Possible differences among codes in the Box Homework 1

Box Simulation Organizing Committee

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Three reasons, at least, of the divergence of collisions numbers by different codes.

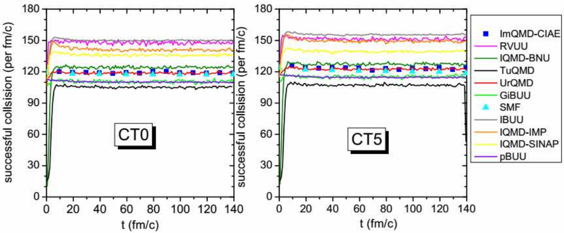
- Relativistic or nonrelativistic. (some effect)
- The Bertsch prescription or a method that automatically reproduces ideal value. (some effect)
- Spuriously repeated collisions are avoided or allowed in the Bertsch prescription. (very important)
- In addition, it should be affected if some codes require additional conditions for two particles to attempt a collision, such as a distance cut for accelerating the code. (can be very important, depending on what is actually done)

Even in the simplest case CT0, many of the calculations are diverging from each other and from the known theoretical value. We must solve this problem.

- Please check the questions in pages 3 - 8.
- Below the questions and after the page 9, we also put some information to show how these points will influence the results.

C mode :

Cascade, only collisions, no Pauli-blocking, no mean field



See the slides by Yongja Wang and Maria Colonna, and the note by Hermann Wolter, for the full description of the current results.

Kinematics

Questions

Is the kinematics in the code relativistic or nonrelativistic?

1. Equation of motion: $d\mathbf{R}_i/dt = \mathbf{P}_i/\sqrt{M^2+\mathbf{P}_i^2}$ or $d\mathbf{R}_i/dt = \mathbf{P}_i/M$.
2. For the judgment of collision attempts.
   - In the relativistic case, the box condition must be first considered for the relative coordinate $\Delta\mathbf{r} = \text{modulo}(\mathbf{r}_i - \mathbf{r}_j + \frac{1}{2}L,\ L) - \frac{1}{2}L$ in the original frame, and then it should be Lorentz transformed to the two-particle center-of-mass frame.
3. Lorentz or Galilei transformation to the frame in which a two-nucleon scattering is isotropic.

Effect in dN_{coll}/dt for CT0: 124[1] (nonrelativistic) → 119 (relativistic): (corrected Bertsch)

Ideal value for Boltzmann: 116.8 (nonrelativistic) → 112.6 (relativistic, by J. Xu)

[1] Simulated results in this document were obtained with a simple cascade code by A. Ono unless otherwise mentioned. It works both in relativistic and nonrelativistic kinematics. The default choice here is nonrelativistic and with a corrected Bertsch prescription that avoids spurious repetition of collisions.

Initialization

Questions

1. What was the value of the Fermi momentum for initialization?
   - The value suggested by HW1: $P_f = 265$ MeV/c.
   - The precise value $P_f = \hbar(\frac{3}{2}\pi^2\rho)^{1/3} = 263.04$ MeV/c.
2. Are there any correlations between different particles?
   - to avoid two particles that are too close to each other in phase space?
   - to have a fixed value of the total energy, avoiding event-by-event fluctuations?

Effect in dN_{coll}/dt for CT0: 124 ($P_f = 265$) $\to$ 123 (precise P_f)

If we are not sure, the value of the total energy should be checked for the results of different codes.

Basic method to judge collision attempts

Questions

1. In the BUU case, do you use the parallel or full ensemble method?

   (In the case of the full ensemble method, the cross section σ below should be suitably replaced by σ/N_{tp}, where N_{tp} is the number of test particles per nucleon.)

