Computer Assisted Mechanics and Engineering Sciences, 7: 421–426, 2000.
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Comparison of upwind and characteristic schemes for solving multiphase diffusion–convection equation

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(Received August 31, 1999)

In this paper the multiphase diffusion–convection problem is solved numerically by using upwind and characteristic schemes. Discretization for the schemes are performed by finite difference method. For solving the algebraic equations on every time level the modified S.O.R. method is used. In the numerical results computing time, number of iterations and accuracy of the schemes are analysed.

1. Introduction

In this paper two different numerical schemes for solving multiphase diffusion–convection equation is presented. Equation considered is involved in many physical problems of practical interest for example in melting, solidification [2], multi-component fluid flows, flows through porous media, meteorology, pollution problems etc. Usually the problems are discretized by using finite difference, finite element or boundary element method in fixed or in moving grid [6, 7, 8].

The physical situation considered here is involved in steel continuous casting problem [3, 5]. In this problem a one-directional time dependent flow of liquid steel, cooled down in a rectangular geometry.

Let Ω be a rectangular domain in $\mathbb{R}^2$ with the boundary $\Gamma = \Gamma_N \cup \Gamma_D$. Let $T > 0$, and $\Omega_T = \Omega \times]0,T[$. We denote by $H(u(x;t);t)$ the enthalpy and by $u(x;t)$ the temperature of steel at the point $(x;t) \in \Omega_T$.

Using enthalpy method we can formulate the continuous casting problem as a following multiphase diffusion–convection equation which we solve numerically in a fixed grid. For all $t \in]0,T[$ find the pair u, H such that

$$(P) \quad \begin{cases} \dfrac{\partial H}{\partial t} - \Delta u + v(t)\dfrac{\partial H}{\partial x_2} = f(x;t) & \text{on } \Omega, \\ u(x;t) = g_D(x;t) & \text{on } \Gamma_D, \\ \dfrac{\partial u}{\partial n} = g_N(x;t) & \text{on } \Gamma_N, \\ H(x;0) = H_0(x) & \text{on } \Omega. \end{cases}$$

The graph of $H(u)$ is a non-decreasing function $\mathbb{R} \to \mathbb{R}$ involving near vertical segments corresponding to the phase transition state. The speed of the fluid flow to direction x_2 is $v(t)$.

2. Discretization of problem (P)

Let us consider the case where the problem (P) is solved in rectangle domain $\Omega =]0, l_1[\times]0, l_2[$, with the boundary Γ divided into two parts: $\Gamma_D = \{(x_1, x_2) \,|\, x_2 = l_2\,,\ x_1 \in [0, l_1]\}$ and $\Gamma_N = \Gamma \setminus \Gamma_D$.

Let the number of the grid points in both x_1 and x_2 directions are N. Hence the grid parameters are respectively h_1 and h_2. The grid parameter in time is denoted by τ.

Denote

$$\bar{\partial}_1 u(x) = h_1^{-1}[u(x_1, x_2) - u(x_1 - h_1, x_2)]$$
$$\partial_1 u(x) = h_1^{-1}[u(x_1 + h, x_2) - u(x_1, x_2)]$$

and similarly for $\bar{\partial}_2$ and ∂_2. By using normal 5-point difference formula the Laplacian Δ can be discretized

$$\Delta_h = \partial_1\bar{\partial}_1 + \partial_2\bar{\partial}_2 .$$

2.1. Upwind scheme

The semi-discrete upwind scheme approximation for the problem (P) is

$$\begin{cases} \dfrac{\partial H}{\partial t} - \Delta_h u + v\partial_2 H = f & \text{on } \Omega\,, \\ u = g_D & \text{on } \Gamma_D\,, \\ \dfrac{\partial u}{\partial n} = g_N & \text{on } \Gamma_N\,, \\ H(x;0) = H_0(x) & \text{on } \Omega, \end{cases}$$

where

$$\frac{\partial u}{\partial n} = \begin{cases} \bar{\partial}_1 u & \text{if } x_1 = 0, \quad x \in \Gamma \\ \bar{\partial}_1 u & \text{if } x_1 = l_1\,, \quad x \in \Gamma \\ \bar{\partial}_2 u & \text{if } x_2 = 0, \quad x \in \Gamma\,. \end{cases}$$

