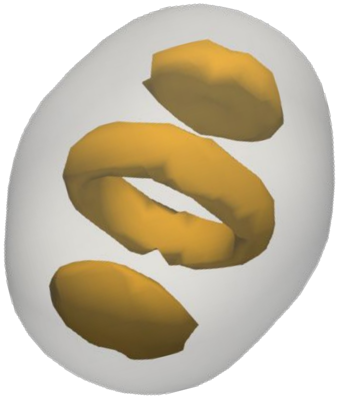
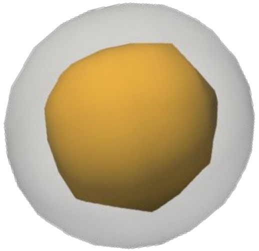
Prospects for Discovery In the Dynamics of Heavy Nuclei and Nuclear Data

Kyle Godbey

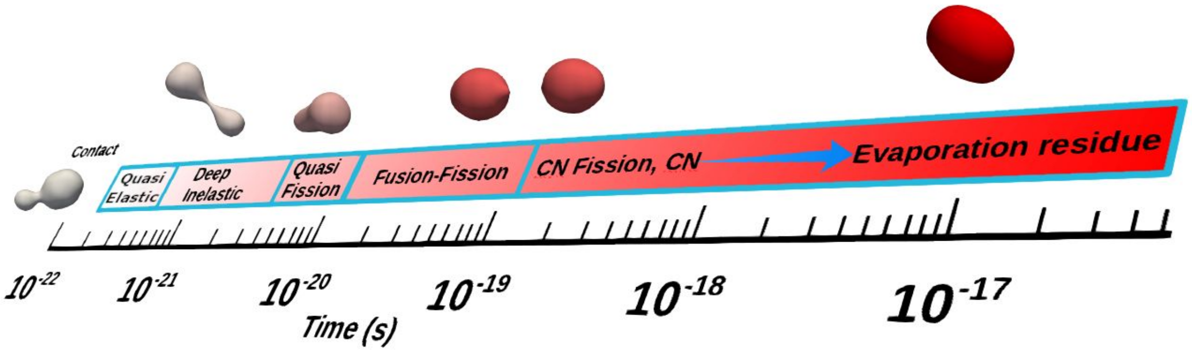


Slides with videos:
https://docs.google.com/presentation/d/1W4TUEMdGKR4zQ5CsnKVykWttvaNX9aRiR_eOjN8vC-A/edit?usp=sharing



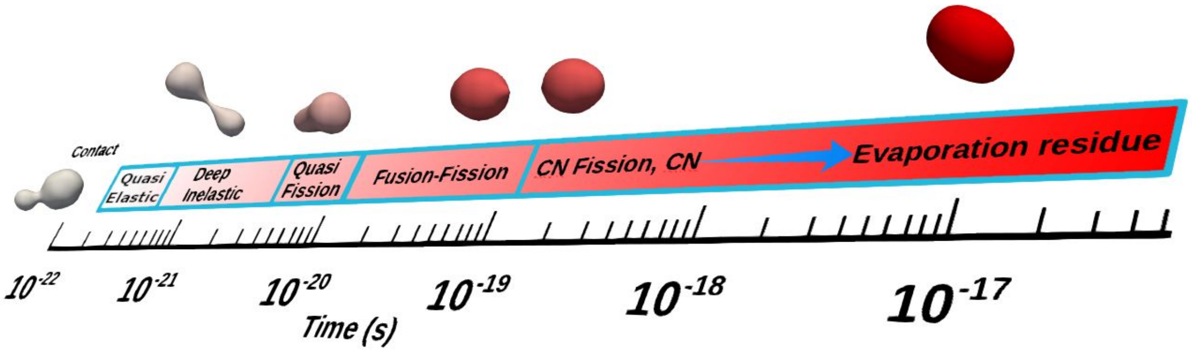
S@INT | S@INT Seminar
October 10, 2023

Heavy-Ion Dynamics

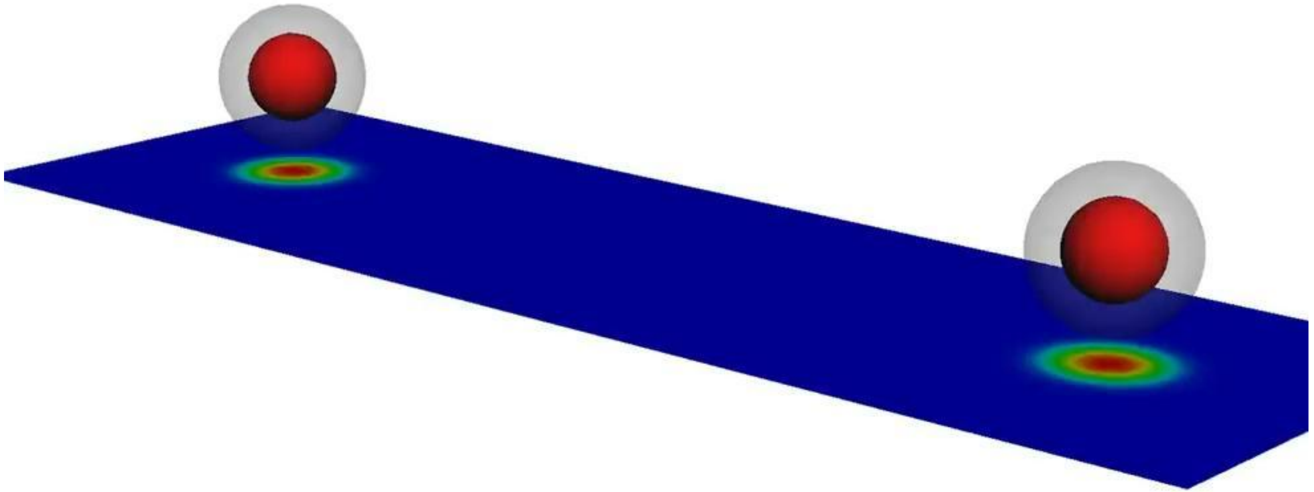


The community is in a good place through the capabilities provided by ARUNA, ATLAS, and FRIB

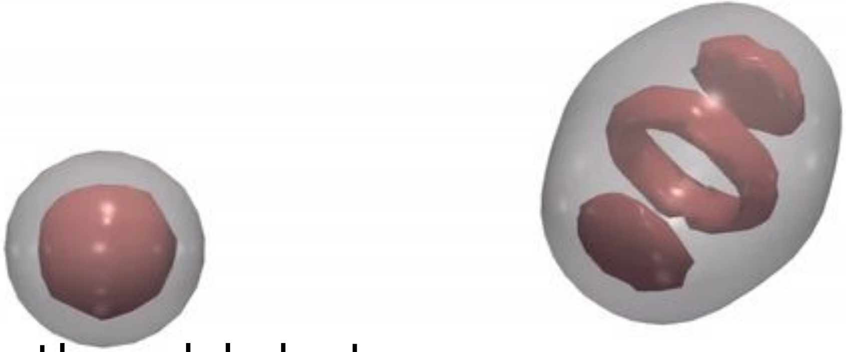
Real-Time Dynamics



Time-dependent, microscopic theories offer a rich depiction of the many complicated things nuclei might do during a reaction



K. Godbey, C Simenel, and A. S. Umar, Absence of hindrance in microscopic 12C + 12C fusion study, Phys. Rev. C 100, 024619 (2019)



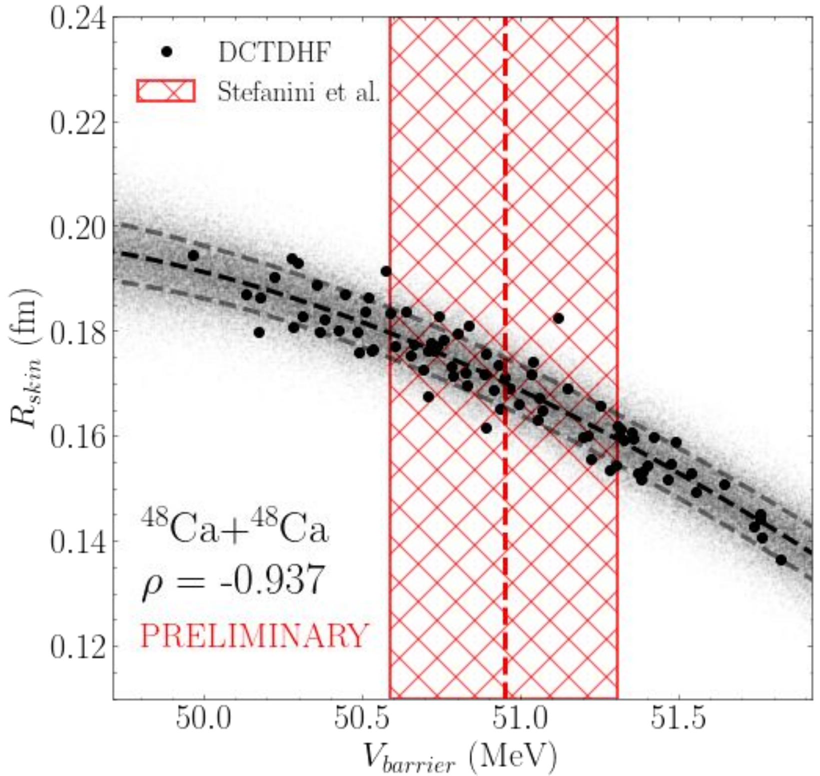
Nuclei are more than blobs!

