Convergence analysis of sectional methods for solving aggregation population balance equations: The cell average technique

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Abstract. The paper deals with the convergence analysis of the cell average technique given by J. Kumar et al. [3] to solve the nonlinear aggregation population balance equations. Similarly to our previous paper Giri et al. [1], which considered the fixed pivot technique, the main emphasis here is to check the convergence for five different types of uniform and non-uniform meshes. First, we observed that the cell average technique is second order convergent on a uniform, locally uniform and non-uniform smooth meshes. Secondly, the scheme is examined closely on an oscillatory and non-uniform random meshes. It is found that the scheme is only first accurate there. In spite of this, the cell average technique gives one order higher accuracy than the fixed pivot technique for locally uniform, oscillatory and random meshes. Several numerical simulations verify the mathematical results of the convergence analysis. Finally the numerical results obtained are also compared with those for the case of the fixed pivot technique.

Keywords: Particles; Aggregation; Cell average technique; Consistency; Convergence.

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1 Introduction

The population balance equations (PBEs) are analytically solvable only for some restricted class of kernels. Because of restrictions, it has been of great interest to develop new numerical methods and assess them by means of mathematical analysis. As noticed by Kostoglou [2] among all numerical sectional methods for solving PBE, the fixed pivot technique [7] is the most popular and widely used in the literature. A new step in the development of sectional methods is due to the recently introduced cell average technique developed by J. Kumar et al. [3]. In a recent paper by Giri et al. [1], convergence analysis of the fixed pivot technique has been discussed for solving aggregation PBE. It has been observed that the fixed pivot technique is second order

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accurate on uniform and non-uniform smooth meshes. Moreover, it has been shown that the scheme is first order accurate on a locally uniform mesh. Quite surprising results have been found on oscillatory and random meshes. The analysis clearly shows that the scheme does not converge on oscillatory and non-uniform random meshes.
The purpose of this work is to demonstrate the convergence analysis of the cell average technique and to compare mathematical as well as numerical results with the fixed pivot technique discussed in [1]. A general idea of the sectional methods and some basic definitions and theorems used in further analysis will be directly taken from [1]. Before proceeding to the next section, it is recommended that readers review the Section 2 in [1].
Let us briefly organize the content of this paper. The mathematical formulation of the cell average technique is reviewed in Section 2. The consistency and convergence are investigated in Section 3 and 4, respectively. Numercial justification of the mathematical results is given in section 5. The all observations presented in this paper are summerized in the last section.

2 The cell average technique

Let us begin with the following truncated version aggregation population balance equation

$$\frac{\partial n(t,x)}{\partial t} = \frac{1}{2}\int_0^x \beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)d\epsilon - \int_0^{x_{\max}} \beta(x,\epsilon)n(t,x)n(t,\epsilon)d\epsilon, \tag{1}$$

with initial condition

$$n(x,0) = n^{\text{in}}(x) \geq 0, \quad x \in \Omega :=]0, x_{\max}].$$

Let I stand for the total number of cells. The total number of particles in the ith cell $\Lambda_i :=]x_{i-1/2}, x_{i+1/2}]$ is given as

$$N_i(t) = \int_{x_{i-1/2}}^{x_{i+1/2}} n(t,x)dx.$$

Integrating the continuous equation (1) over the ith cell we obtain

$$\frac{dN_i}{dt} = B_i - D_i, \quad i = 1, \dots, I,$$

The total birth rate B_i and death rate D_i are given as

$$B_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x \beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)d\epsilon dx. \tag{2}$$

and

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} \beta(x,\epsilon)n(t,\epsilon)n(t,x)d\epsilon dx. \tag{3}$$

The total discrete birth and death rates of particles are calculated by substituting the number density approximation

$$n(t,x) \approx \sum_{i=1}^{I} N_i(t)\delta(x - x_i)$$

into equations (2) and (3) as

$$\hat{B}_i = \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\beta(x_k, x_j)N_j N_k, \tag{4}$$

and

$$\hat{D}_i = N_i \sum_{j=1}^{I} \beta(x_i, x_j)N_j. \tag{5}$$

Here $\hat{B}_i$ and $\hat{D}_i$ denote the discrete birth and death rates in the ith cell respectively. The total volume flux V_i into cell i as a result of aggregation is given by

$$V_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x x\beta(x - \epsilon, \epsilon)n(t, x - \epsilon)n(t, \epsilon)d\epsilon dx. \tag{6}$$

Similarly to the discrete birth rate the discrete volume flux can be obtained as

$$\hat{V}_i = \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\beta(x_k, x_j)N_j N_k(x_j + x_k). \tag{7}$$

Consequently, the average volume $\overline{v}_i \in [x_{i-1/2}, x_{i+1/2}]$ of all new born particles in the ith cell can be evaluated as

$$\overline{v}_i = \frac{\hat{V}_i}{\hat{B}_i}, \quad \hat{B}_i > 0. \tag{8}$$

We do not need volume average $\overline{v}_i$ in case of $\hat{B}_i = 0$. However, for the sake of simplicity of the algorithm, we can set $\overline{v}_i = x_i$ for $\hat{B}_i = 0$. It is assumed that all of the $\hat{B}_i$ particles are assigned temporarily at the average volume $\hat{v}_i$. If the average volume $\hat{v}_i$ is same as the pivot size x_i then the total birth $\hat{B}_i$ can be assigned to the node x_i. But this is rarely possible and hence the total particle birth $\hat{B}_i$ has to be assigned to the neighboring nodes in such a way that the total number and mass remain conserved during this reassignment. Finally, the resultant set of ODEs takes the following form

$$\frac{d\hat{N}_i}{dt} = \hat{B}_i^{CA} - \hat{D}_i^{CA} \tag{9}$$

Let us consider the Heaviside function

$$H(x) := \begin{cases} 1 & \text{if } x > 0, \\ \frac{1}{2} & \text{if } x = 0, \\ 0 & \text{if } x < 0. \end{cases}$$

and

$$\lambda_i^{\pm}(x) = \frac{x - x_{i\pm 1}}{x_i - x_{i\pm 1}}. \tag{10}$$

Then the birth and death terms are given as

$$\begin{aligned} \hat{B}_i^{CA} =& \hat{B}_{i-1}\lambda_i^-(\overline{v}_{i-1})H(\overline{v}_{i-1} - x_{i-1}) + \hat{B}_i\lambda_i^+(\overline{v}_i)H(\overline{v}_i - x_i) \\ &+ \hat{B}_i\lambda_i^-(\overline{v}_i)H(x_i - \overline{v}_i) + \hat{B}_{i+1}\lambda_i^+(\overline{v}_{i+1})H(x_{i+1} - \overline{v}_{i+1}) \end{aligned} \tag{11}$$

