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NUCLEAR TALKS @UCAS

Time-Dependent Density Functional Theory in Low-Energy Nuclear Reaction Dynamics

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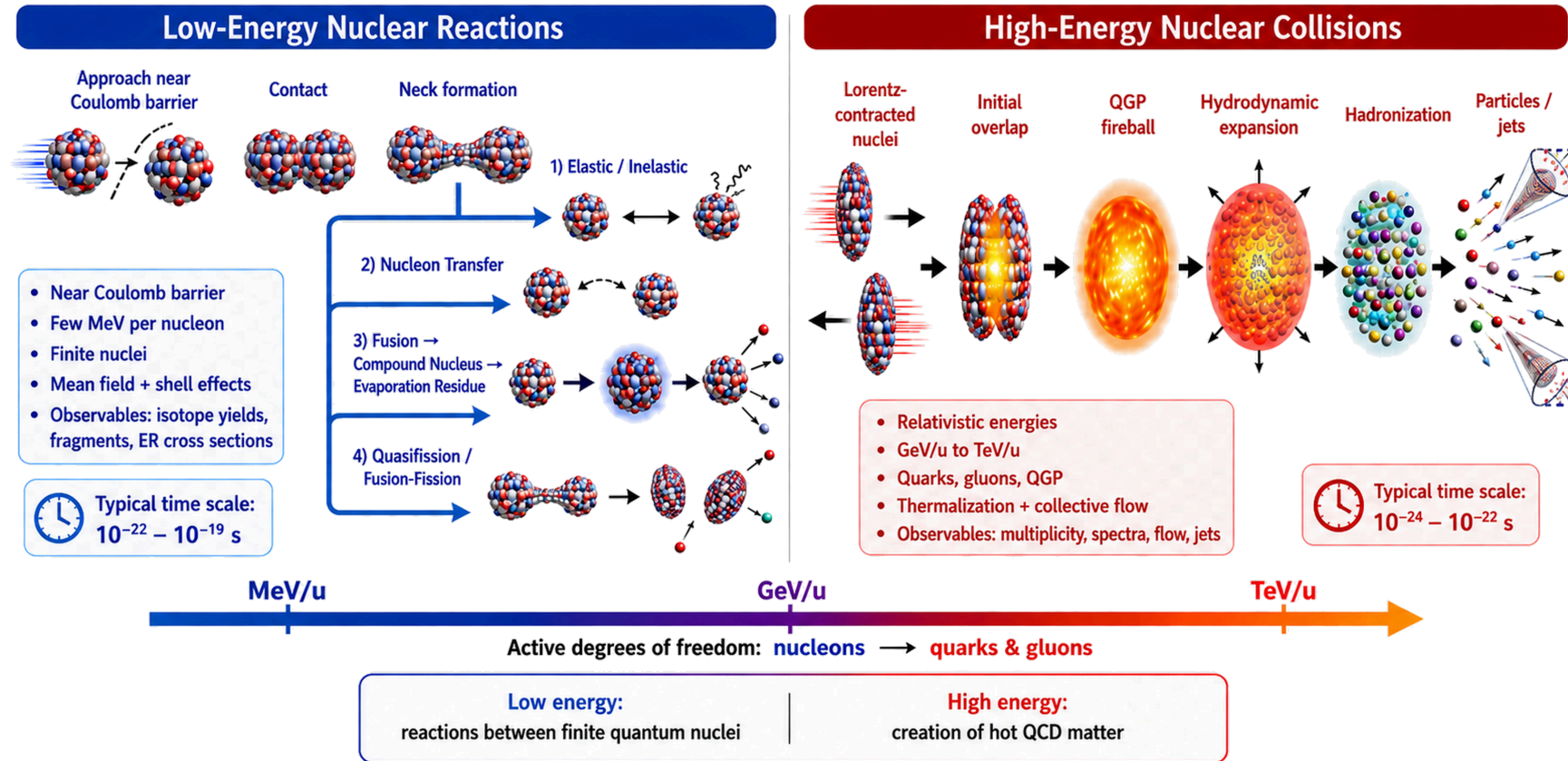
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Low-Energy Reactions Probe Nucleonic Collective Dynamics

- High energy: partons, QGP, thermalization, flow, jets.
- Low energy: nucleons, densities, shapes, shell effects, fragments.
- Low-energy dynamics underpins superheavy-element synthesis, exotic-nuclei production, and r-process modeling.

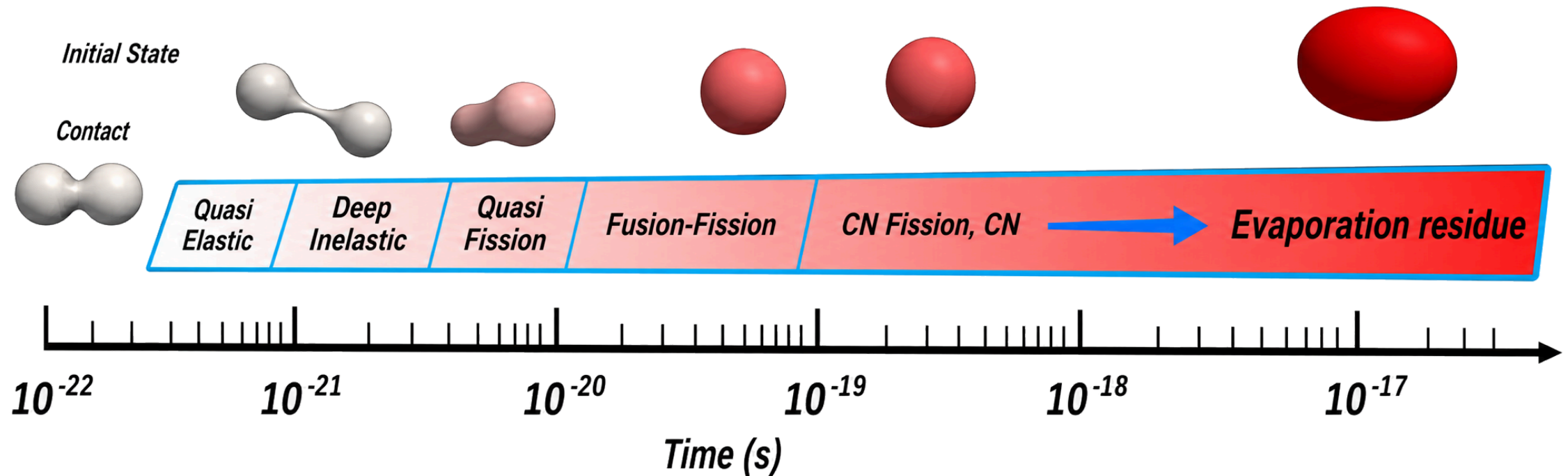
High-Energy Nuclear Collisions vs Low-Energy Nuclear Reactions

Same nuclei, different energy scales, different active degrees of freedom



Near-Barrier Collisions Branch Before Full Equilibration

- Contact occurs on the 10^{-22} s scale.
- Shape evolution, nucleon transfer, dissipation, and shell effects are coupled throughout.
- The system may reseparate, exchange nucleons, or evolve toward a compact mononuclear shape.
- Longer-time evaporation and fission determine the finally measured products.



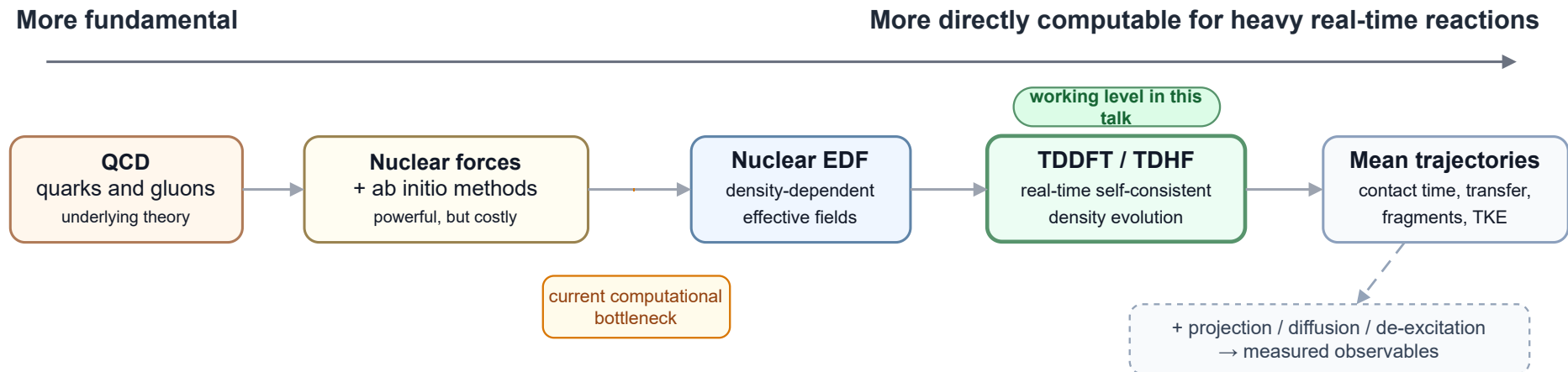
Low-energy heavy-ion collisions branch into different outcomes across several orders of magnitude in time.

Talk Roadmap

- **Method** — Nuclear TDDFT/TDHF: from many-body problem to self-consistent density evolution.
- **Fusion** — Capture, compound-nucleus formation, and superheavy-element survival.
- **Quasifission** — Entrance-channel memory and fusion suppression.
- **Multinucleon transfer** — Isospin equilibration, channel probabilities, and exotic-nuclei production.
- **Fission** — From PES to scission: fragment distributions as an EDF probe.
- **Unified picture** — Shared mechanisms across reaction channels.

Heavy Real-Time Reactions Require an Effective Microscopic Theory

- QCD is the underlying theory.
- Ab initio nuclear theory is powerful but currently limited for heavy real-time reactions.
- Heavy-ion dynamics involves hundreds of nucleons, open channels, and long-time large-amplitude motion.
- The limitation is direct computability, not fundamentality.



