Conference Applications of Mathematics 2013
in honor of the 70th birthday of Karel Segeth.
Jan Brandts, Sergey Korotov, Michal Křížek,
Jakub Šístek, and Tomáš Vejchodský (Eds.),
Institute of Mathematics AS CR, Prague 2013

A PARALLEL METHOD FOR POPULATION BALANCE EQUATIONS BASED ON THE METHOD OF CHARACTERISTICS

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Abstract

In this paper, we present a parallel scheme to solve the population balance equations based on the method of characteristics and the finite element discretization. The application of the method of characteristics transform the higher dimensional population balance equation into a series of lower dimensional convection-diffusion-reaction equations which can be solved in a parallel way. Some numerical results are presented to show the accuracy and efficiency.

1. Introduction

In this paper, we propose a parallel scheme to solve the population balance equation (PBE) based on the application of the method of characteristics and the finite element method. The PBEs aries from the model of the industrial crystallization process (see, e.g., [7, 11, 12] and the references cited therein). Recently, more and more researchers are interested in the numerical methods for PBEs (c.f. [1, 5, 6, 7]). In PBEs, besides the normal space and time variables, the distribution of entities also depends on their own properties which are referred to as internal coordinates. It is a high dimensional system of equations which is a big challenge from the computational point of view. In order to overcome this difficulty, we use the method of characteristics (c.f. [2, 4]) to transfer the original problem to a series of lower-dimensional convection-diffusion-reaction problems which are defined on the characteristics curves and the spatial directions. Based on the data structure for the method of characteristics, a parallel implementation can be applied to do the simulation process that can improve the computational efficiency.

So far, there exists the alternating direction (operator splitting) method for the PBE by decomposing the original problem into two unsteady subproblems of smaller

complexity (see, e.g., [1, 5, 6]). In the two subproblems, the ordering of the data for the solution needs to be different, since they are discretized in different direction (c.f. [1]). It is not so suitable for the parallel implementation and prevents the further improvement of the computation efficiency for the PBE.

In the present paper, we use the method of characteristics to transform the PBE into a series of convection-diffusion-reaction equations on the characteristic curves in each time step. Then the finite element method is applied to solve the series of convection-diffusion-reaction problems. Furthermore, based on the data structure of the numerical scheme, a parallel scheme is constructed to solve the PBE based on the distributed memory. Some numerical results are provided to check the efficiency of this parallel method.

The rest of the paper will go as follows: Section 2 introduces the model problem under consideration and defines some notation. In Section 3, we describe the method of characteristics for solving the PBE. The finite element discretization for the PBE is described in Section 4. Then Section 5 gives the parallel implementation way for the full discrete form of the PBE. The numerical results are given in Section 6 to validate the efficiency of the numerical method proposed in this paper. Some concluding remarks are given in the last section.

2. Model problem

Let $\Omega_{\mathbf{x}}$ be a simply connected domain in $\mathcal{R}^d$ ($d = 2$ or 3) with Lipschitz continuous boundary $\partial\Omega_{\mathbf{x}}$, $\Omega_\ell = [\ell_{\min}, \ell_{\max}] \subset \mathcal{R}$, and $T > 0$. The state of the individual particle in the PBE equation may consists of the external coordinate $\mathbf{x}$ ($\mathbf{x} = (x_1, \ldots, x_d)$), denoting its position in the physical space, and the internal coordinate ℓ, representing the properties of particles, such as size, volume, temperature etc. A PBE for a solid process such as crystallization with one internal coordinate can be described by the following partial differential equation:

