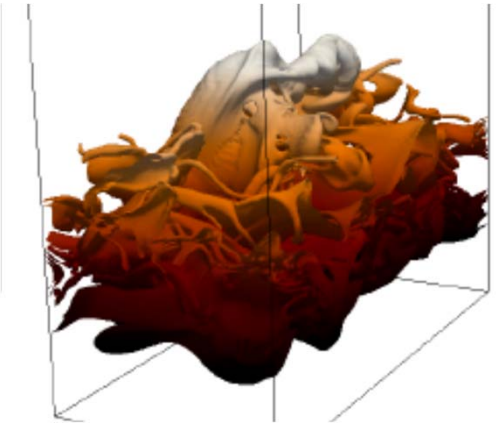

# TPLS 3.0 and Its Use of PETSc

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# Contributors

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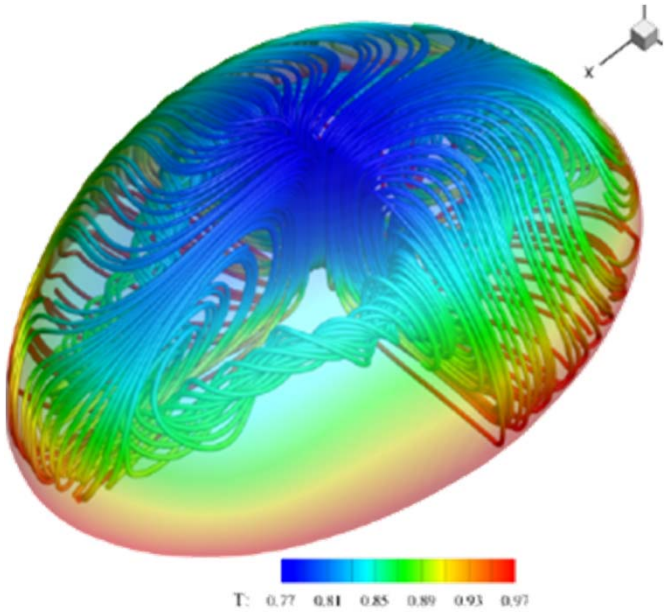



*Evaporating droplets*
*J. Fluid Mech. (2015)*

Funded by EPSRC through the eCSE programme

Portable, Extensible Toolkit for Scientific Computation,
PETSc: https://www.mcs.anl.gov/petsc

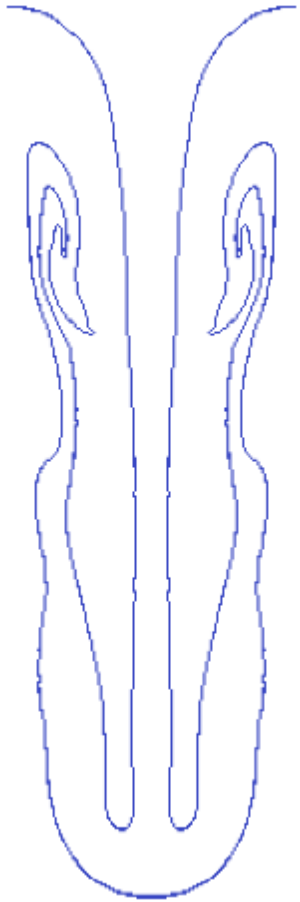
# History of Public Releases

| Year | Version | Notes |
|---|---|---|
| 2013 | 1.0 | Hand coded (generally J-SOR) solvers except for the (PETSc) pressure solver.<br>Serial I/O. |
| 2015 | 2.0 | Parallel I/O (NetCDF).<br>Introduced configuration files.<br>2D domain decomposition. |
| 2017 | 3.0 | 3D domain decomposition.<br>PETSc solvers available for the the momentum calculations.<br>Different densities for the component fluids. |

# TPLS 3.0

- Available from Sourceforge:
  https://sourceforge.net/projects/tpls/

under a BSD-style licence.



# TPLS 3.0 – Density Contrast Flows

- Rayleigh – Taylor instability
  - Two layers of liquid with the upper being the denser.
- Stably stratified, parallel, two-phase flows
  - Two layers of fluid with the upper being the less dense.
  - The fluids are flowing in the same direction.