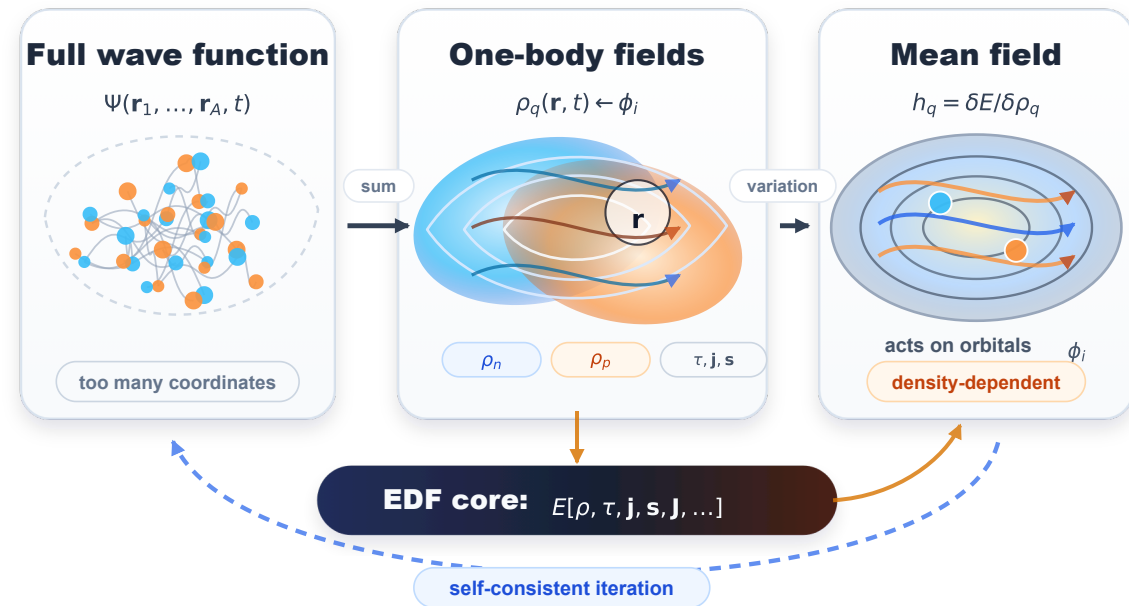
For heavy real-time reactions, the practical starting point is not the most fundamental theory, but the most microscopic theory that remains computable.

Nuclear DFT Trades the Full Wave Function for Density-Dependent Fields

$$\rho_q(\mathbf{r}, t) = \sum_{i \in q} n_i |\phi_i(\mathbf{r}, t)|^2, \quad q = n, p$$

$$E[\rho, \tau, \mathbf{j}, \mathbf{s}, \mathbf{J}, \dots] = \int d^3r \mathcal{H}(\mathbf{r}), \quad h_q(\mathbf{r}, t) = \frac{\delta E}{\delta \rho_q(\mathbf{r}, t)}$$

- The one-body density replaces the full many-body wave function as the working variable.
- An energy-density functional of local densities and currents encodes the effective nuclear interaction.
- Functional variation generates the instantaneous self-consistent mean field.

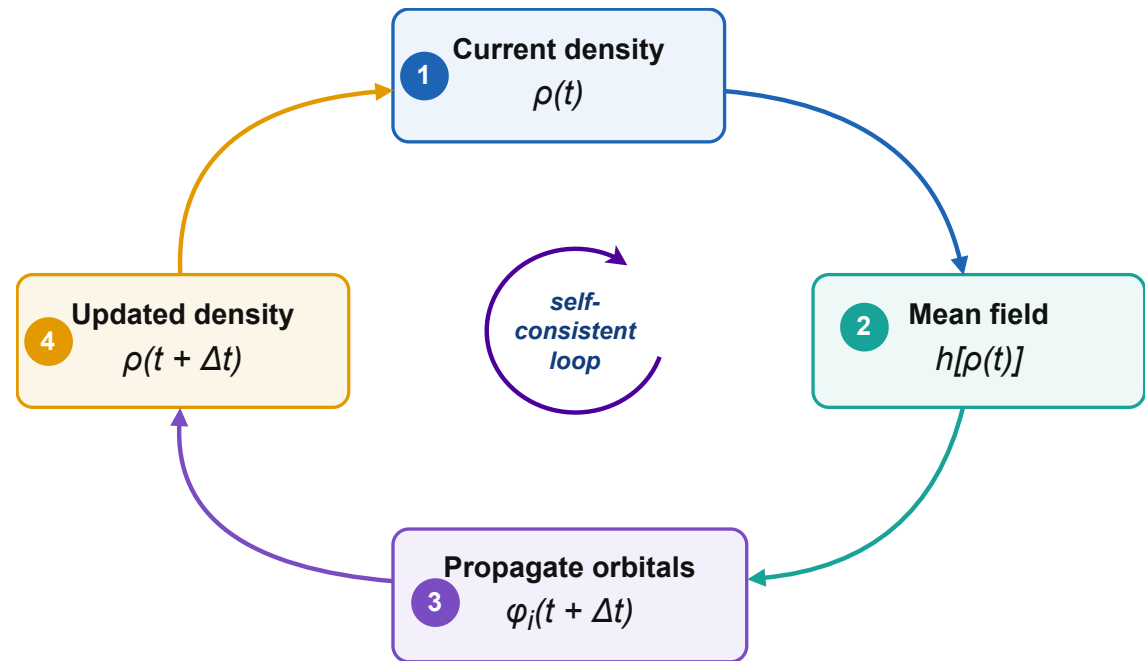


TDHF Propagates the One-Body Density Self-Consistently

$$i\hbar \frac{\partial \phi_i(\mathbf{r}, t)}{\partial t} = h[\rho(t)] \phi_i(\mathbf{r}, t)$$

$$i\hbar\dot{\rho}(t) = [h[\rho(t)], \rho(t)]$$

- Nuclear TDDFT is the umbrella framework in this talk.
- Most real-time cases use Skyrme-TDHF, the mean-field limit of nuclear TDDFT.
- The density and mean field feed back on each other during propagation.



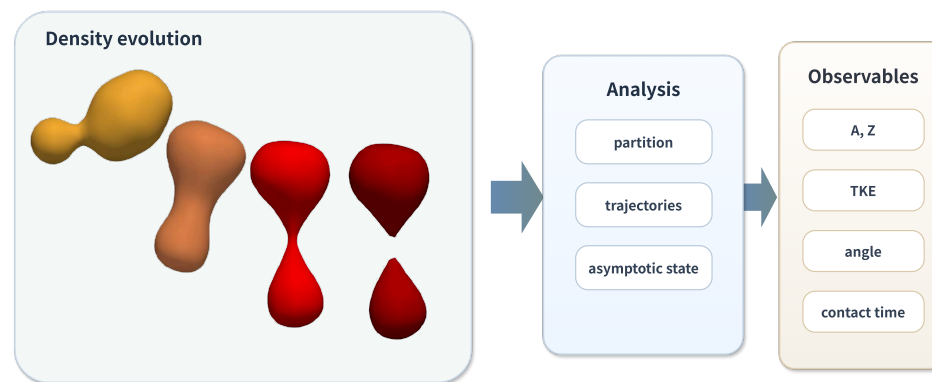
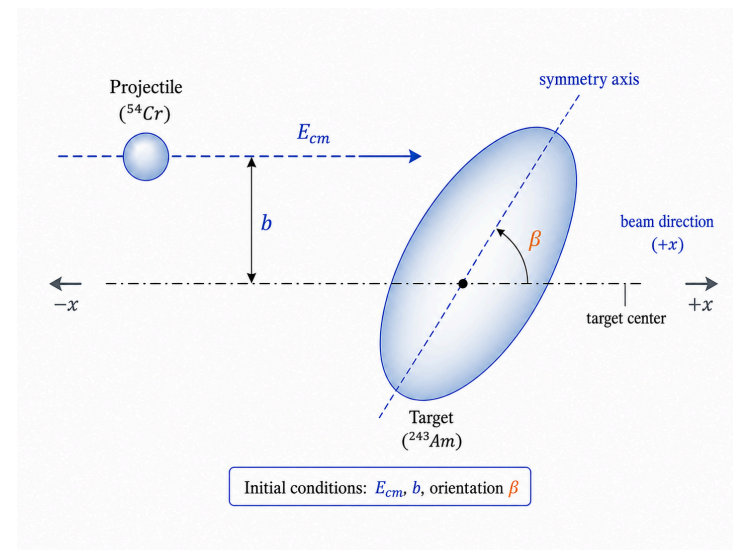
Self-consistent density propagation.

From Initial Boost to Fragment Observables

$$\phi_i^{P/T}(\mathbf{r}, t_0) \rightarrow e^{\pm i\mathbf{k} \cdot \mathbf{r}} \phi_i^{P/T}(\mathbf{r} - \mathbf{R}_{P/T})$$

$$A_F(t) = \int_{V_F} d^3r \rho(\mathbf{r}, t), \quad \text{TKE} \simeq \frac{1}{2} \mu \dot{R}^2 + \frac{Z_1 Z_2 e^2}{R}$$

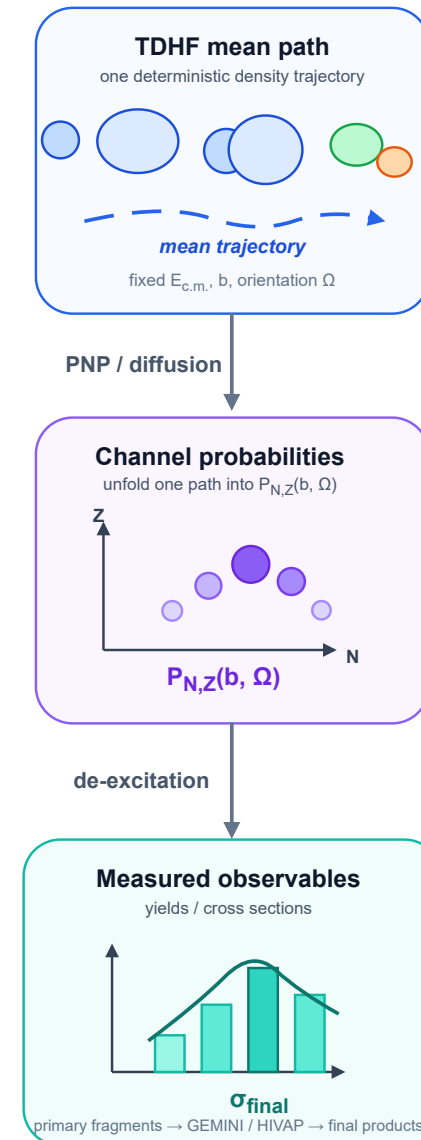
- Prepare HF ground states; a Galilean boost sets the relative motion.
- Initial conditions: $E_{\text{c.m.}}$, impact parameter b , and orientation select one mean trajectory.
- Observables: fragment masses, charges, TKE, and TKEL are extracted from the evolving density.



