PHQMD
(Parton-Hadron-Quantum-Molecular-Dynamics)
- a novel microscopic transport approach to study heavy ion reactions

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- Why a novel approach?
- Basics of the QMD Transport theory
- Inherent Fluctuations and Correlations in QMD
- Fragment Formation

- Comparison with existing data
- Perspectives for BMN/NICA/FAIR/RHIC
Why do we need a novel approach?

At **3 AGeV**, even in central collisions:

20% of the baryons are in clusters

... and baryons in clusters have quite different properties
If we do not describe the **dynamical formation** of fragments

- we cannot describe the nucleon observables \((v_1, v_2, \frac{dn}{dp_T})\)

- we cannot explore the new physics opportunities like
  - hyper-nucleus formation
  - 1\(^{\text{st}}\) order phase transition
  - time development of the phase space density

**Present microscopic approaches** fail to describe fragments at NICA/FAIR energies

VUU(1983), BUU(1983), (P)HSD(96), SMASH(2016) solve the time evolution of the one-body phase space density \(\rightarrow\) **no fragments**

UrQMD solves the n-body theory but has no potential
  \(\rightarrow\) **nucleons cannot be bound to fragments**

(I)QMD solves the n-body theory but is limited to energies \(< 1.5\ \text{AGeV}\)
  \(\rightarrow\) **describes nicely fragments at SIS energies,**
  but conceptually not adapted for NICA/FAIR
QMD (like AMD and FMD) are true N-body theories.

**N-body theory:** Describe the exact time evolution of a system of N particles. All correlations of the system are correctly described and fluctuations correctly propagated.

**Roots in classical physics**

A look into textbooks on classical mechanics: If one has a given Hamiltonian

\[ H(r_1, \ldots, r_N, \ldots, p_1, \ldots, p_N, t) \]

\[ \frac{dr_i}{dt} = \frac{\partial H}{\partial p_i}; \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial r_i} \]

For a given initial condition

\[ r_1(t = 0), \ldots, r_N(t = 0), p_1(t = 0), \ldots, p_N(t = 0) \]

the positions and momenta of all particles are predictable for all times.
Roots in Quantum Mechanics

Remember QM course when you faced the problem

• we have a Hamiltonian
  \[ \hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V \]

• the Schrödinger eq.

  \[ \hat{H} |\psi_j\rangle = E_j |\psi_j\rangle \]

  has no analytical solution

• we look for the ground state energy

Ritz variational principle:

Assume a trial function \( \psi(q, \alpha) \) which contains one adjustable parameter \( \alpha \), which is varied to find a lowest energy configuration:

\[ \frac{d}{d\alpha} <\psi|\hat{H}|\psi> = 0 \]

determines \( \alpha \) for which

is closest to the true ground state wavefunction

and

\[ <\psi|\hat{H}|\psi> > E_0 \]
Extended Ritz variational principle (Koonin, TDHF)

Take trial wavefct with time dependent parameters and solve

\[
\frac{\langle \psi_N | i \frac{d}{dt} \hat{H} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = 0 \quad (1)
\]

QMD trial wavefct for one particle (Gaussian):

\[
\psi_i(q_i, q_{0i}, p_{0i}) = C \exp\left[-(q_i - q_{0i} - \frac{p_{0i}}{m} t)^2 / 4L\right] \cdot \exp[ip_{0i}(q_i - q_{0i}) - i \frac{p_{0i}^2}{2m} t]
\]

For N particles:

\[
\psi_N = \prod_{i=1}^{N} \psi_i(q_i, q_{0i}, p_{0i}) \quad \text{QMD}
\]

\[
\psi_F^N = \text{Slaterdet} \left[ \prod_{i=1}^{N} \psi_i(q_i, q_{0i}, p_{0i}) \right] \quad \text{AMD/FMD}
\]

The QMD trial wavefct eq. (1) yields

\[
\frac{dq}{dt} = \frac{\partial \langle H \rangle}{\partial p} \; ; \; \frac{dp}{dt} = -\frac{\partial \langle H \rangle}{\partial q}
\]

For Gaussian wavefct eq. of motion very similar to Hamilton’s eqs.
VUU, BUU, HSD, SMASH solve a Boltzmann type eq.

\[
\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}
\]