and

$$\hat{D}_i = N_i \sum_{j=1}^{I} \beta(x_i, x_j) N_j. \tag{12}$$

The first and the fourth terms on the right hand side of equation (11) can be set to zero for $i = 1$ and $i = I$ respectively. The numerical approximation of $N_i(t)$ is defined by $\hat{N}_i(t)$. In the rest of this paper, for the sake of simplicity, we suppress the notation of parameter t and use N_i instead of $N_i(t)$. The set of equations (9) is a discrete formulation for solving a general aggregation problem. The form of aggregation kernel and type of grids can be chosen arbitrarily. The set of equations (9) together with an initial condition can be solved with any higher order ODE solver to obtain number of particles in a cell $\hat{N}_i$. An appropriate solver to solve such equations is recommended in Giri et al. [1]. All other details can be found in [3, 4].
By using (4) and (5) the cell average technique (9) can be written as

$$\begin{aligned} \frac{d\hat{N}_i}{dt} =& \lambda_i^-(\overline{v}_{i-1})H(\overline{v}_{i-1} - x_{i-1}) \sum_{x_{i-3/2} \le x_j + x_k < x_{i-1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\beta(x_k, x_j)N_jN_k \\ &+ [\lambda_i^+(\overline{v}_i)H(\overline{v}_i - x_i) + \lambda_i^-(\overline{v}_i)H(x_i - \overline{v}_i)] \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\beta(x_k, x_j)N_jN_k \\ &+ \lambda_i^+(\overline{v}_{i+1})H(x_{i+1} - \overline{v}_{i+1}) \sum_{x_{i+1/2} \le x_j + x_k < x_{i+3/2}}^{j \ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right)\beta(x_k, x_j)N_jN_k \\ &- N_i \sum_{j=1}^{I} \beta(x_i, x_j)N_j. \end{aligned} \tag{13}$$

Before proceeding to the next section let us assume

$$\Delta x_{\min} \le \Delta x_i = x_{i+1/2} - x_{i-1/2} \le \Delta x \quad \text{and} \quad \frac{\Delta x}{\Delta x_{\min}} \le K,$$

where K is a positive constant.

3 Consistency

We need the following lemma to investigate the consistency of the cell average technique.

Lemma 3.1. *If B_i, D_i, $\hat{B}_i$, $\hat{D}_i$, V_i and $\hat{V}_i$ are given by equations (2)-(7) respectively, then we have the following error estimates*
1. $B_i = \hat{B}_i + \mathcal{O}(\Delta x^3)$,
2. $D_i = \hat{D}_i + \mathcal{O}(\Delta x^3) = \hat{D}_i^{CA} + \mathcal{O}(\Delta x^3)$,
3. $V_i = \hat{V}_i + \mathcal{O}(\Delta x^3)$.

Proof. Let us first consider

$$B_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}}\int_0^x \beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)d\epsilon dx.$$

By changing the order of integration we get

$$\begin{aligned}B_i =&\frac{1}{2}\int_0^{x_{i-1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}}\beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)dxd\epsilon\\&+\frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}}\int_{\epsilon}^{x_{i+1/2}}\beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)dxd\epsilon.\end{aligned}$$

This can be rewritten as

$$\begin{aligned}B_i =&\frac{1}{2}\sum_{j=1}^{i-1}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}}\beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)dxd\epsilon\\&+\frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}}\int_{\epsilon}^{x_{i+1/2}}\beta(x-\epsilon,\epsilon)n(t,x-\epsilon)n(t,\epsilon)dxd\epsilon.\end{aligned}$$

Now we apply the midpoint rule to the outer integrals in both terms on the right hand side to obtain

$$\begin{aligned}B_i =&\frac{1}{2}\sum_{j=1}^{i-1}\int_{x_{i-1/2}}^{x_{i+1/2}}\beta(x-x_j,x_j)n(t,x-x_j)dx\cdot n(t,x_j)\Delta x_j\\&+\frac{1}{2}\int_{x_i}^{x_{i+1/2}}\beta(x-x_i,x_i)n(t,x-x_i)n(t,x_i)\Delta x_i dx+\mathcal{O}(\Delta x^3),\end{aligned}$$

and use the relationship $N_i = n(t,x_i)\Delta x_i + \mathcal{O}(\Delta x^3)$ for the midpoint rule to get the form

$$\begin{aligned}B_i =&\frac{1}{2}\sum_{j=1}^{i-1}N_j\int_{x_{i-1/2}}^{x_{i+1/2}}\beta(x-x_j,x_j)n(t,x-x_j)dx\\&+\frac{1}{2}N_i\int_{x_i}^{x_{i+1/2}}\beta(x-x_i,x_i)n(t,x-x_i)dx+\mathcal{O}(\Delta x^3),\\=:&\tilde{B}_i+\mathcal{O}(\Delta x^3).\end{aligned}\tag{14}$$

Let us denote the integral terms in $\tilde{B}_i$ by I_1 and I_2 respectively and evaluate them separately.

The integrals I_1.

We consider the first integral in (14) as

$$I_1 = \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}}^{x_{i+1/2}} \beta(x - x_j, x_j) n(t, x - x_j) dx.$$

By using the substitution $x - x_j = x'$ we obtain

$$I_1 = \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx'. \tag{15}$$

We now define $l_{i,j}$ and $\gamma_{i,j}$ to be those indices such that the following hold

$$x_{i-1/2} - x_j \in \Lambda_{l_{i,j}} \quad \text{and} \quad \gamma_{i,j} := \text{sgn}[(x_{i-1/2} - x_j) - x_{l_{i,j}}] \tag{16}$$

where

$$\text{sgn}(x) := \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x = 0, \\ \text{-1} & \text{if } x < 0. \end{cases}$$

By the definition of the indices $l_{i,j}$ and $\gamma_{i,j}$ in (16), the equation (15) can be rewritten as

$$\begin{aligned} I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t, x') dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(\gamma_{i,j}+1)}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \beta(x', x_j) n(t, x') dx' \\ &+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx'. \end{aligned} \tag{17}$$

