

核破碎反応・シミュレーション計算

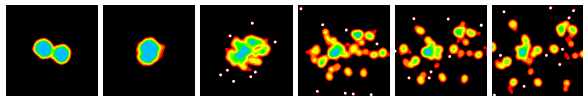
小野章

東北大・理

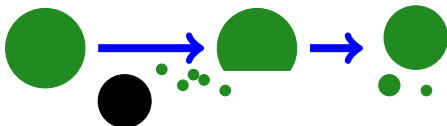
理研ミニワークショップ「核データと核理論」2009年3月25-26日

- 種々の破碎反応の微視的・動力的記述
 - 重イオン衝突（中心衝突）
 - 入射核破碎反応
 - 核子入射
- AMD の最近の進展
 - 計算の高速化（Skyrme 力）
 - クラスタ相関
 - 熱化学平衡の記述

- 重イオン衝突（中心衝突）



- 入射核破碎反応



- 核子入射反応での破碎片生成

核物質の動的過程

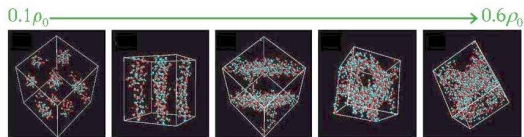
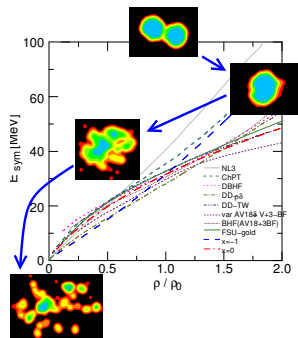
- 平均場・状態方程式
- フロー・膨張
- 液相気相相転移



カスケード+統計計算 (?)

応用上重要

Nuclear Matter in Nuclear Collisions and Neutron Stars



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

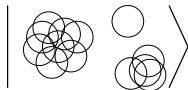
- Inhomogeneous. (fragments, clusters, pasta)
- Excited. (finite temperature and/or dynamic)
- Liquid-gas phase transition.

- Statistical calculations with AMD for finite systems
⇒ Relevance of equilibrium in nuclear collisions (Furuta, Ono)
- Extension of AMD for cluster correlations (Ono)
- AMD study of neutron star (Hasnaoui, Ono, Furuta, Gulminelli, Chomaz)
 - Implementation of Skyrme force in AMD
- Isospin effects etc in heavy-ion collisions

Antisymmetrized Molecular Dynamics

AMD wave function

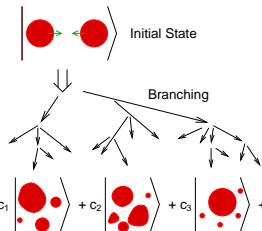
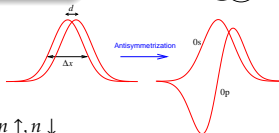
$$|\Phi(Z)\rangle = \det_{ij} \left[\exp \left\{ -v \left(\mathbf{r}_j - \frac{\mathbf{Z}_i}{\sqrt{v}} \right)^2 \right\} \chi_{\alpha_i}(j) \right]$$



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

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 :

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

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

Energy is conserved. No temperature in the equation.

Quantum effects are included.

Mean field + Quantum branching

At each time t_0 , for each wave packet k, \dots

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

+ Branching at $t_0 + \tau$

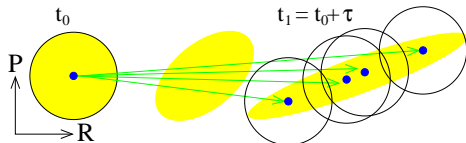
τ : Coherence time

$t = t_0$

$t = t_0 + \tau$

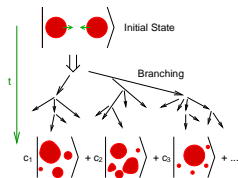
$$|Z_k\rangle\langle Z_k| \xrightarrow{\text{Mean field}} |\psi_k\rangle\langle\psi_k| \xrightarrow{\text{Branching}} \int |z\rangle\langle z| w_k(z) dz$$

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)



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 can be flexible and faster.

