Dynamics of quantum equilibration in low-energy collisions

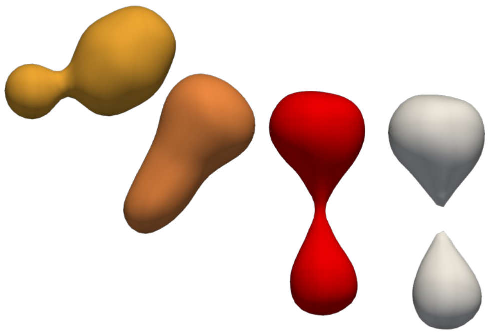
A.S. Umar

Department of Physics & Astronomy

VANDERBILT UNIVERSITY

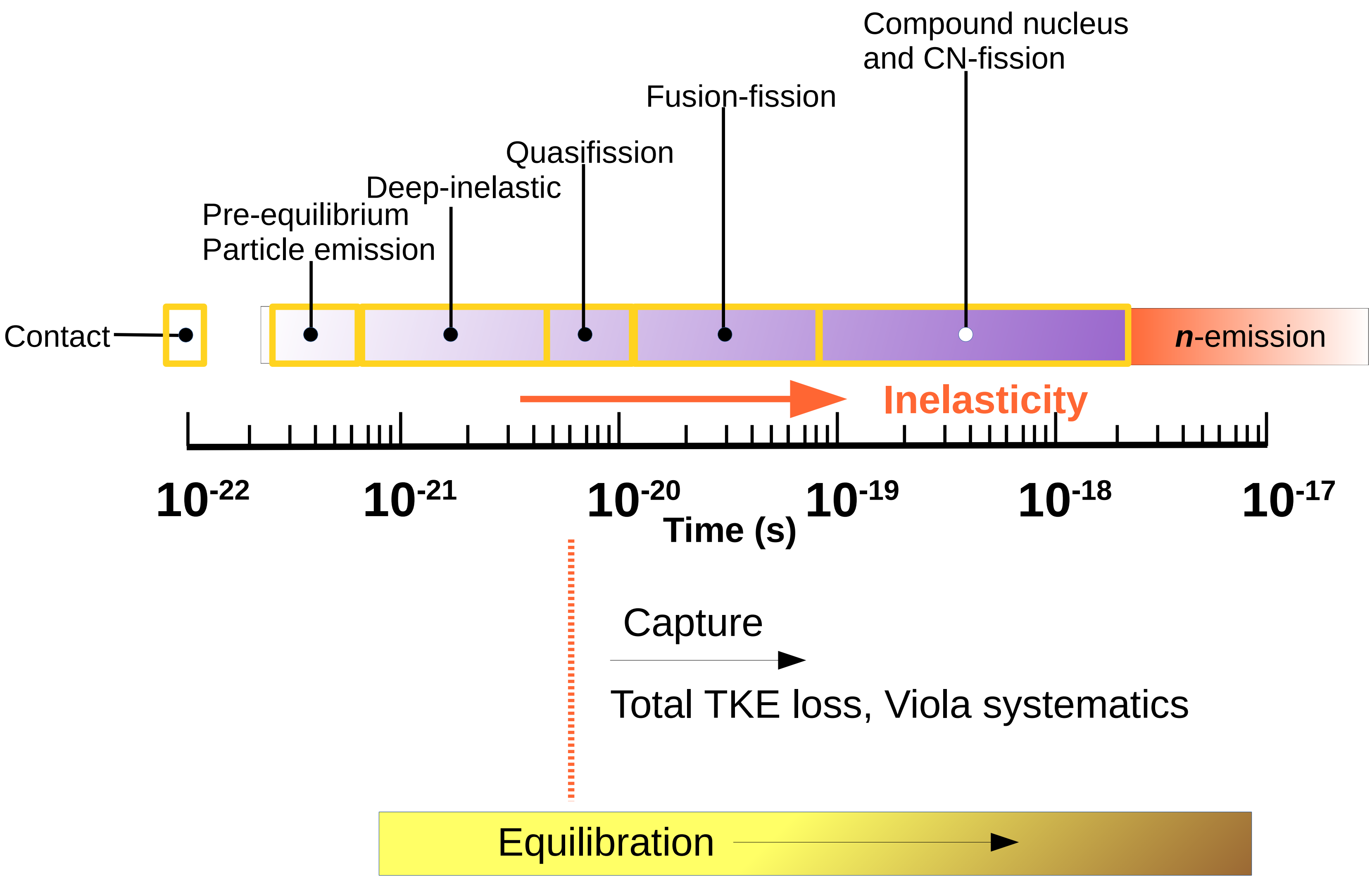
Topics:

Low-energy heavy-ion reactions
TDHF/TDDFT - primer
Equilibration phenomena
Study of collision dynamics and shell effects
Scaled measure for equilibration times

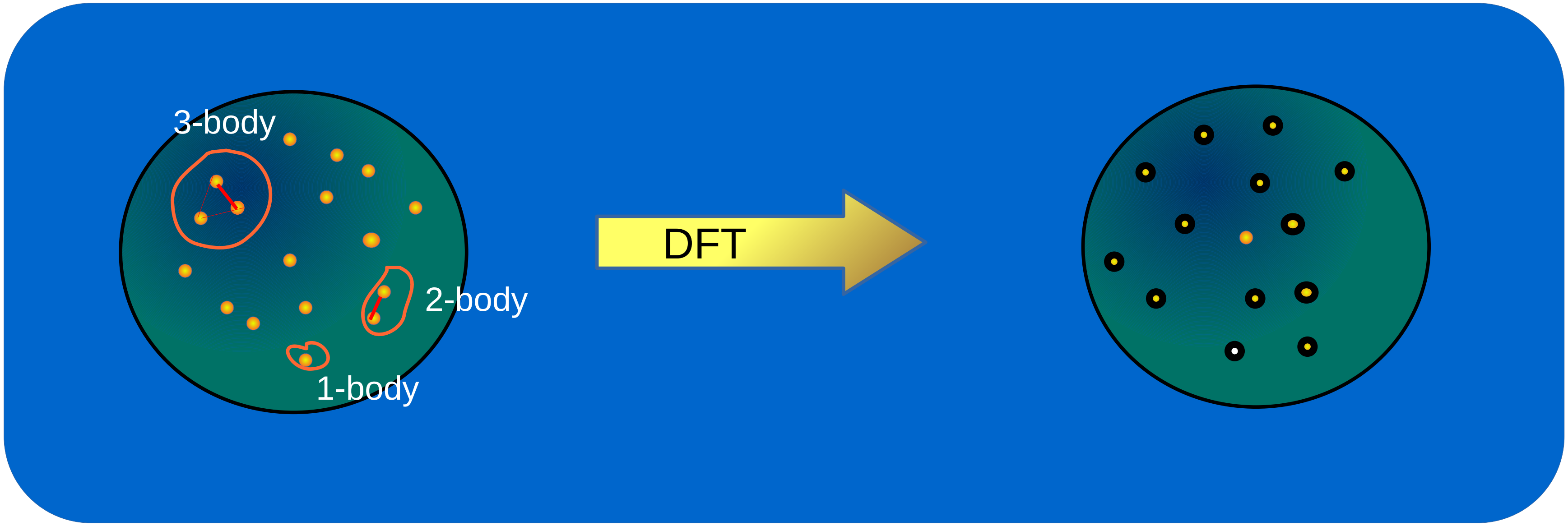


Research supported by: U.S. Department of Energy, Division of Nuclear Physics

Time scales and inelasticity for low-energy nuclear reactions



Density Functional Theory and Energy Density Functional (EDF)



ab-initio

$$\langle \Psi | H | \Psi \rangle = E$$

Mean-field - EDF

$$\Psi \rightarrow \Phi_{Slater}$$

$$H \rightarrow H_{eff}$$

$$E = \langle \Phi | H_{eff} | \Phi \rangle = \int d^3 r \; \{ H(\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu} \; ; \boldsymbol{r}) + H_{Coulomb}(\rho_p) \}$$

Single-(one-) particle density *etc.* in terms of s.p. states

EDF in NP more complicated

$$\rho_q(\boldsymbol{r}) = \sum_{i=1}^{A} \sum_{\sigma} \phi_i^*(\boldsymbol{r}, \sigma, q) \phi_i(\boldsymbol{r}, \sigma, q)$$

$$v = v_{NN-eff} \rightarrow DFT(Hartee - Fock)$$

$$v \neq v_{NN-eff} \rightarrow DFT(Kohn - Sham)$$

Skyrme EDF – Galilean Invariant

$$H_S(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau - \boldsymbol{j}^2)$$

$$-\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2) - \frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho$$

$$+\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n)$$

$$+\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}(\rho_p^2+\rho_n^2)\left(x_3+\frac{1}{2}\right)\right]$$

$$+\frac{1}{4}t_0x_0\boldsymbol{s}^2 - \frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) + \frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2 - \frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)$$

$$+\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2) + \frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2)$$

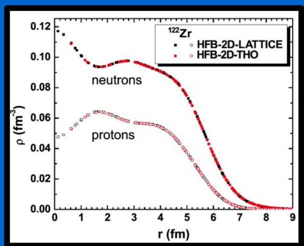
$$-\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\nabla_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]$$

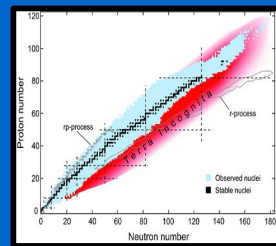
Time-odd terms come in pairs!
Total is T-R invariant

(s,j,T) time-odd, vanish for static HF calculations of even-even nuclei
non-zero for dynamic calculations, odd mass nuclei, cranking etc.

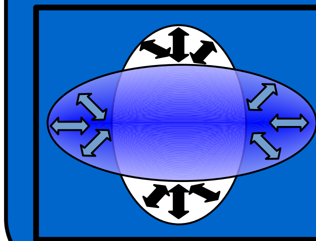
TDDFT- Study Structure and Reactions in Same Framework

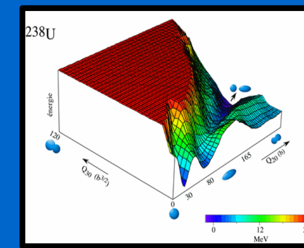
Structure

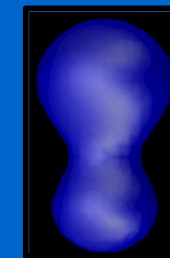




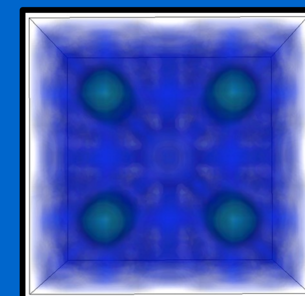
Oscillations, Fusion, Fission

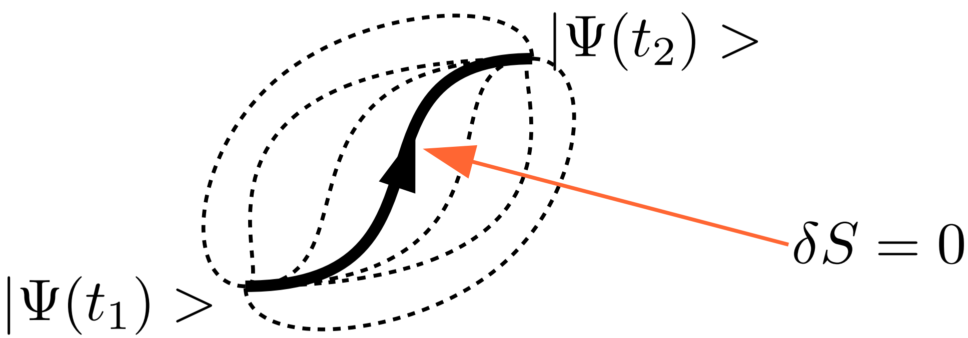






Neutron Star Crust





- TDDFT is the time-dependent generalization of DFT

$$S = \int_{t_1}^{t_2} dt < \Phi(t)|H - i\hbar\partial_t|\Phi(t) >$$

$$i\frac{\partial}{\partial t}\phi_\alpha = h(\rho, \tau, \mathbf{j}, \mathbf{s}, \mathbf{T}, \mathbf{J}_{\mu\nu}; \mathbf{r})\phi_\alpha$$

self-consistent

- Only input is the EDF (structure information only)
- TDDFT gives the *most probable outcome*
- Describe reactions and structure on an equal footing microscopically

Modern TDDFT Codes

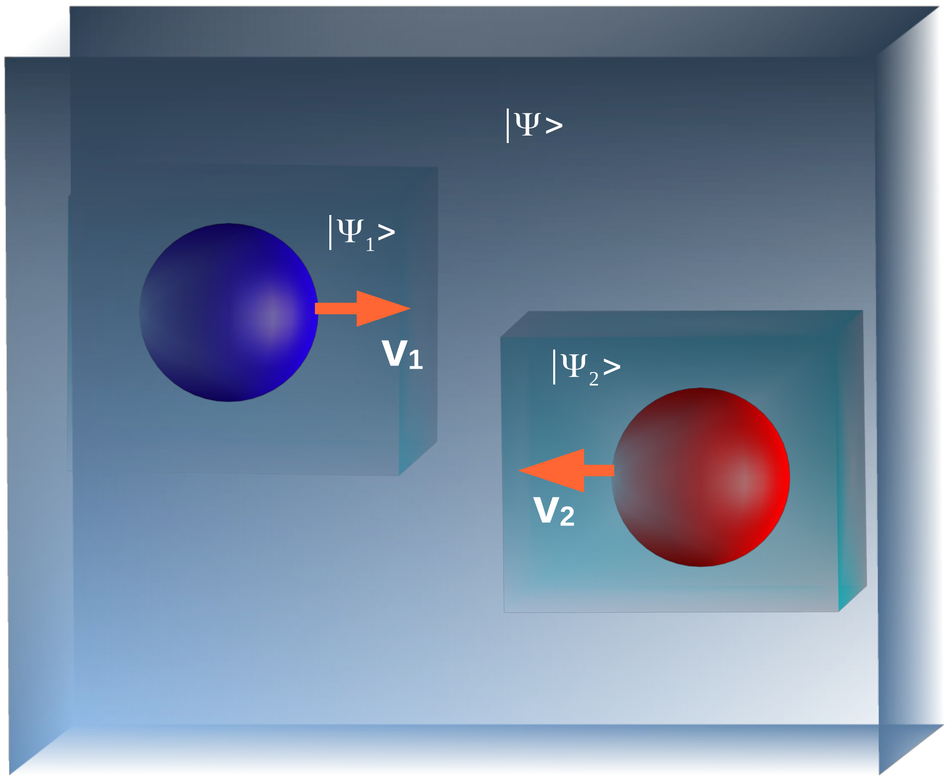
VU-TDDFT Code

- Basis-Spline discretization for high accuracy
- 3-D Cartesian lattice – no geometrical simplification
- Complete EDF including all terms (time-even, full time-odd)
- Coded in Fortran-95 and OpenMP

1. Umar, Oberacker, VU-TDDFT, Phys. Rev. C 73, 054607 (2006)
2. Maruhn, Reinhard, Stevenson, Umar, Sky3D, Comp. Phys. Comm. 185, 2195 (2014)
3. B. Schuetrumpf, *et al.* Sky3D V1.1, Comp. Phys. Comm. 229, 211 (2018)

TDDFT Initial Setup

- Initial approach is determined by Coulomb trajectory up to **R_0**
- The initial DFT Slater determinants boosted by velocities at **R_0**