From Mean Trajectories to Measured Cross Sections

- A single TDHF run gives the mean trajectory: contact time, primary fragment masses, and kinetic energies.
- Particle-number projection and diffusion models supply channel probabilities and fluctuations.
- Statistical de-excitation converts excited primary fragments into measured yields and cross sections.

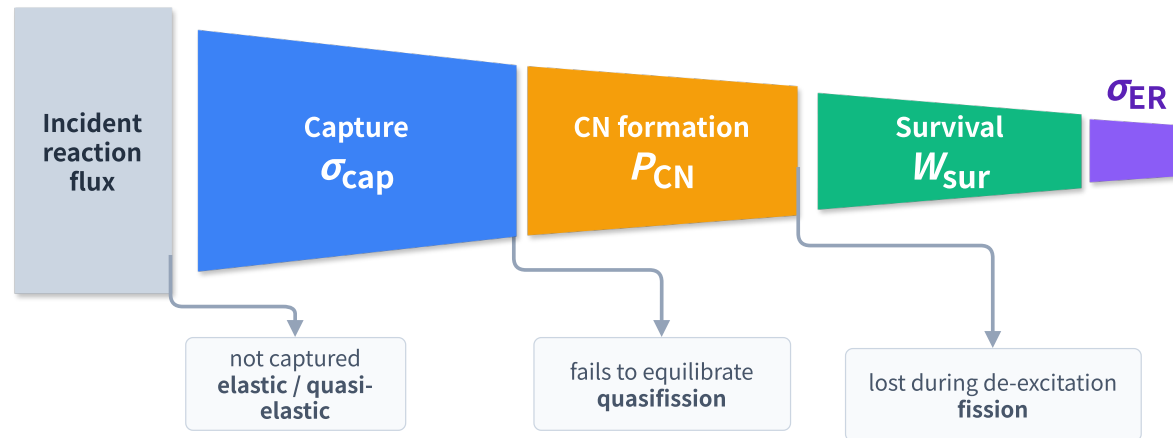
$$\sigma_{N,Z} = \frac{1}{4\pi} \int d\Omega \, 2\pi \int b \, db \, P_{N,Z}(b, \Omega)$$



Superheavy Yields Survive Three Filters: Capture, Fusion, Survival

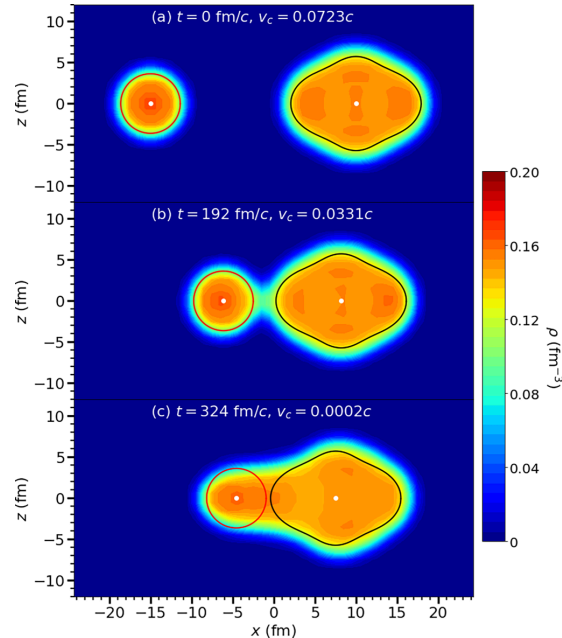
- Capture: overcome the entrance barrier to form a dinuclear configuration.
- Fusion: form the compound nucleus with probability P_{CN} ; quasifission competes.
- Survival: avoid fission during de-excitation with probability W_{sur} .

$$\sigma_{ER}(E) = \sum_J \sigma_{cap}(E, J) P_{CN}(E, J) W_{sur}(E^*, J)$$

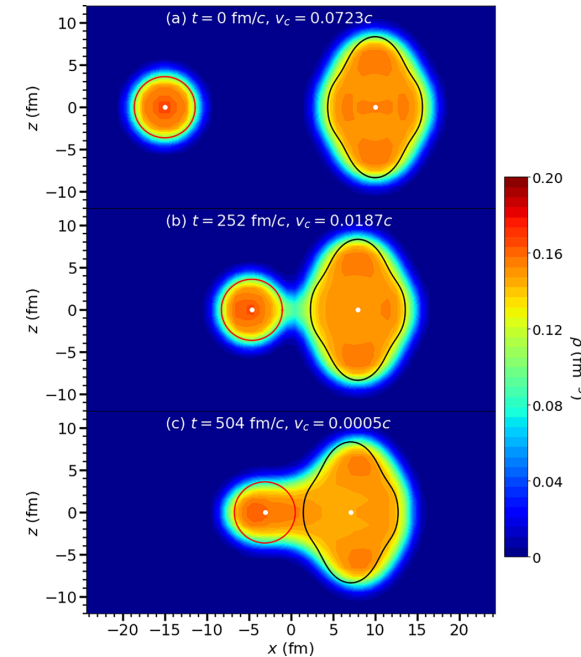


Orientation Changes the Whole Shape-Evolution Path

- The same system follows different dynamical paths.
- Orientation changes contact geometry and dissipation.
- Shape evolution matters beyond a one-dimensional barrier.



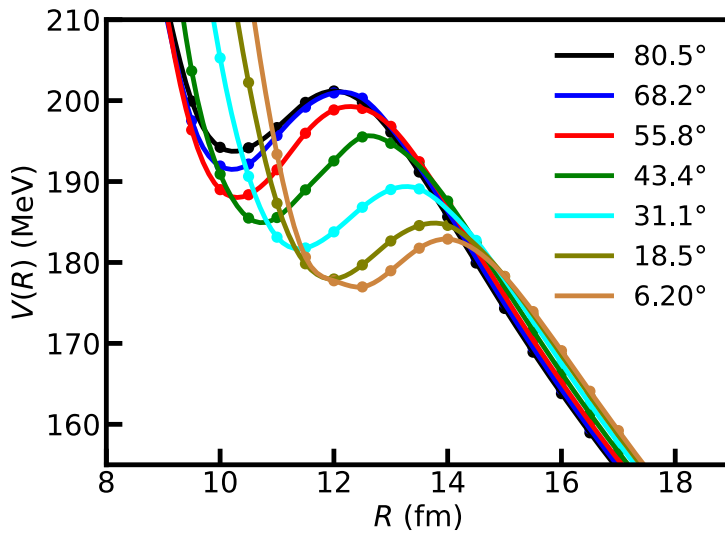
Tip collisions tend to follow a more elongated shape-evolution path.



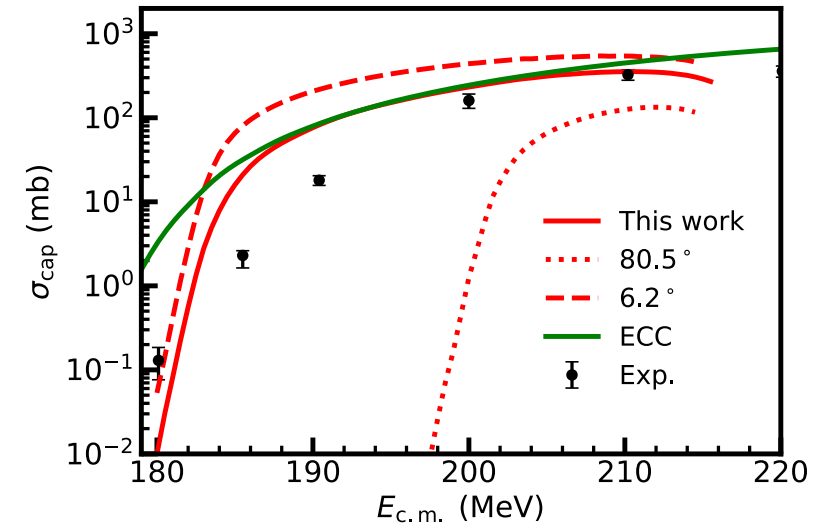
Side collisions can produce a more compact injection configuration.

Tip Lowers the Barrier, Side Favors Compact Configuration

- Tip: lower capture barrier, but more elongated injection.
- Side: higher capture barrier, but more configuration.



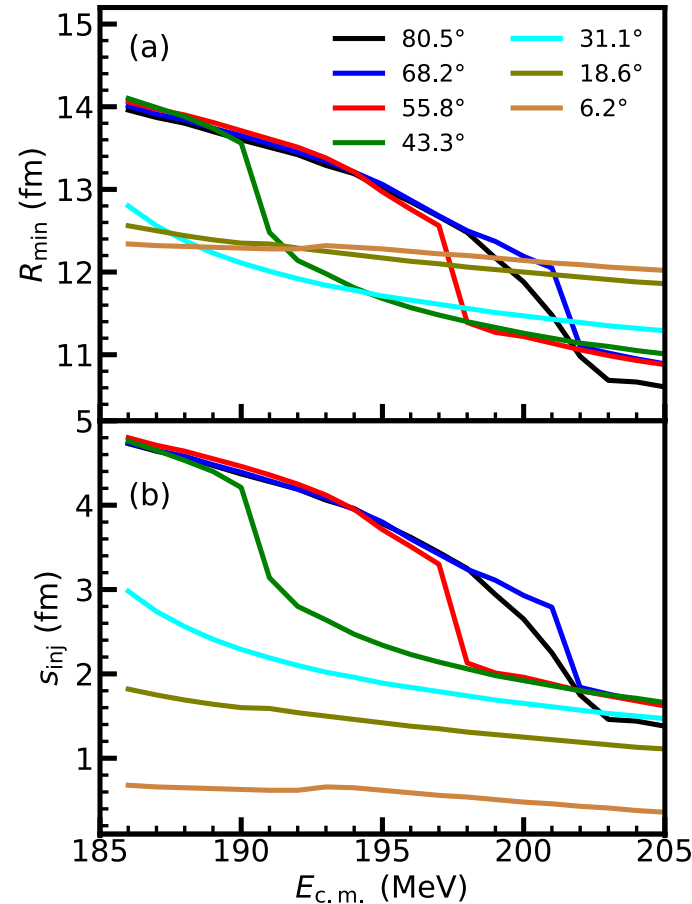
Orientation-dependent ion-ion potentials show different capture barriers.



