

Clustering in AMD

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Workshop on Simulations of Low and Intermediate Energy Heavy Ion Collisions,
ECT*, Trento, Italy, May 11 – 15, 2009

- AMD framework (including some details)
- Cluster correlations in AMD
- Skyrme force with AMD

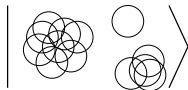
- Gogny force (finite range, density-dependent; $\rho_0 = 0.166 \text{ fm}^{-3}$, $K = 228 \text{ MeV}$)
- The width parameter $\nu = (2.5 \text{ fm})^{-2}$
- \Rightarrow Ground state of the Au nucleus (B.E. = 1537 MeV, $\langle r^2 \rangle^{1/2} = 5.56 \text{ fm}$)
- $\sigma_{\text{NN}} = 40 \text{ mb}$ with isotropic angular distribution. ($\sigma_{\text{NN}} = 0$ if $p_{\text{rel}} < 50 \text{ MeV}/c$.)
- $b = 0$ and $b = 8.376 \text{ fm}$. Initial distance = 15 fm.
- A two-nucleon collision is a scattering of the centroids of two wave packets which have momentum widths.

As the momenta (or \sqrt{s}) of colliding nucleons,

- 1 the momentum centroids are written out (1st result of HW1).
 - 2 the *test particle momenta* taken randomly from the Gaussian distribution $f_W(\mathbf{r}, \mathbf{p})$ are written out (updated result of HW1, and HW2).
- The state is represented by $\{\mathbf{Z}_k, S_{k,ab}; k = 1, \dots, A\}$ in AMD.
100A test particles for output are generated randomly based on $f_S(\mathbf{r}, \mathbf{p})$.
 - Good for the momenta of emitted nucleons.
 - Not good for the internal wave function of nuclei.

AMD wave function

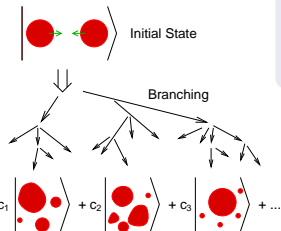
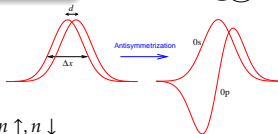
$$|\Phi(Z)\rangle = \det_{ij} \left[\exp \left\{ -v \left(\mathbf{r}_j - \frac{\mathbf{Z}_i}{\sqrt{v}} \right)^2 \right\} \chi_{\alpha_i}(j) \right]$$



$$\mathbf{Z}_i = \sqrt{v} \mathbf{D}_i + \frac{i}{2\hbar \sqrt{v}} \mathbf{K}_i$$

v : Width parameter = $(2.5 \text{ fm})^{-2}$

χ_{α_i} : Spin-isospin states = $p \uparrow, p \downarrow, n \uparrow, n \downarrow$



Stochastic equation of motion for the wave packet centroids Z :

$$\frac{d}{dt} \mathbf{Z}_i = \{ \mathbf{Z}_i, \mathcal{H} \}_{\text{PB}} + \Delta \mathbf{Z}_i(t) + (\text{NN collisions})$$

$$\mathcal{H}(Z^*, Z) = \frac{\langle \Phi(Z) | (T + V) | \Phi(Z) \rangle}{\langle \Phi(Z) | \Phi(Z) \rangle} - \frac{3\hbar^2 v}{2M} A + T_0 (A - \mathcal{N}_F(Z^*, Z))$$

- Mean field (Time evolution of single-particle wave functions)
- Nucleon-nucleon collisions (as the residual interaction)

When do two nucleons collide?

All the nucleon pairs are checked at every time step dt .

Assumptions

- 1 Collision attempt rate is proportional to the density overlap and the relative velocity.

$$P(\mathbf{r})|d\mathbf{r}| = \alpha e^{-\nu r^2} |d\mathbf{r}|, \quad \mathbf{r} = \mathbf{R}_1 - \mathbf{R}_2$$
$$d\mathbf{r} = \mathbf{r}(t) - \mathbf{r}(t - dt) = (\mathbf{v}_1 - \mathbf{v}_2)dt$$

- 2 The two nucleons move on straight lines until they collide, and the total cross section is σ_{NN} .

