Solving Two-Phase Flow Transport Equations Using the Lax-Wendroff Scheme

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INTRODUCTION

Recently high-resolution numerical methods have been successfully applied for the solution of two-phase flow transport equations, in which spatial discretization employs the 2nd-order Central Difference (C-D) with flux limiters while time integration is still of 1st-order accuracy [1, 2]. In this work, the Lax-Wendroff (L-W) scheme [3] has been used to solve the two-phase flow equations. First, a simple 1D linear transport model problem is employed to demonstrate the superiority of the L-W scheme over the C-D scheme. Then the L-W scheme is implemented in TRACE and assessment is focused on evaluating the performance of the L-W scheme in simulation of flow oscillations in a single BWR bundle. It is found that the 2nd-order accuracy can be achieved for both spatial discretization and time integration. In order to remove spurious oscillations, the L-W scheme has to be implemented with nonlinear flux limiters. The motivation of this work is to relax time-step size by using the L-W scheme, and therefore speed up reactor simulation.

FORMULATION OF THE L-W SCHEME FOR TWO-PHASE FLOW TRANSPORT EQUATIONS

In reactor thermal-hydraulics analysis codes such as TRACE, RELAP5, and COBRA, the two-phase flow transport equations are typically discretized on a staggered grid using the finite volume method with a semi-implicit time discretization [4] as

\[
\frac{f^{n+1} - f^n}{\Delta t} + \left( f^{n+1} \right)_{j+1/2} - \left( f^{n+1} \right)_{j-1/2} = R^{n+1}_j
\]  

(1)

where \( f = \alpha \rho \psi \), \( \alpha \) and \( \rho \) are the phase volume fraction and density; \( \psi = 1 \) for the mass equation, \( \psi = u \) for the momentum equation, and \( \psi = e \) (internal energy) for the energy equation; \( u \) the velocity at the cell edge; \( \Delta t \) and \( \Delta x \) the time and space steps; \( n \) and \( j \) the temporal and spatial indices; \( R \) the mass source term for the mass equation, momentum source term, and the heat source term plus the pressure term for the energy equation. The angle brackets denote the fluxes:

\[
\begin{align*}
(f^n u^{n+1})_{j+1/2} &= u^{n+1}_{j+1/2} \\
&+ \phi(r^n_{j+1/2})(1 - v_{j+1/2}) \frac{f^n_{j+1} - f^n_{j}}{2} \quad \text{if } u^{n+1}_{j+1/2} \geq 0 \\
&- \phi(r^n_{j+1/2})(1 - v_{j+1/2}) \frac{f^n_{j+1} - f^n_{j}}{2} \quad \text{if } u^{n+1}_{j+1/2} < 0
\end{align*}
\]

(2a)

\[
\begin{align*}
(f^n u^{n+1})_{j-1/2} &= u^{n+1}_{j-1/2} \\
&+ \phi(r^n_{j-1/2})(1 - v_{j-1/2}) \frac{f^n_{j} - f^n_{j-1}}{2} \quad \text{if } u^{n+1}_{j-1/2} \geq 0 \\
&- \phi(r^n_{j-1/2})(1 - v_{j-1/2}) \frac{f^n_{j} - f^n_{j-1}}{2} \quad \text{if } u^{n+1}_{j-1/2} < 0
\end{align*}
\]

(2b)

where

\[
\begin{align*}
r^n_{j+1/2} &= \begin{cases} 
\frac{f^n_{j+1} - f^n_{j}}{f^n_{j+1} - f^n_{j-1}} & \text{if } u^{n+1}_{j+1/2} \geq 0 \\
\frac{f^n_{j+1} - f^n_{j-1}}{f^n_{j+1} - f^n_{j-1}} & \text{if } u^{n+1}_{j+1/2} < 0
\end{cases}
\]

(3a)

\[
\begin{align*}
r^n_{j-1/2} &= \begin{cases} 
\frac{f^n_{j} - f^n_{j-1}}{f^n_{j} - f^n_{j-2}} & \text{if } u^{n+1}_{j-1/2} \geq 0 \\
\frac{f^n_{j} - f^n_{j-2}}{f^n_{j} - f^n_{j-2}} & \text{if } u^{n+1}_{j-1/2} < 0
\end{cases}
\]