-> Neutron skins
-> Intrinsic deformations
-> Clustering effects

Correlations Between Structure and Reactions

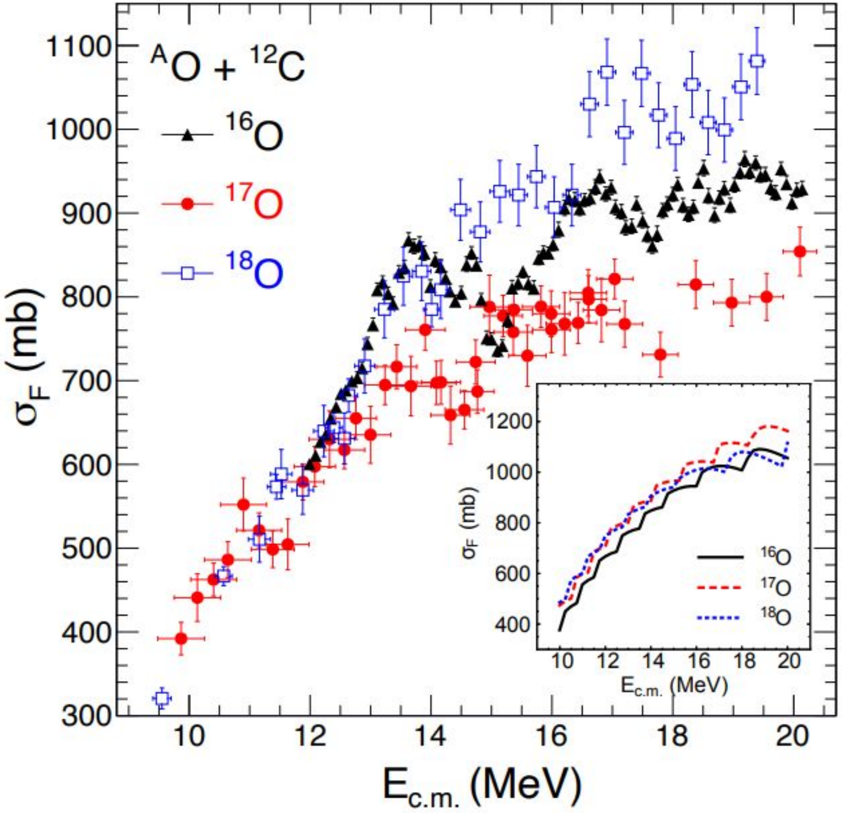
$V_{barrier}$ is a quantity extracted from fusion cross sections

Nothing precludes a comparison to cross sections directly



Structures in Reaction Data

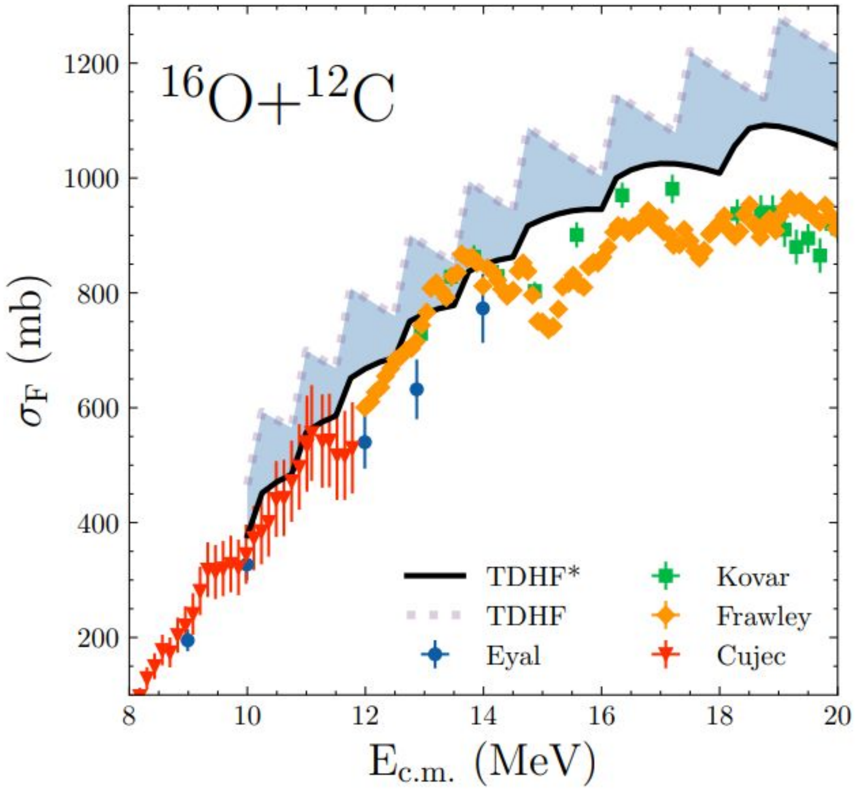
Consider fusion cross sections for a chain of oxygen isotopes and carbon



R. T. deSouza, K. Godbey, S. Hudan, W. Nazarewicz, In search of beyond mean-field signatures in heavy-ion fusion reactions. (submitted) (2023)

Structures in Reaction Data

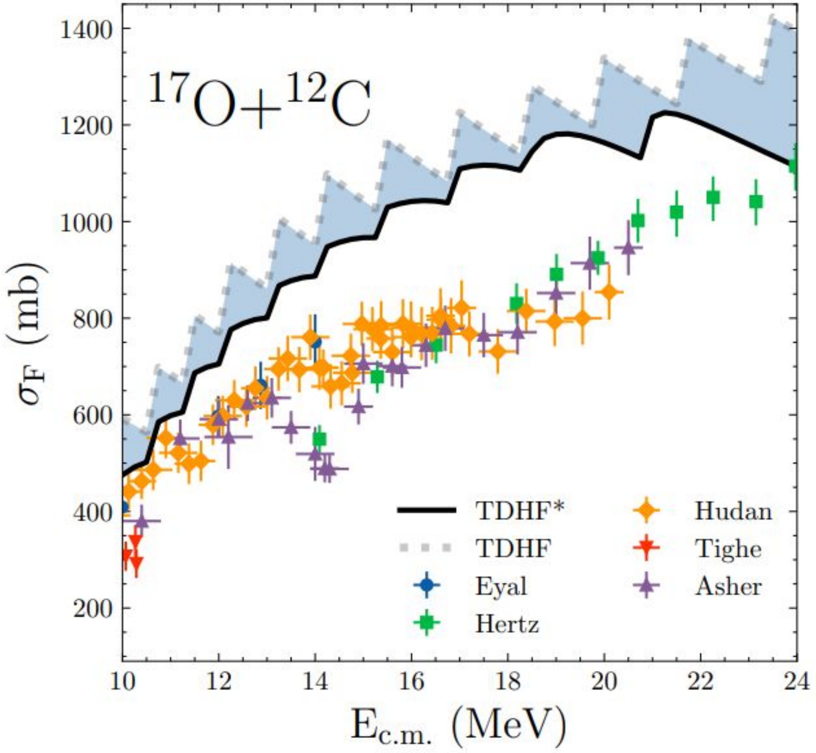
L-wave ratcheting is present in both the theory and experiment, but other features are missing



R. T. deSouza, K. Godbey, S. Hudan, W. Nazarewicz, In search of beyond mean-field signatures in heavy-ion fusion reactions. (submitted) (2023)

Structures in Reaction Data

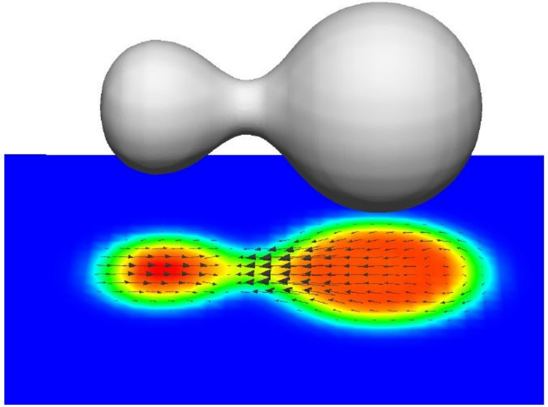
L-wave ratcheting is present in both the theory and experiment, but other features are missing



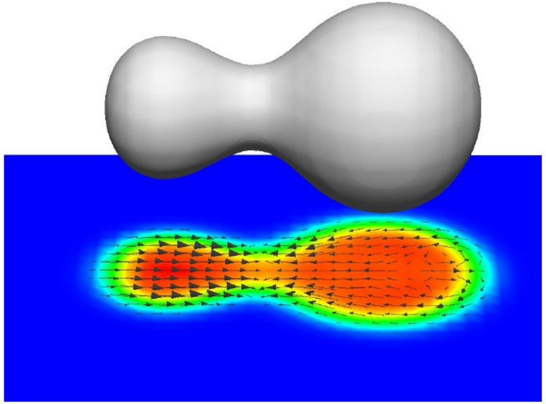
R. T. deSouza, K. Godbey, S. Hudan, W. Nazarewicz, In search of beyond mean-field signatures in heavy-ion fusion reactions. (submitted) (2023)

Transfer and Equilibration too!