Same interaction, not possible classically

\[
\left( \frac{\partial f}{\partial t} \right)_{\text{coll}} = \int \int gI(g, \Omega)[f(p'_A, t)f(p'_B, t) - f(p_A, t)f(p_B, t)] d\Omega d^3p_A d^3p_B.
\]

\(\mathbf{v} \cdot \) differential cross section

Only the test particle method made it possible to solve the BUU equations in complex situations

Test particle method -> replace integrals by sums (MC) integration

\[
f(r, p, t) = \lim_{N \to \infty} \sum_{i=1}^{N} \delta(r - r_i(t)) \delta(p - p_i(t))
\]

test particle \(\neq\) nucleon

If \(N\) small unphysical fluctuations

What means \(N \to \infty\) in reality?
When is $N$ sufficiently large?

One uses delta like forces: $F(r) = \delta(r)$ (Skyrme) but then point-like test particles $f = \Sigma \delta(r-r_i(t))$ do almost never interact. Solution: one uses grids (and introduces the grid size $a$ which plays a similar role as the width in QMD).

**Euler**

Result different if number of test particles is finite (usually $N=100$)

**Lagrange**

Average distance between nucleons 2fm. Grid size $\approx 1$fm (surface). Therefore very many test particles necessary to avoid numerical fluctuations: $100tp \rightarrow 12$ in a cell $\rightarrow 30\%$ fluctuation
Bi+Xe, 28 AMeV  b=5fm

25 test particles/N

Less physical

W. Bauer
U. Schröder

275 test particles/N

More physical

Numbers of test particles must be large enough
Attempts have been made to form clusters in the test particle BUU approach using a coalescence description for test particles

\[
P_d(r_1, r_2, p_1, p_2, t) = \rho^W_d (p_1 - p_2, r_1 - r_2)
\]

deuteron Wigner density

but theoretically not consistent because 1 and 2 are test particles, no nucleons.

In addition:

- result depends on the number of test particles
- result depends on time \( t \) when eq. is applied
- time is different for different particles: PRC56,2109
- no information about the formation process
How does a collision term appear?

The Hamiltonian (Schrödinger and Boltzmann eq.) contains $V = NN$ potential

The NN potential has a hard core, would make transport calculations very unrealistic (Bodmer 75) (independent of the beam energy the participants would thermalize like In a cascade calculation without Pauli blocking)

Solution (taken over from TDHF):
Replace the NN potential $V_{NN}$ by the solution of the Bethe-Salpeter eq. in T-matrix approach (Brueckner)

$$T = V + V_{T}$$

$$T_{\alpha}(E; q, q') = V_{\alpha}(q, q') + \int k^{2} dk\ V_{\alpha}(q, k)\ G^{0}_{QQ}(E, k)\ T_{\alpha}(E; k, q')$$
Consequences:

\[ T_\alpha(E; q, q') = V_\alpha(q, q') + \int k^2 dk \, V_\alpha(q, k) \, G_{QQ}^0(E, k) \, T_\alpha(E; k, q') \]

\[ V_{\text{NN}} \text{ is real} \rightarrow T \text{ is complex} = \text{Re} T + i \text{Im} T \]

\[ \text{corresponds to } V_{\text{NN}} \text{ in Hamiltonian (Skyrme)} \]

\[ \sigma_{\text{elast}} \text{ collisions done identically in BUU (test-particles) and QMD (particles)} \]

To this one adds inelastic collisions

\( \text{(BUU, HSD, SMASH and QMD - the same way)} \)

\( \rightarrow \text{Therefore in BUU and QMD the spectra of produced particles are (almost) identical (intensively checked in the past)} \)
The goal: Dynamical modeling of cluster formation by a combined model

\[ \text{PHQMD} = (\text{QMD & PHSD}) \& \text{SACA (FRIGA)} \]

- Parton-Hadron-Quantum-Molecular-Dynamics - a non-equilibrium microscopic transport model which describes n-body dynamics based on QMD propagation with collision integrals from PHSD (Parton-Hadron-String Dynamics) and cluster formation by the SACA model or by the Minimum Spanning Tree model (MST).

- MST can determine clusters only at the end of the reaction.

