Delivering a Nuclear Science capability at Lawrence Livermore National Laboratory

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Lawrence Livermore National Laboratory

This presentation is intended to be an open discussion so that you learn about LLNL

- LLNL is application focused
- LLNL operates through well-integrated, high performing teams
  - Teams are usually comprised of people with different skill sets
- LLNL is a national leader in Nuclear Science
  - What I will present is only part of the capability

Our mission is to strengthen the nation's security through world-class science, technology, and engineering

Stockpile Stewardship

All-WMD Threat Reduction

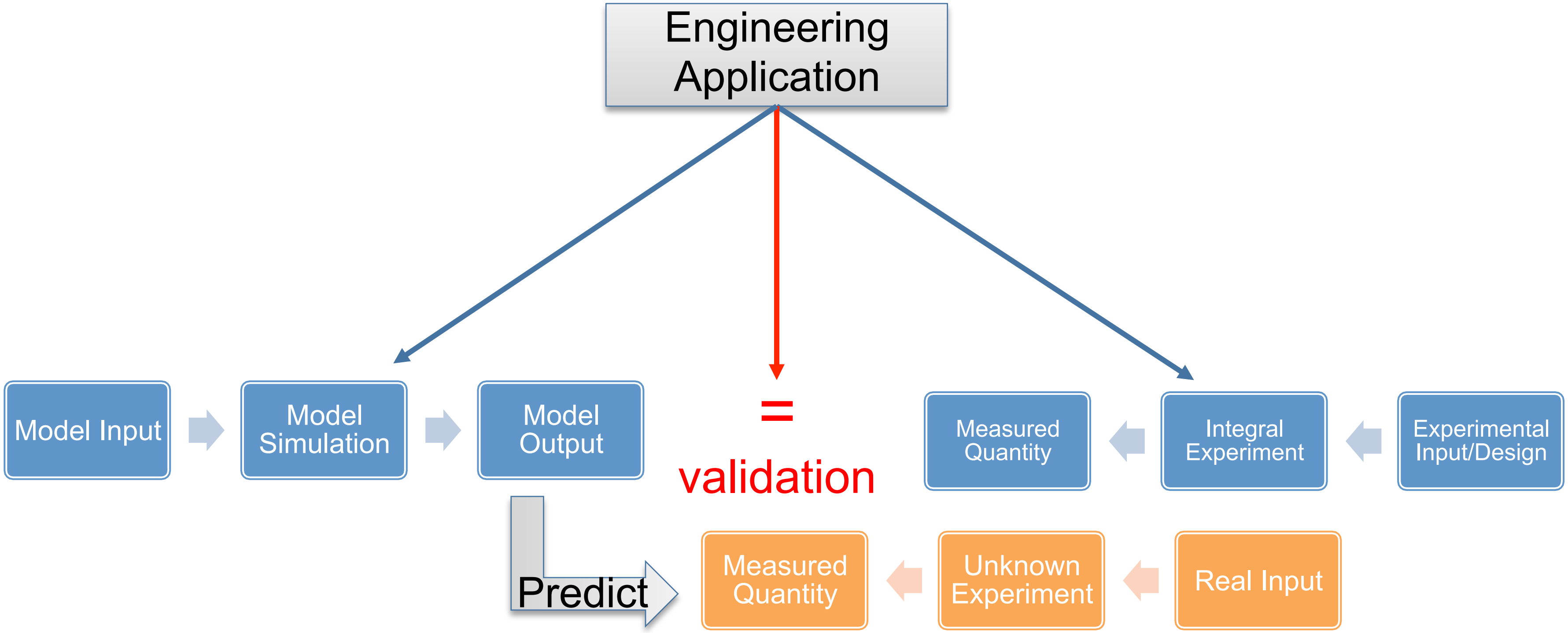
Cross-Domain Deterrence

Energy and Climate Security

"At LLNL, our work is to diminish the likelihood and impact of war, of terrorism, and of natural and man-made disasters through the innovative application of cutting-edge science and technology."