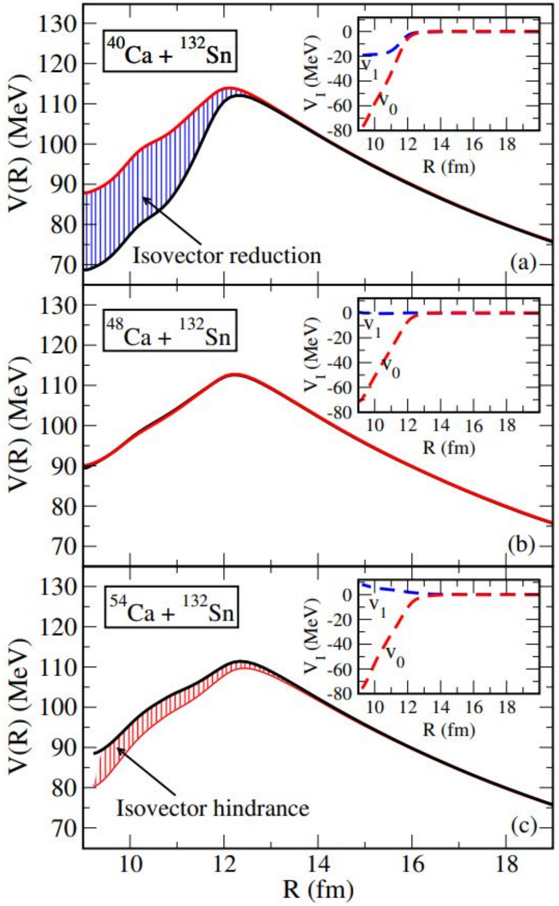
40Ca + 132Sn | **48Ca + 132Sn**



transfer

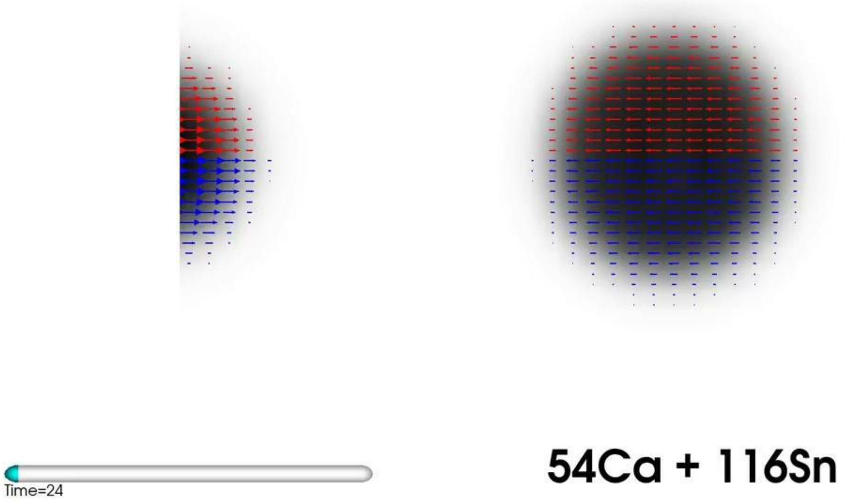


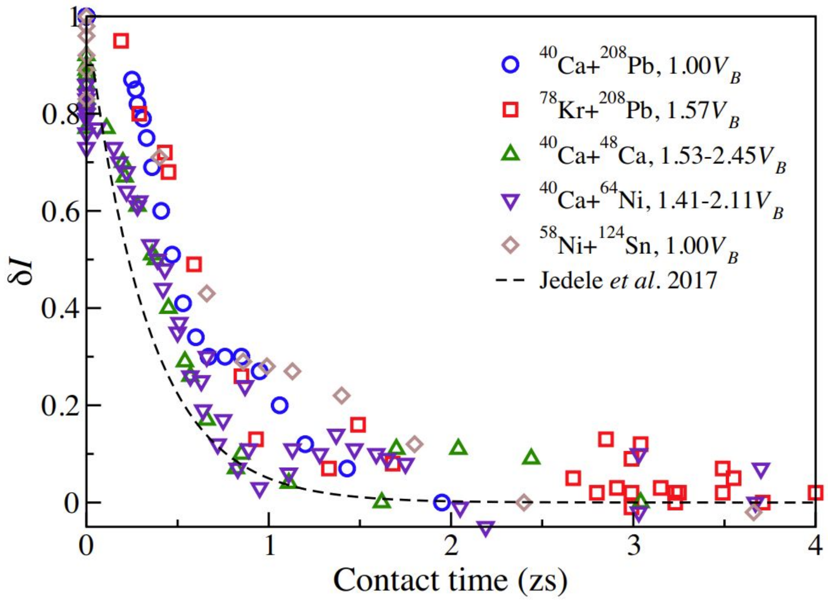
No net transfer



K. Godbey, A. S. Umar, and C. Simenel, “Dependence of fusion on isospin dynamics”, Phys. Rev. C 95, 011601 (Rapid Communication) (2017).

Transfer and Equilibration too!





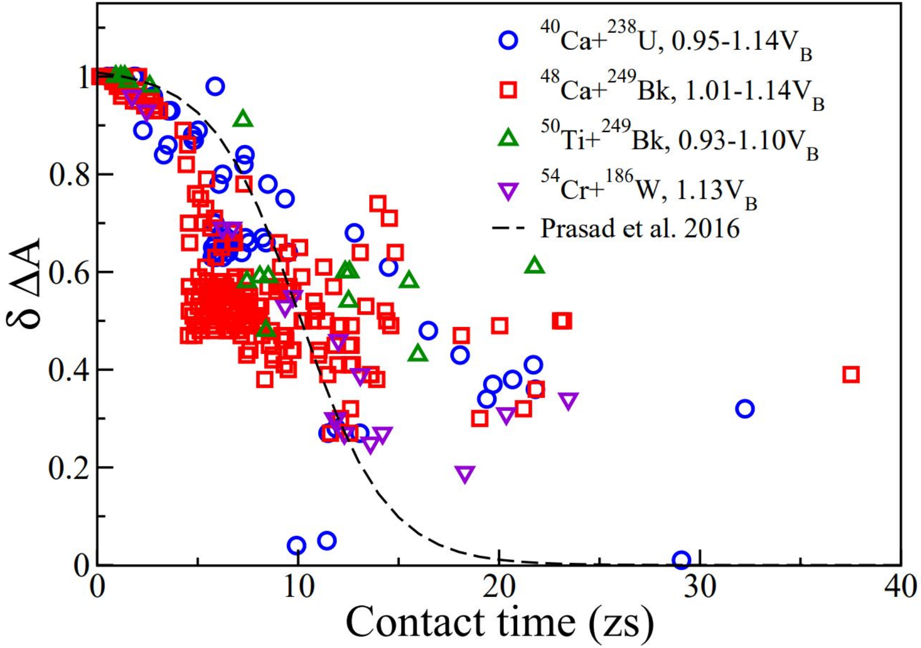
C. Simenel, K. Godbey, and A. S. Umar, Timescales of Quantum Equilibration, Dissipation and Fluctuation in Nuclear Collisions, Phys. Rev. Lett. 124, 212504 (2020)

Transfer and Equilibration too!

- Equilibration of the mass difference between fragments

- Relatively slow!