For time discretization we denote

$$\partial_\tau H = \frac{H^{k+1} - H^k}{\tau}\,.$$

Using implicit Euler method in time and normal difference quotients in space we can write the fully discrete form of equation (P) as follows. For all $k = 0, 1, \ldots, nt-1$ find the pair u^{k+1}, H^{k+1}

$$(P_h) \quad \begin{cases} \partial_\tau H - \Delta_h u^{k+1} + v\partial_2 H^{k+1} = f^{k+1} & \text{on } \Omega\,, \\ u^{k+1} = g_D & \text{on } \Gamma_D\,, \\ \dfrac{\partial u^{k+1}}{\partial n} = g_N & \text{on } \Gamma_N\,, \\ H_0 = H(x;0) & \text{on } \Omega\,. \end{cases}$$

Taking into account boundary conditions and discretizing them by using normal difference quotients we can write the problem (P_h) in the matrix form

$$MH^{k+1} + AU^{k+1} = F^{k+1}. \tag{1}$$

In Eq. (1) the vector H^{k+1} contains the nodal values of the enthalpy and the vector U^{k+1} nodal values of the temperature at the time level $k+1$. The matrix A is the usual 5-point difference approximation for the Laplacian operator, and M is the matrix form for the operator $\partial_\tau + v\partial_2$. The right-hand side vector $F^{k+1} = \bar{F}^{k+1} + \tau^{-1}H^k$ contains all known nodal values of the problem (P_h).

2.2. Characteristic scheme

For the characteristic scheme the discretization of the convection term differs from the upwind scheme. To approximate the term

$$\left(\frac{\partial}{\partial t} + v(t)\frac{\partial}{\partial x_2}\right) H$$

we use the characteristics of this first order differential operator. Namely if (x_1, x_2, t) is the grid point on the time level t we choose the point

$$(x_1, \tilde{x}_2, t-\tau) = \left(x_1, x_2 - \int_{t-\tau}^{t} v(\xi)\,\mathrm{d}\xi, t-\tau\right)$$

on time level $t-\tau$ and approximate the term

$$\left(\frac{\partial}{\partial t} + v(t)\frac{\partial}{\partial x_2}\right) H \approx \frac{H(x_1, x_2, t) - H(x_1, \tilde{x}_2, t-\tau)}{\tau}.$$

Generally the point $(x_1, \tilde{x}_2)$ is not the grid point so we use linear interpolation for the function H. If

$$(x_1, \tilde{x}_2) = \alpha(x_i, x_{j-1}) + (1-\alpha)(x_i, x_j), \qquad \alpha \in (0,1),$$

where (x_i, x_{j-1}) and (x_i, x_j) are grid points, then we put

$$H(x_1, \tilde{x}_2, t-\tau) \equiv \tilde{H}(x_1, x_2, t-\tau) = \alpha H(x_i, x_{j-1}, t-\tau) + (1-\alpha)H(x_i, x_j, t-\tau).$$

Near the boundary $\{x_1 \in [0, l_1], x_2 = 0\}$ it can happen that $(x_1, x_2) \notin \Omega$. In that case we write

$$\tilde{H}(x_1, x_2, t-\tau) = \alpha[2h_2 H(g_i) + H(x_i, x_{j+1}, t-\tau)] + (1-\alpha)H(x_i, x_j, t-\tau).$$

Thus we can write the approximation as

$$\partial_\tau \tilde{H} = \left(\frac{\partial}{\partial t} + v(t)\frac{\partial}{\partial x_2}\right) H \approx \frac{H(x_1, x_2, t) - \tilde{H}(x_1, x_2, t-\tau)}{\tau}.$$

The problem (P) for the characteristic scheme can be written

$$(\tilde{P}_h)\quad \begin{cases} \partial_\tau \tilde{H} - \Delta_h u^{k+1} = f^{k+1} & \text{on } \Omega, \\ u^{k+1} = g_D & \text{on } \Gamma_D, \\ \dfrac{\partial u^{k+1}}{\partial n} = g_N & \text{on } \Gamma_N, \\ H_0 = H(x;0) & \text{on } \Omega, \end{cases}$$

