

Proceedings of the 12th International Conference on
Computational Fluid Dynamics in the Oil & Gas,
Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



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Editors:

Jan Erik Olsen and Stein Tore Johansen

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen



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CONTENTS

PRAGMATIC MODELLING	9
On pragmatism in industrial modeling. Part III: Application to operational drilling	11
CFD modeling of dynamic emulsion stability	23
Modelling of interaction between turbines and terrain wakes using pragmatic approach	29
FLUIDIZED BED	37
Simulation of chemical looping combustion process in a double looping fluidized bed reactor with cu-based oxygen carriers.....	39
Extremely fast simulations of heat transfer in fluidized beds.....	47
Mass transfer phenomena in fluidized beds with horizontally immersed membranes	53
A Two-Fluid model study of hydrogen production via water gas shift in fluidized bed membrane reactors	63
Effect of lift force on dense gas-fluidized beds of non-spherical particles	71
Experimental and numerical investigation of a bubbling dense gas-solid fluidized bed	81
Direct numerical simulation of the effective drag in gas-liquid-solid systems	89
A Lagrangian-Eulerian hybrid model for the simulation of direct reduction of iron ore in fluidized beds.....	97
High temperature fluidization - influence of inter-particle forces on fluidization behavior	107
Verification of filtered two fluid models for reactive gas-solid flows	115
BIOMECHANICS.....	123
A computational framework involving CFD and data mining tools for analyzing disease in carotid artery	125
Investigating the numerical parameter space for a stenosed patient-specific internal carotid artery model.....	133
Velocity profiles in a 2D model of the left ventricular outflow tract, pathological case study using PIV and CFD modeling.....	139
Oscillatory flow and mass transport in a coronary artery.....	147
Patient specific numerical simulation of flow in the human upper airways for assessing the effect of nasal surgery.....	153
CFD simulations of turbulent flow in the human upper airways	163
OIL & GAS APPLICATIONS	169
Estimation of flow rates and parameters in two-phase stratified and slug flow by an ensemble Kalman filter	171
Direct numerical simulation of proppant transport in a narrow channel for hydraulic fracturing application	179
Multiphase direct numerical simulations (DNS) of oil-water flows through homogeneous porous rocks	185
CFD erosion modelling of blind tees	191
Shape factors inclusion in a one-dimensional, transient two-fluid model for stratified and slug flow simulations in pipes	201
Gas-liquid two-phase flow behavior in terrain-inclined pipelines for wet natural gas transportation	207

NUMERICS, METHODS & CODE DEVELOPMENT	213
Innovative computing for industrially-relevant multiphase flows	215
Development of GPU parallel multiphase flow solver for turbulent slurry flows in cyclone.....	223
Immersed boundary method for the compressible Navier–Stokes equations using high order summation-by-parts difference operators	233
Direct numerical simulation of coupled heat and mass transfer in fluid-solid systems	243
A simulation concept for generic simulation of multi-material flow, using staggered Cartesian grids.....	253
A cartesian cut-cell method, based on formal volume averaging of mass, momentum equations.....	265
SOFT: a framework for semantic interoperability of scientific software	273
POPULATION BALANCE	279
Combined multifluid-population balance method for polydisperse multiphase flows	281
A multifluid-PBE model for a slurry bubble column with bubble size dependent velocity, weight fractions and temperature.....	285
CFD simulation of the droplet size distribution of liquid-liquid emulsions in stirred tank reactors	295
Towards a CFD model for boiling flows: validation of QMOM predictions with TOPFLOW experiments	301
Numerical simulations of turbulent liquid-liquid dispersions with quadrature-based moment methods.....	309
Simulation of dispersion of immiscible fluids in a turbulent couette flow	317
Simulation of gas-liquid flows in separators - a Lagrangian approach.....	325
CFD modelling to predict mass transfer in pulsed sieve plate extraction columns	335
BREAKUP & COALESCENCE	343
Experimental and numerical study on single droplet breakage in turbulent flow	345
Improved collision modelling for liquid metal droplets in a copper slag cleaning process	355
Modelling of bubble dynamics in slag during its hot stage engineering.....	365
Controlled coalescence with local front reconstruction method	373
BUBBLY FLOWS	381
Modelling of fluid dynamics, mass transfer and chemical reaction in bubbly flows	383
Stochastic DSMC model for large scale dense bubbly flows.....	391
On the surfacing mechanism of bubble plumes from subsea gas release.....	399
Bubble generated turbulence in two fluid simulation of bubbly flow	405
HEAT TRANSFER	413
CFD-simulation of boiling in a heated pipe including flow pattern transitions using a multi-field concept	415
The pear-shaped fate of an ice melting front	423
Flow dynamics studies for flexible operation of continuous casters (flow flex cc).....	431
An Euler-Euler model for gas-liquid flows in a coil wound heat exchanger.....	441
NON-NEWTONIAN FLOWS.....	449
Viscoelastic flow simulations in disordered porous media	451
Tire rubber extrudate swell simulation and verification with experiments	459
Front-tracking simulations of bubbles rising in non-Newtonian fluids.....	469
A 2D sediment bed morphodynamics model for turbulent, non-Newtonian, particle-loaded flows.....	479