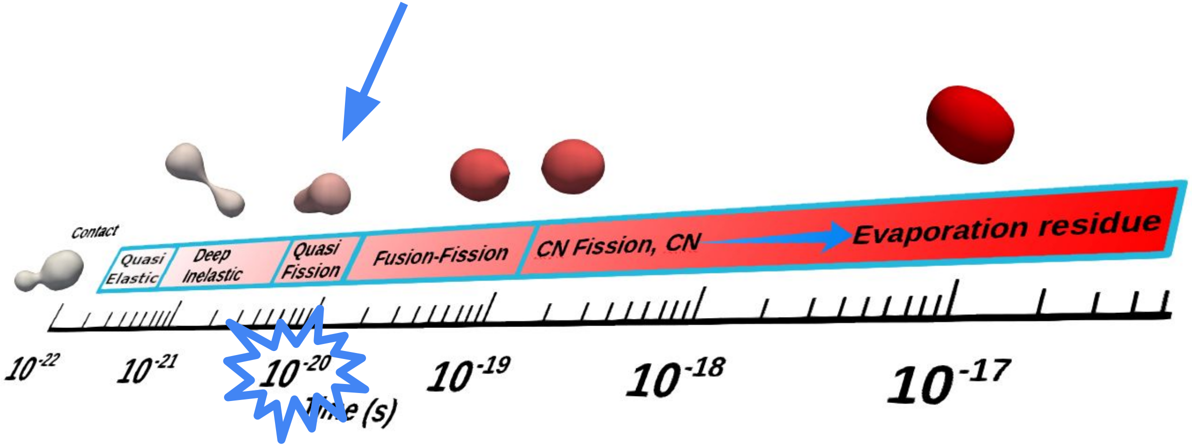
  Equilibration time ~ 10-20 zs



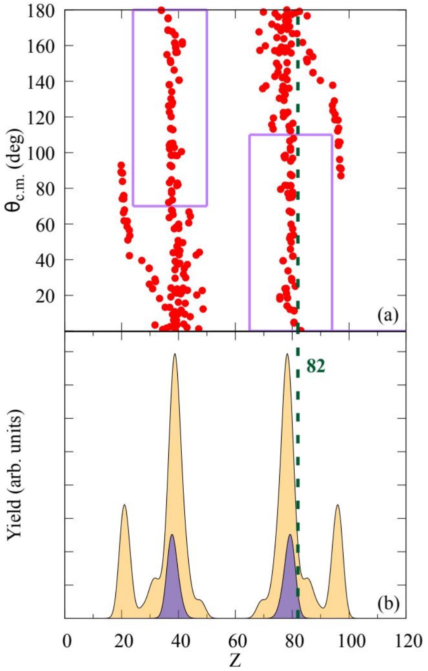
C. Simenel, K. Godbey, and A. S. Umar, Timescales of Quantum Equilibration, Dissipation and Fluctuation in Nuclear Collisions, Phys. Rev. Lett. 124, 212504 (2020)

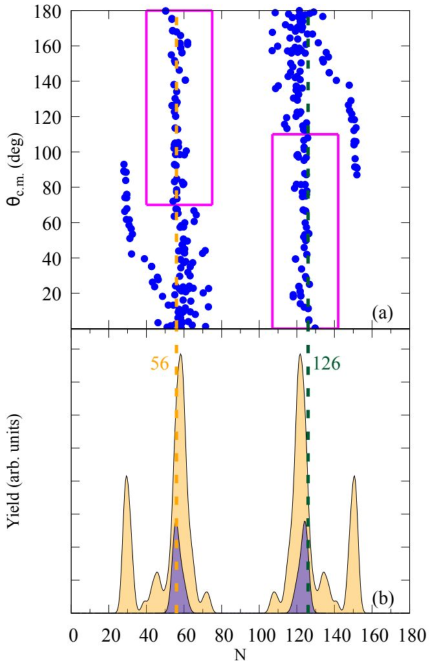
Introducing Quasifission

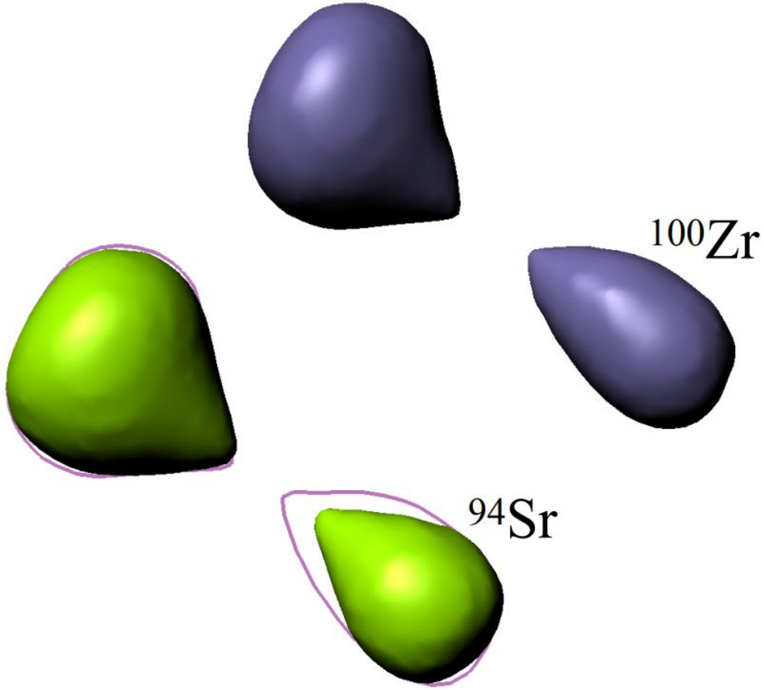
That's 10s of zeptoseconds!



Deformed Shell Effects in Quasifission







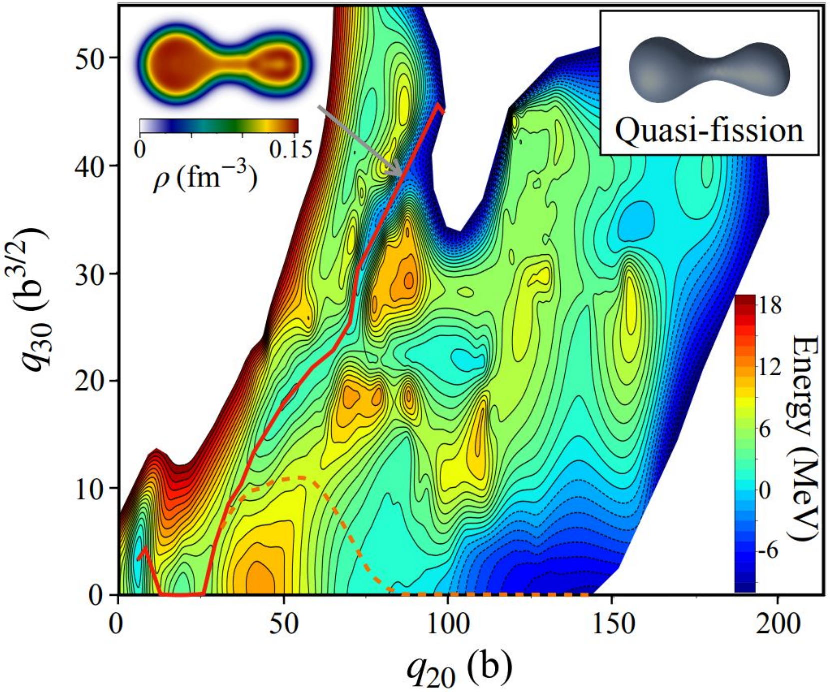
K. Godbey, A. S. Umar, and C. Simenel, "Deformed shell effects in 48Ca+249Bk quasifission fragments", Phys. Rev. C 100, 024610 (2019).

Quasifission as a Probe for Fission

Very similar shapes and dynamics are indeed seen in QF and fission, but to what extent?

Two excellent candidate systems to test/explore this:

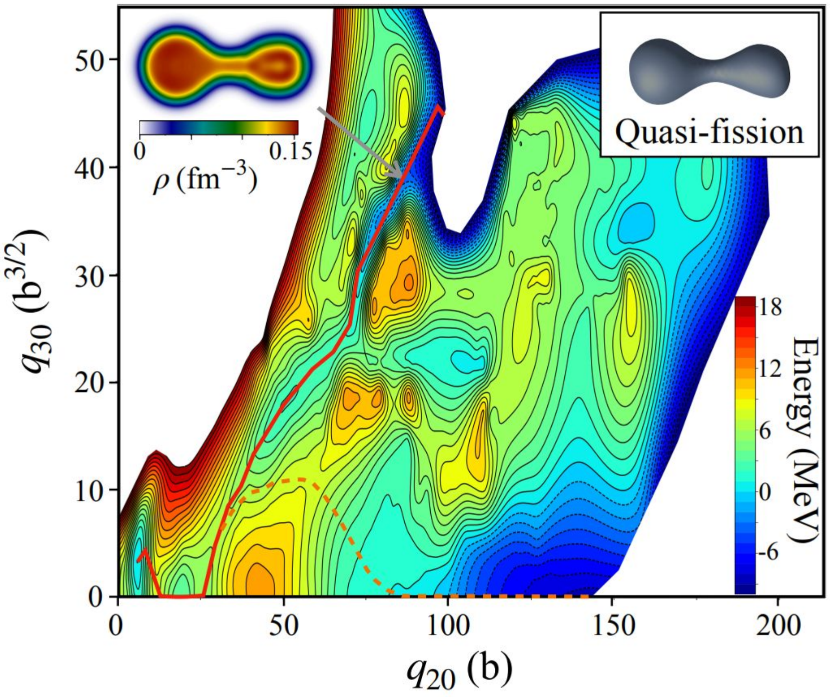
^{48,49,50}Ca + ^{176}Yb -> Some QF
^{16,17,18}O + ^{208}Pb -> No QF



C. Simenel, P. McGlynn, A. S. Umar, and K. Godbey, “Comparison of fission and quasi-fission modes”, Physics Letters B 822, 136648 (2021).