$$\int_0^{\infty} 2\pi b db \left[1 - e^{-\int_{-\infty}^{\infty} P(\mathbf{b}+\mathbf{z}) dz} \right] = \sigma_{\text{NN}}$$

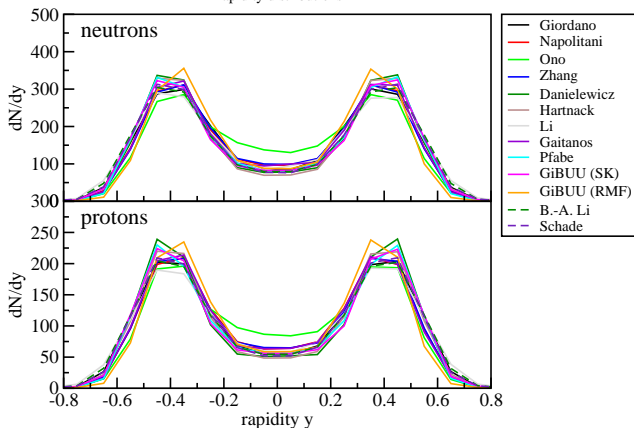
⇒ The coefficient α is given as a function of σ_{NN} and ν .

$$y = \frac{\nu \sigma_{\text{NN}}}{\pi}, \quad x = \alpha \sqrt{\frac{\pi}{\nu}}, \quad y = - \sum_{n=1}^{\infty} \frac{(-x)^n}{n(n!)}$$

Rapidity distribution in peripheral collisions

Au+Au@0.4 AGeV, $b=0.6*b_{\text{max}}$ fm, $t=100$ fm/c

Rapidity distributions



The ^{197}Au nuclei (represented by $f_w(\mathbf{r}, \mathbf{p})$) are too large?

Representations of the state

- ① Original AMD coordinates: $Z = \{\mathbf{Z}_k\}_{k=1,\dots,A}$

$$\mathbf{u} = \sqrt{\nu}\mathbf{r} + \frac{i}{2h\sqrt{\nu}}\mathbf{p}$$

$$|\Phi(Z)\rangle = \det_{ij} [e^{-2(\sqrt{\nu}\mathbf{r}_i - \mathbf{Z}_j)^2}] \Rightarrow f(\mathbf{r}, \mathbf{p}) = 8 \sum_{ij} e^{-2(\mathbf{u} - \mathbf{Z}_i)^* \cdot (\mathbf{u} - \mathbf{Z}_j)} B_{ij} B_{ji}^{-1}$$

Used for expectation values, the deterministic term $\{Z, \mathcal{H}\}_{\text{PB}}$ etc.

- ② Physical coordinates: $\{\mathbf{W}_k\} = \{\sqrt{\nu}\mathbf{R}_k + \frac{i}{2h\sqrt{\nu}}\mathbf{P}_k\}_{k=1,\dots,A}$

$$\mathbf{W}_k = \sum_j \left(\sqrt{Q(Z)} \right)_{kj} \mathbf{Z}_j \Rightarrow f_{\text{W}}(\mathbf{r}, \mathbf{p}) = 8 \sum_{k=1}^A e^{-2\nu(\mathbf{r} - \mathbf{R}_k)^2 - (\mathbf{p} - \mathbf{P}_k)^2 / 2h^2\nu}$$

Used in two-nucleon collisions.

- ③ Deformed Gaussian parameters in phase space: $\{X_{k,a}, S_{k,ab}\}$ $\{X_{k,a}\}_{a=1,\dots,6} = \mathbf{W}_k$

$$f_{\text{S}}(\mathbf{r}, \mathbf{p}) = 8 \sum_{k=1}^A \exp\left[-\frac{1}{2} \sum_{ab} (x_a - X_a) S_{k,ab}^{-1} (x_b - X_b)\right], \quad \{x_a\}_{a=1,\dots,6} = \left\{ \sqrt{\nu}\mathbf{r}, \frac{1}{2h\sqrt{\nu}}\mathbf{p} \right\}$$

Vlasov eq. is solved to evaluate the fluctuation ΔZ and $\frac{d}{dt} S_{k,ab}$.

The momentum width is respected in all the representations.

Mean field + Quantum branching

At each time t_0 , for each wave packet k , ...