Anticipate • Innovate • Deliver

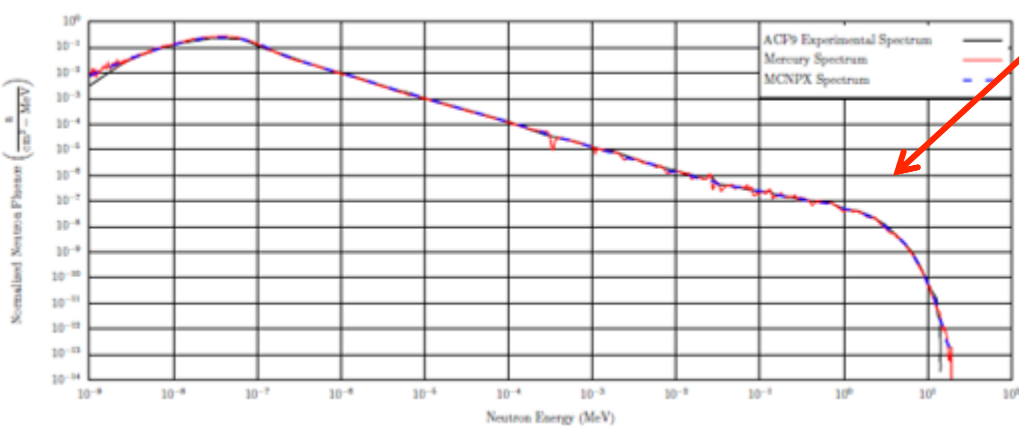
Predictive Science is key to delivering for our mission. What is predictive science?

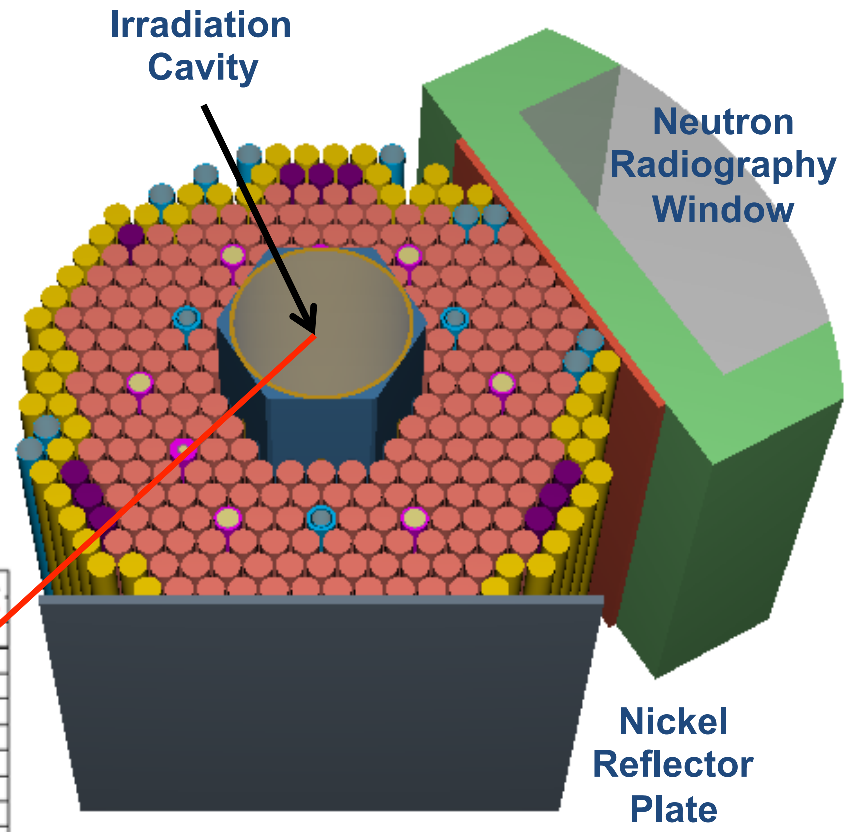


- Goal: Establish a "validated" modeling methodology that allows the application scientist to model or design unknown systems
- Today's applications are often "Inverse Problems", where the Real Input is unknown
- Note: this process aggregates efforts from many areas of expertise