(3b)

\[
\begin{align*}
\nu_{j+1/2} &= \frac{u^{n+1}_{j+1/2} \Delta t}{\Delta x_{j+1/2}} = \frac{u^{n+1}_{j+1/2} \Delta t}{(\Delta x_{j+1} + \Delta x_{j+1/2})/2} \quad \text{local CFL number (4a)} \\
\nu_{j-1/2} &= \frac{u^{n+1}_{j-1/2} \Delta t}{\Delta x_{j-1/2}} = \frac{u^{n+1}_{j-1/2} \Delta t}{(\Delta x_{j-1/2} + \Delta x_{j})/2} \quad \text{(4b)}
\end{align*}
\]

Use of different linear functions for \( \phi(r) \) in Eqs (2a) and (2b) gives the following linear schemes:

- **Upwind:** \( \phi(r) = 0 \)  
- **C-D:** \( \phi(r) = 1 \) and \( \nu_{j\pm 1/2} = 0 \)  
- **L-W:** \( \phi(r) = 1 \)

It is well known that both the C-D and L-W schemes produce spurious oscillations at the location where the solution has large gradients [5, 6]. The fix is to replace \( \phi(r) = 1 \) with nonlinear flux limiters [2], e.g.,

- **Minmod (ENO):** \( \phi(r) = \text{minmod}(1, r) \)
- **MUSCL:** \( \phi(r) = \max\left[0, \min\left(1.5r, \frac{1.5r}{2}, 1.5\right)\right] \)
- **OSPRE:** \( \phi(r) = \frac{1.5(r^2 + r)}{r^2 + 1} \)
- **Van Albada (VA):** \( \phi(r) = \frac{r^2 + 1}{r^2 + 1} \)
**A MODEL PROBLEM**

To demonstrate the applicability and superiority of the L-W scheme as compared with the C-D scheme, it is used to solve a model problem, which is a 1D linear homogeneous transport equation:

\[
\begin{align*}
\{ f_t + f_x &= 0 \\
 f(x, 0) &= \eta(x)
\end{align*}
\]  

(12)

Where

\[
\eta(x) = \begin{cases} 
0 & 0 \leq x < 5 \\
1 & 5 \leq x < 6 \\
1 & 6 \leq x
\end{cases}
\]

(13)

For the linear transport equation, the local truncation errors for the above numerical schemes can be easily obtained as

- **Upwind:** \( \tau = -\frac{1}{2} \left( 1 - \frac{\Delta t}{\Delta x} \right) f_{xx}\Delta x \)  

(14)

- **C-D:** \( \tau = -\frac{1}{6} \left[ 1 - \left( \frac{\Delta t}{\Delta x} \right)^2 \right] f_{xxx}(\Delta x)^2 + \frac{1}{2} f_{xx}\Delta t \)  

(15)

- **L-W:** \( \tau = -\frac{1}{6} \left[ 1 - \left( \frac{\Delta t}{\Delta x} \right)^2 \right] / f_{xxx}(\Delta x)^2 \)  

(16)

It shows that the upwind scheme is 1st-order accurate. The C-D scheme has 2nd-order accuracy in space, but only 1st-order accuracy in time. Only the L-W scheme has 2nd-order accuracy in both space and time.

The above model problem is solved using MATLAB [7]. The problem is discretized on a staggered mesh \( \Delta x = 0.05 \) using the finite volume formulation as discussed previously, and solved using the upwind, C-D, and L-W schemes, respectively. For each scheme, two time step sizes are used to solve Eq. (13): \( \Delta t = 0.05 \) (CFL = 1) and \( \Delta t = 0.0025 \) (CFL = 0.05). For the C-D and L-W schemes, the flux limiter VA is used. The results are shown in Fig. 1. The blue curve is the exact solution and the red curve is the numerical solution.

The 1st-order upwind scheme produces significant numerical diffusion when CFL < 1. The smaller time step the more diffusion. When CFL = 1 the numerical solution agrees with the exact solution.

