# freeCappuccino input file specification guide

March 14th 2021

*Description of input parameters and their default values, possible values, description, discussion on status of the code related to it, etc.*

*The description below refers to fortran namelist file e.g. 'input.nml' that is required to configure the simulation. Not all the parameters have to be present, nor do they have to be in specific order.*

| Parameter key | Values | Description |
|---|---|---|
| title | String<br>e.g. 'Laminar flow in cavity' | Descriptive name of the case which will be written in monitor file. |
| mesh_format | 'nativeMesh'<br>'foamMesh' | Mesh format 'nativeMesh' for native polyMesh format or 'foamMesh' for OpenFOAM polyMesh. |
| lread | T/F | Read restart file - continue simulation from saved state? |
| ltest | T/F | Verbosity for linear solver convergence (for troubleshooting). |
| calcU | T/F | Activate Velocity field calculation? |
| urfU | Real array, size(3),<br>e.g. 0.7, 0.7, 0.7 | Under-relaxation factor for momentum equations. |
| gdsU | Real,<br>e.g. 1.0 | gamma-deferred correction parameter for velocity. |
| cSchemeU | String<br>e.g. 'linearUpwind' | Convection scheme for momentum equation. |
| dSchemeU | String,<br>e.g. 'skewness' | Diffusion scheme for momentum equation |
| nrelaxU | Int,<br>e.g. 1 | Integer parameter for diffusion scheme - advanced |
| lSolverU | Sting,<br>e.g. 'bicgstab' | Linear algebraic solver for momentum equation |

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| Parameter key | Values | Description |
|---|---|---|
| maxiterU | Int,<br>e.g. 10 | Max no of iterations for linear U-V-W equations |
| tolAbsU | Real,<br>e.g. 1e-13 | Absolute tolerance level for residual for linear U-V-W equations |
| tolRelU | Real,<br>e.g. 0.025 | Relative tolerance level for residual for linear U-V-W equations |
| ScndOrderPressIntrp | T/F | Second order (default), or mass flow weighted interpolation of pressure to faces. |
| calcP | T/F | Activate Pressure field calculation? True/False. |
| urfP | Real, eg. 0.3 | Under-relaxation factor for pressure |
| lSolverP | Sting,<br>e.g. 'iccg' | Linear algebraic solver for pressure/pressure correction |
| maxiterP | Int,<br>e.g. 50 | Max no of iterations for pressure/pressure correction |
| tolAbsP | Real,<br>e.g. 1e-13 | Absolute tolerance level for residual for pressure/pressure correction |
| tolRelP | Real,<br>e.g. 0.025 | Relative tolerance level for residual for pressure/pressure correction |
| TurbModel | String,<br>e.g. 'none' | Turbulence model - defined by string code. |
| urf | Real array, size(8),<br>e.g. 8*0.7 | Under-relaxation factors. (Array of 8 values) |
| gds | 8*1.0 | Deferred correction factor. (Array of 8 values) |
| cScheme | String,<br>e.g. 'linearUpwind' | Convection scheme - default is second order upwind. |

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| Parameter key | Values | Description |
|---|---|---|
| dScheme | String, e.g. 'skewness' | Diffusion scheme, i.e. the method for normal gradient at face uncorrected/skewness/offset. |
| nrelax | Int, e.g. 0 | Relaxation parameter non-orthogonal correction for face gradient. {-1/0/1} |
| lSolver | Sting, e.g. 'bicgstab' | Linear algebraic solver. |
| maxiter | Int, e.g. 20 | Max number of iterations in linear solver. |
| tolAbs | Real, e.g. 1e-13 | Absolute residual level. |
| tolRel | Real, e.g. 0.01 | Relative drop in residual to exit linear solver. |
| calcVis | T/F | Activate dynamic viscosity recalculation ( Non-Newtonian flows) |
| non_newtonian_model | String, e.g. 'PowerLaw' | Self-explanatory |
| npow | Real, e.g. 0.4 | Exponent for power-law fluids |
| Consst | Real, e.g. 10.0 | Consistency index for power-law fluids |
| shearmin | Real, e.g. 1e-3 | Lower limit for the shear rate magnitude for power-law fluids |
| Tau_0 | Real | Yield stress |
| megp | Real | Exponential growth parameter |
| muplastic | Real | Plastic viscosity |
| muzero | Real | Zero shear rate viscosity |
| muinfty | Real | Infinity shear rate viscosity |
| lamtime | Real | Natural time - time parameter |
| urfVis | Real, e.g. 0.8 | Under-relaxation parameter |