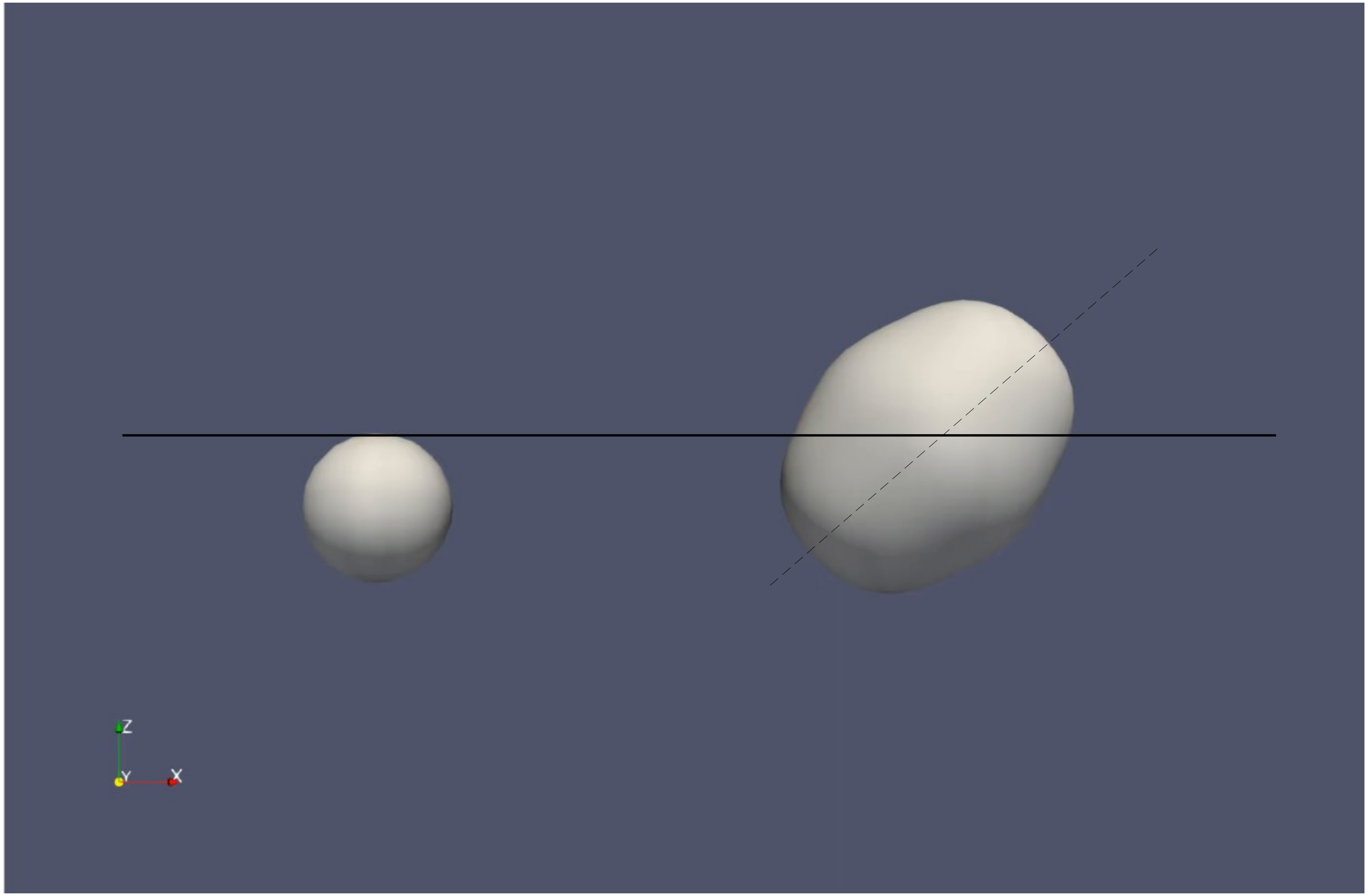


$$|\Psi_j\rangle \rightarrow \exp(i\boldsymbol{k}_j \cdot \boldsymbol{R})|\Psi_j\rangle$$

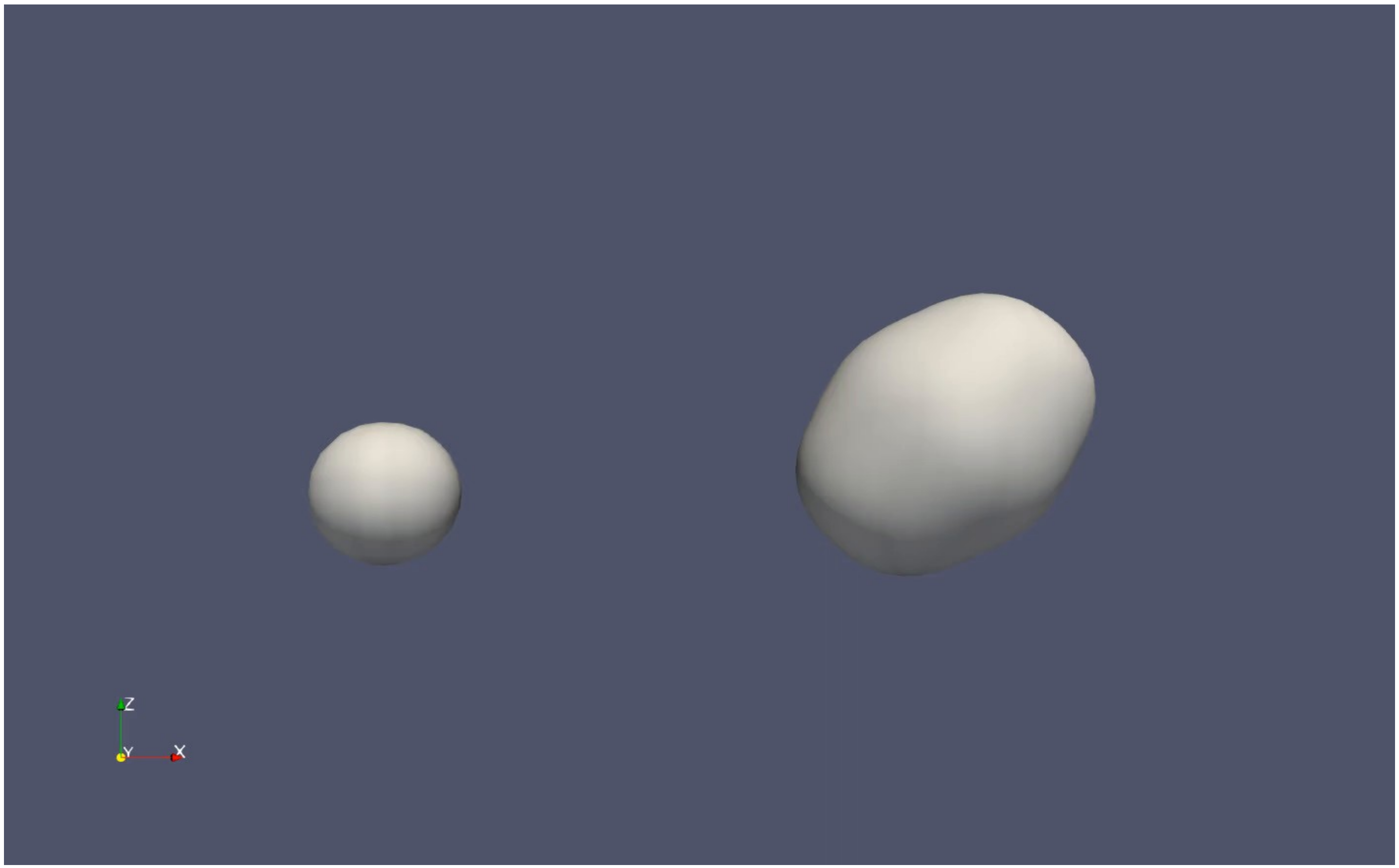
$$\boldsymbol{R} = \frac{1}{A_j}\sum_{i=1}^{A_j} r_i$$

If final stage contains a single fragment – **Fusion**
If final stage contains two fragments – **Deep-inelastic** or **quasifission**

Example: ^{48}Ca + ^{249}Bk (β=135^{o}) @ E_{cm}=234 MeV, L =60$\hbar$



Example: ^{48}Ca + ^{249}Bk (β=135^o) @ E_{cm}=234 MeV, L =60$\hbar$



Final products: ^{94}Sr and ^{203}Au

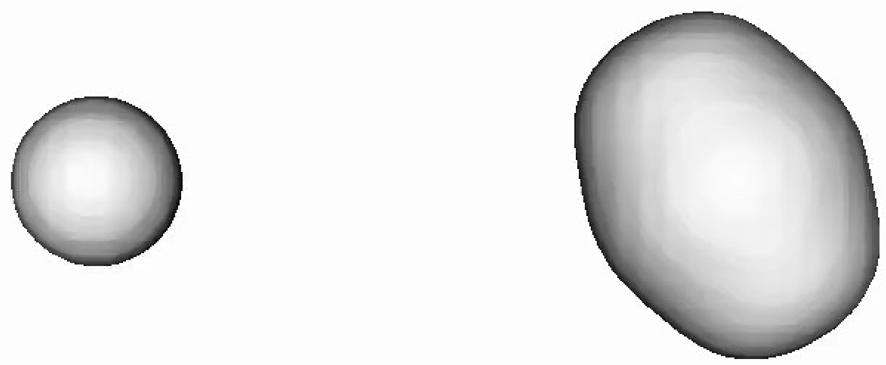
Contact time: 4.8 zs

Computer time: 1.5 days
on a 20 processor workstation

Equilibration dynamics

Equilibration:
Mass
Isospin
Energy
Angular momentum
Fluctuations (beyond TDHF)

Dynamics:
Time scales of reaction
Orientation of deformed nuclei



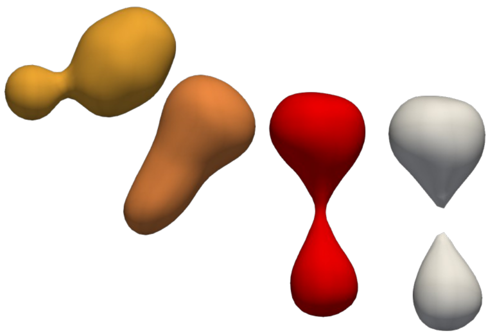
Quantum:
Shell effects

Theory:
TDHF is proven to be an excellent diagnostic tool for low-energy reactions, reproducing many exp features. Fluctuations can be studied with TDRPA and SMF.

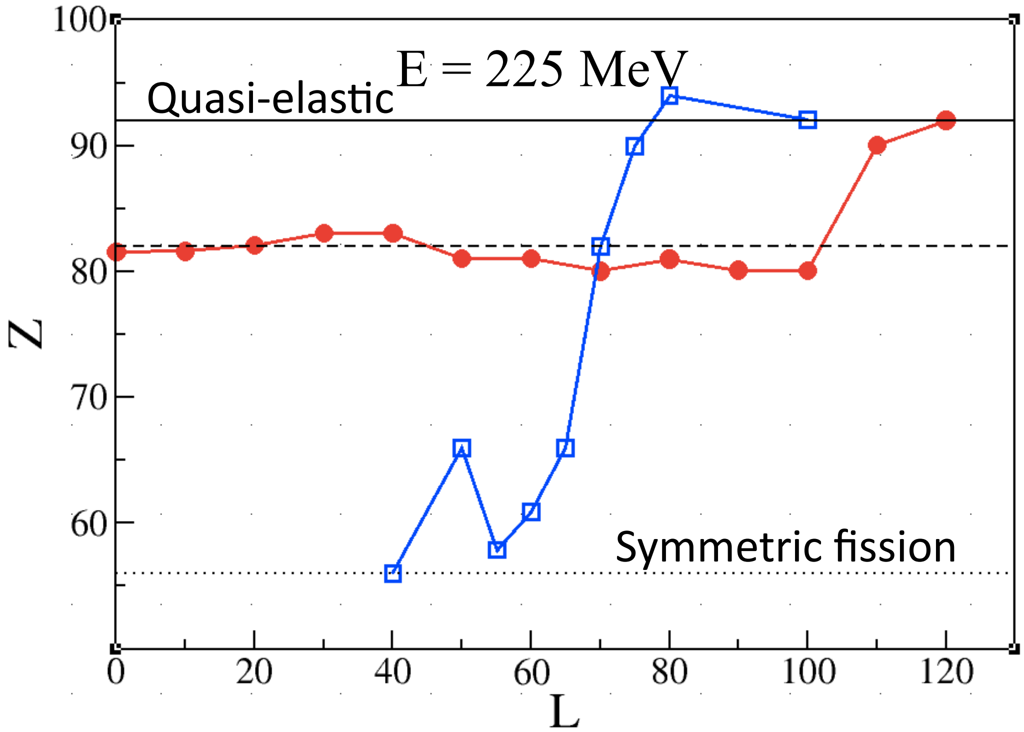
Recent TDHF review - Simenel, Umar, Prog. Part. Nucl. Phys. **103**, 19 (2018)

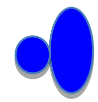
Mass Equilibration

Quasifission

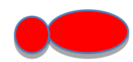


Quasifission – ^{40}Ca + ^{238}U – orientation and shell effects





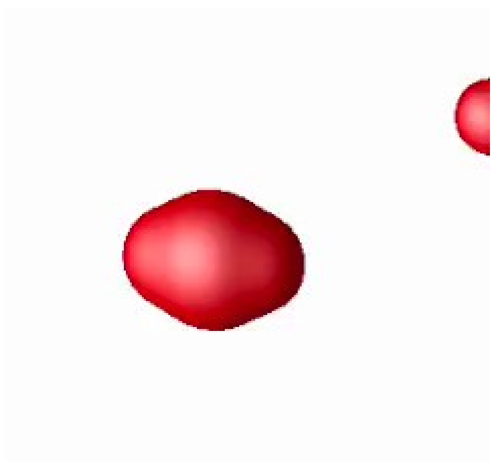
- Fusion and long QF time
- Large mass transfer

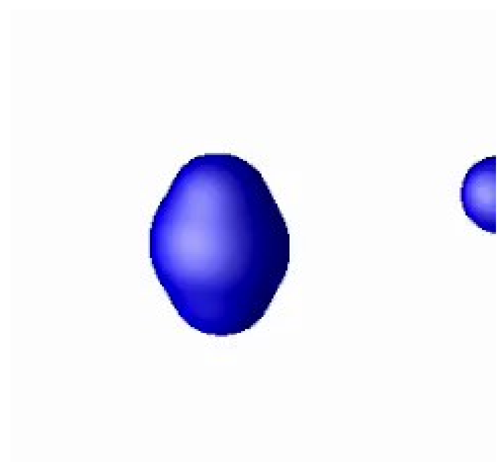


- No fusion, short QF time
- Mass transfer dominated by **quantum shell effects** in the ^{208}Pb region

1 zs = 10^{-21} sec

E=225, L=100 (tip)
Final fragments: ^{78}Ge, ^{200}Hg
c. time < 10 zs

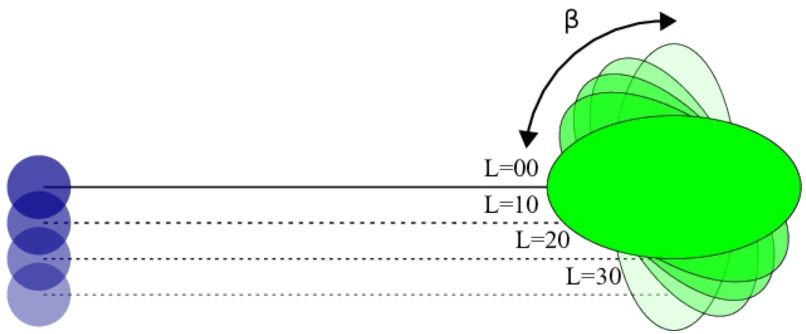




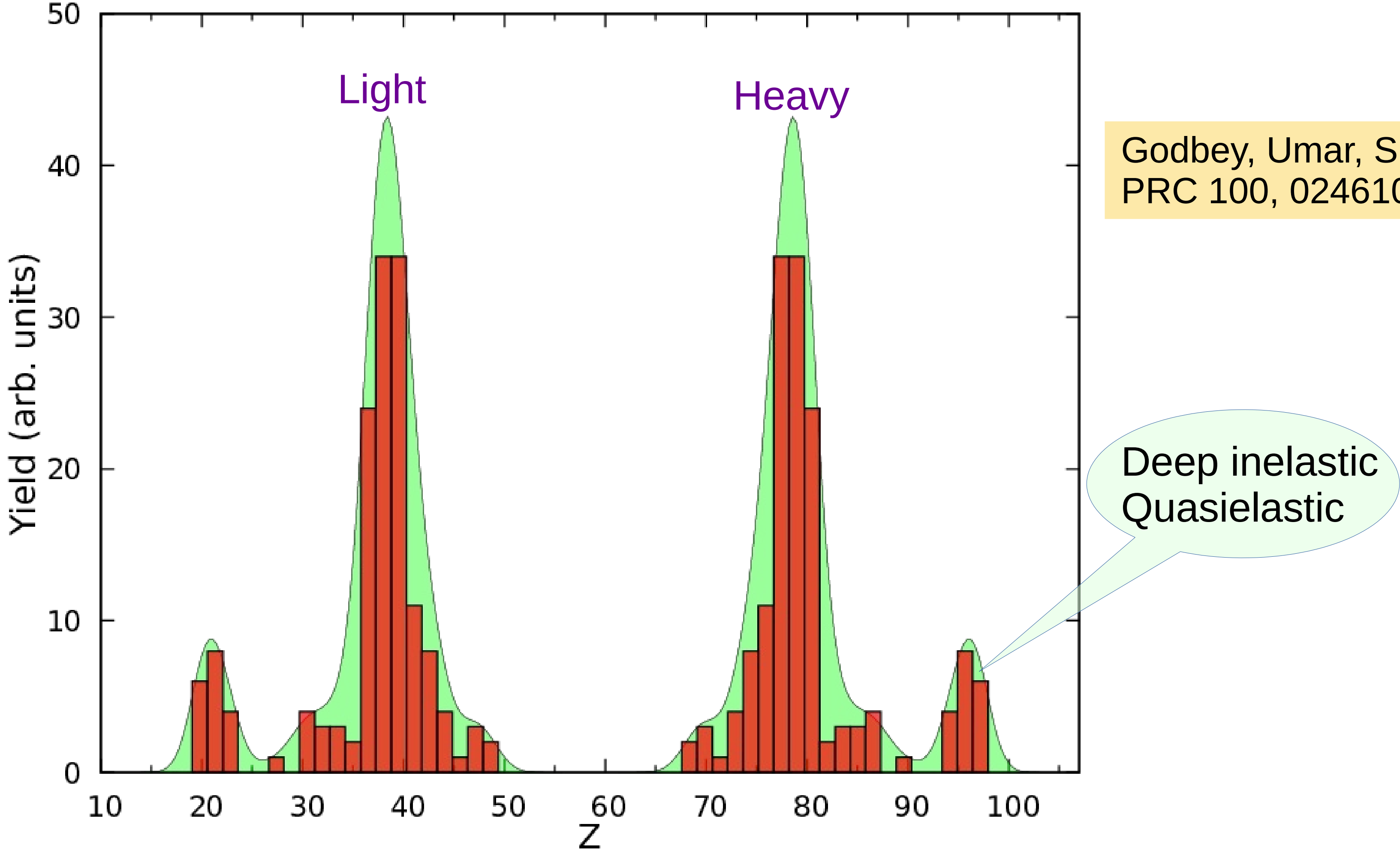
E=225, L=40 (side)
Final framents: ^{140}Ba,^{138}Ba
c. time > 20zs