Taking account boundary conditions and discretizing them by using normal difference quotients we can write the above equation also in the matrix form

$$\tilde{M} H^{k+1} + A U^{k+1} = F^{k+1}. \tag{2}$$

In Eq. (2) the vectors H^{k+1}, U^{k+1} and the matrix A are the same as in Eq. (1). In this case $\tilde{M}$ is a diagonal matrix of the form $M = \tau^{-1} I$, where the I is the identity matrix.

3. Solving algorithm

For solving the problem (P_h) respectively $(\tilde{P}_h)$ at time level $k+1$ by using upwind or characteristic scheme we must solve the corresponding algebraic equation (1) or (2). The following calculation algorithm is used at every time step t^{k+1}, $k = 0, \dots, nt-1$. For each time level t^{k+1}, set the initial guess $u^0 = u(x\,;\, t^{k+1} - \tau)$. Moreover we assume that

$$H(u) = \begin{cases} \alpha_1 u + \gamma_1, & u < u_M - \varepsilon, \\ \alpha_2 u + \gamma_2, & u \in [u_M - \varepsilon,\, u_M + \varepsilon], \\ \alpha_3 u + \gamma_3, & u > u_M + \varepsilon, \end{cases}$$

where u_M is the phase change temperature. For theoretical background of the algorithm see Elliot and Ockendon [1].

1. $j := 0$ (number of iterations)
2. $j := j + 1;\quad i := 0$ (number of node)
3. $i := i + 1$
4. $z_i^j = f_i^{j-1} - \left(\sum_{l<i} A_{il} u_l^j + m_{il} H_l^j\right) - \left(\sum_{l>i} A_{il} u_l^{j-1} + m_{il} H_l^{j-1}\right)$
5. $v_i^j = \begin{cases} \dfrac{z_i^j - m_{ii}\gamma_1}{m_{ii}\alpha_1 + a_{ii}}, & \text{if } z_i^j < (u_M - \varepsilon)(m_{ii}\alpha_1 + a_{ii}) + m_{ii}\gamma_1\,, \\ \dfrac{z_i^j - m_{ii}\gamma_3}{m_{ii}\alpha_3 + a_{ii}}, & \text{if } z_i^j > (u_M + \varepsilon)(m_{ii}\alpha_3 + a_{ii}) + m_{ii}\gamma_3\,, \\ \dfrac{z_i^j - m_{ii}\gamma_2}{m_{ii}\alpha_2 + a_{ii}}, & \text{else} \end{cases}$
6. $u_i^j = u_i^{j-1} + \omega(v_i^j - u_i^{j-1})$
7. if $i < N$ (N = total number of nodes) goto 3
8. if $\|u^j - u^{j-1}\| > \epsilon$ go to 2, else STOP.

4. Numerical example

To illustrate the calculation speed and accuracy of the previous numerical schemes the following numerical example is considered.

Let $\Omega =]0,1[\times]0,1[$, with the boundary Γ divided in two parts $\Gamma_D = \{x_1 \in [0,1],\ x_2 = 1\}$ and $\Gamma_N = \Gamma \setminus \Gamma_D$, moreover let $T = 1$. Let us consider the case where the phase change temperature $u_M = 1$ and the latent heat $L = 1$. Let the phase change interval be $[u_M - \varepsilon,\, u_M + \varepsilon]$, $\varepsilon = 0.01$, and the velocity is $v(t) = \frac{1}{5}$.