Find $z : (0, T] \times \Omega_\ell \times \Omega_{\mathbf{x}} \to \mathcal{R}$ such that

$$\begin{cases} \partial z/\partial t + G(\ell)\partial_\ell z - \varepsilon\Delta_{\mathbf{x}} z + \mathbf{b}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} z = f(t, \ell, \mathbf{x}) & \text{in } (0, T] \times \Omega_\ell \times \Omega_{\mathbf{x}}, \\ z(0, \ell, \mathbf{x}) = z_{\text{init}}(\ell, \mathbf{x}) & \text{in } \Omega_\ell \times \Omega_{\mathbf{x}}, \\ z(t, \ell_{\min}, \mathbf{x}) = z_{\text{bdry}}(t, \mathbf{x}) & \text{on } (0, T] \times \Omega_{\mathbf{x}}, \\ z(t, \ell, \mathbf{x}) = 0 & \text{on } (0, T] \times \Omega_\ell \times \partial\Omega_{\mathbf{x}}, \end{cases} \tag{1}$$

where the diffusion coefficient $\varepsilon > 0$ is a given constant, $\Delta_{\mathbf{x}}$ and $\nabla_{\mathbf{x}}$ denote the Laplacian and gradient with respect to $\mathbf{x}$, respectively, $\mathbf{b}$ is a given velocity and satisfies $\nabla_{\mathbf{x}} \cdot \mathbf{b} = 0$, and f is a source function. Here $G(\ell) > 0$ represents the growth rate of the particles that depends on ℓ but is independent of $\mathbf{x}$ and t. Furthermore, let us assume the data $G(\ell)$, $\mathbf{b}$, f, z_{init} and z_{bdry} are sufficiently smooth functions for our error estimate analysis.

Now we introduce some notation of the function spaces (see [2, 3]). Let $H^m(\Omega_{\mathbf{x}})$ denote the standard Sobolev space of functions with derivatives up to m in $L^2(\Omega_{\mathbf{x}})$ and the norm is defined by

$$\|v\|_{H^m(\Omega_{\mathbf{x}})} = \left(\int_{\Omega_{\mathbf{x}}} \sum_{0 \le |\alpha| \le m}^{m} \left| \frac{\partial^\alpha v}{\partial \mathbf{x}^\alpha} \right|^2 d\mathbf{x} \right)^{1/2},$$

where α denote a non-negative multi-index $\alpha = \{\alpha_1, \ldots, \alpha_d\}$, $|\alpha| = \sum_{1 \le j \le d} \alpha_j$, and

$$\frac{\partial^\alpha v}{\partial^\alpha \mathbf{x}} = \frac{\partial^{\alpha_1 \ldots \alpha_d} v}{\partial x_1^{\alpha_1} \ldots x_d^{\alpha_d}}.$$

We use $(\cdot, \cdot)_{\mathbf{x}}$ and $\|\cdot\|_{L^2(\Omega_{\mathbf{x}})}$ to denote the L^2-inner product and the associated norm in $\Omega_{\mathbf{x}}$, respectively, which are defined as follows

$$(v, w)_{\mathbf{x}} = \int_{\Omega_{\mathbf{x}}} vw d\mathbf{x} \quad \text{and} \quad \|v\|^2_{L^2(\Omega_{\mathbf{x}})} = (v, v)_{\mathbf{x}}.$$

Let X be a Banach space with the norm $\|\cdot\|_X$. Then we define

$$\begin{aligned}
C(\Omega_\ell; X) &= \Big\{ v : \Omega_\ell \to X : \ v \text{ is continuous} \Big\}, \\
W^{m,\infty}(\Omega_\ell; X) &= \Big\{ v : \Omega_\ell \to X : \ \Big\| \frac{\partial^j v}{\partial \ell^j} \Big\|_X < \infty, \ 0 \le j \le m \Big\}, \\
W^{m,\infty}((0,T]; X) &= \Big\{ v : (0,T] \to X : \ \Big\| \frac{\partial^j v}{\partial t^j} \Big\|_X < \infty, \ 0 \le j \le m \Big\},
\end{aligned}$$

where the derivatives $\partial^j v / \partial \ell^j$ and $\partial^j v / \partial t^j$ are understood in the sense of distributions on Ω_ℓ and $(0, T]$, respectively. The norms in the above defined spaces are given as follows

$$\begin{aligned}
\|v\|_{C(\Omega_\ell; X)} &= \sup_{\ell \in \Omega_\ell} \|v(\ell)\|_X, \\
\|v\|_{W^{m,\infty}(\Omega_\ell; X)} &= \max_{0 \le j \le m} \sup_{\ell \in \Omega_\ell} \Big\| \frac{\partial^j v}{\partial \ell^j} \Big\|_X, \\
\|v\|_{W^{m,\infty}((0,T]; X)} &= \max_{0 \le j \le m} \sup_{t \in (0,T]} \Big\| \frac{\partial^j v}{\partial t^j} \Big\|_X.
\end{aligned}$$

