational procedure.

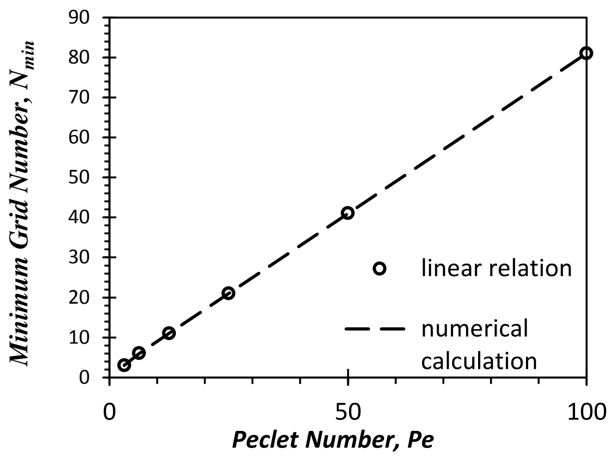

Figure-5. Minimum grid numberN_{min}as a linearfunction ofthe Peclet number Pe.

The key aspect in this research is the formulation of the special function as a collection of ordered pairs of the form $(Pe_i, N_i), i = 1,2, ...,$n for the given CDE. This sheds light on the possibility of a more general framework for the selection of grid type in computational fluid dynamics, the relationship between the flow parameter/s and the grid quality in finite difference numerical scheme, as well as the influence of Pe (e.g. low, transition, high) on the numerical error pattern.

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