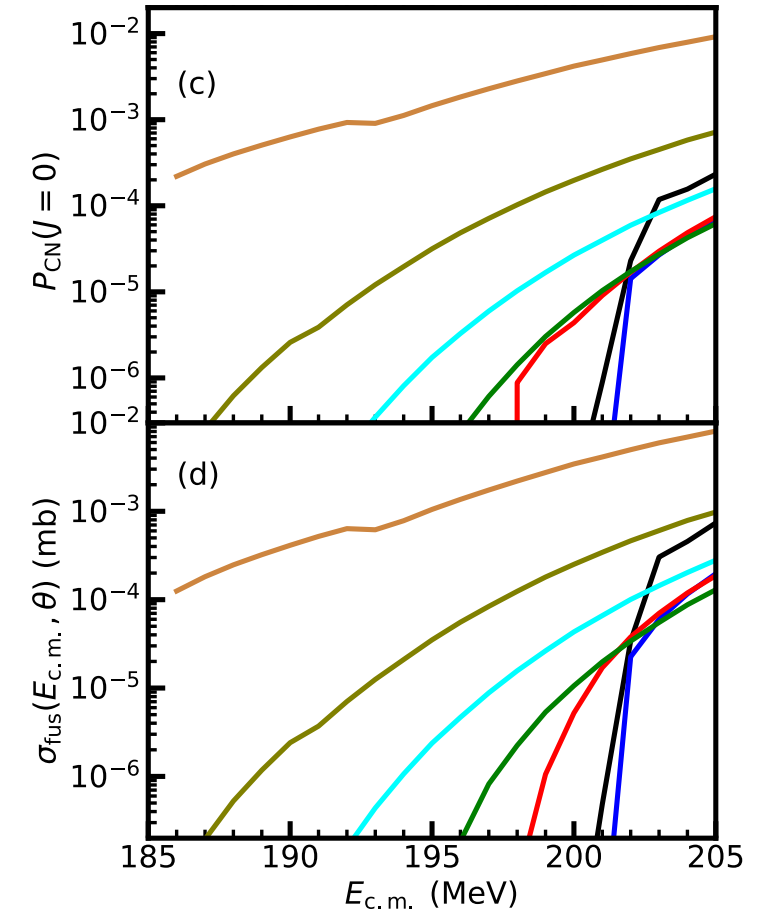
Capture cross sections alone do not determine evaporation-residue yields.

TDHF Supplies the Injection Configuration for Diffusion Models

- The injection distance measures how far the system starts outside a compact mononuclear shape.
- Smaller injection distance generally increases P_{CN} .
- The microscopic trajectory constrains the diffusion model.



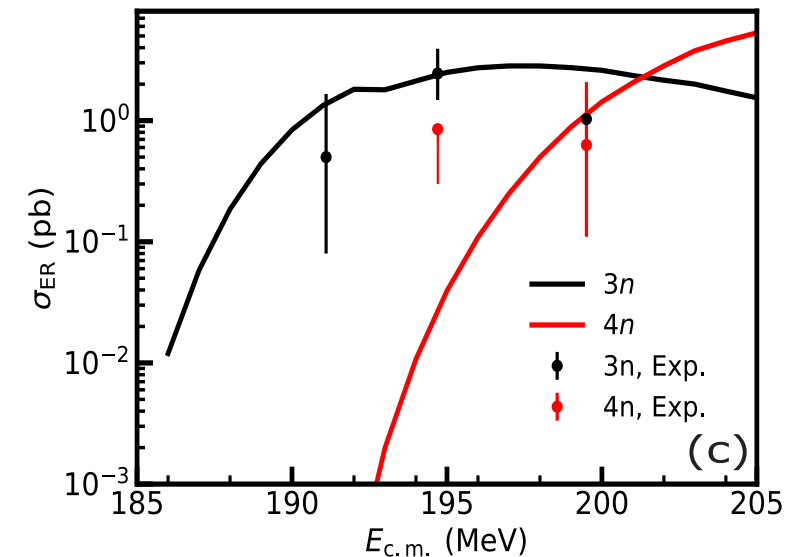
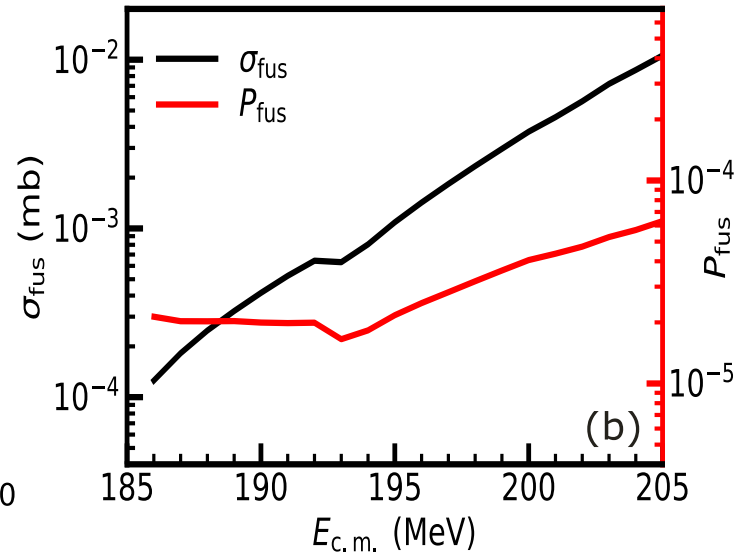
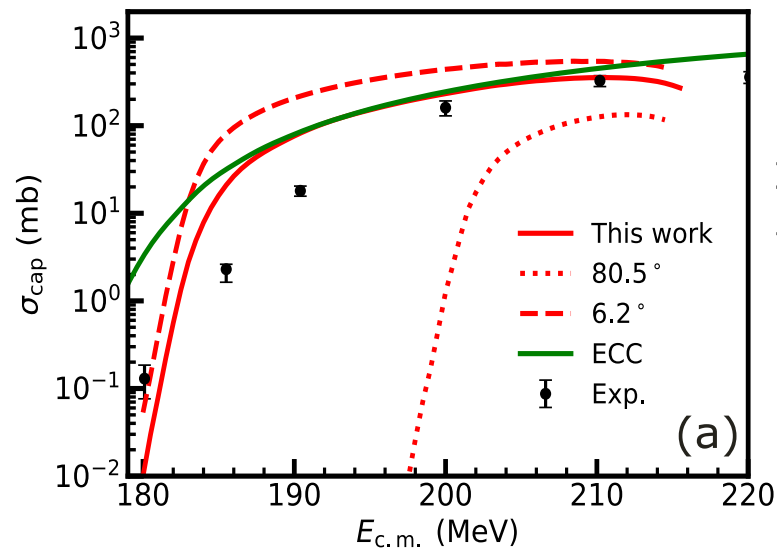
Orientation-dependent injection distances



Fusion probabilities constrained by TDHF trajectories.

Microscopic Injection Inputs Constrain Evaporation-Residue Cross Sections

- Orientation-dependent TDHF trajectories determine injection configurations.
- Diffusion gives P_{CN} .
- Statistical survival gives evaporation-residue yields.



Orientation-averaged fusion probabilities quantify the compound-formation filter.

A Density Movie Visualizes Fusion Evolution

- System: $^{54}\text{Cr} + ^{243}\text{Am}$.
- TDHF follows the real-time density evolution.
- The trajectory becomes compact, but residue formation still requires survival modeling.



A mean-field density movie provides a visual bridge from contact to a compact mononuclear configuration.

Entrance-Channel Memory Distinguishes Quasifission from Fusion-Fission

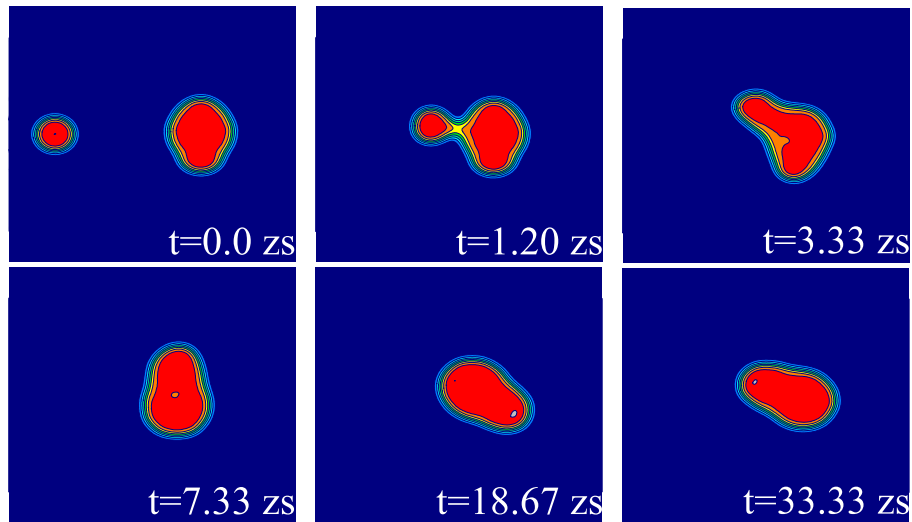
- Quasifission: reseparation before full equilibration.
- Fusion-fission: fission after compound-nucleus formation.
- The final two-fragment topology alone is not sufficient for classification.

