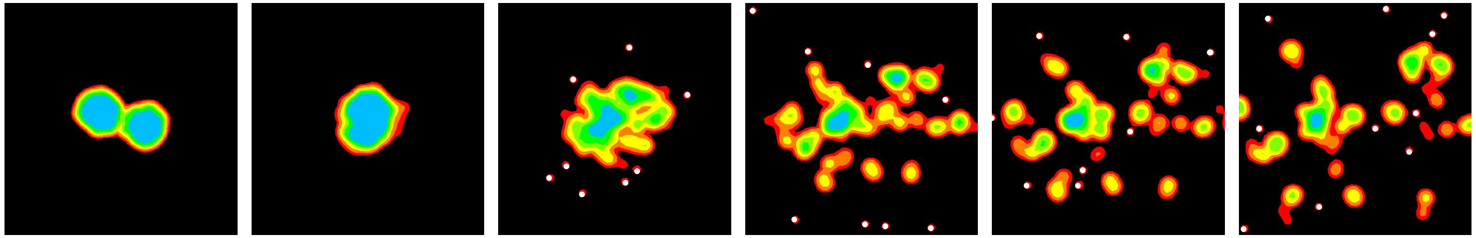
Time-dependent AMD calculations for reactions

Akira Ono (Tohoku University)

AMD solves the time evolution of many-nucleon systems approximately.

- Reactions with complicated mechanisms
- Statistical properties of excited systems

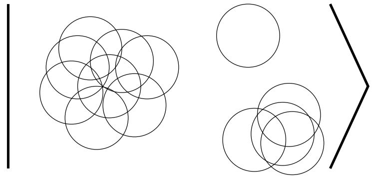
- Framework of AMD
- Typical applications of AMD
- Supercomputing in future



The first version of AMD

A Slater determinant of Gaussian wave packets

$$|\Phi(\mathbf{Z})\rangle = \det_{ij}\left[\exp\left\{-\nu(\mathbf{r}_i - \mathbf{Z}_j/\sqrt{\nu})^2\right\}\chi_{\alpha_j}(i)\right]$$



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

ν : Width Parameter = $(2.5\ \text{fm})^{-2}$

χ_{α_i} : Spin-Isospin States = $p\uparrow, p\downarrow, n\uparrow, n\downarrow$

Time Dependent Variational Principle for $\{\mathbf{Z}_1(t), \ldots, \mathbf{Z}_A(t)\}$

$$\delta\int dt\, \frac{\langle\Phi(\mathbf{Z})|(i\hbar\frac{d}{dt} - H)|\Phi(\mathbf{Z})\rangle}{\langle\Phi(\mathbf{Z})|\Phi(\mathbf{Z})\rangle} = 0 \qquad \Rightarrow \qquad i\hbar\sum_{j\tau} C_{i\sigma,j\tau}\frac{dZ_{j\tau}}{dt} = \frac{\partial\mathcal{H}}{\partial Z^*_{i\sigma}}$$

Wave packet motion in the mean field

H: Effective Hamiltonian (such as the Gogny force and the Skyrme force)

Recent AMD

- Single-particle motions in the mean field

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

- Two-nucleon collisions

$$\mathrm{N}_1(\mathbf{p}_1) + \mathrm{N}_2(\mathbf{p}_2) \to \mathrm{N}_1(\mathbf{p}'_1) + \mathrm{N}_2(\mathbf{p}'_2), \qquad \frac{d\sigma_{\mathrm{NN}}}{d\Omega}$$

- Cluster correlations and formation of fragments

$$\psi_k(\mathbf{r}, t) \to e^{-\nu(\mathbf{r}-\mathbf{Z}_k)^2} \quad \text{(wave packet)}$$

- A huge number of configurations/channels

$$|\Phi(Z_0)\rangle \longrightarrow \begin{cases} |\Phi(Z')\rangle \\ |\Phi(Z'')\rangle \\ \ldots \end{cases}$$

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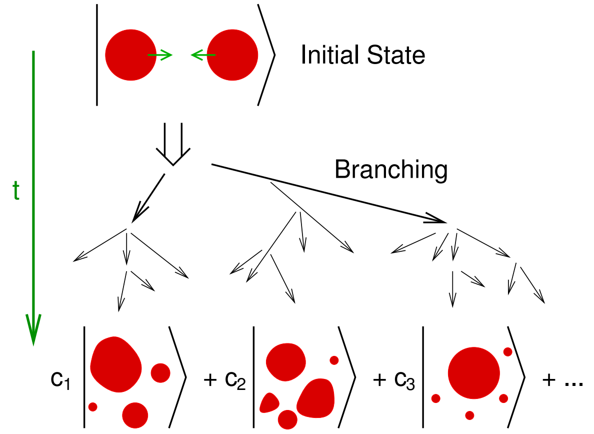
Stochastic eq of motion:

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



$$|\Psi(t)\rangle\langle\Psi(t)| \approx \overline{|\Phi(Z(t))\rangle\langle\Phi(Z(t))|}$$