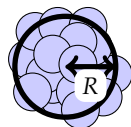
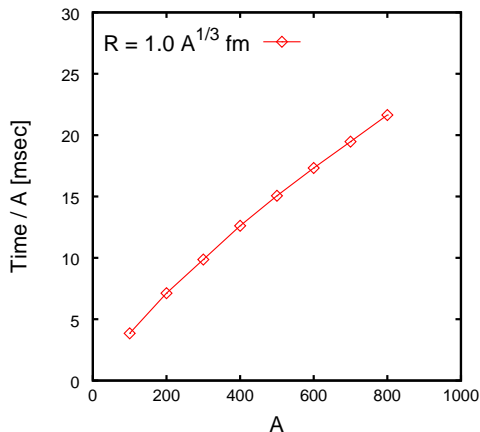
⇒ Applications to heavy systems and stellar matter

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

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

重い系に使えるか？

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



⇔ Naive expectation $\sim A^2 V$

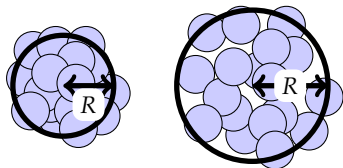
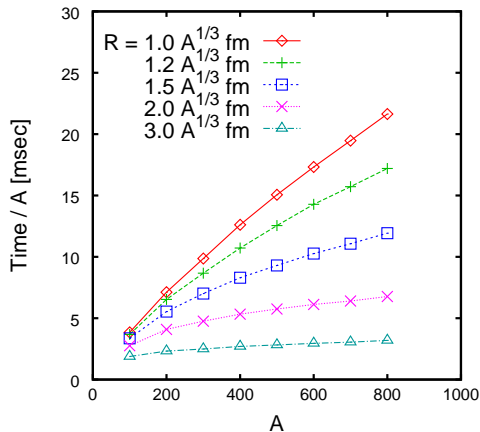
$$\langle V \rangle = \int d\mathbf{r} \mathcal{V}(\rho(\mathbf{r}), \tau(\mathbf{r}), \Delta\rho(\mathbf{r}), \mathbf{j}(\mathbf{r}))$$

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

- 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

重い系に使えるか？

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



⇔ Naive expectation $\sim A^2 V$

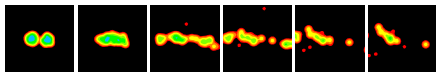
$$\langle V \rangle = \int d\mathbf{r} \mathcal{V}(\rho(\mathbf{r}), \tau(\mathbf{r}), \Delta\rho(\mathbf{r}), \mathbf{j}(\mathbf{r}))$$

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

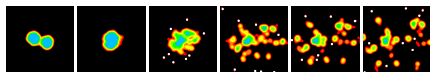
- Mesh size $\Delta r = 0.75$ fm, $Z_{\uparrow} = Z_{\downarrow} = N_{\uparrow} = N_{\downarrow}$
- Xeon E5430 Harpertown 2.66 GHz, Using 1 of 8 cores, Almost no load by other processes

AMD results for multifragmentation (central collisions)

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



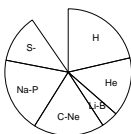
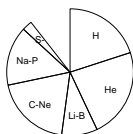
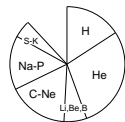
Xe + Sn at 50 MeV/u, $0 \leq b \leq 4$ fm



Experiment

AMD

AMD



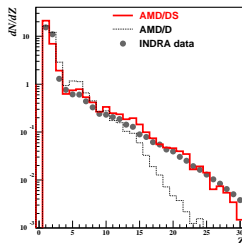
Hagel et al.

