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BOUNDARY AND SOURCE TERM TREATMENT IN THE LARGE TIME STEP METHOD FOR A COMMON TWO-FLUID MODEL

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ABSTRACT

In this paper we present the Large Time Step method based on the Roe scheme applied to a standard two-fluid model. The Large Time Step method was originally developed in the nineteen eighties by Randall LeVeque and has enjoyed increasing popularity in the CFD community in recent years due to its attractive features such as increased accuracy and efficiency compared to its standard low time step counterparts. In terms of efficiency and computation time, one of the main disadvantages in common explicit schemes is the limited time step size imposed by the CFL condition. The idea behind the Large Time Step method is to increase the domain of dependence which leads to a relaxation of the CFL condition, allowing us to use Courant numbers larger than one, i.e. using very large time steps compared to standard explicit methods. It is shown that such an approach notably reduces the computation time and increases the accuracy of the solution. However, the idea of increasing the domain of dependence causes difficulties when it comes to boundary treatment, especially in the presence of source terms. In this paper, we describe and address these difficulties. We extend the standard Roe scheme with the Large Time Step method and apply it to the standard two-fluid model for the water faucet test case, focusing on the treatment of the boundary conditions. Furthermore, we compare the performance of the scheme with the classical Roe scheme in terms of computational time.

Keywords: Two-fluid model, Large Time Step, Boundary treatment, Source term.

NOMENCLATURE

a	speed of sound, $[m/s]$
$\mathbf{A}(\mathbf{U})$	Jacobian matrix
$\hat{\mathbf{A}}$	Roe matrix
$\mathbf{F}$	flux vector
g	gravitational acceleration, $[m/s^2]$
k	phase index, g - gas, l - liquid
p	pressure, $[Pa]$
p^i	interface pressure, $[Pa]$
$\mathbf{Q}$	source term
$\hat{\mathbf{R}}$	matrix of right eigenvectors of Roe matrix
t	time, $[s]$
$\mathbf{U}$	vector of conserved variables
v	velocity, $[m/s]$
x	spatial coordinate $[m]$
α	volume fraction
λ	eigenvalue of Jacobian matrix
$\hat{\Lambda}$	diagonal matrix of eigenvalues of Roe matrix
ρ	density, $[kg/m^3]$

INTRODUCTION

The two-fluid model is a mathematical model in widespread use for the simulation of two phase flow. The model contains difficulties associated with a complicated eigenstructure and non-conservative terms (Jones and Prosperetti, 1985; Flåtten and Morin, 2012; Morin *et al.*, 2013). Despite these difficulties the model has been successfully used in many applications, such as oil & gas (Larsen *et al.*, 1997; Bendiksen *et al.*, 1991) and the nuclear industry (Barre and Bernard, 1990). Current research and improvements of the two-fluid model are based on resolving the mathematical difficulties and further improving the computational performance, in terms of new numerical schemes which aim to increase the accuracy of the solution or reduce the computational time. In the present work we show that the computational time can be reduced and the accuracy can be improved by the Large Time Step (LTS) scheme. The basic idea is to formulate an explicit scheme which will not be limited by the CFL condition, thereby allowing us to use time steps much larger than usually associated with explicit schemes. Such schemes were first introduced by Randall LeVeque in the nineteen eighties (LeVeque, 1985), but have recently seen a revival with applications to the Euler equations (Qian and Lee, 2012) and the shallow water equations (Morales-Hernández *et al.*, 2014; Xu *et al.*, 2013). To the best of our knowledge no application of LTS to two phase flows has yet been published.

Although the results obtained with the LTS scheme are promising, there are certain difficulties when it comes to the treatment of boundary conditions, especially in presence of source terms, such as gravity. In this paper we present two different approaches to treat the boundaries. We show the effect of the different treatments of boundary conditions on the accuracy of the solution depending on the choice of the time step

and the grid size. A performance study demonstrates how the computational time is reduced by increasing the time step in the LTS method.