- Characteristics of the simulations:
  - Flows involving many length and time scales.
  - Flows with sharp changes in interfacial topologies.
  - Transient three-dimensional simulations required over long periods of time

- Require scalable code run at very high resolutions

# TPLS 3.0: The Equations

Two-phase, incompressible, Navier–Stokes equations with interface capturing.

$$\rho(\phi)\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\frac{1}{Re}\nabla\cdot[\mu(\phi)(\nabla\mathbf{u}+\nabla\mathbf{u}^{\mathrm{T}})]+\mathbf{f}_{\mathrm{st}}(\phi)+\rho(\phi)\mathbf{g}$$

where $\nabla\cdot\mathbf{u}=\mathbf{0}$, $\mathbf{g}$ is gravity and $\phi$ is the interface capturing field.

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi=\mathbf{0},\quad \mathbf{f}_{\mathrm{st}}=\delta_{\epsilon}(\phi)\frac{\mathbf{1}}{\mathbf{We}}\hat{\mathbf{n}}\nabla\cdot\hat{\mathbf{n}},\quad \hat{\mathbf{n}}=\frac{\nabla\phi}{|\nabla\phi|}.$$

# TPLS 3.0: The Technicalities

Marker-and-cell discretisation: pressures, densities, viscosities and φ at cell centres, velocities at cell faces.

Finite volumes, with flux-conservative differencing for the momentum equation.

Momentum step: centred differences for the convective derivative, Crank-Nicholson treatment for diffusion, 3rd order Adams-Bashforth for the time evolution.

Projection method: momenta are updated first, followed by a correction step involving a pressure update, thereby enforcing incompressibility.

The levelset function, φ, is carried with the flow (3rd order WENO) but is corrected at each time step ('redistancing').