PRC50(1994)2017

$\tau(\rho)$

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

Charge distribution



● AMD ($\tau \rightarrow 0$)

● AMD ($\tau_{\text{NN-coll}}$)

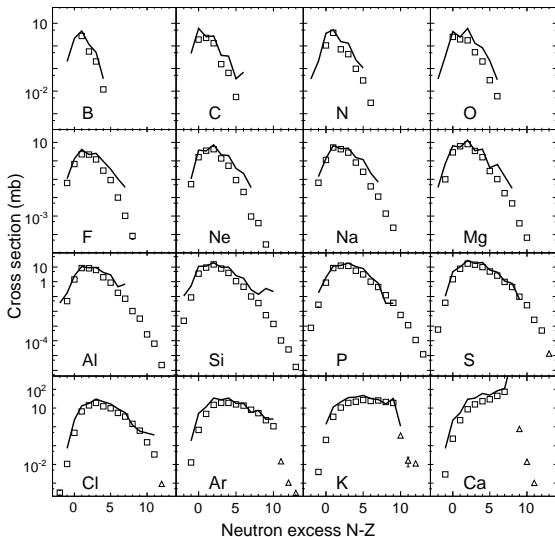
Can we reproduce different data with the same model of branching?

(Cluster correlations?)

Rare isotope production by projectile fragmentation

Mocko, Tsang, AO et al., PRC78(2008)024612.

$^{48}\text{Ca} + ^9\text{Be}$ at 140 MeV/nucleon



AMD (反対称化分子動力学)

核子波束の運動を解くことによる反応のシミュレーション

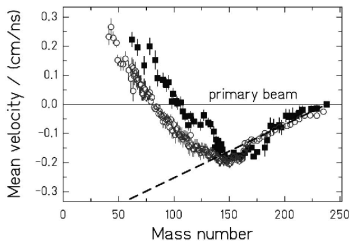
- 平均場の効果
- 二核子衝突 (確率的)
- 励起したフラグメントの統計崩壊
- AMD calc: 17,000 events
⇒ 40 CPU · days
(HPC Center at MSU)
- Experiment: $\sim 10^7$ events

Experimental data of velocity shift

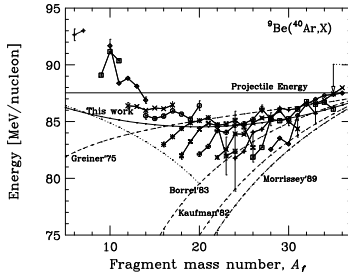
Ricciardi et al., PRL 90 (2003) 212302.

Notani et al., PRC 76 (2007) 044605.