Mean field propagation $t_0 \rightarrow t_0 + \tau$

+ Branching at $t_0 + \tau$

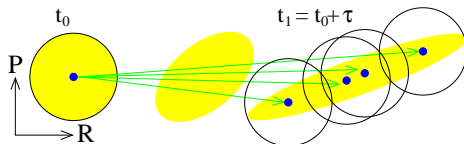
τ : Coherence time

$t = t_0$

$t = t_0 + \tau$

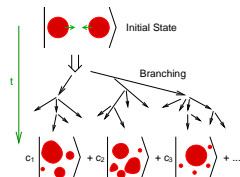
$$|Z_k\rangle\langle Z_k| \xrightarrow{\text{Mean field}} |\psi_k\rangle\langle\psi_k| \xrightarrow{\text{Branching}} \int |z\rangle\langle z| w_k(z) dz$$

for $k = 1, \dots, A$



$$i\hbar \frac{d}{dt} |\psi_k(t)\rangle = h^{\text{HF}} |\psi_k(t)\rangle \quad \text{or} \quad \frac{\partial f_k}{\partial t} = -\frac{\partial h^{\text{HF}}}{\partial \mathbf{p}} \cdot \frac{\partial f_k}{\partial \mathbf{r}} + \frac{\partial h^{\text{HF}}}{\partial \mathbf{r}} \cdot \frac{\partial f_k}{\partial \mathbf{p}}$$

- $\tau \rightarrow 0$ (Strongest branching)
- $\tau = \tau(\rho)$ (Density-dependent)
- $\tau = \tau_{\text{NN-coll}}$ (Decoherence at NN collisions)



Equation of motion for the wave packet centroids

$$\begin{aligned}\frac{d}{dt}\mathbf{Z}_i &= \{\mathbf{Z}_i, \mathcal{H}\}_{\text{PB}} && \text{Mean field} \\ &+ \Delta\mathbf{Z}_i(t) && \text{Mean field \& Branching} \\ &+ \mu(\mathbf{Z}_i, \mathcal{H}') && \text{Dissipation} \\ &+ \text{NN-Collision}\end{aligned}$$

If \mathbf{Z}_i were canonical variables for simplicity,

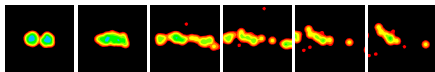
$$\begin{aligned}\{\mathbf{Z}_i, \mathcal{H}\}_{\text{PB}} &= \frac{1}{i\hbar} \frac{\partial \mathcal{H}}{\partial \mathbf{Z}_i^*} \\ \overline{\Delta Z_{ia}(t)} &= 0, \quad \overline{\Delta Z_{ia}(t)\Delta Z_{jb}(t')} = D_{iab}(t)\delta_{ij}\delta(t-t') \\ (\mathbf{Z}_i, \mathcal{H}') &= \frac{1}{\hbar} \frac{\partial \mathcal{H}'}{\partial \mathbf{Z}_i^*}, \quad \mathcal{H}' = \mathcal{H} + \sum_m \beta_m Q_m\end{aligned}$$

- μ is determined by the total energy conservation.
- Lagrange multipliers β_m are determined so that Q_m are not changed by the $(\mathbf{Z}_i, \mathcal{H}')$ term.

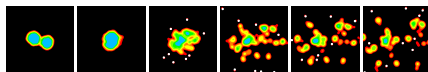
$$\{Q_m\} = \left\{ \left\langle \sum_i \mathbf{r}_i \right\rangle, \left\langle \sum_i \mathbf{p}_i \right\rangle, \left\langle \sum_i \mathbf{r}_i \times \mathbf{p}_i \right\rangle, \left\langle \sum_i r_{i\sigma} r_{i\tau} \right\rangle, \left\langle \sum_i p_{i\sigma} p_{i\tau} \right\rangle \right\} \quad \sigma, \tau = x, y, z$$

AMD results for multifragmentation (central collisions)

$^{40}\text{Ca} + ^{40}\text{Ca}$ at 35 MeV/u, $b = 0$



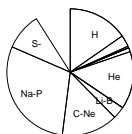
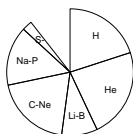
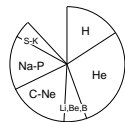
Xe + Sn at 50 MeV/u, $0 \leq b \leq 4$ fm



Experiment

AMD

AMD



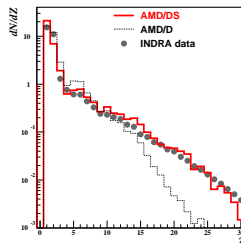
Hagel et al.