MODEL DESCRIPTION

We consider a one-dimensional isentropic equal-pressure two-fluid model without energy equations (Evje and Flåtten, 2003), where we solve separate conservation equations for mass and momentum of two fluids ($k = g, l$):

$$\frac{\partial(\rho_k \alpha_k)}{\partial t} + \frac{\partial(\rho_k \alpha_k v_k)}{\partial x} = 0 \tag{1}$$

$$\frac{\partial(\rho_k \alpha_k v_k)}{\partial t} + \frac{\partial\left(\rho_k \alpha_k v_k^2 + (p - p^i)\alpha_k\right)}{\partial x} + \alpha_k \frac{\partial p^i}{\partial x} = Q_k. \tag{2}$$

Closure relations and thermodynamic submodel

The model is closed by a basic relation between volume fractions:

$$\alpha_g + \alpha_l = 1 \tag{3}$$

and by equation of state for each phase k:

$$\rho_k = \rho_{k,0} + \frac{p - p_{k,0}}{a_k^2} \tag{4}$$

where the speed of sound a is defined as $a_k^2 = \partial p / \partial \rho_k$. The parameters are defined as:

$$\begin{aligned} p_{l,0} &= 10^5 \text{ Pa} & p_{g,0} &= 0 \\ \rho_{l,0} &= 1000 \text{ kg/m}^3 & \rho_{g,0} &= 0 \\ a_l &= 10^3 \text{ m/s} & a_g &= \sqrt{10^5} \text{ m/s}. \end{aligned}$$

Although the model assumes equality of phase pressures, $p_g = p_l$, we need to define an interface pressure term to ensure that the system is hyperbolic:

$$\Delta p = p - p^i = \delta \frac{\alpha_g \alpha_l \rho_g \rho_l}{\rho_g \alpha_l + \rho_l \alpha_g} (v_g - v_l)^2 \tag{5}$$

with $\delta = 1.2$. For details on closure relations and interface pressure modeling we refer to Evje and Flåtten (2003).

NUMERICAL MODEL

The system of equations (1) - (2) can be written in quasilinear form as:

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}(\mathbf{U}) \frac{\partial \mathbf{U}}{\partial x} = \mathbf{Q}(\mathbf{U}). \tag{6}$$

This system is discretized by the explicit Euler method in time and the Roe scheme in non conservative form in space:

$$\mathbf{U}_j^{n+1} = \mathbf{U}_j^n - \frac{\triangle t}{\triangle x}\left(\triangle \mathbf{F}_{j-1/2}^+ + \triangle \mathbf{F}_{j+1/2}^-\right) + \triangle t \mathbf{Q}_j^n \tag{7}$$

where the flux differences $\triangle \mathbf{F}^+$ and $\triangle \mathbf{F}^-$ are:

$$\triangle \mathbf{F}_{j+1/2}^{\pm} = \triangle \mathbf{F}_{j+1/2}^{\pm}\left(\mathbf{U}_j, \mathbf{U}_{j+1}\right) = \hat{\mathbf{A}}_{j+1/2}^{\pm}\left(\mathbf{U}_{j+1} - \mathbf{U}_j\right) \tag{8}$$

Herein, the fundamental component is the construction of a *Roe matrix* $\hat{\mathbf{A}}$ (see Evje and Flåtten (2003) for details), and we define

$$\hat{\mathbf{A}}^{\pm} = \hat{\mathbf{R}} \hat{\Lambda}^{\pm} \hat{\mathbf{R}}^{-1} \tag{9}$$

where $\hat{\mathbf{R}}$ is the matrix of eigenvectors of $\hat{\mathbf{A}}$ and $\hat{\Lambda}$ is the diagonal matrix of eigenvalues. Herein,

$$\lambda^+ = \max(0, \lambda), \tag{10}$$

$$\lambda^- = \min(0, \lambda). \tag{11}$$

In this paper we will refer to this formulation and results obtained with it as "the standard Roe scheme".
A known limititation of this scheme is that the time step must satisfy the constraint $C \leq 1$, where C is the *Courant number*:

$$C = \max|\lambda| \frac{\Delta t}{\Delta x}. \tag{12}$$

Herein, the maximum is taken over all eigenvalues in all computational cells.
In the following, we will describe an extension of the Roe scheme that gets rid of this limitation.

