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References: This code of conduct is based heavily on that of the INT and the APS. We are also grateful to Roxanne Springer for valuable discussion and guidance.

Neck Rupture and Scission Neutrons in Nuclear Fission

INT Rising Researchers Seminar

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University of Washington

Tuesday, March 4, 2025

CENTER FOR EXCELLENCE IN NUCLEAR TRAINING AND UNIVERSITY-BASED RESEARCH

Outline for talk:

- Introduction to fission
- Anatomy of the fission process
- Our results on scission neutrons
- Prospects for experimental detection
- Future work

Paper: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Collaborators on this work:

- **Aurel Bulgac** (PI, UW)
- Ionel Stetcu (LANL)
- Ibrahim Abdurrahman (LANL)

History and Motivation

- **Nuclear fission is a nuclear reaction in which the nucleus of an atom splits into two (or more) smaller nuclei, called "fission fragments" (FFs).**

- The fission reaction also releases light, in the form of gamma rays, and neutrons.

- The reaction produces a lot of energy (when compared to other nuclear and chemical reactions) primarily in the kinetic energy of the emerging FFs.
  - Typical energies for chemical reactions are ~10 eV
  - KE of fission fragments ~170 MeV $= 170 \cdot 10^6$ eV (10 million times more energy per reaction!)

- Discovered experimentally in December 1938 by Otto Hahn and Fritz Strassmann.
  - They bombarded a uranium sample (92 protons per nucleus) with a beam of neutrons and observed barium (56 protons per nucleus)!
  - At the time there was no known mechanism by which such a process could occur.

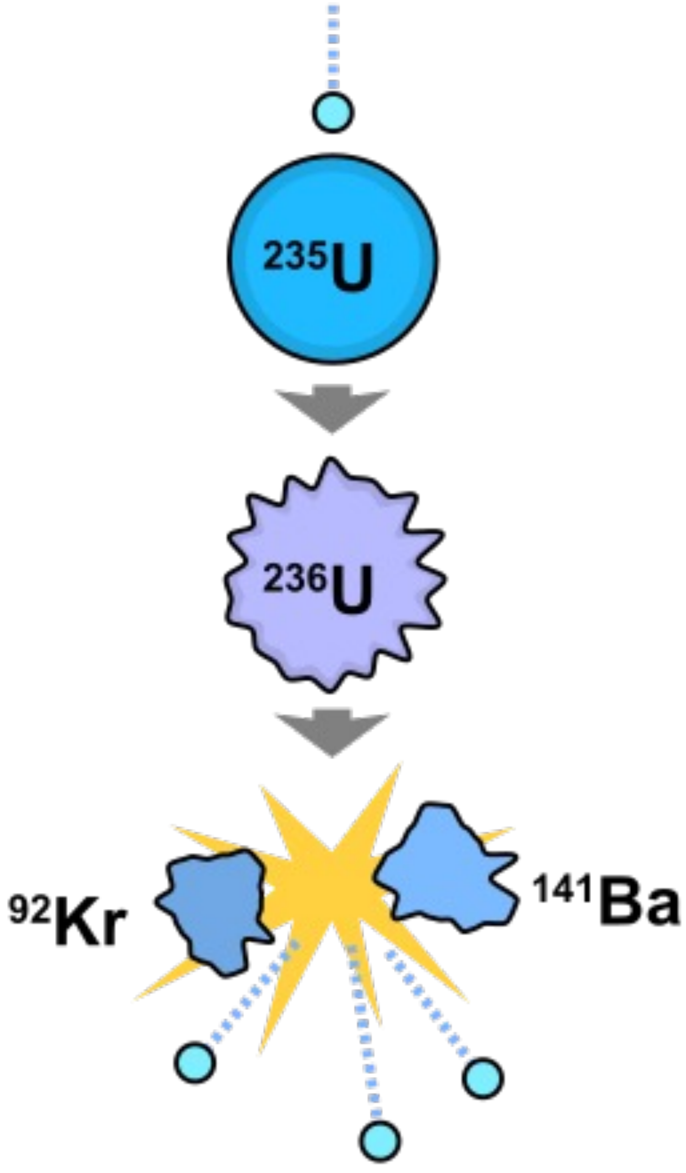


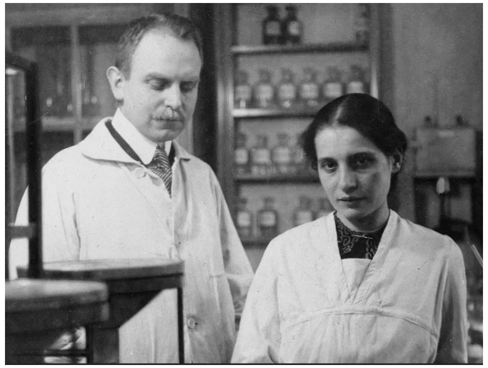
Image source: *https://en.wikipedia.org/wiki/Nuclear_fission*

History and Motivation (Continued)

- One month later, in January 1939, Lise Meitner and Otto Frisch published theoretical explanation, that **the nucleus has split roughly in half**.

- **Since it takes one neutron to induce a fission reaction, and each reaction releases more than one neutron on average, this creates the possibility for a chain reaction.** (Concept due to Leó Szilárd, 1933.)

- Relevance to society:
  - Nuclear fission reactors: controlled chain reactions
    - Produce heat and can thus act as a power source
    - Can produce neutrons, photons, or radioactive isotopes for scientific, engineering, or medical applications
  - Nuclear weapons: uncontrolled chain reactions
  - National security (non-proliferation and detection)
    - Detecting whether someone has detonated a nuclear weapon in the atmosphere or is trying to smuggle one across your border, for example, require a detailed understanding of the fission process.



Otto Hahn and Lise Meitner in 1912

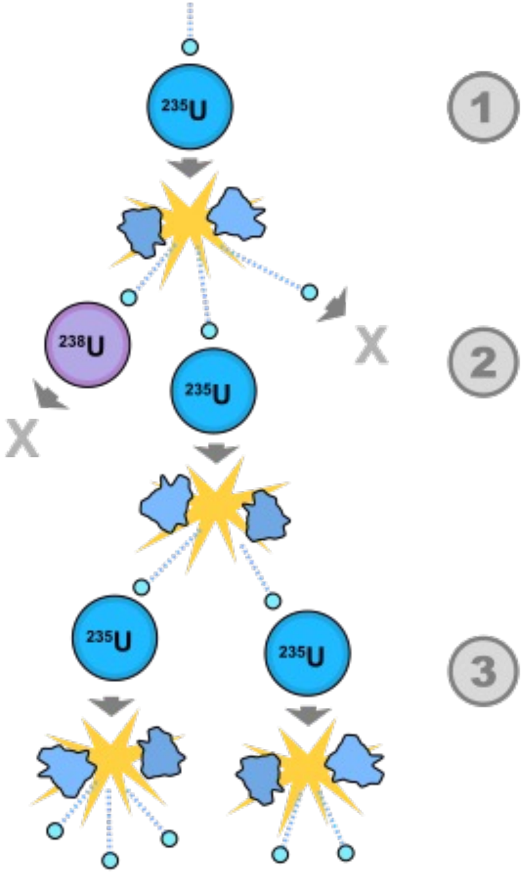


Image source: *https://en.wikipedia.org/wiki/Nuclear_fission*

Relevance of Fission to Modern Physics

As scientists, we are interested in fission because **it is a quantum mechanical phenomenon of immense complexity, still lacking a complete microscopic description to this day**.

"Fundamental" Physics:

- Fission is a strongly-interacting quantum many-body process out of equilibrium.
  - Each color adds immense difficulty (and fun) to the problem: to calculate all properties of the nucleus, its dynamics, and the properties of the emerging "debris" starting from the basic laws of nature.

Astrophysics:

- Collisions between neutron stars and core-collapse supernovas produce large quantities unstable neutron-rich nuclei through the "r-process".
  - Fission is one of the primary decay pathways.
  - The r-process is believed to be responsible for the origin of half the elements heavier than iron in the universe.

Superheavy elements:

- What are the heaviest elements (i.e., nuclei) that can possibly exist in nature?
- Spontaneous fission one of the primary decay pathways of superheavies.