Quasifission and fusion-fission differ by history

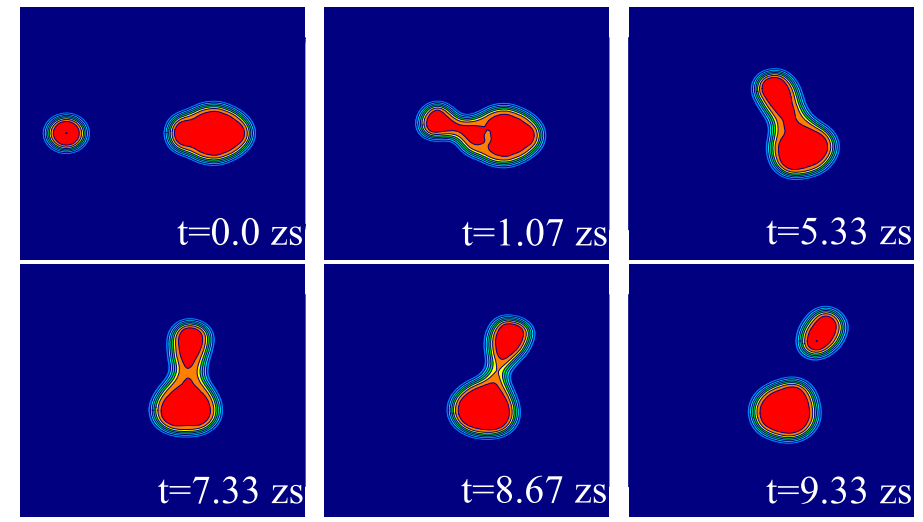


Orientation Decides Between Fusion and Quasifission

- Different Pu isotope targets produce very different superheavy yields — why?
- Side collisions can evolve toward a compact mononuclear configuration (fusion-like).
- Tip collisions often favor elongated shapes and reseparation (quasifission).



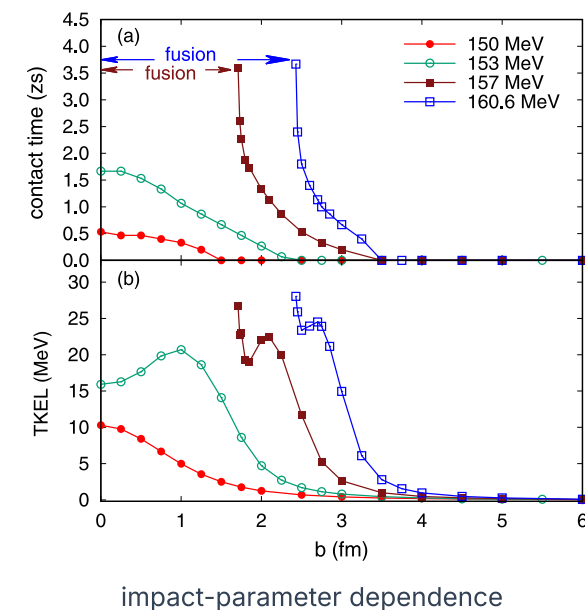
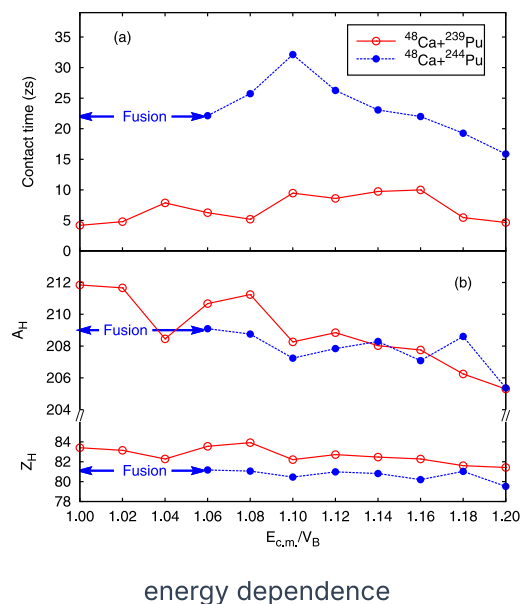
side collision density evolution



tip collision density evolution

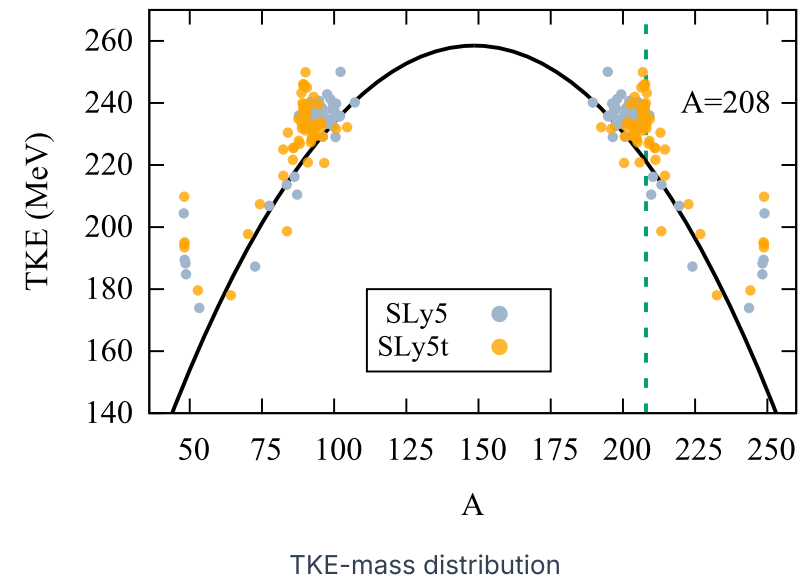
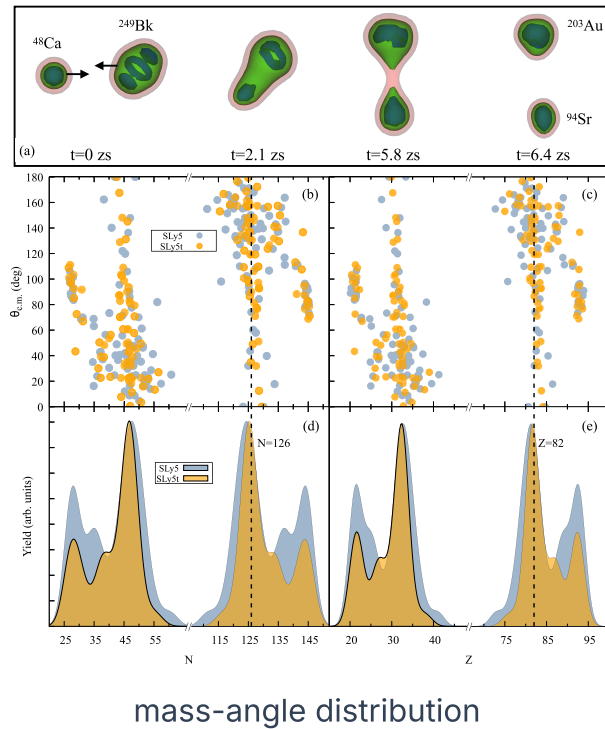
Long Contact and Mass Drift Diagnose Quasifission Dynamics

- Contact time measures how long the system remains connected by a neck.
- Fragment mass and charge reveal nucleon exchange and mass drift.
- TKE and scattering angle encode dissipation.



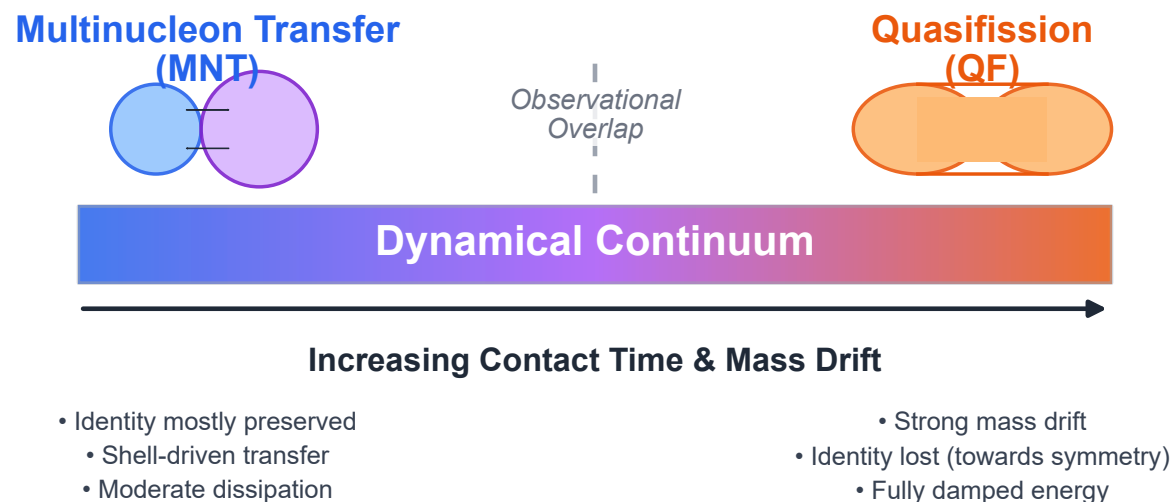
Pb-Like Shell-Favored Fragments Steer the Mass Drift

- Mass drift is not random.
- Shell closures near $Z = 82$ and $N = 126$ guide the heavy fragment.
- Quasifission yields therefore carry information about shell structure.