METALLURGICAL APPLICATIONS.....	491
Experimental modelling of metallurgical processes	493
State of the art: macroscopic modelling approaches for the description of multiphysics phenomena within the electroslag remelting process	499
LES-VOF simulation of turbulent interfacial flow in the continuous casting mold	507
CFD-DEM modelling of blast furnace tapping	515
Multiphase flow modelling of furnace tapholes	521
Numerical predictions of the shape and size of the raceway zone in a blast furnace.....	531
Modelling and measurements in the aluminium industry - Where are the obstacles?	541
Modelling of chemical reactions in metallurgical processes.....	549
Using CFD analysis to optimise top submerged lance furnace geometries	555
Numerical analysis of the temperature distribution in a martensitic stainless steel strip during hardening.....	565
Validation of a rapid slag viscosity measurement by CFD.....	575
Solidification modeling with user defined function in ANSYS Fluent.....	583
Cleaning of polycyclic aromatic hydrocarbons (PAH) obtained from ferroalloys plant.....	587
Granular flow described by fictitious fluids: a suitable methodology for process simulations	593
A multiscale numerical approach of the dripping slag in the coke bed zone of a pilot scale Si-Mn furnace.....	599
INDUSTRIAL APPLICATIONS	605
Use of CFD as a design tool for a phosphoric acid plant cooling pond	607
Numerical evaluation of co-firing solid recovered fuel with petroleum coke in a cement rotary kiln: Influence of fuel moisture	613
Experimental and CFD investigation of fractal distributor on a novel plate and frame ion-exchanger	621
COMBUSTION	631
CFD modeling of a commercial-size circle-draft biomass gasifier.....	633
Numerical study of coal particle gasification up to Reynolds numbers of 1000.....	641
Modelling combustion of pulverized coal and alternative carbon materials in the blast furnace raceway	647
Combustion chamber scaling for energy recovery from furnace process gas: waste to value	657
PACKED BED.....	665
Comparison of particle-resolved direct numerical simulation and 1D modelling of catalytic reactions in a packed bed	667
Numerical investigation of particle types influence on packed bed adsorber behaviour	675
CFD based study of dense medium drum separation processes	683
A multi-domain 1D particle-reactor model for packed bed reactor applications.....	689
SPECIES TRANSPORT & INTERFACES	699
Modelling and numerical simulation of surface active species transport - reaction in welding processes	701
Multiscale approach to fully resolved boundary layers using adaptive grids.....	709
Implementation, demonstration and validation of a user-defined wall function for direct precipitation fouling in Ansys Fluent.....	717

FREE SURFACE FLOW & WAVES	727
Unresolved CFD-DEM in environmental engineering: submarine slope stability and other applications.....	729
Influence of the upstream cylinder and wave breaking point on the breaking wave forces on the downstream cylinder	735
Recent developments for the computation of the necessary submergence of pump intakes with free surfaces	743
Parallel multiphase flow software for solving the Navier-Stokes equations	752
PARTICLE METHODS	759
A numerical approach to model aggregate restructuring in shear flow using DEM in Lattice-Boltzmann simulations	761
Adaptive coarse-graining for large-scale DEM simulations.....	773
Novel efficient hybrid-DEM collision integration scheme.....	779
Implementing the kinetic theory of granular flows into the Lagrangian dense discrete phase model.....	785
Importance of the different fluid forces on particle dispersion in fluid phase resonance mixers	791
Large scale modelling of bubble formation and growth in a supersaturated liquid.....	798
FUNDAMENTAL FLUID DYNAMICS	807
Flow past a yawed cylinder of finite length using a fictitious domain method	809
A numerical evaluation of the effect of the electro-magnetic force on bubble flow in aluminium smelting process.....	819
A DNS study of droplet spreading and penetration on a porous medium.....	825
From linear to nonlinear: Transient growth in confined magnetohydrodynamic flows.....	831

PARALLEL MULTIPHASE FLOW SOFTWARE FOR SOLVING THE NAVIER-STOKES EQUATIONS

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ABSTRACT

A code based on finite element method was built and applied on the variable density incompressible Navier-Stokes equations for accurately simulating immiscible two phase flows. The algorithm simulates the interface between the two liquid phases with high accuracy; it utilizes both the level-set method with a third order strong stability property Runge-Kutta (SSPRK) time integrator and a second-order projection method for the momentum equation. The solver developed is based on deal.II, an open source framework code. Numerical assessments on the transport and momentum equations are presented to verify the code accuracy. Nonconforming manufactured solutions are shown to produce the expected convergence rate of the used numerical schemes. Simulation of classical Rayleigh-Taylor instability was carried out and shown to match those in the published work.

Keywords: CFD, projection methods, level set, LES .

NOMENCLATURE

Greek Symbols

ρ Density
 μ Dynamic viscosity
 ν Kinematic viscosity
 ϕ Level set

Latin Symbols

\mathbf{u} Velocity
 p Pressure
 t Time
 V An appropriate space with proper boundary conditions

All symbols are non-dimensional.

METHOD

The *variable density incompressible Navier-Stokes equations* are defined as follows:

$$\begin{aligned} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) &= 0, & \text{in } \Omega \times (0, T], & (1) \\ \rho[\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}] - 2\mu \operatorname{div}(\nabla^s \mathbf{u}) \\ &+ \nabla p = \rho \mathbf{f}, & \text{in } \Omega \times (0, T], & (2) \\ \operatorname{div}(\mathbf{u}) &= 0, & \text{in } \Omega \times (0, T], & (3) \end{aligned}$$

where $\Omega \subset \mathbb{R}^{2,3}$ and $\partial\Omega$ is the boundary, $\rho(\mathbf{x}, t)$ is the density at $(\mathbf{x}, t) \in \Omega \times [0, T]$, $\mathbf{u}(\mathbf{x}, t)$ is the velocity vector field, μ

is the dynamic viscosity, and $p(\mathbf{x}, t)$ is the pressure. **Bold** variables are vector valued. Equation (1) is referred to as the transport equation, (2) is the momentum equation and (3) is the incompressibility constraint.

