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A CONSISTENT MASS AND MOMENTUM FLUX COMPUTATION METHOD USING RUDMAN-TYPE TECHNIQUE WITH A CLSVOF SOLVER

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ABSTRACT

In this paper, a computational method is presented that addresses the problem of multiphase flow characterized by phases with significant density ratio accompanied by strong shearing. The Coupled Level-Set Volume-of-Fluid (CLSVOF) technique is used for interface tracking, while the momentum transfer is coupled to that of mass by means of momentum fluxes computed using a sub-grid. This is an extended adaptation of Rudman's volume tracking technique [1]. The new method is shown to conserve kinetic energy when applied to cases otherwise unfeasible, such as shear layer with high density ratio.

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Introduction

A large number of atomization processes are characterized by a large density ratio coupled with strong shear, frequently a combination required to destabilize the liquid jet. Examples may be found in cryogenics, where gases injected at high velocities create the spray by breaking up an ergol jet.

When simulating this kind of phenomena, one may encounter an nonphysical accumulation of kinetic energy [1, 2] caused by errors in interface advection that redistribute the mass incorrectly, thus creating artificial momentum in liquid [3]. We illustrate it below while describing a planar shear layer simulation (see Figures 5 and 6). Since the flow is dominated by convection, the terms representing it in Navier-Stokes equation are thought to cause the error as the momentum transfer is not coupled to that of mass. While amplified by the presence of shear, the problem itself is found whenever large density ratios are considered, e.g. water droplet oscillating in air as described

by Raessi [4].

First numerical approaches to high density ratio flows are to be found in applications of the Lattice-Boltzmann method (LBM), by McNamara & Zanetti [5]. Later works by Lee & Lin [6] or Shi et al. [7] have advanced the LBM to the point when simulating a droplet impacting a liquid film became feasible with $1:10^3$ density ratio; still, the method remains relatively complicated in implementation.

A different approach was to use a MAC[1]-type Navier-Stokes solver with a interface tracking method. In 1998 Rudman [1] proposed using VOF technique to transfer both mass and momentum, ensuring energy conservation. His FGVT[2] method allowed e.g. for decreasing "parasitic currents" phenomenon compared to contemporary schemes in simulation of a $1:1000$ density ratio stationary droplet, and at the same time kept the kinetic energy one order of magnitude lower than that obtained using the Continuum Surface Force [8] schemes. Continuing in this vein were the works of Bussmann et al. [9], who generalized the approach to non-structured, collocated meshes.

To enable more accurate surface tension calculations and simplify certain implementation aspects the Level Set (LS) methods [10] were brought into the scope, beginning with works of Sussman [11], who obtained stable solutions of $1:1000$ density ratio flows using velocities extrapolated off the liquid – which was facilitated by having the gradients of the level-set distance function readily available. The work kept VOF coupled to the LS as well. Building up on this were the works of Li et al. [12], F. Xiao [13] and F. Xiao et al. [14], where similar methodology was applied to model primary breakups and atomization.

Employing a technique similar to Rudman's [1] is not ruled out even in the domain of Level Set method alone, as was shown by works of Desjardins & Moureau [15] or Raessi & Pitsch [2]. Authors of the latter have presented a distance function-based momentum flux calculation concept which yields both an improvement in test cases such as the gravitational collapse of a water column[3] or oscillating droplet as well as the ability to include staggering density ratios such as $1:10^6$. However, the momentum flux calculations introduced therein were one-dimensional, and the geometrical orientation of the interface was not accounted for. Staying withing the LS formulation (without VOF) Ghods & Herrmann [3] introduced a two-dimensional CRMT[4] method that was claimed to be easily generalized to three-dimensional space. It utilized density fluxes based on LS distance function ϕ (via quasi-fraction function computed from it). This approach permitted the authors of [3] to obtain results similar to [2].

In this paper, we present a CLSVOF code [16–18] enabling us a choice between LS-based and VOF-based momentum fluxes calculation. We settle on the latter, since they are much more accurate that LS-based [18], limiting the possibility of introducing error this way. The momentum fluxes are calculated using a sub-grid, while possible errors resulting from interpolation of velocity are limited by using a WENO5 [19] scheme. Two-dimensional results are presented in the paper, with three-dimensional simulations to follow in later publications.