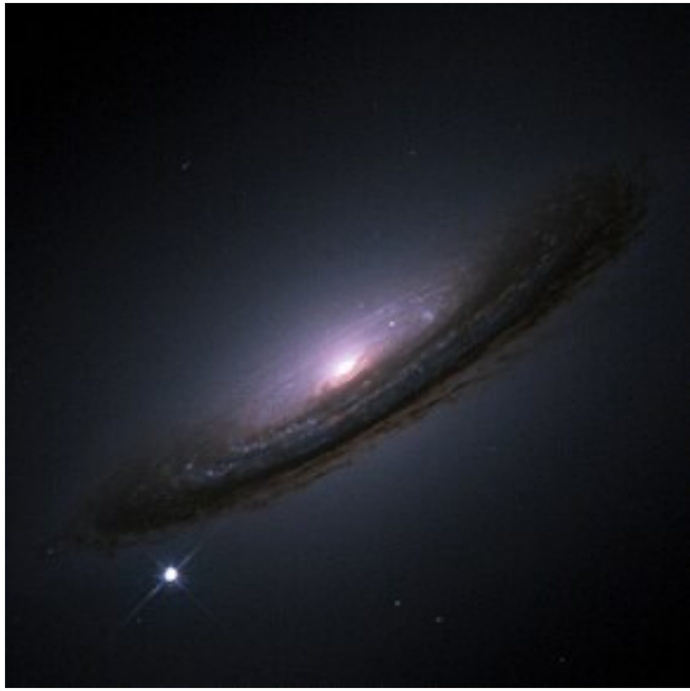
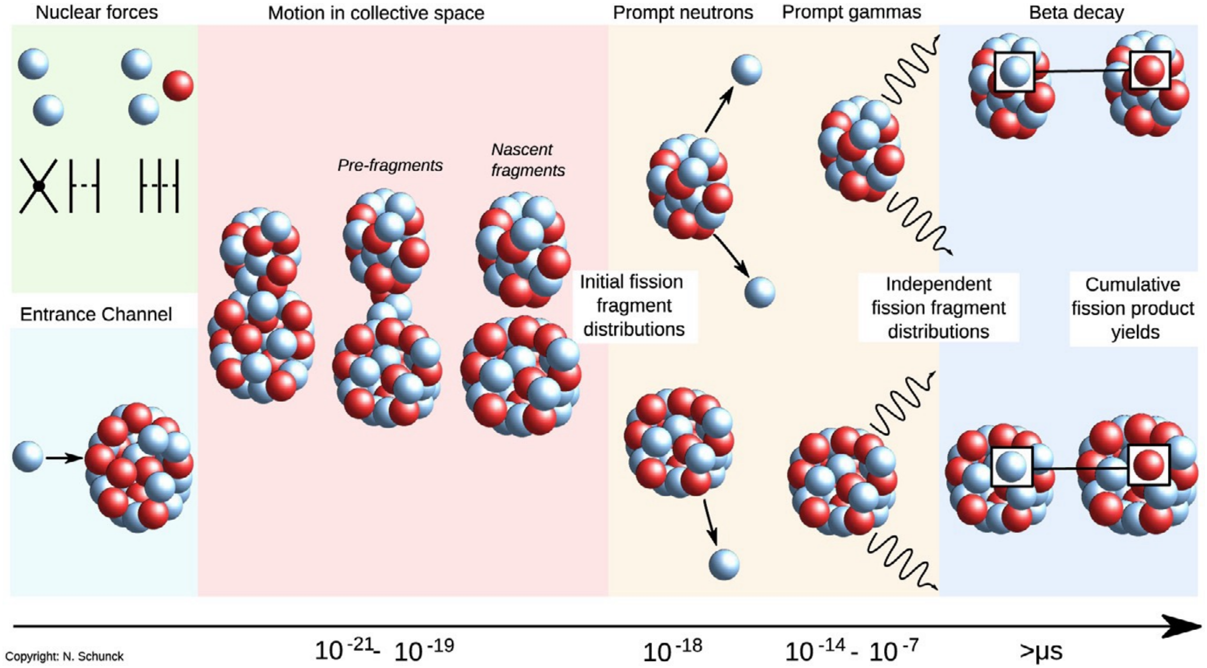


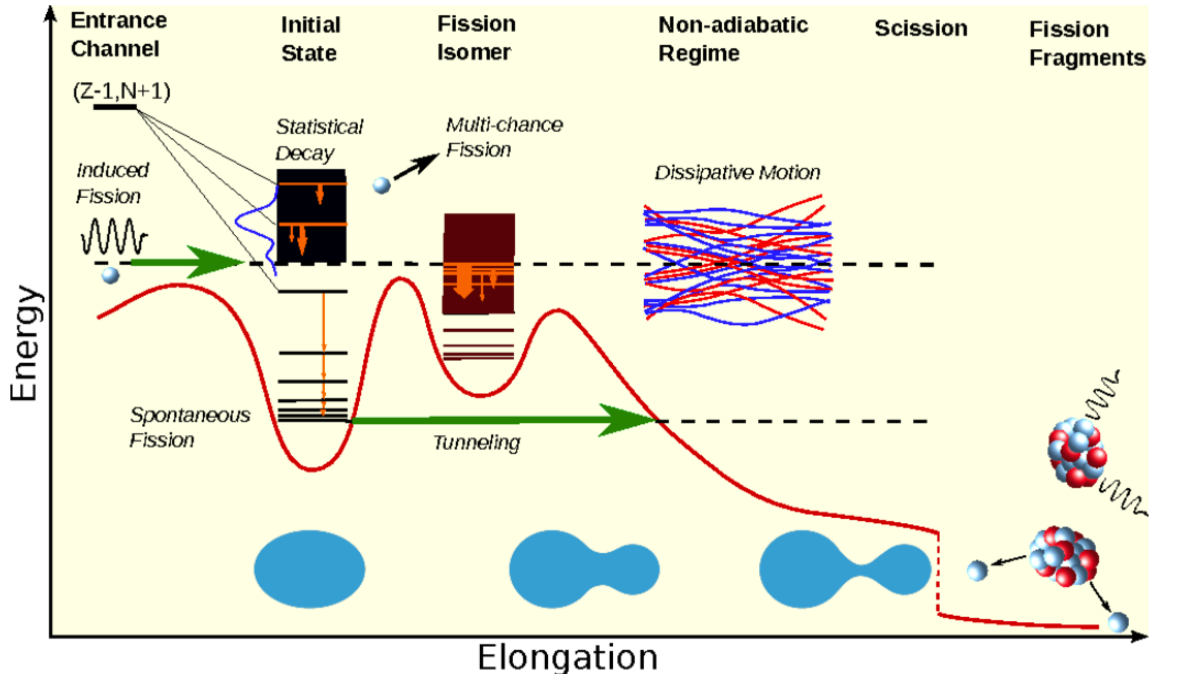
Image Source: Wikipedia/Supernova

Image Source: Wikipedia/Neutron star merger

Anatomy of the Fission Process

- Nucleus of a heavy atom absorbs a neutron, moves to "outer saddle point"
  - 10^{-14} s
  - Quasi-equilibrium process
  - Ground state cold with a small spin
- Saddle to scission
  - 5×10^{-21} s
  - Highly non-equilibrium
  - Collective velocity small
  - Nucleus heats up
- Scission/neck rupture
  - 10^{-22} s
  - Highly non-equilibrium
  - ***Scission neutrons released***
  - Fastest stage of fission dynamics