- Simulated Annealing Clusterization Algorithm - cluster selection according to the largest binding energy (extension of the SACA model -> FRIGA which includes hypernuclei). FRIGA allows to identity fragments very early during the reaction.
The potential interaction is most important in two rapidity intervals:

- at beam and target rapidity where the fragments are initial - final state correlations and created from spectator matter
- at midrapidity where - at a late stage - the phase space density is sufficiently high that small fragments are formed

In both situations we profit from the fact that the relative momentum between neighboring nucleons are small and therefore nonrelativistic kinematics can be applied.

Potential interaction between nucleons

\[ U_{ij}(r, r') = U_{\text{Skyrme}} + U_{\text{Coul}} \]
\[ = \frac{1}{2} t_1 \delta(r - r') + \frac{1}{\gamma + 1} t_2 \delta(r - r') \rho^{\gamma-1}(r) \]
\[ + \frac{1}{2} \frac{Z_i Z_j e^2}{\rho(r)} \]  

\[ (3) \]

\( t_1 \), \( t_2 \) and \( \gamma \) adjusted to reproduce a given nuclear equation of state
To describe the potential interactions in the spectator matter we transfer the Lorentz-contracted nuclei back into the projectile and target rest frame, neglecting the small time differences.

\[
\langle U(\mathbf{r}_i) \rangle = \sum_j \int d^3r d^3r' d^3p d^3p' U_{ij}(\mathbf{r}, \mathbf{r}') f_i(\mathbf{r}, p, t) f_j(\mathbf{r}', p', t)
\]

\[
\langle U_i(\mathbf{r}_i, t) \rangle = \alpha \left( \frac{\rho_{int}}{\rho_0} \right) + \beta \left( \frac{\rho_{int}}{\rho_0} \right)^\gamma.
\]

For the midrapidity region \( \gamma \to 1 \). and we can apply nonrelativistic kinematics as well.

All elastic and inelastic collisions are treated as in PHSD - therefore the spectra of produced particles are very similar to PHSD results.
Results
First Results of PHQMD

Produced particles are well reproduced at SIS/NICA/FAIR energies

(dominated by collisions \(\rightarrow\) similar to PHSD)
How to define fragments in transport theories which propagate nucleons?

A) **Minimum Spanning Tree (MST)** is a cluster recognition method applicable for the (asymptotic) final state where coordinate space correlations may only survive for bound states. The MST algorithm searches for accumulations of particles in coordinate space:

1. Two particles are **bound** if their distance in coordinate space fulfills

   \[ |\vec{r}_i - \vec{r}_j| \leq 2.5 \text{ fm} \]

2. A particle is **bound to a cluster** if it is bound with at least one particle of the cluster.

   ![Diagram of Minimum Spanning Tree](image)

   Additional momentum cuts (coalescence) change little:
   Large relative momentum
   -> finally not at the same position

B) SACA and FRIGA see talk of V. Kireyev
There are two kinds of fragments

- formed from **spectator matter**
  close to beam and target rapidity
  initial-final state correlations
  HI reaction makes spectator matter unstable
  can be identified by MST or SACA → Kireyev

- formed from **participant matter**
  created during the expansion of the fireball
  “ice” ($E_{\text{bind}} \approx 8 \text{ MeV/N}$) in “fire” ($T \geq 100 \text{ MeV}$)
  origin not known yet
  seen from SIS to RHIC
  can be only identified by MST presently
  (quantum effects are important)
**First Results of PHQMD**

**Spectator Fragments**

experm. measured up to $E_{\text{beam}} = 1\text{AGeV}$ (ALADIN)

agreement for **very complex fragment observables** like the
- energy independent “rise and fall”
- largest fragment ($Z_{\text{bound}}$)

$rms(p_t)$ shows $\sqrt{Z}$ dependence
Protons at midrapidity well described

midrapidity fragment production increases with decreasing energy

1.5 AGeV central

> 30% of protons bound in cluster
First Results of PHQMD

There are all kinds of fragments at midrapidity and they are stable (MST finds at 60fm/c the same fragments as at 90fm/c)
First Results of PHQMD

- Fragments are stable from 30 fm/c -> 90 fm/c
- Hyper-nuclei are produced in number

