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High-resolution method for numerically solving PDEs in process engineering

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Abstract

Abrupt phenomena in modelling real-world systems indicate the importance of investigating systems with steep gradients. However, it is difficult to solve such systems either analytically or numerically. In 1993, Koren developed a high-resolution numerical computing scheme to deal with compressible fluid dynamics with Dirichlet boundary condition. Recently, Qamar adapted this scheme to numerically solve population balance equations without diffusion terms. This paper extends Koren’s scheme for partial differential equations (PDEs) that describe both nonlinear propagation and diffusive effects, and for PDEs with Cauchy or Neumann boundary condition. Accurate and convergent numerical solutions to the test problems have been obtained. The new results are also compared to those obtained by wavelet-based methods. It is shown that the method developed in this paper is more efficient.

1 Introduction

Modelling real-world systems such as chemical processes and physical phenomena generally results in a set of partial differential equations (PDEs). The solutions of such systems are important for understanding the physical meaning of the processes and the relationship among the process variables, and also for optimising the system performance. However, the tools for getting analytical solutions, or even numerical ones, are not sufficient for obtaining efficient

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solutions. In recent years, much effort has been made in this research direction for various methods, such as wavelet-based methods and finite difference approaches [1]-[11]. For most PDEs with regular solutions, all these methods work well. However, it is still challenging to develop more effective methods for numerically solving PDEs with steep gradients or irregular solutions.

In 1993, Koren [6] posed an algorithm for numerically solving PDEs with Dirichlet boundary condition, especially, for systems with advection, diffusion and source terms. Later, this method was adapted for population balance equations (PBEs) with Dirichlet boundary conditions [5,10]. The known results have shown the advantages of this method. However, our recent investigation indicates that the success of this method largely depends on how the boundary conditions are dealt with. Many engineering systems such as those in chemical processes are governed by PDEs with Cauchy or Neumann boundary conditions, e.g., the fixed-bed multicomponent adsorption model and nonisothermal catalytic reactor models in [4]. Therefore, effort has to be made to deal with various boundary conditions in order to make use of Koren's idea in a wider range of real-world systems. This paper aims to extend Koren’s scheme to the process engineering research sector for a wider range of PDEs, especially the ones with Cauchy/Neumann boundary conditions. For this purpose, two schemes will be developed based on Koren’s work: Flux-Interpolation and State-Interpolation. In order to highlight the advantages of these two schemes, the Burger’s equation and a Non-Steady-State Model for a Chromatographic Column are used as the test problems.

Let us start with a brief review of Koren’s high-resolution scheme, which was originally posed for numerically solving PDEs with Dirichlet boundary condition [6].

2 Koren’s High-Resolution Scheme

Consider the following PDE

\[
\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} + \beta \frac{\partial^2 u}{\partial x^2} = 0. \tag{1}
\]

Let us start from the mesh discretization of interval \([a, b]\). Divide the entire interval into \(N\) subintervals \(\Omega_i = [x_{i-1/2}, x_{i+1/2}], i = 1, \cdots, N\), with \(x_{1/2} = a, x_{N+1/2} = b\), and let \(x_i = \frac{x_{i-1/2}+x_{i+1/2}}{2}, \Delta x_i = x_{i+1/2} - x_{i-1/2}\). It follows that \(x_i = x_{i-1/2} + \Delta x_i/2\). Following [10], approximate the unknown \(u\) in \(\Omega_i\) as follows

\[
u_i(t) = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t)dx. \tag{2}
\]
Integrating equation (1) on both sides for $x$ from $x_{i-1/2}$ to $x_{i+1/2}$ gives the semi-discrete equation

$$\frac{\partial u_i(t)}{\partial t} + \frac{1}{\Delta x_i} (f_{i+1/2} - f_{i-1/2}) + \frac{1}{\Delta x_i} \beta \frac{\partial u}{\partial x} |_{x_{i+1/2}} - \frac{\partial u}{\partial x} |_{x_{i-1/2}} = 0. \quad (3)$$

For a good numerical method, it should give better approximations for $f_{i+1/2}$ and $\frac{\partial u}{\partial x} |_{i+1/2}, i = 0, \cdots, N$. In the following, we will focus on how to approximate them.