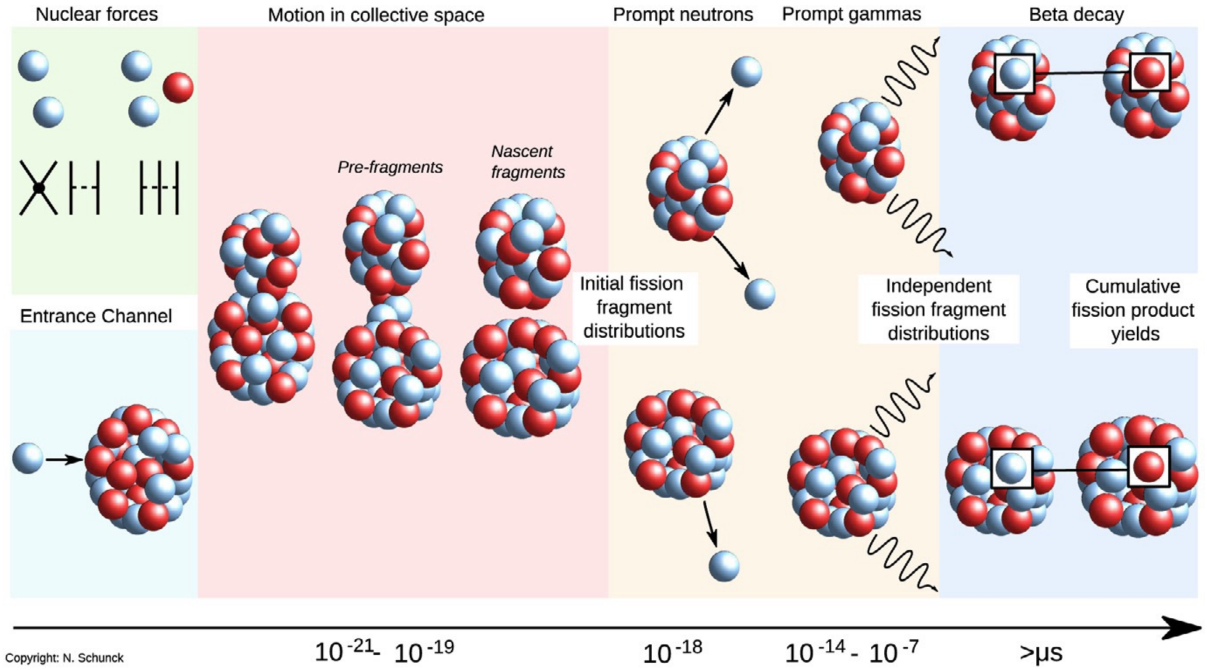


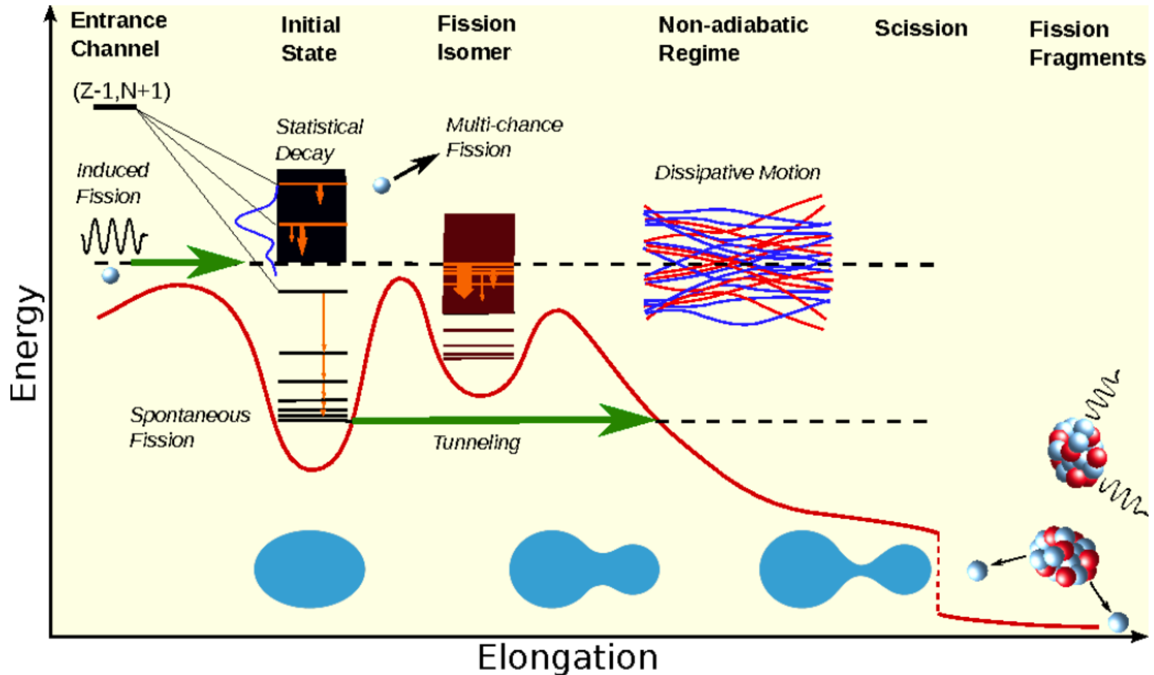


Source: *Future of Nuclear Fission Theory*, Bender *et al.* Journal of Physics G: Nuclear and Particle Physics(2020)

Anatomy of the Fission Process (Continued)

- FFs accelerate due to Coulomb interaction
  - 10^{-18} s
  - Quasi-equilibrium
  - Shapes relax
  - Fragments now hot, rotating rapidly
- Prompt neutron emission
  - Up to 10^{-14} s
  - Evaporation
- Gamma emission
  - Up to 10^{-3} s
  - De-excitation
- Subsequent beta decays
  - Can take very long time, in extreme cases up to age of the universe
- Up to 40 orders of magnitude in time scales!





Source: *Future of Nuclear Fission Theory*, Bender *et al.* Journal of Physics G: Nuclear and Particle Physics(2020)

Theoretical Approach — "TDSLDA"

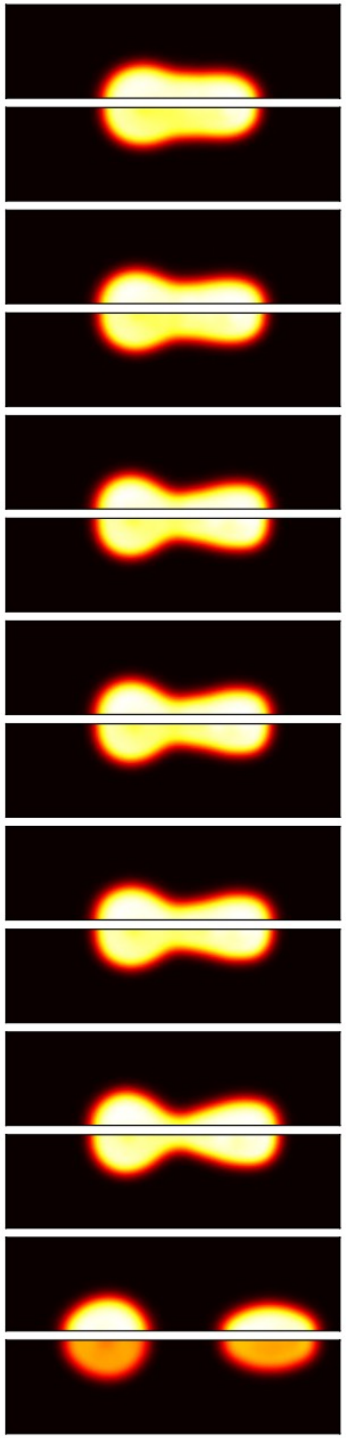
- Stands for "time-dependent superfluid local density approximation"

- **Density functional theory is a general theory for interacting fermionic many-body systems.**
  - Hohenberg and Kohn + Kohn and Sham ~ 143,000 citations!
  - "Time dependent density functional theory can be viewed as an exact reformulation of time-dependent quantum mechanics, where the fundamental variable is no longer the many-body wave function, but the density." Marques and Gross, Ann. Rev. Phys. Chem. (2004)

- TDSLDA is an extension of time-dependent density functional theory to superfluid systems

- Most advanced theoretical approach for studying nuclear fission dynamics
  - Also for nuclei more generally, cold atoms, neutron star crusts, quantum turbulence, etc.
  - Equilibrium and non-equilibrium

- **Only 8 (well-known) parameters**
  - Each nuclear parameter has been known for decades. All of them unrelated to nuclear fission.



Past Successes of TDSLDA

- **Single formalism can be applied to calculate static and dynamical properties of nuclei at low energies across the entire nuclear chart** (all nuclei heavier than oxygen or so).

- Using the "SeaLL1" functional, provides among the best descriptions of a variety of nuclear properties:
    - Masses
    - Charge radii
    - Compressibility
    - Surface tension
    - Isospin symmetry
    - Shell structure
    - Pairing gaps
    - Two-nucleon separation energies
    - Etc.

