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Title: Investigation of fission yields in a time-dependent superfluid local density approximation

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Investigation of fission yields in a time-dependent superfluid local density approximation

PI: Ionel Stetcu (T-2)

Highlight from first microscopic calculation of ^{240}Pu fission:

- **Fully unrestricted 3D calculation with full nuclear energy density functional**
- **Long evolution times from outer fission saddle to full scission**
- **TKE predicted within 3% of expected values**
- **Light fission fragment heavily deformed, heavy fission fragment spherical (as expected)**
- **Demonstrated the essential role played by pairing correlations in nuclear shape evolution**

IC's Moonlight was used for small-scale testing

Bulgac et. al, Physical Review Letters 116, 122504 (2016)

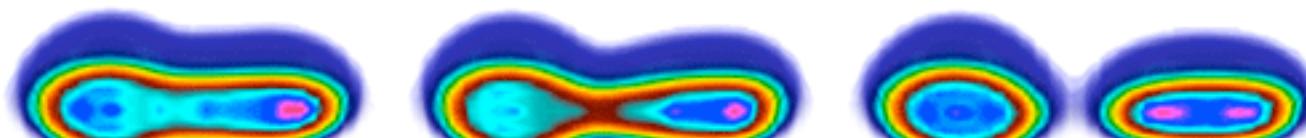
Time-Dependent Density Functional Theory with Nuclear Energy Density Functional a la Skyrme

Construct constrained initial state near the outer fission barrier

Evolve in time beyond the scission point

Full characterization of fission fragment properties as a function of initial excitation energy of the fissioning nucleus (neutron incident energy):

- Average mass, charge, excitation energy, and angular momentum
- TKE of fission fragments

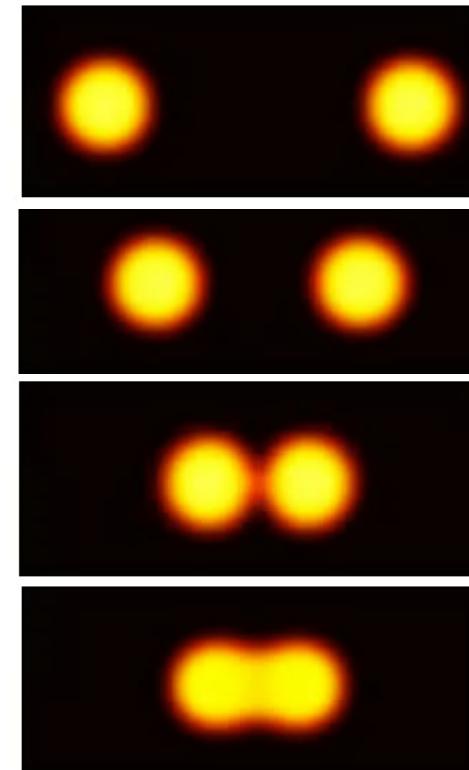
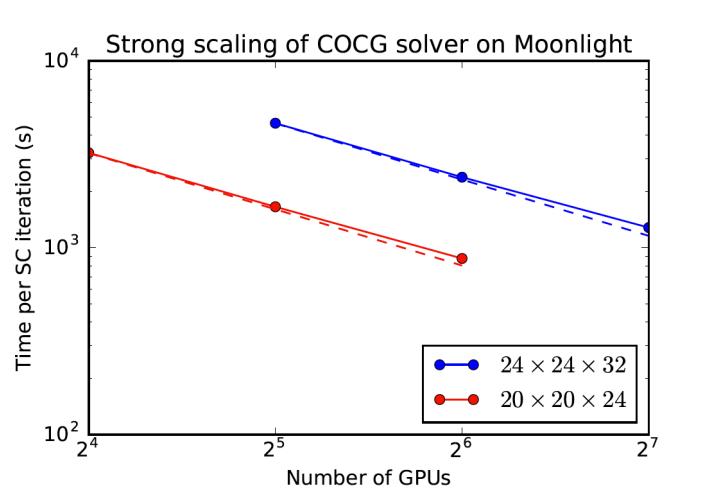


<http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.116.122504>

Development of new capabilities

Shifted Conjugate-Orthogonal Conjugate-Gradient (COCG) method for superfluid many-fermion systems:

- Calculating local densities without obtaining the quasiparticle-wfs from a given HFB Hamiltonian.
- Highly effective implementation on GPU
- Flexibility of using spatial symmetry of lattices.
- Will allow for an efficient preparation of initial states for fission and fusion/collision calculations



Work in progress

Shi Jin et al, arXiv:1608:03711 (2016), submitted to Phys. Rev. C

Microscopic simulations that include all relevant degrees of freedom