Wakhle *et al.*, PRL **113**, 182502 (2014)

Quasifission – ^{48}Ca + ^{249}Bk – orientation and shell effects

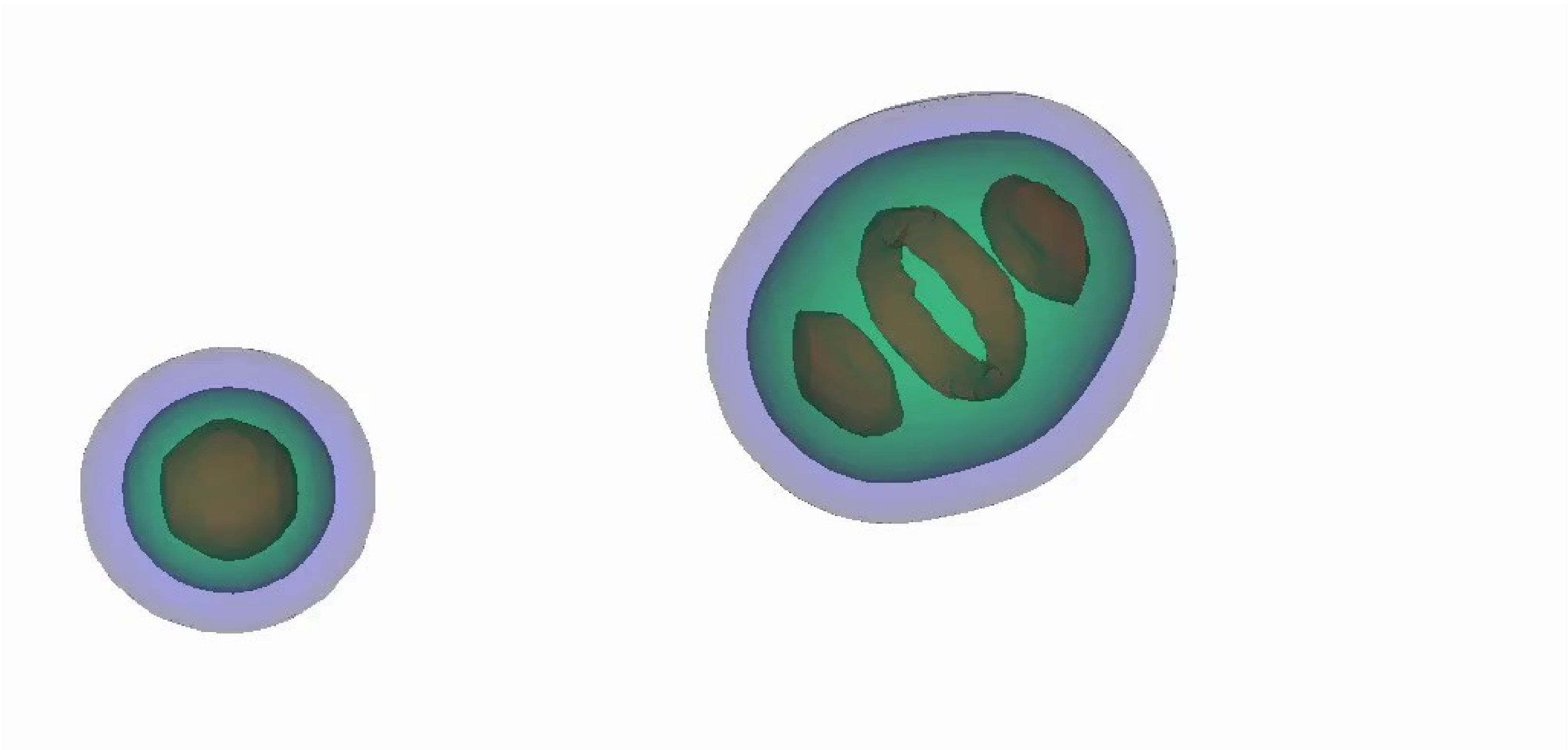


- Most comprehensive QF calculation
- All β in range (0°,180°) Δβ=15°
- Entire L range for each β
- A total of 148 collisions
- Each (β,L) run takes 1-3 days on 20 core CPU



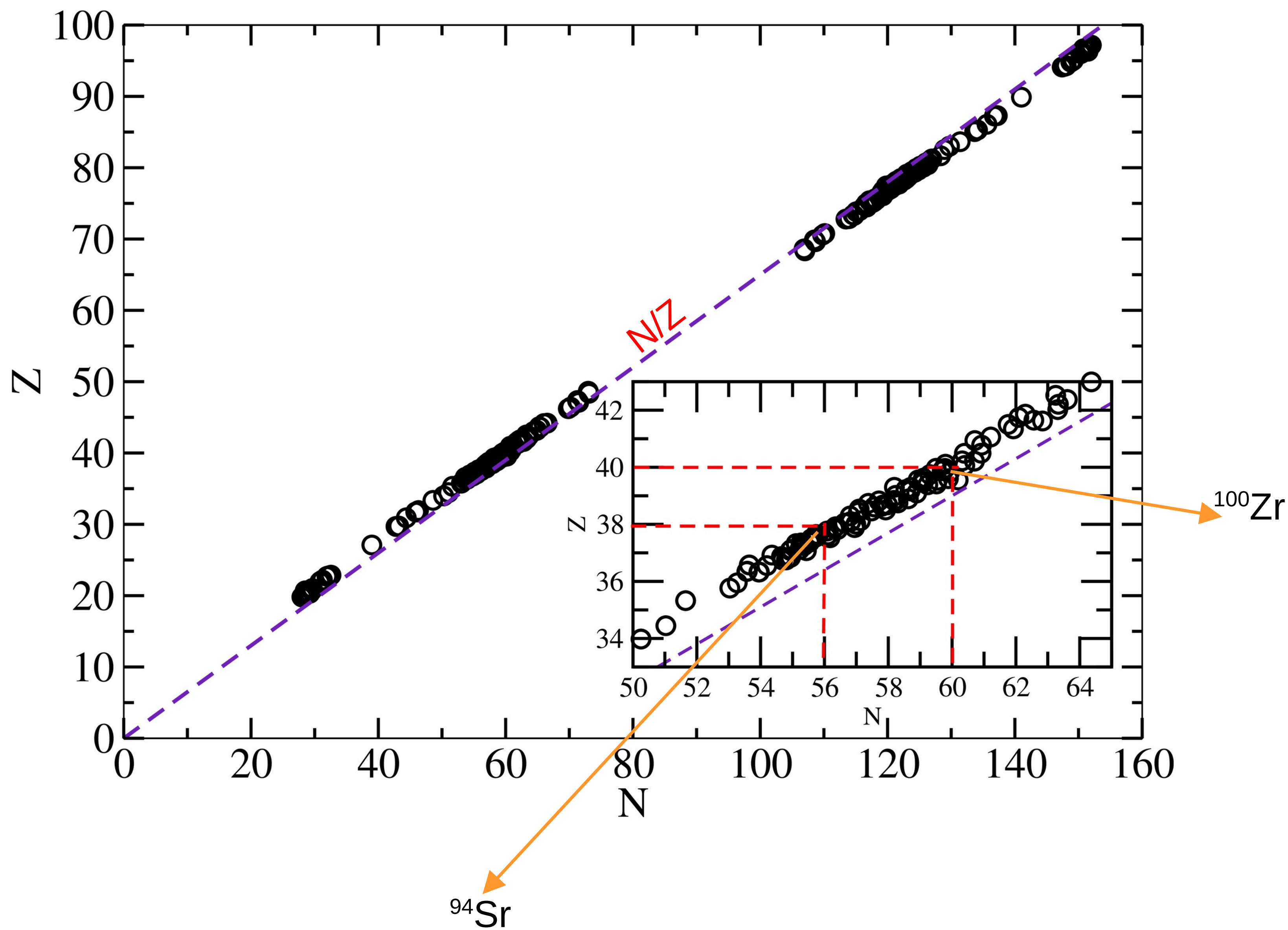
Godbey, Umar, Simenel, PRC 100, 024610 (2019)

Quasifission – ^{48}Ca + ^{249}Bk – orientation and shell effects



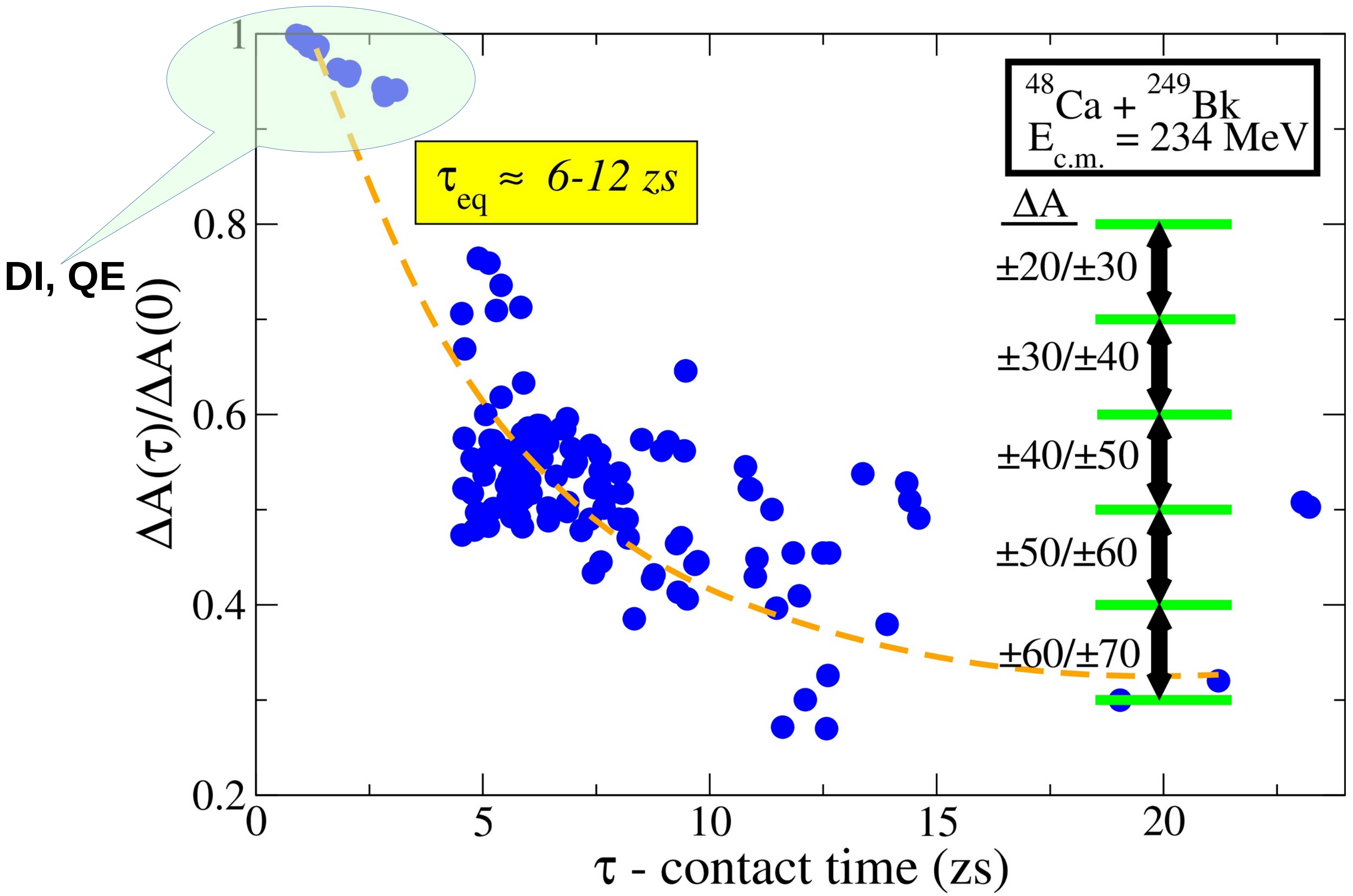
$E_{c.m.}$= 234 MeV, L=90$\hbar$, β=150^o
Final fragments: ^{99}Zr, ^{198}Ir
contact time 8 zs

Quasifission – ^{48}Ca + ^{249}Bk – orientation and shell effects



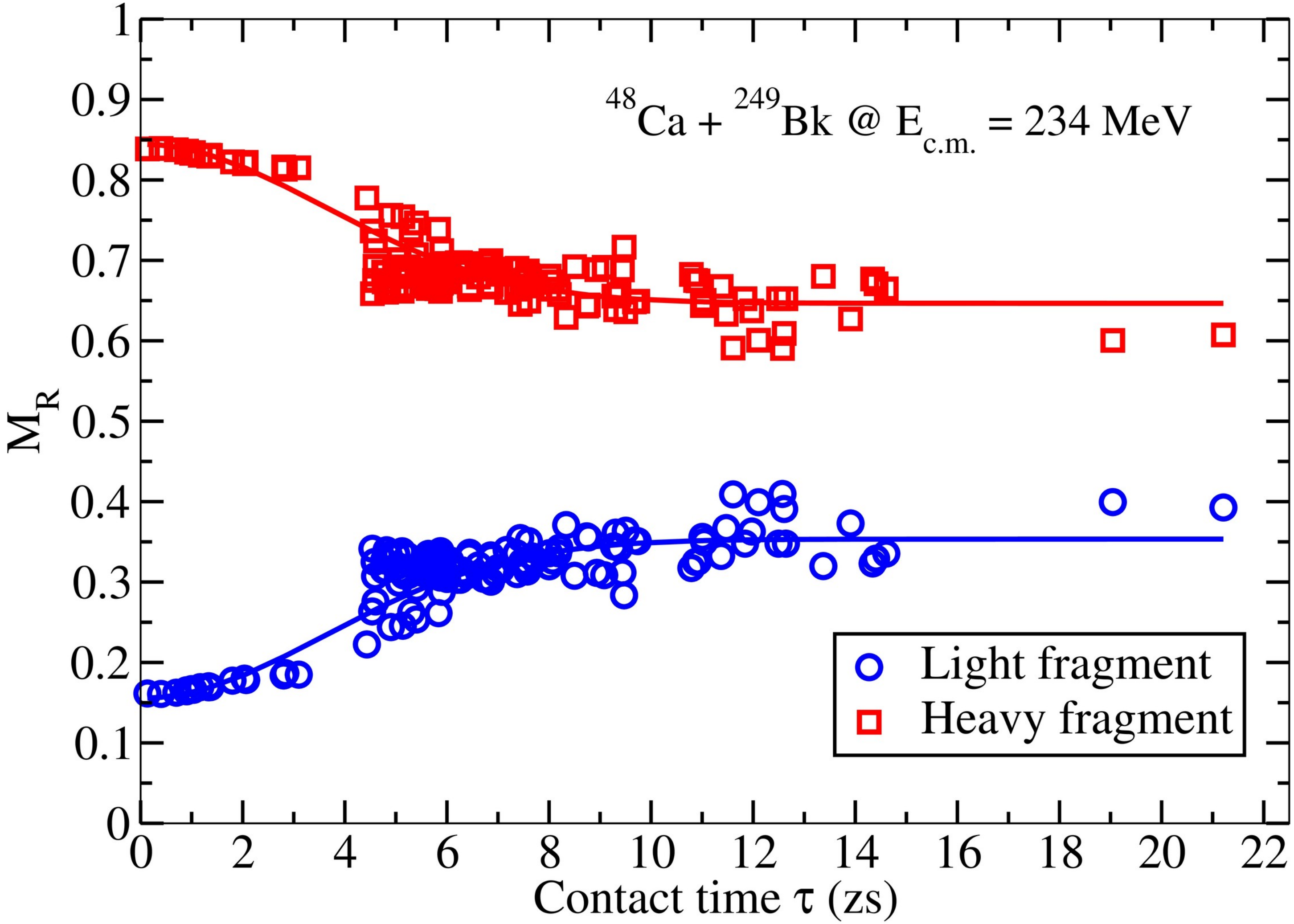
Quasifission in ^{48}Ca + ^{249}Bk – equilibration time

$$\Delta A(t) = A_{TLF}(t) - A_{PLF}(t)$$



Quasifission in ^{48}Ca + ^{249}Bk – equilibration time

$$M_R = \frac{M_{frag}}{M_1 + M_2}$$



Summary for mass equilibration

- ~ >**12 zs** to reach mass equilibrium
  (Toke *et al.* PRC 1985, du Rietz *et al.*, PRC 2013)