PRC50(1994)2017

$\tau(\rho)$

$\tau_{\text{NN-coll}}$

Charge distribution



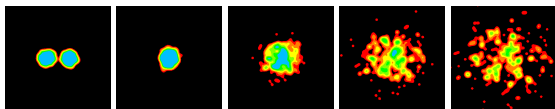
● AMD ($\tau \rightarrow 0$)

● AMD ($\tau_{\text{NN-coll}}$)

Can we reproduce different data with the same model of branching?

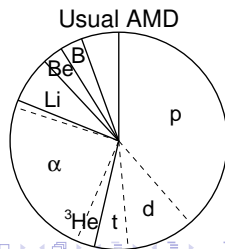
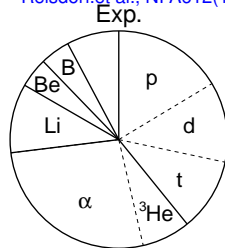
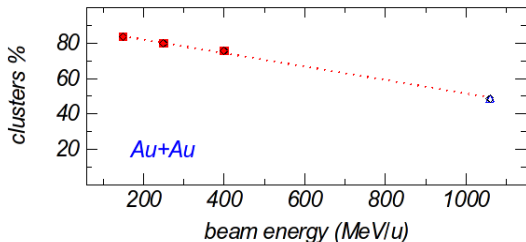
(Cluster correlations?)

Cluster correlations in heavy-ion collisions



$^{197}\text{Au} + ^{197}\text{Au}$ at 150 MeV/u

Reisdorf et al., NPA612(1997)493.



Example: Four nucleons in the gas at $T = 10$ MeV

- Uncorrelated: $\langle E \rangle = \frac{3}{2}T \times 4 = 60$ MeV
- α cluster: $\langle E \rangle = \frac{3}{2}T \times 1 - 28.3$ MeV = -13.3 MeV

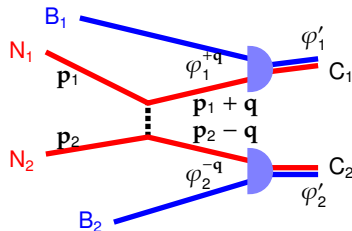
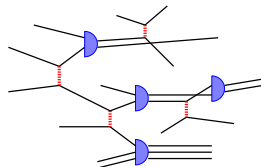
During the time evolution of AMD,

- Cluster formation
- Propagation /definition of cluster
- Breakup

$$N_1 + B_1 + N_2 + B_2 \rightarrow C_1 + C_2$$

- N_1, N_2 : Colliding nucleons
- B_1, B_2 : Spectator nucleons/clusters
- C_1, C_2 : $N, (2N), (3N), (4N)$

$$\frac{d\sigma}{d\Omega} = F_{\text{kin}} |\langle \varphi'_1 | \varphi_1^{+q} \rangle|^2 |\langle \varphi'_2 | \varphi_2^{-q} \rangle|^2 \left(\frac{d\sigma}{d\Omega} \right)_{\text{NN}}$$

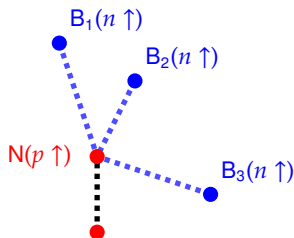


c.f. Danielewicz et al., NPA533 (1991) 712.

How much is the probability that the scattered nucleon N_1 is a part of a cluster after the momentum transfer q ?

Probability of forming a cluster

The probability for a scattered nucleon **N** to form a cluster is not as simple as $|\langle \varphi' | \varphi^a \rangle|^2$, when there are many possible combinations of cluster formation.



$|\Phi^a\rangle$: The state of the left figure.

$|\Phi'_B\rangle$: The state when **N** and **B** are placed at the same phase space point.