### 2.1 Approximation of $f_{i\pm1/2}$

Two schemes were given to approximate $f_{i+1/2}$ in [6]:

1. Upwind scheme, which is a first-order approximation

   $$f_{i+1/2} = f_i, \quad \text{and} \quad (4)$$

   the so-called $\kappa$–flux interpolation scheme

   $$f_{i+1/2} = f_i + \frac{1 + \kappa}{4} (f_{i+1} - f_i) + \frac{1 - \kappa}{4} (f_i - f_{i-1}), \kappa \in [-1, 1]. \quad (5)$$

2. Remark 1 If function $f(u)$ is linear with respect to $u$, e.g., $f(u) = u$, the approximation equation (5) is equivalent to the following state interpolation

   $$f_{i+1/2} = f \left( f_i + \frac{1 + \kappa}{4} (u_{i+1} - u_i) + \frac{1 - \kappa}{4} (u_i - u_{i-1}) \right), \quad (6)$$

   which was posed in [6] for the case of linear $f(u)$. In this paper, both the flux interpolation expressed in equation (5) and the state interpolation shown in equation (6) will be used for numerically solving our testing problems. The high resolution schemes based on flux interpolation and state interpolation will be denoted as $HR_1$ and $HR_2$, respectively later in this paper.

If $\kappa = 1/3$, we may use the following optimized $\kappa$–interpolation approximation

$$f_{i+1/2} = f_i + \frac{1}{2} \left( \frac{1}{3} + \frac{2}{3} r_i^+ \right) (f_i - f_{i-1}), \quad (7)$$

or

$$f_{i+1/2} = f_i + \frac{1}{2} \Phi(r_i^+) (f_i - f_{i-1}), \quad (8)$$

where the flux limited function $\Phi$ is defined by

$$\Phi(r) = \max \left( 0, \min \left( 2r, \min \left( \frac{1}{3} + \frac{2}{3} r, 2 \right) \right) \right), \quad (9)$$
and the upwind ratio of two consecutive flux gradients is defined by

$$r_i^+ = \frac{f_{i+1} - f_i + \epsilon}{f_i - f_{i-1} + \epsilon},$$

(10)

where $\epsilon$ is a small parameter for avoiding division by zero.

### 2.2 Approximation of $\frac{\partial u}{\partial x} |_{i+1/2}$

The backward and forward difference approximations will be used to approximate $\frac{\partial u}{\partial x} |_{i+1/2}$:

$$\frac{\partial u}{\partial x} \bigg|_{x_{i+1/2}} = \frac{u_{i+1} - u_i}{\Delta x_i}, \quad \frac{\partial u}{\partial x} \bigg|_{x_{i-1/2}} = \frac{u_i - u_{i-1}}{\Delta x_i}.$$  

(11)

It is known that all the approximations mentioned above work well at the internal subintervals, e.g., for $\Omega_i$, $i = 2, \ldots, N-1$. The difficulties lie in dealing with the boundary conditions. For instance, there is no $f_{-1}$ when $i = 0$. In the following section we will address this subject corresponding to different boundary conditions.

### 2.3 Schemes for solving PDEs with Dirichlet boundary conditions

This subsection is based on the results of [6]. Assuming that equation (1) has the following Dirichlet boundary conditions:

$$u(t, a) = u_{in}(t) =: u_{in},$$

(12a)

$$u(t, b) = u_{out}(t) =: u_{out},$$

(12b)

which implies that for both upwind scheme and $\kappa$–interpolation scheme, we have the exact values for $f_{1/2}$ and $f_{N+1/2}$:

$$f_{1/2} = f(u(t, a)) = f(u_{in}),$$

(13a)

$$f_{N+1/2} = f(u(t, b)) = f(u_{out}).$$

(13b)

For $i = 1$, noting that formula (5) is only valid for $\kappa = 1$. From the work in [6] and [10], we will use the 1–flux interpolation scheme instead of the normal $\kappa$–flux interpolation scheme for $f_{3/2}$, implying that

$$f_{3/2} = \frac{f_1 + f_2}{2} \text{ or } f \left( \frac{u_1 + u_2}{2} \right),$$

(14)

Since there is no information on $\frac{\partial u}{\partial x}$ from the boundary conditions in this case, the biased second-order accuracy difference will be employed to approximate
the values of $\frac{\partial u}{\partial x} \big|_{i+1/2}$ at the left and right ends of the interval $[a, b]$. This gives

$$\frac{\partial u}{\partial x} \big|_{1/2} = -8u(t, a) + 9u_1 - u_2 \over 3\Delta x_0,$$

(15)

and

$$\frac{\partial u}{\partial x} \big|_{N+1/2} = \frac{8u(t, b) - 9u_N + u_{N-1}}{3\Delta x_N}.$$

(16)

3 Schemes for solving PDEs with Cauchy or Neumann boundary conditions

In this section, Koren’s scheme will be extended for numerically solving the PDEs with Cauchy or Neumann boundary conditions.

