**1. DESCRIPTION**

PUReIBM-PS2D-FD1D is a three-dimensional psudeo-spectral particle-resolved direct numerical simulation solver for detailed analysis of homogeneous fixed and freely evolving fluid-particle suspensions. PUReIBM-PS2D-FD1D is a continuum Navier-Stokes solver based on Cartesian grid that utilizes Immeresed Boundary method to represent particle surfuces.

**2. REQUIRED PACKAGES**

In PUReIBM-PS2D-FD1D, Fourier transforms are handles using the FFTW library. Therefore, it is required that this package be downloaded from "www.fftw.org" website and compiled as prior to compiling PUReIBM. It is recommended that the latest version of FFTW be used for this purpose. Then, the address to the "include" directory of the FFTW should be modified on top of the file "SRC/FLO/fftw3\_interface.F90". Note that in the serial and parallel modes, the files "fftw3.f03" and "fftw3-mpi.f90" should be used.

The parallelization of PUReIBM-PS2D-FD1D is done by two-dimensional domain decomposition technique along the x directions in the physical space.

**3. COMPILATION**

One list of file dependencies and two scripts are used to generate the makefile required for compiling PUReIBM-PS2D-FD1D. The files lists are "src\_flo\_scal" and "src\_post" that which include the name of files needed for compiling, respectively, the main code and post-processor. If any additional file is added in future to the source code, it should also be included in these file lists.

The first script that is used to generate the makefile is called "xdomake" that is the main directory. It calls another script called "domake" that is located in the folder "DOMAKE". Prior to compiling the code, it is required that the path to FFTW library directory in front of "FFTW\_LIBDIR", and also the path to MPI lirary directory "MPI\_LIBDIR" be changed in "domake" file. Note that we have successfully compiled and tested PUReIBM-PS2D-FD1D with Intel FORTRAN compiler. On machines where several Fortran compilers are installed, it is always safe to explicitly define the path to the compiler and linker in the "domake" file in front of "CC" and "LINK".

Once the "domake" file is modified, the makefiles can be generated by running the following in the main folder:

$ ./xdomake OPTIM flo\_scale ibm.exe ifc

In the above command, "OPTIM" means optimal mode. If the debug mode compilation is needed, it should be replace with "DEBUG". "flo\_scal" refers to the file list "src\_flo\_scal". If you intend to generate the makefile for post-processor, replace it with "post". "ibm.exe" is the name of the executable file. "ifc" is the name of the compiler that refers to Intel FORTRAN compiler. In the "DOMAKE" folder, there is a file titles "f77\_opt\_ifc" that defines the switches known by Intel compiler. There are also other files that contain switches for other compilers such as gfortran, path, Portland Group, but they have not been tested for PUReIBM-PS2D-FD1D.

The script also asks if the makefile for parallel simulation is needed to generate. Once the make files are made, the code is compiled as:

$ make -f MAKE/OPTIM\_ifc\_makeflo\_scal

If everything goes well, an execution file is generated in the main folder.

**4. Run case**

Once the complication is done, one can use “ibm.exe” to run a case as follows.

$ ./ibm.exe test > print&

In the above command line, “test” is a file name which is called “test\_floparam.in”. This file contains the flow parameters that related to flow, turbulent, or heat transfer. The run\_name should be added to the beginning in "[floparam.in](http://floparam.in)" as shown above. One example is shown as follows:

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&FLOANDGRID

NPROCY = 1 !number of processors in y direction

NPROCZ = 1………………….!number of processors in z direction

TEND = 2.000000000000000 , !not important

NERR\_STEPS = 100, !not important

WTIME\_MAXHRS = 47.5, !the maximum wall time you want to run your code. if

!you run freely evolving suspensions, this is how long

!your simulations run. For fixed assemblies, if the

!simulation converges, it stops before this time.

SAVEFORRES\_TIME = 6.d0 , !time interval for saving the restart files

TOL\_FERROR = 1.0E-06, !the tolerance for convergence criterion based on

!relative error of the average drag force

VIS = 0.012, !viscosity of the fluid. irrelevant because it is

!changed such that the mean slip velocity becomes 1

! while the Reynolds number is maintained as desired

RE = 20.0, !desired mean slip Reynolds number

RHOF = 1.000000000000 , !density of the fluid

CPF = 4179.00000000000 , !thermal heat capacity of the fluid. not relevant

!because I have not finished the heat transfer part

KF = 0.613000000000000 , !not relevant

CFL = 0.1, !the CFL number, usually set to 0.1. you can try

!higher values if you want a fast result, at

!the of expense loosing some accuracy.

RET = 0.000000000000000 , !the initial Reynolds number based on square root of granular temperature

FLO\_ANG = 0.d0, 90.d0, 90.d0 !The angles of the mean flow direction w.r.t. xyz

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&PART\_PROPT

NBODY = 1, !irrelevant

F1 = 1.600000000000000 , !irelevant

F2 = 1.600000000000000 , !a parameter used to determine the number of

!points on a particle surface. not less than 1.6

LYBYD = 6, !length of the computational box compared to the particle diameter

DBYDX = 40, !grid resolution per particle

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&SCAL\_PROPT

SETPHIMEAN = F,

NSPMX = 1,

PHISTREAM = 1.000000000000000 , !! initial fluid temperature

PHISURF = 0.0000000000000000 , !!! surface temperature

LUMPED\_CAP = F,

PR\_OR\_SC\_NU = 0.7D0 , !! Prandtl number or Schmit number

ZERO\_FLOW\_IN\_SOLID = F,

sourcepresent = F

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For example, “NBODY” represent the number of solid spheres in any simulation. More details of the parameters and the name list can be found in the source file “SRC/FLO/initialize.F90”.

5.Q & A

Any question relate to PUReIBM can be sent to [mehr@iastate.edu](mailto:mehr@iastate.edu) and [sciam@iastate.edu](mailto:sciam@iastate.edu) .