Transport equation weak formulation

The weak formulation for the transport equation is: Find $\rho(\mathbf{x}, t) \in V(\Omega)$ such that:

$$\int_{\Omega} v \left(\frac{\partial}{\partial t} \rho + \mathbf{u} \cdot \nabla \rho \right) dx = 0, \quad \forall v \in V(\Omega), \quad (4)$$

$$\rho(\mathbf{x}, t) = \rho_{\partial\Omega}, \quad \text{in } \partial\Omega_-, \quad (5)$$

$$\rho(\mathbf{x}, 0) = \rho_0, \quad \rho_0 > 0, \quad (6)$$

where V is an appropriate space for the transport equation with appropriate boundary conditions.

To accurately capture the density field ρ , we choose the 3rd order time integration method "Strong Stability Preserving Runge-Kutta" with three steps (abbreviated as SSPRK(3,3)) as described by (Gottlieb, 2005). The SSPRK(3,3) steps are:

$$y^{(1)} = y^k + \Delta t f(t^k, y^k), \quad (7)$$

$$y^{(2)} = \frac{1}{4} \left(3y^k + y^{(1)} + \Delta t f(t^{k+1}, y^{(1)}) \right), \quad (8)$$

$$y^{k+1} = \frac{1}{3} \left(y^k + 2y^{(2)} + 2\Delta t f(t^{k+\frac{1}{2}}, y^{(2)}) \right). \quad (9)$$

The strong stability preserving property is $\|y^{k+1}\| \leq \|y^k\|$. This makes it attractive in the transport equation case. The SSP property comes from the maximum principle preserving property of the Forward Euler method.

The Level Set Model

The fluid mixture we are interested in modeling with the transport equations has two phases: oil, and water. Each has a different density value ρ . Since they do not mix, it is important that each phase must be distinct when modeled and the volume of each phase in Ω be conserved. Otherwise, the incompressibility condition $\operatorname{div}(\mathbf{u}) = 0$ will be violated. As a consequence, when solving the approximation of the transport equation, one needs to make sure the interface between two phases is tracked with enough accuracy. There are many methods to achieve such accuracy, which can be divided into two classes. In the first one, the interface is implicitly tracked by a function defined on the whole domain. Such methods include the level set method, and volume of fluid method. In

the second class, the interface is explicitly tracked with front-tracking methods. We will use the level set method between two phases.

The level set method was first introduced by (Osher and Sethian, 1988) to evolve the interface with speeds depending on the curvature of a given velocity field. The interface is tracked with a function $\Phi(\mathbf{x})$ to represent the $n - 1$ dimensional interface $\Gamma \subset \Omega$ separating Ω into two phases Ω_1 and Ω_2 . There are many ways to define Γ but we are going to use the tanh function with the interface at $\Phi(\mathbf{x}) = 0.5$. The tanh function is defined as:

$$\Phi(\mathbf{x}) := \frac{1}{2} \left(1 + \tanh \left(\frac{d(\mathbf{x})}{\gamma} \right) \right), \quad (10)$$

where d is a distance from the interface function and γ controls how steep the interface is. To describe the evolution of an interface that is transported along with a fluid, we can use Φ instead of ρ in (4):

$$\int_{\Omega} v \left(\frac{\partial}{\partial t} \Phi + \mathbf{u} \cdot \nabla \Phi \right) dx = 0, \quad \forall v \in V(\Omega), \quad (11)$$

$$\Phi(\mathbf{x}, t) = \Phi_{\partial\Omega}, \quad \text{in } \partial\Omega, \quad (12)$$

$$\Phi(\mathbf{x}, 0) = \Phi_0, \quad \Phi_0 > 0. \quad (13)$$

This essentially transports the Φ function instead of the density ρ . To reconstruct ρ from Φ , we use the function $H(\Phi)$:

$$H(\Phi(\mathbf{x})) = \begin{cases} \rho_1, & \Phi(\mathbf{x}) < 0.5, \\ \rho_2, & \Phi(\mathbf{x}) \geq 0.5, \end{cases} \quad (14)$$

where ρ_1, ρ_2 are the densities of the fluids in Ω_1 and Ω_2 respectively ($\rho_1 < \rho_2$). $H(\Phi)$ will produce density fields that have discontinuous transitions between phases, which are undesirable when dealing with PDEs that expect smooth enough functions. There are many functions that create smoother transitions such as:

$$H(\Phi(\mathbf{x})) = \frac{\rho_2 - \rho_1}{2} + \frac{\rho_2 + \rho_1}{2} \tanh \left(\frac{\Phi(\mathbf{x})}{\gamma} \right), \quad (15)$$

where α controls how steep the transition between the two densities is. The advantage of this reconstruction is that it produces the closest density field close to (14) with some retained smoothness. Another candidate H function is:

$$H(\Phi(\mathbf{x})) = (\rho_2 - \rho_1)\Phi(\mathbf{x}) + \rho_1, \quad (16)$$

which is a linear scaling of the level set to the densities in Ω . It is robust but translates the undesirable oscillations that extends beyond $\Phi(\mathbf{x}) > 1$ or $\Phi(\mathbf{x}) < 0$. This issue may be solved by clipping the reconstruction at a certain radius α around 0.5 ($0 \leq \alpha \leq 0.5$):

$$H(\Phi(\mathbf{x})) = \begin{cases} \rho_1, & \Phi(\mathbf{x}) \leq 0.5 - \alpha, \\ \rho_2, & \Phi(\mathbf{x}) \geq 0.5 + \alpha, \\ (\Phi(\mathbf{x}) - (0.5 - \alpha)) \frac{\rho_2 - \rho_1}{2\alpha} + \rho_1, & \text{otherwise.} \end{cases} \quad (17)$$

