Box calculations

Following the discussions during and after the transport simulation workshop at Shanghai in 2014, we have realized that it is very important to perform simulations in a periodic box because, under suitable conditions, the results can be better understood and checked against analytical predictions. We would like to use the box calculations to test accurately the critical ingredients entering the description of heavy-ion collisions such as:
  - Collision integral
  - Pauli blocking
  - Mean field dynamics
For box simulations, the problems linked to initialization and Pauli-blocking implementation, which we found to be a big source of discrepancies between the different codes, are much less crucial, and the above effects can be studied in a decoupled way (unlike in a full collision of finite nuclei). Also, in some cases analytical results are available, which allow one to check the results in a model independent way. In homework1 we will only address the first two ingredients, i.e. collision integral and Pauli blocking. The test of the mean field in box calculations will be the subject of a later homework.

The box calculations should be performed with **periodic boundary conditions (BC)**. Indeed, considering reflecting BC would imply the presence of edge effects, which only become unimportant in the limit of very large boxes. In contrast, with periodic BC the box can be kept relatively small.

1) Details of periodic boundary conditions
Let us consider a box of volume $V = L_1*L_2*L_3$, where the system is confined. The position of the center of box is $(L_1/2, L_2/2, L_3/2)$. (In later homework with mean field propagation it is useful to have a box extended in one direction, so if you reprogram, take this generality already into account now.) In order to calculate the spatial density and the mean-field potential, one usually deals with distances (in coordinate space) between particles or space points. Periodic BC can be introduced in an elegant way by redefining the position of particles moving out the box and the distance metric between two points (or particles) as it follows:
- In order to keep all particles inside the box, a particle leaving the box has to enter it on the opposite side, keeping the same momentum.
  Thus, indicating with $r_i(k)$ (k=1,2,3) the original coordinate of the particle i and with $r_{i,new}(k)$ the modified coordinate , this condition implies:
  - if $r_i(k) > L_k$ then $r_{i,new}(k) = r_i(k) - L_k$
  - if $r_i(k)<0$ then $r_{i,new}(k) = r_i(k) + L_k$
  In Fortran, this can be written as $r_{i,new}(k) = modulo(r_i(k), L_k)$.
- Let us indicate with $dr(k) = r_i(k) - r_j(k)$ the three components of the distance vector between points i and j. Then, when periodic BC are imposed:
  - if $dr(k) > L_k/2$ then $dr_{new}(k) = dr(k) - L_k$

- if dr(k) < -L$_k$/2 then dr$_{new}$(k) = dr(k) + L$_k$
This condition can be implemented as
dr$_{new}$(k) = modulo(dr(k) + L$_k$/2, L$_k$) - L$_k$/2.

2) Details of nuclear interaction and N-N cross section

The same simplified force and N-N cross section employed for the calculations of transport 2014 (Shanghai) should be considered (for homework 1 the mean field is actually not needed, but we give it here already for later homeworks):

- For non-relativistic transport codes: use a standard soft Skyrme parametrization (without momentum dependence) with the following parameters: a = -209.2 MeV, b = 156.4 MeV, τ=1.35, M_n=M_p=938 MeV and a symmetry potential energy with linear density dependence $S_{pot}*(\rho/\rho_0)$, S_{pot} =18 MeV.
  The total single-particle potential is then:

$$U_{\frac{n}{p}} = a\left(\frac{\rho}{\rho_0}\right) + b\left(\frac{\rho}{\rho_0}\right)^\tau \pm 2S_{pot}\frac{\rho}{\rho_0}\delta.$$

$$U_{\frac{n}{p}} = a\left(\frac{\rho}{\rho_0}\right) + b\left(\frac{\rho}{\rho_0}\right)^\tau \pm 2S_{pot}\frac{\rho}{\rho_0}\delta; \quad \delta = (\rho_n - \rho_p)/\rho$$