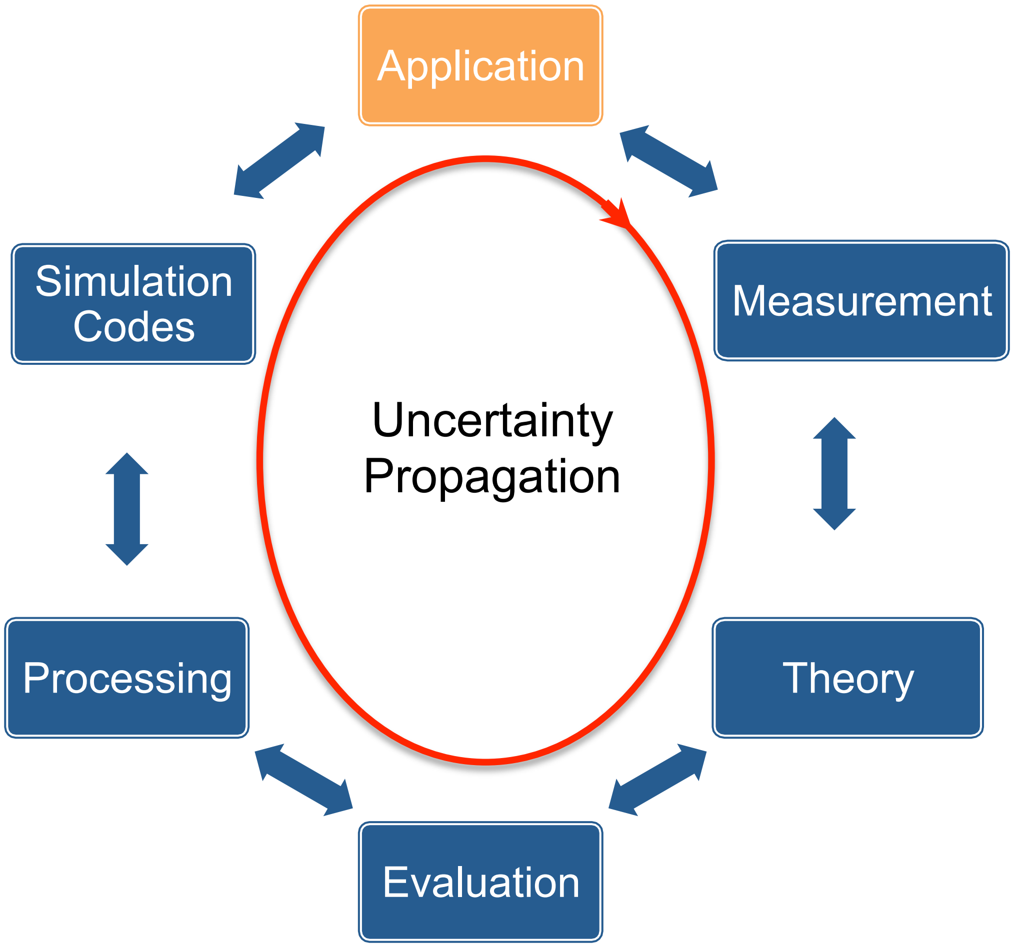
Example: Reactor modeling supports safe operations as well as material science experiments

- ACRR: water-moderated pool research reactor that can be operated in steady-state or pulsed mode
- Reactor core: 236 element array of uranium dioxide/beryllium oxide (enriched to 35 weight percent) with stainless steel cladding
- ACRR has a dry irradiation cavity in center of core that can be used to expose experiments to neutron and gamma fluxes





LLNL maintains a complete nuclear data pipeline to support our Predictive Science capability



Our priorities are data driven, through development of sophisticated UQ methodology