MNT and Quasifission Form a Dynamical Continuum

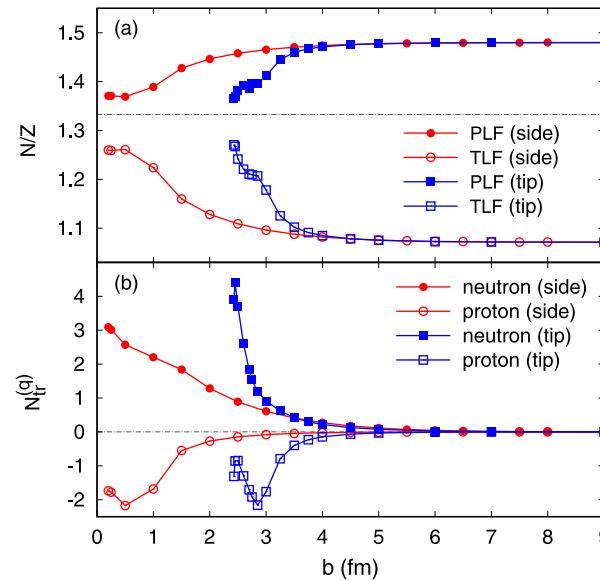
- During neck formation, nucleons are exchanged between the two fragments.
- Both MNT and quasifission involve contact, exchange, dissipation, and reseparation.
- MNT focuses on transfer channels.
- Quasifission focuses on fusion suppression and large mass drift.



The boundary is dynamical and observational, not a simple mass cut.

The N/Z Gradient Drives Opposite Neutron and Proton Flows

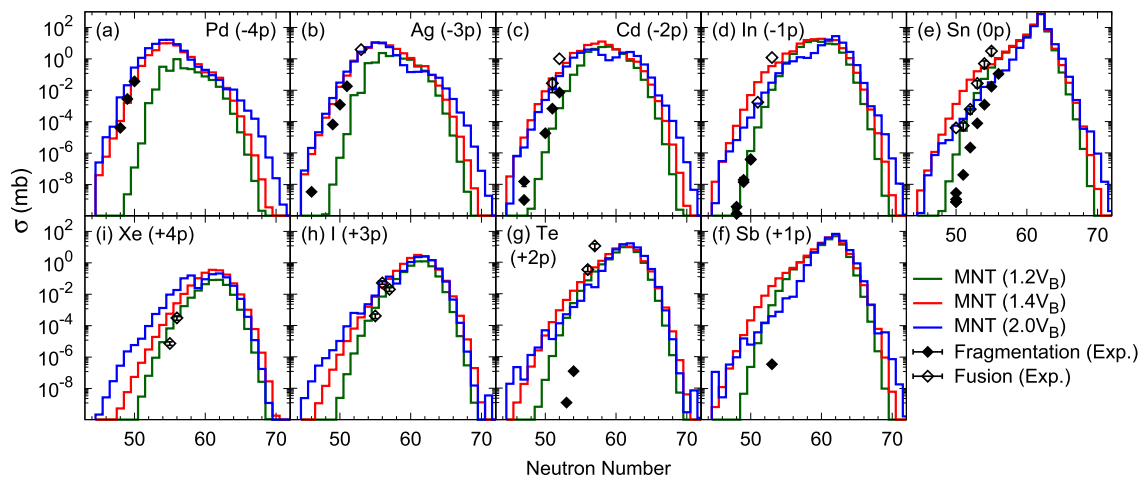
- ^{58}Ni ($N/Z \simeq 1.07$) + ^{124}Sn ($N/Z = 1.48$): large initial N/Z imbalance.
- Neutrons transfer toward the Ni-like fragment.
- Protons transfer toward the Sn-like fragment.
- Both fragments move toward a common N/Z (isospin equilibration).



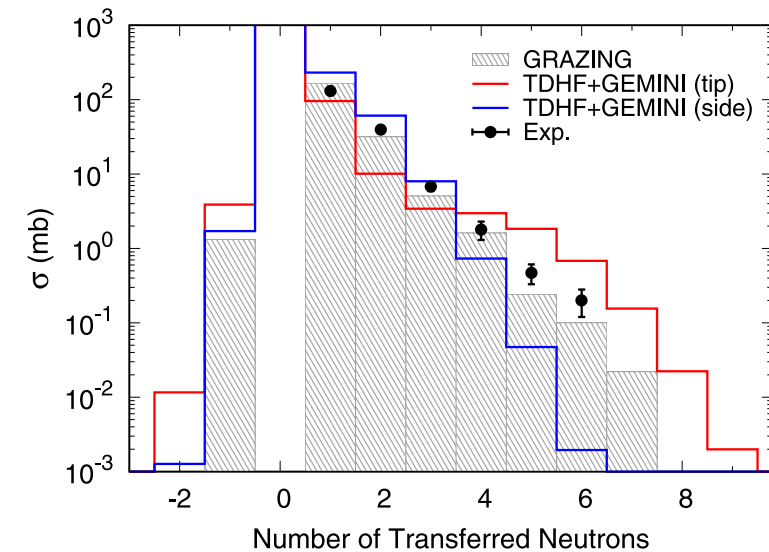
Neutron and proton transfer reduce the initial N/Z imbalance in $^{58}\text{Ni} + ^{124}\text{Sn}$.

PNP and GEMINI Connect Primary Transfer to Measured Yields

- TDHF gives primary fragments and mean transfer.
- PNP gives channel probabilities $P_{N,Z}(b)$.
- GEMINI propagates excited primary fragments to secondary products.
- $\sigma_{N,Z} = 2\pi \int b db P_{N,Z}(b)$.



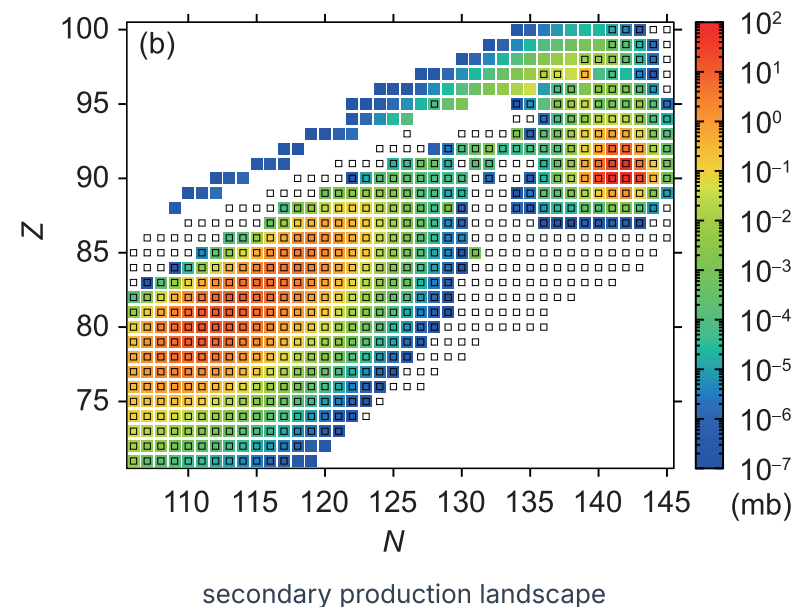
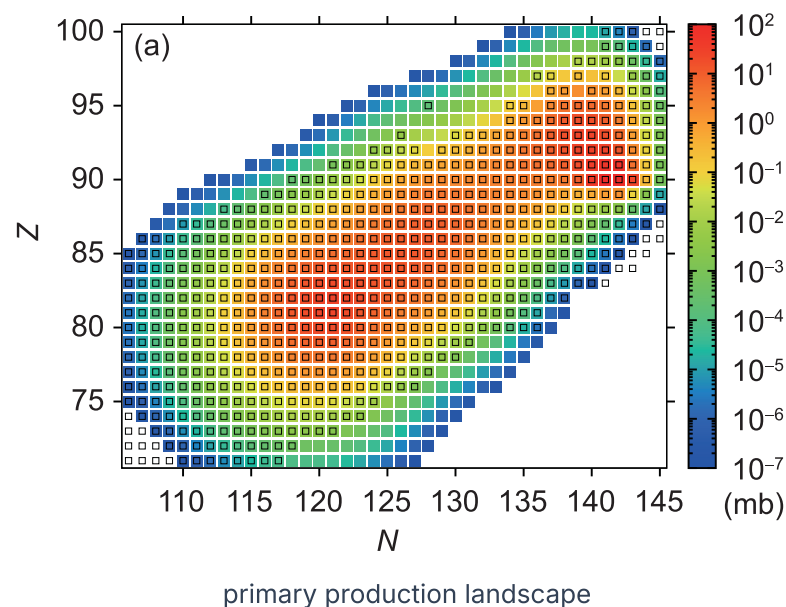
GEMINI converts excited primary fragments into secondary yields.



Channel cross sections can be compared with measured products after de-excitation.

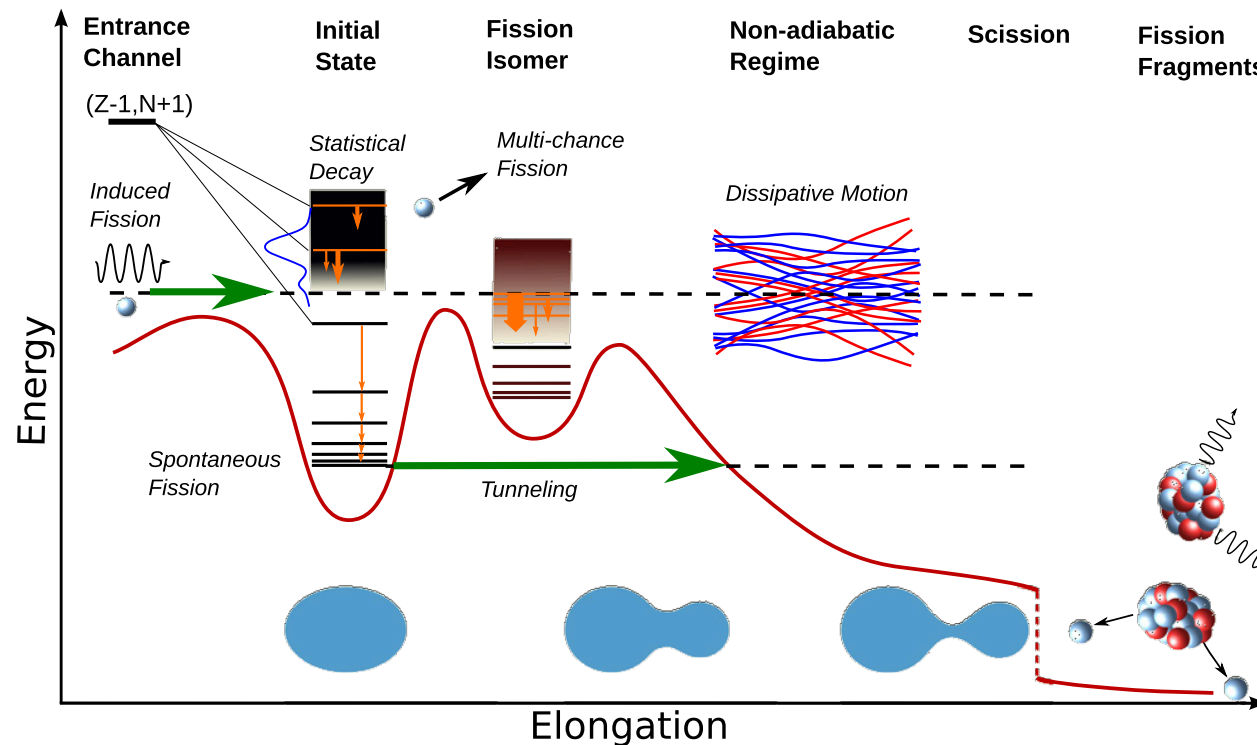
Reaction Dynamics Guides Production of Exotic Nuclei

- MNT can access proton-rich or neutron-rich regions.
- Production maps depend on both primary transfer and secondary survival.
- TDHF-based modeling helps screen reaction choices.