  (Properties of this parameterization: compressibility K_0=240 MeV, saturation density ρ_0 =0.16 fm^{-3} , binding energy at saturation density E_0= -16 MeV, symmetry energy $S(\rho_0)$~30.3 MeV)

- For relativistic transport codes:
  use a nonlinear σ-ω-ρ RMF parameterization "NLρ" (see parameter set I in PRC65, 045201, by Liu B et al.)
  (Properties of this parameterization: K_0=240 MeV, ρ_0=0.16 fm^{-3} , E_0=-16 MeV, $S(\rho_0)$~30.3 MeV)

- Turn off the Coulomb interaction

- Use a constant isotropic elastic cross section of 40 mb.
  There should be no restriction on the collisions times and energies. i.e. a particle that has already collided in a time step can collide again. There should also be no threshold for the collision energy.
  (If your usual procedure in the calculation of a heavy ion collision is different, e.g. having a threshold for the collision energy, or not allowing a collision of the same particle in the same time step, and you do not want to change your code, then you could also provide results for this procedure, but indicate this clearly.)

- Turn off all inelastic collisions

Homework 1

We should use a cubic box, of size L_k = 20 fm.
Particles interact only through two-body collisions, i.e. the mean-field interaction is suppressed.
The simulation should be followed until t=140 fm/c, with a recommended step of Δt=0.5 or 1.0 fm/c.

1) **Initialization:**
   - Uniform density ρ_0=0.16 fm^{-3}, with isospin asymmetry equal to zero. With the above size of the box this corresponds to 1280 nucleons, 640 neutrons and 640 protons. Particle positions are initialized randomly from 0 to L_k.
   - In momentum space we consider two cases, corresponding to the temperature T=0 and T=5 MeV.
     Particle momenta are initialized randomly in a sphere with Fermi momentum p_F=265 MeV/c (T=0 case) or with the Fermi distribution,
     $f=1/(1+\exp((E-\mu)/T))$, with $E=p^2/2m$ (relativistically
     $E=\sqrt{p^2+m^2}$), corresponding to T = 5 MeV.
     The chemical potential can be estimated in the non-relativistic case from the expression:
     $\mu(T)\approx\mu(0)(1-\frac{\pi^2}{12}\left(\frac{T}{\mu(0)}\right)^2)$, where $\mu(0)$ is the Fermi energy.
     At the density considered, we have $\mu(0)$ = 37.39 MeV and μ(T=5 MeV) = 36.84 MeV.
     In the relativistic case it has to be obtained from the normalizing
     Condition $2\int f\, d^3p=\rho_{n,p}$ for neutrons and protons, respectively.

2) **Pauli-blocking:**
   In order to better investigate the consequences of the Pauli-blocking treatment in the different codes, the simulations should be performed with two options:
   - OP1: Just consider your standard treatment, that you usually adopt in your simulations;

- OP2: In the evaluation of the Pauli blocking factor $P_{block} = (1 - f_1)(1 - f_2)$, calculate the distribution function f (in the final states 1 and 2) following the analytical expression given by the Fermi-Dirac distribution .
  This simulation will provide an estimate of the exact number of collisions associated with the temperature considered.
  Of course, in the T = 0 case the distribution function is equal to 1(0) inside (outside) the Fermi sphere and the number of successful collisions should be rigorously equal to zero.

3) **Number of runs:**
   BUU-like: 100 test particles per nucleon, 10 runs
   MD: 200 runs

The following calculation modes should be considered:

C: No-blocking cascade mode: only collisions, no Pauli-blocking, no mean field.

CB: Blocking cascade mode: collisions with Pauli blocking, no mean field.

Altogether there will be 6 calculations: 2 modes (C,CB), 2 options (OP1/2) and 2 temperatures (T0,T5). (only 6, because for mode C the two options do not enter). Please provide the results in the following sequence using the above nomenclature (CT0, CT5, CBOP1T0, CBOP2T0, CBOP1T5, CBOP2T5).
The calculation CBOP2T0 should be the free collisionless propagation of a Fermi gas and thus trivial, but a good check anyway. Here only one run for both BUU and MD is sufficient.