Mean field + Qauntum branching

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

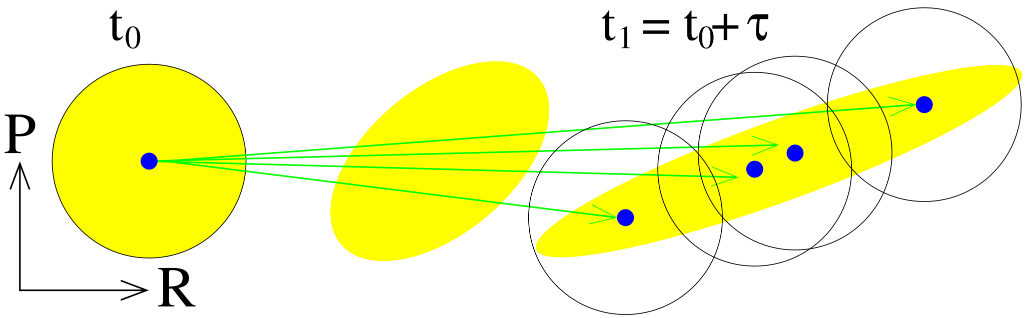
$\boxed{\text{Mean field propagation } t_0 \to t_0 + \tau}$ + $\boxed{\text{Branching at } t_0 + \tau}$ τ: Coherence time

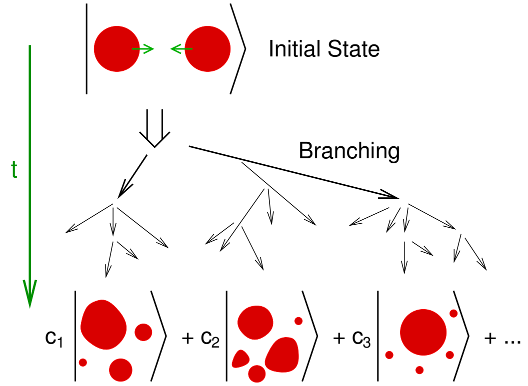
$$t = t_0 \qquad\qquad t = t_0 + \tau$$

$$|\mathbf{Z}_k\rangle\langle\mathbf{Z}_k| \xrightarrow[\text{Mean field}]{} |\psi_k\rangle\langle\psi_k| \xrightarrow[\text{Branching}]{} \int |\mathbf{z}\rangle\langle\mathbf{z}|\, w_k(\mathbf{z}) d\mathbf{z} \qquad \text{for } k = 1, \ldots, A$$

$$i\hbar \frac{d}{dt}|\psi_k(t)\rangle = h^{\text{HF}}|\psi_k(t)\rangle$$

$$\frac{\partial f_k}{\partial t} = -\frac{\partial h^{\text{HF}}}{\partial \mathbf{p}} \cdot \frac{\partial f_k}{\partial \mathbf{r}} + \frac{\partial h^{\text{HF}}}{\partial \mathbf{r}} \cdot \frac{\partial f_k}{\partial \mathbf{p}}$$





- A choice of τ: Branching at each NN collision

Required computation

$$\frac{d}{dt}\mathbf{Z}_i = \{\mathbf{Z}_i, \mathcal{H}\}_{\mathrm{PB}} \ni \frac{\partial}{\partial \mathbf{Z}_i^*}\frac{\langle\Phi|V|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \frac{\partial}{\partial \mathbf{Z}_i^*}\sum_{j=1}^{A}\sum_{k=1}^{A}\sum_{m=1}^{A}\sum_{n=1}^{A}\langle jk|v|mn\rangle(B^{-1}_{mj}B^{-1}_{nk} - B^{-1}_{nj}B^{-1}_{mk})$$

- Analytic computation $\propto A^4$
- Triple loop approximation $\Rightarrow 12A^3$ [AO, PRC 59 (1999) 853]
- Orthogonalize the single-particle states $\Rightarrow$?

Current limitation of application

- Heavy-ion collisions ($A \lesssim 400$) are feasible. (The number of events may be limited.)
- Nuclear matter calculations ($A \gg 1000$) are not possible.