Quasifission as a Probe for Fission

Quasifission as a surrogate for fission can be instrumental near the dripline, particularly in heavy nuclei



C. Simenel, P. McGlynn, A. S. Umar, and K. Godbey, “Comparison of fission and quasi-fission modes”, Physics Letters B 822, 136648 (2021).

Enabling Progress

Explosion of interest in principled uncertainty quantification across nuclear physics in recent years as well as continued investment in novel computational paradigms

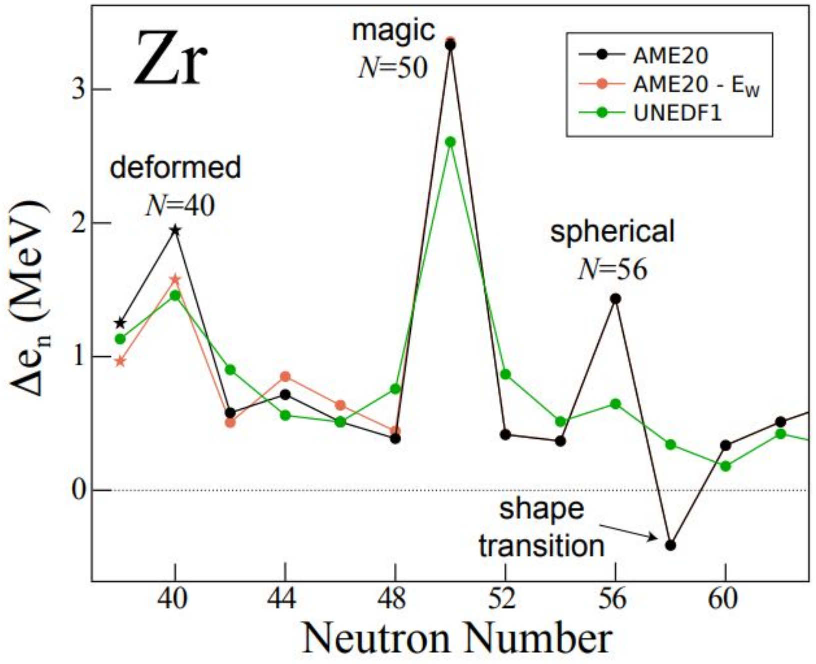
Now we can leverage that interest in collaboration with applied mathematicians, statisticians, and computer scientists

Going Data Mining

There is a lot of published data in nuclear physics going back many decades – let's extract some insights!

With respect to masses, one can consider mass filters such as:

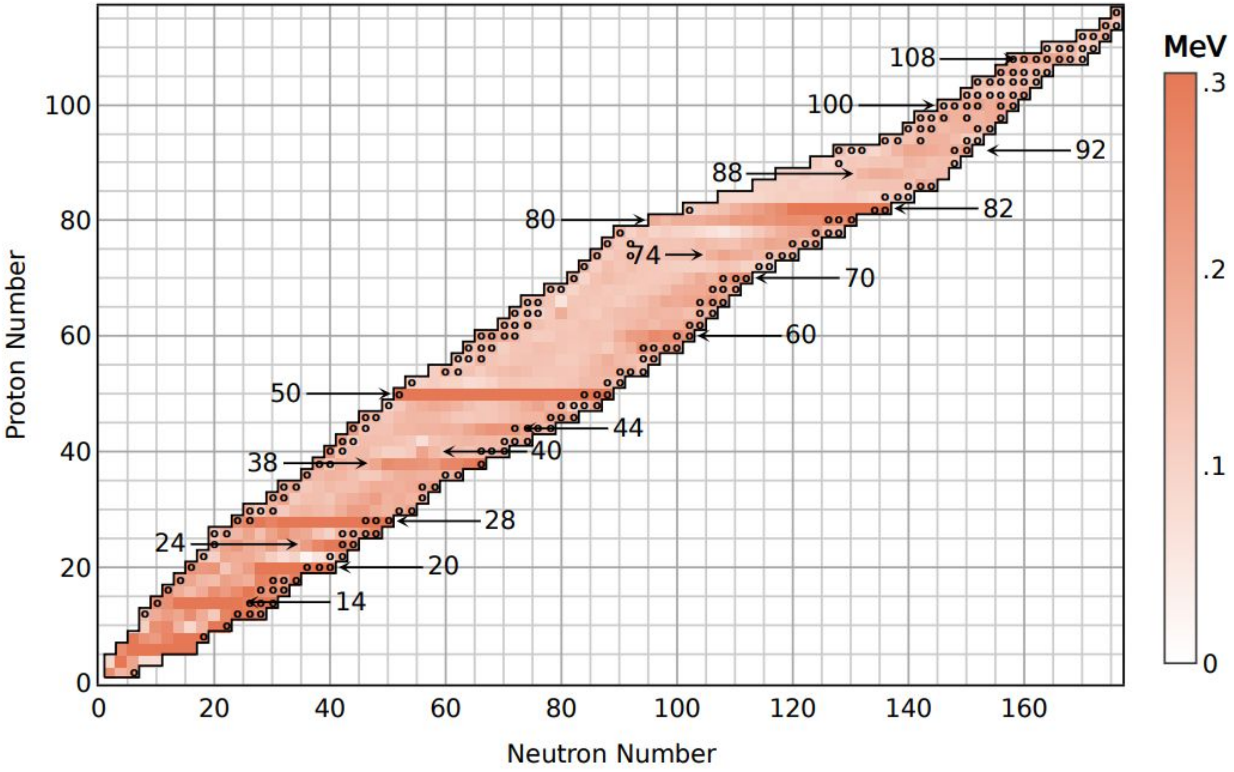
$$\Delta e_n(N = 2k, Z) = S_n(N, Z) - S_n(N+2, Z)$$