Equations

Usually, we solve the Navier-Stokes equation in the non-conservative form (Eq. 1):

$$\begin{cases} \bigtriangledown.(u) = 0 \\ \frac{\partial u}{\partial t} + (u.\bigtriangledown)u = \frac{1}{\rho}(-\bigtriangledown P + \bigtriangledown.(2\mu D) + F_V) \end{cases} \tag{1}$$

And we transport the interface, thanks to the CLSVOF method [16, 20]

$$\frac{\partial \phi}{\partial t} + \bigtriangledown.u\phi = 0 \tag{2}$$

where ϕ represents the interface characterized by VoF or level-set function.

The resolution of Navier-Stokes equations is done by a projection's method:
We first determine intermediate velocity u^* , by solving Navier Stokes equations without the pressure term.

$$u^* = u^n + \Delta t(-(u.\bigtriangledown)u + \frac{1}{\rho}(\bigtriangledown.(2\mu D) + F_V) \tag{3}$$

This velocity doesn't satisfy the mass conservation (the velocity field is not divergence free). We want to obtain u^{n+1} satisfying $\bigtriangledown.(u^{n+1}) = 0$.

$$u^{n+1} + \frac{\Delta t}{\rho^{n+1}}(\bigtriangledown P^{n+1}) = u^* \tag{4}$$

We then apply the divergence operator($\bigtriangledown.$)

$$\bigtriangledown.(\frac{\bigtriangledown P^{n+1}}{\rho^{n+1}}) = \frac{\bigtriangledown.u^*}{\Delta t} \tag{5}$$

We solve Poisson's equation (Eq. 5) to obtain the pressure. We then write:

$$u^{n+1} = u^* - \Delta t(\frac{\bigtriangledown P^{n+1}}{\rho^{n+1}}) \tag{6}$$

[1]Marker-And-Cell
[2]Fine Grid Volume Tracking
[3]This test case is known also as "broken dam" or "dam-break".
[4]Consistent Re-scaled Momentum Transport

The convection term is discretized by a WENO scheme [19]. For the diffusion term, we implemented the Sussman approach [20] which was adapted to a staggered grid by Lalanne [21]. The ghost fluid method (GFM) [22] is used to describe the jump of scalar variables at the interface.
As it has been discussed before, the previous formulation of the convection term leads to unstable behaviours. That is why we decide to solve the convection term in the conservative form. To be consistent, we simultaneously solve the transport of mass.

First, we determine an intermediate velocity u^* by adding only the convection term in the Navier Stokes equations. We solve

$$(\rho u)^* = (\rho u)^n + \bigtriangledown.(\rho uu) \tag{7}$$

leading to

$$u^* = \frac{(\rho u)^*}{\rho^{n+1}} \tag{8}$$

We go back to the usual projection method in the non conservative form of the Navier Stokes equations without the convection term.

$$u^{**} = u^* + \frac{\Delta t}{\rho}(\bigtriangledown.(2\mu D) + F_V) \tag{9}$$

The crucial point of the method is the discretization of the momentum fluxes.

How to make flux calculation consistent with mass transport?

The basis of the method is to use mass transport flux to compute momentum flux, which will make them consistent. In Fig. 1, we show the points for mass flux (A,B,C,D) , and momentum flux(A',B',C',D').

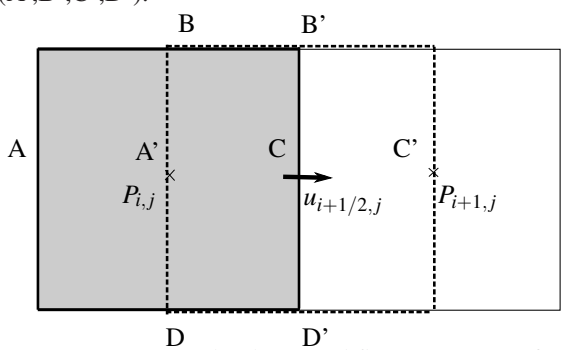

FIGURE 1: Control volume and flux momentum faces

Fluxes are deduced from VoF fluxes of the discretized equation (Eq. 11).

$$F_{i,j}^{n+1} = F_{i,j}^n + \frac{\Delta t}{\Delta x}(G_{i-1/2,j} - G_{i+1/2,j}) + \frac{\Delta t}{\Delta y}(\tilde{G}_{i,j-1/2} - \tilde{G}_{i,j+1/2}) \tag{10}$$

where $\tilde{G}_{i,j-1/2}, \tilde{G}_{i,j+1/2}, G_{i-1/2,j}, G_{i+1/2,j}$ are the four VoF fluxes through the four faces of the cell centered on i,j,k, computed with a split method.