Still activity in spectator matter after 30 fm/c
At RHIC

hyper-nuclei also from spectator matter
Z=2 fragments at midrapidity

\( \sqrt{s} = 200 \text{ AGeV AuAu } b=2\text{fm hard} \)
Conclusions

We presented a new model, PHQMD, for the NICA/CBM energies which allows - in contrast to all other models - to predict the
dynamical formation of fragments

- allows to understand the proton spectra and the properties of light fragments (\(dn/dp_Tdy, v_1, v_2, \) fluctuations)
- allows to understand fragment formation in participant and spectator region
- allows to understand the formation of hypernuclei

Very good agreement with the presently available fragment data as well as with the AGS single particle spectra

But a lot has still to be done!!
Back up
Fragments - the most interesting n-body observables

QMD has been constructed to study multifragmentation. Fragments are N-body correlations -> not accessible in BUU.

In QMD fragments are preserved initial state correlations.

Fragment nucleons come from a well defined subspace of the initially populated phase space.
How to define fragments in transport theories which propagate nucleons?

History:

- **Minimum spanning tree** (possible at the end of the reaction)
  - Study of fragmentation mechanism impossible
- **SACA** or ECRA determines fragments very early
  - Possible to study reaction mechanism
- **New SACA** (talk of A. LeFevre) allows for studying isotope yields and hypernuclei (including symmetry energy, pairing and shell effects)
If we want to identify fragments earlier one has to use momentum space info as well as coordinate space info.


a) Take the positions and momenta of all nucleons at time $t$.
b) Combine them in all possible ways into all kinds of fragments or leave them as single nucleons.
c) Neglect the interaction among clusters.
d) Choose that configuration which has the highest binding energy.

Simulations show: Clusters chosen that way at early times are the **prefragments** of the final state clusters because **fragments are** not a random collection of nucleons at the end but **initial-final state correlations**
How does this work?
Simulated Annealing Procedure: PLB301:328, 1993
later SACA

Take randomly 1 nucleon out of a fragment

Add it randomly to another fragment

\[ E = E_{\text{kin}}^1 + E_{\text{kin}}^2 + V^1 + V^2 \]
\[ E' = E'_{\text{kin}}^1 + E'_{\text{kin}}^2 + V'^1 + V^2 \]

If \( E' \) < \( E \) take the new configuration
If \( E' \) > \( E \) take the old with a probability depending on \( E' - E \)
Repeat this procedure very many times

→ Leads automatically to the most bound configuration
ECRA or SACA can really identify the fragment pattern very early as compared to the Minimum Spanning Tree (MST) which requires a maximal distance in coordinate space between two nucleons to form a fragment.

At 60 fm/c $A_{\text{max}}$ and multiplicities of intermediate mass fragments are determined.
Evidence for early cluster formation

Strong correlation between $\beta/\beta_{\text{proj}}$ and $N/Z$

Aladin supports this (LeFevre)

Can only be explained if fragments are formed early and gets therefore full Coulomb boost

Statistical models cannot at all explain this result
Fluctuations due to collision term

The collisions term causes fluctuations (in density and momentum space) because it removes particles from their phase space cell.

In BUU these fluctuations are $1/N$ times smaller than in QMD and therefore negligible for large $N$ (number of test particles).

In QMD these fluctuations are responsible for fragmentation (especially for spectator fragments, dominant for $E > 100$ AMeV).

(and also for single nucleon spectra because one has to subtract fragment nucleons to obtain measured single part spectrum)

Because fluctuations are important: attempts to introduce additional fluctuations in BUU
• take a small number of test particles ($N_1$):
  - mathematically this is then **not a correct solution** of the differential (BUU) equation
  - in practise problems with **energy and momentum conserv.**
  - assumes,relations between physical ($\sigma, T, \rho$) and mathematical fluctuations ($1=\overline{N}$) which are difficult to justify

• add a fluctuating force to the BUU equation
  Colonna, Suraud, Ayik.......  
  - mathematically correct
  - difficult to determine these fluctuations
    size in $\Delta r$ and $\Delta p$, dependence of $T, \rho, (as \ effectively \ in \ QMD)$.???

• move in BUU several testparticles simultaneously (Bertsch..)
  - how many and which ones?
  - in which way?