- Orientation dependence effects time-scales
  - slow QF versus fast QF

First exp. evidence

- Shell effects influence/hinder equilibration (Z=82)
  - 40Ca+238U (Wakhle *et al.* + TDHF)
  - 48Ti + 238U (M. Morjean *et al*. PRL 119, 222502 (2017))

- Deformed shell effects observed in TDHF
  - preference for neutron rich Zr isotopes (strongly deformed and bound)
  - optimal pair that minimizes energy

Godbey, Umar, Simenel, PRC 100, 024610 (2019)

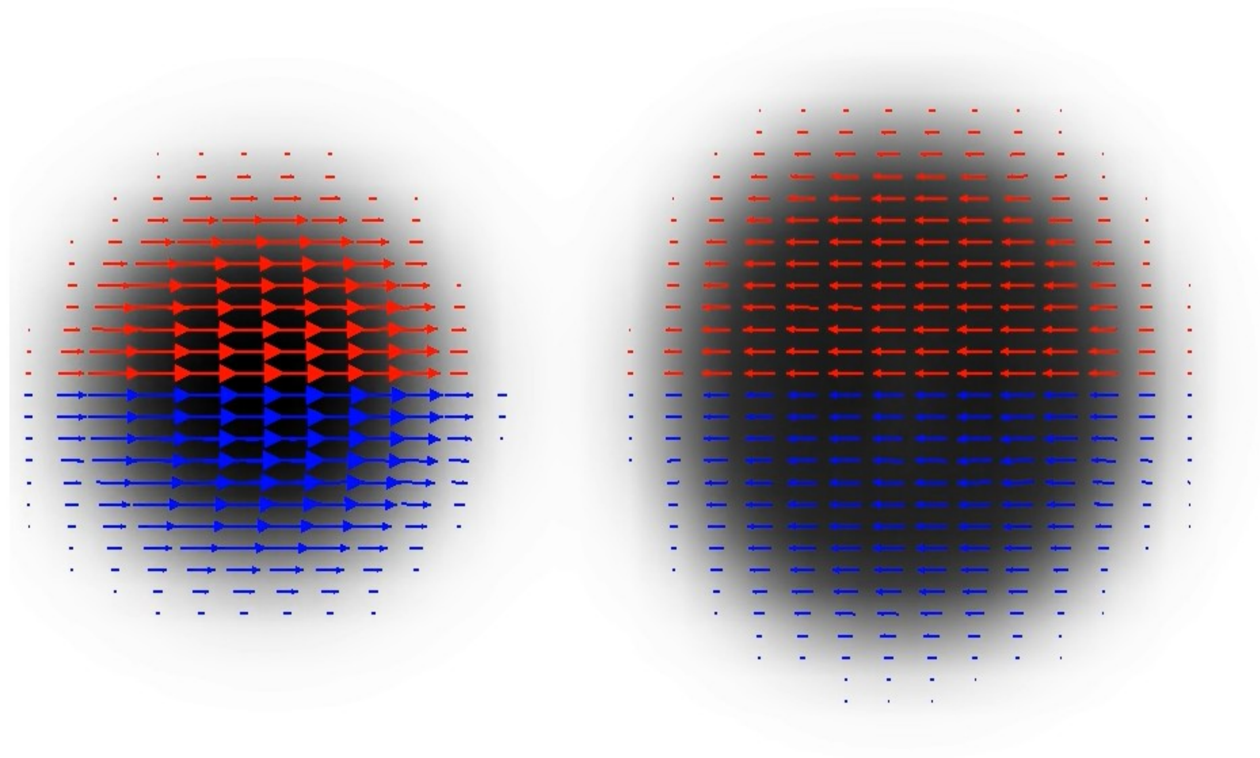
Isospin Equilibration

Deep-inelastic reactions

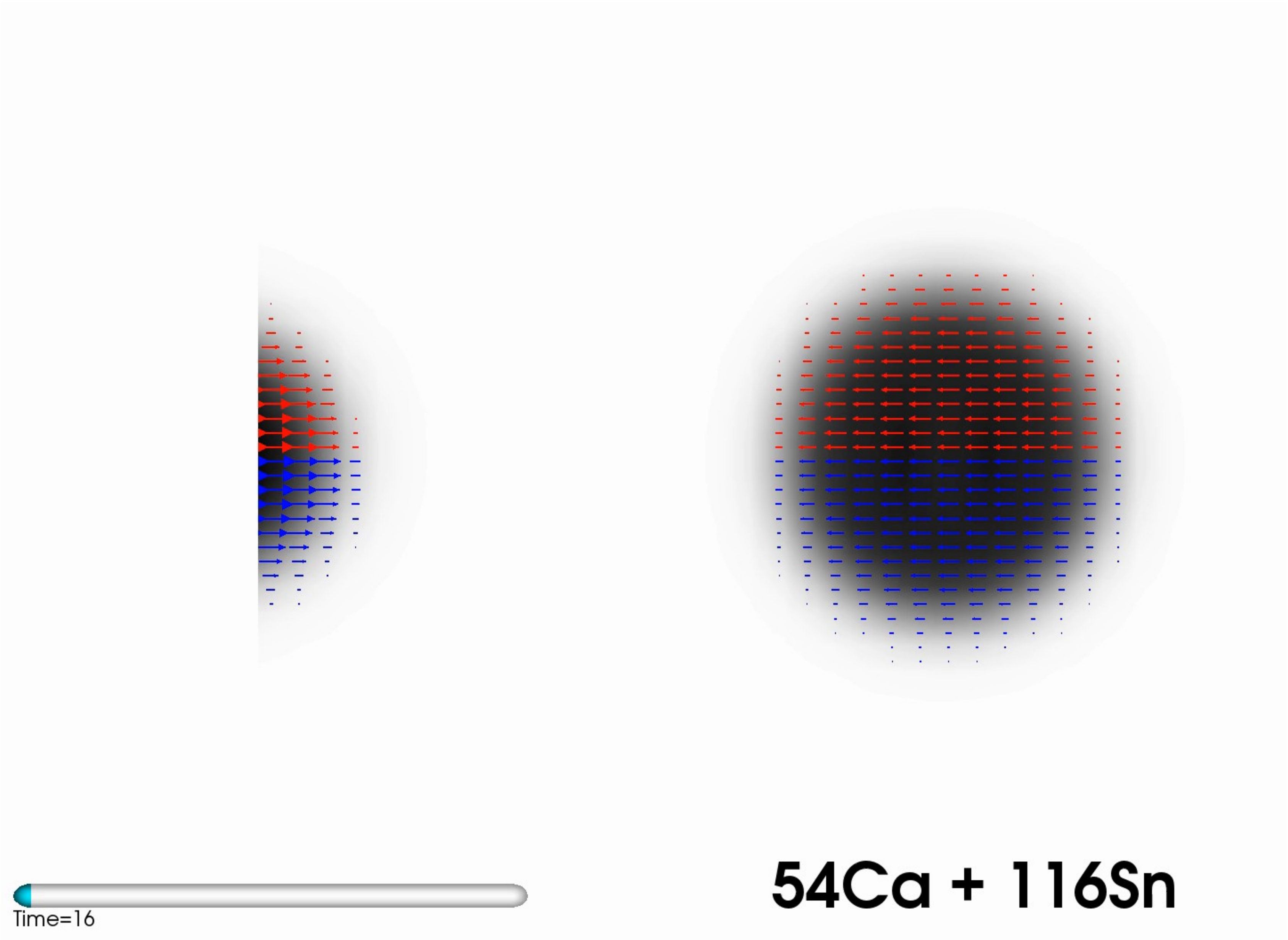
Isospin equilibration

- Connection with symmetry energy, isospin dependence of EoS
- Much faster than mass equilibration: Equilibration ~ exp(**-t/0.3zs**) from experiments at Fermi energy (Jedele *et al.*, PRL 118, 2017)
- Needs faster reaction mechanisms than quasifission
- Deep-inelastic collisions
  (Planeta *et al.*; deSouza *et al.*, PRC 1988, K. Stiefel *et al*, PRC 2014)
- Will be studied with RIBs

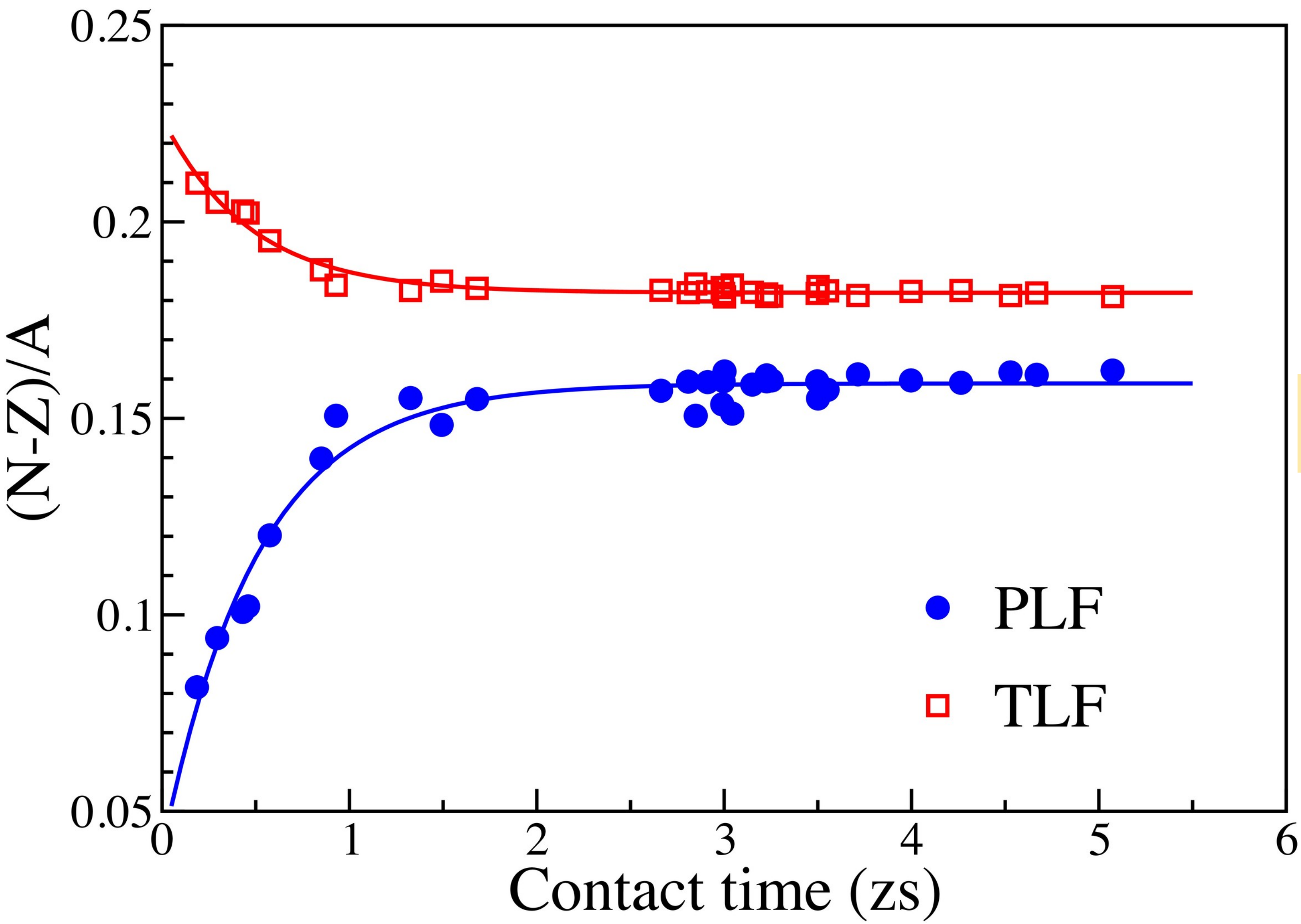
Isospin equilibration in fusion – $^{54}Ca+^{116}Sn$ (E_{cm} = 120 MeV)



Isospin equilibration in fusion – $^{54}Ca+^{116}Sn$ (E_{cm} = 120 MeV)



Isospin equilibration in DI – $^{78}Kr+^{208}Pb$ – 8.5 MeV/A

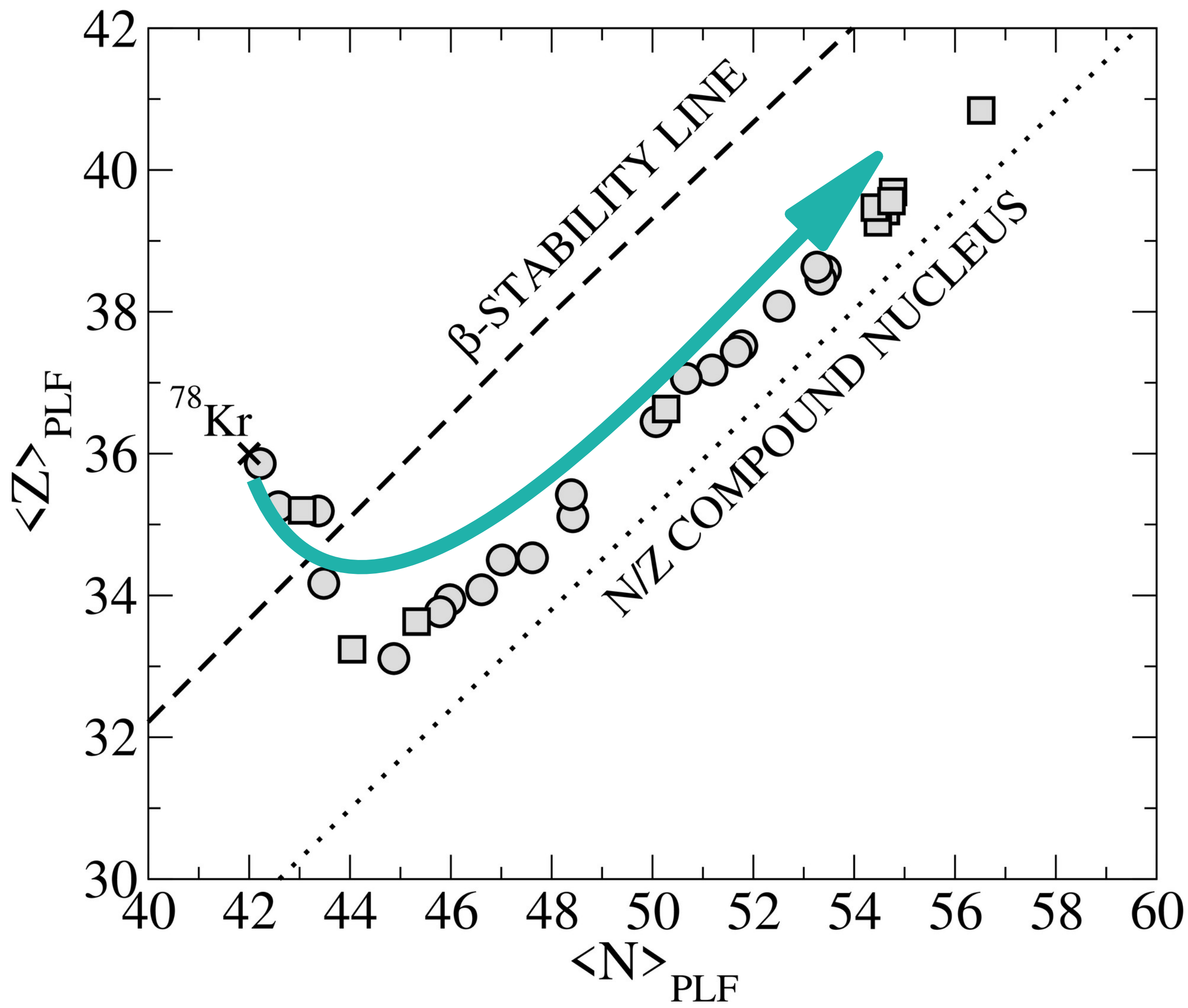


Umar, Simenel, Ye
PRC 96, 024625 (2017)