Large Time Step Scheme

To extend the standard Roe scheme to the LTS Roe scheme we use the approach proposed by LeVeque (1985).
As stated earlier, the basic idea of the LTS method is to increase the domain of dependence. Since the information from the domain of dependence with which we update cell state $\mathbf{U}_j^{n+1}$ is delivered in terms of fluxes through the cell faces, we reformulate the flux differences to include all flux differences in the domain of dependence. Hence we modify (8) as follows:

$$\mathbf{F}_{j+1/2}^+ = \sum_{i=0}^{\infty} \hat{\mathbf{A}}_{j+1/2-i}^{i+}\left(\mathbf{U}_{j+1-i} - \mathbf{U}_{j-i}\right) \tag{13}$$

$$\mathbf{F}_{j+1/2}^- = \sum_{i=0}^{\infty} \hat{\mathbf{A}}_{j+1/2+i}^{i-}\left(\mathbf{U}_{j+1+i} - \mathbf{U}_{j+i}\right) \tag{14}$$

where the matrices $\hat{\mathbf{A}}^{i\pm}$ are defined as:

$$\hat{\mathbf{A}}^{i\pm} = \hat{\mathbf{R}}^{i\pm} \hat{\Lambda}^{i\pm} \left(\hat{\mathbf{R}}^{i\pm}\right)^{-1} \tag{15}$$

$$\hat{\Lambda}^{i\pm} = \text{diag}\left(\lambda^{i\pm}\right) \tag{16}$$

$$\lambda^{i+} = \max\left(0, \min\left(\lambda^i - i\frac{\triangle x}{\triangle t}, \frac{\triangle x}{\triangle t}\right)\right) \tag{17}$$

$$\lambda^{i-} = \min\left(0, \max\left(\lambda^i + i\frac{\triangle x}{\triangle t}, -\frac{\triangle x}{\triangle t}\right)\right). \tag{18}$$

The infinite sum from equations (13) and (14) will contain only a finite number of nonzero terms, because the term $\lambda^i - i\frac{\triangle x}{\triangle t}$ becomes negative, and the term $\lambda^i + i\frac{\triangle x}{\triangle t}$ becomes positive at some point.
Due to limited length of the paper the reader is referred to the forthcoming journal article for more extensive explanation of the LTS method.

BOUNDARY CONDITIONS

Increasing the domain of dependence leads to a difficulty when it comes to the definition of boundary cells. In the standard Roe scheme we must provide only one boundary cell at each boundary, because the first cell in the domain is updated only from its neighboring cells, i.e. the Roe scheme is a three-point scheme:

$$\mathbf{U}_j^{n+1} = f\left(\mathbf{U}_{j-1}^n, \mathbf{U}_j^n, \mathbf{U}_{j+1}^n\right) \tag{19}$$

For the first cell in the domain this leads to:

$$\mathbf{U}_1^{n+1} = f\left(\mathbf{U}_{LBC}, \mathbf{U}_1^n, \mathbf{U}_2^n\right) \tag{20}$$

with $\mathbf{U}_{LBC}$ being $\mathbf{U}$ in the left boundary cell. From the way the LTS Roe scheme is formulated it is clear that the value at any cell may depend on more than three cells:

$$\mathbf{U}_j^{n+1} = f\left(..., \mathbf{U}_{j-2}^n, \mathbf{U}_{j-1}^n, \mathbf{U}_j^n, \mathbf{U}_{j+1}^n, \mathbf{U}_{j+2}^n, ...\right) \tag{21}$$

where the particular size of the domain of dependence depends on the local Courant number. Clearly, this leads to a difficulty when it comes to the definition of numerical boundary conditions, since (for example at the left boundary) we do not have cells associated with $\mathbf{U}_{j-2}^n$, $\mathbf{U}_{j-3}^n$, etc. We now suggest two different ways to define these boundary cells in the presence of source terms.

Extrapolated boundary conditions

Assume that we apply a Courant number C, i.e. we will need $M = \text{ceil}(C)$ numerical ghost cells at each boundary to directly apply the LTS Roe scheme. The straightforward way to provide these additional cells is to simply extrapolate the values of the original boundary condition cell. In this way, all additional cells in the boundary zone will have the same values as the original boundary cell:

$$\mathbf{U}_p^n = \mathbf{U}_{LBC}^n \quad \forall \quad p < LBC \tag{22}$$

$$\mathbf{U}_p^n = \mathbf{U}_{RBC}^n \quad \forall \quad p > RBC \tag{23}$$

where *LBC* and *RBC* denote the indices of the left and right boundary cells, respectively. Assuming N cells in the interior domain, we will use the convention that $LBC = 0$ and $RBC = N + 1$.