For spaces X, Y and Z, we use the short notation $Z(Y(X)) := Z((0, T]; (Y(\Omega_\ell; X))$ in this paper.

3. Method of characteristics

In this section, we describe the method of characteristics (c.f. [2, 4, 9]) for the PBE (1). The reason we adopt this method for the discretization in the product space

$(0,T]\times\Omega_\ell$ is that it has the suitable data structure for the parallel implementation which will be discussed in the following sections.

First we set

$$\psi(t,\ell) \;=\; (1+G(\ell)^2)^{1/2}.$$

Let the characteristic direction associated with the hyperbolic part of (1), $\partial z/\partial t + G(\ell)\partial z/\partial \ell$, be denoted by $s(t)$. Then

$$\frac{\partial}{\partial s} \;=\; \frac{1}{\psi}\frac{\partial}{\partial t} + \frac{G(\ell)}{\psi}\frac{\partial}{\partial \ell}. \tag{2}$$

Then (1) can be written as

$$\begin{cases} \psi\partial z/\partial s - \varepsilon\Delta_{\mathbf{x}} z + \mathbf{b}(\mathbf{x})\cdot\nabla_{\mathbf{x}} z = f & \text{in } (0,T]\times\Omega_\ell\times\Omega_{\mathbf{x}},\\ z(0,\ell,\mathbf{x}) = z_{\text{init}}(\ell,\mathbf{x}) & \text{in } \Omega_\ell\times\Omega_{\mathbf{x}},\\ z(t,\ell_{\min},\mathbf{x}) = z_{\text{bdry}}(t,\mathbf{x}) & \text{on } (0,T]\times\Omega_{\mathbf{x}},\\ z(t,\ell,\mathbf{x}) = 0 & \text{on } (0,T]\times\Omega_\ell\times\partial\Omega_{\mathbf{x}}. \end{cases} \tag{3}$$

We use uniform partitions for the time interval $(0,T]$ and the internal coordinate interval Ω_ℓ, respectively. Let $\tau = T/N$, $\iota = (\ell_{\max}-\ell_{\min})/M$, $t^n = n\tau$, $n = 0,1,\ldots,N$ and $\ell_m = \ell_{\min} + m\iota$, $m = 0,1,\ldots,M$. In order to satisfy the stability condition, we set

$$\tau \le \frac{\iota}{\max_{\ell_{\min}\le\ell\le\ell_{\max}} G(\ell)}. \tag{4}$$

Then starting with $z(0,\ell,\mathbf{x}) = z_{\text{init}}$, $z(t,\ell_{\min},\mathbf{x}) = z_{\text{bdry}}(t,\mathbf{x})$, the equation (3) can be discreted in each sub-intervals $(t^{n-1},t^n]\times(\ell_{m-1},\ell_m]\times\Omega_{\mathbf{x}}$ ($n = 1,2,\ldots,N$ and $m = 1,2,\ldots,M$) as follows.