Let us assume there are total p terms in

$$\sum_{k=l_{i,j}+\frac{1}{2}(\gamma_{i,j}+1)}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \beta(x', x_j) n(t, x') dx'$$

and set

$$l_{i,j} + \frac{1}{2}(\gamma_{i,j} + 1) =: k_1.$$

By using the definition of the indices $l_{i,j}$ and $\gamma_{i,j}$ in (16), we can write

$$\Delta x_{k_2} + \Delta x_{k_3} + \ldots + \Delta x_{k_{p-1}} \leq \Delta x_i \leq \Delta x$$

which implies that

$$(p-2) \leq \frac{\Delta x}{\Delta x_{\min}} \leq K \Rightarrow p \leq K + 2.$$

This means the above sum has finite number of terms. So one can apply the midpoint rule in the second term on the right hand side to get

$$\begin{aligned}
I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t, x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{k=l_{i,j}+\frac{1}{2}(\gamma_{i,j}+1)}^{l_{i+1,j}+\frac{1}{2}(\gamma_{i+1,j}-1)} \beta(x_k, x_j) n(t, x_k) \Delta x_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx' + \mathcal{O}(\Delta x^3).
\end{aligned}$$

This can be further rewritten as

$$\begin{aligned}
I_1 =& \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t, x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \sum_{x_{i-1/2} \le (x_j + x_k) < x_{i+1/2}} \beta(x_k, x_j) N_k \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx' + \mathcal{O}(\Delta x^3).
\end{aligned} \quad (18)$$

The integrals I_2.

Let us consider the second integral in (14) as

$$I_2 = \frac{1}{2} N_i \int_{x_i}^{x_{i+1/2}} \beta(x - x_i, x_i) n(t, x - x_i) dx.$$

By using the substitution $x - x_i = x'$ we obtain

$$I_2 = \frac{1}{2} N_i \int_{0}^{x_{i+1/2}-x_i} \beta(x', x_i) n(t, x') dx.$$

Again by the definition of the indices $l_{i,j}$ and $\gamma_{i,j}$ in (16) we split the above integral as

$$\begin{aligned}
I_2 =& \frac{1}{2} N_i \sum_{k=1}^{l_{i+1,i}+\frac{1}{2}(\gamma_{i+1,i}-1)} \int_{x_{k-1/2}}^{x_{k+1/2}} \beta(x', x_i) n(t, x') dx' \\
&+ \frac{1}{2} N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1/2}-x_i} \beta(x', x_i) n(t, x') dx'.
\end{aligned}$$

Analogously as before, one can easily show that the summation in the first term on the right hand side has finite number of terms. So one can apply the midpoint rule in the first term to obtain

$$\begin{aligned}I_2 =& \frac{1}{2} N_i \sum_{k=1}^{l_{i+1,i}+\frac{1}{2}(\gamma_{i+1,i}-1)} \beta(x_k, x_i) n(t, x_k) \Delta x_k \\ &+ \frac{1}{2} N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1/2}-x_i} \beta(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

This can be further rewritten as

$$\begin{aligned}I_2 =& \frac{1}{2} N_i \sum_{x_i+x_k<x_{i+1/2}} \beta(x_k, x_i) N_k \\ &+ \frac{1}{2} N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1/2}-x_i} \beta(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned} \tag{19}$$

By substituting (18), (19) into (14) we get

$$\begin{aligned}B_i =& \frac{1}{2} \sum_{j=1}^{i-1} N_j \sum_{x_{i-1/2}\le(x_j+x_k)<x_{i+1/2}} \beta(x_k, x_j) N_k \\ &+ \frac{1}{2} N_i \sum_{x_i+x_k<x_{i+1/2}} \beta(x_k, x_i) N_k \\ &+ \frac{1}{2} \sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t, x') dx' \\ &+ \frac{1}{2} \sum_{j=1}^{i-1} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx' \\ &+ \frac{1}{2} N_i \int_{x_{l_{i+1,i}+\frac{1}{2}\gamma_{i+1,i}}}^{x_{i+1/2}-x_i} \beta(x', x_i) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

The terms on the right hand side can be combined as

$$\begin{aligned}B_i =& \sum_{x_{i-1/2}\le x_j+x_k<x_{i+1/2}}^{j\ge k} \left(1 - \frac{1}{2}\delta_{j,k}\right) \beta(x_k, x_j) N_j N_k \\ &+ \frac{1}{2} \sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t, x') dx' \\ &+ \frac{1}{2} \sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t, x') dx' + \mathcal{O}(\Delta x^3).\end{aligned}$$

i.e.

$$
\begin{aligned}
B_i = &\hat{B}_i + \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \beta(x', x_j) n(t,x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \beta(x', x_j) n(t,x') dx' + \mathcal{O}(\Delta x^3).
\end{aligned}
$$

Using the properties $\lambda_i^+(x'+x_j) + \lambda_{i+1}^-(x'+x_j) = 1$, the integral terms on the right hand side can be rewritten as

$$
\begin{aligned}
B_i = &\hat{B}_i + \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)\beta(x', x_j) n(t,x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_{i+1}^-(x'+x_j)\beta(x', x_j) n(t,x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \lambda_i^+(x'+x_j)\beta(x', x_j) n(t,x') dx' \\
&+ \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \lambda_{i+1}^-(x'+x_j)\beta(x', x_j) n(t,x') dx' + \mathcal{O}(\Delta x^3). \qquad (20)
\end{aligned}
$$

Let us denote the remaining integrals on the right hand side in (20) by $E_1, \ldots, E_4$ respectively and calculate them separately.

The integrals E_1 and E_2.

$$
E_1 = \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}-x_j}^{x_{l_{i,j}+\frac{1}{2}\gamma_{i,j}}} \lambda_i^+(x'+x_j)\beta(x', x_j) n(t,x') dx'. \qquad (21)
$$

By the definition of the indices $l_{i,j}$ in (16) we can write the following inequality

$$
|E_1| \leq \frac{1}{2}\sum_{j=1}^{i-1} N_j \int_{x_{l_{i,j}-\frac{1}{2}}}^{x_{l_{i,j}-\frac{1}{2}}+2\overline{\Delta}_1} \lambda_i^+(x'+x_j)\beta(x', x_j) n(t,x') dx'.
$$

where $\overline{\Delta}_1 = (x_{i+1} - x_j) - x_{l_{i,j}-1/2}$. By applying the midpoint rule and using $\lambda_i^+(x_{i+1}) = 0$, we get

$$
|E_1| \leq 0 + \mathcal{O}(\Delta x^3).
$$

Similarly as before in E_1, we use $\overline{\Delta}_2 = (x_i - x_j) - x_{l_{i,j}-1/2}$ in place of $\overline{\Delta}_1$ and $\lambda_{i+1}^-(x_i) = 0$ to get

$$
|E_2| \leq 0 + \mathcal{O}(\Delta x^3).
$$

The integral E_3.