2. How is it judged whether two particles (i, j) attempt a collision during a time step Δt?
   - The Bertsch prescription $2|\mathbf{r}\cdot\mathbf{v}| < \mathbf{v}^2\delta t$ and $\mathbf{r}^2 - (\mathbf{r}\cdot\mathbf{v})^2/\mathbf{v}^2 < \sigma/\pi$, where $\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$ and $\mathbf{v} = \mathbf{v}_i - \mathbf{v}_j$ are the relative coordinate and velocity in some frame.
     1. Nonrelativistic. $\mathbf{r}$ and $\mathbf{v}$ are the Galilei-invariant relative coordinate and velocity. $\delta t = \Delta t$.
     2. Relativistic. $\mathbf{r}$ and $\mathbf{v}$ are calculated in the two-particle c.m. frame. $\delta t = \Delta t$.
     3. Relativistic. $\mathbf{r}$ and $\mathbf{v}$ are calculated in the two-particle c.m. frame. $\delta t = \gamma\Delta t$ with the γ factor.
   - The mean free path prescription
   - anything else

Effect in dN_{coll}/dt for CT0: Nonrelatitivtic: 117 (ideal Boltzmann) → 124 (corrected Bertsch)
Relativistic: 112.6 (ideal Boltzmann) → 118 (corrected Bertsch, both Y. Zhang and J. Xu)
Is this a kind of many-body effect? (See Slide 13)

More on the method to judge collision attempts

Questions

1. Are there any additional conditions that a pair of two nucleons should not attempt a collision? (Conditions on the distance, on $\sqrt{s}$, etc.)
2. In the QMD case, does the wave packet width play any role in two-particle collisions, or do you use only the information of the centroids?
3. After a particle i collide with j in a time step, it will further attempts collisions in the same time step with other particles k. Is the collision (i, k) judged by using the momentum $\mathbf{P}_i$ before the first collision (i, j) or after it?
4. Are the pairs of two particles checked always in the same order at different time steps? (E.g., (1,2) is always the first and (1279, 1280) is always the last.)

Spuriously repeated collisions in the Bertsch prescription

Question

If you faithfully follow the Bertsch prescription, when two nucleons have approached to each other within the interaction range, they can repeat several collisions before they move a way from each other (see Slide 9).

- Does your code do any trick to avoid such spuriously repeated collisions? (see Slide 12 for an example of how to avoid them.)

Effect in dN_{coll}/dt for CT0: 124 (avoid spurious) → 161 (allow spurious, $\Delta t = 0.5$ fm/c)

Both Y. Zhang and J. Xu also got fully consistent results on this effect of the spurious collisions.

All the codes should be modified to avoid spuriously repeated collisions, to see whether the divergence of the results disappears.

Time step

Questions

1. What was your choice of the time step Δt, 0.5 or 1 fm/c?
2. Did you (or will you) check that the results don't depend on the choice of Δt?

In some cases, the convergence of the results for $\Delta t \to 0$ is very slow. For example, when the spuriously repeated collisions are allowed,

dN_{coll}/dt for CT0: 149 ($\Delta t = 1.0$ fm/c), 161 ($\Delta t = 0.5$ fm/c), 171 ($\Delta t = 0.2$ fm/c)

This Δt dependence is now consistent with both calculations by Y. Zhang and J. Xu.
See also Slide 11 for more about the Δt dependence.

The Δt dependence is not so strong and $\Delta t = 0.5$ fm/c is sufficient, if the spuriously repeated collisions are avoided by a suitable method.

The Bertsch prescription

Bertsch prescription (nonrelativistic version)

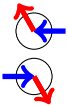
Two nucleons may collide

- when the relative distance is minimum during a time step, $2|\mathbf{r}\cdot\mathbf{v}| < \mathbf{v}^2\Delta t$,
- and when the minimum distance is $\mathbf{r}^2 - (\mathbf{r}\cdot\mathbf{v})^2/\mathbf{v}^2 < \sigma/\pi$,

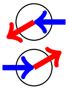
where $\mathbf{r}$ and $\mathbf{v}$ are the relative coordinate and velocity, respectively, at the current time t.

There is not anything more.

Then the same pair of two particles can collide more than once, as in the second example.



- By the collision, the momenta are changed from the blue to the red arrows. After the collision, the particles are moving away from each other ($\mathbf{r}\cdot\mathbf{v} > 0$), so they will never collide again.



- After the collision (red arrows), the particles are again approaching to each other ($\mathbf{r}\cdot\mathbf{v} < 0$) and the distance is $|\mathbf{r}| < \sqrt{\sigma/\pi}$, so they will collide again at a later time.