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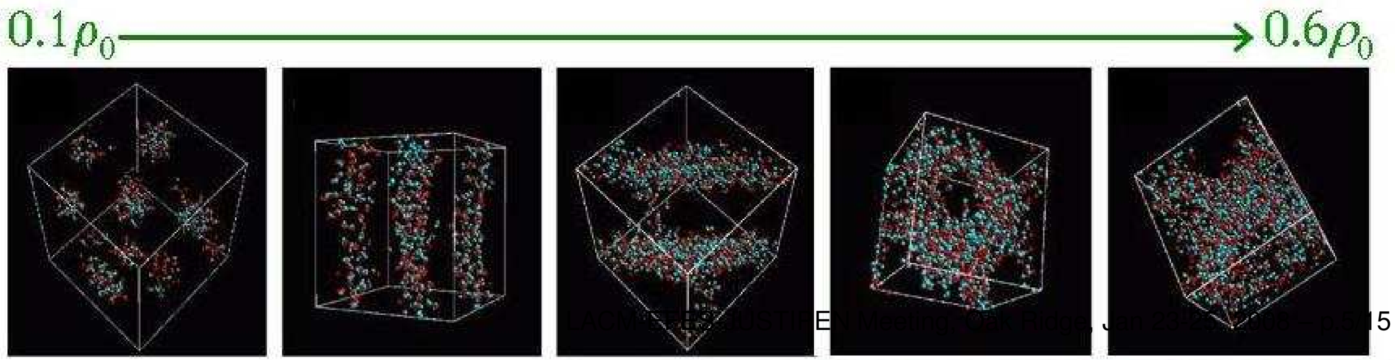
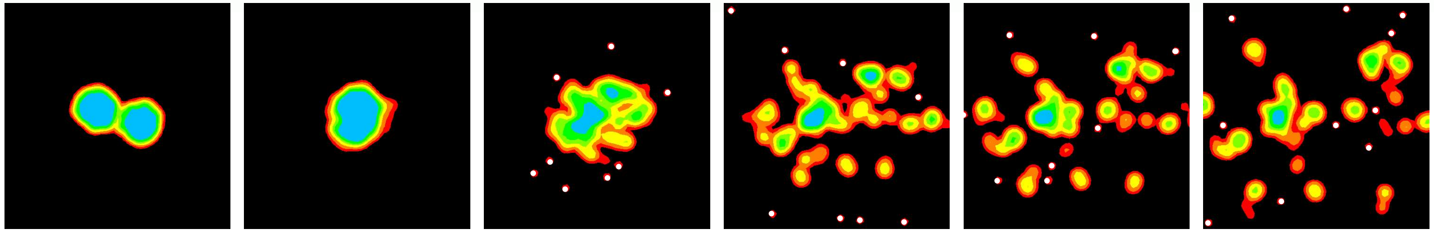
c.f. QMD simulation of nuclear pasta. G. Watanabe et al., PRC 68 (2003) 035806.