LLNL supports a wide range of high fidelity Nuclear Physics Experiments

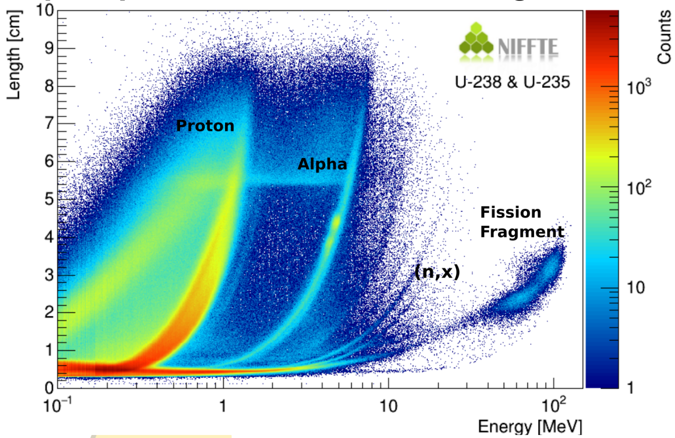
Experiment	Purpose	Facility
fissionTPC LLNL + LANL	Fission cross sections (n,f) [$\chi\nu\sigma_f$] is the fission source term driving neutron reactivity	LANSCE
Chi-Nu LANL+LLNL	Prompt Fission Neutron Spectra (PFNS) is key part of fission source	LANSCE
Fission Product Yields LLNL + many collaborators	^{239}Pu, ^{238}U, ^{235}U Cumulative and Independent FPY	TUNL (& NCERC)
Branching Ratio LLNL + TAMU + ANL + UC Irvine	Fission product β-delayed branching ratios	CARIBU/ANL, Texas A&M
Surrogate: Hyperion LLNL + TAMU	Surrogate (p,d) for (n,γ) reactions	Texas A&M cyclotron
Surrogate: NeutronStars LLNL + TAMU	Surrogate (α,α') for (n,xn) reactions	Texas A&M cyclotron
NIF doped capsules*	Test reactions with large 14 MeV neutron source	NIF
Scoping studies on Scattering*	Understand neutron elastic and inelastic scattering	Undetermined

*not discussed further in this presentation

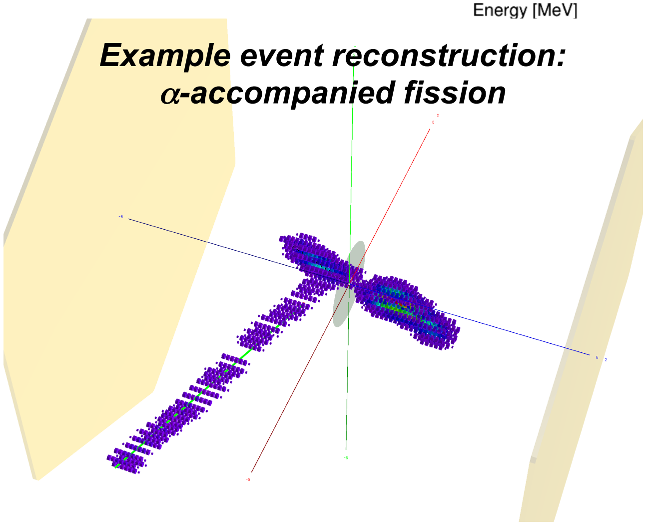
The fissionTPC detector is currently used for (n,f) Cross Section Measurement

- **Targets are two-sided to make ratio measurements**
  - Result is only as good as benchmark
- **High fidelity data provides greater detail than previous methods**
  - 3D particle tracking and identification
  - Reduction and detailed quantification of uncertainties
  - Beam and target non-uniformities
  - Detection Efficiency
  - Spontaneous decay pile-up
- **Cross Section Milestones, data collection and analysis**
  - U238/U235 delivered
  - Final Pu239/U235 this year
  - Li6/U235 data this year
  - Li6/U235 & Li6/Pu239 2020-22

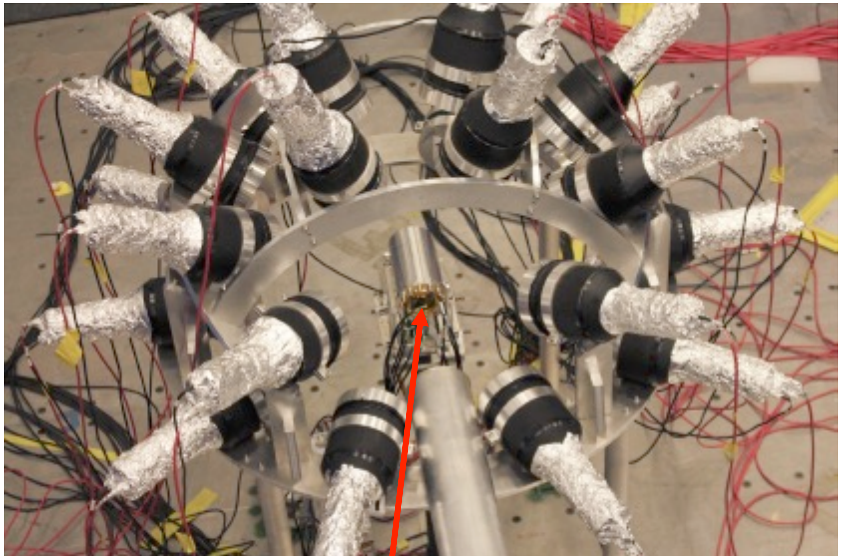
Excellent Particle ID effectively eliminates pileup and beam induced background