First we compute

$$\check{\ell}_m \;=\; \ell_m - \tau G(\ell_m). \tag{5}$$

Actually, this is a first order discretization to obtain the approximation at the time level $t = t^{n-1}$ for the following characteristic ordinary differential equation (c.f. [4]):

$$\begin{cases} d\ell/dt \;=\; G(\ell) & \text{in } [t^{n-1},t^n),\\ \ell(t^n) \;=\; \ell_m. \end{cases} \tag{6}$$

From the condition (4), we have $\check{\ell}_m \ge \ell_{\min}$ for $m \ge 1$. Then we compute the direction differential $\psi\frac{\partial z}{\partial s}$ at the node (t^n,ℓ_m) in the following way

$$\begin{aligned} \psi(t^n,\ell_m)\frac{\partial z}{\partial s}(t^n,\ell_m,\mathbf{x}) \;&\approx\; \psi(t^n,\ell_m)\frac{z(t^n,\ell_m,\mathbf{x}) - \check{z}(t^{n-1},\check{\ell}_m,\mathbf{x})}{(\tau^2+(\ell_m-\check{\ell}_m)^2)^{1/2}}\\ &=\; \frac{z(t^n,\ell_m,\mathbf{x}) - \check{z}(t^{n-1},\check{\ell}_m,\mathbf{x})}{\tau}, \end{aligned} \tag{7}$$

where $\check{z}\left(t^{n-1},\check{\ell}_m,\mathbf{x}\right) := \alpha_m^n\, z\left(t^{n-1},\ell_{m-1},\mathbf{x}\right) + \left(1-\alpha_m^n\right) z\left(t^{n-1},\ell_m,\mathbf{x}\right)$ with $\alpha_m^n = (\ell_m - \check{\ell}_m)/\iota$.

In order to give the semi-discrete form of the PBE, we set $z_m^n(\mathbf{x}) \approx z(t^n,\ell_m,\mathbf{x})$. Then the semi-discrete form of the PBE can be defined as follows:

$$\begin{cases} \frac{z_m^n(\mathbf{x})-\check{z}_m^n(\mathbf{x})}{\tau} - \varepsilon\Delta_{\mathbf{x}} z_m^n(\mathbf{x}) + \mathbf{b}(\mathbf{x})\nabla_{\mathbf{x}} z_m^n(\mathbf{x}) = f_m^n(\mathbf{x}) & \text{in } \Omega_{\mathbf{x}}, \\ z_m^0(\mathbf{x}) = z_{\text{init}}^m(\mathbf{x}) & \text{for } x \in \Omega_{\mathbf{x}}, \\ z_0^n(\mathbf{x}) = z_{\text{bdry}}(t^n,\mathbf{x}) & \text{for } (0,T]\times\Omega_{\mathbf{x}}, \\ z_m^n(\mathbf{x}) = 0 \text{ for } m = 1,2,\ldots,M & \text{on } \partial\Omega_{\mathbf{x}}\,, \end{cases} \tag{8}$$

where $f_m^n(\mathbf{x}) = f(t^n,\ell_m,\mathbf{x})$, $\check{z}_m^n(\mathbf{x}) = \alpha_m^n z_{m-1}^{n-1}(\mathbf{x}) + (1-\alpha_m^n) z_m^{n-1}(\mathbf{x})$.

From the Taylor expansion method, we can derive the following error estimate for the semi-discrete form (8)

$$\|z(t^n,\ell_m,\mathbf{x}) - z_m^n(\mathbf{x})\|_{C(X)} \;\leq\; C\tau \|z(t,\ell,\mathbf{x})\|_{W^{2,\infty}(W^{1,\infty}(X))}, \tag{9}$$

where the space X can be $L^2(\Omega_{\mathbf{x}})$ or $H^1(\Omega_{\mathbf{x}})$.

4. Finite element method

In this section, we give the fully discrete form of the PBE by the finite element method. Let V_h be a finite element subspace of $H_0^1(\Omega_{\mathbf{x}})$ which has the k-th order of accuracy (c.f. [2, 3]):

$$\inf_{v_h\in V_h} \|u - v_h\|_{H^1(\Omega_{\mathbf{x}})} \leq Ch^k \|u\|_{H^{m+1}(\Omega_{\mathbf{x}})} \quad \forall u \in H^{m+1}(\Omega_{\mathbf{x}}). \tag{10}$$

and

$$\inf_{v_h\in V_h} \|u - v_h\|_{L^2(\Omega_{\mathbf{x}})} \leq Ch^{k+1} \|u\|_{H^{m+1}(\Omega_{\mathbf{x}})} \quad \forall u \in H^{m+1}(\Omega_{\mathbf{x}}). \tag{11}$$

