

#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)

p50_s001.udf			
constitutive_eq	struct		-
sel type	select	Shear_Two_fluid	
Shear_Two_fluid	struct		-
DX	double		1.0
RHO	double		1.0
ETA	double		1.0
kBT	double		0.0
alpha_v	double		1.0
alpha_o	double		1.0
Phase_separation	struct		-
tau	double		0.6
u	double		0.6
K	double		0.6
W	double		0.6
xai	double		1.2
L	double		0.1
Mean_Bulk_concentration	double		0.0
External_field	struct		-
sel type	select	DC	
DC	struct		-
Shear_rate	double		0.01

○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 $\phi_A + \phi_B$, 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.)

($\times \text{Max}(\text{tau}, \text{u}) \times L$ 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.”

object_type	struct	-	-
sel type	select	spherical_particle	-
spherical_particle	struct	-	-
Particle_spec[]	struct array	-	-
Particle_spec[0]	struct	-	-
Particle_number	int		50
MASS_RATIO	double		1.0
Surface_charge	double		0.0
A_XI	double		2.0
A	double		3.0

○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 of 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

mesh	struct	-	-
NPX	int		7
NPY	int		7
NPZ	int		3

NPX: Defines the size of simulation box in x-direction as $L_x = 2^{\text{NPX}}$

NPY: Defines the size of simulation box in y-direction as $L_y = 2^{\text{NPY}}$

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

#Switch

switch	struct	-	-
sel ROTATION	select	ON	-
sel HYDRO_int	select	Correct	-
sel Stokes	select	with advection	-
sel LJ_truncate	select	ON	-
INIT_distribution	struct	-	-
sel type	select	uniform_random	-
FIX_CELL	struct	-	-
pin	struct	-	-

○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

output	struct	-	-
i GTS	int	100	-
i Num_snap	int	300	-
sel AVS	select	ON	-
ON	struct	-	-
s Out_dir	string	avs_50_s	-
s Out_name	string	data	-
sel FileType	select	BINARY	-
sel UDF	select	ON	-

○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