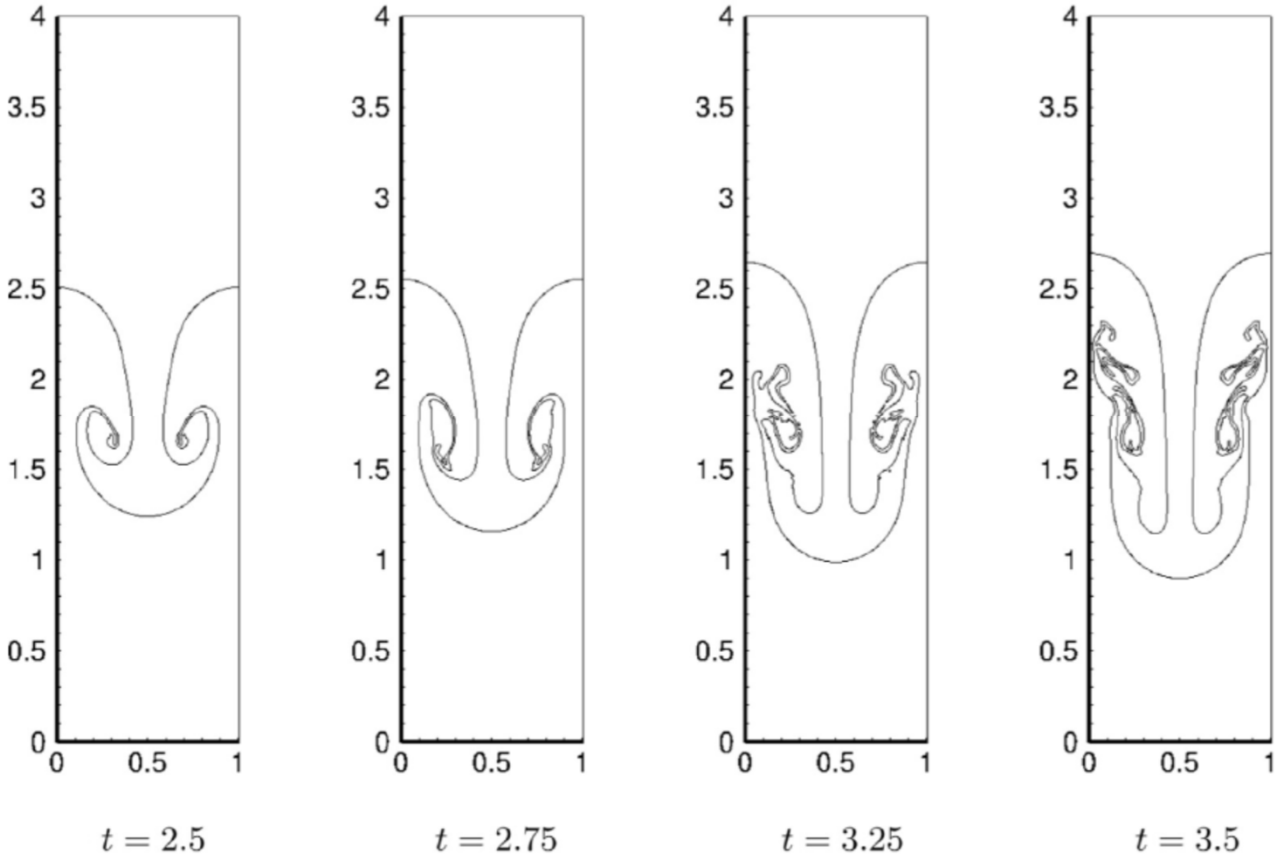
# TPLS 3.0: Rayleigh-Taylor Instability

- Heavy fluid sitting on top of a light fluid (gravity acting downwards)
- System starts from rest with a sinusoidal perturbation to the interface
- Heavy fluid accelerates downwards forming complicated interfacial structures due to rollup of vorticity
- System parametrised by the Atwood number

$$\mathrm{At} = (\rho_{\mathrm{heavy}} - \rho_{\mathrm{light}})/(\rho_{\mathrm{heavy}} + \rho_{\mathrm{light}}),$$

- In simulations, $\rho_{\mathrm{heavy}} = 3\rho_{\mathrm{light}}$

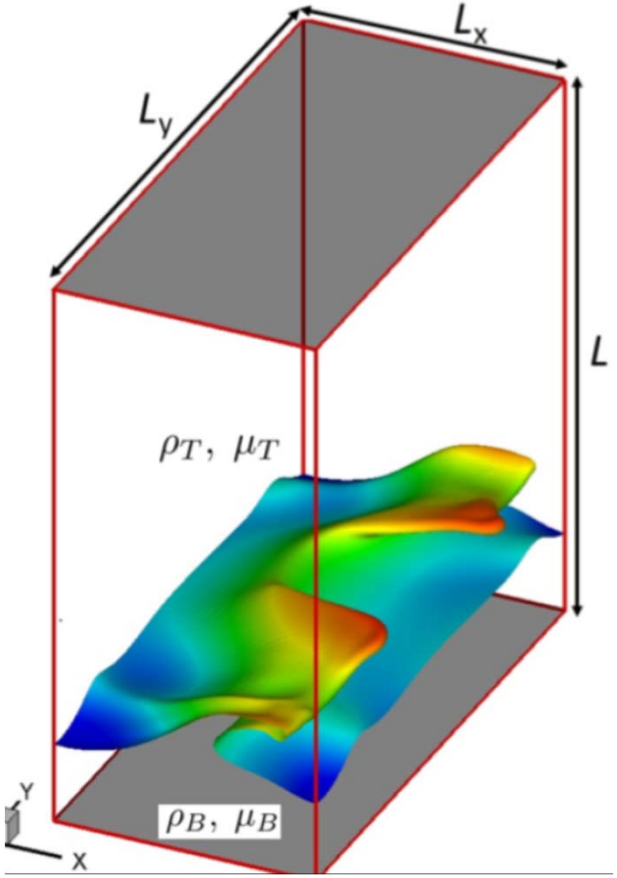
# TPLS 3.0: Rayleigh-Taylor Instability




See Z. Solomenko *et al.* (2017) Int J Multiphase Flow, 95, 235.

# TPLS 3.0: Stratified Flows

- A pressure-driven channel flow with two stably stratified phases
- At high flow rates (Reynolds numbers), an unstable equilibrium sets in
- Interfacial waves develop and can evolve to breaking waves, ligaments, billows, droplets etc.
- The density ratio, *r* (bottom phase vs top phase) is a key parameter