Based on the finite element space V_h, we can define the fully discrete form for the PBE as follows:

For the n-th time step $t = t^n$ and $m = 0,1,\ldots,M$, find $z_{m,h}^n \in V_h$ such that

$$\begin{cases} \left(\frac{z_{m,h}^n - \check{z}_{m,h}^n}{\tau}, v_h\right) + a(z_{m,h}^n, v_h) = (f_m^n(\mathbf{x}), v_h) & \forall v_h \in V_h, \\ a_0(z_{m,h}^0, v_h) = a_0(z_{\text{init}}(\ell_m,\mathbf{x}), v_h) & \forall v_h \in V_h,\ m = 1,\ldots,M, \\ a_0(z_{0,h}^n, v_h) = a_0(z_{\text{bdry}}(t^n,\mathbf{x}), v_h) & \forall v_h \in V_h, \end{cases} \tag{12}$$

where $\check{z}_{m,h}^n = \alpha_m^n z_{m-1,h}^{n-1} + (1-\alpha_m^n) z_{m,h}^{n-1}$ with α_m^n being defined in Section 3 and

$$\begin{aligned} a(u,v) &= \int_{\Omega_{\mathbf{x}}} \left(\varepsilon\nabla u\cdot\nabla v + \mathbf{b}(\mathbf{x})\cdot\nabla u\; v\right) d\mathbf{x}, \\ a_0(u,v) &= \int_{\Omega_{\mathbf{x}}} \nabla u\cdot\nabla v d\mathbf{x}. \end{aligned}$$

From the standard error estimate theory of the finite element method (c.f. [2, 3]), the fully discrete form (12) has the following error estimates

$$\max_{1\le m\le M}\|z(T,\ell_m,\mathbf{x})-z_{m,h}^N\|_{H^1(\Omega_{\mathbf{x}})}\le C(\tau+h^k)\|z\|_{W^{2,\infty}(W^{1,\infty}(H^{k+1}(\Omega_{\mathbf{x}})))} \tag{13}$$

and

$$\max_{1\le m\le M}\|z(T,\ell_m,\mathbf{x})-z_{m,h}^N\|_{L^2(\Omega_{\mathbf{x}})}\le C(\tau+h^{k+1})\|z\|_{W^{2,\infty}(W^{1,\infty}(H^{k+1}(\Omega_{\mathbf{x}})))}. \tag{14}$$

5. A parallel way

In this section, we present a parallel scheme to solve the PBE (1) based on the full discrete (12). Fortunately, from (12), we can find that the finite element equation is independent for each m in any time step t^n. Based on this property, we can construct a type of parallel scheme to implement the full discretization of the fully discrete form (12).

Assume we use P processors to compute the PBE. Decompose the set $\{0,1,2,\ldots,M\}$ into P subsets $\mathbf{m}_1,\mathbf{m}_2,\ldots,\mathbf{m}_P$ such that $\mathbf{m}_1=\{0,1,\ldots,m_1-1\}$, $\mathbf{m}_p=\{m_{p-1},m_{p-1}+1,\ldots,m_p-1\}$ $(p=2,\ldots,P-1)$ and $\mathbf{m}_P=\{m_{P-1},\ldots,m_P-1\}$. In the p-th processor, the equation (12) is solved on the sub-intervals $(t^{n-1},t^n]\times(\ell_{m_{p-1}},\ell_{m_p-1}]\times\Omega_{\mathbf{x}}$ $(n=1,2,\ldots,N,\ p=1,2,\ldots,P,\ \ell_0=\ell_{\min}$ and $\ell_M=\ell_{\max})$. Because the growth rate of the particles $G(\ell)$ is positive, the dependence of each point ℓ_m is on the left $(\ell<\ell_m)$. This means that the solution $z_{m_p-1,h}^{n-1}$ in the p-th processor as the initial condition for the $(p+1)$-th processor computing at the time step t^n.