$|\langle \Phi'_B | \Phi^a \rangle|^2$ is not the probability because of the non-orthogonality: $N_{BB'} \equiv \langle \Phi'_B | \Phi'_{B'} \rangle \neq \delta_{BB'}$

The probability that **N** forms a cluster with one of **B**'s:

$$P = \langle \Phi^a | \hat{X} | \Phi^a \rangle \quad \hat{X} = \sum_{BB'} |\Phi'_B\rangle N_{BB'}^{-1} \langle \Phi'_{B'}|$$
$$= \sum_B |\langle \tilde{\Phi}'_B | \Phi^a \rangle|^2 \quad |\tilde{\Phi}'_B\rangle = (N^{-1/2})_{BB'} |\Phi'_{B'}\rangle$$

$|\langle \tilde{\Phi}'_B | \Phi^a \rangle|^2$ is regarded as the probability that **N** forms a cluster with **B**.

Clustering probability – Is it a well-defined concept?

G. Röpke and H. Schulz, NPA477 (1988) 472.

... we introduce creation and annihilation operators for bound states

$$a_{A\alpha}^{\dagger}(\mathbf{p}) = \sum_{1\dots A} \psi_{A\alpha,\mathbf{p}}^*(1\dots A) a^{\dagger}(1)\cdots a^{\dagger}(A).$$

Here $\psi_{A\alpha,\mathbf{p}}(1\dots A)$ denotes the wave function of the A -nucleon cluster state with total momentum \mathbf{p} and internal quantum number α ...

... the operator

$$n_{A\alpha}(\mathbf{p}, \mathbf{r}) = \int \frac{d^3k}{(2\pi\hbar)^3} e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} a_{A\alpha}^{\dagger}(\mathbf{p} - \frac{1}{2}\mathbf{k}) a_{A\alpha}(\mathbf{p} + \frac{1}{2}\mathbf{k})$$

is the Wigner transform of the density associated with a cluster of mass number A . The mean values

$$f_{A\alpha}(\mathbf{p}, \mathbf{r}, t) = \langle n_{A\alpha}(\mathbf{p}, \mathbf{r}) \rangle^t$$

represent the Wigner distribution functions of the corresponding clusters. In this way, clusters are considered as new species like in a chemical picture.

Clustering probability (?)

Is it true that the number of clusters is obtained by

$$N_{A\alpha}(t) = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{d^3r}{(2\pi\hbar)^3} f_{A\alpha}(\mathbf{p}, \mathbf{r}, t) = \int \frac{d^3p}{(2\pi\hbar)^3} \langle a_{A\alpha}^\dagger(\mathbf{p}) a_{A\alpha}(\mathbf{p}) \rangle^t \quad ?$$

Consider $(A\alpha) = \text{deuteron}$, and choose $\psi_{d,p}(1, 2) = e^{i\mathbf{p}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\hbar} \left(\frac{v}{\pi}\right)^{\frac{3}{4}} e^{-\frac{1}{2}v(\mathbf{r}_1-\mathbf{r}_2)^2}$.

For an AMD wave function $|\Phi(Z)\rangle$ (of nucleons with the same spin), N_d is calculated as

$$N_d = \sum_{ik}^{\text{proton}} \sum_{jl}^{\text{neutron}} e^{-\frac{1}{2}(\mathbf{Z}_i^* - \mathbf{Z}_j^*) \cdot (\mathbf{Z}_k - \mathbf{Z}_l)} B_{ik} B_{jl} B_{ki}^{-1} B_{lj}^{-1}$$

In the case of a single proton (at \mathbf{Z}_p) and many neutrons,

$$N_d = \sum_{jl}^{\text{neutron}} e^{-\frac{1}{2}(\mathbf{Z}_p^* - \mathbf{Z}_j^*) \cdot (\mathbf{Z}_p - \mathbf{Z}_l)} B_{jl} B_{lj}^{-1} \neq F(\mathbf{Z}_p) = \sum_{jl}^{\text{neutron}} e^{-(\mathbf{Z}_p^* - \mathbf{Z}_j^*) \cdot (\mathbf{Z}_p - \mathbf{Z}_l)} B_{jl} B_{lj}^{-1}$$

$F(\mathbf{r}, \mathbf{p})$ is the Husimi function satisfying $0 \leq F(\mathbf{r}, \mathbf{p}) \leq 1$, but N_d easily exceeds 1.

Conclusion: This N_d is not what we want!