This reconstruction introduces relatively sharp changes in the density gradient and affects the stability of simulation runs. Finally, the last reconstruction we are going to introduce has the property of having slope zero at the $0.5 \pm \alpha$ points and

being a transition polynomial of third degree ($0 \leq \alpha \leq 0.5$):

$$H(\Phi(\mathbf{x})) = \begin{cases} \rho_1, & \text{if } \Phi(\mathbf{x}) \leq 0.5 - \alpha, \\ \rho_2, & \text{if } \Phi(\mathbf{x}) \geq 0.5 + \alpha, \\ \frac{(4\alpha - 2\Phi(\mathbf{x}) + 1)(2\alpha + 2\Phi(\mathbf{x}) - 1)^2}{32\alpha^3}, & (18) \\ (\rho_2 - \rho_1) + \rho_1, & \text{otherwise.} \end{cases}$$

Compared to the clipped reconstruction (17), the above has smooth gradient transitions and was found to have a stabilizing effect when used in the simulations below. This transition is comparable to the Heaviside function (14) in (Sussman and Fatemi, 1999) but has the advantage of being polynomial in nature.

Entropy-Viscosity

The Entropy-Viscosity is (at least) a second-order stabilization term introduced by (Guermont *et al.*, 2011a) and (Guermont and Pasquetti, 2011). It has the advantage of having a less diffusive effect on the solution and thus allowing the construction of stabilized second order numerical schemes. Using the transport equation weak form:

$$\int_{\Omega} v_h \left(\frac{\partial \rho_h}{\partial t} + \mathbf{u}_h \cdot \nabla \rho_h - \text{div} (v \nabla \rho) \right) dx = 0, \quad \forall v_h \in V_h(\Omega), \quad (19)$$

and v is calculated for each cell separately as follows. Define $E(\phi)$ as convex functions that satisfies the differential inequality:

$$\partial_t E(\phi) + \mathbf{u} \cdot \nabla E(\phi) < 0, \quad (20)$$

where ϕ is the level set function mentioned in section and $E(\phi)$ is the entropy function. For examples, one can use:

$$E(\phi) = \begin{cases} \frac{1}{p} (\phi - \frac{1}{2})^p \text{ where } p = 1, 2, \dots, \\ -\log(|\phi(1 - \phi)| + 10^{-14}). \end{cases} \quad (21)$$

In the fully discretized setting, use ϕ^n, ϕ^{n-1} and compute the following values for each quadrature points q_k, q_f in cell k and face f :

$$R^{n+1/2}(q_k) = \frac{\Pi_{\mathcal{T}_h} E(\phi^n) - \Pi_{\mathcal{T}_h} E(\phi^{n-1})}{\Delta t} + \quad (22)$$

$$\frac{1}{2} (\mathbf{u}^n \cdot \nabla \Pi_{\mathcal{T}_h} E(\phi^n) + \mathbf{u}^{n-1} \cdot \nabla \Pi_{\mathcal{T}_h} E(\phi^{n-1}))$$

$$J^n(q_f) = \mathbf{u}^n \cdot \mathbf{n} [\partial_n \Pi_{\mathcal{T}_h} E(\phi^n)]|_f. \quad (23)$$

Then get the maximum $R_k^{n+1/2} = \max_{q_k \in k} |R^{n+1/2}(q_k)|$ and $J_k^n = \max_{f \in k} \max_{q_f \in f} |J^n(q_f)|$. Note that we are using the Crank-Nicolson scheme to calculate R giving us a second order accurate value for R . The viscosity ν_k will then be:

$$\nu_k = \min \left(C_m h |\mathbf{u}|_{L^\infty}, C_e h^2 \frac{R^{n+1/2} + J_k^n}{\|E(\phi^n) - \overline{E(\phi^n)}\|_{L^\infty(\Omega)}} \right), \quad (24)$$

where $\overline{E(\phi)} = \frac{1}{|\Omega|} \int_{\Omega} E(\phi)$ and $\|E(\phi^n) - \overline{E(\phi^n)}\|_{L^\infty(\Omega)}$ is a normalization factor. The amount of artificial viscosity is proportional to the entropy production but bounded from above by the linear artificial viscosity. If the solution is smooth and entropy production is very small, little or no artificial viscosity is added. Some disadvantages remain such as coefficients C_e, C_m to tune and the ambiguity of h .

Compression for the Level Set

For the level set method to work, the curved shape of the level set function over the boundary must be maintained to prevent adding non-physical effects to the model. The stabilization viscosity diffuses the level set interface as the simulation marches in time. Consequently, with the presence of the diffusion term, we add the compression (or anti-diffusion) term $\text{div}\left(C_K \frac{\mathbf{v}}{h} (1 - \phi_h) \phi_h \frac{\nabla \phi_h}{|\nabla \phi_h|}\right)$ to the transport equation (4):

$$\int_{\Omega \times [0, T]} \frac{\partial}{\partial t} \phi_h + \mathbf{u} \cdot \nabla \phi_h - \text{div}\left(\mathbf{v} \nabla \phi_h - C_K \frac{\mathbf{v}}{h} \phi_h (1 - \phi_h) \frac{\nabla \phi_h}{|\nabla \phi_h|}\right) dxdt = 0, \quad (25)$$

where the level set $\phi \in [0, 1]$ and defined at $\phi = 0.5$. This compression term eliminates the need for a separate reinitialization step. In practice, it has been observed that the compression term in (25) induces “fingering” effect in simulations. It is the result of perturbations in the initial level set that the compression term gradually propagates resulting in the level set extending like fingers. To mitigate that, a smoothed out ϕ_h^* is used in the normal of the compression front $\frac{\nabla \phi_h}{|\nabla \phi_h|}$ where ϕ_h^* is the solution to $\phi_h^* - h^2 \Delta \phi_h^* = \phi$, $\nabla \phi_h^* \cdot \mathbf{n} = 0$ on $\partial\Omega$. We will denote S as the operator that maps ϕ to the corresponding ϕ^* (i.e. $S\phi_h = \phi_h^*$).