Source: *Wikipedia, Table of Nuclides*

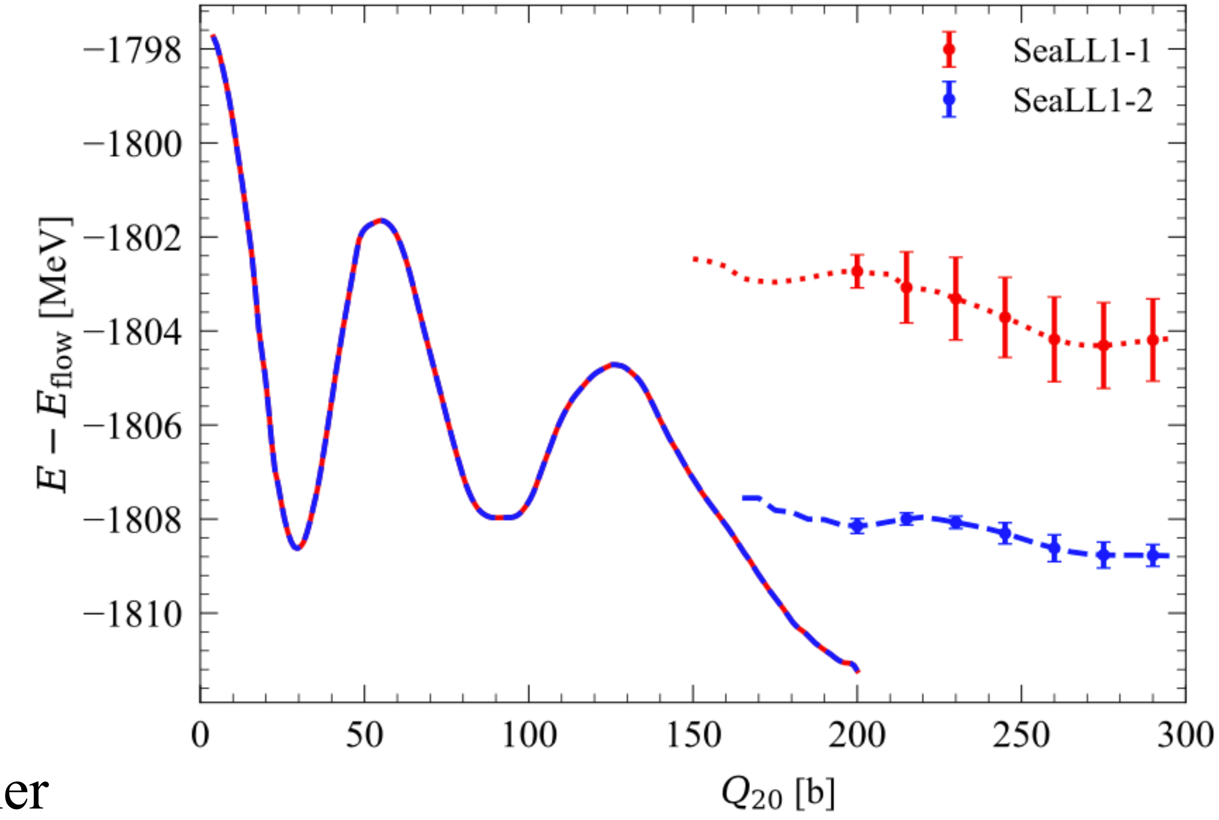
Source: *Minimal nuclear energy density functional*, A. Bulgac, M. M. Forbes, S. Jin, R. N. Perez, N. Schunck, Physical Review C (2019)

Past Successes of TDSLDA

- **Scission achieved starting from outer saddle with very little excitation energy** (because pairing treated properly)
  - i.e., nucleus actually breaks apart.
  - Pairing allows for repopulation of states as nucleus elongates.

- Adiabatic approximation strongly violated
  - Approximation formerly widely invoked in the literature.
  - Otherwise, energy would follow closely the constrained PES to the right.

- Light FF emerges from fission hotter and with higher angular momentum than the heavy fragment.
- FF intrinsic spins not perpendicular to fission axis.
  - Both previous points contradict assumptions used by other leading phenomenological models.



Source: *Fission Dynamics of ^{240}Pu from Saddle To Scission and Beyond*, A. Bulgac, S. Jin, K. Roche, N. Schunck, I. Stetcu, Physical Review C (2019)

<u>Scission Neutrons (SNs)</u>

- SNs conjectured to exist as early as 1939 by N. Bohr and J. Wheeler, same year fission discovered.

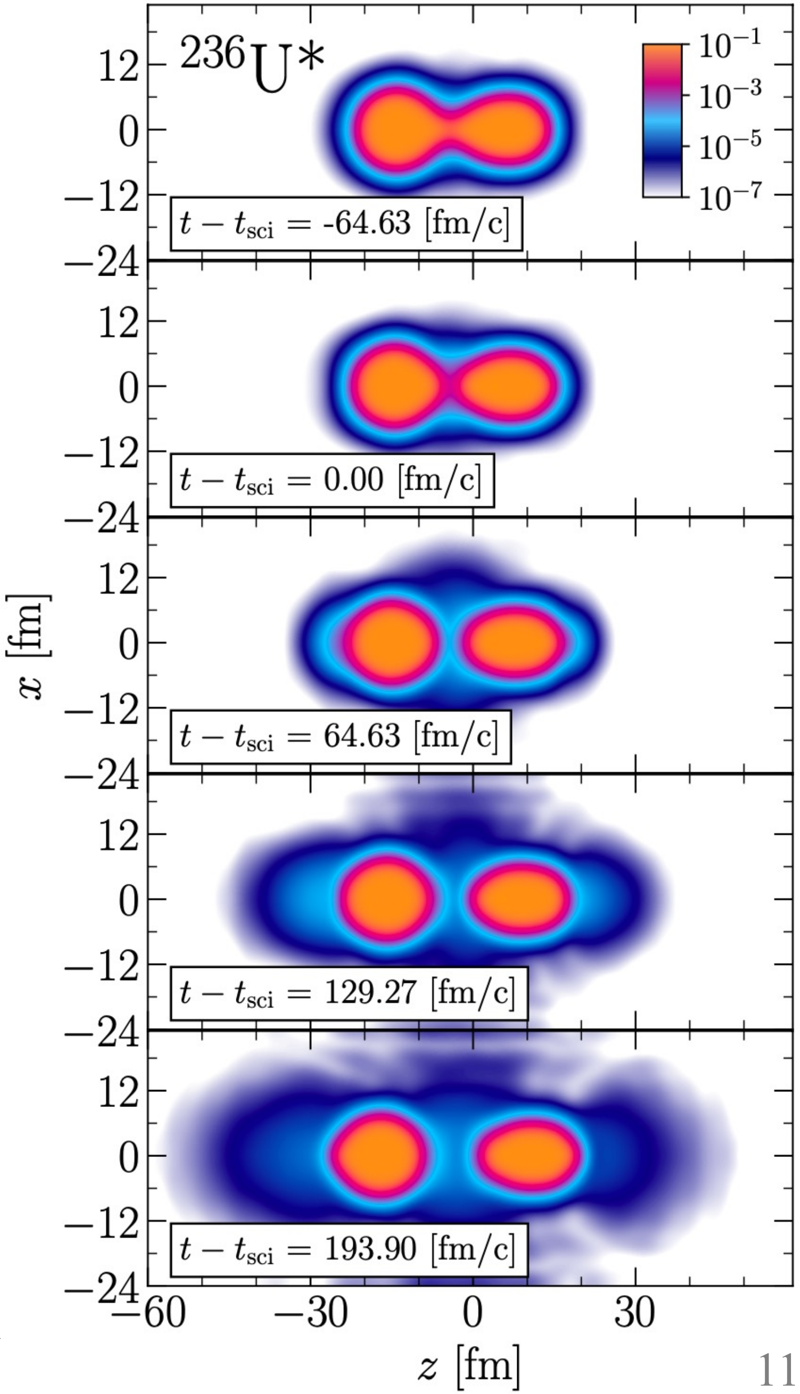
> "…**attention may be called to observations on the manner in which a fluid mass of unstable form divides into two smaller masses of greater stability; it is found that tiny droplets are generally formed in the space where the original enveloping surface was torn apart**."

- Contentious history: **no consensus in the literature from experiment or theory whether they should exist, even now.**

- We present arguably the first fully microscopic time-dependent simulation of the phenomenon.

- Scission neutrons clearly present, "for free" (i.e., no kicks or perturbations required).

