

New atom style

```
atom_style      bio
atom_modify     map array sort 10000 1e-5
boundary        pp pp pp
newton          off
communicate     single vel yes
read_data       IC5nut.in
```

```
group HET type 1 group AOB type 2 group NOB type 3 group EPS type 4 group inert type 5
```

```
neighbor        1.0e-5 bin neigh_modify delay 0
```

Group definitions

Neighbour list definitions

```
pair_style      gran/hooke/history 200000000 NULL 15000000 NULL 0.5 1
pair_coeff       * *
timestep        1
velocity        all set 0.0 0.0 0.0 units box
fix             1 all nve/sphere
fix             2 all gravity 9.8 vector 0 -1 0 # spherical 90.0 -180.0
fix            3 all fdrag
```

Physical interaction box

Variable definitions

```
variable KsHET equal 0.01 variable Ko2HET equal 0.81 variable Kno2HET equal 0.0003 variable Kno3HET equal 0.0003 variable Knh4AOB equal 0.001 variable Ko2AOB equal 0.0005
variable Kno2NOB equal 0.0013 variable Ko2NOB equal 0.00068
```

```
variable MumHET equal 0.00006944444 variable MumAOB equal 0.00003472222 variable MumNOB equal 0.00003472222 variable etaHET equal 0.6
variable bHET equal 0.00000462962 variable bAOB equal 0.00000127314 variable bNOB equal 0.00000127314 variable bEPS equal 0.00000196759
variable YEPS equal 0.18 variable YHET equal 0.61 variable EPSdens equal 30 variable EPSratio equal 1.25 variable factor equal 2.0
```

```
fix g1 all nugrowth 1 v_KsHET v_Ko2HET v_Kno2HET v_Kno3HET v_Knh4AOB v_Ko2AOB v_Kno2NOB v_Ko2NOB v_MumHET v_MumAOB v_MumNOB v_etaHET v_bEPS v_YEPS v_YHET v_EPSdens
```

```
fix dt1 HET death 1 v_bHET v_factor 1952467
```

```
fix dt2 AOB death 1 v_bAOB v_factor 1234312
```

```
fix dt3 NOB death 1 v_bNOB v_factor 1325352
```

```
fix d1 all divide 1 v_EPSdens 2.0 1242242
```

```
fix e1 HET eps_extract 1 v_EPSratio v_EPSdens 1242242
```

Death model

Division model

EPS extraction model

Growth model

```
dump          id1 HET custom 2000 HET.bubblemd radius outerradius
#dump         id2 HET custom 172800 HETdeath.bubblemd type radius outerradius mass outermass
#dump         id2 EPS custom 1000 snapshot2.bubblemd id type diameter mass x y z vx vy vz
dump          id all custom 2000 snapshot.bubblemd id type radius vx vy vz x y z outerradius outermass
```

Outputting the information

```
thermo_style   custom step atoms ke vol
#thermo_style  granular # not work. syntax change?
#thermo_style  one    # granular does not work
thermo         1
thermo_modify  lost error
#restart       1000000 restart.*.bubblemd
```

```
run 172800
```

Running the case for 172800 sec = 2 days