TBFsol user guide

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Structure of a test case

- 0 **folder**: contains the input fields, including initial and boundary conditions, that will be read as input by the solver. These files are stored in binary format. An example of how to generate the initial fields is given in the file `initGen.f90`. The boundary conditions are specified by the following integer values:

    – type 1: fixed value
    – type 2: fixed normal gradient
    – type 3: periodic
    – type 6: hydrophobic-like contact angle (only used for the volume fraction field)

    Boundary type 4 and 5 are used internally by the solver.

- **specs folder**: contains the parameters of the simulation. Possible user entries are: integer, real (double precision) and logical. Each entry is specified by an identification name followed by one blank space and its value. Note: do not use a 'tab' or more than one blank space to separate the parameter name by its value.

    List of input files:

    – decompose:
        – `px` (integer): number of cores along the x-direction
        – `py` (integer): number of cores along the y-direction
        – `pz` (integer): number of cores along the z-direction
        – `wrap_x` (logical): TRUE if the x-direction is periodic; FALSE otherwise.
        – `wrap_y` (logical): TRUE if the y-direction is periodic; FALSE otherwise.
        – `wrap_z` (logical): TRUE if the z-direction is periodic; FALSE otherwise.
    – initBubbles:
        – `method` (integer): three different methods to initialise bubbles are available:
            – 1: single bubble
            – `R` (real): bubble radius
            – `x0` (real): initial bubble position along x-direction
            – `y0` (real): initial bubble position along y-direction
            – `z0` (real): initial bubble position along z-direction
            – `nref` (integer): number of grid refinement to compute the initial bubble field. The higher the number the more accurate the initial volume fraction field will be.

- 2: two bubbles. Same parameters as the previous items. The parameters of the two bubbles are identified by _b1 and _b2.
  - 3: array of bubbles
    - R (real): bubbles radius
    - nix (integer): number of bubbles along the x-direction
    - nby (integer): number of bubbles along the y-direction
    - nbz (integer): number of bubbles along the z-direction
    - nref (integer): number of grid refinement to compute the initial bubble field. The higher the number the more accurate the initial volume fraction field will be.
    - random_distr (logical): if TRUE an initial random distribution of the bubbles is set. If FALSE the bubbles are uniformly distributed along the cartesian directions.
- mesh
  - Lx (real): length of the domain along the x-direction
  - Ly (real): length of the domain along the y-direction
  - Lz (real): length of the domain along the z-direction
  - isXunif (logical): TRUE sets the grid distribution along the x-direction to be uniform; FALSE sets the grid distribution to follow an hyperbolic tangent profile.
  - isYunif (logical): TRUE sets the grid distribution along the y-direction to be uniform; FALSE sets the grid distribution to follow an hyperbolic tangent profile.
  - isZunif (logical): TRUE sets the grid distribution along the z-direction to be uniform; FALSE sets the grid distribution to follow an hyperbolic tangent profile.
  - nx (integer): number of grid points along the x-direction
  - ny (integer): number of grid points along the y-direction
  - nz (integer): number of grid points along the z-direction
- parameters
  - rhol (real): liquid mass density.
  - rhog (real): gas mass density.
  - mul (real): liquid dynamic viscosity.
  - mug (real): gas dynamic viscosity.
  - sigma (real): surface tension.
  - gCH (real): gravity force acting along the x-direction in the vertical channel flow configuration.
  - g (real): gravity force.
- pcg_solver
  - nLevels (integer): number of multigrid levels.
  - nPreeSweep (integer): number of pre-smoothing sweeps.
  - nPostSweep (integer): number of post-smoothing sweeps.

- – tolMG (real): multigrid solver tolerance.
- – maxIterMG (integer): maximum number of iterations of the multigrid solver.
- – fullInfoMG (logical): TRUE: output of each multigrid solver iteration. FALSE: output only converged multigrid solver iteration.
- – tolPCG (real): conjugate gradient solver tolerance.
- – maxIterPCG (integer): maximum number of iterations of the conjugate gradient solver.
- – fullInfoPCG (logical): TRUE: output of each conjugate gradient solver iteration. FALSE: output only converged conjugate gradient solver iteration.
- – schemes
  - – time_scheme (integer):
    - – 0: Adams-Bashforth 2 time integration.
    - – 1: Runge-Kutta 3 time integration.
  - – k (real):
    - – 1: central differencing scheme for momentum convection.
    - – 0.5: QUICK scheme for momentum convection.
- – timeControl
  - – Tf (real): final simulation time.
  - – dt (real): time-step size.
  - – writeInterval (integer): an output folder is written every writeInterval number of time-steps.
  - – dtout (real): an output folder is written every dtout time units. If you use this parameter, set writeInterval to −1.
  - – input_folder (integer): number of folder to start the simulation from. Note: the restart of the VOF solver is still not available.
  - – adaptiveTimeStep (logical): TRUE: the time-step size will be adjusted according to cflMax. FALSE: a constant time-step size is imposed.
  - – cflMax (real): maximum CFL number of the simulation. It works only when adaptiveTimeStep is set to TRUE.
  - – Ts (real): staring time of statistical averaging.
  - – Tr (real): ramp-up interval (in time units) of the material properties.
  - – isRampUp (logical): TRUE: the material properties will be ramped-up from time 0 to Tr. FALSE: the material property are assigned to a fixed value as prescribed in the file 'parameters'.
  - – vofBlocksRedInterval (real): time interval (in time units) of the block redistribution routine.