Miniature version of KAPSEL(AIST version) Manual　(2013/May/13)

AIST Hideki Kobayashi
and Hiroshi Morita

#0. Validation

We checked that this Kapsel program can work on CentOS6.4, and we do not test on other OSs.

#1. How to run

You can run Kapsel almost along the original Kapsel.
>./kapsel -I[*input.udf] -Ddefine_rev0.udf -O[*output.udf] -R[*restart.udf]

Procedure　(sample file: p50_s001.udf)

1. Put in the same directory these files, kapsel,define_rev0.udf,p50_s001.udf.
   If you put at $HOME/kapsel/exe,
2. make directory “avs_50_s” at $HOME/kapsel/exe
   > mkdir avs_50_s
3. make directory “avs_50_s/avs” at $HOME/kapsel/exe

> mkdir avs_50_s/avs

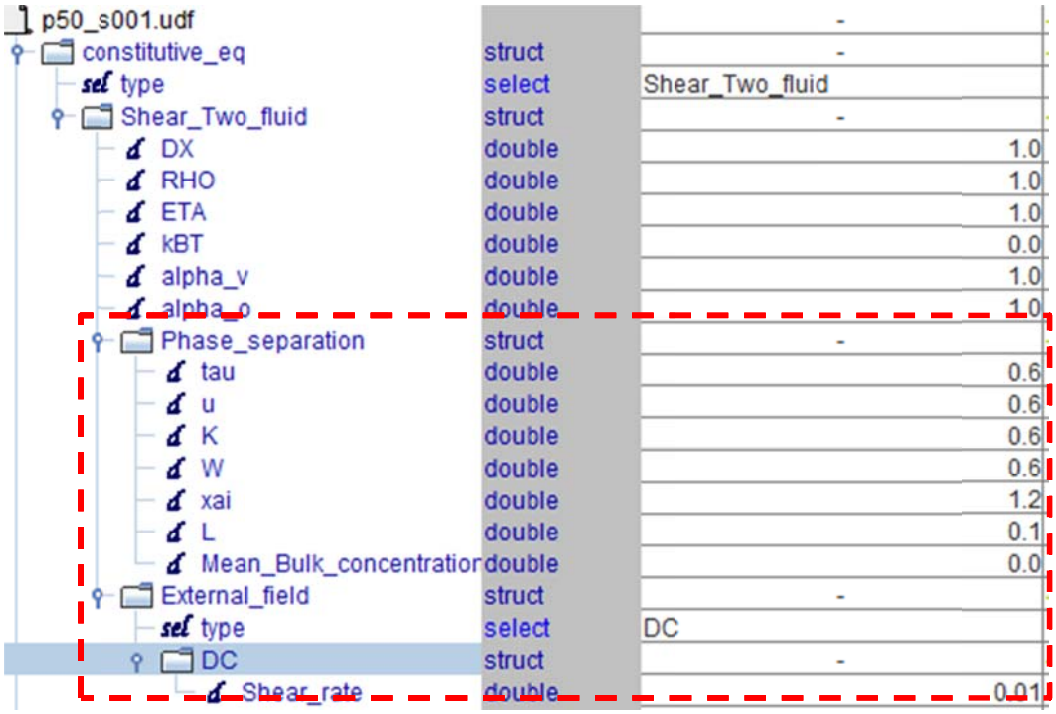
4. Please run Kapsel.

>kapsel -Ddefine_rev0.udf -Ip50_s001.udf -Ooutput.p50_s001.udf -Rrestart.p50_s001.udf

#2. Principal changeable parameters

＃Constitutive_eq

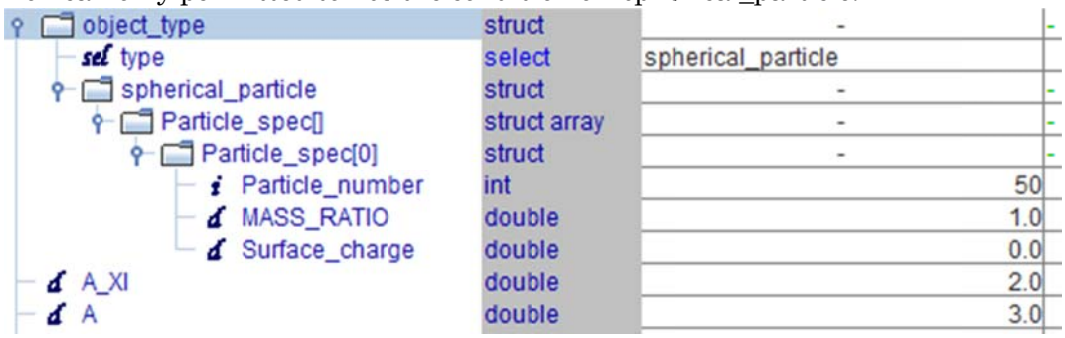
You can run only by the condition of “Shear_Two_fluid”
;with the condition of Newton fluid +two phase fluid+ shear(periodic boundary)



○Phase_separation:

tau: The factor of 2nd order in Ginzburg-Landau model
u: The factor of 4th order in Ginzburg-Landau model
K: Interfacial tension
W: Wetting interaction
xai: coupling constant
L: Mobility
Mean_Bulk_concentration: Mean bulk concentration(= Average of φ_A+φ_B, where φ_i is a concentration of i-phase. For example, when A-phase = 0.7 and B-phase = 0.3, Mean bulk concentration equal 0.4.)
(※Max(tau,u)×L is less than 0.18. A recommendation value is 0.06.)
○External_field: You can choose one from below two items.
DC: Steady shear (DC)
AC:Oscillatory shear (AC)

＃Object_type
You can only permitted to use the condition of "spherical_particle."

