Formulation of Low Peclet Number Based Grid Expansion Factor for the Solution of the Convection-Diffusion Equation

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***Abstract*—Convection-diffusion problems, due to its fundamental nature, are found in various science and engineering applications. In this research, the importance of the relationship between grid structure and flow parameters in such problems is emphasized. In particular, we propose a systematic technique in the selection of the grid expansion factor based on its logarithmic relationship with low Peclet number. Such linear mathematical connection between the two non-dimensional parameters serves as a guideline for 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. Results confirm the effectiveness of the new approach.**

Keywords-convection-diffusion equations; finite difference method; non-uniform grid; grid-expansion factor; Thomas algorithm

I. INTRODUCTION

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

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

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)

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

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

$$D_t(\rho\varphi) = \partial_t(\rho\varphi) + \partial_{x_j}\left(\rho u_j \varphi\right) \quad (3)$$

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 $\partial_{x_j}\left(\rho u_j \varphi\right)$ (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

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

In case of 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

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

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 expansion factor r_e based grid structure in finite difference

numerical scheme, and formulate the mathematical relationship between r_e and Pe which is necessary in achieving numerical accuracy in the solution of the equation, thus unify the deduction of heuristic selections of grid expansion factor for solving the contaminated fluids problem that leads to less pre-computation time. Note that the relatively smaller grid expansion factor does not unconditionally lead to higher numerical accuracy.

II. CONVECTION DIFFUSION PROBLEMS

Various numerical methods for solving CDE are by now well formulated and many useful schemes can be found such as finite differences, finite elements, spectral procedures, and the method of lines [1-12]. For instance, [1] presented a comparative study between the two most popular Lattice Boltzmann (LB) models for CDE (i.e. those in two dimensions with five and nine discrete lattice velocities, respectively). Other variants include multiple-relaxation-time LB model for the axisymmetric, as well as isotropic and anisotropic diffusion processes whose both applicability and accuracies have been investigated by [2] and [3] respectively. For the latter case, [4] proposed a finite-difference LB model for nonlinear equations. In the problem where no scalar or flux jump exists, [5] introduced a numerical scheme for dealing with curved interfaces with second-order spatial accuracy in conjunction with the LB method. Authors in [6] summarized well-known a priori error estimates for the discontinuous Galerkin approximation which carry over to the subspace of the discontinuous piecewise-quadratic space, while authors in [7] proposed the approximation of high order alternating evolution. Both [8] and [9] considered compact difference scheme for solving CDE. Authors in [8] claimed that the fourth-order scheme requires only 15 grid points, while authors in [9] successfully proved that it is computationally more efficient than the standard second-order central difference scheme. Recent methods include those that solve nonlinear fractional CDE, as homotopy analysis transform and homotopy perturbation Sumudu transform methods whose reliability and efficiency were clearly demonstrated in [10], and that based on the operational matrices of shifted Jacobi polynomials of high accuracy [11]. Author in [12] introduced a Schwarz waveform relaxation algorithm for the CDE that converges without overlap of the subdomains.

The choice of suitable computational grid to discretize the governing partial differential equations (e.g. by means of polynomial fitting, Taylor series expansion and compact scheme to obtain approximations to the derivatives of the variables with respect to the coordinates) is necessary at the onset of numerical modeling of the convection-diffusion problems as in [1-17]. It is worth noting that the variable values at locations other than the defined grid nodes can also be determined by interpolation. Another important aspect is the method to solve the discretized algebraic equations. The solution is obtained via either direct [18-20] or iterative [21-24] methods. In this paper, the steady one-dimensional CDE is discretized by finite difference techniques on non-uniform grids with a defined number of nodes, and the solutions are obtained by using Thomas' algorithm (i.e. direct method).

III. DISCRETIZATION AND SOLUTION

The starting point is the CDE in differential form as given by (5). Defining the boundary conditions as

$$\begin{aligned} \varphi(0) &= 0, \\ \varphi(1) &= 1 \end{aligned} \tag{6}$$

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 [25]. The φ profiles for different ranges of Pe are illustrated in Figure 1.

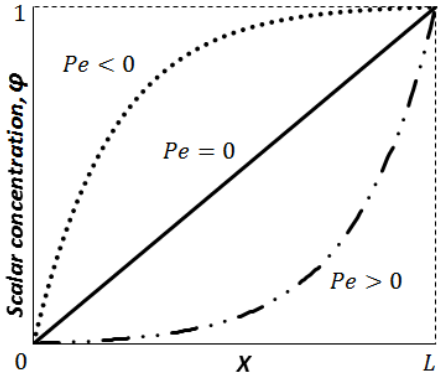

Fig. 1. Boundary conditions and solution profiles as a function of the Peclet number.

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

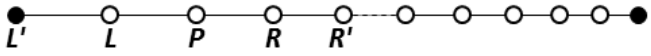

Fig. 2. Computational molecules.

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 unknown. The equation system of is expressed by

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

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;

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

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

$$\begin{aligned}C_P &= C_P^{conv} + C_P^{diff}\\ &= -\left(C_R^{diff} + C_L^{diff}\right)\end{aligned}$$

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

$$\rho = 1.0, u = 1.0, N = 11. \tag{12}$$

IV. SEQUENCES OF THE PECLET NUMBERS AND THE GRID EXPANSION FACTORS

The range of low Peclet numbers Pe is $[0,100]$. The mathematical relationship between Pe and grid expansion factors r_e is represented by a set of ordered pairs $\left(Pe_i, r_{e_i}\right), i = 1,2, \ldots, n$.