Now we consider

$$E_3 = \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \lambda_i^+(x'+x_j)\beta(x',x_j)n(t,x')dx'.$$

By the definition of the indices $l_{i,j}$ in (16) one can write

$$|E_3| \leq \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}-1/2}}^{x_{l_{i+1,j}-1/2}+2\overline{\Delta}_3} \lambda_i^+(x'+x_j)\beta(x',x_j)n(t,x')dx'$$

where $\overline{\Delta}_3 = (x_{i+1}-x_j) - x_{l_{i+1,j}-1/2}$. By applying the midpoint rule and using $\lambda_i^+(x_{i+1}) = 0$, we obtain

$$|E_3| \leq 0 + \mathcal{O}(\Delta x^3).$$

The integral E_4.

$$E_4 = \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+\frac{1}{2}\gamma_{i+1,j}}}^{x_{i+1/2}-x_j} \lambda_{i+1}^-(x'+x_j)\beta(x',x_j)n(t,x')dx'.$$

By the definition of the indices $l_{i,j}$ in (16) we obtain

$$|E_4| \leq \frac{1}{2}\sum_{j=1}^{i} N_j \int_{x_{l_{i+1,j}+1/2}-2\overline{\Delta}_4}^{x_{l_{i+1,j}+1/2}} \lambda_{i+1}^-(x'+x_j)\beta(x',x_j)n(t,x')dx'$$

where $\overline{\Delta}_4 = x_{l_{i+1,j}+1/2} - (x_i - x_j)$. By applying the midpoint rule and using $\lambda_{i+1}^-(x_i) = 0$, we obtain

$$|E_4| \leq 0 + \mathcal{O}(\Delta x^3).$$

Finally all these values can be substituted in equation (20)

$$B_i = \hat{B}_i + \mathcal{O}(\Delta x^3).$$

Now we consider the integrated death term as

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} \beta(x,\epsilon)n(t,\epsilon)n(t,x)d\epsilon dx.$$

This can be rewritten as

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \sum_{j=1}^{I} \int_{x_{j-1/2}}^{x_{j+1/2}} \beta(x,\epsilon)n(t,\epsilon)n(t,x)d\epsilon dx.$$

Applying the midpoint rule in both integrals, we obtain

$$D_i = N_i \sum_{j=1}^{I} \beta(x_i, x_j) N_j + \mathcal{O}(\Delta x^3).$$

Thus,

$$D_i = \hat{D}_i + \mathcal{O}(\Delta x^3) = \hat{D}_i^{CA} + \mathcal{O}(\Delta x^3).$$

Now we consider the volume flux

$$V_i = \frac{1}{2} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x x\beta(x-\epsilon, \epsilon) n(t, x-\epsilon) n(t, \epsilon) d\epsilon dx.$$

Proceeding as in B_i one can get

$$\begin{aligned} V_i =& \frac{1}{2} \sum_{j=1}^{i-1} N_j \int_{x_{i-1/2}}^{x_{i+1/2}} x\beta(x-x_j, x_j) n(t, x-x_j) dx \\ &+ \frac{1}{2} N_i \int_{x_i}^{x_{i+1/2}} x\beta(x-x_i, x_i) n(t, x-x_i) dx + \mathcal{O}(\Delta x^3), \\ =:& \tilde{V}_i + \mathcal{O}(\Delta x^3). \end{aligned} \tag{22}$$

Analogously, we can easily obtain

$$V_i = \hat{V}_i + \mathcal{O}(\Delta x^3).$$

□

Now we simplify the each term in (11) separately. Consider the first term without Heaviside function $H(x)$ and substitute the value of λ from the expression (10), we get

$$\lambda_i^-(\overline{v}_{i-1}) \hat{B}_{i-1} = \frac{\overline{v}_{i-1} - x_{i-1}}{x_i - x_{i-1}} \hat{B}_{i-1} = \frac{2}{\Delta x_i + \Delta x_{i-1}} [(\overline{v}_{i-1} - x_{i-1}) \hat{B}_{i-1}]. \tag{23}$$

Let us take

$$\begin{aligned} (\overline{v}_{i-1} - x_{i-1}) \hat{B}_{i-1} =& (\overline{v}_{i-1} - x_{i-1})(\tilde{B}_{i-1} + \mathcal{O}(\Delta x^3)) \\ =& \overline{v}_{i-1} \tilde{B}_{i-1} - x_{i-1} \tilde{B}_{i-1} + \mathcal{O}(\Delta x^4) \\ =& \frac{\hat{V}_{i-1}}{\hat{B}_{i-1}} \tilde{B}_{i-1} - x_{i-1} \tilde{B}_{i-1} + \mathcal{O}(\Delta x^4). \end{aligned} \tag{24}$$

Since $\hat{V}_{i-1} = \tilde{V}_{i-1} + \mathcal{O}(\Delta x^3)$, $\hat{B}_{i-1} = \tilde{B}_{i-1} + \mathcal{O}(\Delta x^3)$ and $\tilde{B}_{i-1}$, $\hat{B}_{i-1} \neq 0$, then

$$\frac{\hat{V}_{i-1}}{\hat{B}_{i-1}} = \frac{\tilde{V}_{i-1}}{\tilde{B}_{i-1}} + \mathcal{O}(\Delta x^3).$$

Substituting this value in (24), we obtain

$$\begin{aligned}(\overline{v}_{i-1}-x_{i-1})\hat{B}_{i-1} =&\tilde{V}_{i-1}-x_{i-1}\tilde{B}_{i-1}+\tilde{B}_{i-1}\mathcal{O}(\Delta x^3)+\mathcal{O}(\Delta x^4)\\ =&\tilde{V}_{i-1}-x_{i-1}\tilde{B}_{i-1}+[\hat{B}_{i-1}+\mathcal{O}(\Delta x^3)]\mathcal{O}(\Delta x^3)+\mathcal{O}(\Delta x^4)\\ =&\tilde{V}_{i-1}-x_{i-1}\tilde{B}_{i-1}+\mathcal{O}(\Delta x^4)\end{aligned}$$

because $\hat{B}_{i-1}$ is of first order. Now we put this value in (23) to get

$$\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1}=\frac{2}{\Delta x_i+\Delta x_{i-1}}[\tilde{V}_{i-1}-x_{i-1}\tilde{B}_{i-1}+\mathcal{O}(\Delta x^4)].$$