The corresponding output file extensions are listed in the following table:

	T=0	T = 5 MeV
C	*.CT0	*.CT5
CB+OP1	*.CBOP1T0	*.CBOP1T5
CB+OP2	*.CBOP2T0	*.CBOP2T5

4) Output files:
a) (Test) particle files (please name your file as "particle.*"): for these files only one run for BUU codes and 100 runs for MD codes,
at times **0,20,40,60,80,100,120,140** fm/c the following information for each (test) particle:
ID=0, charge (0 or 1), mass [GeV], (x,y,z) [fm], (px,py,pz) [GeV]

The variables "charge" and "ID" are *integer* variables, the others are *real*. (The variable ID, used previously to identify proj and target nucleons, is not needed in a box calculation. We keep it anyway, to have the structure of the files the same as before.)

b) Collisions (please name your file "collision.*"): here we think of two options:
i) Provide for each of the above 6 calculations (for mode CB separately for attempted and successful collisions)
(1) the collision rate $\Delta N_{coll}/\Delta t$ as a function of time (from 0 to 140 fm/c, with a step of 10 fm/c, i.e Δt = 10 fm/c), and please name your file as "dNdt_attempted.*", "dNdt_successful.*"
(2) the collision energy distribution $\Delta N_{coll}/\Delta E_{tot}$ as a function of the total energy of the colliding pair including the rest masses (or sqrt(s) relativistically) in the interval from 1.8 to 2.0 GeV with bin size ΔE_{tot}=0.01 GeV. Please name your file as "dNdE_attempted.*", "dNdE_successful.*"

ii) Alternatively send collision files, as in the earlier homework:
write for each run for each attempted collision for the two colliding particles
**time of coll [fm/c], ID1, charge1, mass1, px1,py1,pz1**
ID2, charge2, mass2, px2,py2,pz2, isuccess
The variables *ID, charge* and *isuccess* are *integer* variables, the others are *real*. "isuccess" is 0(1) if the collision is Pauli blocked (not Pauli blocked).

c) Figures:
If possible, please also generate, for each calculation mode, option and temperature figures representing the collision rate $\Delta N_{coll}/\Delta t$ and collision energy distribution $\Delta N_{coll}/\Delta E_{tot}$, in order to avoid misunderstandings, from our side, when analyzing your output files (for mode CB separately for attempted and successful collisions). Following is an example.
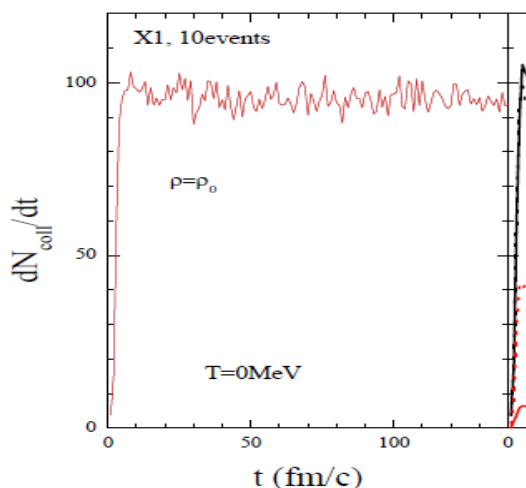
5) Reading program and uploading
a) Please provide a simple Fortran program to read your files, and check that this program indeed works. This sounds simple, but in Trento we had considerable difficulties. This may be caused by trivial things like a blank line between runs or a line with the time or impact parameter.
b) Compress your files using "gzip" or "bzip2", otherwise we will have again problems to uncompress your files. The files will be very large!

PLEASE send your results before Jan. 16, 2016.
Many thanks for your efforts,
and many greetings,
the Box Simulation Organizing Committee
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