**Question:** Why not start directly from a N-body theory where fluctuations are (better) under control ?  
(Width L fixed by nucl. density profile etc.)
Early fragment formation reproduces data quantitatively

Example: Bimodality

\[
a_2(t) = \frac{Z_{\text{max}(t)} - Z_{\text{max} - 1(t)}}{Z_{\text{max}(t)} + Z_{\text{max} - 1(t)}}
\]

mean value as well as the distribution (arXiv:0708.3639)
With ECRA we can trace back the fragment formation. Can calculate $a_2(t)$:

$$a_2(t) = \frac{Z_{\text{max}}(t) - Z_{\text{max}-1}(t)}{Z_{\text{max}}(t) + Z_{\text{max}-1}(t)}$$

Fragment pattern is created very early.
How to determine the width L?
- **surface** of the nucleus -> L not too large
- **correlations** of the relative 2-part. wavefct in a nucleus (healing distance) \( \approx 2 \text{fm} \)
- **range** of nuclear potential \( \approx 2 \text{ fm} \)

\[
L = 4.33 \text{ fm}^2
\]

Where \( L \) shows up in the observables?
- initially the **average over many simulations** gives the same \( \rho(r) \) as BUU \( \int d^3p f (r; p; t) \)
  - **but** the density in each simulation fluctuates around \( \rho(r) \)
  - **Initial state fluctuations depend on** \( L \)
- \( L \) determines the local density change if a nucleons is kicked out by a hard collision (spectator fragmentation)
- **L influences spectator fragmentation**
- \( L \) plays also a role when fragments are formed from prefr. in **participant fragmentation** (via binding energies)
The QMD trial wavefct eq. (1) yields

\[ \frac{dq}{dt} = \frac{\partial <H>}{\partial p} \quad ; \quad \frac{dp}{dt} = -\frac{\partial <H>}{\partial q} \]

very similar to classical Hamilton eq. (H-><H>)
AMD/FMD equations much more complicated

Of course trial wavefct is our choice and nothing prevents us to assume that also the width L is time dependent.

In QMD L is assumed to be constant

It’s value has not changed since the first publication in 1985
Influence of L on fragment yield (Y. Leifels)

AuAu 150 AMeV

There are differences but they are modest
How one should this imagine?
Easiest Way: percolation model (Bauer)

Divide the nucleus in phase space cells. Inside the nucleus initially all cells are filled by a nucleon.

Filled cell (model in 2 dim)

Collisions with large mom transfer between proj and targ nucleons remove nucleons from their orig.cells

Connected occupied cells become prefragments

Completely opposite to statistical models:
No initial final state correlations, nucleons are formed very late at densities less than $< 0.2 \rho_0$. 
Collisions in BUU and QMD

BUU and QMD describe the (measured) one particle density

\[ \Psi(r) = \int d^3p \, f(r; p; t) = \bigcirc = \sum_{i=1}^{N} \tilde{A}_i(r; t) \]

BUU \hspace{1cm} QMD

and the measured Fermi distribution with

\[ \tilde{A}_i(r; r_{i0}(t); p_{i0}(t); t) = \exp[i \cdot (r_{i0}(t) \cdot p_{i0}(t)t = m)^2 - 4L] \]

Therefore \( f(r; p_1; t)f(r; p_2; t) \propto (p_1; p_2 \neq p_3; p_4) \) is the same and consequently the collisions should be very similar

Parallel ensemble method: subroutines are even identical

BUT: In AMD and FMD cross section cannot be defined that way \( \rightarrow \) FMD: no coll, AMD rather arbitrary
BUU/LV/VUU

```
f (r_1 ; p_1 ; t) = f (1)
```

Can predict correlations only if

```
f (2) = f (1) f (1)
```

- deuteron density
  - if neutron density \* proton density
    (what is rarely the case)
- if the system is in global equilibrium

Parameters: grid size

consequences: Trento workshop

Summary

```
f^{(N)} (r_1 ; r_2 ; \cdots ; r_N ; p_1 ; p_2 ; \cdots ; p_N ; t) = f^{(N)}
```

Can predict any correlation

```
f (2) = \int d^3 r_i d^3 p_i f^{(N)}
```

allows predictions of fragments

HBT correlations

QMD/IQMD/AMD

We expect that

- 1 body observables like \((p,n), \Lambda, K, \pi\) spectra are identical
  - This has extensively been checked (Init. Fluc not important)
- N body observables differ