Broad range of fast contact times

$(N-Z)/A = \alpha + \beta e^{-\tau/\mathbf{0.5zs}}$ ~ **1 zs** to reach isospin equilibrium

Isospin equilibration – $^{78}Kr+^{208}Pb$ – 8.5 MeV/A

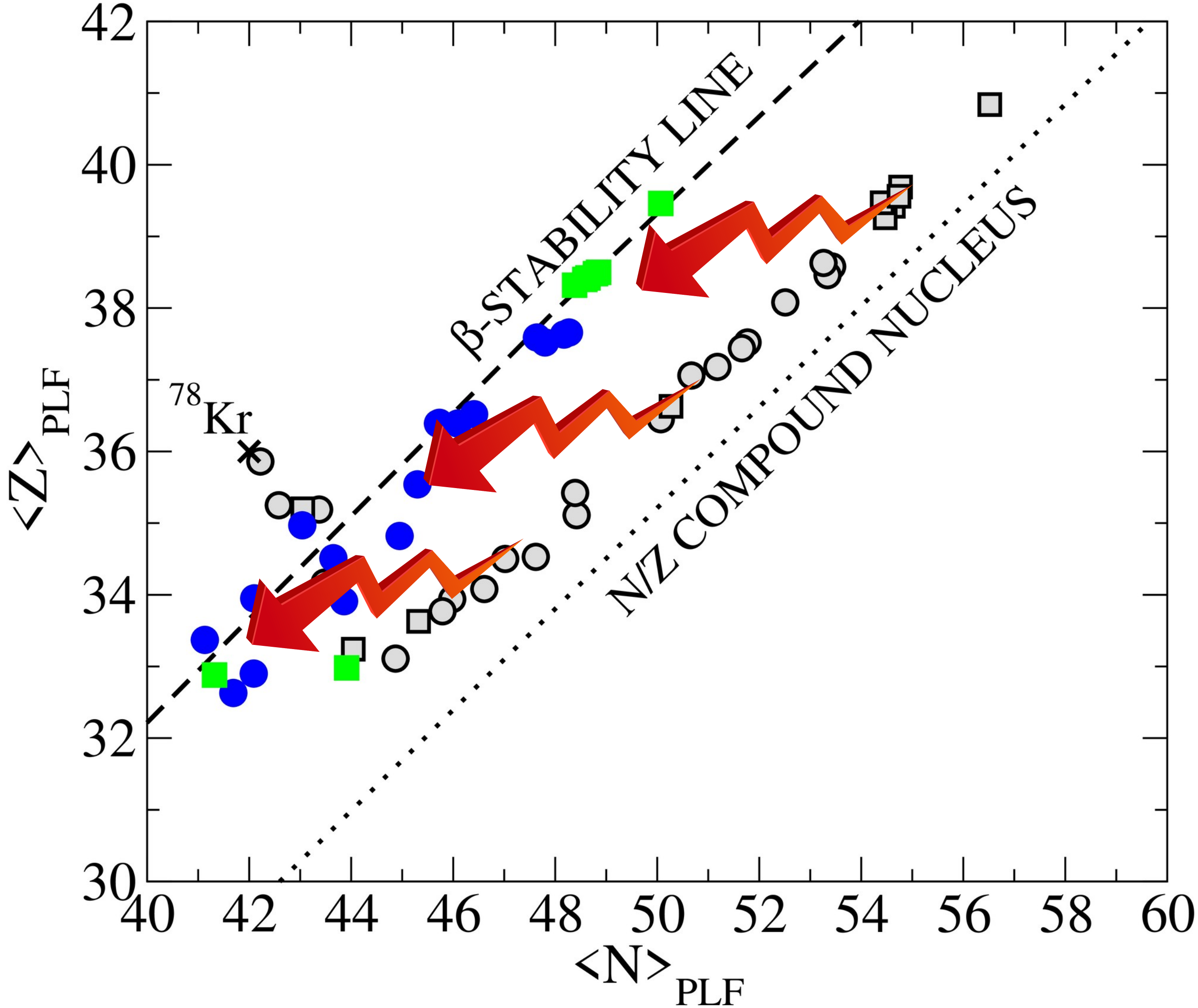


Umar, Simenel, Ye
PRC 96, 024625 (2017)

Isospin and mass equilibration (TDHF)

Need reconstrucution of the primary fragments (statistical codes)

Isospin equilibration – ^{78}Kr+^{208}Pb – 8.5 MeV/A

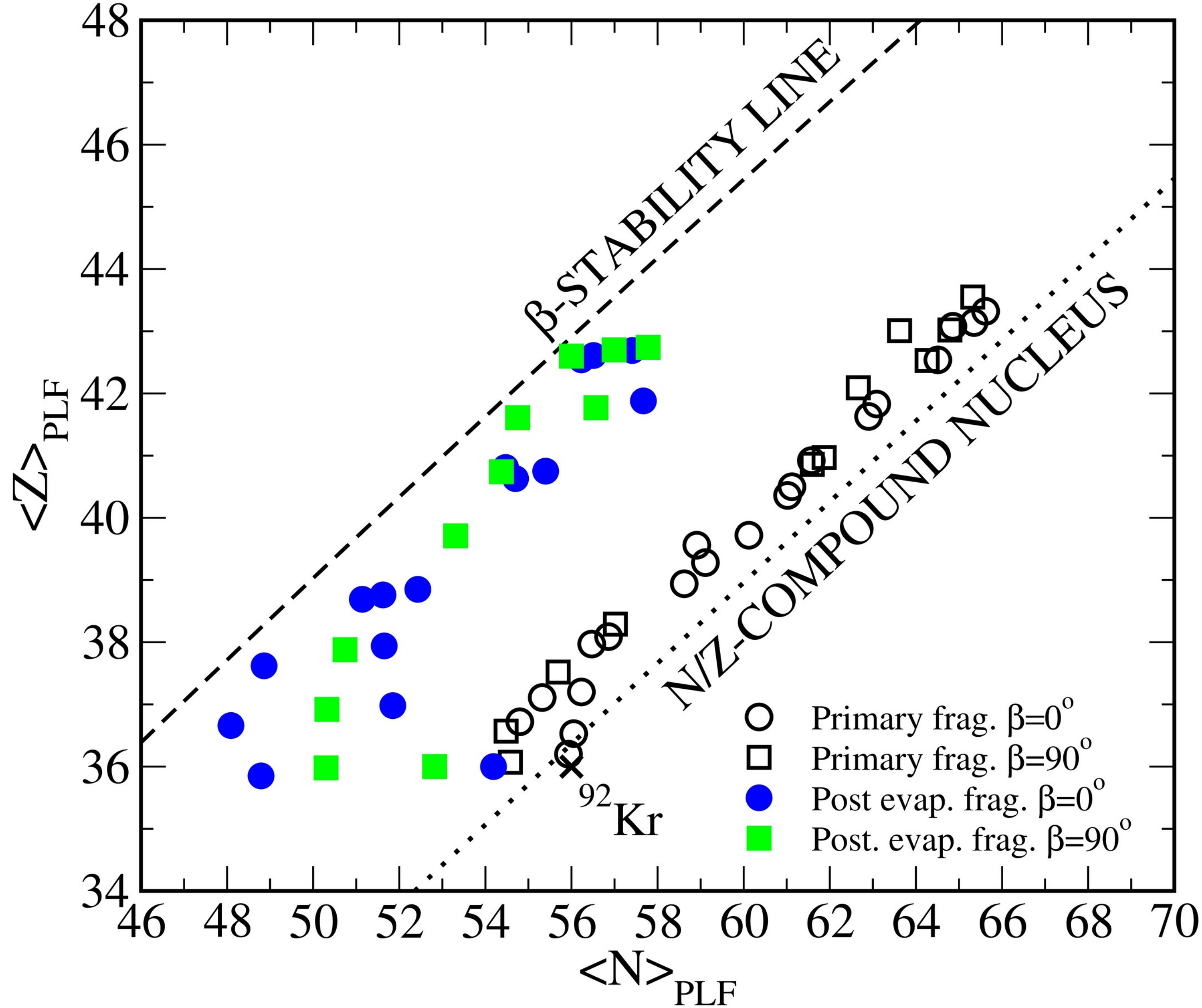


Umar, Simenel, Ye
PRC 96, 024625 (2017)

Isospin and mass equilibration (TDHF)

Statistical deexcitation (GEMINI)

Isospin equilibration – $^{92}Kr+^{208}Pb$ – 8.5 MeV/A

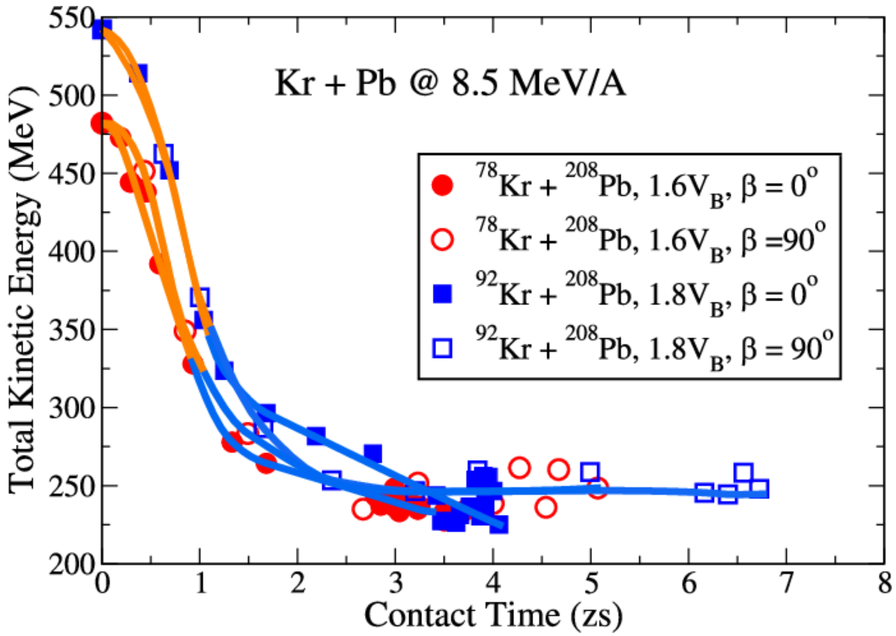


TKE Equilibration

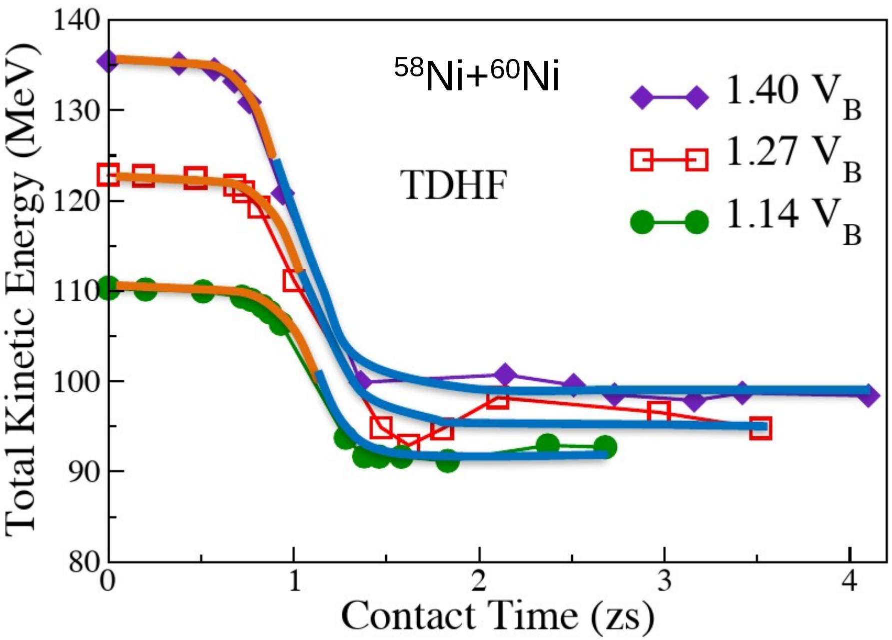
Deep-inelastic reactions

Energy dissipation

Umar, Simenel, Ye PRC **96**, 024625 (2017)



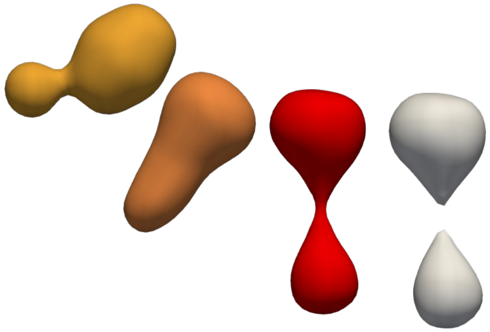
Williams et al., PRL **120**, 022501 (2018)



≈ 1.5zs to reach equilibrium (full energy dissipation)

Systematic Study

- Introduce a scaled measure
- Study many diverse systems
- Range of diverse energies
- Use three different codes



Simenel, Godbey, Umar, Phys. Rev. Lett. **124**, 212504 (2020)

Scaled measure

- Rather than plotting for each system separately create a approximately **scaled measure** as a function of contact time τ

$$\delta X(\tau) = \frac{X(\tau) - X_\infty}{X_0 - X_\infty}$$

τ - Time of two fragments linked together by a neck $(\rho \simeq 0.08 \text{ fm}^{-3})$

$\mathrm{X}(\tau)$ - The quantity used to characterize equilibration at contact time

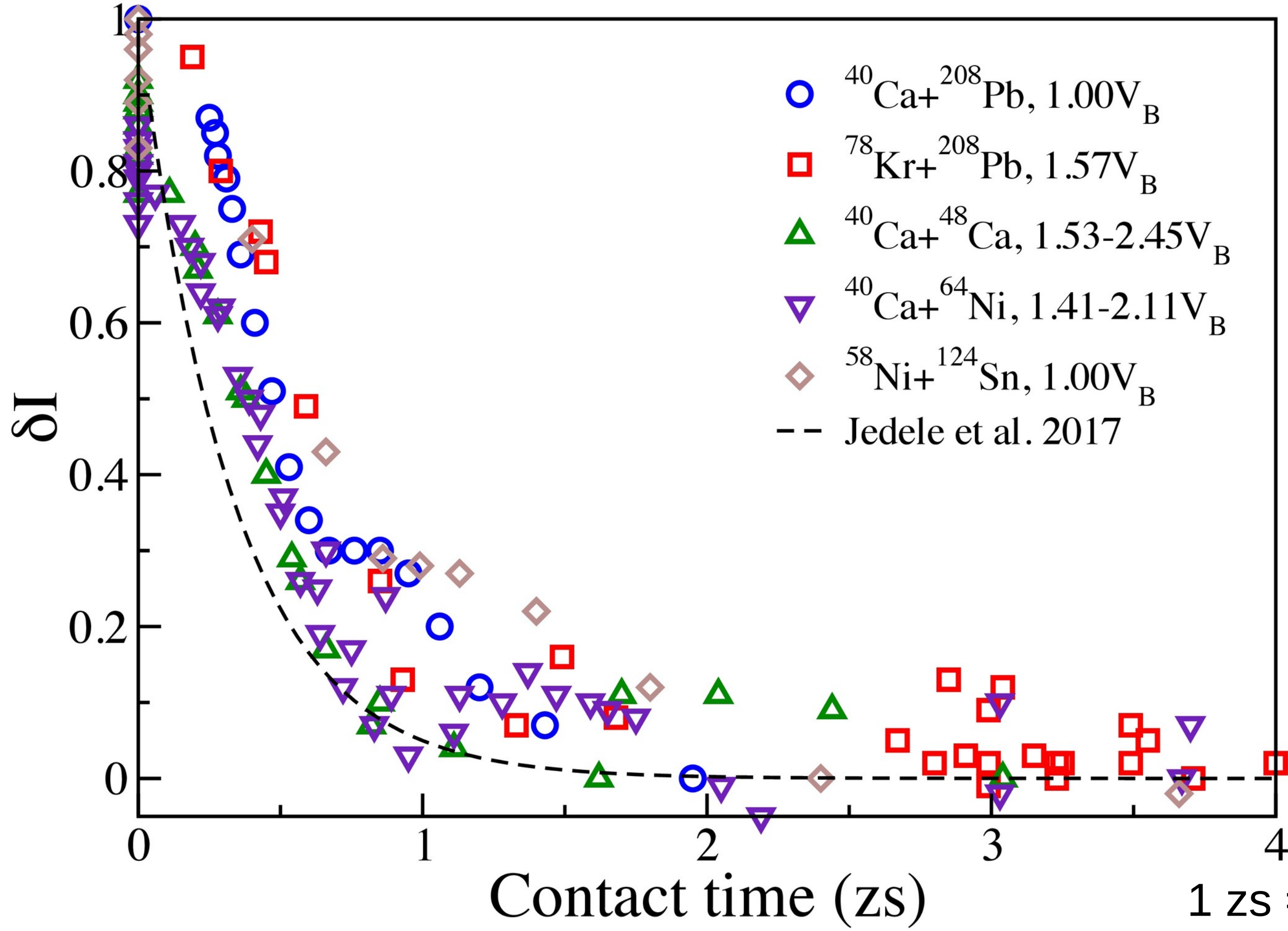
X_0 - Initial value of this quantity

X_∞ - Saturation value at long contact times

Simenel, Godbey, Umar, Phys. Rev. Lett. **124**, 212504 (2020)