L. Buskirk, K. Godbey, W. Nazarewicz, W. Satula, Nucleonic Shells and Nuclear Masses, (submitted) (2023).

Going Data Mining

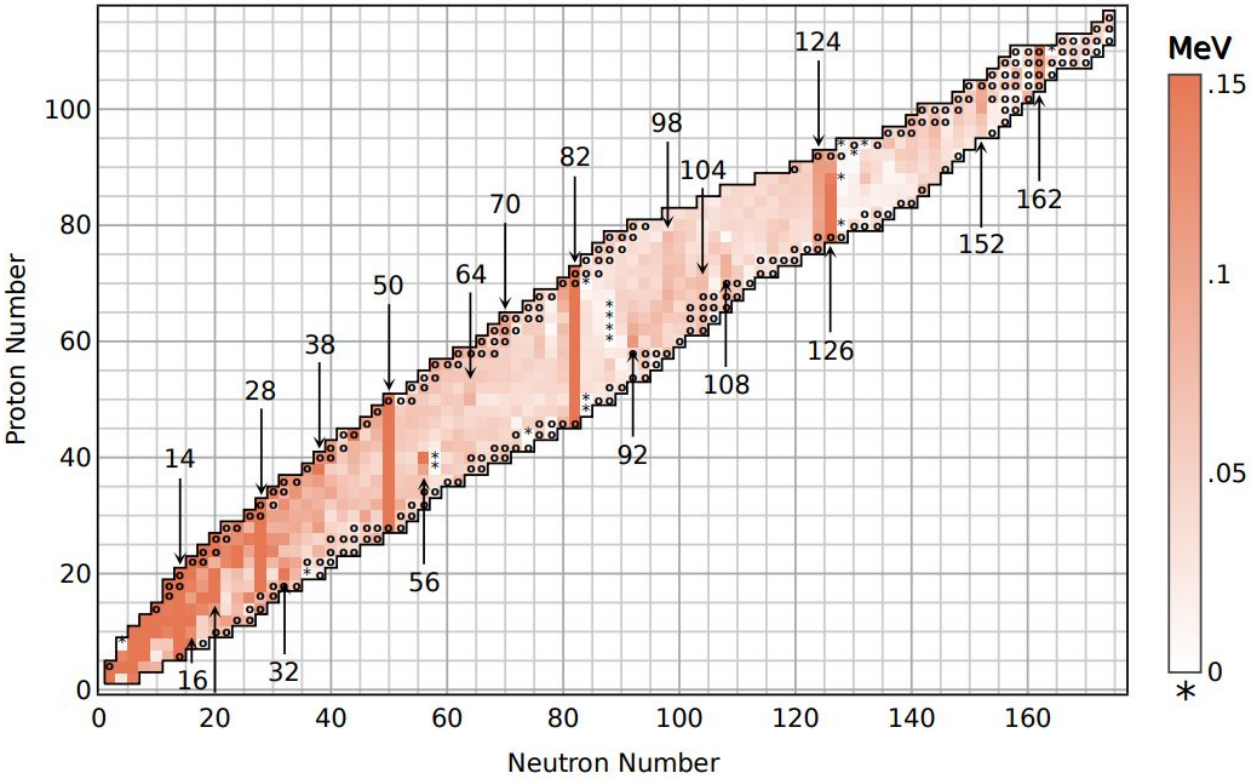
$$\Delta\tilde{e}_p$$



L. Buskirk, K. Godbey, W. Nazarewicz, W. Satula, Nucleonic Shells and Nuclear Masses, (submitted) (2023).

Going Data Mining

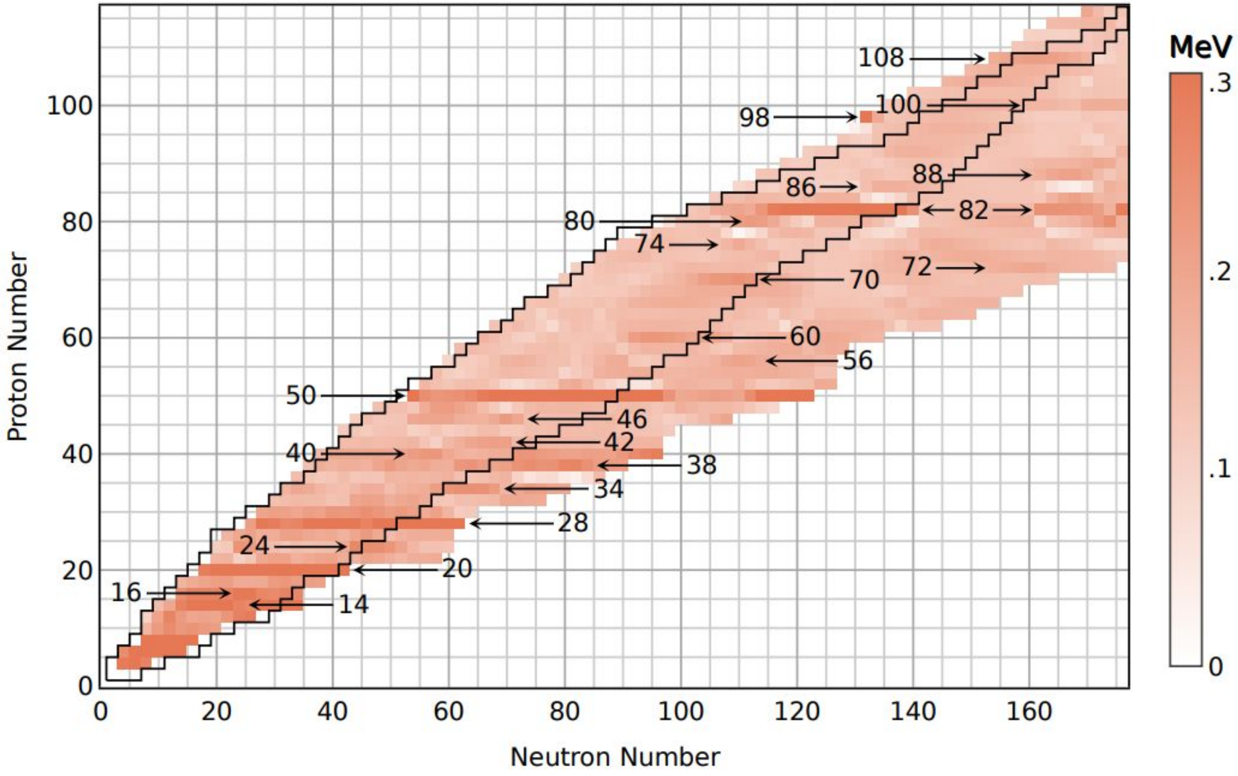
$\Delta\tilde{e}_n$



L. Buskirk, K. Godbey, W. Nazarewicz, W. Satula, Nucleonic Shells and Nuclear Masses, (submitted) (2023).

Going Data Mining

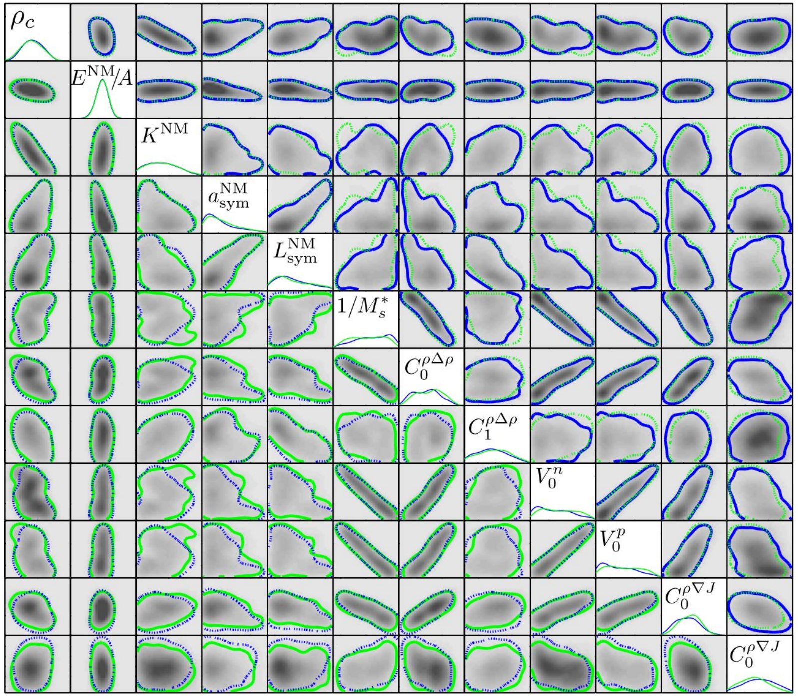
$$\Delta\tilde{e}_p$$



L. Buskirk, K. Godbey, W. Nazarewicz, W. Satula, Nucleonic Shells and Nuclear Masses, (submitted) (2023).

L. Buskirk, K. Godbey, W. Nazarewicz, W. Satula, Nucleonic Shells and Nuclear Masses, (submitted) (2023).

Reproducibility and Accessibility



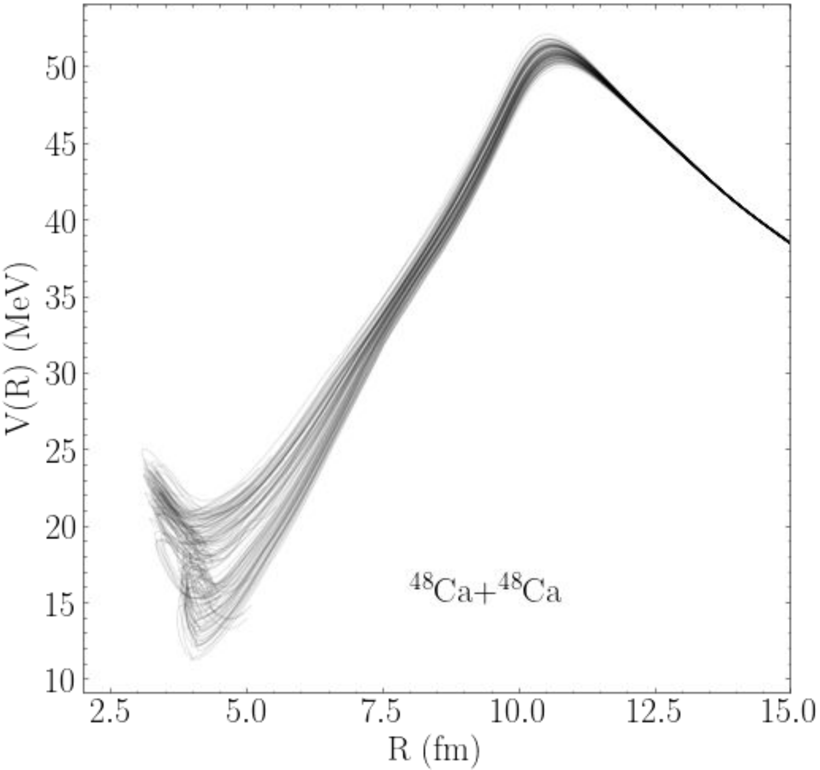


Image Credit:
J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz, Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements, Phys. Rev. Lett.114, 122501 (2015).