● Formation

- $(d\sigma/d\Omega)_{NN} \Rightarrow$ Cluster formation cross section
- Clusters: $N, 2N, 3N, 4N = (0s)^n$
- Pauli-blocking factor: $\prod_{i \in C} (1 - f_i)$
- Avoid double countings of final states
- Take care of the non-orthogonality of final states

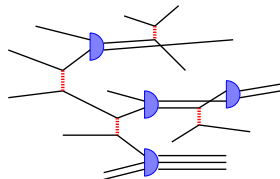
● Propagation

Nucleons i in a cluster C are propagated as usual, except that the internal fluctuations are turned off:

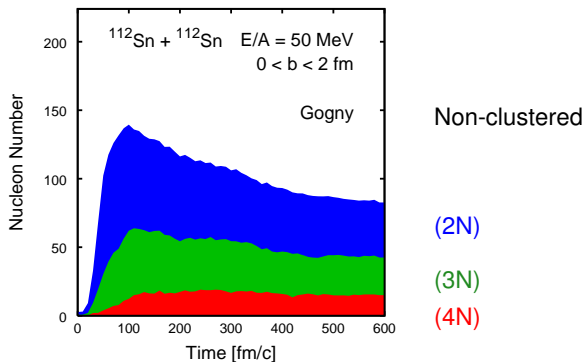
$$\frac{d}{dt} \mathbf{Z}_i = \{\mathbf{Z}_i, \mathcal{H}\}_{\text{PB}} + \Delta \mathbf{Z}_i(t), \quad \Delta \mathbf{Z}_i(t) := \frac{1}{C} \sum_{j \in C} \Delta \mathbf{Z}_j(t)$$

● Breakup

A cluster C is broken when a nucleon in C collides with another nucleon.



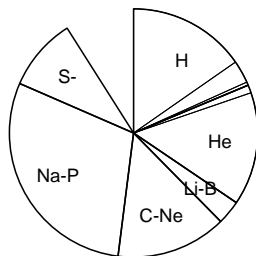
Number of nucleons in correlated clusters



Effects of cluster correlations

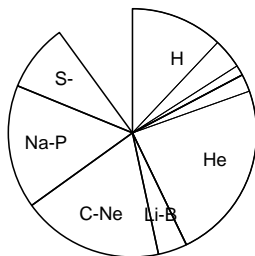
$^{40}\text{Ca} + ^{40}\text{Ca}$, $E/A = 35$ MeV, filtered violent collisions

w/o cluster correlations



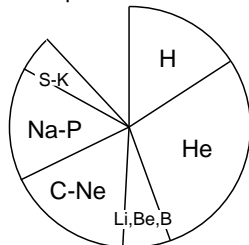
p	6.7
d	1.5
t	0.3
^3He	0.3
α	2.7

with cluster correlations



p	4.4
d	1.8
t	0.5
^3He	0.6
α	5.0

experiment



Effects of clusters

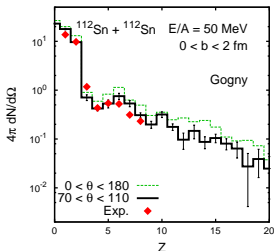
- $M_p \downarrow$
- $M_\alpha \uparrow$
- $\sum_{\text{IMF}} Z \downarrow$

Coherence time: $\tau_{\text{NN-coll}}$

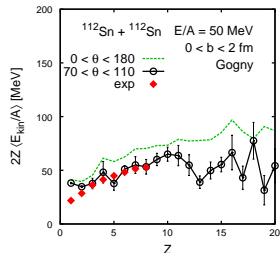
Results for Sn + Sn system

$^{112}\text{Sn} + ^{112}\text{Sn}$ at $E/A = 50$ MeV/nucleon, $0 < b < 2$ fm

With cluster correlations $\Sigma Z(70^\circ < \theta < 110^\circ) = 22.6$



n	27.3
p	10.4
d	6.4
t	3.0
^3He	1.2
α	12.2



Xe+Sn, INDRA data

p	8.4
d	4.4
t	3.3
^3He	0.9
α	10.1

multiplicities of detected particles

- So far AMD calculations are done with the Gogny force.

$$v_{ij} = \sum_{k=1,2} (W_k + B_k P_\sigma - H_k P_\tau - M_k P_\sigma P_\tau) e^{-(\mathbf{r}_i - \mathbf{r}_j)^2 / a_k^2} + t_\rho (1 + P_\sigma) \rho(\mathbf{r}_i)^\sigma \delta(\mathbf{r}_i - \mathbf{r}_j)$$

$$\langle V \rangle = \frac{1}{2} \sum_{i=1}^A \sum_{j=1}^A \sum_{k=1}^A \sum_{l=1}^A \langle ij | v | kl - lk \rangle B_{ki}^{-1} B_{lj}^{-1} \quad \sim A^4$$

- Skyrme force is applicable in principle.
(May be advantageous for heavy systems.)

