Hunting nuclear clusters

Cluster finding using Coalescence, MST and Simulated Annealing

V. Kireyeu, 63rd meeting of the PAC for Particle Physics

CCL Common Clusterization Library

1. Common Clusterization Library

- **Box-like coalescence:** proximity Δr, Δp at the freeze-out time.
- **Minimum Spanning Tree (MST):** spatial proximity in the cluster COM frame, optional momentum-space cuts, binding-energy stability checks.
- **Smart MST (sMST):** continuous tracking of stable MST clusters throughout the reaction.
- **Simulated Annealing chain:** binding energy minimisation via a Metropolis-type criterion, effective at early stages where MST fails.
- **Configurability:** Rich set of tuneable parameters (temperature schedule, step modes, momentum cuts, E_{bind} cuts, QMD EoS parameters, Skyrme potential form etc).
- **Unified codebase:** all algorithms share the same particle/energy infrastructure and parameter set.

Open source for open science!

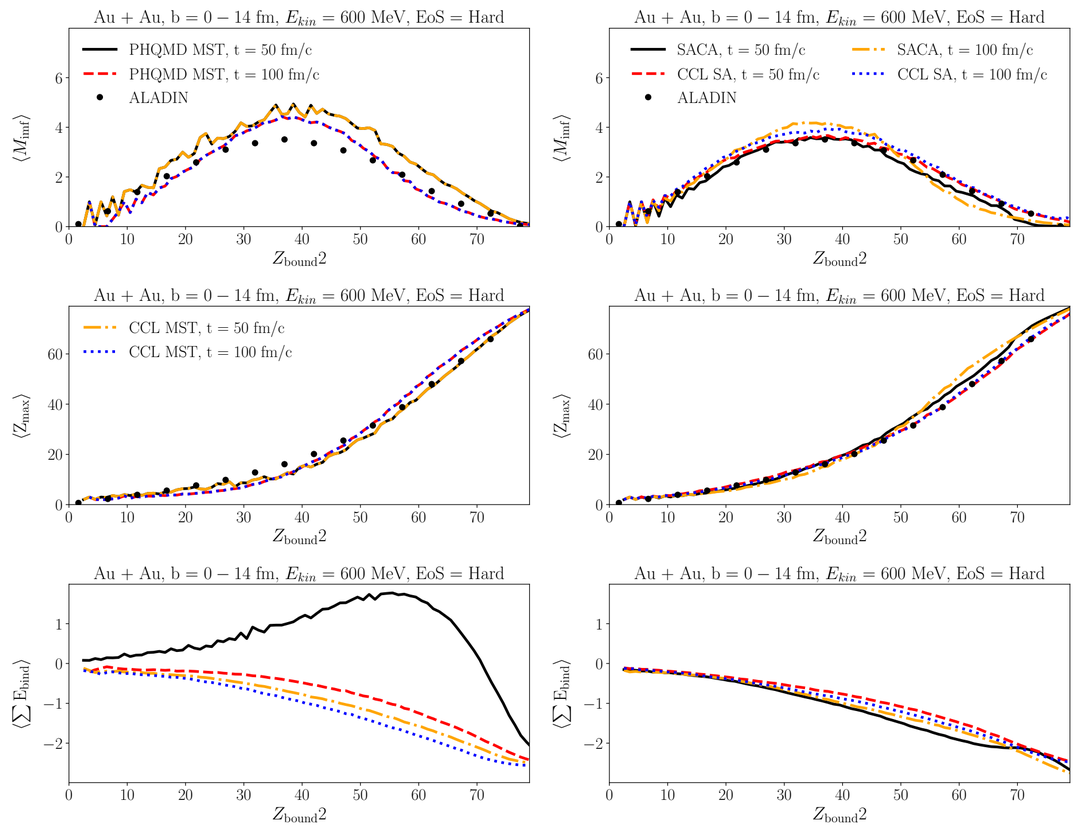
https://github.com/vkireyeu/ccl

2. Still no consensus on the mechanism

- **Coalescence:** all clusters are formed during kinetic **freeze-out**, occurring after the hadronic expansion phase. If the neighbouring nucleons with the appropriate charge are found within the coalescence radius in both coordinate and momentum space, these nucleons are deemed to form a deuteron or part of a light cluster.
- **Potential mechanism:** the potential interaction among nucleons in the hadronic phase gives rise to bound clusters of various sizes, and their multiplicity is contingent upon the specifics of the expansion of the hot interaction zone and its composition.
- **Kinetic mechanism** (not available in CCL)**:** light clusters, such as deuterons, can be generated through inelastic reactions involving hadrons, such as NNπ → dπ and NNN → dN, where a pion or a nucleon acts as a 'catalyst' during the hadronic phase of heavy-ion collisions.

Same clustering logic applied to different models makes differences attributable to physics without algorithmic bias.