The C-D scheme becomes unstable when \( \Delta t = 0.05 \) (CFL = 1). It is found that for this model problem the time step size \( \Delta t \) has to be less than 0.03, i.e., CFL < 0.6. The result of \( \Delta t = 0.025 \) largely overshoots the gradient due to relatively large numerical error in 1st-order time stepping, although it is 2nd-order accurate in space. For acceptable accuracy, a small time step has to be used.

The L-W scheme is stable for CFL up to 1 as shown in Fig. 1. The L-W scheme can use as large a time step size as with CFL=1. So the L-W performs much better than the C-D in terms of accuracy and efficiency, which will significantly speed up calculations.

**IMPLEMENTATION OF THE L-W SCHEME INTO TRACE**

In this study, the L-W scheme has been implemented in the mass and energy transport equations in TRACE Version 5.0 Patch 4 (V5.0p4). The coding work is trivial since it only requires that \( (1 - v_{i+1/2}) \) be inserted into the existing C-D scheme as shown in Eqs (2a) and (2b).

In this study, the flux limiter VA is applied for both the C-D and L-W schemes. Assessment is focused on evaluating the performance of the L-W scheme in simulation of flow oscillations in a single-CHAN model as shown in Fig. 2. The single-CHAN model consists of a CHAN, an inlet BREAK, and an outlet BREAK. The CHAN component is representative of a typical BWR fuel assembly with 24 uniform axial nodes in the powered section. The single-CHAN model is renodalized with 120 fine nodes for the powered section, which is used as a reference case. The flow is determined by the differential pressure between the inlet and outlet BREAKs. Flow oscillations are induced by a rapid pressure perturbation at the outlet BREAK in a one-second period between 50 and 51 s.

The inlet flow oscillations predicted with the upwind, C-D, and L-W schemes are plotted in Figs 3, 4 and 5, respectively. The time step \( \Delta t = 0.0189s \) is the largest value allowed by the CFL limit. Indeed, it is determined by the vapor velocity in the top node where the vapor velocity reaches its maximum value in the fuel bundle. Therefore, the CFL numbers in all other nodes below the top are less than one. It is shown in Fig. 3 that the upwind significantly underpredicts the magnitude of oscillations because of its numerical diffusion. In addition, the scheme does not predict the steady-state flow rate very well because of the same reason. It can be seen in Fig. 4 that the C-D results exhibit some sensitivity to the time step. The error in time becomes dominant when the time step size is large. Again, the L-W converges well even with the time step at the CFL limit as shown in Fig. 5.

**CONCLUSIONS**

This study has shown the superior performance of the Lax-Wendroff scheme (with a flux limiter) as compared with the Central Difference scheme: 2nd-order accuracy in both time and space, which can speed up reactor simulation by using a relatively large time step up to the CFL limit. In addition, the Lax-Wendroff scheme is easy of implementation and does not incur significant computational cost. The method can effectively improve the numerical solution of two-phase flow transport equations and scalar transport in the fluid. While the tests in this paper are all 1D, the implementation in TRACE also permits applications on 2D and 3D meshes.

However, it is important to note that the Central-Difference scheme belongs to the class of the method of
lines, which is flexible to use other time stepping schemes and useful for multidimensional problems.

Fig. 1. Model Problem Results

Fig. 2. TRACE Single-CHAN Model

Outlet

\[ P_{\text{out}} = 7.0 \times 10^6 \text{ Pa} \]

\[ Q = 4.5 \text{ MW} \]

Inlet

\[ P_{\text{in}} = 7.05 \times 10^6 \text{ Pa} \]

\[ T_{\text{in}} = 543 \text{ K} \]

Fig. 3. Upwind Results

C-D with Flux Limiter VA

\[ \text{Reference fine mesh} \]

\[ dt = 0.0189s \]

\[ dt = 0.01s \]

\[ dt = 0.005s \]

Fig. 4. C-D Results

L-W with Flux Limiter VA

\[ \text{Reference fine mesh} \]

\[ dt = 0.0189s \]

\[ dt = 0.01s \]

\[ dt = 0.005s \]

Fig. 5. L-W Results

REFERENCES