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| Parameter key | Values | Description |
|---|---|---|
| calcT | T/F | Activate Temperature equation calculation? True/False. |
| urfT | Real, e.g. 0.7 | Under-relaxation factors. |
| gdsT | Real, e.g. 1.0 | Deferred correction factor. |
| cSchemeT | String, e.g. 'linearUpwind' | Convection scheme - default is second order upwind. |
| dSchemeT | String, e.g. 'skewness' | Diffusion scheme, i.e. the method for normal gradient at face skewness/offset. |
| nrelaxT | Int, e.g. 0 | Relaxation parameter non-orthogonal correction for face gradient. Advanced. |
| lSolverT | String, e.g. 'bicgstab' | Linear algebraic solver. |
| maxiterT | Int, e.g. 20 | Max number of iterations in linear solver. |
| tolAbsT | Real, e.g. 1e-15 | Absolute residual level. |
| tolRelT | Real, e.g. 0.01 | Relative drop in residual to exit linear solver. |
| sigt | Real, e.g. 0.9 | sigma_t - Prandtl-Schmid number for temperature. |
| calcEn | T/F | Activate Energy field calculation? True/False. |
| urfEn | Real, e.g. 0.9 | Under-relaxation factors. |
| gdsEn | Real, e.g. 1.0 | Deferred correction factor. |
| cSchemeEn | String, e.g. 'linearUpwind' | Convection scheme - default is second order upwind. |

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| Parameter key | Values | Description |
|---|---|---|
| dSchemeEn | String, e.g. 'skewness' | Diffusion scheme, i.e. the method for normal gradient at face skewness/offset. |
| nrelaxEn | Int, e.g. 0 | Relaxation parameter non-orthogonal correction for face gradient. |
| lSolverEn | String, e.g. 'bicgstab' | Linear algebraic solver type (see list below). |
| maxiterEn | Int, e.g. 20 | Max number of iterations in linear solver. |
| tolAbsEn | Real, e.g. 1e-15 | Absolute residual level. |
| tolRelEn | Real, e.g. 0.01 | Relative drop in residual norm to exit linear solver. |
| sigtEn | Real, e.g. 0.9 | Prandtl-Schmid number for energy equation. |
| solveTotalEnergy | T/F | What we solve here - default is total energy, but other options are... |
| solveInternalEnergy | T/F | internal energy, or... |
| solveEnthalpy | T/F | enthaply. |
| addViscDiss | T/F | Add viscous dissipation term? True/False. |
| lbuoy | T/F | Buoyancy activated? True/False. |
| boussinesq | T/F | Bousinesq approximation for buoyancy. |
| tref | Real, e.g. 300.0 | Reference temperature for buoyant flows. |
| gravx | Real, e.g. 0.0 | Three components of gravity vector. |
| gravy | Real, e.g. -9.81 | - |

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| Parameter key | Values | Description |
|---|---|---|
| gravz | Real, e.g. 0.0 | - |
| calcCon | T/F | Activate passive scalar concentration field calculation? True/False. |
| urfCon | Real, e.g. 0.7 | Under-relaxation factors. |
| gdsCon | Real, e.g. 1.0 | Deferred correction factor. |
| cSchemeCon | String, e.g. 'linearUpwind' | Convection scheme - default is second order upwind. |
| dSchemeCon | String, e.g. 'skewness' | Diffusion scheme, i.e. the method for normal gradient at face skewness/offset. |
| nrelaxCon | Int, e.g. 0 | Type of non-orthogonal correction for face gradient minimal/orthogonal/over-relaxed. 1/0/-1. |
| lSolverCon | String, e.g. 'bicgstab' | Linear algebraic solver. |
| maxiterCon | Int, e.g. 20 | Max number of iterations in linear solver. |
| tolAbsCon | Real, e.g. 1e-15 | Absolute residual level. |
| tolRelCon | Real, e.g. 0.01 | Relative drop in residual to exit linear solver. |
| sigCon | Real, e.g. 0.9 | Prandtl-Schmidt number for passive scalar concentration |
| calcEpot | T/F | Activate Electric potential field calculation? True/False. |
| urfEpot | Real, e.g. 0.8 | Under-relaxation factor. |
| gdsEpot | Real, e.g. 1.0 | Deferred correction factor. |