To obtain mass flux at the same face than for momentum, Rudman's method consists in transporting the mass on a sub-grid twice smaller than the Navier Stokes grid.The sub-grid is presented in Fig. 2.

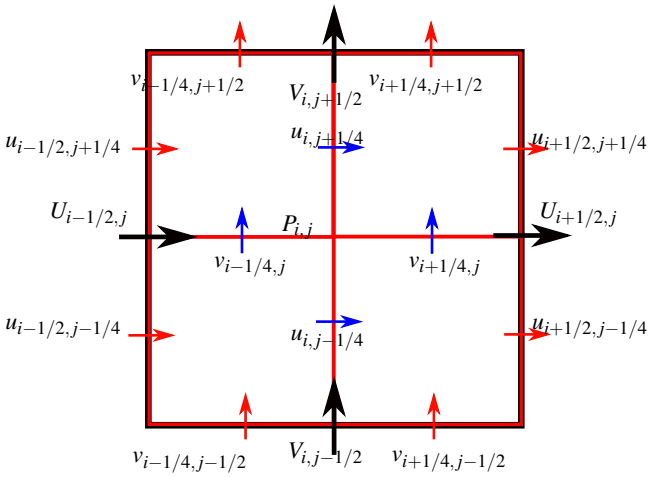

FIGURE 2: Sub-grid scheme

To obtain velocities on the sub-grid, an interpolation is needed. Whereas Rudman used a simple centered average interpolation, we use a more sophisticated scheme. Different approaches exist to obtain a more accurate interpolation [23], [24] and we choose the Toth's scheme. This interpolation takes into account the velocity gradient for velocities that are located on a face of the coarse grid. For velocity on the coarse grid, Toth imposed two conditions: divergence free in each sub-grid cell (necessary to conserve mass) and with the same vorticity one the refined and coarse grid.

In order to illustrate the interpolation influence, we present some results on the Zalesak test case. It consists in a rigid body rotation (Zalesak's disk) in a constant rotating velocity field. We use analytic velocity field definition only on coarse grid, it is subsequently interpolated onto sub-grid. We compare the centered average interpolation with the interpolation purposed by Toth.

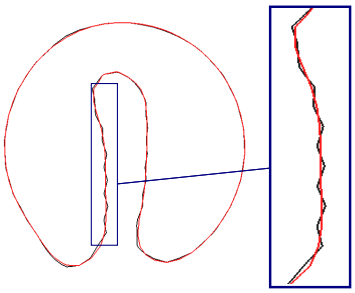

FIGURE 3: Zalesak's disk after one rotation with the two interpolation scheme.
The black represents the interface position when we use a simple centered average interpolation.
In red the position interface when we use the more sophisticated scheme.

With the simple approximation, we can see that some "teeth" appear, which is not the case with the Toth's interpolation.

From the velocity field on the fine grid, it is now possible to estimate mass fluxes.

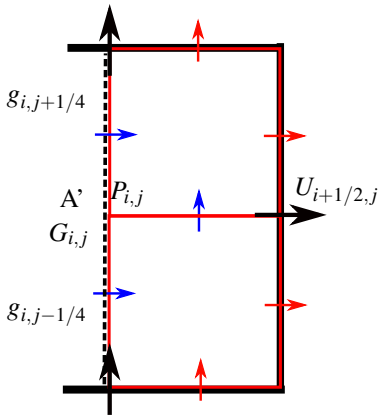

FIGURE 4: Relation between fluxes on coarse and refined grid

During VoF advection on the refined grid,the fluxes $g_{i,j-1/4}$ and $g_{i,j+1/4}$ are computed and we can easily obtain the flux $G_{i,j}$ through the face A' (Fig. 4) by writing $G_{i,j} = g_{i,j-1/4} + g_{i,j+1/4}$. These fluxes are VoF fluxes (G for coarse grid and g for the sub-grid) and it is straightforward to compute in the same way all the mass fluxes we need.(We will use H for mass flux of coarse grid and h for mass flux of the sub-grid). We can then write the momentum term (Eq. 11)

$$\nabla \cdot (\rho uu)_{i+1/2,j} = \frac{H_{i+1,j}U^{conv}_{i+1,j} - H_{i,j}U^{conv}_{i,j}}{dx}, \qquad (11)$$