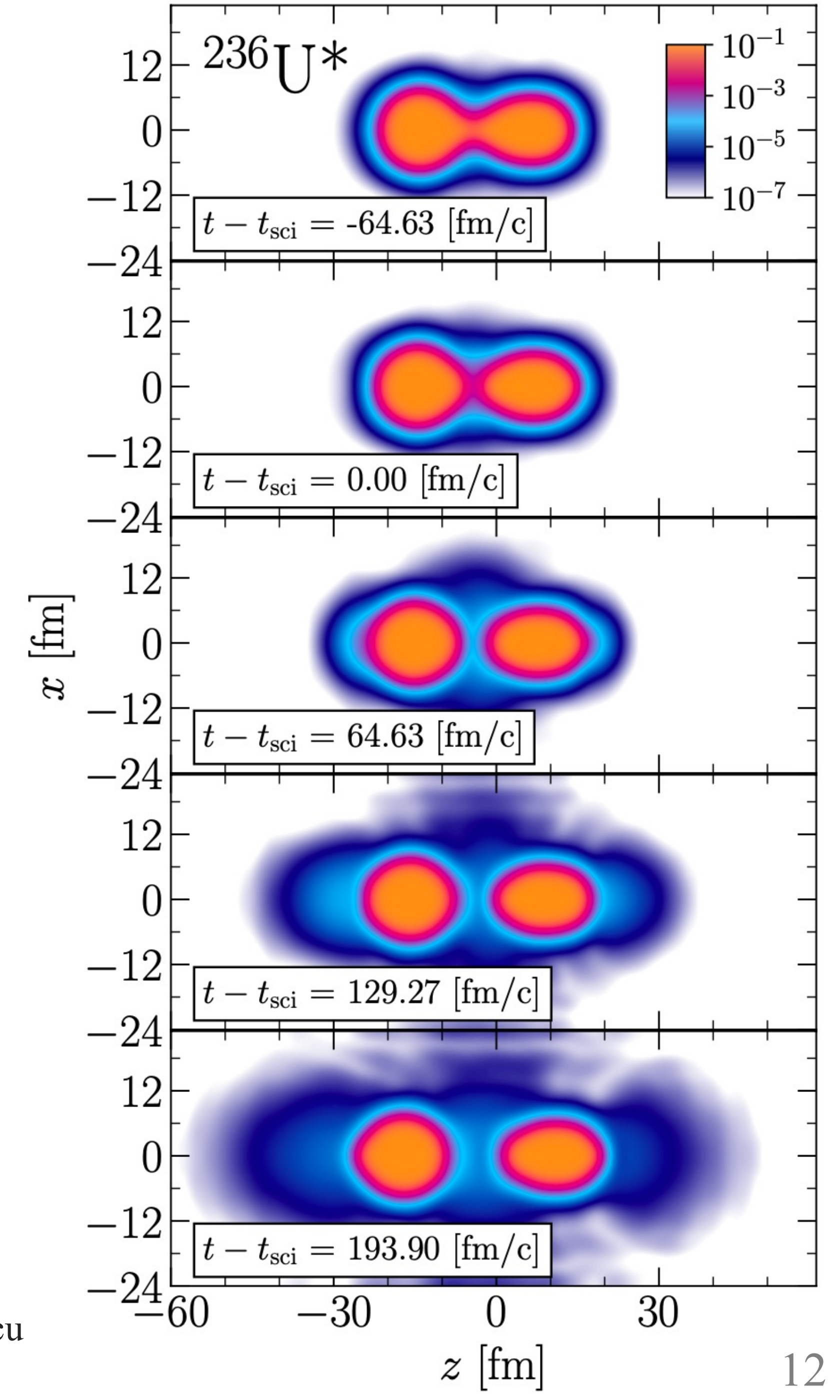
- SNs observed in all TDSLDA fission calculations to date.



Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Scission Neutrons (SNs)

- **Distinctive angular distribution, with roughly equal numbers of neutrons emitted perpendicular to axis and along fission axis.**
    - Differs from the prompt neutron angular distribution, thought to be emitted isotropically in the rest frame of each fragment.
    - SNs are released from an essentially stationary compound, hence unaffected by Coulomb acceleration
- **Same angular distribution observed for all nuclei and trajectories considered**: ^{235}U(n,f), ^{239}Pu(n,f), ^{252}Cf(sf)
- Numbers amount to 9-14% of total emitted neutrons during the fission process



Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Scission Neutrons (SNs)

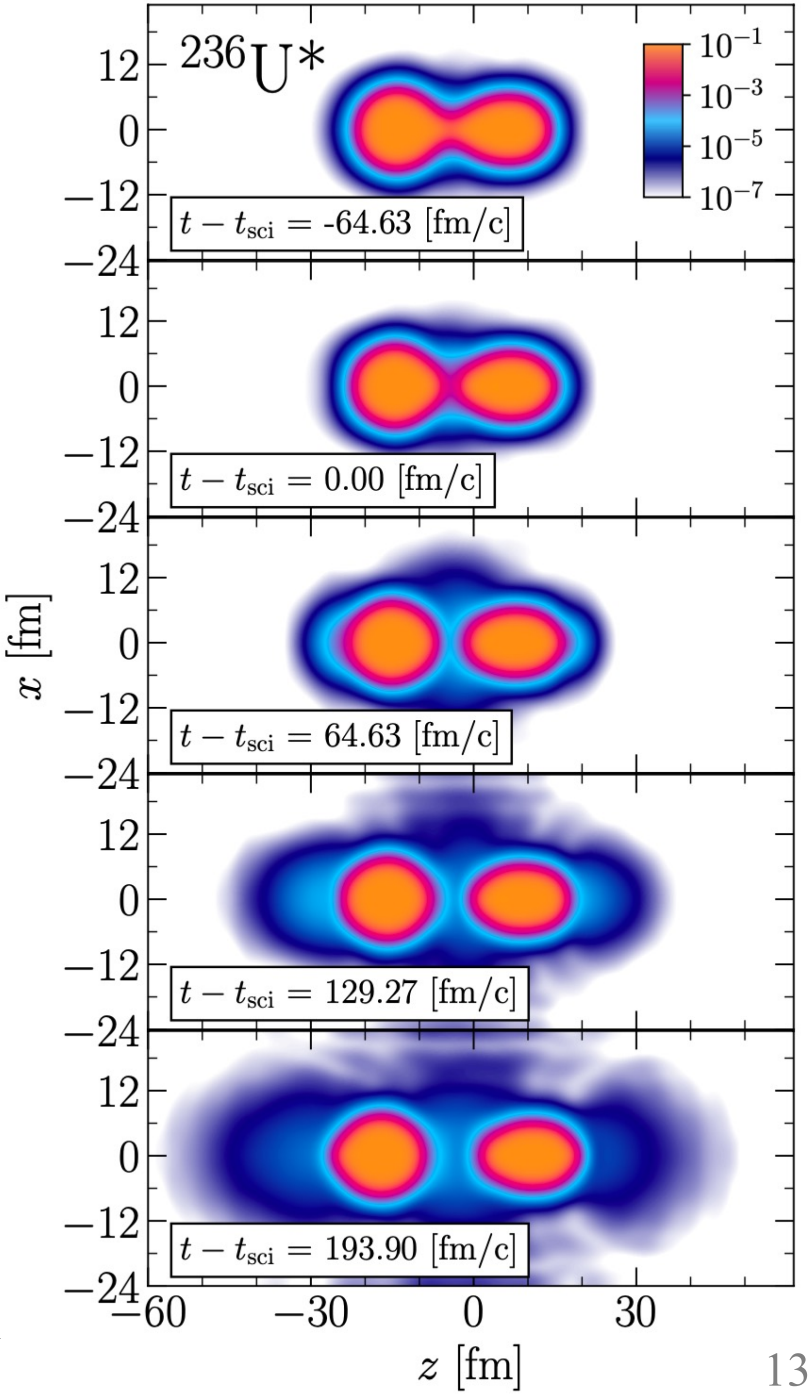
- SNs released during small interval while neck "heals" imperfectly after rupture.

- (So, Bohr and Wheeler's conjectured mechanism is wrong.)