Fission Evolves from Collective Deformation to Scission and Fragments

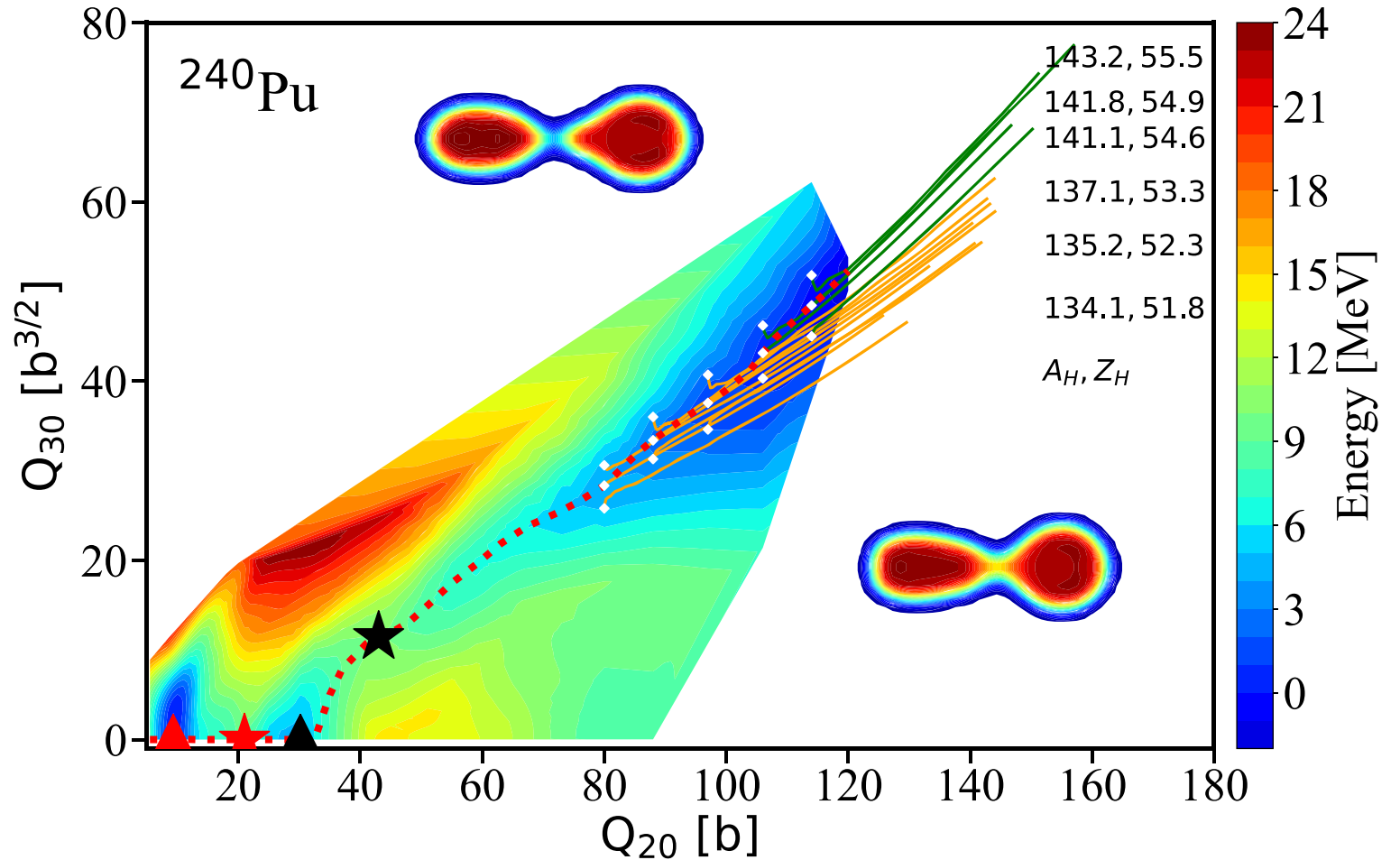
- Barriers and tunneling set the entrance to fission.
- Scission creates excited primary fragments.
- Beyond the barrier, dissipative motion drives large-amplitude shape evolution.
- Prompt neutron and gamma emission modify measured fragment observables.



Fission is not only a barrier problem; the key physics is the path from initial state to scission and fragments.

Two Asymmetric Valleys Generate Distinct Fragment Channels

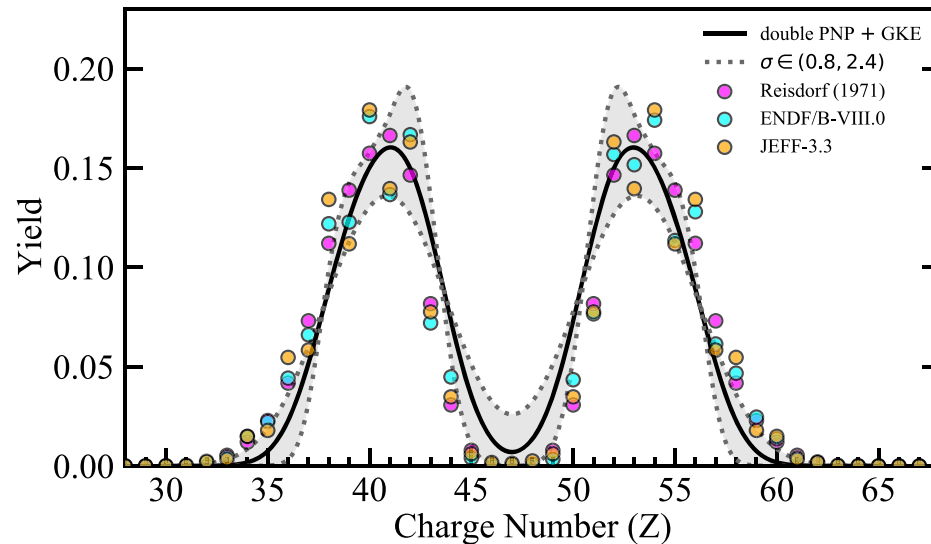
- Benchmark system: ^{240}Pu ; initial configurations sampled along the fission valley.
- The 2D PES is organized by Q_{20} and Q_{30} .
- Dynamical TDHF trajectories follow different asymmetric valleys.
- The channels lead to different heavy-fragment masses and charges.



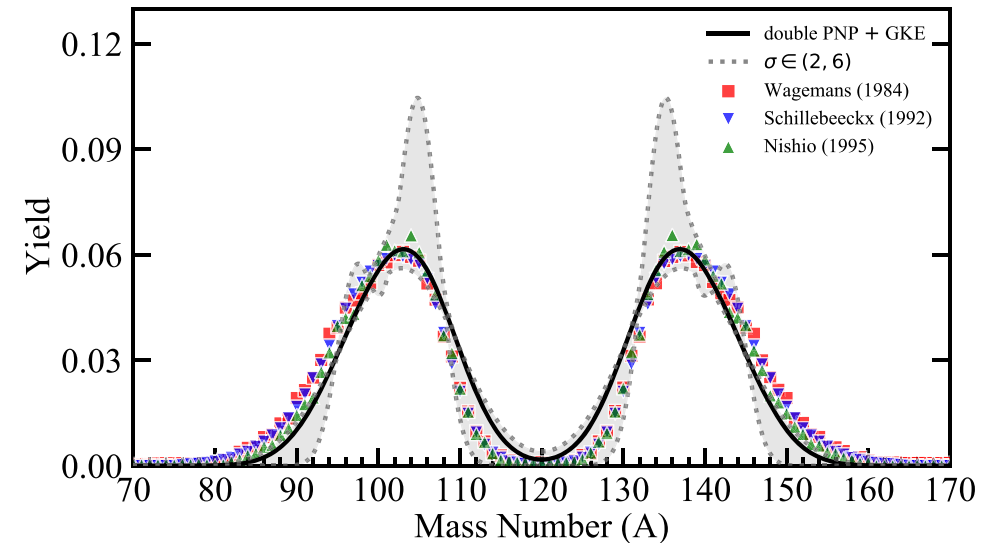
2D PES and TDDFT trajectories of ^{240}Pu with two asymmetric fission channels.

Double PNP Converts Scission Densities into Charge and Mass Distributions

- Standard TDDFT gives mean fragment properties.
- Double PNP assigns probabilities to fragment neutron and proton numbers.
- Summed trajectories generate charge and mass distributions.