Interpolation of the convected velocity

The convected velocity needs to be interpolated on two locations ((i,j) and $(i,j+1/2)$). Both, Raessi et al. [2] and Desjardins et al. [15] used an upwind scheme when nodes are crossing the interface and a centered interpolation in either case.

Note that we use a WENO 5 scheme [19] to ensure a higher interpolation order of the convected velocity even close to the interface. The code remains stable with this interpolation even for high density ratio.

Results

2D sheet layer

In order to illustrate our purpose a simple test case has been studied, a 2D sheet layer with high density ratio(Fig. 5). The domain is a square 0.003m x 0.003m. The shear layer is $300\mu m$ thick. The sheet(in blue) has a density of $1000kg/m^{-3}$ and the air a density of $1kg/m^{-3}$. There is no diffusion, no gravity and no surface tension. Initially, the velocity of the gas is $U_{gas} = 30ms/s$ and $U_{liquid} = 2m/s$ in the liquid. We give a small perturbation in the vertical velocity. $v(x,y) = 0.01U_{liquid} * sin(2\pi/(xmax - xmin) * exp(-(2y/a))$
Periodic conditions are used. Under these conditions, kinetic energy should be conserved.

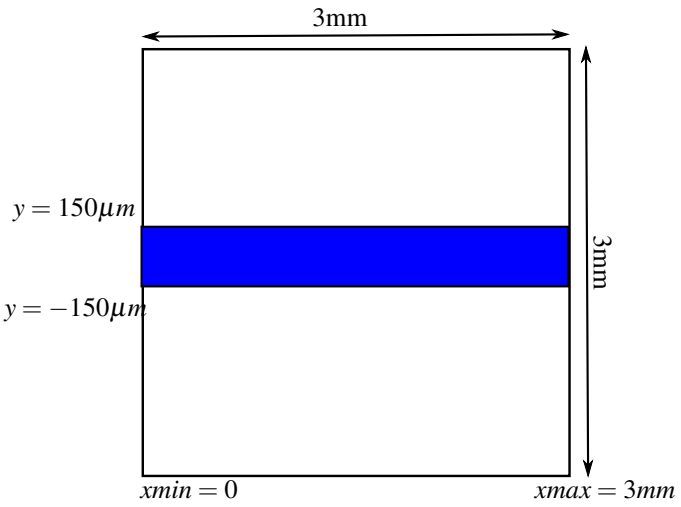

FIGURE 5: 2D shear layer

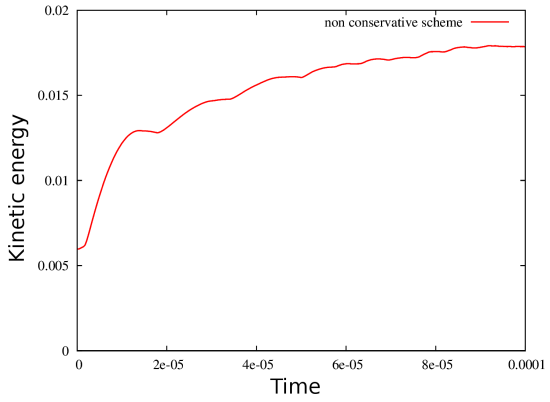

FIGURE 6: Kinetic energy for the non conservative scheme

We observe in Fig. 6 that kinetic energy is growing, whereas it should remain approximately constant. The error seems to come from the inconsistent transport between mass (thanks to level-set or VoF function) and velocity [2, 15].