Let us detail the algorithm for solving (25):

1. Initialize the level set by normalizing the initial density scalar field.

$$\phi_h^0 = \frac{\rho_h^0 - \rho_{\min}}{\rho_{\max} - \rho_{\min}},$$

2. For each of the SSPRK(3,3) steps below, we need to solve the following:

$$L^n(\mathbf{u}_h, \phi_h, \phi_h^*) = -\mathbf{u}_h \cdot \nabla \phi_h - \text{div}\left(\mathbf{v} \nabla \phi_h - C_K \frac{\mathbf{v}}{h} \phi_h (1 - \phi_h) \frac{\nabla \phi_h^*}{|\nabla \phi_h^*|}\right), \quad (26)$$

when solved for each of the three steps below, the values are

$$\phi_h^{(1)} = \phi_h^n + \Delta t L^n(\mathbf{u}_h^n, \phi_h^n, S\phi_h^n), \quad (27)$$

$$\phi_h^{(2)} = \frac{1}{4} \left(3\phi_h^n + \phi_h^{(1)} + \Delta t L^{n+1}(2\mathbf{u}_h^n - \mathbf{u}_h^{n-1}, \phi_h^{(1)}, S\phi_h^{(1)}) \right), \quad (28)$$

$$\phi_h^{n+1} = \frac{1}{3} \left(\phi_h^n + 2\phi_h^{(2)} + 2\Delta t L^{n+\frac{1}{2}} \left(\frac{1}{2} [3\mathbf{u}_h^n - \mathbf{u}_h^{n-1}], \phi_h^{(2)}, S\phi_h^{(2)} \right) \right). \quad (29)$$

3. Lastly, we “denormalize” the level set with a reconstruction function such as:

$$\rho_h^{n+1} = H(\phi_h)(\rho_{\max} - \rho_{\min}) + \rho_{\min}. \quad (30)$$

It is worth mentioning that when the entropy-viscosity vanishes in well resolved regions of the solution, the compression stops working and the sharpness of the level set interface is lost. This may be remedied by using some “antivanish” viscosity $\mathbf{v}_{\text{antivanish}} = \mathbf{v} + \mathbf{v}_\epsilon$ where \mathbf{v}_ϵ is a small positive amount of viscosity that maintains the balance between diffusion and compression and, thus, maintains the slope of the level set.

Projection method for the momentum equation

Initialize the algorithm with $\rho^0 = \rho_0$, $\mathbf{u}^0 = \mathbf{u}_0$, $p^0 = p_0$, $\phi^0 = q^0 = 0$ then proceed as follows:

1. Setup intermediate variables:

$$\begin{aligned} \rho^* &= \rho^{n+1} + \frac{1}{6} \text{BDF}_2(\rho^{n+1}), \\ &\quad \text{where } \text{BDF}_2(\phi^{n+1}) = 3\phi^{n+1} - 4\phi^n + \phi^{n-1}, \\ p^* &= p^n + \frac{1}{3} \left(4\delta\psi^n - \delta\psi^{n-1} \right), \\ \mathbf{u}^* &= 2\mathbf{u}^n - \mathbf{u}^{n-1}. \end{aligned}$$

2. Prediction:

$$\begin{aligned} &\frac{3\rho^* \mathbf{u}^{n+1} - 4\rho^{n+1} \mathbf{u}^n + \rho^{n+1} \mathbf{u}^{n-1}}{2\Delta t} - \rho^{n+1} \mathbf{u}^* \cdot \nabla \mathbf{u}^{n+1} \\ &+ \frac{1}{2} \text{div}(\rho^{k+1} \mathbf{u}^*) \mathbf{u}^{n+1} - \mu \Delta \mathbf{u}^{n+1} + \nabla p^* = \rho^{n+1} \mathbf{f}^{n+1}, \\ &\quad \mathbf{u}^{n+1}|_{\partial\Omega} = 0, \end{aligned}$$

3. Projection:

$$\begin{aligned} \Delta \delta\psi^{n+1} &= \frac{3\rho_{\min}}{2\Delta t} \text{div}(\mathbf{u}^{k+1}), \quad \partial_n \delta\psi^{n+1} = 0, \\ \delta q^{n+1} &= -\text{div}(\mathbf{u}^{n+1}), \end{aligned}$$

4. Pressure correction: $p^{n+1} = \psi^{n+1} - \mu q^{n+1}$.

where BDF stands for Backwards Difference Formula.

This variable density projection method is shown to have an error of $O(\Delta t^2)$ in the L^2 norm. The stability proof can be found in (Guermont and Salgado, 2011, §5.4)

Large Eddy Simulation

The Large Eddy Simulation (LES) is based on the – at least – 2nd order entropy-viscosity method (Guermont *et al.*, 2011b). The concept behind LES is separating the flow into large – or resolved – and small – or subgrid – scales. For a good overview of LES, see (John, 2004).