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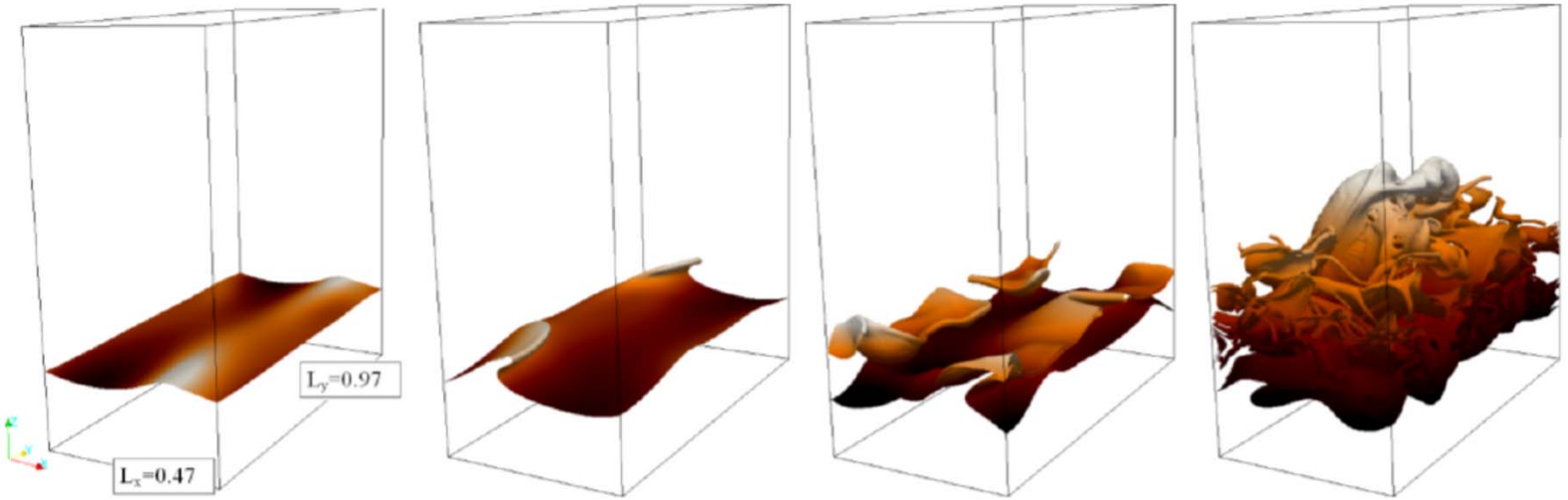
# TPLS 3.0: Stratified Flows




(a) $t = 0.4$ (b) $t = 0.5$ (c) $t = 0.6$ (d) $t = 0.7$

Interface shape evolution from DNS for a case at moderate density ratio, $r = 10$. Other parameters: $(m = 50, h_0 = 0.2, \mathcal{G} = 0.1, \mathrm{We} = 10)$, and $\mathrm{Re} = 500$.

# How to Use TPLS

- Describe the initial configuration
  - initial_config.opt
- Generate the initial configuration
  - run ./create_initial_configuration
- Configure how the program works (non-PETSc options)
  - tpls_config.opt
- PETSc run-time configuration
  - .petscrc

# initial_config.opt

- ## Domain grid
- # Number of grid points in X (l), Y (m) and Z (n) directions.
- maxl 257
- maxm 145
- maxn 153

- ## Interface detection method.
- # Options:
- # lsm - level-set method (default)
- # dim - diffuse interface method
- idm lsm

- ## Flow type.
- # Options:
- # channel - channel flow
- # rti - Rayleigh Taylor Instability
- flow_type channel

# initial_config.opt (cont.)

- ## Fluid flow

- # Reynolds number.
- re 1.0

- # Viscosity and density of the lower fluid.
- mu_minus 1.0
- rho_minus 1.0
- # Viscosity and density of the upper fluid.
- mu_plus 1.0
- rho_plus 3.0

- # Interface height, or height of lower liquid layer, expressed as
- # a proportion where 0 <= height <= 1.
- height 0.5

# initial_config.opt (cont.)

- # Pressure gradient.
- dpdl -1.0

- # Gravity.
- Grav 1.0
- gz -1.0

- # Surface tension scaling parameter.
- scap 0.01

- # Time step (>0).
- dt 0.0001

- # Smooth width scale factor.
- smooth_width_scale 1.5

# tpls_config.opt

- ## Process grid
- # Number of processes in the X, Y and Z dimensions, which defines the
- # process grid which overlays the domain grid.
- # The following conditions need to be respected:
- #  Number of processes available = num_procs_x * num_procs_y * num_procs_z
- #  num_procs_x is a divisor of (maxl - 1)
- #  num_procs_y is a divisor of (maxm - 1)
- #  num_procs_z is a divisor of (maxn - 1)
- #  num_procs_x >= 1
- #  num_procs_y >= 1
- #  num_procs_z >= 1
- # TPLS will raise an error if these conditions do not hold.
- num_procs_x 16
- num_procs_y 6
- num_procs_z 8

# tpls_config.opt (cont)

- ## Selection of PETSc or original equation solvers.
- # T or F for PETSc or original.
- petsc_solver_u T
- petsc_solver_v T
- petsc_solver_w T
- petsc_solver_p T

- ## Is a solver to be monitored?
- # T or F.
- u_monitoring_on F
- v_monitoring_on F
- w_monitoring_on F
- p_monitoring_on F

# tpls_config.opt (cont)

- ## Original momentum equation solver configuration
- # Number of iterations in solvers for u, v and w velocities (>= 1).
- mom_u 30
- mom_v 30
- mom_w 30
- ## Level-set equation solver configuration
- # Number of iterations in solver (>= 1).
- levelset 10