$^{238}\text{U} + \text{Pb}$ and $^{238}\text{U} + \text{Ti}$
at 1 GeV/nucleon

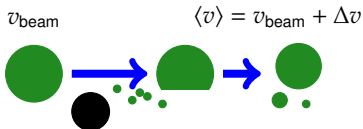


$^{40}\text{Ar} + ^9\text{Be}$
about 90A MeV



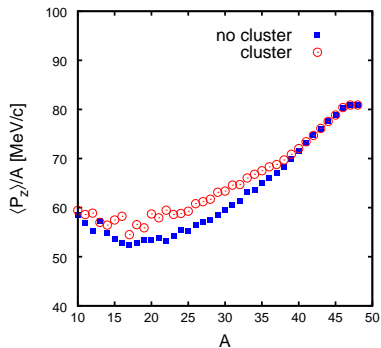
Dashed line: Morrissey systematics

$$\Delta v_{\parallel} \propto \Delta A$$

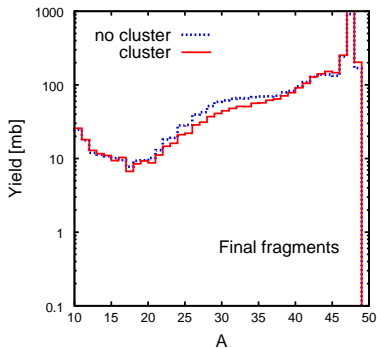


Fragment mean velocity and yield

フラグメントの速度（運動量）の平均値



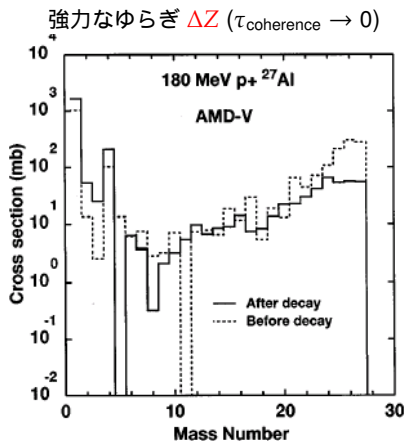
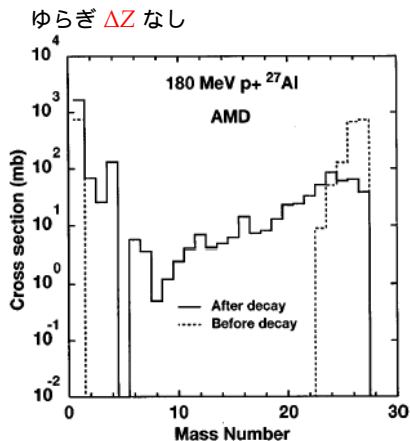
フラグメントの質量数分布



なぜ、フラグメントの速度のピークががビームより速くなり得るのか、計算では説明できていない。

$p + {}^{27}\text{Al}$ at 180 MeV

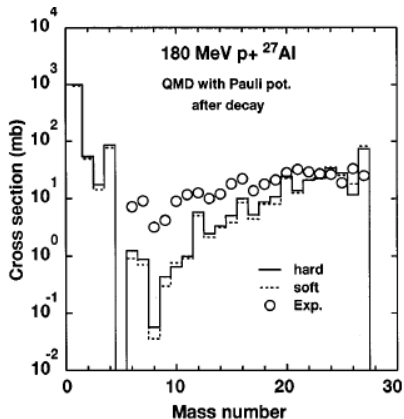
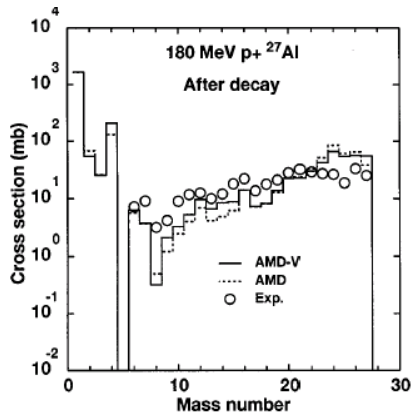
Y. Tosaka, A. Ono, H. Horiuchi, PRC60 (1999) 064613.



核子による標的核破碎

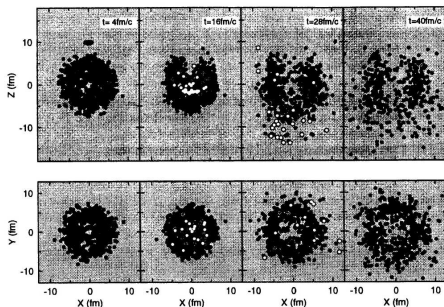
$p + {}^{27}\text{Al}$ at 180 MeV

Y. Tosaka, A. Ono, H. Horiuchi, PRC60 (1999) 064613.



AMD も QMD も $A \sim \frac{1}{2}A_{\text{projectile}}$ のフラグメントを過小評価している。

フラグメントの角度分布に側方ピーク



シミュレーション計算の実状：

- α (5 GeV/u) + Au

Tomoyuki Maruyama et al, PTP 97 (1997) 579.

