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**COMPUTER LABORATORY SESSION**

**SETTING UP AND RUNNING A SIMULATION WITH UPI**

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*These are preliminary lecture notes, intended only for distribution to participants.*



## Setting up and running a simulation with UPI

- **OCSET**: to build the input file for UPI
- **UPI**: to perform the simulation
- **REPORT**: to perform a post-simulation statistical analysis

## OCSET

- NEEDED FILE: [qid.dm](#) approved density matrix table.

- INTERACTING SESSION:

in UPI/setup/

```
>> ocset
```

```
64 bit Linear Congruential Generator with Prime Addend
```

```
seed = 985456376, stream_number = 0 parameter = 0
```

```
input name of run
```

```
RUN1
```

```
input dm file
```

```
He4.nd
```

```
input: nparts
```

```
32
```

```
input density
```

```
0.02179
```

```
input crystal number of unit cells in each direction
```

```
crystal:1=sc,2=bcc,3=hcp,4=fcc(3d),3=triangular(2d)
```

```
4 2 2 2
```

```
computing 32 lattice sites dimensionality 3 number density 0.21790E-01
```

```
face-centered cubic lattice
```

```
q displs      0.00000    0.00000    0.00000
q displs      0.00000    0.50000    0.50000
q displs      0.50000    0.00000    0.50000
q displs      0.50000    0.50000    0.00000
npuc  4 nvacancies      0 box size 0.11367E+02 0.11367E+02 0.11367E+02
number of cells in each direction      2      2      2
nearest and next nearest neighbor distance  0.40187E+01 0.56833E+01
possible fits= 3
possible tslice  10.  20.  40.  80.  160.  320.  640.
input physical temperature, tslice
5 160
nslices = 32 temp 5.
enter initial random displacements
1.0
input: nspins nppss
0
input blocks passes, levels for omove
100 20 4
input blocks, passes, levels, hitsfor select
0 0 0 0
```

- OUTPUT FILES:

- *qid.sy*: the input file for UPI

```
UNITS K A
  ENORM      0.32000000E+02
BOXSIZE 0.1136660887E+02  0.1136660887E+02  0.1136660887E+02
  VTAIL      -0.11397509E+02
  PTAIL      -0.24835173E+00
  BETA       0.20000000E+00
NSLICES  32
TYPE He4  0.605961500E+01    0    32 run1.He4.ic
POT PAIR  He4    He4    He4.nd.dm
  GAMMA 3 He4    32.
  CUTK    0.86585950E+00
RESTART
OMOVE  100  20  4
```

- *qid.label.ic*: initial coordinates for paths

- HINT: This is a minimal setting for running, not necessarily the best one. Look at the UPI-Commands notes for other useful keywords.

# UPI

- INPUT FILES:

- *qid.sy*
- *qid.dm*
- *qid.label.ic*

- OUTPUT FILES:

- *qid.bsc*: binary data for statistical analysis
- *qid.cyc*: cycle length probability [*length*,  $P(\textit{length})$ ]
- *qid.dat*: formatted output file for DataSpork package
- *qid.em*: effective mass [ $t$ ,  $m/m^*$ , *error*] (fig 28 of Rev.Mod.Phys.)

– *qid.acc*: acceptance probability for all different kinds of moves

\* Simple case: no permutations  $T = 10K$

```

gate      nmovers acc.ratio trials
acceptance for particle He4
winding   1  0.00000      276907          0
  bisect  1  0.86533      320000      276907  0.86533
displace  1  0.55877      159906      89351
nsets= 1 nblocks  500

```

\* More complex case of permuting particles:  $T = 0.5K$

```

gate      nmovers acc.ratio trials
acceptance for particle He4
winding   1  0.00000      8653          0
  bisect  1  0.25086      34494      8653  0.66040  0.65483  0.58008
permute   2  0.63009       319          201
winding   2  0.05970       201          12
  bisect  2  0.00974      32749      319  0.15594  0.24555  0.25439
permute   3  0.50963       675          344
winding   3  0.69477       344          239
  bisect  3  0.01202      56151      675  0.17157  0.26168  0.26775
permute   4  0.29114        79          23
winding   4  0.69565        23          16
  bisect  4  0.00541      14606      79  0.13885  0.20809  0.18720
displace  1  0.12874      11504      1481
nsets= 3 nblocks  230

```

– *qid.ev*: virial estimator data [ $t, E_k, err, E_t, err, P, err$ ]