- # Maxu
- maxu 10.0

# tpls_config.opt (cont)

- ## TPLS operation
- # PHI channel .dat file output frequency (>= 1).
- phi_dat_frequency 1000
- # UVW channel .dat file output frequency (>= 1).
- uvw_dat_frequency 1000
- # Backup channel .dat file output frequency (>= 1).
- backup_frequency 1000
- # Backup files in netCDF hdf5 format (= T or F).
- backup_hdf5_format T
- # Number of timesteps (>= 1).
- num_timesteps 1000

- ## DIM equation solver configuration
- #  Number of iterations
- max_iteration_dim 18

# Run-Time Configuration of PETSc
# .petscrc

- -u_ksp_rtol 0.00000007
- -u_ksp_final_residual
- -v_ksp_rtol 0.000001
- -v_ksp_final_residual
- -w_ksp_rtol 0.0000002
- -w_ksp_final_residual
- -p_ksp_rtol 0.00009
- -p_ksp_type minres
- -p_pc_type sor
- -p_pc_sor_omega 1.5
- -p_ksp_final_residual

- Note that one can configure the PETSc (Krylov) solvers individually through a prefix to the configuration options. For example the generic option ksp_rtol becomes u_ksp_rtol, etc. As we shall see, the prefixes are specified in the code.

# Why Use PETSc

- PETSc provides support for structured grids.

```
call DMDACreate3d(PETSC_COMM_WORLD,                                &
        DM_BOUNDARY_PERIODIC,                                      &
        DM_BOUNDARY_PERIODIC,                                      &
        DM_BOUNDARY_NONE,                                          &
        DMDA_STENCIL_BOX,                                          &
        global_dim_x, global_dim_y, global_dim_z+2,                &
        num_procs_x, num_procs_y, num_procs_z,                     &
        dof, stencil_width,                                        &
        petsc_x_lengths,                                           &
        PETSC_NULL_INTEGER,                                        &
        petsc_z_lengths_p,                                         &
        da_s, ierr)
```

- This creates `da_s` which may then be used to create PETSc vectors.

# Why Use PETSc (cont.)

- Two sorts of array may be created: global, distributed arrays and local arrays.

```
    call DMGetGlobalVector(da_s, pres_vec, ierr)
    call DMGetLocalVector(da_s, pres_lvec, ierr)
```

- A local vector includes room for the appropriate ghost (halo) points.

- It is simple to populate a local vector (including its halo points) given a global vector.

```
call DMGlobalToLocalBegin(da_s, pres_vec, INSERT_VALUES, pres_lvec, ierr)
call DMGlobalToLocalEnd(da_s, pres_vec, INSERT_VALUES, pres_lvec, ierr)
```

- Note the absence of MPI calls. The movement of data is done behind the scenes by PETSc.

# Why Use PETSc (cont.)

- Distributed matrices may also be created from DMs and used in conjunction with KSPs to solve linear systems.

```
call DMCreateMatrix(da_s, A, ierr)
call compute_rhs_p(ksp_pres, b_vec, ierr)
call compute_matrix_p(ksp_pres, A, A, ierr)
call KSPSetOperators(ksp_pres, A, A, ierr)
call KSPSolve(ksp_pres, b_vec, pres_vec, ierr)
call MatDestroy(A, ierr)
```

This requires that a relationship has been established between the DM and the KSP.

# Why Use PETSc (cont.)

- KSPs provide access to PETSc linear solvers. A KSP may be associated with a DM as illustrated here.

```
call KSPCreate(PETSC_COMM_WORLD, ksp_u, ierr)
call KSPSetOptionsPrefix(ksp_u, 'u_', ierr)
call KSPSetFromOptions(ksp_u, ierr)
call KSPSetComputeInitialGuess(ksp_u, set_initial_guess_u,
                               PETSC_NULL_OBJECT, ierr)
call KSPSetDM(ksp_u, da_u, ierr)
call KSPSetDMActive(ksp_u, PETSC_FALSE, ierr)
```

- One can see that a prefix has been associated with the KSP so that it can have its own run-time, configuration options.

# TPLS 3.0 Performance

- 3D decomposition accelerates speed (2 x TPLS2.0 on 1,536 cores)
- Krylov solvers do not lead to an increase in performance but have different termination criteria
- Density contrast doubles the execution time
- Refer to the eCSE report for full performance analysis

# Further Work

- Merge existing code on counter-current flows and droplet formation.
- Include heat transfer, mass transfer with reaction and interfacial phase change.
- Implement complex geometries.