3. MST vs Simulated Annealing

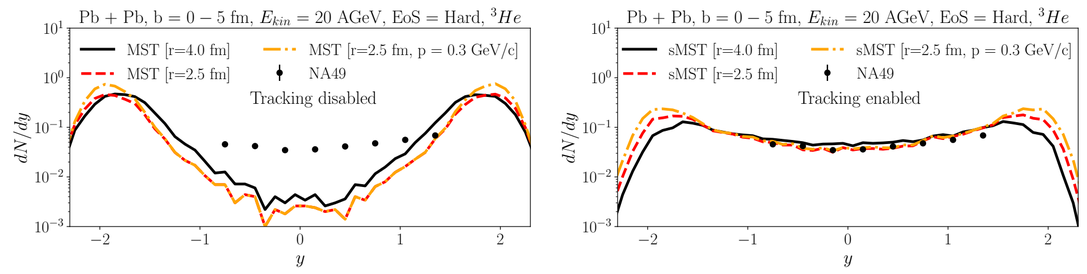


$\langle M_{\rm imf}\rangle$ — mean multiplicity of the forward emitted intermediate mass fragments (3 ≤ Z ≤ 30).
$\langle Z_{\rm max}\rangle$ — average maximal charge of the single fragment in the event.
$Z_{\rm bound}2$ — total number of bound charges (Z ≥ 2) within the forward-emitted clusters in event.

MST: slightly overestimates the experimental «rise and fall» curve. While it's curve is reproduced at all time steps, the mean binding energy at the earlier time is mostly positive for lighter IMF clusters, that means they are not «bound».

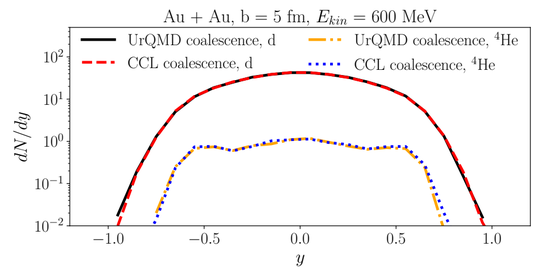
SACA, SA: at earlier time original SACA and CCL SA procedures succeeds to describe the ALADIN experimental data, however, CCL SA shows a bit better agreement. Similar behaviour is true for the $\langle Z_{\rm max}\rangle$ observable: slight overestimation by SACA and the perfect agreement with the data by CCL SA procedure.

4. Smart MST



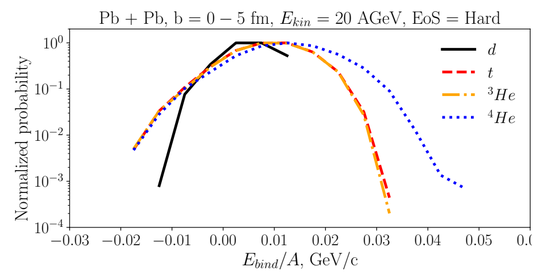
The QMD dynamics propagates single baryons and thus if MST finds a stable cluster, on the next time step it can dissolve without collision occurred even if the corresponding quantum system must be stable.
sMST allows to track stable clusters during the system evolution using only the information about the current step time and the last collision tame of the clusters constituent particles. Applied at all time steps this procedure recovers «lost» clusters automatically.

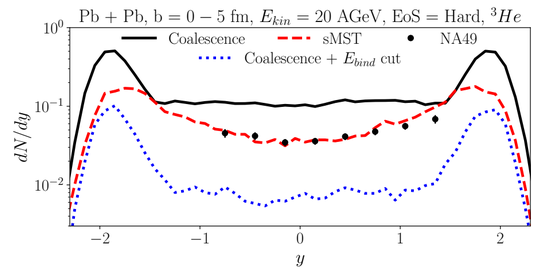
5. Coalescence?



More than half of a century passed since the coalescence approach was firstly proposed to describe the deuterons production in emulsions, then modified to describe the light nuclei production in relativistic heavy-ion reactions. The CCL implements the «box-like» coalescence proposed and successfully used by the authors of the UrQMD transport approach.

It is also possible within the CCL library to check the binding energy of the produced «coalescence» nuclei by the exactly same way used for SA procedure.
The picture is: more than 85% of the each «coalescence» nuclei would be considered as «not bound» within «sMST» or SA-based approaches as their binding energy $E_{bind} > 0$.





The coalescence overestimates the NA49 experimental data within |y| < 1 rapidity window. When applying additional negative binding energy cut, the Helium-3 yields drops down drastically. sMST applied to the same data set describe shows the perfect agreement with the data.

Summary

- The MST-based clusterization reproduce ALADiN observables quite well, however, the application of the SACA and/or SA procedures reduces the total system E_{bind} at earlier times and yields into the better agreement with the experimental data.
- At the later times the mean binding energy of the system $\langle E_{bind}\rangle$ for the MST-based clusterization is similar to the SACA and SA procedures. This could be explained by the fact that at the later times the system is so dilute, so baryons with high relative velocities/momentum are well separated in space, so the found by the proximity criteria MST clusters can be already bound enough.
- The stable clusters tracking procedure «smart MST» («sMST») allows for the noticeable reparation of the nuclei artificially «lost» due to QMD operation features.
- The coalescence based on the spin-isospin combinatorial factor can describe the experimental data, however, more than than 85% of found nuclei are not bound with positive binding energy $E_{bind} > 0$. Addition of the negative binding energy criterion to the «box-like» coalescence strongly suppress the yields of nuclei.
- **The Helium-3 nuclei found by the MST-based cluster finding procedure and the coalescence algorithm applied on top of the exactly the same set of baryons was presented for the first time and compared to the NA49 experimental data. Results favours the «sMST» procedure.**

Modifications in clusterization procedures for heavy-ion collisions: minimum spanning tree, simulated annealing, coalescence, V. Kireyeu, arXiv:2512.02084