Our numerical example is

$$\begin{cases} \dfrac{\partial H}{\partial t} - \Delta K + v(t)\,\dfrac{\partial H}{\partial x_2} = f(x;t) & \text{on } \Omega, \\ u(x_1\,,1\,;\,t) = \left(x_1 - \dfrac{1}{2}\right)^2 + \dfrac{5}{4} - \dfrac{1}{2}e^{-4t} & \text{on } \Gamma_D\,, \\ \dfrac{\partial u}{\partial n} = 1 & \text{on } \Gamma_N\,, \\ u(x_1\,,x_2\,;\,0) = \left(x_1 - \dfrac{1}{2}\right)^2 + \left(x_2 - \dfrac{1}{2}\right)^2 + \dfrac{1}{2} & \text{on } \Omega, \end{cases}$$

where

$$H(u) = \begin{cases} 2u & u < u_M - \varepsilon\,, \\ \left(\dfrac{1+8\varepsilon}{2\varepsilon}\right)(u-1) + \dfrac{5+4\varepsilon}{2} & u \in [u_M - \varepsilon\,,\, u_M + \varepsilon]\,, \\ 6u - 3 & u > u_M + \varepsilon\,, \end{cases}$$

and

$$K(u) = \begin{cases} u & u < u_M - \varepsilon\,, \\ \dfrac{3}{2}u - \dfrac{1-\varepsilon}{2} & u \in [u_M - \varepsilon\,,\, u_M + \varepsilon]\,, \\ 2u - 1 & u > u_M + \varepsilon\,. \end{cases}$$

Furthermore

$$f(x;t) = \begin{cases} 4e^{-4t} + \dfrac{1}{5}(4x_2 - 2) - 4 & u < u_M\,, \\ 12e^{-4t} + \dfrac{1}{5}(12x_2 - 6) - 8 & u > u_M \end{cases}$$

The exact solution of our problem is

$$u(x_1\,, x_2\,, t) = \left(x_1 - \frac{1}{2}\right)^2 + \left(x_2 - \frac{1}{2}\right)^2 - \frac{1}{2}e^{-4t} + 1$$

The numerical test was run in the Sun Ultra Enterprise 4000 for different grid parameters h and τ. In Table 1 the maximum iteration number, maximum CPU-time and maximum L_2-error of time levels $k = 1, \dots, nt$ is presented as a function of parameter values.

Table 1. The comparison of upwind and characteristic methods. The parameters ite, CPU and L_2-error are the maximum number of iterations, calculation time and L_2-error of the time levels, respectively

		Upwind scheme			Characteristic scheme		
h	τ	ite	CPU [s]	L_2-error	ite	CPU [s]	L_2-error
$\frac{1}{4}$	$\frac{1}{8}$	23	$2.61 \cdot 10^{-2}$	$4.285 \cdot 10^{-2}$	21	$1.156 \cdot 10^{-2}$	$9.077 \cdot 10^{-2}$
$\frac{1}{8}$	$\frac{1}{16}$	43	0.115	$2.178 \cdot 10^{-2}$	40	$6.919 \cdot 10^{-2}$	$3.340 \cdot 10^{-2}$
$\frac{1}{16}$	$\frac{1}{32}$	76	0.346	$1.122 \cdot 10^{-2}$	74	0.246	$1.498 \cdot 10^{-2}$
$\frac{1}{32}$	$\frac{1}{64}$	127	0.647	$9.199 \cdot 10^{-3}$	127	0.427	$7.053 \cdot 10^{-3}$
$\frac{1}{64}$	$\frac{1}{128}$	205	0.794	$9.056 \cdot 10^{-3}$	205	0.623	$4.915 \cdot 10^{-3}$

In this case it turned out that the both schemes need approximately the same amount of iterations to achieve the required accuracy of stopping criterion in the calculation algorithm. However, the characteristic scheme was at least 30% faster than the upwind scheme. The main reason for that is the difference of the numerical approximation of the convection term. In the characteristic method the convection term is included in time derivative and, hence, updated only once at every time level. In the upwind scheme the convection term is updated at every iteration step.

The both schemes seems to converge properly with respect to the change of grid parameters. The slower convergence of the upwind method, when the grid parameters are small, is probably due to the round off errors in the computer program.

5. Conclusions

The problem considered here is closely involved in continuous casting of metal alloys (steel, copper, aluminium). The study of fast calculation methods has practical interest because of the development of large and realistic simulation models which can be used in process simulation, control and optimization. Our future work is related to the study of the domain decomposition method (DDM) for solving the continuous casting problem [4]. The DDM is suitable for calculating the solution in multiprocessor computer.

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