Again, Substituting the values of $\tilde{B}_{i-1}$ from (14) and $\tilde{V}_{i-1}$ from (22) into the preceding equation we obtain

$$\begin{aligned}\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1}=\frac{1}{\Delta x_i+\Delta x_{i-1}}\Bigg[&\sum_{j=1}^{i-2}N_j\int_{x_{i-3/2}}^{x_{i-1/2}}(x-x_{i-1})\beta(x-x_j,x_j)n(t,x-x_j)dx\\ &+\int_{x_{i-1}}^{x_{i-1/2}}(x-x_{i-1})\beta(x-x_{i-1},x_{i-1})n(t,x-x_{i-1})n(t,x_{i-1})\Delta x_{i-1}dx\\ &+\mathcal{O}(\Delta x^4)\Bigg].\end{aligned}$$

Set $f(x,y):=\beta(x,y)n(t,x)$. Then the above equation becomes

$$\begin{aligned}\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1}=\frac{1}{\Delta x_i+\Delta x_{i-1}}\Bigg[&\sum_{j=1}^{i-2}N_j\int_{x_{i-3/2}}^{x_{i-1/2}}(x-x_{i-1})f(x-x_j,x_j)dx\\ &+\int_{x_{i-1}}^{x_{i-1/2}}(x-x_{i-1})f(x-x_{i-1},x_{i-1})n(t,x_{i-1})\Delta x_{i-1}dx\\ &+\mathcal{O}(\Delta x^4)\Bigg].\end{aligned}\tag{25}$$

We use Taylor series expansions about x_{i-1} of each integrand in equation (25)as

$$\begin{aligned}(x-x_{i-1})f(x-x_j,x_j) =&0+f(x_{i-1}-x_j,x_j)(x-x_{i-1})+f_x(x_{i-1}-x_j,x_j)(x-x_{i-1})^2\\ &+\mathcal{O}(\Delta x^3),\\ (x-x_{i-1})f(x-x_{i-1},x_{i-1}) =&0+f(x_{i-1}-x_{i-1},x_{i-1})(x-x_{i-1})+\mathcal{O}(\Delta x^2).\end{aligned}$$

The substitution of the above Taylor series expansion in equation (25) gives

$$\begin{aligned}\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1}=\frac{1}{\Delta x_i+\Delta x_{i-1}}\Bigg[&\frac{1}{12}\sum_{j=1}^{i-2}N_jf_x(x_{i-1}-x_j,x_j)\Delta x_{i-1}^3\\ &+\frac{1}{8}f(x_{i-1}-x_{i-1},x_{i-1})n(t,x_{i-1})\Delta x_{i-1}^3+\mathcal{O}(\Delta x^4)\Bigg].\end{aligned}$$

This can be further simplified using Taylor series expansion as

$$\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1} = \frac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}}\Bigg[\frac{1}{12}\sum_{j=1}^{i-2} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3).$$

Now we consider the second term

$$\lambda_i^+(\overline{v}_i)\hat{B}_i = \frac{\overline{v}_i - x_{i+1}}{x_i - x_{i+1}}\hat{B}_i = \left(1 - \frac{\overline{v}_i - x_i}{x_{i+1} - x_i}\right)\hat{B}_i = \hat{B}_i - \frac{2}{\Delta x_{i+1} + \Delta x_i}[\overline{v}_i\hat{B}_i - x_i\hat{B}_i].$$

Proceeding as before we obtain the following simplified form

$$\lambda_i^+(\overline{v}_i)\hat{B}_i = \hat{B}_i - \frac{\Delta x_i^3}{\Delta x_{i+1} + \Delta x_i}\Bigg[\frac{1}{12}\sum_{j=1}^{i-1} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3).$$

Similarly the other two terms can be easily obtained as

$$\lambda_i^-(\overline{v}_i)\hat{B}_i = \hat{B}_i + \frac{\Delta x_i^3}{\Delta x_i + \Delta x_{i-1}}\Bigg[\frac{1}{12}\sum_{j=1}^{i-1} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3),$$

and

$$\lambda_i^+(\overline{v}_{i+1})\hat{B}_{i+1} = -\frac{\Delta x_{i+1}^3}{\Delta x_{i+1} + \Delta x_i}\Bigg[\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3).$$

Without loss of generality the summation appearing in all four terms can be taken up to i since the terms we are adding are third order accurate. Further if use Lemma 3.1 then all the terms can be rewritten in a more simplied form as

$$\lambda_i^-(\overline{v}_{i-1})\hat{B}_{i-1} = \frac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}}\Bigg[\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3). \tag{26}$$

$$\lambda_i^+(\overline{v}_i)\hat{B}_i = B_i - \frac{\Delta x_i^3}{\Delta x_{i+1} + \Delta x_i}\Bigg[\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i)\Bigg] + \mathcal{O}(\Delta x^3). \tag{27}$$

$$\lambda_i^-(\overline{v}_i)\hat{B}_i = B_i + \frac{\Delta x_i^3}{\Delta x_i + \Delta x_{i-1}}\left[\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t,x_i)\right] + \mathcal{O}(\Delta x^3), \tag{28}$$

$$\lambda_i^+(\overline{v}_{i+1})\hat{B}_{i+1} = -\frac{\Delta x_{i+1}^3}{\Delta x_{i+1} + \Delta x_i}\left[\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t,x_i)\right] + \mathcal{O}(\Delta x^3). \tag{29}$$

Let us calculate the local discretization error in the case $\overline{v}_{i-1} > x_{i-1}$, $\overline{v}_i > x_i$ and $\overline{v}_{i+1} \geq x_{i+1}$ as

$$\hat{B}_i^{CA} = B_i + \left(\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t,x_i)\right) \times \left(\frac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}} - \frac{\Delta x_i^3}{\Delta x_{i+1} + \Delta x_i}\right) + \mathcal{O}(\Delta x^3). \tag{30}$$

Similarly for the case $\overline{v}_{i-1} \leq x_{i-1}$, $\overline{v}_{i+1} < x_{i+1}$ and $\overline{v}_i < x_i$ we have

$$\hat{B}_i^{CA} = B_i + \left(\frac{1}{12}\sum_{j=1}^{i} n(t,x_j)\Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t,x_i)\right) \times \left(\frac{\Delta x_i^3}{\Delta x_i + \Delta x_{i-1}} - \frac{\Delta x_{i+1}^3}{\Delta x_{i+1} + \Delta x_i}\right) + \mathcal{O}(\Delta x^3). \tag{31}$$

We need the following useful corollary to investigate the order of consistency.

Corollary 3.2. *Let $\beta(x,\epsilon) : \mathcal{C}(\Omega^2) \to \mathbb{R}$ and $n(t,\epsilon) : \mathcal{C}(\mathbb{R},\Omega) \to \mathbb{R}$. If the function*

$$B(t,x) = \frac{1}{2}\int_0^x \beta(x-\epsilon,\epsilon) n(t,x-\epsilon) n(t,\epsilon) d\epsilon.$$

has finitely many oscillations (at the most a finite number of maxima and minima) in Ω at any time t, then the expression $x_i - \bar{v}_i, i = 1,\ldots,I$ defined using (4), (7) and (8) by

$$x_i - \bar{v}_i = \frac{x_i\hat{B}_i - \hat{V}_i}{\hat{B}_i}$$

changes its sign at most finitely many times for Δx sufficiently small.