- "Slingshot"/"catapult" mechanism (Mädler, 1985) responsible for longitudinal emission with slight delay
  - **reabsorption of neck into fragments pushes matter through the fragment and out the other side, with a delay.**

- **SNs velocity high enough when released that FFs will never catch them, meaning they escape to infinity and are in principle measurable.**

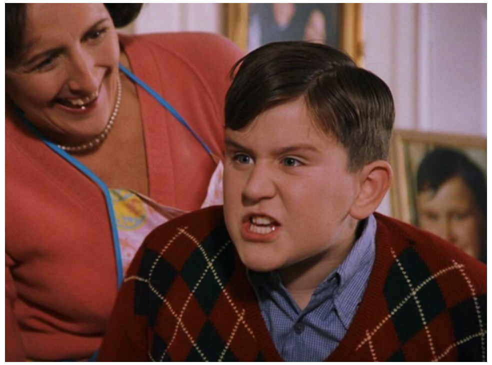
- Cloud of SNs is essentially non-interacting, so condensation into a third nucleus *appears* unlikely. (Note: Our formalism cannot describe condensation.)



Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

How many are there?

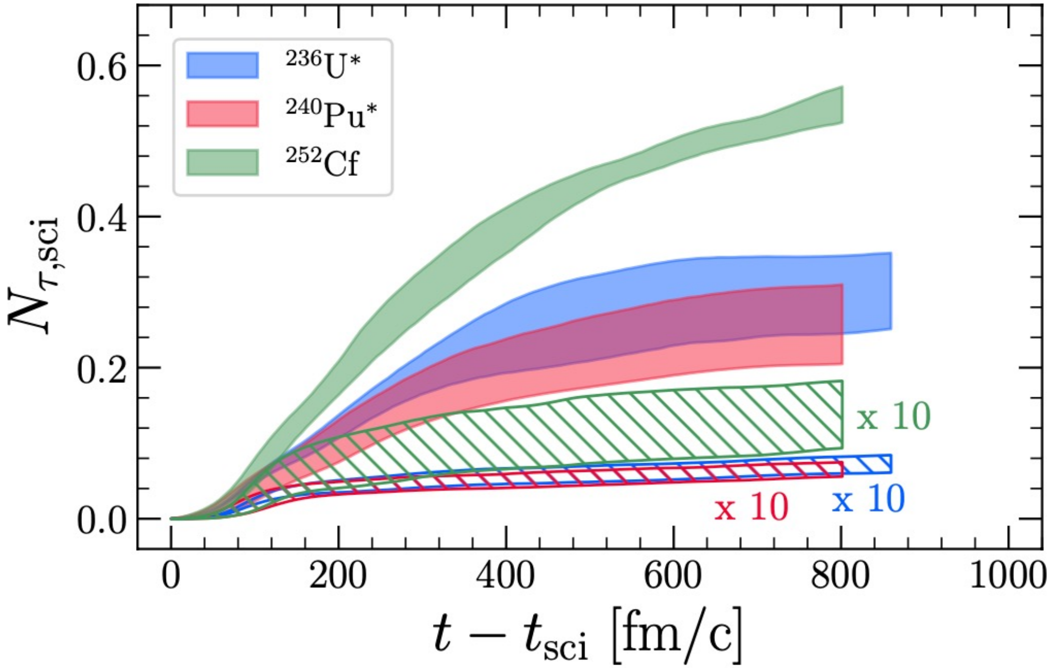
- Average number of emitted scission neutrons per fission event
  - ^{236}U: 0.30 ± 0.05
  - ^{240}Pu: 0.26 ± 0.05
  - ^{252}Cf: 0.55 ± 0.02

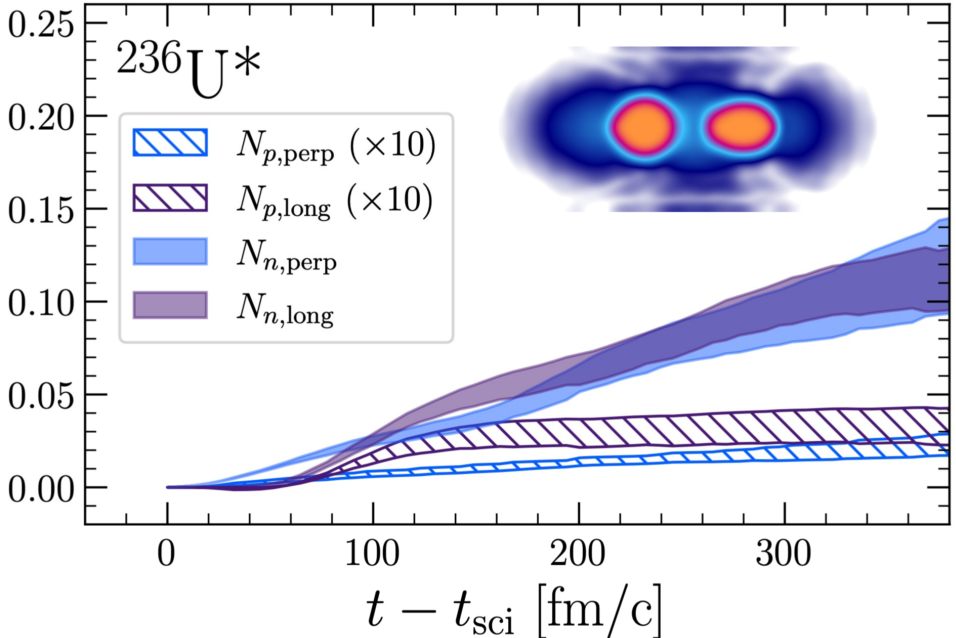


- Proton emission about 1/50th of neutron emission

- Some of the curves for $N(t)$ are still increasing, meaning the estimate that SNs constitute **9-14% of total emitted neutrons during the fission process is likely conservative**.

- **Roughly equal numbers emitted along fission axis and in a ring-shaped cloud perpendicular to the axis**.





Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

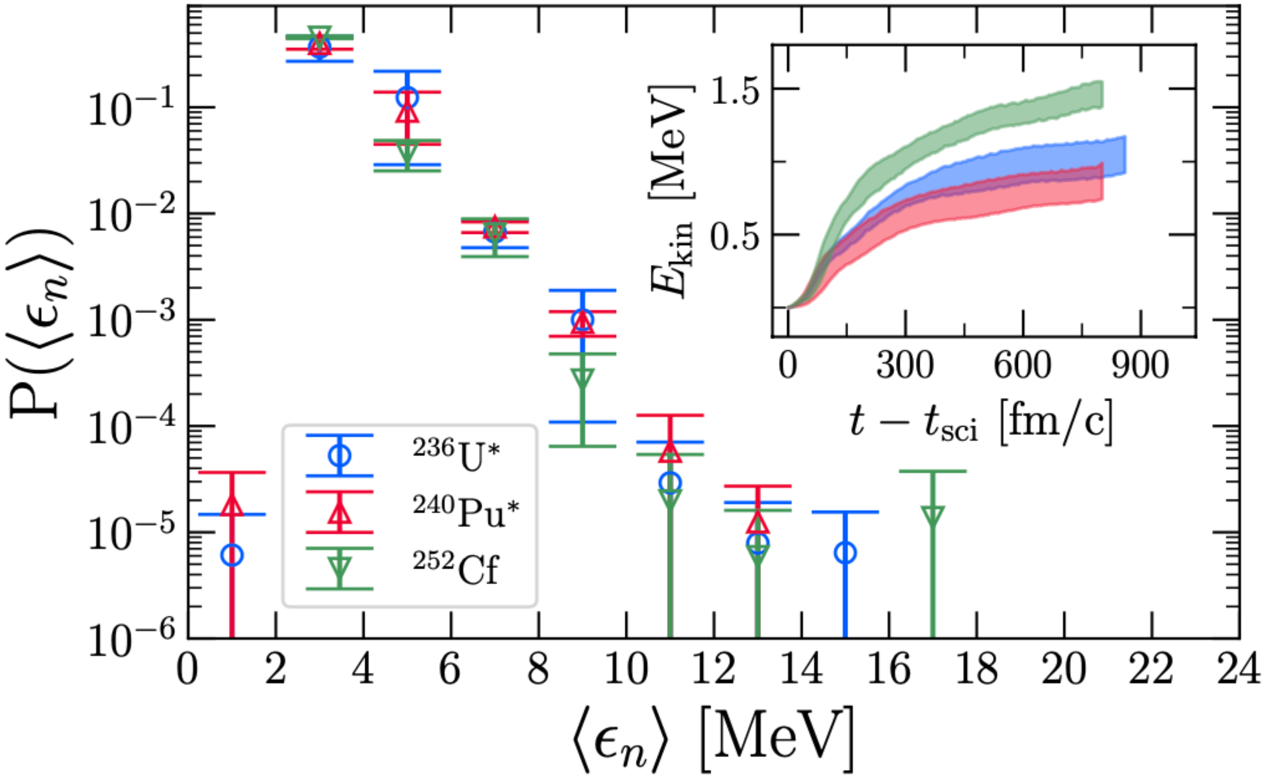
Kinetic Energy of Scission Neutrons

- Average KE per neutron for SNs
  - ^{236}U: 3.51 ± 0.25 MeV
  - ^{240}Pu: 3.42 ± 0.27 MeV
  - ^{252}Cf: 2.67 ± 0.24 MeV

- Kinetic energy distribution shows a small fraction of SNs carry up to 17 MeV of kinetic energy.