When dealing with the Navier-Stokes equations, LES is added as a cell-wise viscosity $\mathbf{v}_K \geq 0$ to the term $-2\mathbf{v} \text{div}(\nabla^s \mathbf{u})$. The result is a viscosity $\mathbf{v} + \mathbf{v}_K$. The classical Smagorinsky model ((Smagorinsky, 1963)) uses:

$$\mathbf{v}_K := C_s \delta_K^2 \|\nabla^s \mathbf{u}\|,$$

where C_s is the Smagorinsky constant and δ_K is the width of the filter (which is proportional to h_K). (Guermont *et al.*, 2011c) proposed the following Entropy-Viscosity approach:

$$\mathbf{v}_K := \min \left(C_m h_K |\mathbf{u}|, C_e h_K^2 \frac{|D_h(\mathbf{x}, t)|}{\|\mathbf{u}_h^2\|_{L^\infty(\Omega)}} \right),$$

where

$$\begin{aligned} D_h(\mathbf{x}, t) &:= \\ \partial_t \left(\frac{1}{2} \mathbf{u}_h^2 \right) + \text{div} \left(\left(\frac{1}{2} \mathbf{u}_h^2 + p_h \right) \mathbf{u}_h \right) - Re^{-1} \Delta \left(\frac{1}{2} \mathbf{u}_h^2 \right) \\ &\quad + Re^{-1} (\nabla \mathbf{u}_h)^2 - \mathbf{f} \cdot \mathbf{u}_h \end{aligned} \quad (31)$$

where h_K is the mesh size locally, $\|\mathbf{u}_h^2\|_{L^\infty(\Omega)}$ is a normalizing term, and C_m, C_e are appropriate constants. The first term $C_m h_K |\mathbf{u}|$ is the first order artificial viscosity. When the mesh is fine enough to simulate all the scales, $h_K^2 |D_h(\mathbf{x}, t)|$ is much smaller than the first-order artificial viscosity. This makes \mathbf{v}_K a consistent viscosity that vanishes when scales of all levels are resolved.

NUMERICAL RESULTS

We test the schemes discussed in the previous sections numerically and present them here.

Validation

Here, we will present the validation of the projection method with density $\rho(\mathbf{x}, t) = 1$. This is a constant density test performed on a variable density equation for validation purposes. Using $\Omega = (0, 1)^d$ domain with a uniform mesh and cell-wise $[\mathbb{Q}_2]^d$ continuous finite elements, we introduce the following simple linear polynomial manufactured solution for the momentum equation:

$$\mathbf{u}(\mathbf{x}, t) = (1+t) \begin{pmatrix} x+y \\ x-y \end{pmatrix}, \quad p(\mathbf{x}, t) = (1+t)xy, \quad (32)$$

$$\mathbf{u}(\mathbf{x}, t) = (1+t) \begin{pmatrix} 1+z \\ 1+x \\ 1+y \end{pmatrix}, \quad p(\mathbf{x}, t) = (1+t)xyz. \quad (33)$$

for $d = 2, 3$ respectively. We solve the equation (2) with $\mu = 1$ running until final time $T = 1$. The projection step is disabled, which means that the exact pressure is interpolated every time step. The boundary condition $\mathbf{u}|_{\partial\Omega} = \mathbf{u}(\mathbf{x}, t)|_{\partial\Omega}$ is enforced. The time step is changed to roughly achieve a Courant-Friedrichs-Lewy condition (CFL) of 0.25. As expected, table 1 shows that the error is machine epsilon which means that the algorithm reproduces the conforming manufactured solutions exactly.

	cells	\mathbf{u}_{dofs}	Δt	$\ e_{\mathbf{u}}\ _{L2}$	$\ e_{\mathbf{u}}\ _{H1}$	CFL_{max}
2D	16	162	8E-03	3E-13	1E-12	0.2621
	64	578	4E-03	1E-15	2E-14	0.2606
	256	2178	2E-03	1E-14	8E-14	0.2607
3D	8	375	3E-02	9E-16	1E-14	0.2601
	64	2187	1E-02	5E-15	3E-14	0.2614
	512	14739	7E-03	7E-15	7E-14	0.2613

Table 1: Error values for running conforming manufactured solutions in a unit cube. We get the expected value of machine epsilon.

Projection Scheme

Using $\Omega = (0, 1)^d$ domain with a uniform mesh and cell-wise $[\mathbb{Q}_2]^d/\mathbb{Q}_1$ Taylor-Hood continuous finite elements, we introduce the following simple linear polynomial manufactured solution for the momentum equation:

$$\mathbf{u}(\mathbf{x}, t) = (1+t) \begin{pmatrix} x+y \\ x-y \end{pmatrix}, \quad p(\mathbf{x}, t) = (1+t)xy, \quad (34)$$

$$\mathbf{u}(\mathbf{x}, t) = (1+t) \begin{pmatrix} 1+z \\ 1+x \\ 1+y \end{pmatrix}, \quad p(\mathbf{x}, t) = (1+t)xyz. \quad (35)$$

with $d = 2, 3$ respectively. We solve the equation (2) with $\mu = 1$ running until final time $T = 1$. The projection step is disabled, which means that the exact pressure is interpolated from the exact solution to the discrete space every time step. We enforce the following boundary condition $\mathbf{u}|_{\partial\Omega} = \mathbf{u}(\mathbf{x}, t)|_{\partial\Omega}$. The source term is modified to reflect the exact solutions. As expected, table 2 shows that the error is machine epsilon (~ 0), which means that the algorithm reproduces the conforming manufactured solutions exactly.

	cells	\mathbf{u}_{dofs}	Δt	$\ e_{\mathbf{u}}\ _{L2}$	$\ e_{\mathbf{u}}\ _{H1}$
2D	16	162	1E-02	8E-16	1E-14
	64	578	5E-03	6E-15	4E-14
	256	2178	3E-03	2E-14	1E-13
3D	8	375	2E-02	1E-15	1E-14
	64	2187	1E-02	3E-15	3E-14
	512	14739	5E-03	9E-15	8E-14

Table 2: Error values for running conforming manufactured solutions in a unit cube. We get a machine epsilon as expected.