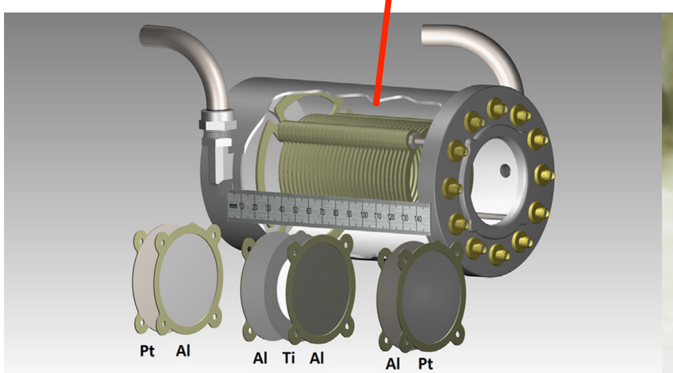


Example event reconstruction: α-accompanied fission

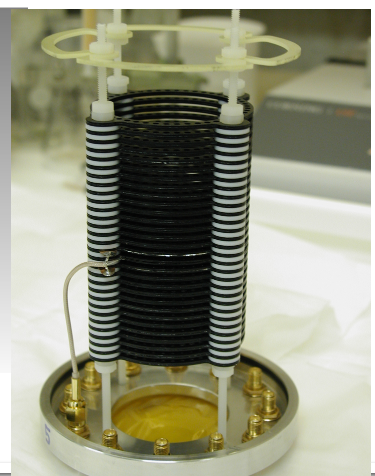


Chi Nu measures Prompt Fission Neutron Spectrum for the major actinides



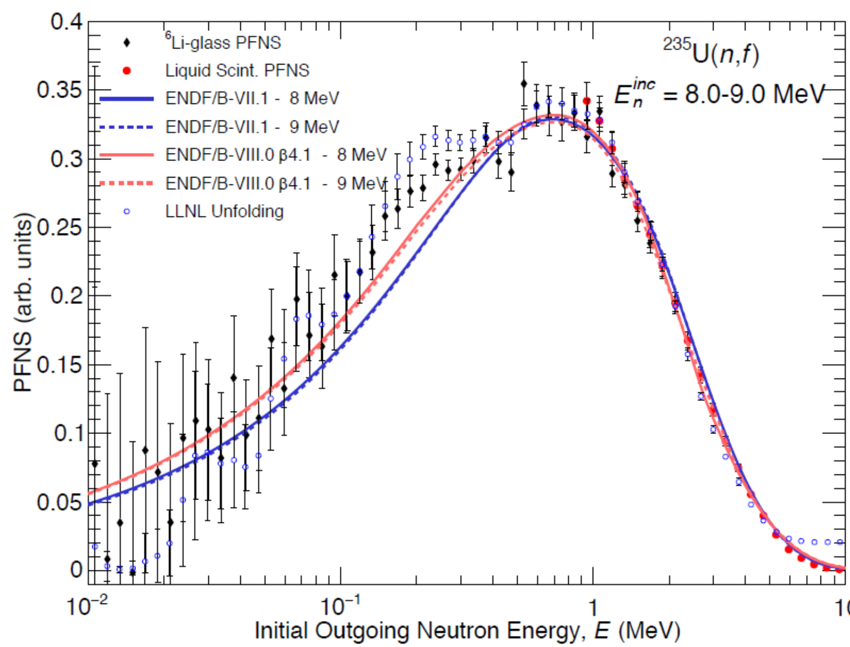


Metal foils on aluminum frames



10 PPACs assembly

The double-hump structures in PFNS at near and above the second-chance fission observed using the ratio-of-ratio method (LANL) and Bayesian unfolding technique (LLNL)