- **Potentially relevant for prompt fission neutron spectra**, where the high energy part underpredicted relative to experiment in leading statistical codes such as CGMF.

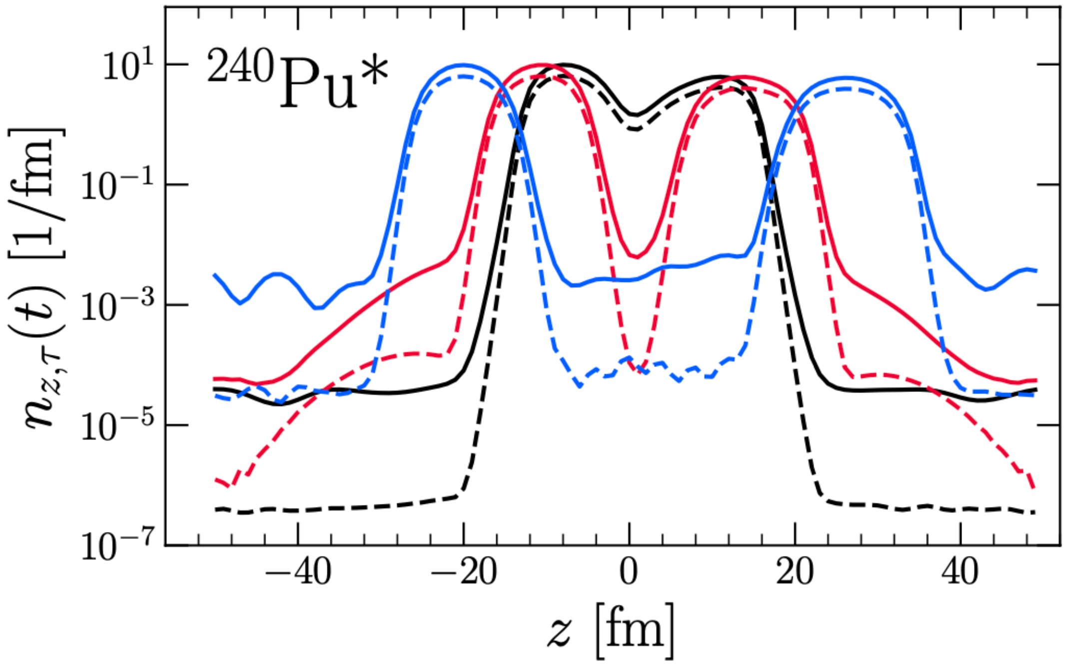
- **Evaporation of neutron by fully accelerated fragments cannot produce neutrons of this energy.**

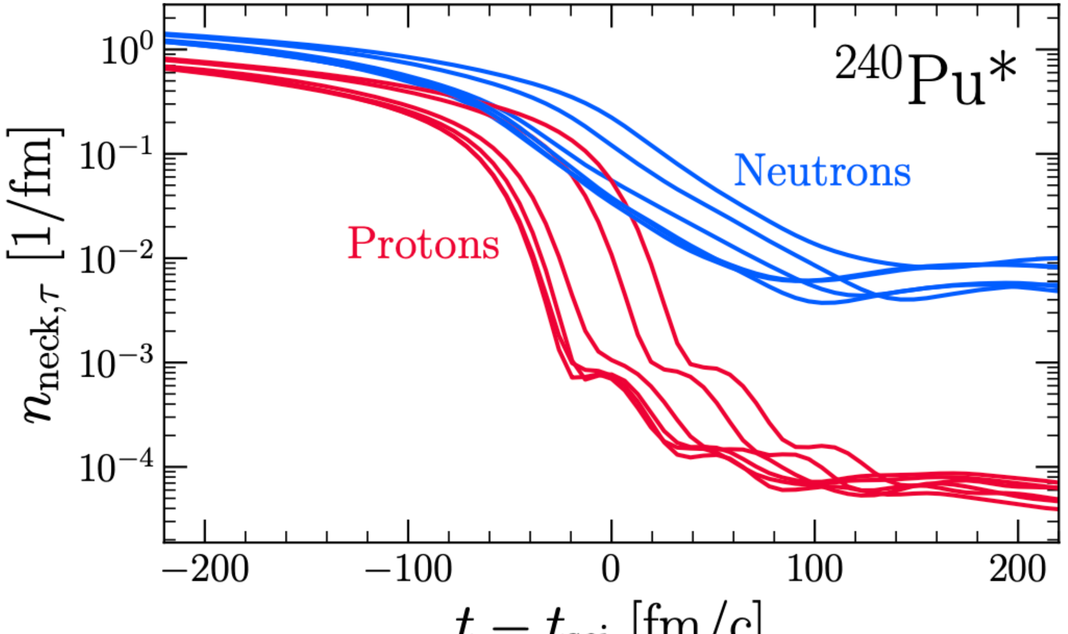


Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Dynamics of the Neck

- **Neck location determined early, near outer barrier, and does not move with time.**
  - Contradicts widely used phenomenological Brosa model, which assumes neck ruptures at random location.
- Once a critical neck diameter of ~3 fm is reached, nuclear surface can no longer withstand Coulomb repulsion between fragments, and neck ruptures.
- **Neck exhibits "universal"* dynamics during rupture**:
  - Different curves correspond to different initial deformations.
  - Rupture times are 35.0 ± 2.2 fm/c for neutrons and 15.3 ± 0.3 fm/c for protons.
  - Proton neck ruptures before neutron neck by 50-100 fm/c.
  - Time for fastest information to communicate between fragments would be ~160 fm/c.





Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Numerical Calculations

- **Largest simulation boxes ever considered** in order to follow emitted particles for as long as possible.