Now, we validate the scheme by running a convergence rate test. We use the same 2D setup as before with the following nonconforming manufactured solutions:

$$\mathbf{u}(\mathbf{x}, t) = \begin{pmatrix} \cos(x) + \cos(y+t) \\ \sin(x) + \sin(y+t) \end{pmatrix}, \quad (36)$$

$$p(\mathbf{x}, t) = \cos(x+y+t).$$

We see in table 3 that we get the $O(\Delta t^2)$ in the L^2 norm as expected. The H^1 norms are a bit higher than the expected $O(\Delta t^{\frac{3}{2}})$.

\mathbf{u}_{dofs}	Δt	$\ e_{\mathbf{u}}\ _{L2}$	rate	$\ e_{\mathbf{u}}\ _{H1}$	rate
4802	2E-02	1.54E-04	-	1.04E-03	-
18818	1E-02	4.28E-05	1.85	3.11E-04	1.75
74498	5E-03	1.14E-05	1.9	9.01E-05	1.79
296450	2.5E-03	2.98E-06	1.94	2.57E-05	1.81

\mathbf{u}_{dofs}	Δt	$\ e_p\ _{L2}$	rate	$\ e_p\ _{H1}$	rate
4802	2E-02	1.37E-03	-	2.22E-02	-
18818	1E-02	4.10E-04	1.74	8.63E-03	1.36
74498	5E-03	1.18E-04	1.8	3.27E-03	1.4
296450	2.5E-03	3.31E-05	1.83	1.22E-03	1.42

Table 3: Convergence rate for the constant density projection method. The CFL_{max} is at 0.64.

Realistic Models

In this section, we will study the applications of variable density projection scheme on a more realistic model; the Rayleigh-Taylor instability test. We compare our results with the work of (Guermont *et al.*, 2011a). Specifically in the early times before turbulent behavior.

Rayleigh-Taylor Instability

We now apply the method to a more realistic problem. We use the Rayleigh-Taylor instability test that (Tryggvason, 1988) used. Two fluids are initially at rest in the 2D domain $(-d/2, d/2) \times (-2d, 2d)$ and the heavier fluid is on top. The transition of the phase-field variable ρ is as follows:

$$\rho(x, y, t = 0) = \frac{\rho_{\text{max}} + \rho_{\text{min}}}{2} + \frac{\rho_{\text{max}} - \rho_{\text{min}}}{2} \tanh\left(\frac{y + \mu(x)}{\alpha d}\right), \quad (37)$$

where $\alpha \approx 0.04$ and the initial interface is slightly perturbed as follows:

$$\mu(x) = 0.1 \cos(2\pi x/d). \quad (38)$$

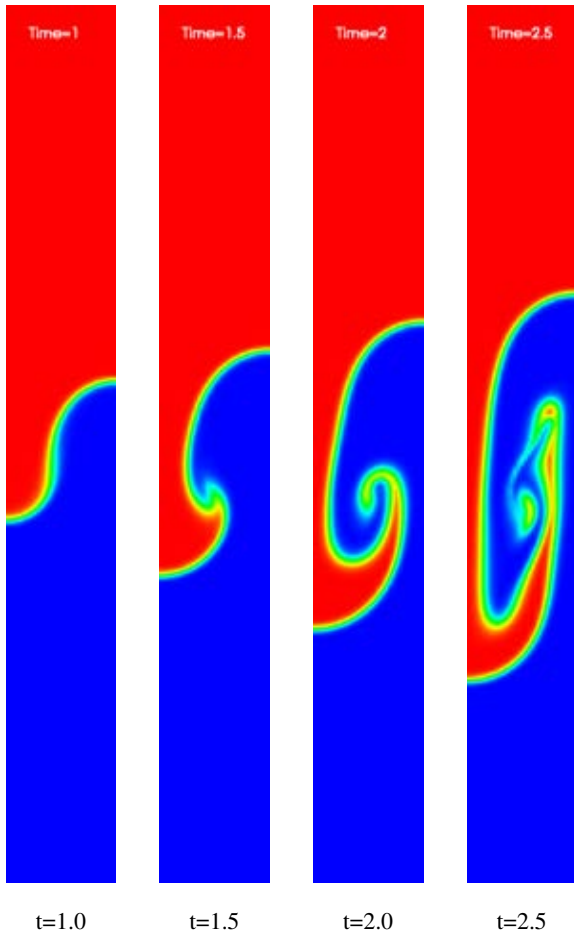


Figure 1: The Rayleigh-Taylor instability with density ratio of 3.