Proof. The proof can be done in the same manner as Corollary 2.4 in [6]. □

Let us now go back to the discussion of the local discretization error $\sigma_i(t) = (B_i - D_i) - (\hat{B}_i^{CA} - \hat{B}_i^{CA})$. From the equations (26-31) we can estimate that

$$\sigma_i(t) = \begin{cases} C_i \left(\dfrac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}} - \dfrac{\Delta x_i^3}{\Delta x_{i+1} + \Delta x_i} \right) + \mathcal{O}(\Delta x^3), & \bar{v}_{i-1} > x_{i-1}, \bar{v}_i > x_i, \bar{v}_{i+1} \geq x_{i+1} \\ C_i \left(\dfrac{\Delta x_i^3}{\Delta x_i + \Delta x_{i-1}} - \dfrac{\Delta x_{i+1}^3}{\Delta x_{i+1} + \Delta x_i} \right) + \mathcal{O}(\Delta x^3), & \bar{v}_{i-1} \leq x_{i-1}, \bar{v}_i < x_i, \bar{v}_{i+1} < x_{i+1}, \\ \mathcal{O}(\Delta x^3), & \bar{v}_{i-1} \leq x_{i-1}, \bar{v}_i = x_i, \bar{v}_{i+1} \geq x_{i+1}, \\ \mathcal{O}(\Delta x^2), & \text{elsewhere } (i = I_1, \ldots, I_m, 1, I). \end{cases}$$

where

$$C_i = \left(\frac{1}{12} \sum_{j=1}^{i} n(t, x_j) \Delta x_j f_x(x_i - x_j, x_j) + \frac{1}{8} f(x_i - x_i, x_i) n(t, x_i) \right).$$

We have four cases for the order of the local error. The last case comes due to the sign change of $x_i - \bar{v}_i$ and due to boundaries. As discussed before in Corollary 3.2, the number of sign changes depends on the properties of birth rate function $B(t, x)$ and is finite for finitely oscillating function. Here due to the sign change of $x_i - \bar{v}_i$ we have taken m cells, say $I_1, \ldots, I_m$, in which the order may deteriorate. Since this number m remians finite, this does not lower the order of the scheme. For simplicity let us denote set of indices in each case as follows

$$\begin{aligned} \mathfrak{J}_1 &= \{ i \in \mathbb{N} \,|\, \bar{v}_{i-1} > x_{i-1}, \bar{v}_i > x_i, \bar{v}_{i+1} \geq x_{i+1} \}, \\ \mathfrak{J}_2 &= \{ i \in \mathbb{N} \,|\, \bar{v}_{i-1} \leq x_{i-1}, \bar{v}_i < x_i, \bar{v}_{i+1} < x_{i+1} \}, \\ \mathfrak{J}_3 &= \{ i \in \mathbb{N} \,|\, \bar{v}_{i-1} \leq x_{i-1}, \bar{v}_i = x_i, \bar{v}_{i+1} \geq x_{i+1} \}, \\ \mathfrak{J}_4 &= \{ i \in \mathbb{N} \,|\, i = I_1, \ldots, I_m, 1, I \}. \end{aligned}$$

Then, the order of consistency is given by

$$\begin{aligned} \|\sigma(t)\| &= \sum_{i \in \mathfrak{J}_1} |\sigma_i(t)| + \sum_{i \in \mathfrak{J}_2} |\sigma_i(t)| + \sum_{i \in \mathfrak{J}_3} |\sigma_i(t)| + \sum_{i \in \mathfrak{J}_4} |\sigma_i(t)| \\ &= \sum_{i \in \mathfrak{J}_1} C_i \left(\frac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}} - \frac{\Delta x_i^3}{\Delta x_{i+1} + \Delta x_i} \right) \\ &\quad + \sum_{i \in \mathfrak{J}_2} C_i \left(\frac{\Delta x_i^3}{\Delta x_i + \Delta x_{i-1}} - \frac{\Delta x_{i+1}^3}{\Delta x_{i+1} + \Delta x_i} \right) + \mathcal{O}(\Delta x^2). \end{aligned} \tag{32}$$

As stated before we consider the order of consistency on five different meshes. Details can be found in J. Kumar and Warnecke [6].

Uniform mesh: For a uniform mesh, $\Delta x_i = \Delta x$ for any $i = 1, \ldots, I$, the equation (32) clearly gives

$$\|\sigma(t)\| = \mathcal{O}(\Delta x^2). \tag{33}$$

Similarly to the fixed pivot technique, the cell average technique is second order consistent.

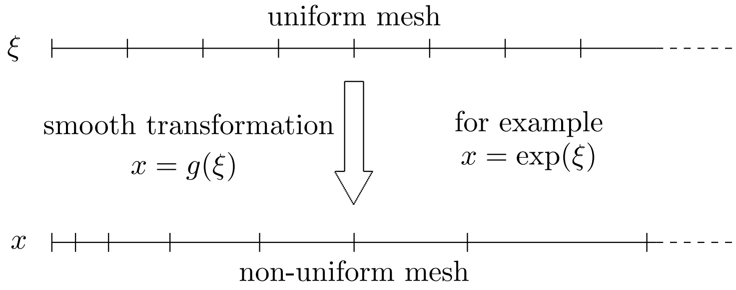

Figure 1: Non-uniform smooth mesh.

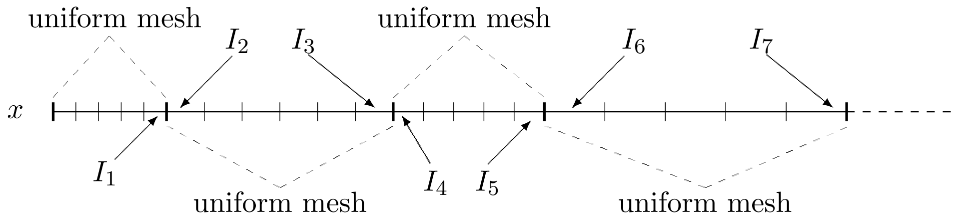

Figure 2: Locally uniform smooth mesh.