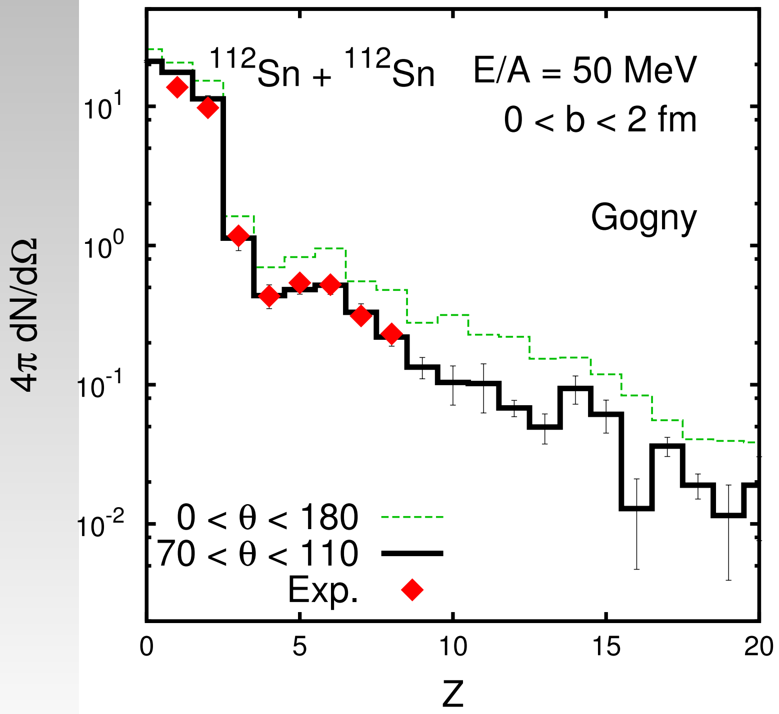
AMD results for multifragmentation

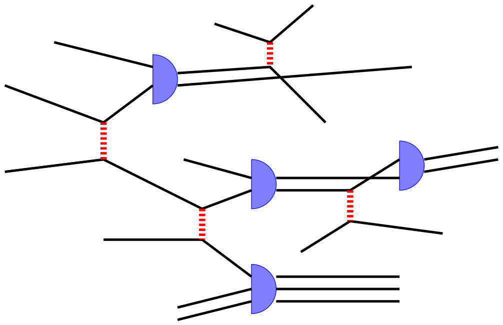


$^{112}Sn + ^{112}Sn$ central collisions

144 events, 20 CPU · days

Distribution of fragment Z





During the time evolution of AMD,

- Cluster formation
- Propagation
- Breakup

Fragment charge correlations

39 MeV/u central Xe + Sn collisions

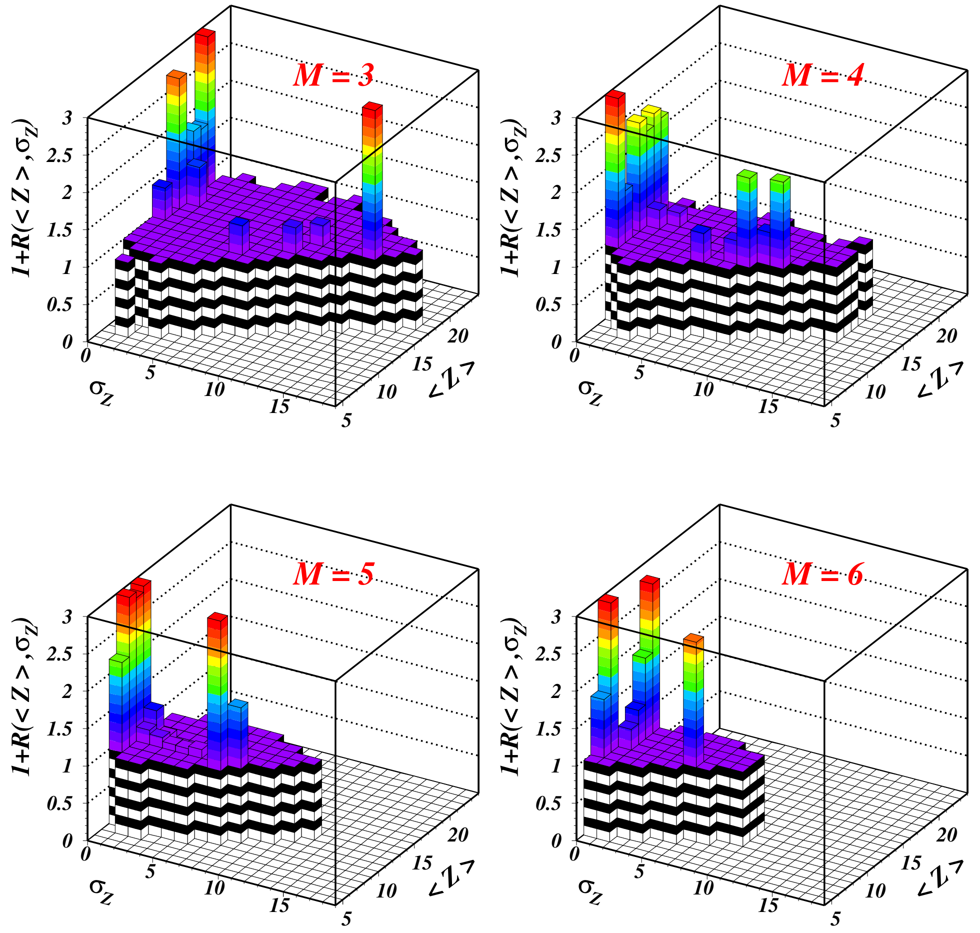
Tabacaru, Borderie et al., EPJA 18 (2003) 103.

M: fragment multiplicity

Look for events with $Z_1 = Z_2 = \cdots = Z_M$

$$\langle Z \rangle = \frac{1}{M} \sum_{i=1}^{M} Z_i$$

$$\sigma_Z^2 = \frac{1}{M} \sum_{i=1}^{M} (Z_i - \langle Z \rangle)^2$$



Enhancement of events with $\sigma_Z \lesssim 1$.

(events with almost equal-sized fragments.)

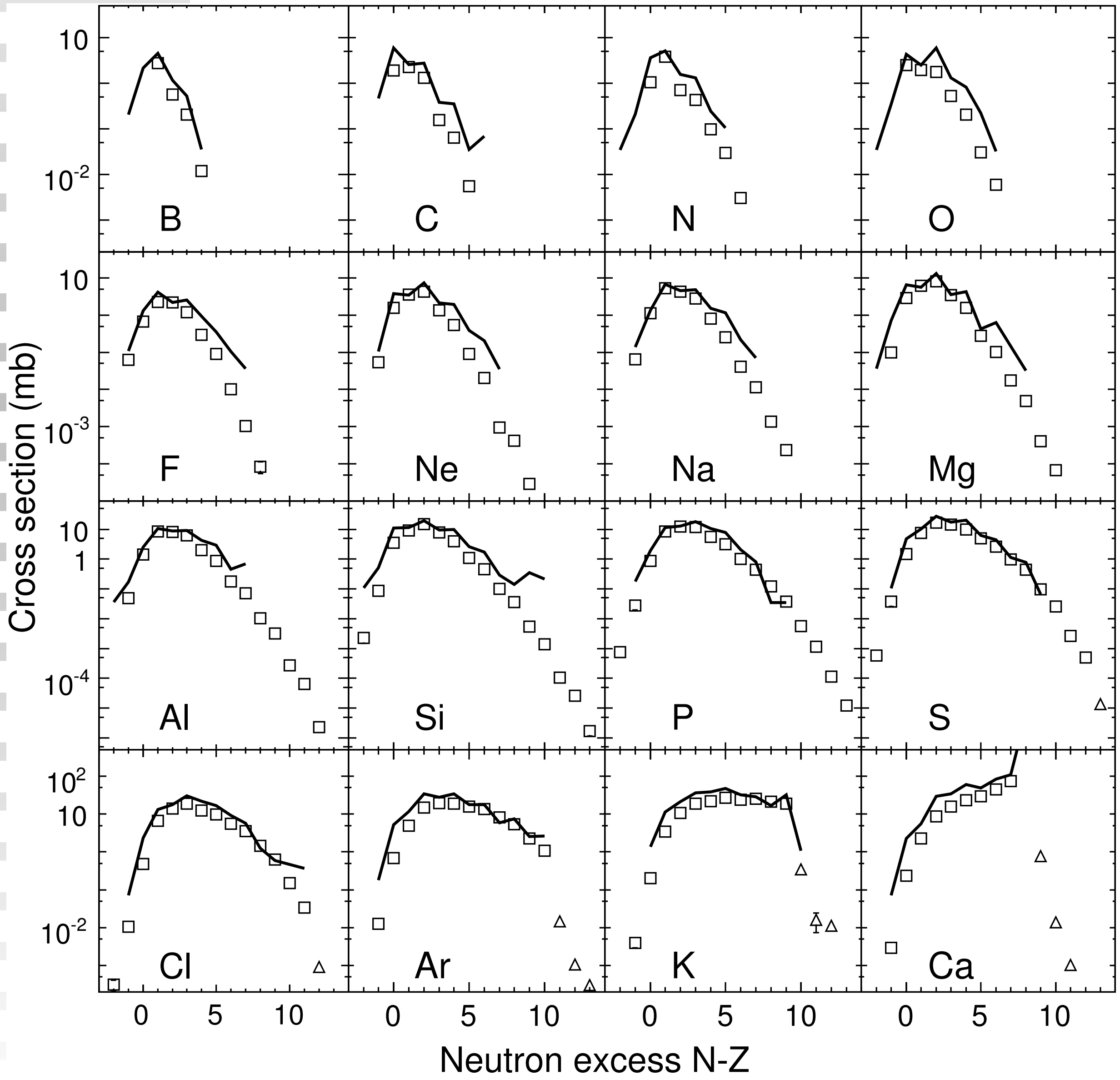
About 0.1 – 0.8% of the total.