We will refer to this formulation as *EBC*, i.e. extrapolated boundary conditions. If there are no source terms present in the computational domain this approach will be very effective, and very accurate results may be obtained. For reference we advise the reader of the forthcoming journal article by the same authors.

Herein, there are a number of ways of constructing the values of the primary *LBC* and *RBC* cells, depending on the physics of the prescribed problem. Most rigorous are the *characteristic boundary conditions*, see for instance Fjelde and Karlsen (2002).

However, regardless of our choice of updating $\mathbf{U}_{LBC}$ and $\mathbf{U}_{RBC}$ we are left with a central problem associated with the *EBC* as given by (22)–(23) in the presence of source terms. Assuming the constant boundary conditions, the assumption of locally uniform data corresponds to a valid steady state solution in the *absence* of source terms. Consequently, the application of (22)–(23) may be viewed as follows:

- Calculate $\mathbf{U}_{LBC}$ and $\mathbf{U}_{RBC}$ by some boundary scheme, for instance by extrapolation of the characteristic or primitive variables.
- Solve the steady-state *homogeneous* problem

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}(\mathbf{U})\frac{\partial \mathbf{U}}{\partial x} = 0 \tag{24}$$

  in an artifical domain extended at the boundaries (the solution is simply $\mathbf{U} = \text{const.}$)
- Transport the solution in this artificial domain into the actual computational domain through the LTS scheme.

Comparing (6) to (24), we see that under this point of view the EBC approach introduces an *artifical discontinuity* of the source term at the boundaries. Applying a Courant number $C > 1$, we will then see this manifest itself as a discontinuity in the numerical solution, propagating C cells per time step away from the boundary. Clearly, this is a numerical artifact arising from our extrapolation being faster than the interaction between transport and source term effects in each cell. This issue is the main topic of our current paper, and we will illustrate this phenomenon in the numerical section. We now proceed to propose a natural modification that will remedy this.

Steady state boundary condition

To overcome the problem discussed above, we simply replace our equation (24) by (6) to instead solve the steady state problem:

$$\mathbf{A}(\mathbf{U})\frac{d\mathbf{U}}{dx} = \mathbf{Q}(\mathbf{U}). \tag{25}$$

By solving this for $\frac{d\mathbf{U}}{dx}$ we obtain:

$$\frac{d\mathbf{U}}{dx} = (\mathbf{A}(\mathbf{U}))^{-1}\mathbf{Q}(\mathbf{U}). \tag{26}$$

Now, by solving this equation at the left and the right boundary cells we obtain the slopes $\delta_x\mathbf{U}_L$ and $\delta_x\mathbf{U}_R$ (left and right, respectively) which we then use to formulate the additional boundary cells as:

$$\mathbf{U}_{-q}^n = \mathbf{U}_{LBC}^n - q\triangle x\delta_x\mathbf{U}_L \quad \forall \quad q \in [0, \ldots, M] \tag{27}$$

at the left boundary zone and:

$$\mathbf{U}_{N+q}^n = \mathbf{U}_{RBC}^n + (q-1)\triangle x\delta_x\mathbf{U}_R \quad \forall \quad q \in [1, \ldots, M] \tag{28}$$

at the right boundary zone. These equations then replace our previous equation (22) and (23). We will refer to this formulation as *SSBC*, i.e. steady state boundary conditions.
In the following, we will present some numerical simulations highlighting the differences between *EBC* and *SSBC*.

NUMERICAL RESULTS

As a test case to compare our implementations of the boundary conditions we use a simplified water faucet problem proposed by Ransom (1987). We consider a vertical pipe 12 meters long with initial data:

$$\alpha_l = 0.8, \quad v_l = 10 \text{ m/s}, \quad v_g = 0 \text{ m/s}, \quad p = 10^5 \text{ Pa}.$$

The source term Q_k is limited to gravity and defined as:

$$Q_k = \rho_k \alpha_k g.$$

The following boundary conditions are given:

Inlet: $\alpha_l = 0.8, \quad v_l = 10$ m/s, $\quad v_g = 0$ m/s,
Outlet: $p = 10^5$ Pa.