Non-uniform smooth mesh: If we chose the mesh fulfilling the following conditions

$$\left(\frac{\Delta x_i^3}{\Delta x_{i+1}+\Delta x_i} - \frac{\Delta x_{i-1}^3}{\Delta x_i + \Delta x_{i-1}}\right) = \mathcal{O}(\Delta x^3),$$
$$\text{and } \left(\frac{\Delta x_{i+1}^3}{\Delta x_{i+1}+\Delta x_i} - \frac{\Delta x_{i}^3}{\Delta x_i + \Delta x_{i-1}}\right) = \mathcal{O}(\Delta x^3),$$

then we will get again the second order consistency. An example of such mesh was already given in [5].Let us consider a variable ξ with uniform grids and a smooth transformation $x = g(\xi)$ to get non-uniform smooth mesh, see Figure 1. The equations (32) can be simplified by using Taylor series expansion in the smooth transformation, see J. Kumar and Warnecke [6]. So analogously to the uniform mesh we obtain $\|\sigma(t)\| = \mathcal{O}(\Delta x^2)$, i.e. the technique is second order consistent.

Locally uniform mesh: Similar to the fixed pivot and the cell average techniques discussed in [1, 5, 6], according to the Figure 2 we obtain

$$\sigma_i(t) = \begin{cases} \mathcal{O}(\Delta x^2), & i = 1, I, I_1, I_2, \ldots \\ \mathcal{O}(\Delta x^3), & \text{elsewhere.} \end{cases}$$

Therefore we have $\|\sigma(t)\| = \mathcal{O}(\Delta x^2)$. In this case the consistency order differs that what we got in the case of fixed pivot technique in [1] for such grids. The cell average technique becomes one order higher consistent than the fixed technique in case of pure aggregation also.

Oscillatory mesh: Let us now consider oscillatory mesh i.e.

$$\Delta x_{i+1} := \begin{cases} 2\Delta x_i & \text{if } i \text{ is odd,} \\ \frac{1}{2}\Delta x_i & \text{if } i \text{ is even.} \end{cases}$$

From the equations (32), we have $\|\sigma(t)\| = \mathcal{O}(\Delta x)$. Thus the cell average technique is only first order consitent on oscillatory meshes.

Non-uniform random mesh: From the equation (32) it is clear that the technique is again only a first order consistent method i.e., $\|\sigma(t)\| = \mathcal{O}(\Delta x)$. It should be pointed out here that the fixed pivot technique was inconsistent on oscillatory and non-uniform random meshes.

4 Convergence

First of all we shall prove the Lipschitz condition on $\hat{\mathbf{B}}(\mathbf{N}(t))$ and $\hat{\mathbf{D}}(\mathbf{N}(t))$ as follows:
Let us consider the birth term for $0 \le t \le T$ and for all $\mathbf{N}$, $\tilde{\mathbf{N}} \in \mathbb{R}^I$, we get from (11)

$$\begin{aligned}\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\tilde{\mathbf{N}})\| \le & \sum_{i=1}^{I} \lambda_i^-(\overline{v}_{i-1}) H(\overline{v}_{i-1} - x_{i-1}) |\hat{B}_{i-1}(\mathbf{N}) - \hat{B}_{i-1}(\tilde{\mathbf{N}})| \\ & + \sum_{i=1}^{I} [\lambda_i^+(\overline{v}_i) H(\overline{v}_i - x_i) + \lambda_i^-(\overline{v}_i) H(x_i - \overline{v}_i)] |\hat{B}_i(\mathbf{N}) - \hat{B}_i(\tilde{\mathbf{N}})| \\ & + \sum_{i=1}^{I} \lambda_i^+(\overline{v}_{i+1}) H(x_{i+1} - \overline{v}_{i+1}) |\hat{B}_{i+1}(\mathbf{N}) - \hat{B}_{i+1}(\tilde{\mathbf{N}})|.\end{aligned}$$

The definitions of $\lambda_i^{\pm}(x)$ and $H(x)$ give $0 \le \lambda_i^{\pm}(x)H(x) \le 1$ and by using this upper bound the above inequality becomes

$$\begin{aligned}\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\tilde{\mathbf{N}})\| \le & \sum_{i=1}^{I} |\hat{B}_{i-1}(\mathbf{N}) - \hat{B}_{i-1}(\tilde{\mathbf{N}})| + \sum_{i=1}^{I} |\hat{B}_i(\mathbf{N}) - \hat{B}_i(\tilde{\mathbf{N}})| \\ & + \sum_{i=1}^{I} |\hat{B}_{i+1}(\mathbf{N}) - \hat{B}_{i+1}(\tilde{\mathbf{N}})|.\end{aligned}$$

Using $\beta_{j,k} \le C$, due to the continuity of β and the finiteness of the domain, we obtain from (4)

$$\begin{aligned}\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\tilde{\mathbf{N}})\| \le & \frac{1}{2} C \sum_{i=1}^{I} \sum_{j=1}^{i-1} \sum_{x_{i-3/2} \le x_j + x_k < x_{i-1/2}} |N_j N_k - \tilde{N}_j \tilde{N}_k| \\ & + \frac{1}{2} C \sum_{i=1}^{I} \sum_{j=1}^{i} \sum_{x_{i-1/2} \le x_j + x_k < x_{i+1/2}} |N_j N_k - \tilde{N}_j \tilde{N}_k| \\ & + \frac{1}{2} C \sum_{i=1}^{I} \sum_{j=1}^{i+1} \sum_{x_{i+1/2} \le x_j + x_k < x_{i+3/2}} |N_j N_k - \tilde{N}_j \tilde{N}_k| \\ \le & \frac{3}{2} C \sum_{j=1}^{I} \sum_{k=1}^{I} |N_j N_k - \tilde{N}_j \tilde{N}_k|.\end{aligned}$$

Now we apply a useful equality $N_j N_k - \tilde{N}_j \tilde{N}_k = \frac{1}{2}[(N_j + \tilde{N}_j)(N_k - \tilde{N}_k) + (N_j - \tilde{N}_j)(N_k + \tilde{N}_k)]$ to get

$$\|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\tilde{\mathbf{N}})\| \le \frac{3}{4} C \sum_{j=1}^{I} \sum_{k=1}^{I} \Big[|(N_j + \tilde{N}_j)||(N_k - \tilde{N}_k)| + |(N_j - \tilde{N}_j)||(N_k + \tilde{N}_k)| \Big]. \tag{34}$$

It can be easily shown that the total number of particles decreases in a coagulation process, i.e.

$$\sum_{j=1}^{I} N_j \le N_T^0 := \text{Total number of particles which are taken initially.}$$

The equation (34) can be rewritten as

$$\begin{aligned} \|\hat{\mathbf{B}}(\mathbf{N}) - \hat{\mathbf{B}}(\tilde{\mathbf{N}})\| &\le \frac{3}{2} N_T^0 C \Big[\sum_{k=1}^{I} |(N_k - \tilde{N}_k)| + \sum_{j=1}^{I} |(N_j - \tilde{N}_j)| \Big] \\ &\le 3 N_T^0 C \|\mathbf{N} - \tilde{\mathbf{N}}\|. \end{aligned} \tag{35}$$

Similarly as before we can easily show the Lipschitz condition for death term as

$$\|\hat{\mathbf{D}}(\mathbf{N}) - \hat{\mathbf{D}}(\tilde{\mathbf{N}})\| \le 3 N_T^0 C \|\mathbf{N} - \tilde{\mathbf{N}}\|. \tag{36}$$

So we can apply Theorem 2.3 in [1] to check the positivity of the solution obtained by the cell average technique.