$\Rightarrow$ Requires many events of simulations.

Rare isotope production by projectile fragmentation

M. Mocko, M.B. Tsang, AO et al.

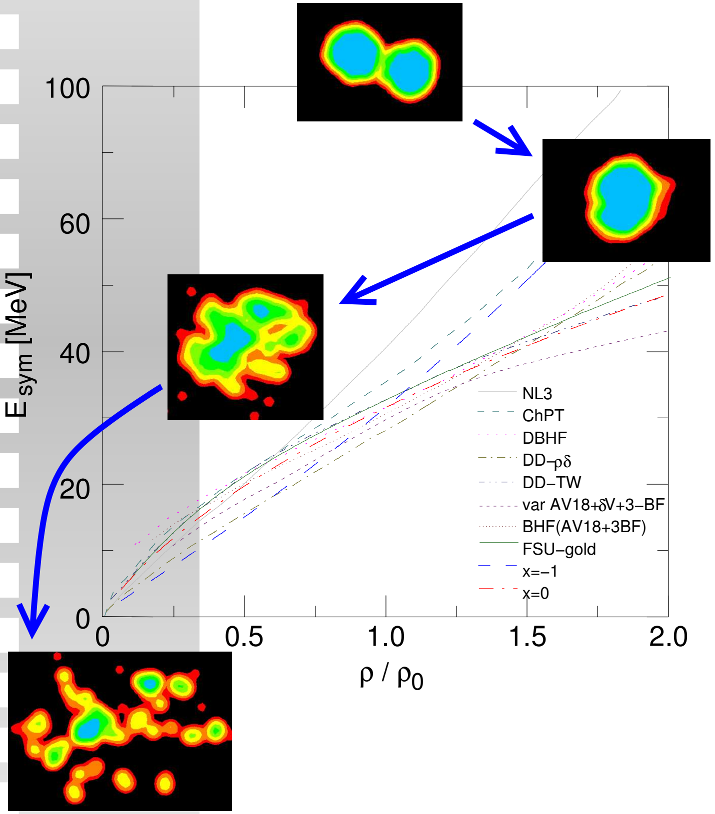
$^{48}Ca + {}^{9}Be$ at 140 MeV/nucleon



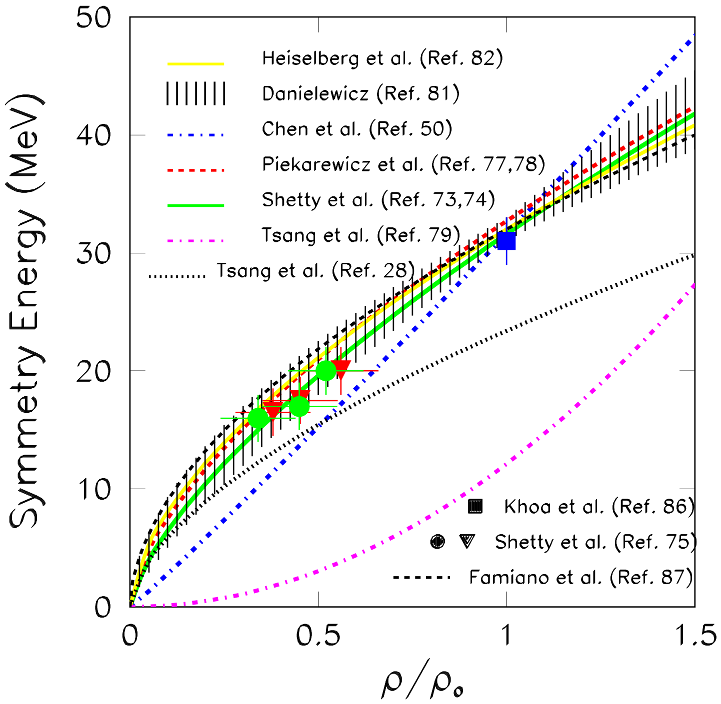
- AMD calc: 17,000 events
  $\Rightarrow$ 40 CPU $\cdot$ days
  (HPC Center at MSU)
- Experiment: $\sim 10^7$ events
- Dependence on target?
  e.g. Ca + ^{181}Ta