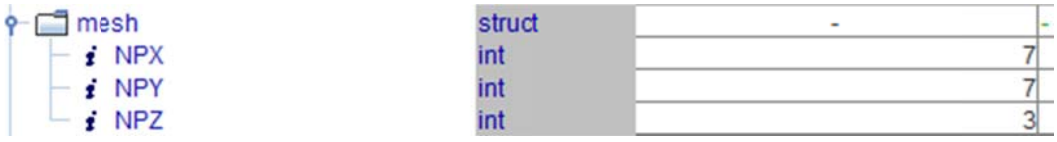


○spherical_particle:
▽Particle_spec[]
Particle_spec[0]: (0 means the 1st component)
Particle_number: Number of particles
MASS_RATIO: Density of particle / density of fluid
Surface_charge: Valency of particles (total charge carried by a single particle in unit of electron charge)

＃A_XI: Thickness of the particle-fluid boundary
＃A: Radius pd particles or beads

＃EPSILON: Energy unit of Lennard-Jones potential
＃LJ_powers: Set of power exponents of the Lennard-Jones potential;
12:6 or 24:12 or 36:18

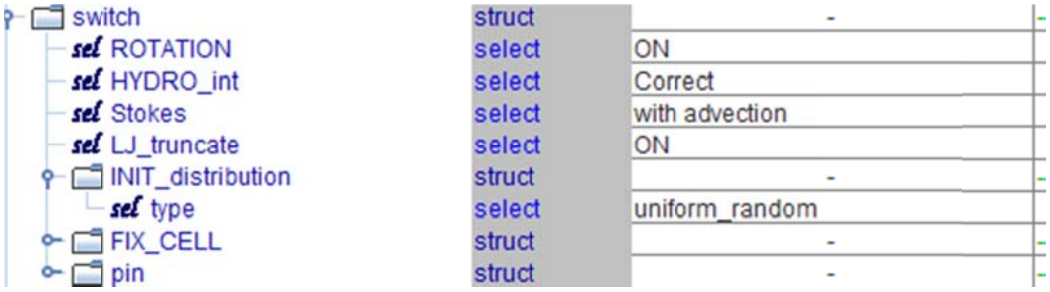
#Mesh



NPX: Defines the size of simulation box in x-direction as Lx=2^NPX
NPY: Defines the size of simulation box in y-direction as Ly=2^NPY

NPZ: Defines the size of simulation box in z-direction as Lz=2^NPZ
(※NPX must equal NPY.)

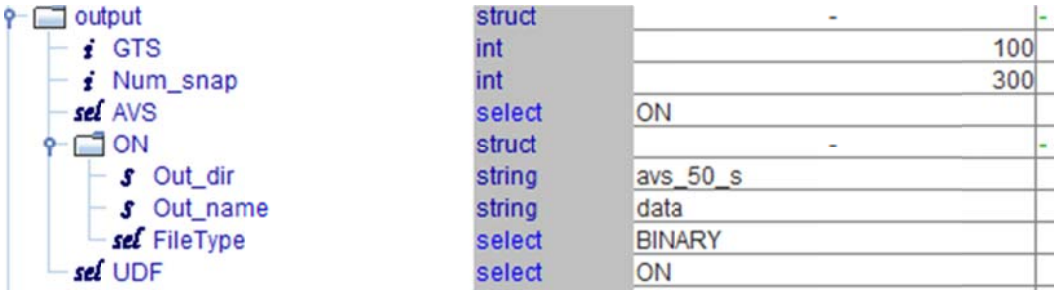
#Switch



○ROTATION: Set ON: solve rotational motion of particles properly
○HYDRO_int: Set Correct (other options are obsolete)
○Stokes: Set with advection (other options are obsolete)
○LJ_truncate:Set ON: LJ without attraction (WCA potential)
○INIT_distribution: Select from below five items.
uniform_random: randomly generate initial particle positions
random_walk: add some deviations to a perfect FCC lattice
FCC: place particles on FCC lattice
BCC: place particles on a BCC lattice
user_specify: Set initial particle positions and velocities manually
(If object_type = chain, all the above options are omitted and initial chain configurations are generated by self-avoided random walk unless user_specify is selected.)

#boundary_condition: Set full_periodic

#output



○GTS: Number of intervals between data saving
○Num_snap: Number of data saving. Total number of simulation step is GTS * Num_snap.
○AVS: Set ON if AVS data is needed. Huge disk space is used if ON.
○ON
Out_dir: Name of subdirectory in which AVS data is saved. Make subdirectories ./"Out_dir" and ./"Out_dir"/avs in advance to run KAPSEL.
Out_name: Set a name of AVS field data file "Out_name".fld
File_Type: Select a file format of AVS data from BINARY or ASCII
○UDF: Set ON