Isospin equilibration

$$I = (N_1 - Z_1) - (N_2 - Z_2)$$



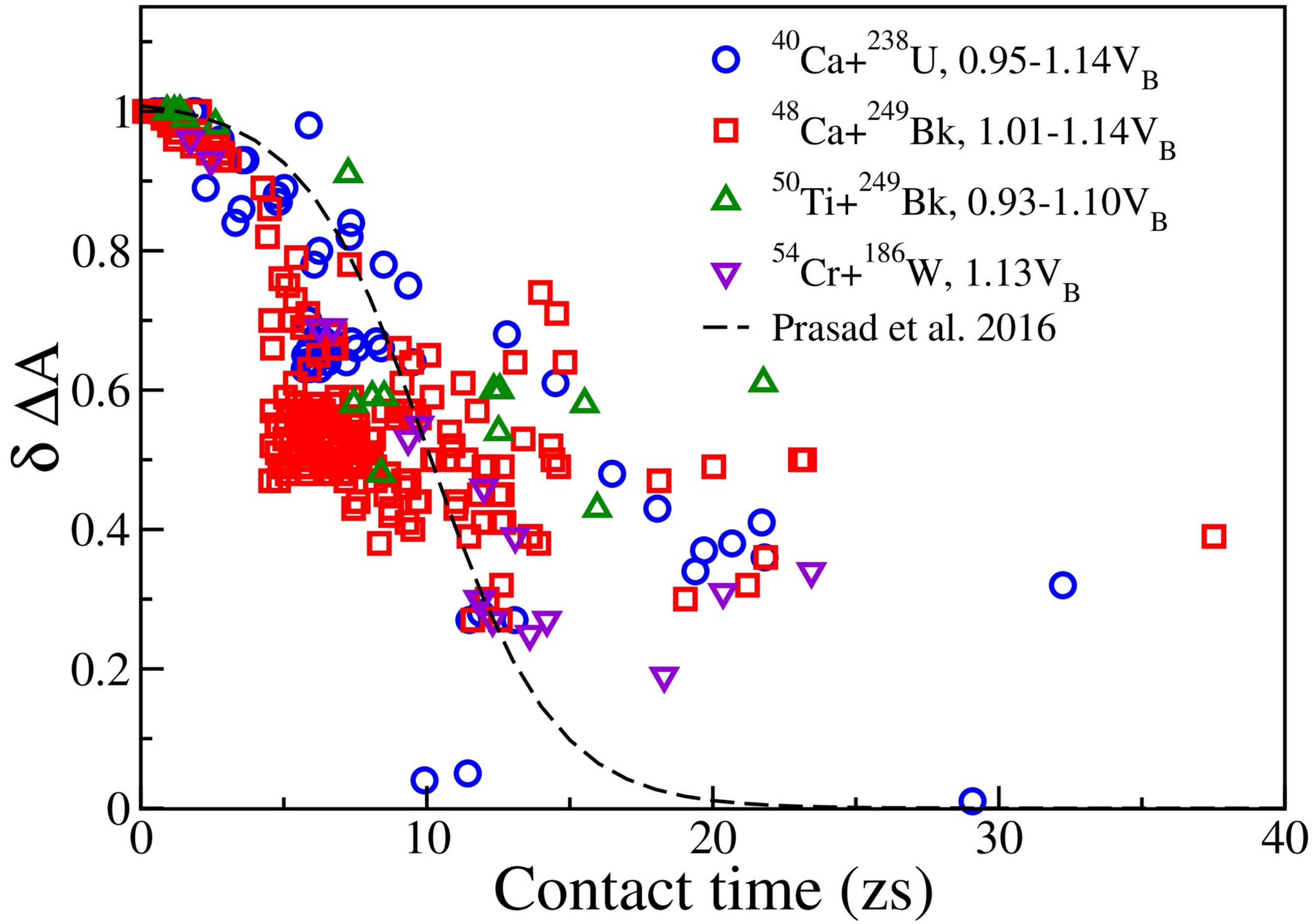
1 zs = 10^{-21} sec

- - - Expected equilibration assuming a rate constant of 3 zs^{-1} determined experimentally by Jedele *et al.*, PRL 118, 062501 (2017) (^{70}Zn+^{70}Zn @ 35 MeV/A)

Recent exp. review: McIntosh and Yennello, Prog. Part. Nucl. Phys. **108**, 103707 (2019)

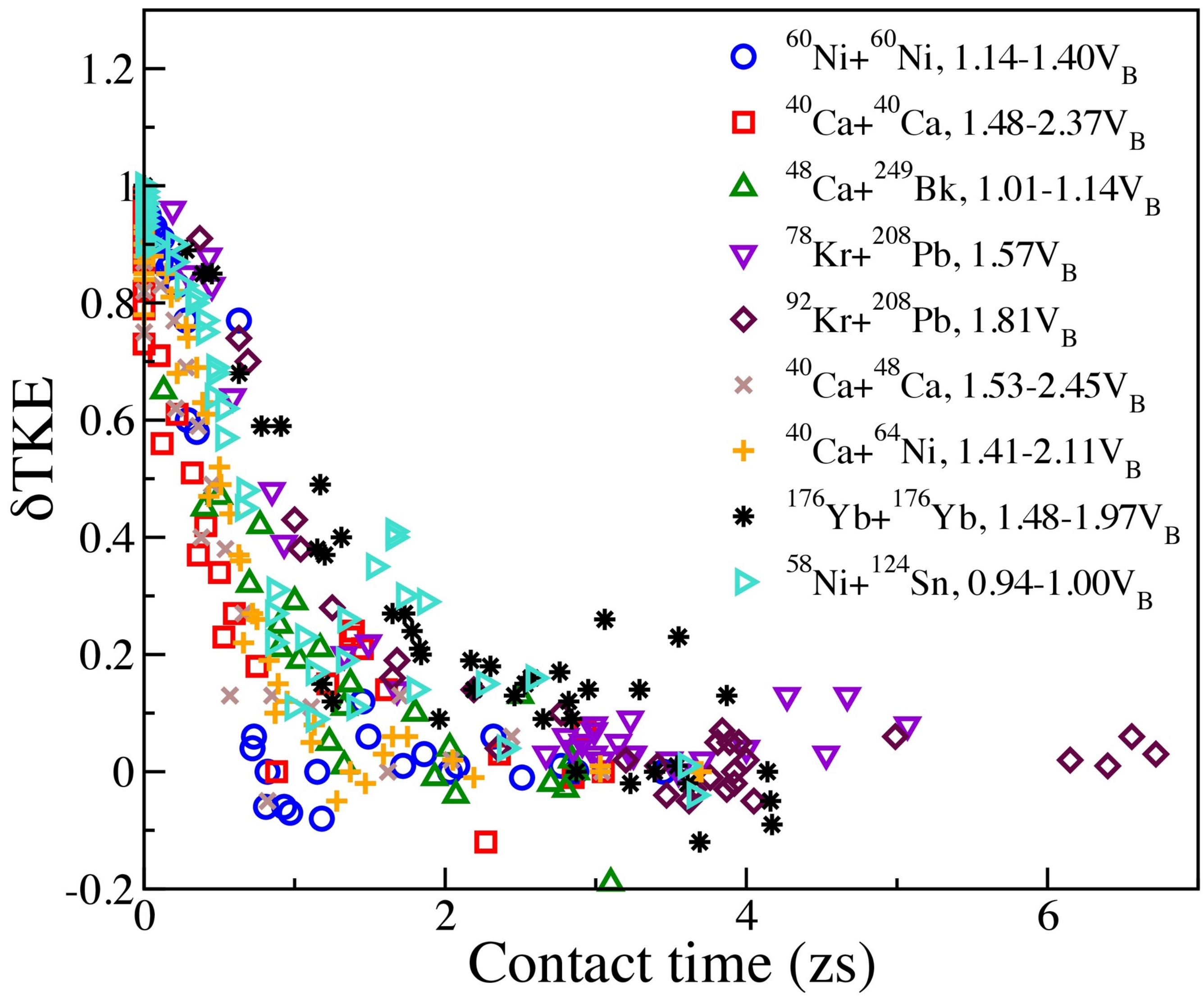
Mass equilibration (quasifission reactions)

$$\Delta A \equiv A_1 - A_2$$



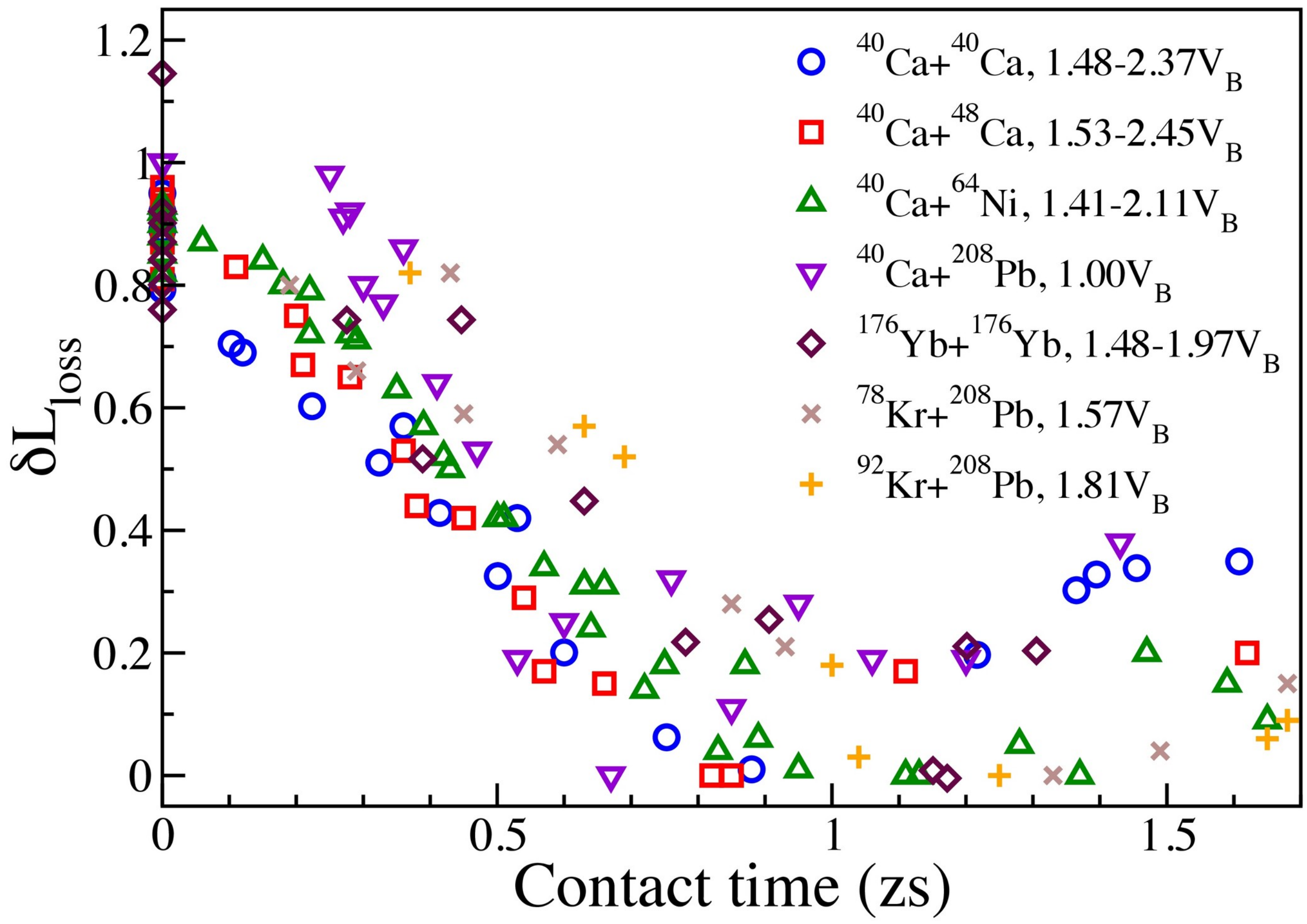
- - - - Expected equilibration assuming Fermi type mass drift Prasad *et al.*, PRC 93, 024607 (2016) ($^{34}S+^{232}Th$)

TKE equilibration



Angular momentum loss

$$\mathrm{L}_{loss}(\tau) = L_0 - L(\tau)$$

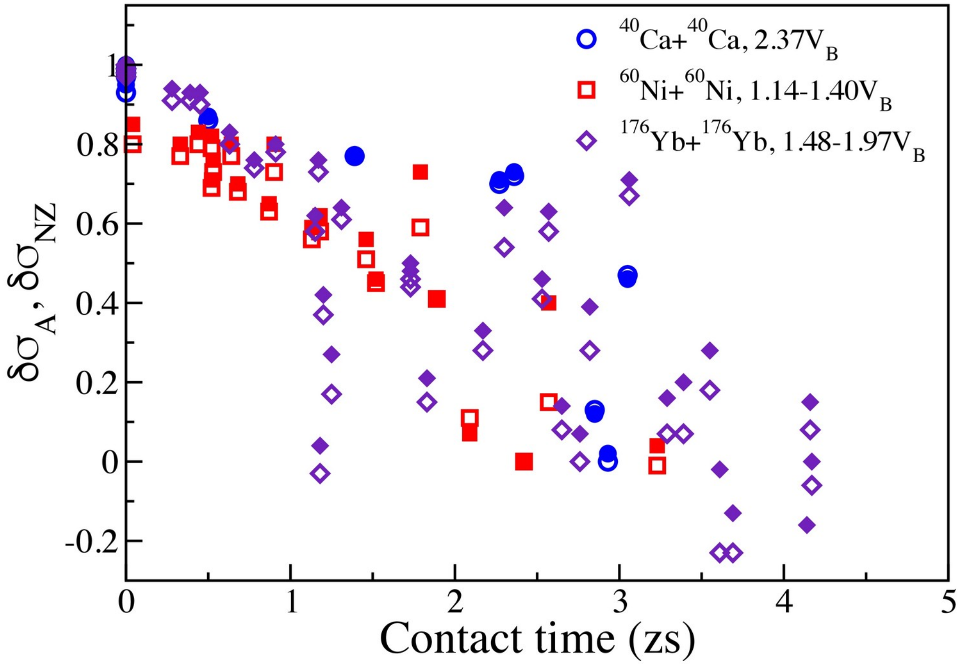


Fluctuations - TDRPA

$$\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2} \qquad \sigma_{NZ} = \sqrt{\langle \hat{N}\hat{Z} \rangle - \langle \hat{N} \rangle \langle \hat{Z} \rangle}$$

Â, N and Ẑ - fragment values, $\sigma_{A_0} = \sigma_{NZ_0} = 0$ (symmetric systems)