Boundary values are then simply obtained by extrapolating the missing variables from the computational domain, more precisely

$$\mathbf{W}^n_{LBC} = \begin{bmatrix} p \\ \alpha_l \\ v_g \\ v_l \end{bmatrix}_{LBC} = \begin{bmatrix} p^n_1 \\ 0.8 \\ 0 \\ 10 \text{ m/s} \end{bmatrix} \tag{29}$$

and

$$\mathbf{W}^n_{RBC} = \begin{bmatrix} p \\ \alpha_l \\ v_g \\ v_l \end{bmatrix}_{RBC} = \begin{bmatrix} 10^5 \text{ Pa} \\ (\alpha_l)^n_N \\ (v_g)^n_N \\ (v_l)^n_N \end{bmatrix}. \tag{30}$$

All the results discussed above are computed at time $t = 0.6s$. The analytical solution for the liquid volume fraction and liquid velocity can be found in Evje and Flåtten (2003), while the complete procedure is available in Trapp and Riemke (1986). The reference solution for the remaining variables is obtained by the standard Roe scheme with superbee wave limiter on a mesh with 10 000 cells and $\triangle t = 3.5294 \cdot 10^{-6}$.
For the actual Roe scheme, we use the exactly the same procedure as described in Evje and Flåtten (2003). Herein, we replace the original discretization (8) by our Large Time Step extension (13)–(18). Note in particular that (13)–(18) reduces to (8) in the event that $C \leq 1$.

Effect of time step

We consider a domain with a fixed number of cells (100) and compare the pressure, volume fraction and velocity profiles for different time steps and different implementations of the boundary conditions, see figure 1.
It can be seen that the solution obtained with SSBC is smoother than the solution obtained with EBC for corresponding time steps, especially for larger time steps. That is expected since the boundaries defined with SSBC introduce a smaller error and provide a smoother transition between the boundary zone and the rest of the domain.
The solutions for the gas volume fraction are very similar among each other which is not surprising because the liquid and gas velocities are more than an order of magnitude smaller than the velocity of the pressure waves. Because of that, the Courant number corresponding to the volume fraction waves is actually smaller than 1 at all times. Further, it can be seen that the accuracy of the solution for the gas volume fraction and liquid velocity is actually *increased*. This is because the larger time step leads to fewer time steps in total, which reduces the numerical diffusion introduced each time we average a cell state. More rigorous insight can be gained through the modified equation analysis, see for instance Harten *et al.* (1976).

Effect of mesh refinement

We also compare the effect of grid refinement starting with a mesh of 100 cells and a time step $\triangle t = 0.00176$ which corresponds to $C \approx 5$. For each refined mesh we keep the Courant number constant, i.e. the ratio $\triangle t / \triangle x = 0.01467 =$ const., see figure 2.
We again note the *SSBC* provides smoother profiles than *EBC*. However, this effect becomes less significant as the mesh is refined. This is to be expected, as the number of boundary cells remains constant as the total number of grid cells is increased. Hence their relative influence becomes smaller.
Nevertheless, practical simulations are often performed on coarse grids due to computational efficiency constraints. Here the results may be sensitive to the different treatments of the boundary conditions presented here.

Performance analysis

The last numerical experiment (see figure 3) shows how the computational time depends on the increased time steps for different grid sizes. The abscissa shows the Courant number. The ordinate shows the relative computational time normalized to one for $C = 1$. The approach used for the treatment of the boundary conditions is SSBC.
Each profile is the averaged results of 10 simulations performed in MATLAB.
It can be seen that the gain in computational time for different mesh sizes shows a similar trend, with the gain being smaller for larger meshes. A precise explanation of this phenomenon would require a careful code profiling beyond the scope of the current paper. However, it should be noted that a relative slow-down