3.1 Dealing with PDEs with Cauchy boundary conditions

From the results described in section 2.1, this sub-section aims to develop a scheme for numerically solving PDEs with Cauchy boundary conditions. Assuming equation (1) has the following Cauchy boundary conditions:

$$u(t, a) + \alpha \frac{\partial u(t, x)}{\partial x} \big|_{x=a} = u_{in}(t) =: u_{in},$$

(17a)

$$\frac{\partial u(t, x)}{\partial x} \big|_{x=b} = u_{out}(t) =: u_{out}.$$  

(17b)

In the internal subintervals, $\Omega_i, i = 2, \ldots, N-1$, the formulae given in section (2.1) can be used to approximate the unknowns.

However, new schemes are developed to deal with the boundary conditions. Our main task is to find suitable replacements to approximate the formulae in equations (13), (15) and (16). Recall that the biased second-order accuracy difference at $x = a$ yeilds

$$\frac{\partial u}{\partial x} \big|_{x=a} = -8u(t, a) + 9u_1 - u_2 \over 3\Delta x_1.$$

(18)

Then combining equations (18) and (17a) gives

$$u(t, a) = \frac{3\Delta x_1 u_{in} - 9\alpha u_4 + \alpha u_2}{3\Delta x_1 - 8\alpha},$$

(19)
which gives the following approximations for \( f \) and \( \partial u / \partial x \) at \( x = a \)

\[
\begin{align*}
\left. f \right|_{1/2} &= f(u(t, a) + \frac{1}{2}(u_1 - u(t, a))), \quad \text{or} \quad (20a) \\
\left. f \right|_{1/2} &= f(u(t, a)) + \frac{1}{2}(f(u_1) - f(u(t, a))), \quad (20b)
\end{align*}
\]

and

\[
\left. \frac{\partial u}{\partial x} \right|_{1/2} = \frac{-8u_1 + 9u_1 - u_2}{3\Delta x_1 - 8\alpha}. \quad (21)
\]

Because of the same reason as mentioned in the previous section, for \( i = 1 \), we have

\[
\begin{align*}
\left. f \right|_{3/2} &= \frac{f_1 + f_2}{2} \text{ or } f \left( \frac{u_1 + u_2}{2} \right). \quad (22)
\end{align*}
\]

Considering the boundary condition (17b), since there is no \( u_{N+1} \), we will use the \(-1\)-interpolation formula instead of the general \( \kappa \)-interpolation to approximate \( f \) and \( \partial u / \partial x \) at \( x = b \), which is given by

\[
\begin{align*}
\left. f \right|_{N+1/2} &= f(u_N + \frac{1}{2}(u_N - u_{N-1})), \quad \text{or} \quad (23a) \\
\left. f \right|_{N+1/2} &= f(u_N) + \frac{1}{2}(f(u_N) - f(u_{N-1})), \quad (23b)
\end{align*}
\]

and

\[
\left. \frac{\partial u}{\partial x} \right|_{N+1/2} = u_{out}. \quad (24)
\]

### 3.2 Dealing with PDEs with Neumann boundary condition

In this sub-section, it is assumed that equation (1) has the following Neumann boundary conditions:

\[
\begin{align*}
\left. \frac{\partial u(t, x)}{\partial x} \right|_{x=a} &= u_{in}(t) =: u_{in}, \quad (25a) \\
\left. \frac{\partial u(t, x)}{\partial x} \right|_{x=b} &= u_{out}(t) =: u_{out}. \quad (25b)
\end{align*}
\]

Similar to the derivation in Section 3.1, the formulae given in section (2.1) is used to approximate the unknowns in the internal subintervals, \( \Omega_i, i = 2, \cdots, N - 1. \) The goal of this sub-section is to find suitable replacements to approximate the formulae in equations (13), (15) and (16). Using the biased second-order accuracy difference at \( x = a \) again gives

\[
u(t, a) = \frac{-3\Delta x_1 u_{in} + 9u_1 - u_2}{8}, \quad (26)\]
which gives the following approximations for $f$ at $x = a$

\[ f \bigg|_{1/2} = f(u(t, a) + \frac{1}{2}(u_1 - u(t, a))), \text{ or} \quad (27a) \]

\[ f \bigg|_{1/2} = f(u(t, a)) + \frac{1}{2}(f(u_1) - f(u(t, a))). \quad (27b) \]

Because of the same reason as mentioned in the previous section, for $i = 1, N$, we have

\[ f_{3/2} = \frac{f_1 + f_2}{2} \text{ or } f \left( \frac{u_1 + u_2}{2} \right), \quad (28) \]

\[ f \bigg|_{N+1/2} = f(u_N + \frac{1}{2}(u_N - u_{N-1})), \text{ or} \quad (29a) \]

\[ f \bigg|_{N+1/2} = f(u_N) + \frac{1}{2}(f(u_N) - f(u_{N-1})), \quad (29b) \]

and

\[ \frac{\partial u}{\partial x} \bigg|_{N+1/2} = u_{out}. \quad (30) \]

Now we have developed new schemes for dealing with PDEs with Cauchy and Neumann boundary conditions. In the following, The developed schemes will be verified through some test problems.