Heavy-ion collisions and EOS

Nuclear matter EOS: $E(\rho,\delta)/A = E(\rho,0)/A + E_{\mathrm{sym}}(\rho)\delta^2, \qquad \delta = (\rho_n - \rho_p)/\rho$

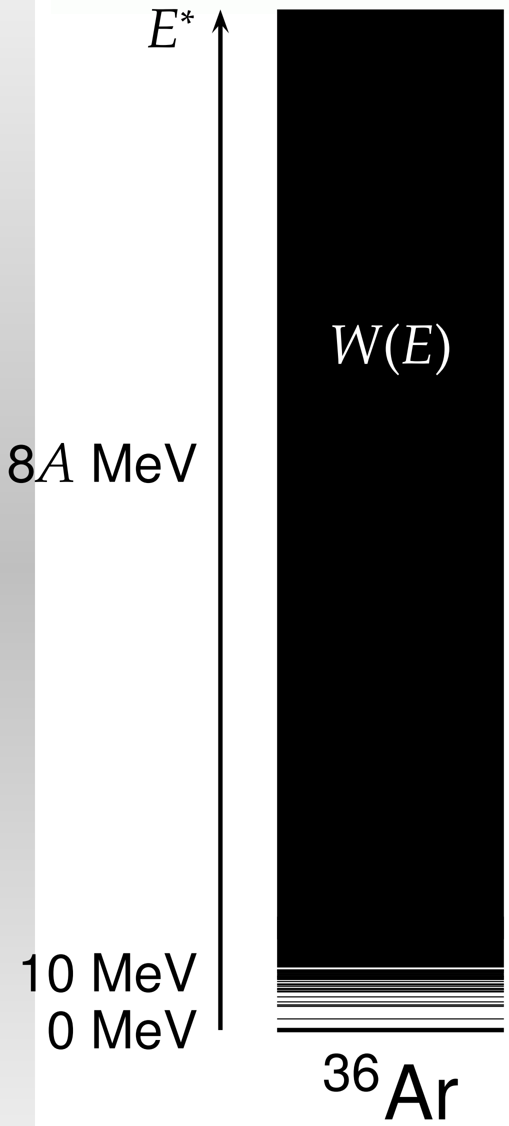


Shetty et al., PRC 76 (2007) 024606



Observables: Isoscaling, Isospin diffusion,
Neutron/proton emission ratio, Giant resonances,
Binding energy and neutron skin,
Neutron star calc., ...

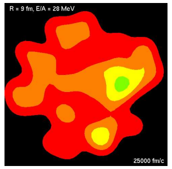
Excited states of ^{36}Ar



Gas

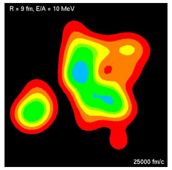
(nucleons + clusters)

$E^* = 28A$ MeV

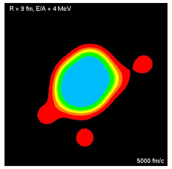


Liquid-gas
phase transition

$E^* = 10A$ MeV



$E^* = 4A$ MeV

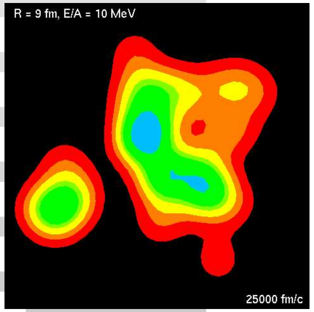


$W(E) \approx e^{2\sqrt{aE^*}}$

Volume $V = \frac{4}{3}\pi(9\ \mathrm{fm})^3$

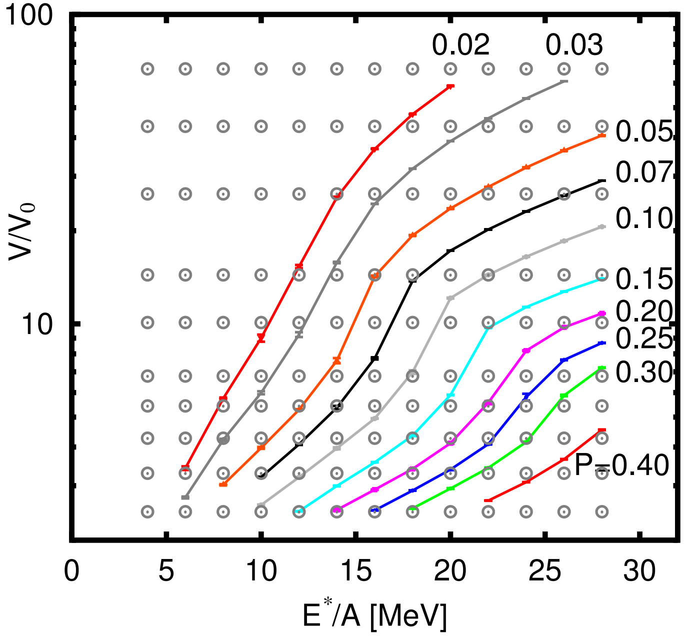
Equilibrium ensembles and caloric curves