We allocate the memory in the p-th processor $(p=1,\ldots,P)$ to save the solutions $z_{m_{p-1},h}^n,\ldots,z_{m_p-1,h}^n$ and the p-th processor $(p=1,\ldots,P-1)$ should send its saved solutions to the next $(p+1)$-th processor after each time step computation. Obviously, for $p=1$, we need to use the boundary condition $z_{\mathrm{bdry}}(t,\mathbf{x})$. Similarly for $p=P$, the sending of solutions is not required since it is the last processor. Based on this distribution of the memory and the computation of the scheme (12), we can construct the following parallel algorithm for the PBE.

Algorithm 5.1. *Parallel algorithm for PBE*

For $n=1,2,\ldots,N$ do

1. *On each processor, compute the solution $z_{m,h}^n$ for $m\in\mathbf{m}_p$ $(p=1,2,\ldots,P)$ in sub-interval $(t^{n-1},t^n]\times(\ell_{m_{p-1}},\ell_{m_p-1}]$.*
2. *For $p=1,2,\ldots,P-1$, send the solutions obtained in the p-th processor $z_{m,h}^n$ $(m\in\mathbf{m}_p)$ to the $(p+1)$-th processor.*
3. *If $n<N$, set $n:=n+1$ and go to Step 1. Else stop.*

6. Numerical results

In this section, we provide some numerical results to validate the numerical scheme proposed in this paper. Let $\Omega_{\mathbf{x}} = [0,1] \times [0,1]$, $\Omega_\ell = [0,1]$, $T = 1$, $\varepsilon = 1$, and $\mathbf{b}(\mathbf{x}) = (1,1)^T$. We chose the functions $f(t,\ell,\mathbf{x})$, $z_{\text{init}}(\ell,\mathbf{x})$ and $z_{\text{bdry}}(t,\mathbf{x})$ such that the exact solution is

$$z(t,\ell,x,y) = \mathrm{e}^{-at}\sin(\pi\ell)\sin(\pi x)\sin(\pi y)$$

with $a = 0.1$. The growth rate of the particles is $G(\ell) = \frac{1}{2} + 2(1-\ell)\ell$.

First, we check the convergence order for the error estimates

$$\|e\|_0 = \max_{1\le m\le M} \|z(T,\ell_m,\mathbf{x}) - z^n_{m,h}\|_{L^2(\Omega_{\mathbf{x}})} \tag{15}$$

and

$$\|e\|_1 = \max_{1\le m\le M} \|z(T,\ell_m,\mathbf{x}) - z^n_{m,h}\|_{H^1(\Omega_{\mathbf{x}})}. \tag{16}$$

The convergence order of the linear and quadratic finite element method for the discretization in $\Omega_{\mathbf{x}}$ is shown in Tables 1 and 2. We see that the experimental results of convergence approach to the theoretically predicated values both for linear and quadratic elements.

mesh size h	$\|e\|_0$		$\|e\|_1$	
	error	order	error	order
2^{-2}	4.5702E-01		2.6897E-00	
2^{-3}	1.4872E-01	1.6197	1.5128E-00	0.8302
2^{-4}	4.0481E-02	1.8773	7.8083E-01	0.9541
2^{-5}	1.0318E-02	1.9721	3.9359E-01	0.9883
2^{-6}	2.7230E-03	1.9219	1.9720E-01	0.9970

Table 1: Errors (15) and (16) and the corresponding rates of convergence for linear element with $\tau = \iota = h^2$.

mesh size h	$\|e\|_0$		$\|e\|_1$	
	error	order	error	order
2^{-1}	6.0137E-01		2.5073E-00	
2^{-2}	6.3958E-02	3.2331	8.5316E-01	1.5552
2^{-3}	7.4660E-03	3.0987	2.3528E-01	1.8584
2^{-4}	9.5200E-04	2.9713	6.0522E-02	1.9588