Proposition 4.1. *The numerical solution by the cell average technique is non-negative.*

Proof. The proof is same as Proposition 5.1 in [1]. □

Now we shall prove the following convergence theorem.

Theorem 4.2. *Let us assume that the Lipschitz conditions on $\hat{\mathbf{B}}(\mathbf{N}(t))$ and $\hat{\mathbf{D}}(\mathbf{N}(t))$ are satisfied for $0 \le t \le T$ and for all $\mathbf{N}$, $\hat{\mathbf{N}} \in \mathbb{R}^I$ where $\mathbf{N}$ and $\hat{\mathbf{N}}$ are two different solutions respectively. More precisely, there exists a Lipschitz constant $L := 3N_T^0 C < \infty$ such that (35) and (36) hold. Then a consistent discretization method is also convergent and the convergence is of the same order as the consistency.*

Proof. The proof is same as Theorem 5.1 in [1]. □

5 Numerical Examples

This section deals with a few numerical examples where we evaluate the experimental order of convergence (EOC) to validate our mathematical observations. Similarly to the mathematical analysis we consider five different type of meshes for the computation. All test cases are taken from [1]. All numerical results of convergence from [1] are repeated to see the difference between two techniques. All computational details of the test case can be found in [1]. Here we discuss only numerical results for the test cases presented in [1].
Let us begin with the first test case of a uniform mesh. The numerical results are presented

in Table 1. As expected from the mathematical analysis both techniques show convergence of second order. In case of uniform mesh, the cell average and the fixed pivot techniques are same for aggregation problems. Since analytical solutions are not available in this case we can see the relative errors in numerical results are same for both the schemes.

Now we consider the second test case of non-uniform smooth meshes. The numerical results of the convergence analysis have been summarized in Table 2. Once again, as expected, both the techniques clearly converge to second order.

The third test case has been performed on a locally uniform mesh. The EOC for both the techniques has been summarized in Table 3. As estimated from the mathematical analysis, the table clearly shows that the cell average technique is of second order while the fixed pivot technique is only first order accurate.

Now let us consider the fourth case of an oscillatory mesh. The numerical results have been shown in Table 4. As expected from the mathematical analysis, the table shows that the cell average technique is first order convergent while the fixed pivot technique is not convergent.

Now we consider the fifth case of random grids. The numerical results of convergence analysis have been summarized in Table 5. We obtain the same result as in case of oscillatory grids.

6 Conclusions

In this paper, we have presented a detailed convergence analysis of the cell average technique for aggregation PBEs. The mathematical and numerical results are compared with those for the case of the fixed pivot technique in [1]. It is remarked that the cell average technique is second order convergent on uniform, non-uniform smooth and locally uniform meshes. However, it gives only a first order convergence on oscillatory and random meshes. It should be pointed out that the fixed pivot technique is only first order convergent on locally uniform mesh and zero order convergent on oscillatory and random meshes. All mathematical observation have been justified numerically.

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References

[1] A.K. Giri, J. Kumar, and G. Warnecke. Convergence analysis of sectional methods for solving aggregation population balance equations: The fixed pivot technique. *Submitted.*

[2] M. Kostoglou. Extended cell average technique for the solution of coagulation equation. *J. Colloid Interface Sci.*, 306:72–81, 2007.

[3] J. Kumar, M. Peglow, G. Warnecke, and S. Heinrich. An efficient numerical technique for solving population balance equation involving aggregation, breakage, growth and nucleation. *Powder Technol.*, 179:205–228, 2007.

[4] J. Kumar, M. Peglow, G. Warnecke, S. Heinrich, and L. Mörl. Improved accuracy and convergence of discretized population balance for aggregation: The cell average technique. *Chem. Eng. Sci.*, 61:3327–3342, 2006.

[5] J. Kumar and G. Warnecke. Convergence analysis of sectional methods for solving breakage population balance equations - I: The fixed pivot technique. *Numer. Math.*, 111:81–108, 2008.

[6] J. Kumar and G. Warnecke. Convergence analysis of sectional methods for solving breakage population balance equations - II: The cell average technique. *Numer. Math.*, 110:539–559, 2008.

[7] S. Kumar and D. Ramkrishna. On the solution of population balance equations by discretization - I. A fixed pivot technique. *Chem. Eng. Sci.*, 51:1311–1332, 1996.

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
200	-	-	-	-
400	0.0598	-	0.0598	-
800	0.0178	1.75	0.0178	1.75
1600	5.0E-3	1.82	5.0E-3	1.82
3200	1.3E-3	1.95	1.3E-3	1.95

Table 1: Uniform grids

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	6.4E-3	-	6.1E-3	-
120	1.6E-3	1.98	1.7E-3	1.86
240	4.0E-4	1.98	5.0E-4	1.88
480	1.0E-4	1.99	1.0E-4	1.87

Table 2: Non-uniform smooth grids

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0303	-	0.025	-
120	0.0156	0.96	8.8E-3	1.51
240	7.7E-3	1.02	2.1E-3	2.08
480	3.8E-3	1.03	5.0E-4	2.15

Table 3: Locally uniform grids

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	-	-	-	-
120	0.0565	-	0.08E-3	-
240	0.0580	-0.03	0.02E-3	1.54
480	0.0655	-0.17	0.01E-3	1.34
960	0.0824	-0.33	0.05E-4	1.05

Table 4: Oscillatory grids

(a) Fixed pivot technique			(b) cell average technique	
Grid Points	Relative Error L_1	**EOC**	Relative Error L_1	**EOC**
60	0.0174	-	0.0127	-
120	0.0220	-0.34	8.3E-3	0.61
240	0.0263	-0.25	4.2E-3	0.99
480	0.0325	-0.30	2.6E-3	0.70

Table 5: Non-uniform random grids