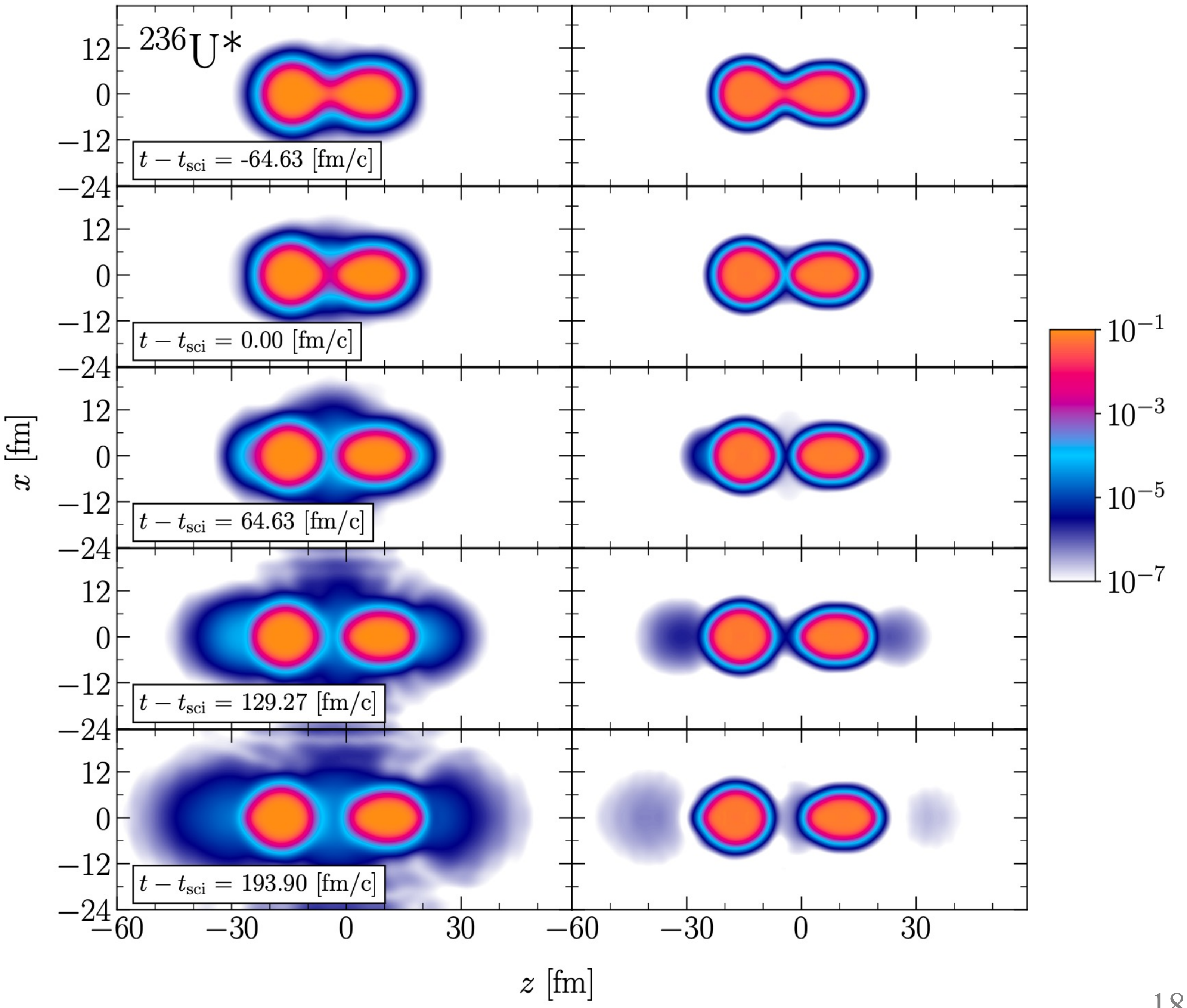
- **Enormous simulations required, 27,648 GPUs for 15 hours straight for a single trajectory!**
  - Used entirety of Summit supercomputer.
  - Required repeatedly diagonalizing a matrix of size 1.1M × 1.1M
  - 4.4M coupled, nonlinear, complex PDEs in 3+1D for 40,000 time steps
  - ~89 TB of new wave function data at each step
  - $\frac{\Delta E}{E(t=0)} < 5\times10^{-5}, \frac{\Delta N}{N(t=0)} < 10^{-9}$

Source: *Neck Rupture and Scission Neutrons in Nuclear Fission*, I. Abdurrahman, **M. Kafker**, A. Bulgac, I. Stetcu - Physical Review Letters, 2024

Image Source: https://www.olcf.ornl.gov/olcf-resources/compute-systems/summit/

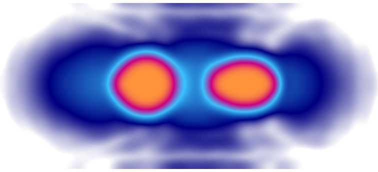
Scission Protons

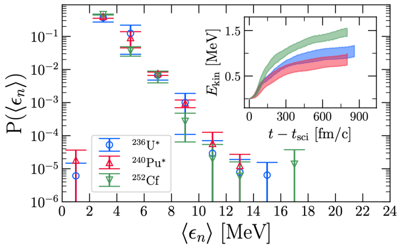
- Scission protons also predicted at 1/50th the level as the neutrons
- Primarily emitted longitudinally.
- This is a problem! Almost certainly not observed in experiments.
- Why might this be the case?
  - Neutron skin?
  - Lack of proton-neutron correlations?
  - Framework does not treat three-particle collisions, hence condensation.



Prospects for Experimental Detection

So, we have a prediction. How can we find out if we're right?





- **Distinctive angular distribution**:
  - In contrast to prompt neutrons evaporated from the hot fragments, and thus spherical in the rest from of each fragment, SN cloud has distinctive non-spherical shape in the lab frame.
  - Would require simultaneous determination of the fission axis, hence fission fragment detectors as well as neutron detectors.
  - Tricky measurement, as it requires several kinds of detectors operating in synchrony.
  - Several experimentalists interested in this: Grisha Rogachev (TAMU), Lee Sobotka (Wash U)
  - But it's early days.

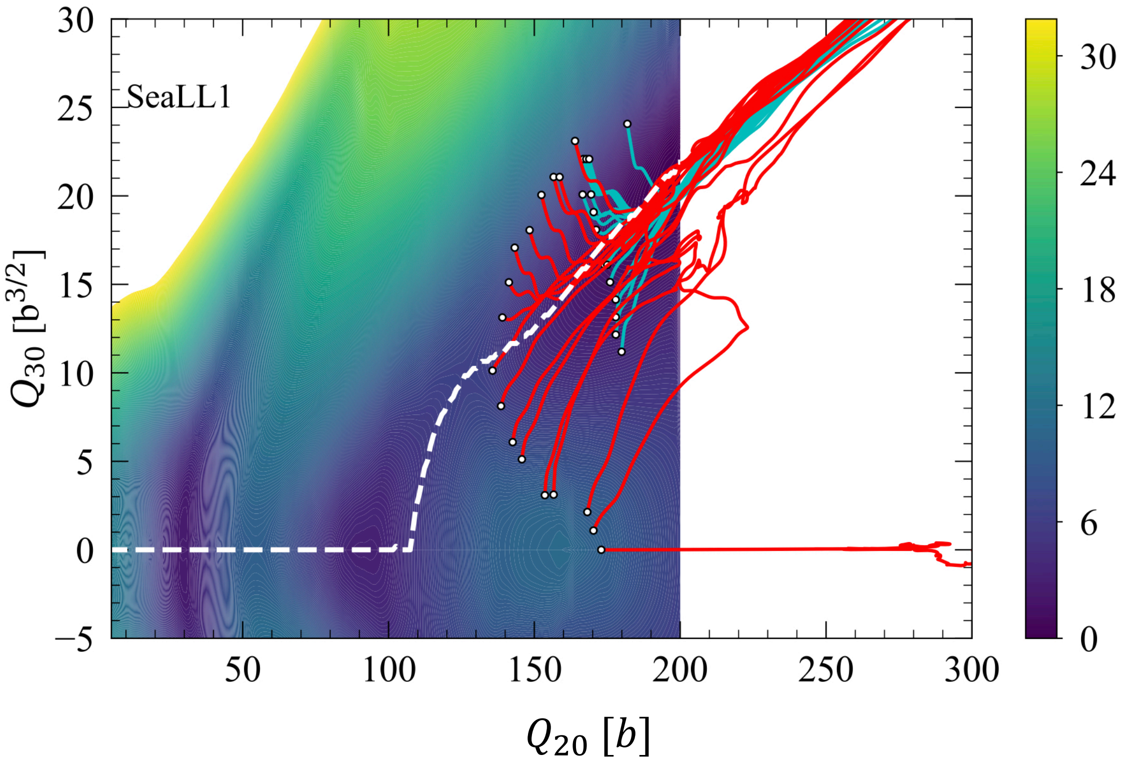
- **High energy neutrons:**
  - Tail of kinetic energy per neutron distribution reveals a small fraction of neutrons emerge with very high kinetic energy.
  - Such high energy neutrons would not be seen from evaporation neutrons from the hot FFs
  - <u>There is experimental evidence for fission neutrons up to 30 MeV, with no other proposed explanation</u>.
- **Scission protons?** Phys. Rev. C **109**, 054616 (2024)
  - Likely would already have been seen…

An experimental detection would offer a direct window into the fastest processes in fission!

Future Directions

- Scission protons—what's the deal?
  - The neutron skin is controlled by the density dependence of symmetry energy. There is room within the parameters of the SeaLL1 functional to try to match the neutron skin thickness measured in experiment.

- Beyond density functional theory: The Enhanced Generator Coordinate Method (A. Bulgac, https://arxiv.org/pdf/2408.02173)
  - Although TDDFT is quantum mechanical, the collective motion is semi-classical in nature.
  - This new approach would allow for mixing, interference and entanglement of many trajectories.
  - It would thus incorporate proton-neutron correlations, beyond-mean-field effects, and **more accurate calculation of scission neutron properties**.



Thank you for listening!

Questions?