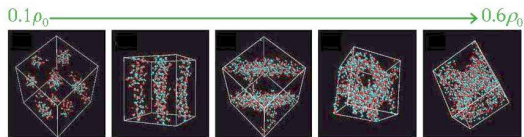
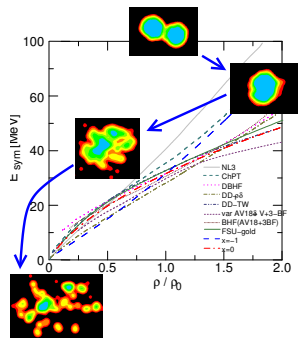
$$v_{ij} = t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}) + \frac{1}{2} t_1 (1 + x_1 P_\sigma) [\delta(\mathbf{r}) \mathbf{k}^2 + \mathbf{k}^2 \delta(\mathbf{r})] \quad \mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$$

$$+ t_2 (1 + x_2 P_\sigma) \mathbf{k} \cdot \delta(\mathbf{r}) \mathbf{k} + t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{r}_i)]^\alpha \delta(\mathbf{r}) \quad \mathbf{k} = \frac{1}{2\hbar} (\mathbf{p}_i - \mathbf{p}_j)$$

$$\langle V \rangle = \int \mathcal{V}(\rho(\mathbf{r}), \tau(\mathbf{r}), \Delta\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})) d\mathbf{r} \quad \sim A^2 V \quad (+\epsilon A^3)$$

$$\rho(\mathbf{r}) = \left(\frac{2\nu}{\pi}\right)^{3/2} \sum_{i=1}^A \sum_{j=1}^A e^{-2\nu(\mathbf{r} - \mathbf{R}_{ij})^2} B_{ij} B_{ji}^{-1}, \quad \mathbf{R}_{ij} = \frac{1}{2\sqrt{\nu}} (\mathbf{Z}_i^* + \mathbf{Z}_j)$$

Nuclear Matter in Nuclear Collisions and Neutron Stars



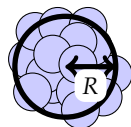
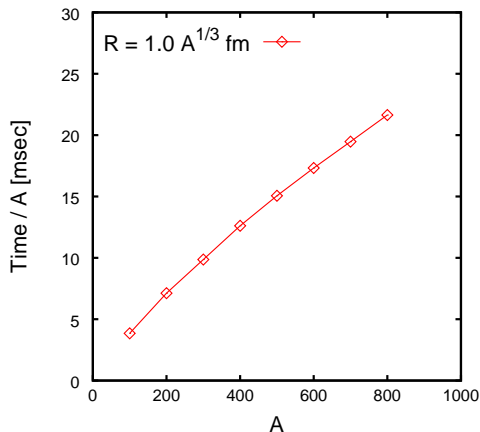
QMD simulation of nuclear pasta. G. Watanabe et al.

- Inhomogeneous. (fragments, clusters, pasta)
- Excited. (finite temperature and/or dynamic)
- Liquid-gas phase transition.

with Hasnaoui, Furuta, Gulminelli, Chomaz

Application to heavy systems with Skyrme force

System size dependence of the CPU time for an evaluation of $\left\{ \frac{\partial}{\partial Z_k} \langle V \rangle; k = 1, 2, \dots, A \right\}$