Table 2: Errors (15) and (16) and the corresponding rates of convergence for quadratic element with $\tau = \iota = h^3$.

size of internal coordinate ι	$\|e\|_0$ error	order	$\|e\|_1$ error	order
2^{-2}	6.3862E-01		2.8423E-00	
2^{-3}	3.4562E-01	0.8858	1.5382E-00	0.8858
2^{-4}	1.7650E-01	0.9695	7.8427E-01	0.9718
2^{-5}	8.8689E-02	0.9928	3.9404E-01	0.9930
2^{-6}	4.4398E-02	0.9983	1.9726E-01	0.9980

Table 3: Errors (15) and (16) and the corresponding rates of convergence in the internal coordinate for the quadratic element with $h = \iota$ and $\tau = \iota^2$.

number of processors	8	16	32	64	128
time (in seconds)	28103.01	13555.03	6832.26	3708.71	1840.43
rate of speed up	1.00	2.07	4.11	7.57	15.26

Table 4: Strong parallel test with linear element $h = 1/256$, $\tau = 1/512$ and $\iota = 1/512$.

number in ℓ	1	2	4	8	16
8	9.30	15.30	27.51	55.28	116.42
16	9.91	15.44	28.44	59.44	117.24
32	9.85	16.98	32.02	60.93	118.89
64	10.01	17.28	32.66	63.88	121.96
128	10.21	17.98	33.55	64.27	127.63

Table 5: Weak parallel test with linear element $h = 1/256$: average time in seconds.

number in ℓ	1	2	4	8	16
8	11.19	16.10	27.60	60.52	120.26
16	11.26	16.43	31.54	61.36	120.83
32	12.73	18.50	35.29	68.18	131.98
64	11.20	19.63	36.39	75.43	133.55
128	12.86	20.28	38.01	73.63	146.01

Table 6: Weak parallel test with linear element $h = 1/256$: maximum time in seconds.

We also check the convergence order for the method of characteristics developed in Section 3. The corresponding numerical result are provided in Table 3. From this table, we can find the convergence order is 1 which is the same as in (9).

Now we come to check the efficiency of the parallel scheme of Algorithm 5.1. For this aim, we set the discretization parameters $h = 1/256$, $\tau = \iota = 1/512$ and use the linear finite element method. The run-time (in seconds) is shown in Table 4. From Table 4, we can find that the parallel Algorithm 5.1 has a good expansibility.

We also check the run-time in each processor for different scale in each processor. For each test, we run 8 time steps ($N = 8$). Tables 5 and 6 show the corresponding run-time (in seconds) for the average time and maximum time, respectively, for all the processors. These two tables also show that Algorithm 5.1 has good parallel properties.

7. Concluding remarks

In this paper, we are concerned with the parallel numerical method for the PBEs with one internal coordinate posed on the domain $(0, T] \times \Omega_\ell \times \Omega_{\mathbf{x}}$ with the dimension $1 + 1 + d$. The parallel scheme is based on the method of characteristics and the finite element discretization. Some numerical results are also provided in Section 6 to demonstrate the efficiency of the proposed method.

Here, for the simplicity of the description of the numerical method, we assume the diffusion coefficient ε to be large enough such that the diffusion is dominated. For the convection dominated case (c.f. [1, 10, 13]), we will combine the method of characteristics and the stabilized finite element methods (c.f. [1, 2, 13, 10]) and this is our future work. Furthermore, the parallel method should also be applied to the simulation of the industrial crystallization process (c.f. [11, 12]) and other similar models (c.f. [7]).

Acknowledgements

This work is supported in part by the National Science Foundations of China (NSFC 11001259, 2011CB309703 and 2010DFR00700) and Croucher Foundation of Hong Kong Baptist University, the national Center for Mathematics and Interdisciplinary Science, CAS, the President Foundation of AMSS-CAS. The second author gratefully acknowledges the support from the MBF-Project SimParTurS under the grant 03TOPAA1 and the Institute for Analysis and Computational Mathematics, Otto-von-Guericke-University Magdeburg.

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