Reproducibility and Accessibility

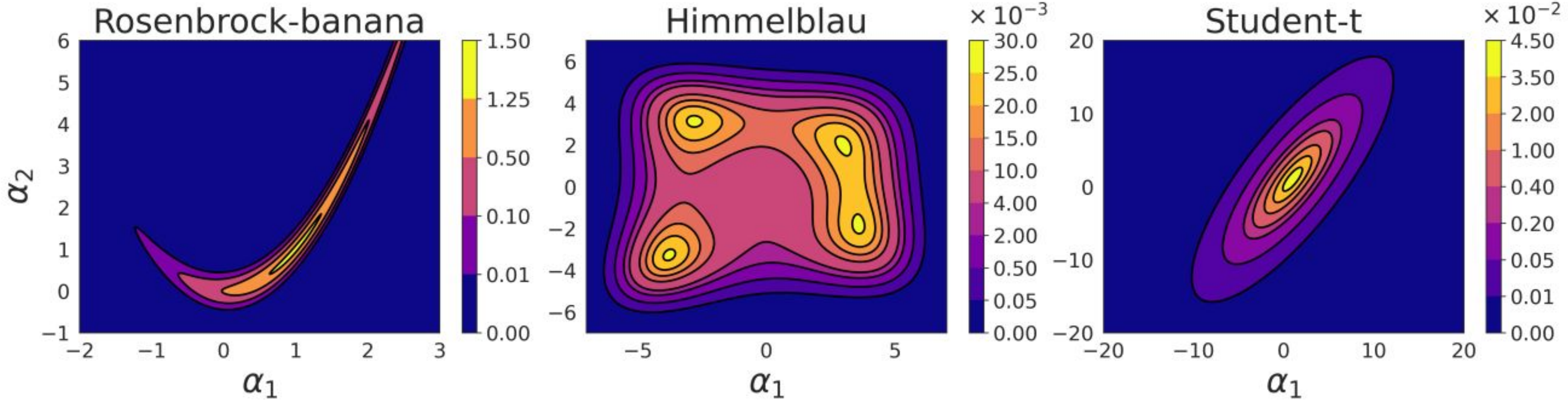
A few challenges include:

- Agility in the face of new data
- Efficiency of calibration
- Distribution of Bayesian posteriors (not just samples!)
- Traceability and reproducibility of results

Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

Reproducibility and Accessibility

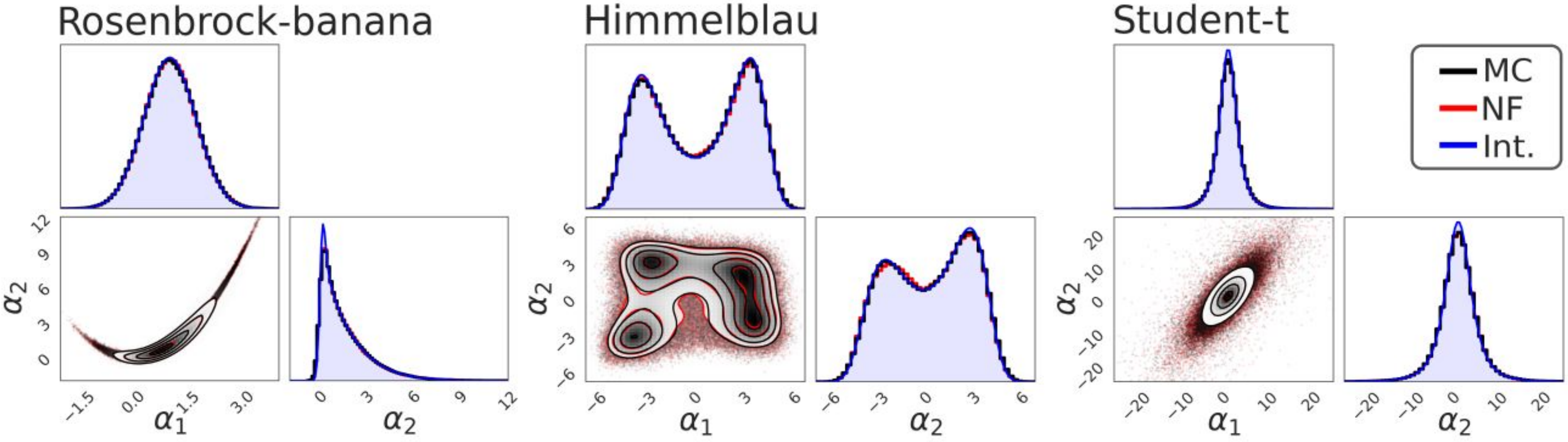
Our approach: use an ML approach to learn normalizing flows for the high-dimensional posterior distributions



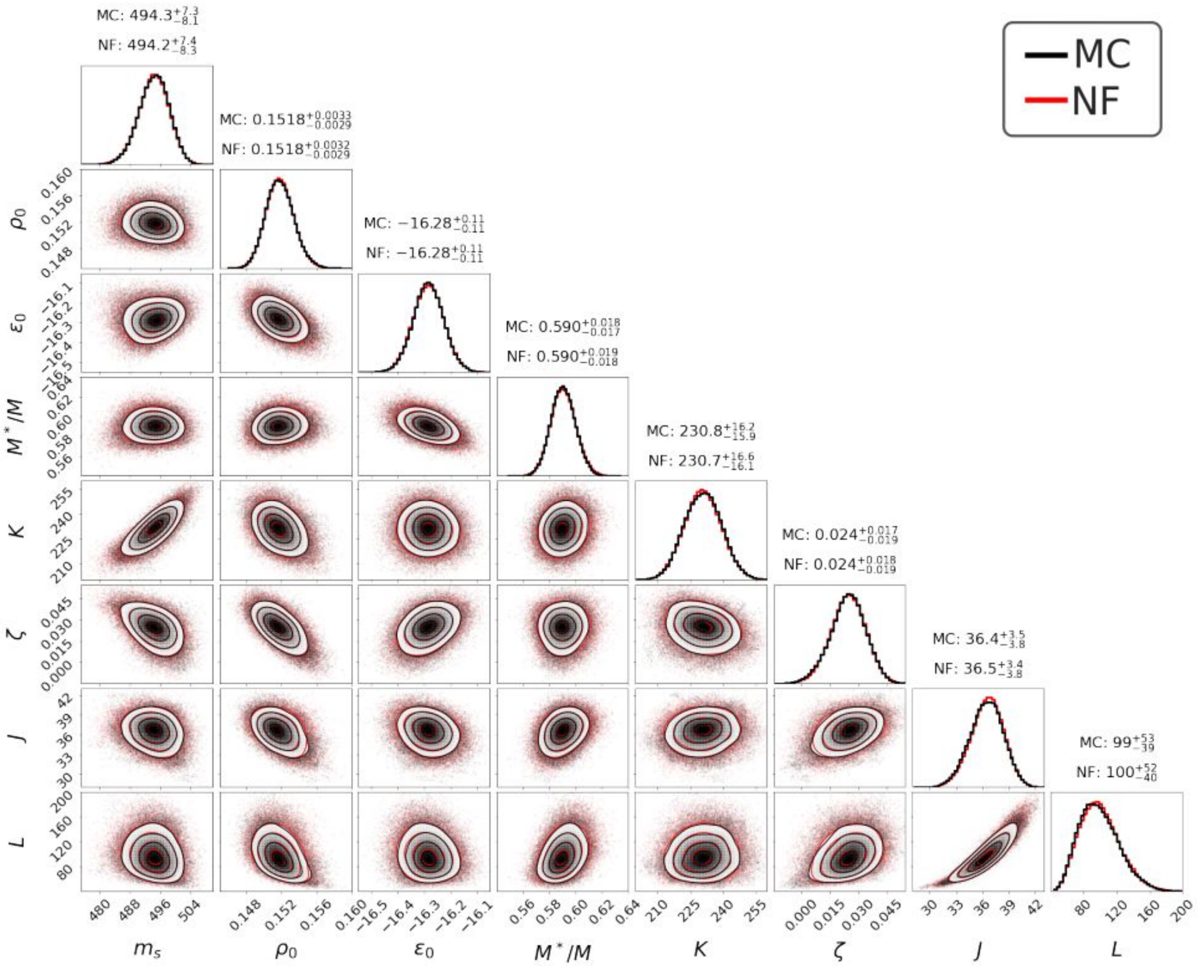
Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

Reproducibility and Accessibility

Our approach: use an ML approach to learn normalizing flows for the high-dimensional posterior distributions



Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

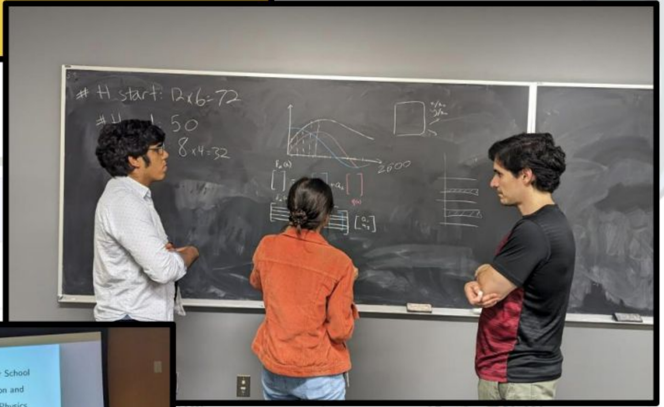


Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

https://github.com/ascsn/2023-FRIB-TA-Summer-School



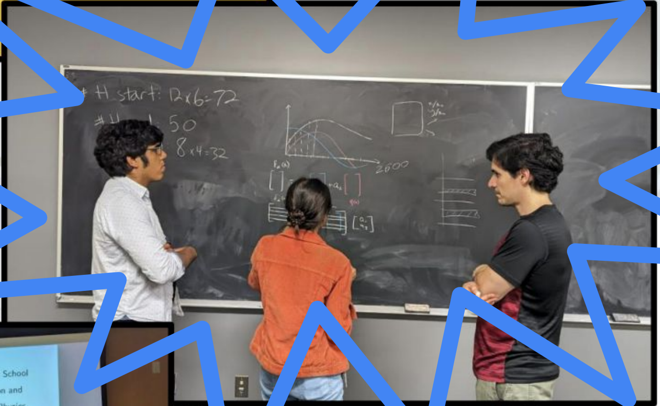
~60 participants spanning a wide audience

