united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

SMR 1595 - 22

Joint DEMOCRITOS - ICTP School on

CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

COMPUTER LABORATORY SESSION

SETTING UP AND RUNNING A SIMULATION WITH UPI

***Carlo PIERLEONI**
Universita' di L'Aquila, L'Aquila, Italy

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 dispacements
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 [$length, P(length)$]
  - *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    0.32000000E+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    0.10000000E+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     0number 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*.skk: 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
```