⇒ QMD では、幅の狭い波束を使って、相互作用のレンジを小さくする必要がある。

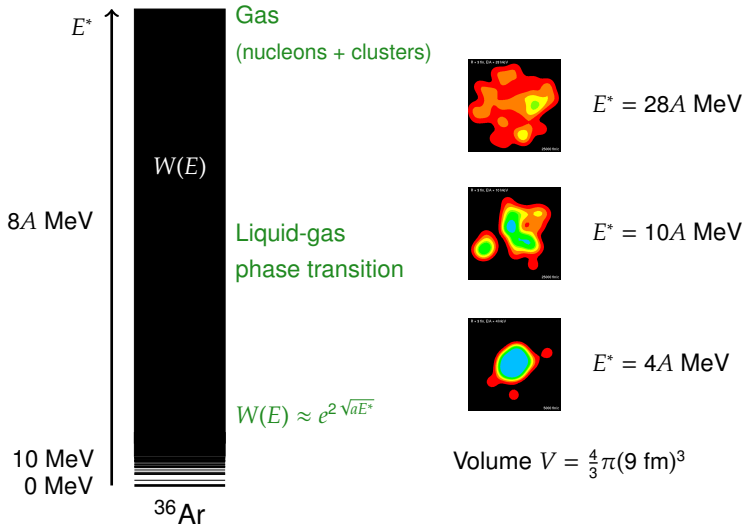
- p (11.5 GeV) + Au

Y. Hirata et al, NPA 707 (2002) 193.

⇒ 微視的な計算 (JAM/MF) に、パーコレーションモデルを組み合わせる必要がある。

少し励起した原子核（膨張が弱い）の崩壊を微視的に記述するのは難しいのか？

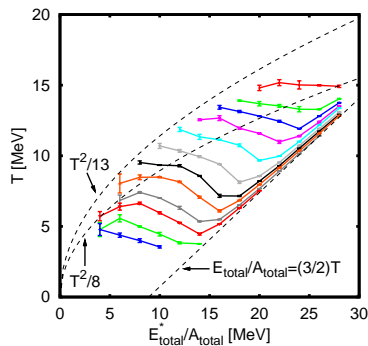
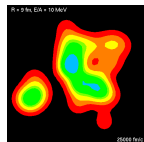
Excited low-density system



Equilibrium ensembles and caloric curves

分子動力学は励起した核子多体系（熱平衡）を適切に記述できるのか？

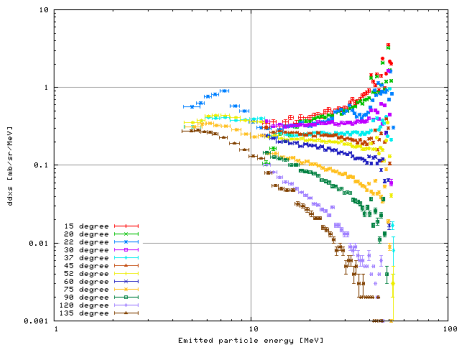
- Ono & Horiuchi
- Ohnishi & Randrup
- Schnack & Feldmeier
- Sugawa & Horiuchi
- Furuta & Ono
- Hasnaoui et al.



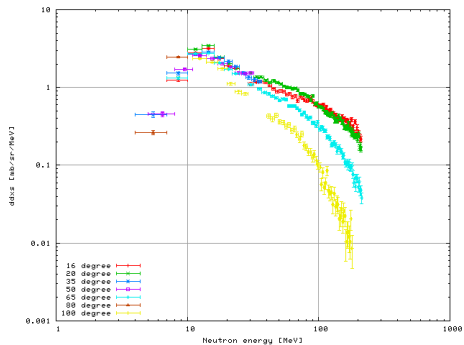
Furuta and Ono,
PRC79 (2009) 014608;
PRC74 (2006) 014612.

Production of light charged particles

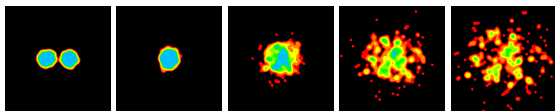
$p(62 \text{ MeV}) + \text{Fe} \rightarrow d$



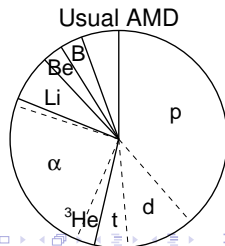
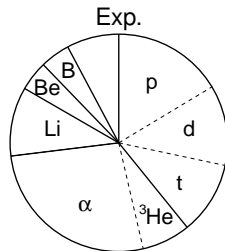
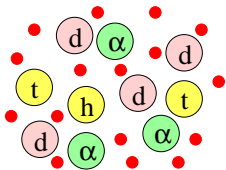
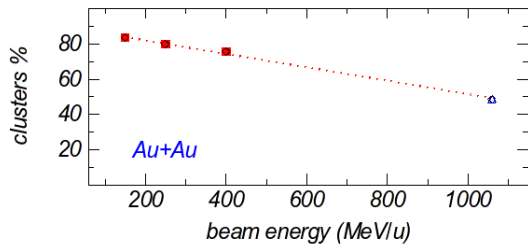
$p(1200 \text{ MeV}) + \text{Au} \rightarrow d$