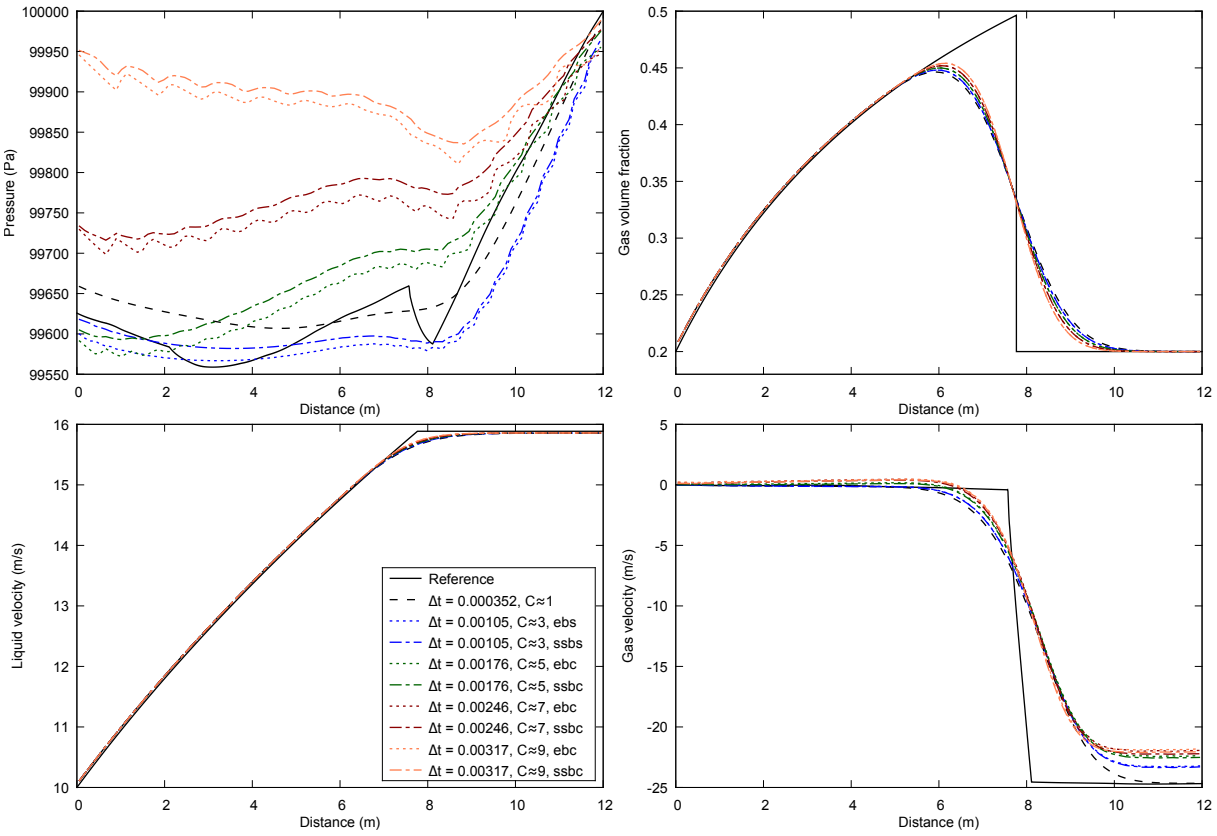

Figure 1: Effect of increasing time step on mesh with 100 cells

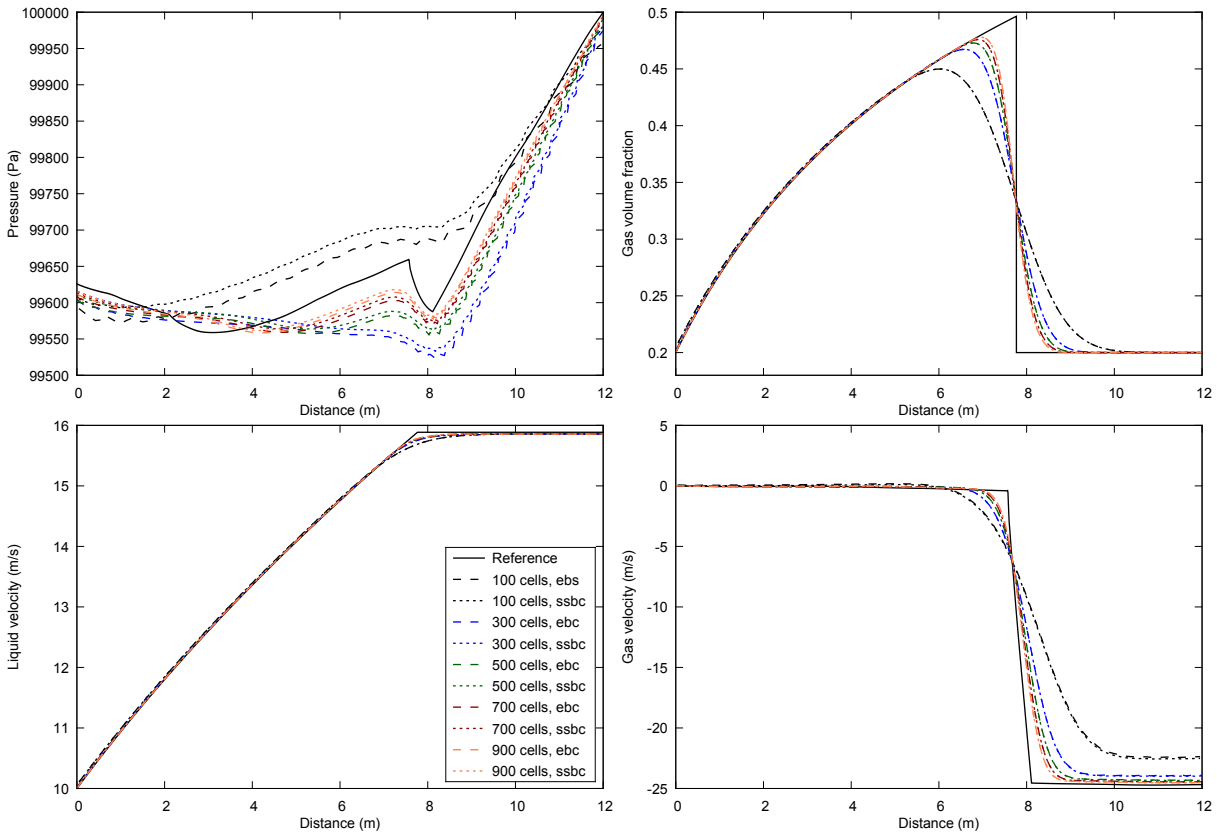

Figure 2: Effect of mesh refinement with $\triangle t / \triangle x =$ const., (C ≈ 5)

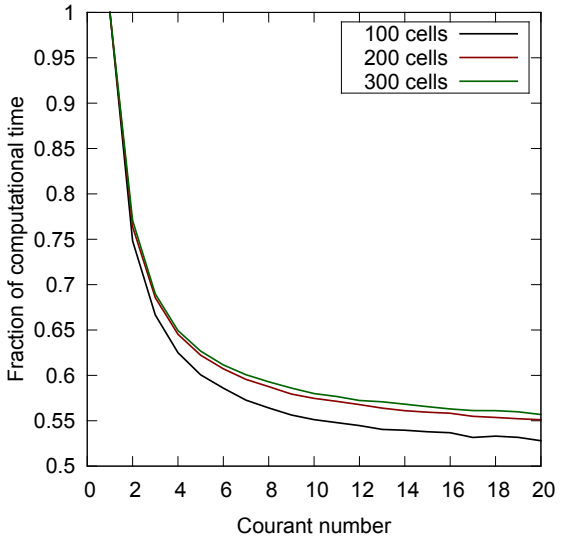

Figure 3: Relative computational time with respect to $C = 1$ vs. Courant number

of the code would be expected for high Courant numbers for coarse meshes, as the values in the artificial boundary cells will then influence a significant part of the domain. The figure indicates that this effect is not detrimental.

CONCLUSION

We extended the standard Roe scheme to a Large Time Step Roe scheme and showed that the two-fluid model can be resolved with an explicit method not limited by the CFL condition.

Increasing the time step size leads to less accurate pressure and gas velocity, but to increased accuracy in volume fractions and liquid velocity. The numerical error associated with pressure waves can be partially reduced by imposing steady state boundary conditions (SSBC) to determine the flow variables in the ghost cells compared to a simple extrapolation boundary treatment. In particular, the SSBC approach will reduce oscillations and lead to smoother profiles. This observation is the main contribution of the current paper.

Grid refinement shows that the error introduced by a larger time step decreases with decreased grid spacing.

A performance study shows that the relative gain in computational time is highly dependant on the Courant number, and that the gain is largest immediately after increasing the time step above the CFL limit.

The proposed method shows promising potential, especially in the two following cases. First, in problems with a large number of grid cells where additional ghost cells introduced by the LTS method cause relatively small increase in computational time compared to the reduction of computational time gained by increasing the time step (i.e. reducing the number of time steps). Second, in problems where the velocities of the phases are much smaller than the acoustic wave speeds and we are not interested in maximum accuracy of the pressure field compared to the accuracy required for volume fractions and velocities.

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