Slide from Pablo Giuliani

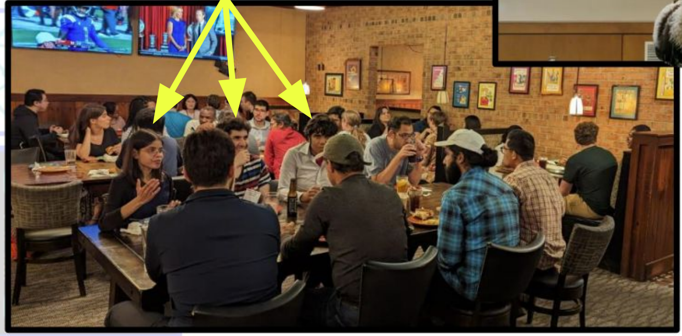
FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

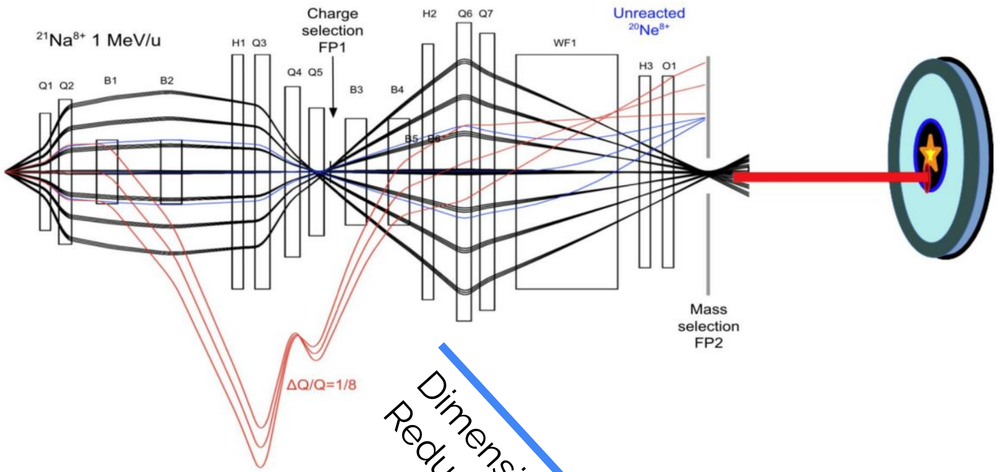
https://github.com/ascsn/2023-FRIB-TA-Summer-School



Social, too!



Slide from Pablo Giuliani



Dimensionality Reduction

PRELIMINARY

# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error (ax)
3	(9.7 ± 0.3) ms*	1 µm	1 nrad
10	(10.9 ± 0.6) ms*	0.01 µm	7.5 prad
15	(12.1 ± 0.2) ms*	0.7 nm	0.3 frad

Fast

Accurate

Dimensionality Reduction in
Nuclear Physics
Presented by ASCSN

Aplication 5: Black-Box Methods

Efficient Emulation of SECAR Beam

Non-linear and non-affine problem

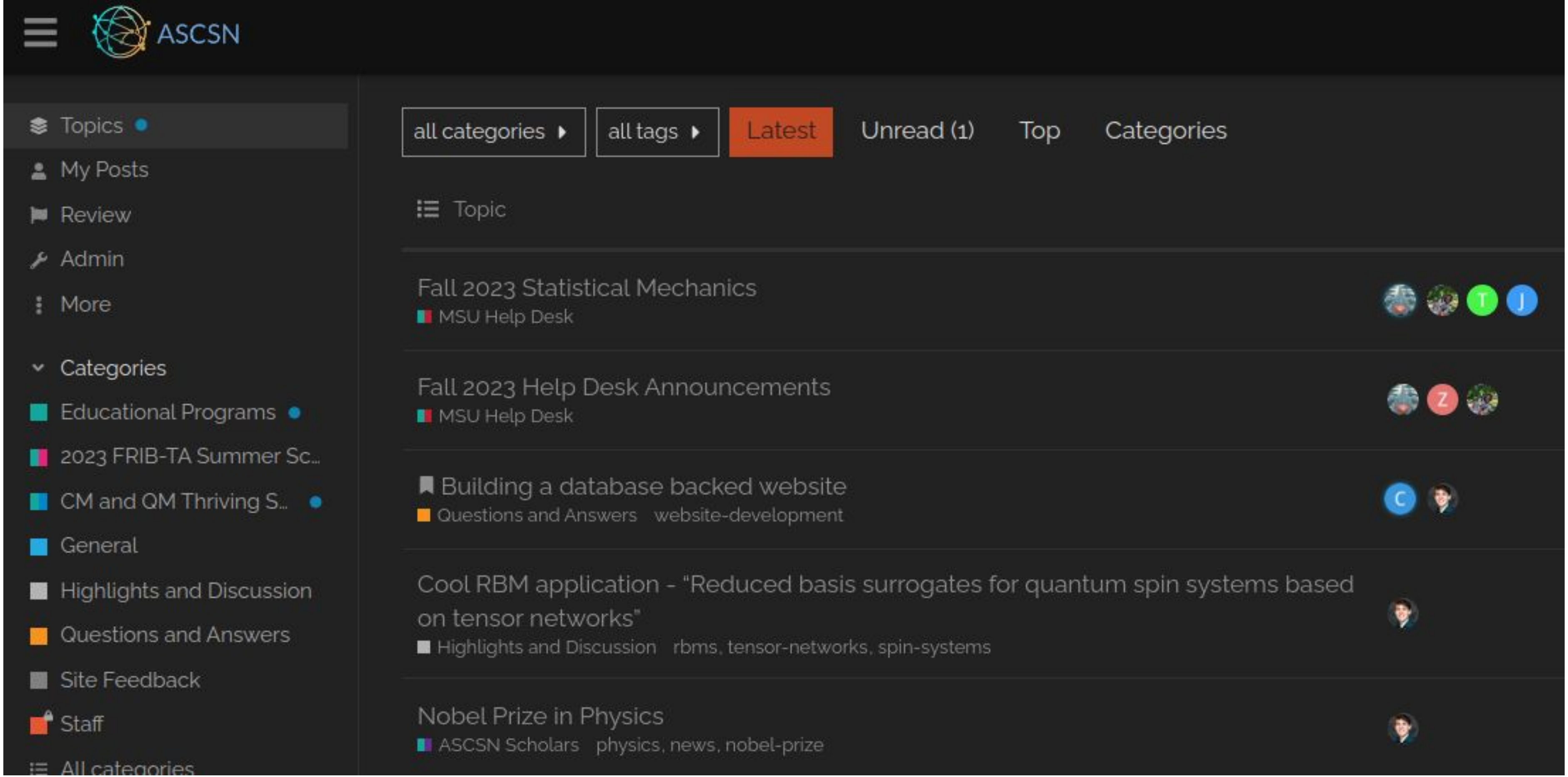
Always accepting new examples!

https://dr.ascsn.net

Dimensionality Reduction in
Nuclear Physics
Presented by ASCSN

Introduction to Dimensionality Reduction in Nuclear Physics

- Introduction
- Application 1: The Quantum Harmonic Oscillator
- Application 2: Two body single channel nuclear scattering
- Application 3: The Empirical Interpolation Method
- Application 4: Time Dependent Systems (evolution in the reduced space)
- Aplication 5: Black-Box Methods
- Contributors



https://forum.ascsn.net

Path(s) Forward

Continued developments in time-dependent microscopic many-body theory are vital to capitalize on the wealth of information accessible through low-energy, heavy-ion dynamics

Deep engagement with the technical domains is also a necessity in today's computational climate

Path(s) Forward

Investments in pedagogy and mentoring are required to ensure we have broad participation and engagement in nuclear science

This includes a specific focus on accessibility and belonging for all individuals in the workforce

Immense Gratitude to All Collaborators!

Funding

DOE NNSA Grant No. DE-NA0004074
DOE Grant Nos. DE-SC0013365, DE-SC0023175
NSF CSSI Program No. 2004601

Computing Resources

Australian National Computational Infrastructure Raijin and Gadi
Oak Ridge Leadership Computing Facility Summit and Frontier
Argonne Leadership Computing Facility Polaris
Texas A&M High Performance Research Computing Terra and Ada
Michigan State University HPCC

Current Ideas for Dynamics

Exploring multiple approaches, including Neural Implicit Flow and Fourier Neural Operators

Now at Nvidia

FOURIER NEURAL OPERATOR FOR PARAMETRIC PARTIAL DIFFERENTIAL EQUATIONS

Zongyi Li zongyili@caltech.edu
Nikola Kovachki nkovachki@caltech.edu
Kamyar Azizzadenesheli kamyar@purdue.edu
Burigede Liu bgl@caltech.edu
Kaushik Bhattacharya bhatta@caltech.edu
Andrew Stuart astuart@caltech.edu
Anima Anandkumar anima@caltech.edu

Director of ML research at Nvidia

Current Ideas for Dynamics