Cluster correlations in heavy-ion collisions



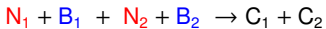
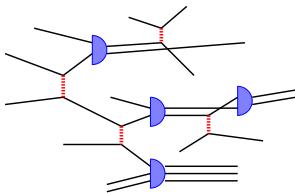
$^{197}\text{Au} + ^{197}\text{Au}$ at 150 MeV/u



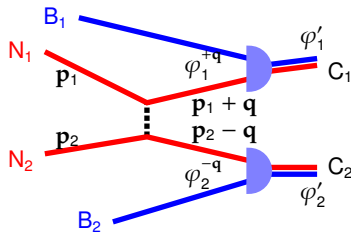
Cluster formation

During the time evolution of AMD,

- Cluster formation
- Propagation
- Breakup



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

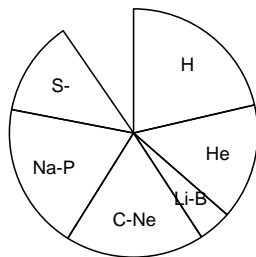


$$\frac{d\sigma}{d\Omega} = F_{\text{kin}} |\langle \varphi'_1 | \varphi_1^{+q} \rangle|^2 |\langle \varphi'_2 | \varphi_2^{-q} \rangle|^2 \left(\frac{d\sigma}{d\Omega} \right)_{\text{NN}}$$

Effects of cluster correlations

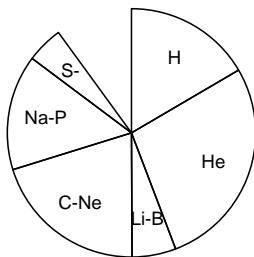
$^{40}\text{Ca} + ^{40}\text{Ca}$, $E/A = 35$ MeV, filtered violent collisions

w/o cluster correlations



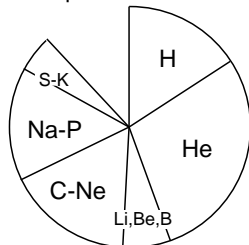
p	6.7
d	1.5
t	0.3
^3He	0.3
α	2.7

with cluster correlations



p	4.4
d	1.8
t	0.5
^3He	0.6
α	5.0

experiment



Effects of clusters

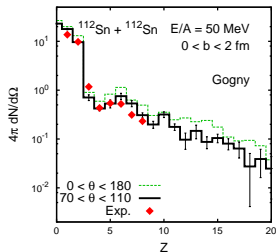
- $M_p \downarrow$
- $M_\alpha \uparrow$
- $\sum_{\text{IMF}} Z \downarrow$

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

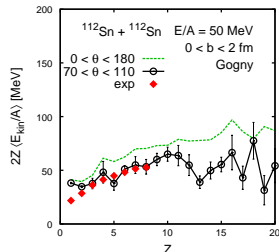
Results for Sn + Sn system

$^{112}\text{Sn} + ^{112}\text{Sn}$ 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

AMD 計算の最近の進展

- 熱平衡（液相気相相転移）の記述の確認
- Skyrme 力の場合の計算の高速化
- クラスタ関連の導入

動力学と熱力学の統一的記述へ
核物質・中性子星の計算へ
粒子ベース \leftrightarrow クラスタ関連

破碎反応の微視的記述（AMD）

- 重イオン衝突（中心衝突）での多重破碎
- 入射核破碎反応
- 核子入射による標的核破碎

破碎しすぎる傾向

破碎が足りない傾向