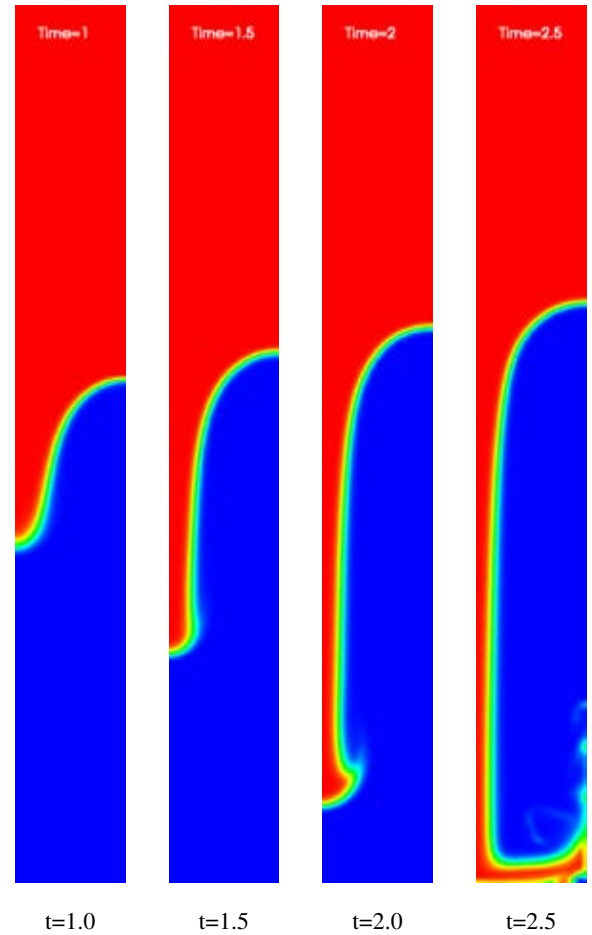


Figure 2: The Rayleigh-Taylor instability with density ratio of 100.

The time is also scaled using the Atwood number in Tryggvason as $t_{\text{Tryg}} = t\sqrt{A_t}$

$$A_t = \frac{\rho_0^{\max} - \rho_0^{\min}}{\rho_0^{\max} + \rho_0^{\min}}, \quad (39)$$

where $\rho_0^{\max} := \max_{\mathbf{x} \in \Omega} \rho_0(\mathbf{x})$ and $\rho_0^{\min} := \min_{\mathbf{x} \in \Omega} \rho_0(\mathbf{x})$. As the system progresses at $t > 0$, the heavy fluid will fall into the lighter fluid as a result of having the momentum equation gravity source term is $\rho \mathbf{g}$

We non-dimensionalize the equations as follows. We divide by: ρ_0^{\min} for the density ρ , d for length, and $d^{1/2}/|\mathbf{g}|^{1/2}$ for time. Consequently, $d^{1/2}|\mathbf{g}|^{1/2}$ is the velocity reference and the Reynolds number is $Re = \rho_0^{\min} d^{1/2} |\mathbf{g}|^{1/2} d / \mu$. We will restrict ourselves to the domain $(0, d/2) \times (-2d, 2d)$ because we assume that the symmetry of the initial setup continues as time progresses. The top and bottom parts have no-slip boundary conditions and the left and right sides have $\mathbf{u} \cdot \mathbf{n} = 0$, $(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{v} \nabla \mathbf{u} = 0$ boundary conditions (known as symmetry or free boundary conditions).

Remark. Note that we must integrate the pressure term by parts in the weak form for p to be in L^2 . In this experiment, we tested both integrating by parts and leaving the pressure term as is. This leads to different boundary conditions for each case: $(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{v} \nabla \mathbf{u} - \mathbf{I} p) = 0$, and $(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{v} \nabla \mathbf{u} = 0$ respectively. In this experiment, both were numerically stable and gave almost exactly the same results when compared to previous papers. By not integrating by parts, p will be in H^1 and we have to answer the question: Is the discrete Ladyzhenskaya-Babuska-Brezzi (LBB) condition sat-

isfied for the space pair H^1, H^1 ? In this experiment specifically, the numerical scheme seems to be stable but we cannot generalize to all possible cases without a rigorous proof.

As hyperbolic equations need stabilization, we do so with the nonlinear entropy viscosity (Guermond *et al.*, 2011a) using the entropy function $E(x) = -\log |\rho(1 - \rho) + 10^{-14}|$. In figure 1, the evolution of the density field of ratio 3 at times 1, 1.5, 2, and 2.5 in Tryggvason time scale $t_{\text{Tryg}} = t\sqrt{A_t}$ with $Re = 1000$. The same times are shown in figure 2 with density ratio of 100. There are 8484 Q_2 degrees of freedom for ρ with uniform mesh size of 2048 cells. The time stepping is variable and maintains a maximum CFL of 0.4.

Now, we want to conduct a more challenging test. Specifically, we will test with density ratio 100 to check the robustness of the scheme – see, for example, (Sussman *et al.*, 1994). As figure 2 shows, the simulation holds nicely. Also, when figure 1 is visually compared with the results in (Guermond *et al.*, 2015), they are visually almost identical.

CONCLUSION

The Navier-Stokes equations were solved using a code developed based on finite element method to accurately simulate immiscible two phase flows. A proprietary massively parallel Navier-Stokes solver code based on the open source software deal.II was successfully implemented to simulate the interface between the two liquid phases with good accuracy. The utilization of both the level set method with a third order strong stability property Runge-Kutta (SSPRK) time integrator and a second-order projection method for the momentum equation was deemed successful. Numerical val-

idations of the transport and momentum equations were presented; they confirmed the code accuracy. The convergence rate of the numerical schemes selected for modeling the non-conforming manufactured solutions were shown to be within expected convergence rate values. Classical Rayleigh-Taylor instability results were shown to be in good agreement with previously published work.

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