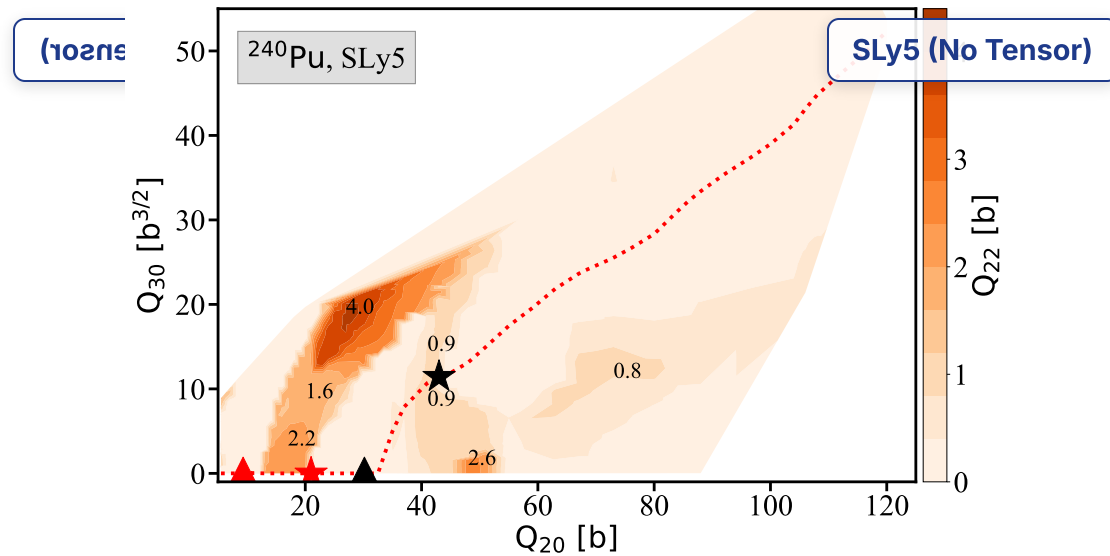
charge distribution with double PNP



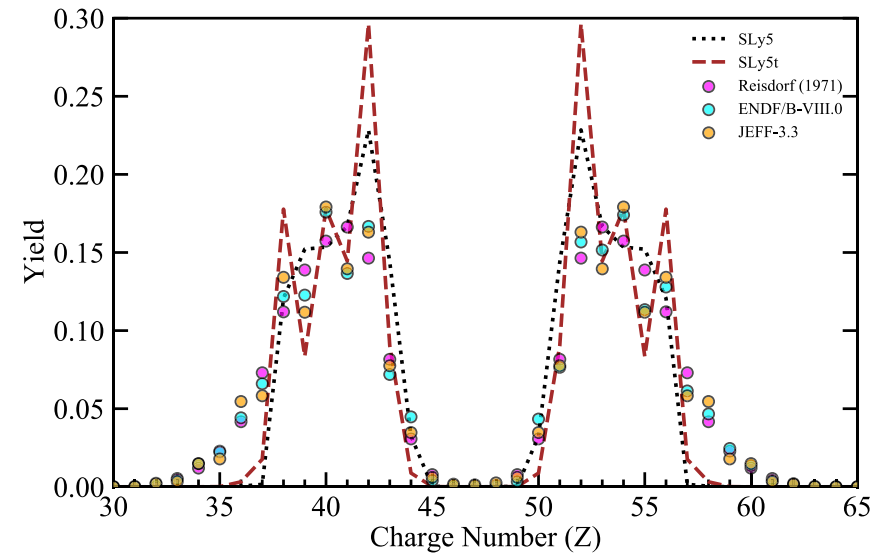
mass distribution after GKE

Tensor Terms Modify Shell Structure and Fragment Yields

- Tensor terms change the PES and single-particle shell structure.
- Shell effects select fission valleys and fragment distributions.
- Fission observables can therefore test EDF ingredients.



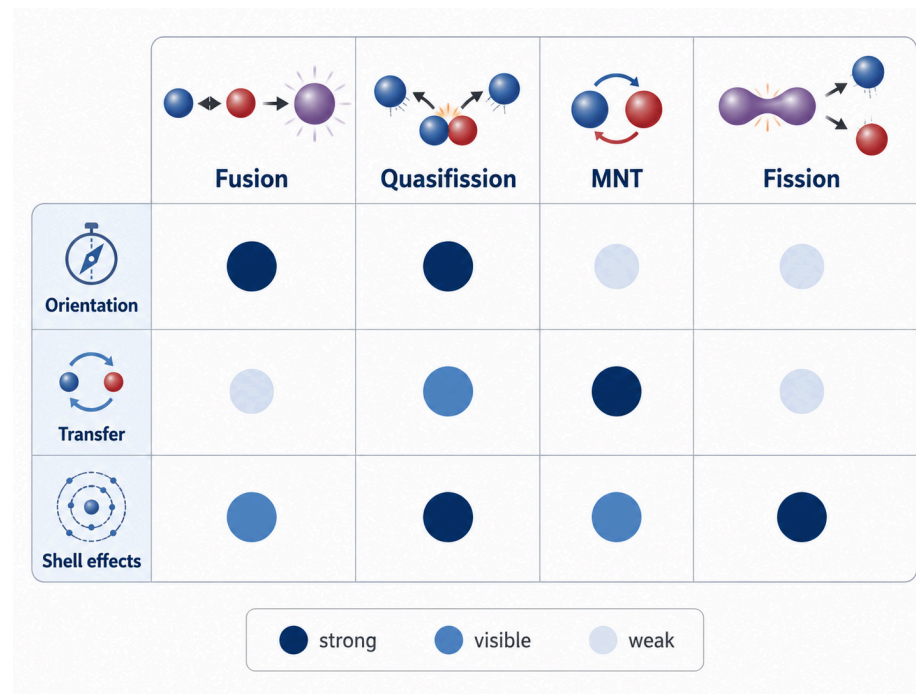
PES topology changes with tensor terms



charge distribution with tensor-force comparison

The Same Mechanisms Recur Across Low-Energy Reaction Channels

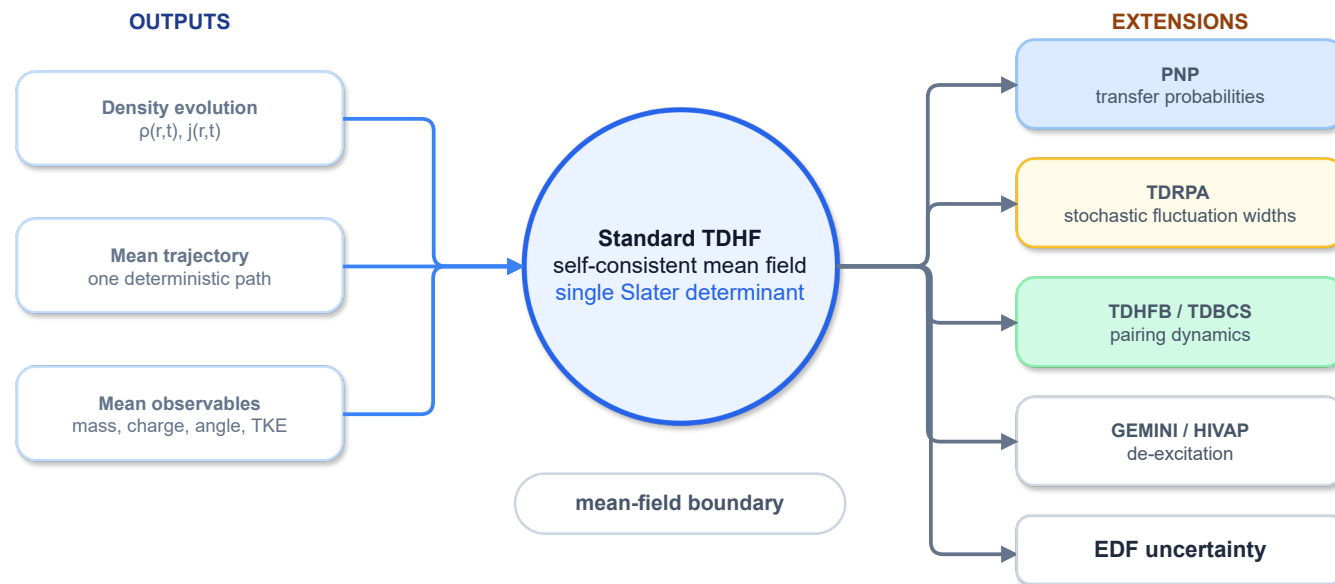
- Orientation is most visible in fusion and quasifission.
- Transfer dominates MNT but also appears in quasifission.
- Shell effects shape mass drift, fission valleys, and fragment yields.



A compact map of which mechanisms are most visible in each process.

Predictive Reaction Theory Needs Fluctuations, Pairing, and De-excitation

- Fluctuations and distribution widths.
- Pairing dynamics: TDHFB / TDBCS.
- Finite temperature and dissipation.
- Statistical de-excitation coupling.
- EDF uncertainty and surrogate models.



TDHF: method boundaries and extensions

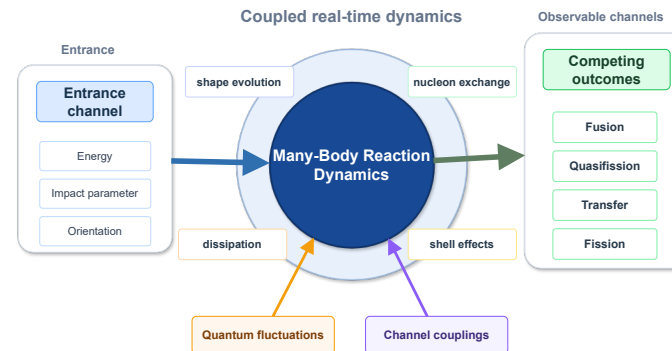
TDDFT Connects Microscopic Mechanisms to Measurable Observables

- Low-energy nuclear reactions are real-time large-amplitude dynamics of finite quantum many-body systems.
- Nuclear TDDFT/TDHF provides a self-consistent density trajectory for fusion, quasifission, multinucleon transfer, and fission.
- Measured yields require projection, diffusion, and statistical de-excitation models beyond the mean trajectory.

Thank you!

Shape, Transfer, Dissipation, and Shells Evolve Together

- The neck couples the two nuclei into one finite quantum system.
- Nucleon exchange and dissipation occur during shape evolution.
- Shell effects can steer the real-time path.
- Small changes in entrance conditions or shell structure can redirect the reaction path.



The neck region couples shape, transfer, dissipation, and shell structure.