4 Numerical Results

In order to demonstrate the advantages of high-resolution schemes developed in this paper, two test problems are selected: Burger’s equation and a non-steady-state model.

4.1 Burger’s Equation

Firstly, let us consider Burger’s equation, one of the simplest PDEs describing both nonlinear propagation and diffusive effects. The equation will be solved using Koren’s scheme. The model was also studied in [1,8] using wavelet-based methods. Burger’s equation is given by

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2}, \quad (31) \]

where $Re$ is the Reynolds number.

Consider the discontinuous initial and boundary conditions used in [1,8]
Boundary conditions
\[ u(t, -1) = 1, \]
\[ u(t, 1) = 0. \] (32)

Initial conditions
\[ u(0, x) = \begin{cases} 1 & \text{for } -1 \leq x \leq 0, \\ 0 & \text{for } 0 < x \leq 1. \end{cases} \] (33)

This is a Dirichlet boundary value problem. So, the numerical scheme posed in sub-section 2.3 is used for numerically solving the Burger’s equation. Here, take \( \kappa = 1/3 \) for the \( k \)-interpolation. The Reynolds number employed here is \( Re = 100 \). The uniform step with step size \( h = 1/N, N = 200 \) is used. The results obtained from both the flux interpolation \( (HR_1) \) and state interpolation \( (HR_2) \) are shown in Figure 1. For comparison, the results obtained from wavelet-Galerkin methods are given in Figure 2, where the top one is from [8] and the bottom one is from [1]. It is seen from Figures 1 and 2 that better results have been obtained from the developed high-resolution method, especially at the ends of the considered interval.

![Graph showing HR-based numerical solutions of the Burger's equation](image)

Fig. 1. HR-based Solutions of Burger’s equation with Re=100

4.2 A Non-Steady-State Model for a Chromatographic Column

The test problem with Cauchy boundary conditions is taken from [3,7], where the model was investigated using the wavelet-collocation method. Consider the following model equation

\[ \frac{\partial y}{\partial t} + \frac{\partial y}{\partial x} = \frac{1}{Pe} \frac{\partial^2 y}{\partial x^2} \] (34)

with initial condition:

\[ y(0, x) = 0, \] (35)
Fig. 2. Wavelet-Galerkin Solution of Burger’s equation with Re=100.

and boundary conditions:

\[ x = 0, \quad \frac{1}{Pe} \frac{\partial y}{\partial x} = y - y_{in}(t), \quad (36a) \]
\[ x = 1, \quad \frac{\partial y}{\partial x} = 0. \quad (36b) \]

Because this is a Cauchy boundary problem, the scheme developed in Section 3 will be employed for numerically solving the test problem. The numerical results are shown in Figures (3) and (4).

In order to compare the results with the known ones, the impulse function used in this case is chosen as the same as the one used in [3,7], which is given as

\[ y_{in} = \delta(t) = \begin{cases} \frac{1}{T}, & 0 \leq t \leq T, \\ 0, & t > T \end{cases}, \quad T = 10^{-3} \]

and the Daubechies wavelets with \( L = 6 \) and \( j = 7, 8, 9 \) are used. The param-
eter and numerical performance are tabulated in Table 1. The CPU time is measured for MATLAB execution on a PC with Windows XP professional 2002 using standard ODE15s solver. It is seen from Table 1 that a more accurate numerical solution with less computing time is obtained by using the developed high-resolution method (HR method).

Table 1
Parameters and numerical performance

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Fig. 3. HR Solution of Chromatographic model at x=1

Fig. 4. HR Solutions of Chromatographic model at t = 0.2 and t = 0.8
## 5 Conclusion

High-resolution schemes for numerically solving PDEs with Cauchy or Neumann boundary conditions have been developed in this paper. Accurate and convergent numerical solutions have been obtained for the test problems. The results obtained from the developed methods are also compared with those obtained from the wavelet-based methods. It is shown that the high-resolution method outperforms the wavelet methods for the test problems. The primary advantage of the newly developed schemes is that they are easy to be adapted for solving different systems without the need of any preliminary work compared to other numerical methods such as wavelet-based methods, where the connection coefficients must be computed first.

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