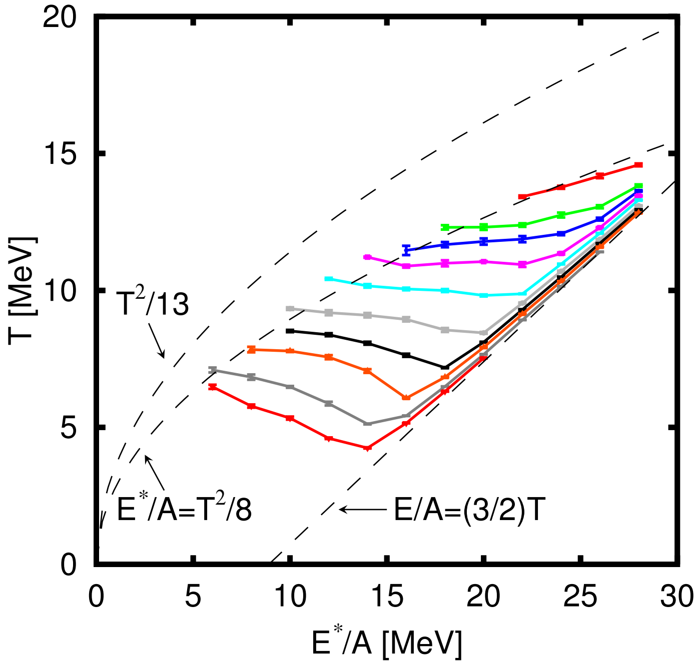
Microcanonical ensemble $\Leftarrow$ Simply solve the time evolution for a long time



- Total energy: E
- Volume: $V = \frac{4}{3}\pi R^3$ (reflections at the wall of container)
- Neutron and proton numbers: $N = 18$, $Z = 18$

$\Rightarrow$ Temperature $T(E, V)$ and Pressure $P(E, V)$



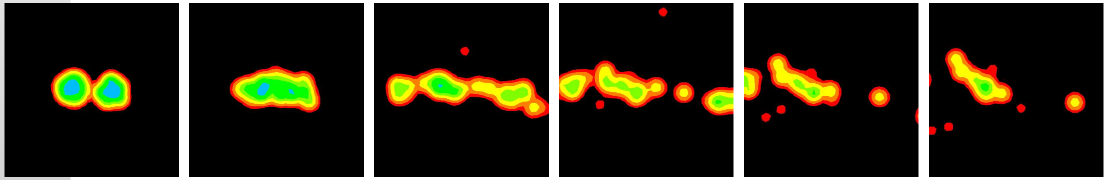


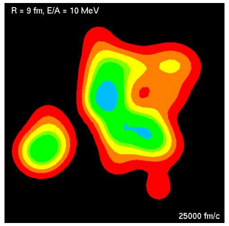
25,000 fm/c $\times$ 130 combinations of (E, V) $\Rightarrow$ 300 CPU $\cdot$ hours