- *qid.gr*: pair distribution function  $g(r)$  in internal format
- *qid.grr*: pair distribution function  $g(r)$  [ $r, g(r)$ ]
- *qid.gv*: reciprocal space vectors in internal format
- *qid.lsc*: label for output quantities
- *qid.out*: standard output

```

output file already exists
time = Mon Oct 22 20:50:34 host h
run id he4.4   Mon Oct 22 20:50:34
trying to open file he4.4.sy
1 CMD: UNITS K A
1 CMD:   ENORM   0.320000000E+02
1 CMD: BOXSIZE 0.1136660887E+02 0.1136660887E+02 0.1136660887E+02
volume of box 1468.56356 minimum side 5.68330444
half box size 5.68330444 5.68330444 5.68330444
2*pi/ell 0.552775727 0.552775727 0.552775727
1 CMD:   VTAIL  -0.11397509E+02
1 CMD:   PTAIL  -0.24835173E+00
1 CMD:   BETA   0.100000000E+00
beta = 0.1 inverse K
temperature = 10. K
1 CMD: NSLICES 4
1 CMD:TYPE He4 0.605961500E+01 0 32 he4.32.He4.ic

```

beginning read from file he4.32.He4.ic

```
input for particle      1
number      32 hbs2m      6.059615
      density =      0.02179
nspins      0 number of particles/state
      first and last particle of this type      1      32
dimensionality of this type  0
1 CMD: POT PAIR He4 He4 He4.nd.dm
addpot beginning read from file He4.nd.dm
ntermact ntermeng  3 6
number of grid points 100 range  0.2  5.5
finished reading potential
number records skipped  4 levels defined  3 terms read  3
number records skipped  4 levels defined  3 terms read  6
number records skipped  4 levels defined  3 terms read  2
number records skipped  4 levels defined  3 terms read  2
set up potential between pairs  1 1 3
1 CMD: GAMMA 3 He4      32.
1 CMD: DISPLACE He4 1.0  0.5
1 CMD: VWINDOW 1 4 0.04
virial window= 1 4
1 CMD: EFFMASS
1 CMD:      CUTK      0.86585950E+00
nshlls      2  50 nvects      9  600
spara, rknorm and cumulative mult      1      3 0.55278E+00
spara, rknorm and cumulative mult      2      9 0.78174E+00
1 CMD: RESTART

total number of particles  32
```

```

minimum nslices= 1
idebug ifleak ifdiag ifsamp 0 1 1 1
  nlamb cutk 2 0.8658595
nparts nslices ntypes 32 4 1
beta enorm 0.1 32.
vtail -11.397509ptail -0.24835173
iref 0 irev 0
npfilen= 1 nlvld= 3
hop 1.
number of projections= 0
g(r) table limit 9.84377204
1 CMD: OMOVE 500 20 1
starting new set with 500 blocks
number of single particle steps/block 20
levels 1
maximum drift 0.28417E+01
gamma= 1.
time = Mon Oct 22 20:50:35s host s
spill id he4.4 nsets 1 ndone 1 Mon Oct 22 20:50:35s
.....
.....
spill id he4.4 nsets 1 ndone 500 Mon Oct 22 20:58:20s
block time 0.94000E+00 secs total time = 0.46130E+03
end of simulation

```

– *qid.rs*: restart file

– *qid.sk*: structure factor [ $k, S(k)$ ]

- INPUT FILES FOR TODAY'S LAB:

- PARTS 1 & 2

```
UNITS K A
  ENORM      0.32000000E+02
BOXSIZE 0.1136660887E+02  0.1136660887E+02  0.1136660887E+02
  VTAIL     -0.11397509E+02
  PTAIL     -0.24835173E+00
  BETA       0.10000000E+00
NSLICES  32
TYPE He4  0.605961500E+01    0    32 he4.32.He4.ic
POT PAIR  He4    He4    He4.nd.dm
  GAMMA 3 He4    32.
DISPLACE He4 0.8  0.5
VWINDOW 1 32 0.04
EFFMASS
  CUTK      0.86585950E+00
RESTART
OMOVE  500  10  4
```