\Leftrightarrow Naive expectation $\sim A^2 V$

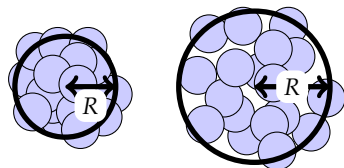
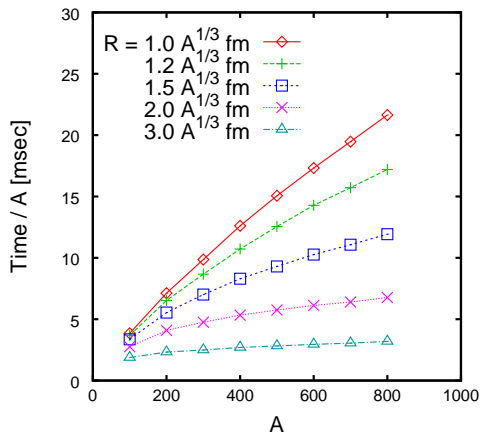
$$\langle V \rangle = \int d\mathbf{r} \mathcal{V}(\rho(\mathbf{r}), \tau(\mathbf{r}), \Delta\rho(\mathbf{r}), \mathbf{j}(\mathbf{r}))$$

$$\rho(\mathbf{r}) = \left(\frac{2\nu}{\pi}\right)^{3/2} \sum_{i=1}^A \sum_{j=1}^A e^{-(\mathbf{r}-\mathbf{R}_{ij})^2} B_{ij} B_{ji}^{-1}$$

- Mesh size $\Delta r = 0.75$ fm, $Z_{\uparrow} = Z_{\downarrow} = N_{\uparrow} = N_{\downarrow}$
- Xeon E5430 Harpertown 2.66 GHz, Using 1 of 8 cores, Almost no load by other processes

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Cluster correlations in AMD

- $N_1 + B_1 + N_2 + B_2 \rightarrow C_1 + C_2$, based on $(d\sigma/d\Omega)_{NN}$
- A problem how to count the number of clusters.
- Cluster correlations have systematic effects on M_p , M_α , and $\sum_{\text{IMF}} Z$.
- Consistent reproduction of various multifragmentation data may be improved.

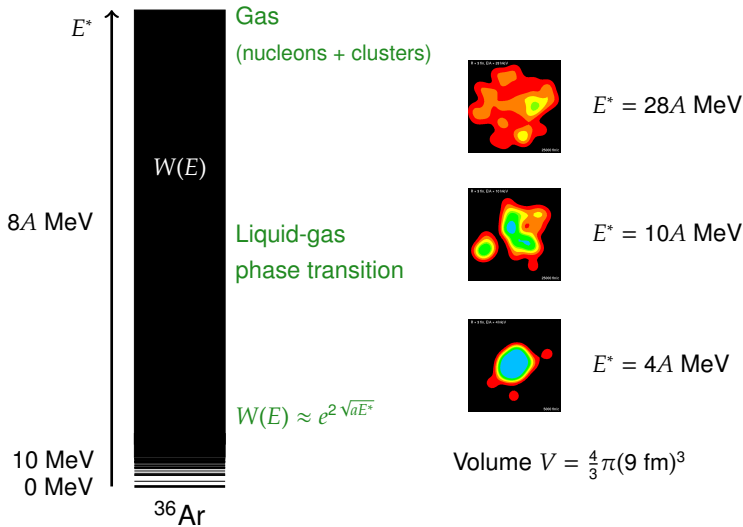
AMD with Skyrme force

- In progress.
- May be applicable to neutron star problems.

Reaction and Equilibrium — A unified study with AMD

- Equivalence for fragment observables
at each reaction time [$80 \lesssim t < (300+) \text{ fm}/c$]
- Some dynamical effects

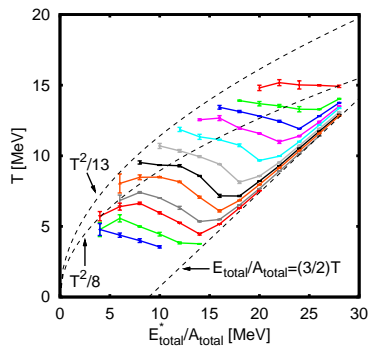
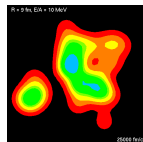
Excited low-density system



Equilibrium ensembles and caloric curves

Can molecular dynamics describe excited nuclear many-body systems in equilibrium?

- Ono & Horiuchi
- Ohnishi & Randrup
- Schnack & Feldmeier
- Sugawa & Horiuchi
- Furuta & Ono
- Hasnaoui et al.



Furuta and Ono,
PRC79 (2009) 014608;
PRC74 (2006) 014612.