We define a sequence of Pe by

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

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

Next, defining a sequence of r_e by

$$\begin{aligned}&re_i,\\ &re_{i+1} = re_i + q,\\ &re_{i+2} = re_{i+1} + q,\\ &re_{i+3} = re_{i+2} + q,\\ &\quad\cdot\\ &\quad\cdot\\ &\quad\cdot\\ &re_n = re_{n-1} + q,\end{aligned} \tag{14}$$

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, r_e). Note that Pe and r_e 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 r_e in X such that (Pe, r_e) 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, r_e) and (Pe, r_e') are both among the ordered pairs that make up the function, then $r_e = r_e'$. This means that every element of the domain has at most one value under g. The function g is therefore a mechanism that assigns to each element Pe of the domain a unique element $g(Pe)$ of the target.

We write

$$r_e = g(Pe),$$

indicating that the ordered pair (Pe, r_e) 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

$$i = 1, n = 6, Pe_1 = 100, re_1 = 0.5, p = 2 \text{ and } q = 0.1 \tag{15}$$

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

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

and

$$0.5, 0.6, 0.7, 0.8, 0.9, 1.0$$

respectively.

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

$$\begin{aligned}&\{(Pe_1, re_1), (Pe_2, re_2), \ldots\ldots, (Pe_6, re_6)\}\\ &= \{(100, 0.5), (50, 0.6), (25, 0.7), (12.5, 0.8),\\ &\quad (6.25, 0.9), (3.125, 1.0)\}.\end{aligned}$$

Proposition b If $0 \leq Pe \leq 3.125$, then the ordered pair $(Pe,\ r_e) = (Pe,\ 1)$.

V. RESULTS OF CALCULATIONS

The boundary conditions and other parameter settings for CDE (i.e. equation in (5)) are given in (6), (12), (13), and (15). The concentration φ profiles which are numerically calculated for Pe of interest are plotted in Figure 3, and show good agreement with the exact solutions. 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 to Pe.

Note that since $r_e = 1.0$ matches $Pe = 3.125$, then $r_e = 1.0$ is appropriate for $0 \leq Pe \leq 3.125$ where φ profile is close to linearity with respect to x. The uniform grid is therefore sufficient for the correct prediction of Pe within the range. Proposition b is thus proven.

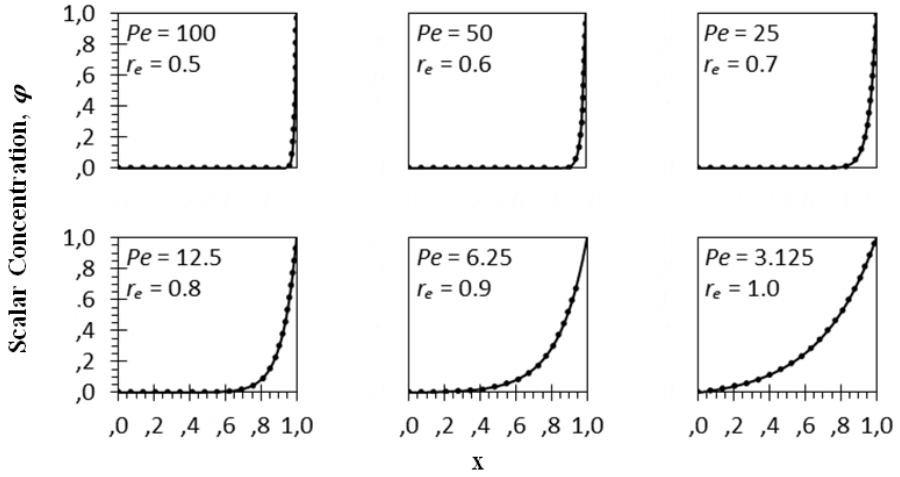

Fig. 3. Concentration profiles

In this numerical calculation of a low Peclet number convection-diffusion flow, it is found that the expansion factor r_e is inversely proportional to the logarithm of Pe as shown in Figure 4.

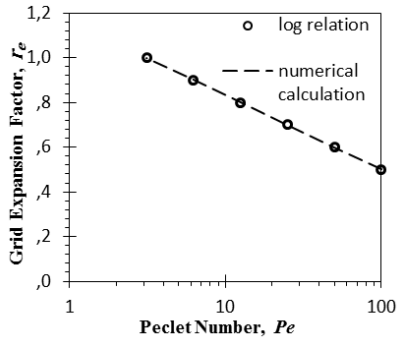

Fig. 4. Grid expansion factor r_e as a function of logarithm of the Peclet number Pe

Theorem Let $0 \leq \mathrm{Pe} \leq 100$, the grid expansion factor $\mathrm{r_e}$ for solving the convection-diffusion equation in (5), with the flow conditions in (6) and (12), is expressed as a linear function of $\lg \mathrm{Pe}$;

$$\mathrm{r_e} = \mathrm{m} \lg \mathrm{Pe} + \mathrm{b},$$

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

$$\mathrm{r_e} = 1$$

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

VI. FINAL REMARKS

A new technique in the determination of grid expansion factor r_e 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 on the grid expansion factor r_e formes a basis for a more effective approach in the selection of grid type for the computational procedure. The key aspect in this research is the formulation of the special function as a collection of ordered pairs of the form $(Pe_i, r_{e_i}), i = 1,2,...,n$ 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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