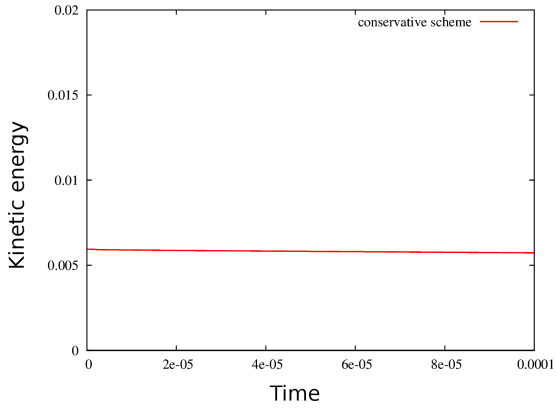

FIGURE 7: Kinetic energy for the conservative scheme

When the shear layer is simulated with the new approach, we observe (see Fig. 7) that kinetic energy is now well conserved. The small decrease of kinetic energy can be explained by the numerical diffusion.

A droplet with $10^6 : 1$ density ratio

The convection of a 2D droplet of high density (10^6) in a gas with density 1 is a well known test case to validate study [2,3,15]. Initially the droplet (0.2 diameter) is centered on a domain 1x1. Periodic limit conditions are used. The velocity of the droplet is 1 and the gas is initially at rest. There is no surface tension, no diffusion and no volume force. Regarding the large inertia of the droplet, it should remain circular during its motion. We present in Fig 8 the shape of the droplet after being advected one period through the domain for different meshes.

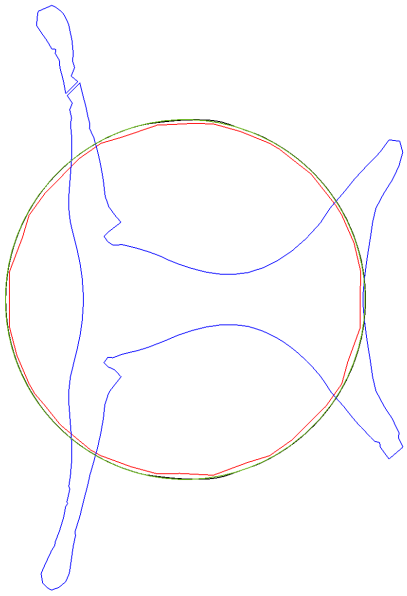

FIGURE 8: Convection of a 2D droplet of high density $10^6 kg.m^{-1}$; in black the analytic solution; in red 32x32 grid with conservative method; in green 128x128 grid with conservative method; in blue 128x128 grid with the non conservative method

We observe (Fig. 8) that the analytic solution(in black), is very close to the green curve corresponding to the convection of the droplet with the new scheme on a 128x128 grid. In red, the result for the new scheme on a 32x32 grid. The most deformed droplet(in blue) corresponds to the convection on a 128x128 grid using the non conservative(WENO convection scheme). It is clear that the new method shows a better conservation of the circular shape of the droplet. Moreover, the new conservative scheme converges very well to the analytic solution.

Dam-break

The geometry of the test case is presented in Fig. 9 and simulation data given in Table 1. This geometry corresponds to the experimental configuration of Martin and Moyce [25]. In this case, body and convective force have a strong influence on the results. Many authors [2, 3, 26] present this test case to show the validity of the discretization convection term.

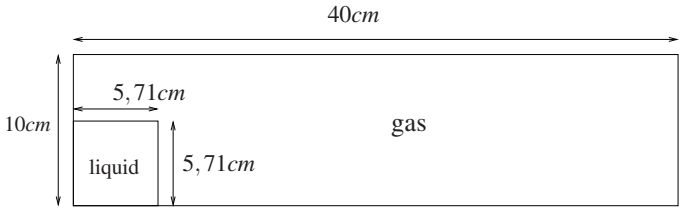

FIGURE 9: Dam-break's configuration

Physical parameters	Dam break
$\rho_1(kg/m^3)$	1000
$\rho_2(kg/m^3)$	1.226
$\mu_1(Pa.s^{-1})$	$1.137*10^{-3}$
$\mu_2(Pa.s^{-1})$	$1.78*10^{-5}$
$g(m.s^{-2})$	9.81
$\sigma(N.m^{-1})$	0.0728

TABLE 1: Dam-break data

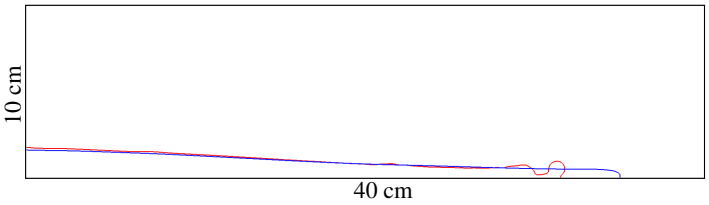

FIGURE 10: liquid/interface at time T=3
in red the shape interface using the usual convection term
in blue the shape interface using the new convection term

In Fig. 10, we observe that momentum errors leads in the non conservative form of Navier Stokes equation to non physical shape of the interface, whereas the new method gives a realistic shape.