Comparison of reaction and equilibrium

T. Furuta, Doctor Thesis, Tohoku University, 2007.

^{40}Ca + ^{40}Ca, E/A = 35 MeV, b = 0



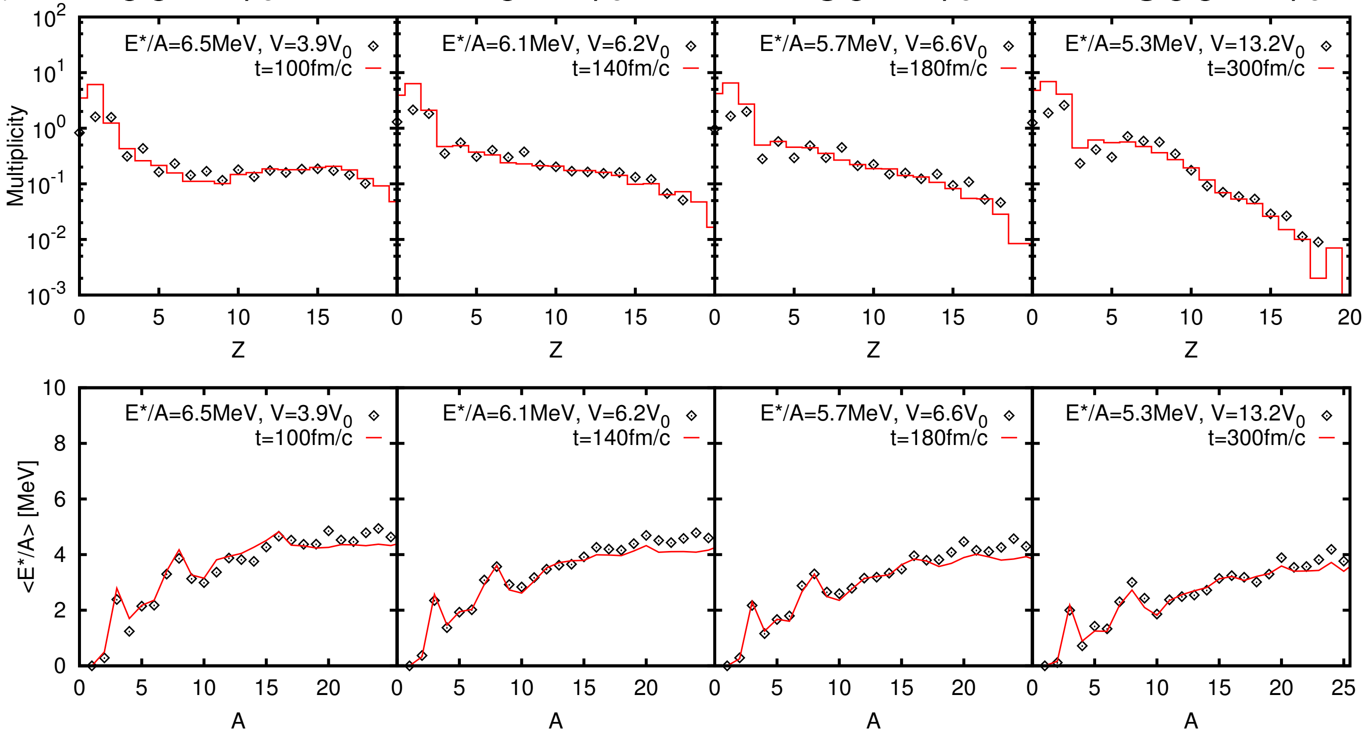


$\{\text{States at the reaction time } t\} \quad = \overset{?}{=} = \quad \text{Equilibrium ensemble}(E, V, A)$

t = 100 fm/c 140 fm/c 180 fm/c 300 fm/c

$M(Z)$

$\langle E^*/A \rangle$



Supercomputing in future

- Many events
  - High statistics demanded by applications
  - Rare phenomena, such as in fragment mass correlations
- Large systems
  - Nuclear matter, Neutron-star matter
- Without triple-loop approximation ($12A^3 \rightarrow A^4$)
  - for better consistency with ground states

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- Couple AMD with TDHF (instead of Vlasov)
- TDHF-based calculations (with stochastic terms)

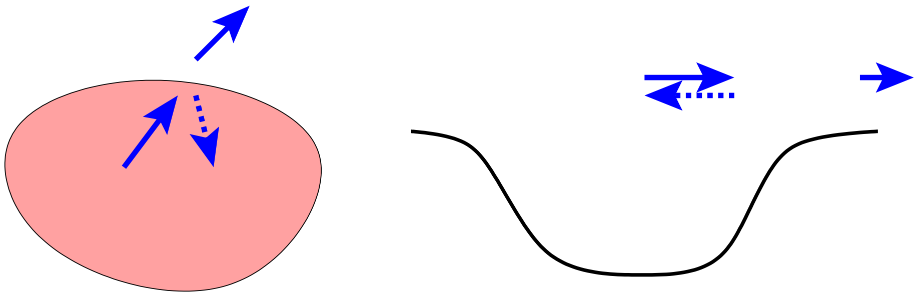
$$|\Psi(t)\rangle\langle\Psi(t)| = \overline{|\Phi_{[\omega]}(t)\rangle\langle|\Phi_{[\sigma]}(t)|} \approx \overline{|\Phi_{[\sigma]}(t)\rangle\langle|\Phi_{[\sigma]}(t)|}$$

- Microscopically derive the NN cross sections and the effective interaction
- ...

Qauntum single-particle motions

A problem in the Vlasov (semiclassical) dynamics:

Reflection by the potential step is not taken into account.



$\Rightarrow$ TDHF with some extensions

$$i\hbar\frac{\partial}{\partial t}\varphi_k(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r}) + \hat{\sigma}\right]\varphi_k(\mathbf{r},t)$$

$\hat{\sigma}$: A stochastic term which may be determined by the idea of AMD.

- Two-nucleon collisions
- Localization of the single-particle distribution

$$|\Psi(t)\rangle\langle\Psi(t)| \;\rightarrow\; \overline{|\Phi_{[\sigma]}(t)\rangle\langle|\Phi_{[\sigma]}(t)|}$$

Summary

- AMD for heavy-ion collisions has been
  - a microscopic event/state generator
  - practical (with reasonable choices of approximations)
  - requiring intensive computation
- Good balance of
  - ‘quantum’ and ‘classical’
  - ‘mean field’ and ‘cluster’
- Supercomputing in future
  - Straightforward applications to
    - rare phenomena (with many simulated events)
    - heavy systems, including $A \to \infty$
  - More precise calculations
    - link AMD with TDHF
    - ...