- PARTS 3

```
UNITS K A
  ENORM      0.32000000E+02
BOXSIZE 0.1136660887E+02  0.1136660887E+02  0.1136660887E+02
  VTAIL     -0.11397509E+02
  PTAIL     -0.24835173E+00
  BETA       2.00000000E+00
NSLICES  80
```

```
TYPE He4 0.605961500E+01 0 32 T2.5.He4.ic
POT PAIR He4 He4 He4.nd.dm
GAMMA 1 He4 1.
GAMMA 2 He4 10.
GAMMA 3 He4 10.
;GAMMA 4 He4 10.
DISPLACE He4 .6 .5
VWINDOW 1 80 0.1
CUTK 0.86585950E+00
RESTART
OMOVE 20 20 3
SELECT 100 20 3 30
SELECT 1000 20 3 30
```

- **HINTS:** read the UPI-Commands notes for the meaning of the various entries

## REPORT

- This code reads the file `qid.bsc` and produces a file `qid.rep` with all statistical averages listed with errors and corrected errors.
  - `Qid.rep` for distinguishable particles  $T = 10K$

```
report for run he4.32
blocks/set 500
value units          mean          cor-err          uncor-err  efficiency  cor-time
ke_He4      K          0.250319E+02    0.372995E+00    0.331069E+00    1.000      1.269
ke_He4.s    K          0.237952E+02    0.371372E+00    0.329964E+00    1.000      1.267
ke_He4.u    K          0.123945E+01    0.174644E-01    0.766888E-02    1.000      5.186
ke_He4.f    K          -0.276167E-02    0.317446E-03    0.279083E-03    1.000      1.294
V_He4He4    K          -0.340306E+03    0.160853E+01    0.111640E+01    1.000      2.076
P_1_He4     K          0.100000E+01    0.000000E+00    0.000000E+00    1.000      0.000
K_virial    K          0.250319E+02    0.372995E+00    0.331069E+00    1.000      1.269
KE_tot      K          0.250319E+02    0.372995E+00    0.331069E+00    1.000      1.269
PE_tot      K          -0.220321E+02    0.502665E-01    0.348876E-01    1.000      2.076
E_tot       K          0.299985E+01    0.366522E+00    0.328324E+00    1.000      1.246
pressure    K          0.256547E+00    0.105360E-01    0.651194E-02    1.000      2.618
D_R         s-1        0.412052E+01    0.202065E-01    0.191823E-01    0.999      1.110
```

– *Qid.rep* for superfluid helium  $T = 0.5K$

```

report for run T0.5
  blocks/set  20 100 230
  value  units          mean          cor-err          uncor-err  efficiency  cor-time
ke_He4    K          0.143336E+02  0.688717E+00  0.971878E-01  1.000      50.218
ke_He4.s  K          0.943971E+01  0.600885E+00  0.894998E-01  1.000      45.075
ke_He4.u  K          0.483299E+01  0.692245E-01  0.276086E-01  1.000       6.287
ke_He4.f  K          0.609094E-01  0.204884E-01  0.624072E-02  1.000     10.778
V_He4He4  K         -0.340086E+03  0.602818E+01  0.124149E+01  1.000     23.577
rs_He4_x  K          0.518420E+00  0.139587E+00  0.377758E-01  1.000     13.654
df_He4_x  K          0.553768E-01  0.111384E+00  0.589976E-01  1.000       3.564
rs_He4_y  K          0.818084E+00  0.266340E+00  0.543102E-01  1.000     24.050
df_He4_y  K         -0.138188E+00  0.140207E+00  0.609474E-01  1.000       5.292
rs_He4_z  K          0.578592E+00  0.311323E+00  0.620829E-01  1.000     25.147
df_He4_z  K         -0.571739E-01  0.118126E+00  0.587535E-01  1.000       4.042
P_1_He4   K          0.156095E+00  0.288351E-01  0.509895E-02  1.000     31.980
K_virial  K          0.143336E+02  0.688717E+00  0.971878E-01  1.000     50.218
KE_tot    K          0.143336E+02  0.688717E+00  0.971878E-01  1.000     50.218
PE_tot    K         -0.220252E+02  0.188381E+00  0.387964E-01  1.000     23.577
E_tot     K         -0.769158E+01  0.470732E+00  0.799051E-01  1.000     34.706
pressure  K         -0.241181E-01  0.125688E-01  0.318336E-02  1.000     15.589
D_R       s-1          0.730832E+00  0.249589E-01  0.208142E-01  0.984       1.438
D_P       s-1          0.211240E+01  0.131936E+00  0.111331E+00  0.984       1.404

```