Nature of this problem doesn't depend on Δt. Namely, the problem exists in the limit $\Delta t \to 0$.

Analytic case of the problem

For a scattering of two particles with the initial impact parameter $b < \sqrt{\sigma/\pi}$, the probability P_n that collisions occur n times is given by

$$P_n = \frac{1}{2^n} \tag{1}$$

under the assumptions that

- there are no other particles, and
- the Pauli blocking probability is zero, and
- angular distribution is isotropic (as in the homework).

Proof is straightforward. After the first collision, because the direction of $\mathbf{v}$ is isotropic, the particles are approaching ($\mathbf{r}\cdot\mathbf{v} < 0$) with the 50% probability so that the second collision will occur at a later time.

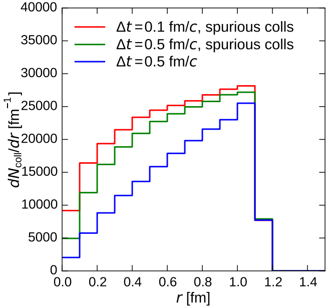
In this case, a single scattering is actually 'double'-counted. The average number of collisions is

$$\langle n \rangle = \sum_{n=1}^{\infty} n P_n = 2 \tag{2}$$

What happens when repeated collisions are allowed? (case CT0)

Distribution of the distance r

between the scattered nucleons



- A good triangular shape (blue) when spurious repetition is avoided.
- Collisions with smaller r increase (green and red) if spurious repetition is allowed.
- Convergence for $\Delta t \to 0$ is slow when spurious repetition is allowed, in particular, for small r.

‘Attractive’ effect

The second collision spuriously occurs only when the first collision happened to be ‘attractive’ ($\mathbf{r}\cdot\mathbf{v}' < 0$ after the collision). Therefore, the two-particle distance at the second collision is always smaller than that at the first collision. (The same argument is continued until a ’repulsive’ collision happens.)

Δt dependence

With a finite Δt, the second collision is sometimes missed if it should happen in the same time step. The missing occurs when $0 < -\mathbf{r}\cdot\mathbf{v}' \lesssim \frac{1}{2}|\mathbf{v}'|^2\Delta t$, where $\mathbf{v}'$ is the relative velocity after the first collision. Therefore, the missing (i.e., underestimation of N_{coll}) is more serious with small $\mathbf{r}$, large $\mathbf{v}$ and large Δt.

How to avoid spurious repeated collisions

Principle

After a collision happened for a pair of particles (i, j), the same pair should not collide again until one of i and j collides with some other particle.

Each particle should carry the ID of the last experienced collision. CID(i)

- Initialize CID(:) at the beginning of each event.

```
CID(:) = -1
```

- When a collision occurred, a collision ID is generated, which can be a random number. The collision ID's of the collided particles are updated by this new collision ID.

```
call random_number(CID(i))
CID(j) = CID(i)
```

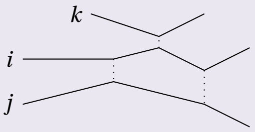
- Two particles carrying the same collision ID do not attempt collisions.

```
if (CID(i).ge.0 .and. CID(i).eq.CID(j)) cycle ! don't attempt a collision
```

Many-body effects?

$dN_{\text{coll}}/dt = 124$ may be larger than the ideal value 119 (both are for nonrelativistic case) due to the following process.

The discussion here is for the exact limit of $\Delta t \to 0$, so that different collisions do not happen at the same time.



When two particles i and j approach to each other, they can collide more than once due to the existence of another particle k.

On the other hand, if there were no other particles, the second collision between i and j is not allowed by our prescription.

For the quantum mechanical three-body scattering, such a diagram should be included in the scattering amplitude, where each interaction corresponds to a T- or G-matrix. If it is allowed to replace the process by an incoherent sequence of three two-body scatterings, our prescription to avoid the spurious collisions is justified. However, we probably don't claim that this is the correct description of the quantum three-body scattering. In any case, due to our choice of the prescription, this kind of many-body effect (i.e., the effect due to the third particle) is likely to increase the two-particle collision number.