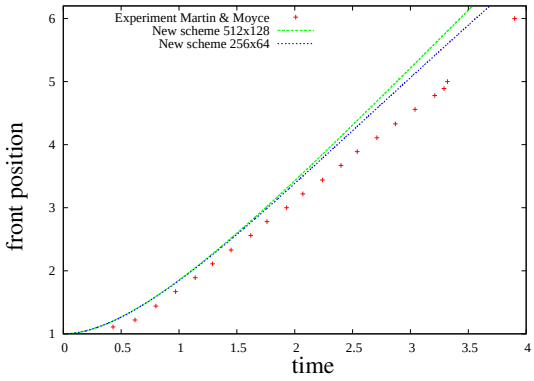

FIGURE 11: Front position

The nondimensional front position is drawn as a function of nondimensionnal time in Fig. 11. Good agreement is observed although a small shift remains on the beginning of the front displacement (0.1 in non dimensional time).

2D liquid sheet

We perform a simulation of a 2d liquid/gas shear layer. The density ratio is 815:1 (typically air/water) . Details of the configuration are shown in Fig 12 and simulation data in Table 2. Liquid is injected at 35 m/s, and gas at 0.6m/s. This configuration corresponds to an experiment that is carried out in the Laboratory of Geophysical and Industrial Flows(LEGI) in Grenoble.

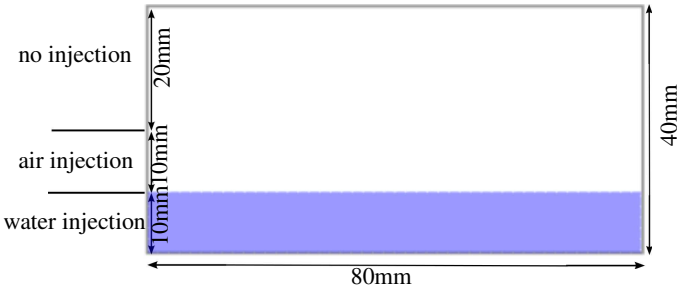

FIGURE 12: geometry 2d liquid sheet

Physical parameters	2d sheet
$\rho_1(kg/m^3)$	1000
$\rho_2(kg/m^3)$	1.226
$\mu_1(Pa.s^{-1})$	$1.137*10^{-3}$
$\mu_2(Pa.s^{-1})$	$1.78*10^{-5}$
$\sigma(N.m^{-1})$	0.0728

TABLE 2: Physical parameters

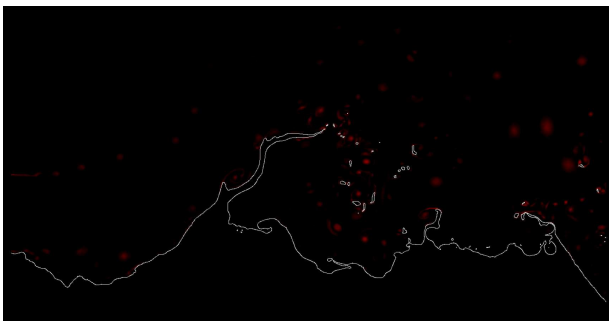

FIGURE 13: 2D liquid sheet simulation (2048x1024)

Without the new scheme, the simulation was unstable and led to nonphysical velocity overshoot. With the new implemented scheme, our code remains stable as we observe in Fig. 13.

First observations, gives results accordingly well with the macroscopic behaviour of the flow. Quantitative comparisons with experimental data will be made in the coming months .

Conclusion

We have implemented Rudman's method for calculation of the convective term, improving velocity interpolation onto the sub-grid. Simple computational tests show clear improvement over previous method formulations. More sophisticated, physical flow simulations which we've performed so far, yield encouraging results, although even more comparative work is planned. Additionally, we continue the work by tacking the problem of large computational costs of using Rudman-type sub-grids, results of which are to be published later.

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