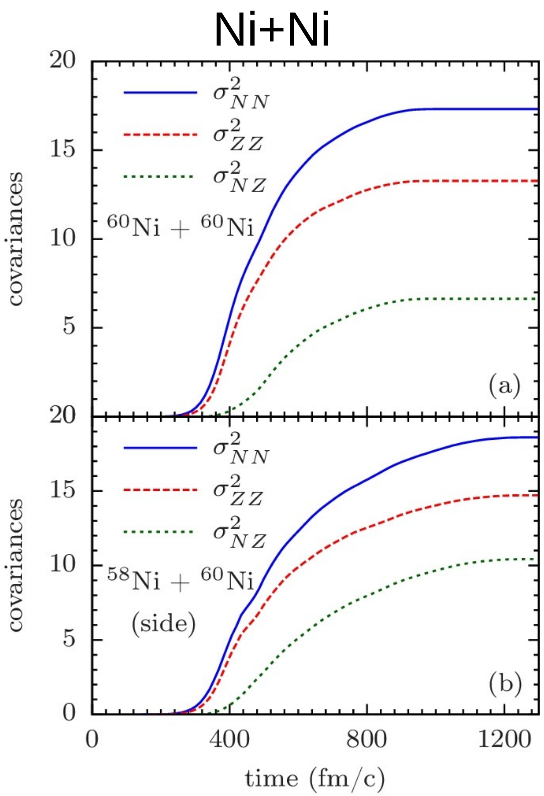
σ_{A,NZ_∞} - average values from TDRPA



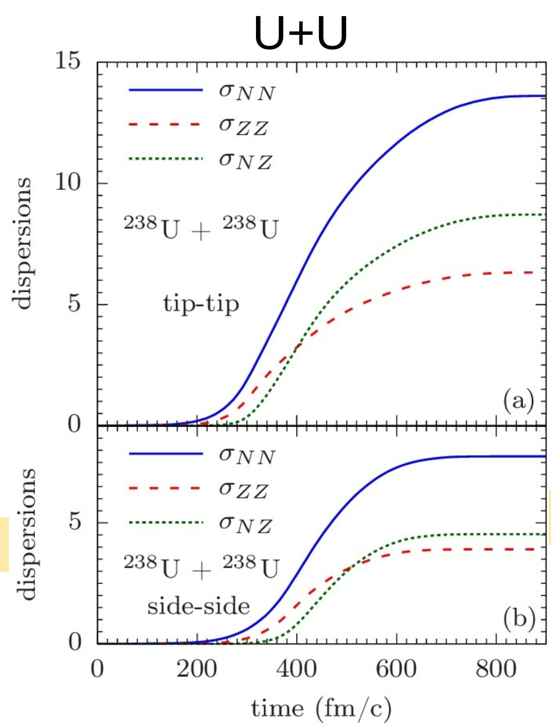
- Need more results for definitive conclusions

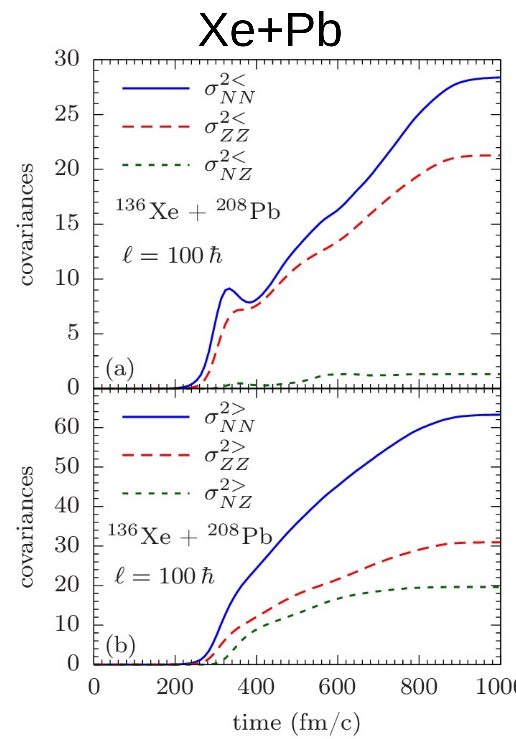
Godbey, Simenel, Umar, PRC 101, 034602 (2020)

Fluctuations – stochastic mean-field (SMF)



Yilmaz, Ayik, Umar, PRC 98, 034604 (2018)





Ayik, Yilmaz, Yilmaz, Umar, PRC 100, 014609 (2019)

Ayik, Yilmaz, Yilmaz, Umar, PRC 102, 024619 (2020)

Quantum equilibration dynamics

	Time to equilibrium	
Mass	~ 20 zs	QF
Isospin	~ 1 zs	DIC
Angular momentum	~ 1 zs	DIC
Energy	~ 1-2 zs	DIC
Mass Fluctuations	~ 3 zs	DIC

Need more systematics……..

Collaborators

PHYSICAL REVIEW LETTERS **124**, 212504 (2020)

Timescales of Quantum Equilibration, Dissipation and Fluctuation in Nuclear Collisions

C. Simenel*, K. Godbey†, and A. S. Umar‡

PHYSICAL REVIEW C **101**, 034602 (2020)

Microscopic predictions for the production of neutron-rich nuclei in the reaction $^{176}Yb + ^{176}Yb$

K. Godbey[1,*], C. Simenel[2,†], and A.S. Umar[3,‡]

PHYSICAL REVIEW C **102**, 024619 (2020)

Merging of transport theory with the time-dependent Hartree-Fock approach: Multinucleon transfer in U+ U collisions

S. Ayik[1,*], B. Yilmaz[2], O. Yilmaz[3], and A.S. Umar[4]

PHYSICAL REVIEW C **100**, 024610 (2019)

Deformed shell effects in 48Ca + 249Bk quasifission fragments

K. Godbey[1,*], A.S. Umar[2,†], and C. Simenel[3,‡]

EXTRA SLIDES
Isospin Dynamics and Fusion Barriers

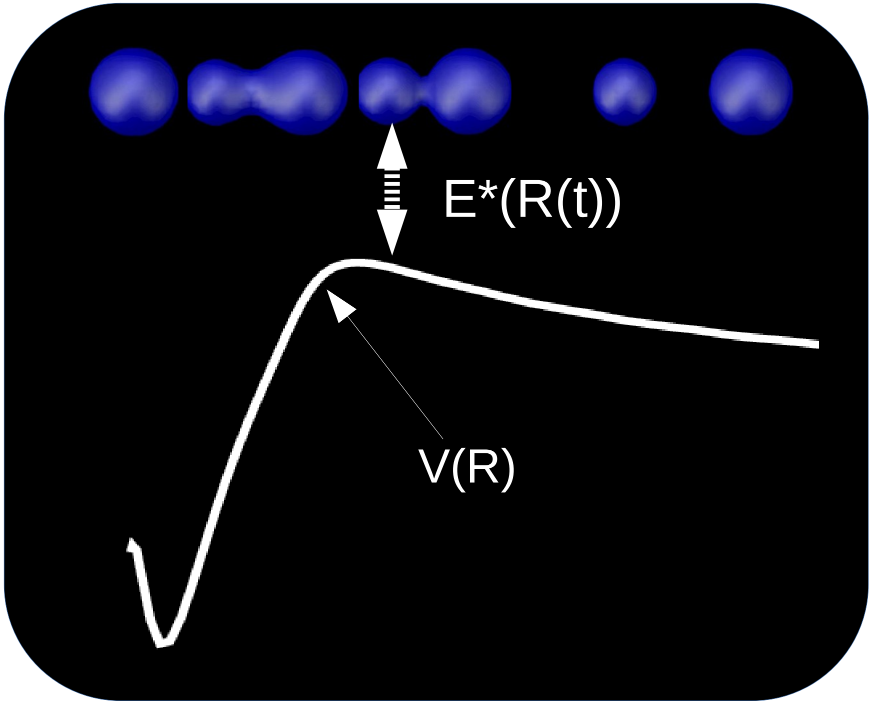
TDDFT + Density Constraint = Internuclear Potentials

- Minimize energy with density constraint during unhindered TDDFT

$$E_{DC}(t) = min_{\rho}\left\{E[\rho_n,\rho_p] + \int d^3r\lambda_n(\mathbf{r})[\rho_n(\mathbf{r}) - \rho_n^{tdhf}(\mathbf{r},t)] + \int d^3r\lambda_p(\mathbf{r})[\rho_p(\mathbf{r}) - \rho_p^{tdhf}(\mathbf{r},t)]\right\}$$

- Microscopic dynamical internuclear potential – can calculate subbarrier fusion, capture

$$V(R) = E_{\mathrm{DC}}(R) - E_{A_1} - E_{A_2}$$



- Parameter-free, only depends on chosen EDF
- Dynamical, energy-dependent
- Calculate E*(t) and M(R)
- Extensively applied to fusion barrier calculations

DC-TDHF + isospin decomposition

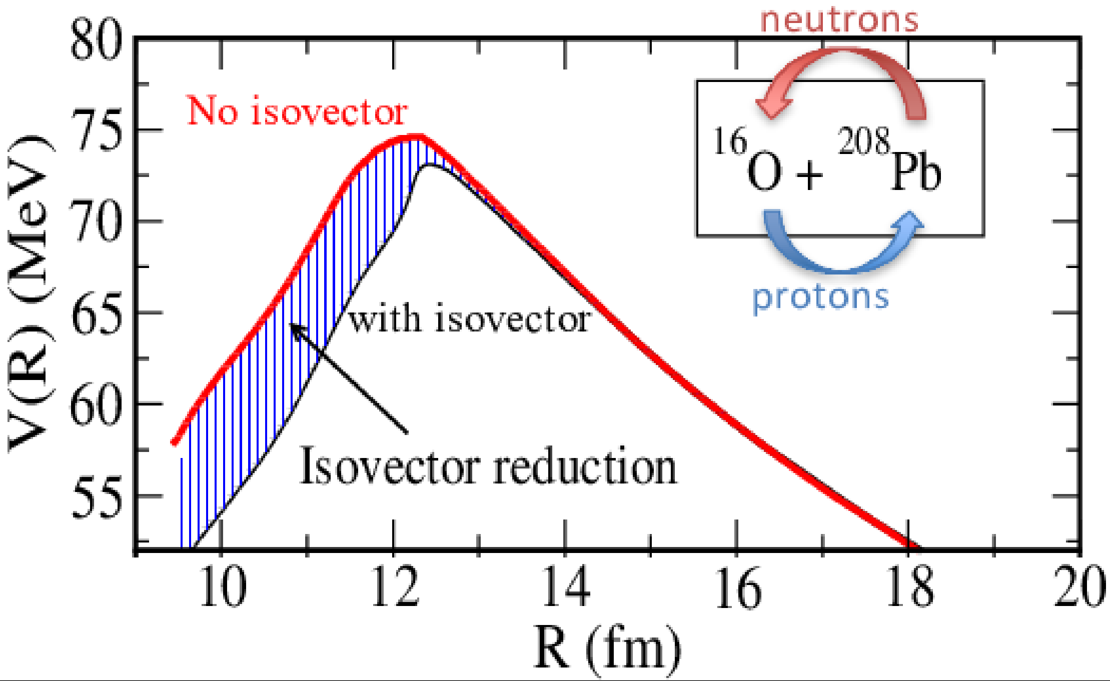
Skyrme EDF

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_{I=0}(\mathbf{r}) + \mathcal{H}_{I=1}(\mathbf{r}) + \mathcal{H}_C(\mathbf{r})$$

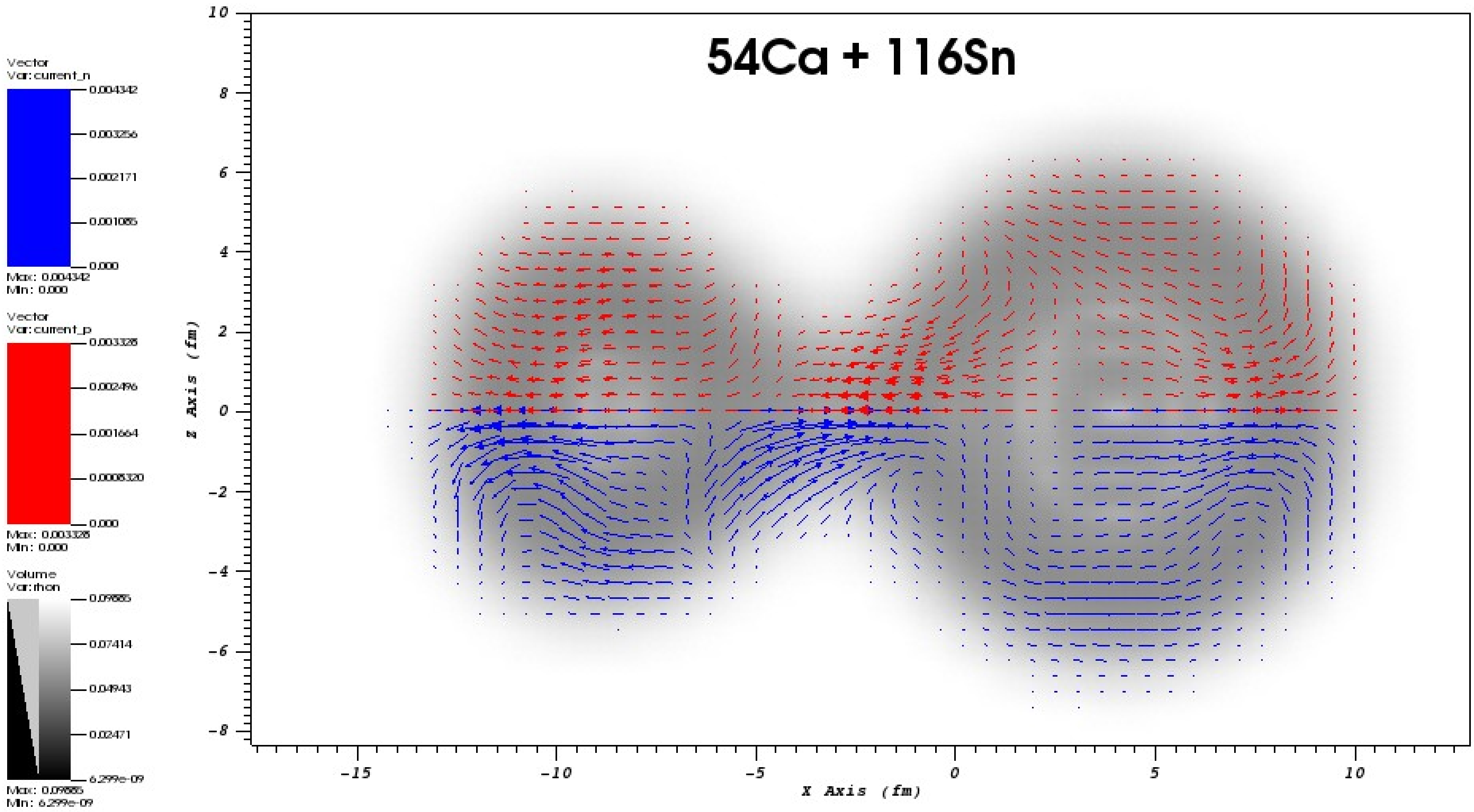
Allows for isospin decomposed ion-ion interaction barrier

$$\mathrm{V(R)} = \mathrm{V_{I=0}}(R) + V_{\mathrm{I=1}}(R) + V_C(R)$$

- Minimize energy with density constraint during unhindered TDHF
- Microscopic internuclear potential
- Parameter-free, only depends on chosen EDF
- Dynamical, energy-dependent
- Extensively applied to fusion barrier calculations



Isospin dynamics and fusion barriers



Energy density functional - Skyrme

Energy written in terms of the Energy Density Functional (EDF)

$$\mathrm{E} = \int d^3\mathbf{r}\, \mathcal{H}(\mathbf{r})$$

Skyrme EDF

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_{I=0}(\mathbf{r}) + \mathcal{H}_{I=1}(\mathbf{r}) + \mathcal{H}_{C}(\mathbf{r})$$