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| Parameter key | Values | Description |
|---|---|---|
| lSolverEpot | Sting, e.g. 'iccg' | Linear algebraic solver. |
| maxiterEpot | Int, e.g. 20 | Max number of iterations in linear solver. |
| tolAbsEpot | Real, e.g. 1e-15 | Absolute residual level. |
| tolRelEpot | Real, e.g. 0.01 | Relative drop in residual to exit linear solver. |
| densit | Real, e.g. 1.0 | Fluid density. |
| viscos | Real, e.g. 1e-2 | Molecular dynamic viscosity. |
| pranl | Real, e.g. 0.71 | Prandtl coefficient for specific fluid. |
| beta | Real, e.g. 1e-3 | Thermal expansion coefficient. |
| lsgdh | T/F | Simple gradient hypothesis for heat-fluxes, or... |
| lggdh | T/F | Generalized gradient hypothesis for heat fluxes, or... |
| lafm | T/F | Algebraic flux modelling for heat fluxes. |
| facnap | Real, e.g. 1.0 | Under-relaxation factor for Reynolds stresses. |
| facflx | Real, e.g. 1.0 | Under-relaxation factor for heat fluxes. |
| ltransient | T/F | Unsteady simulation True/False and chose ONE algorithm below |
| bdf | T/F | Backward-Euler; First-Order Implicit, or... |
| bdf2 | T/F | Second-Order Backward Euler; Second-Order Implicit, or... |
| bdf3 | T/F | Third-order backard, or... |

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| Parameter key | Values | Description |
|---|---|---|
| CN | T/F | Crank-Nicolson. |
| lstsq | T/F | Gradient approximation, chose ONE: Unweighted Least-Square gradient approximation, or... |
| lstsq_qr | T/F | Least square gradients based on thin QR decomposition, or... |
| lstsq_dm | T/F | Distance-square weighted version of Least-Square Gradient, or... |
| gauss | T/F | Cell based Gauss gradient with simple linear interpolation. |
| nigrad | Int, e.g. 1 | Number of iterations for Gauss gradient approximation. |
| limiter | String, e.g. 'Venkatakrishnan' | Gradient limiter - global for all gradients (none, Barth-Jespersen, Venkatakishnan, MDL) |
| SIMPLE | T/F | Pressure-velocity coupling method - SIMPLE, or... |
| PISO | T/F | Pressure-velocity coupling method - PISO. |
| ncorr | Int, e.g. 1 | Number of PISO corrections - only relevant for PISO. |
| npcor | Int, e.g. 1 | Number of iterations for pressure/pressure correction equation - Number of Nonorthogonal corrections. |
| pRefCell | Int, e.g. 1 | Reference cell for setting pressure level (since we have pure Neumann problem) |
| tolerance | Real, e.g. 1e-5 | Desired level of convergence for SIMPLE iterations. |
| numstep | Int, e.g. 1000 | Total number of timesteps. |

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| Parameter key | Values | Description |
|---|---|---|
| timestep | Real, e.g. 1e-3 | Timestep size - also known as dt. |
| nzapis | Int, e.g. 100 | Program writes output files every NZAPIS timesteps. |
| maxit | Int, e.g. 1 | Number of iterations in SIMPLE or PISO sequential equation solution loop. |
| CoNumFix | T/F | Adaptive timestep size based on target Courant number? True/False. |
| CoNumFixValue | Real, e.g. 1.0 | If CoNumFix=True then set target maximum Courant number here. |
| const_mflux | T/F | Do we have constant mass flow in the domain? True/False. |
| magUbar | Real, e.g. 1.0 | If const_mflux=True then set target bulk velocity for constant mass flow situation. |

Possible **linear algebraic solvers** are: 'gauss_seidel', 'dpcg', 'iccg', 'bicgstab'. Most computational effort goes into solution of pressure Poisson equation, which is symmetric, positive definite. Use Incomplete Cholesky Conjugate Gradient (ICCG) for that one. For other transport equations with non-symmetric matrices Bi-CGStab is good option. Using LIS library enables greater choice for precodnitioner/solver combinations, when necessary.

Possible **convection schemes** are: 'cds', 'central', 'linearUpwind', etc.