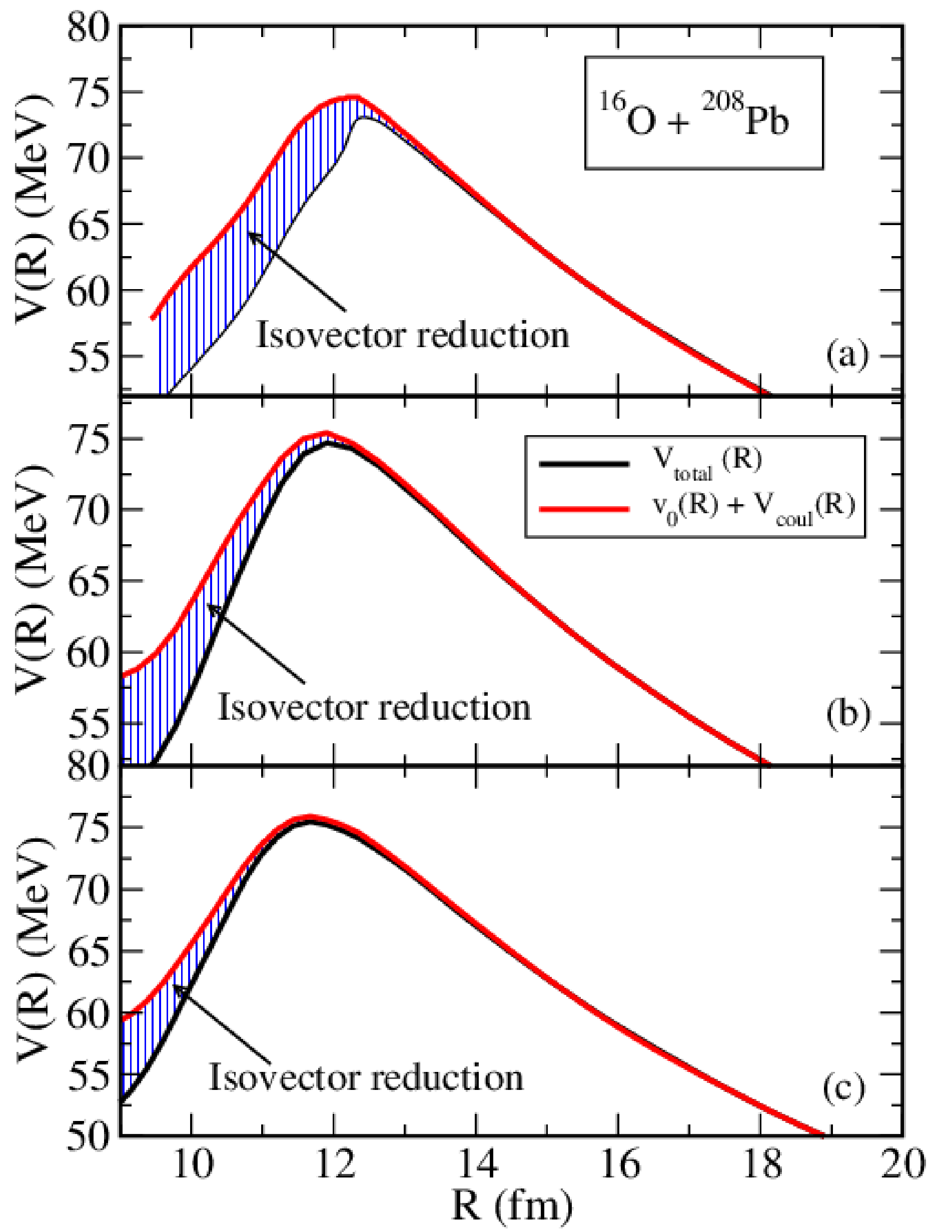
$$\mathrm{H_I}(\mathbf{r}) = C_{\mathrm{I}}^{\rho}\rho_{\mathrm{I}}^2 + C_{\mathrm{I}}^{s}\mathbf{s}_{\mathrm{I}}^2 + C_{\mathrm{I}}^{\Delta\rho}\rho_{\mathrm{I}}\Delta\rho_{\mathrm{I}} + C_{\mathrm{I}}^{\Delta s}\mathbf{s}_{\mathrm{I}}\cdot\Delta\mathbf{s}_{\mathrm{I}} +$$
$$\mathrm{C}_{\mathrm{I}}^{\tau}\left(\rho_{\mathrm{I}}\tau_{\mathrm{I}} - \mathbf{j}_{\mathrm{I}}^2\right) + C_{\mathrm{I}}^{T}\left(\mathbf{s}_{\mathrm{I}}\cdot\mathbf{T}_{\mathrm{I}} - \overleftrightarrow{J}_{\mathrm{I}}^{2}\right) +$$
$$\mathrm{C}_{\mathrm{I}}^{\nabla J}\left(\rho_{\mathrm{I}}\nabla\cdot\mathbf{J}_{\mathrm{I}} + \mathbf{s}_{\mathrm{I}}\cdot(\nabla\times\mathbf{j}_{\mathrm{I}})\right)$$

Allows for isospin decomposed ion-ion interaction barrier

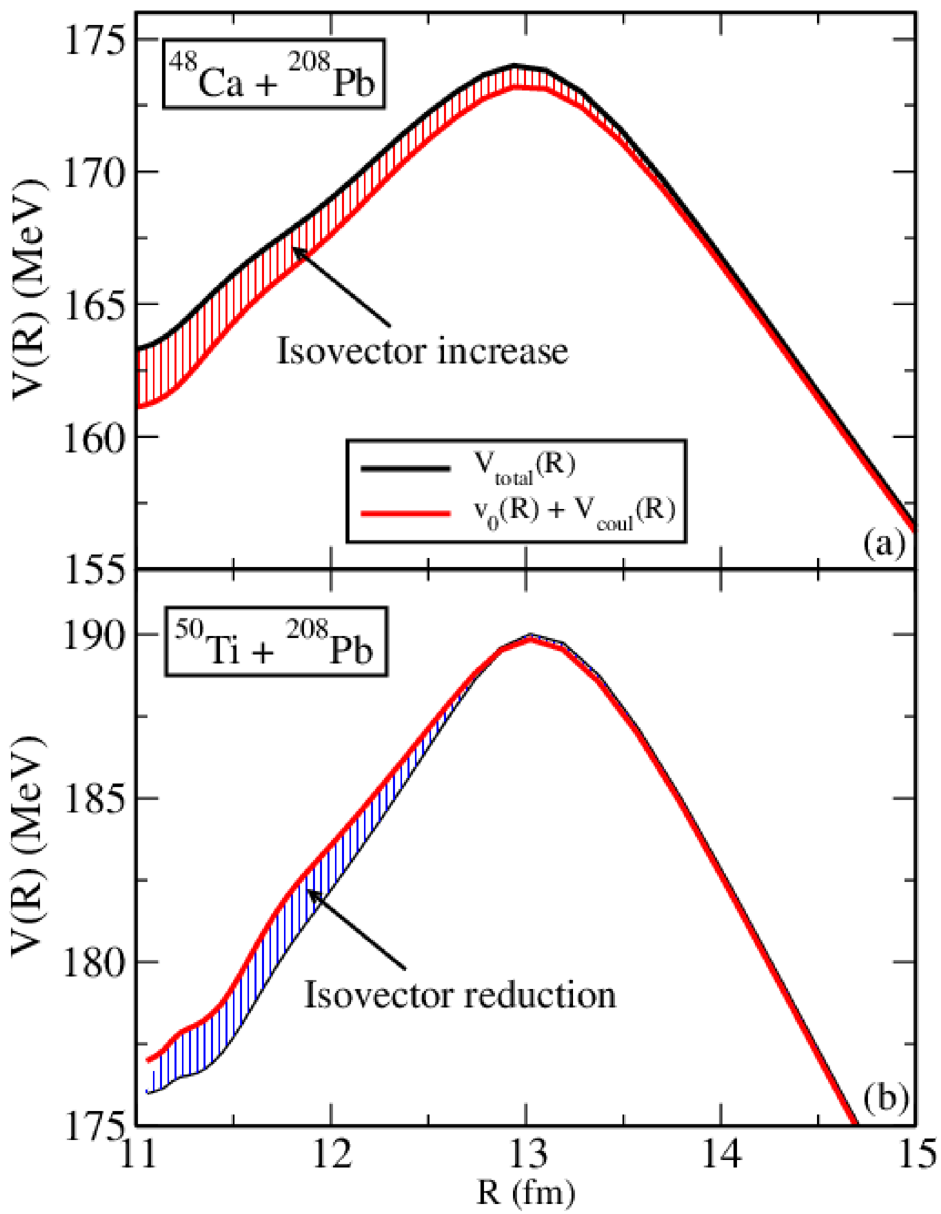
$$\mathrm{V(R)} = \mathrm{E_{DC}}(R) - E_{\mathrm{A}_1} - E_{\mathrm{A}_2}$$

$$\mathrm{V(R)} = \mathrm{V_{I=0}}(R) + V_{\mathrm{I=1}}(R) + V_C(R)$$

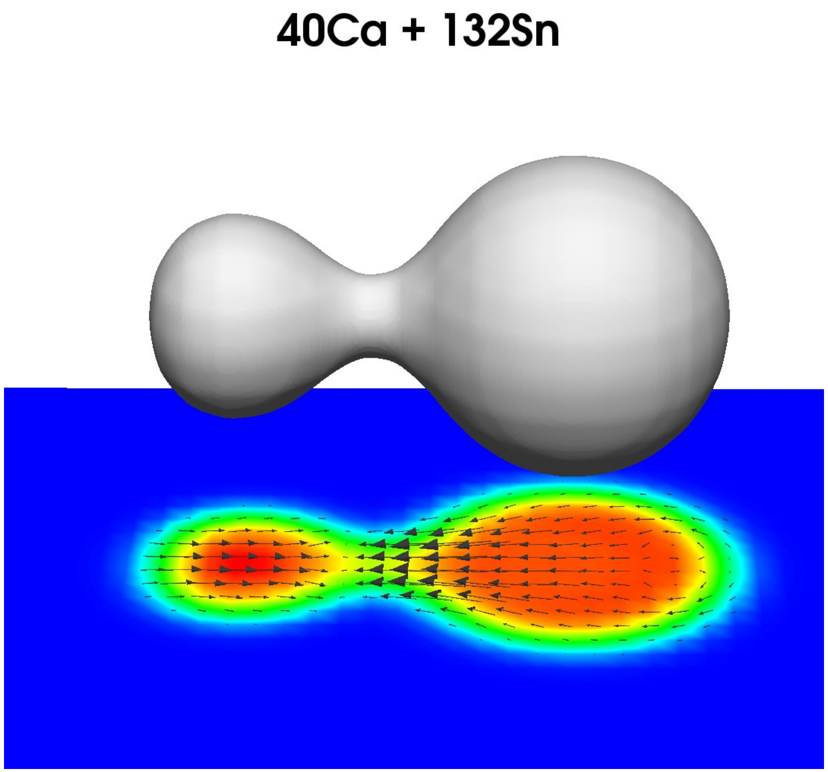
Isospin Decomposition – $^{16}O + ^{208}Pb$



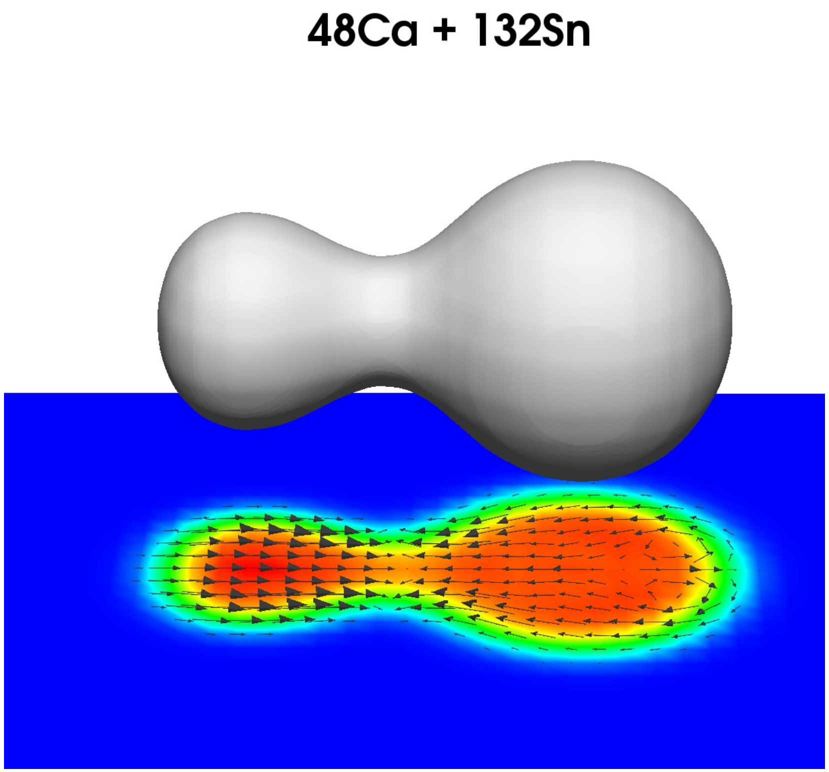
Isospin Decomposition – ^{48}Ca, ^{50}Ti + ^{208}Pb



$^{40}Ca+^{132}Sn$ versus $^{48}Ca+^{132}Sn$

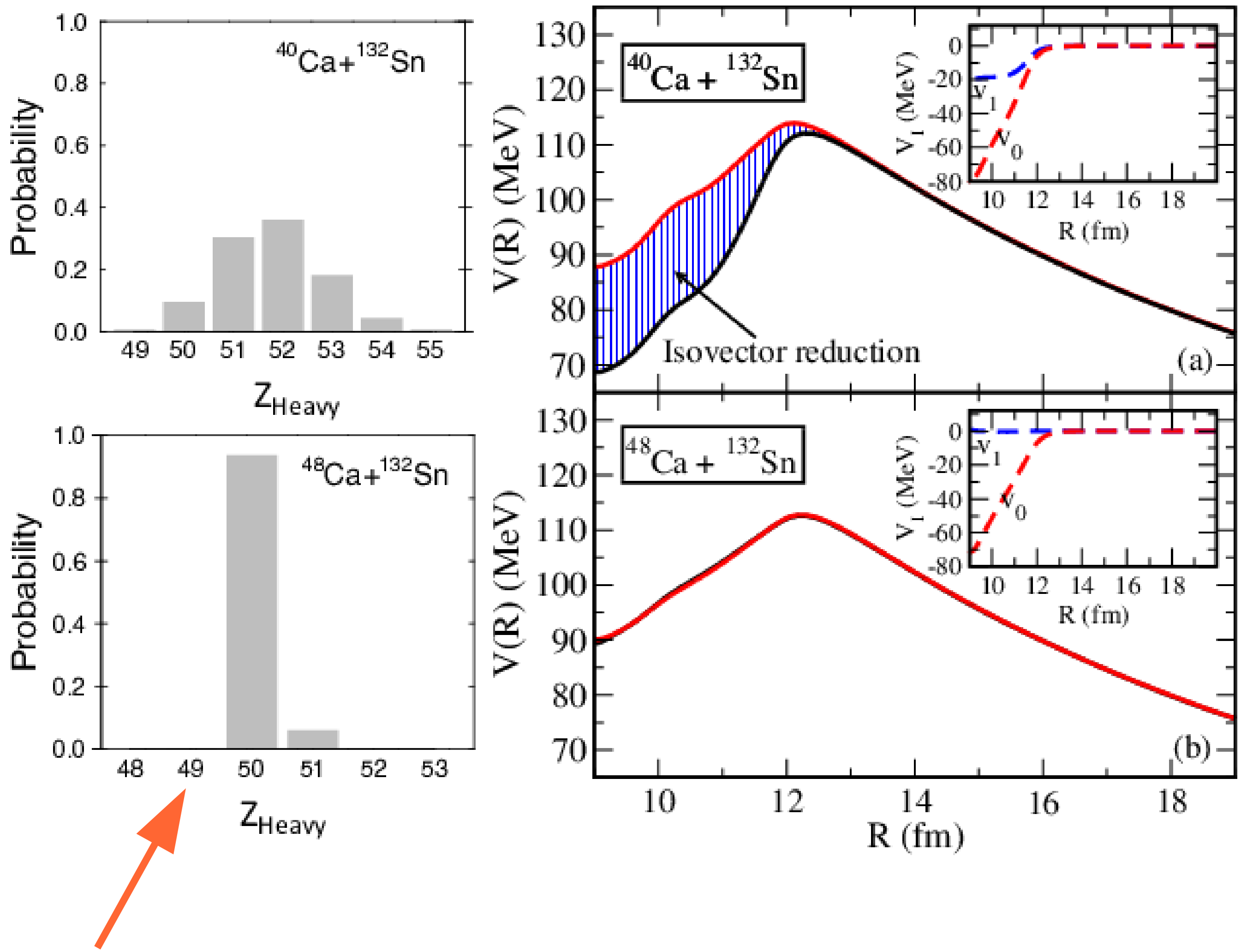


transfer



No net transfer

^{40}Ca+^{132}Sn versus ^{48}Ca+^{132}Sn – Q-value transfer channels



Particle number projection just below the barrier

Isospin Decomposition – $^{40,48,54}Ca+^{132}Sn$