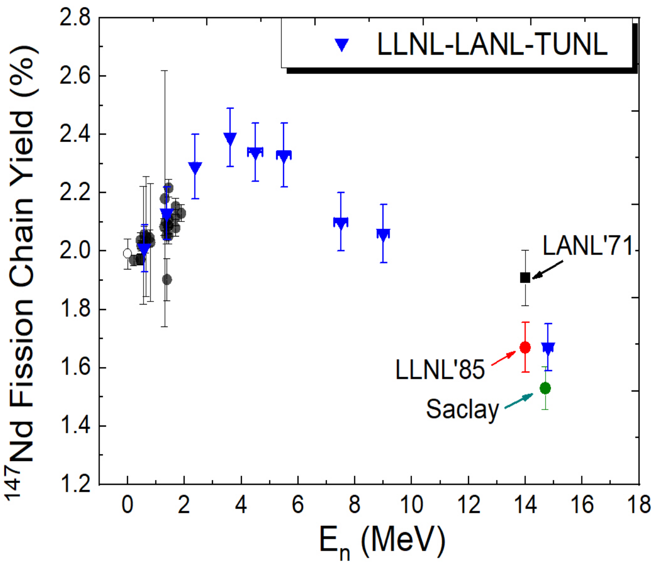


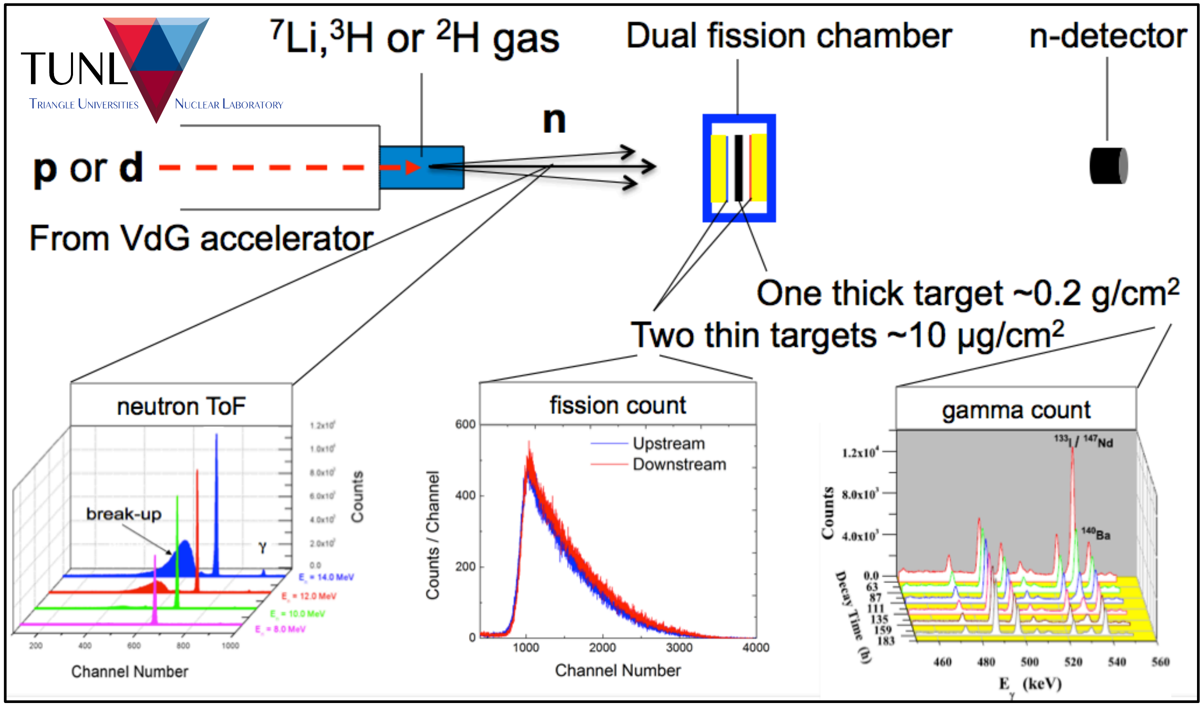
Energy dependence of Fission Product Yield is being measured at TUNL

- Peculiar energy dependency
- Positive slope of the ^{147}Nd FPY from 0.5 to ~4.0 MeV:

  $\Delta Y(^{147}Nd)/\Delta E_n = (5.8 \pm 1.5)\%/MeV$

- At higher energies the FPY for ^{147}Nd turns over and decreases





Strong Partnerships with the TUNL Stockpile Stewardship Academic Alliance Group

Los Alamos NATIONAL LABORATORY EST.1943

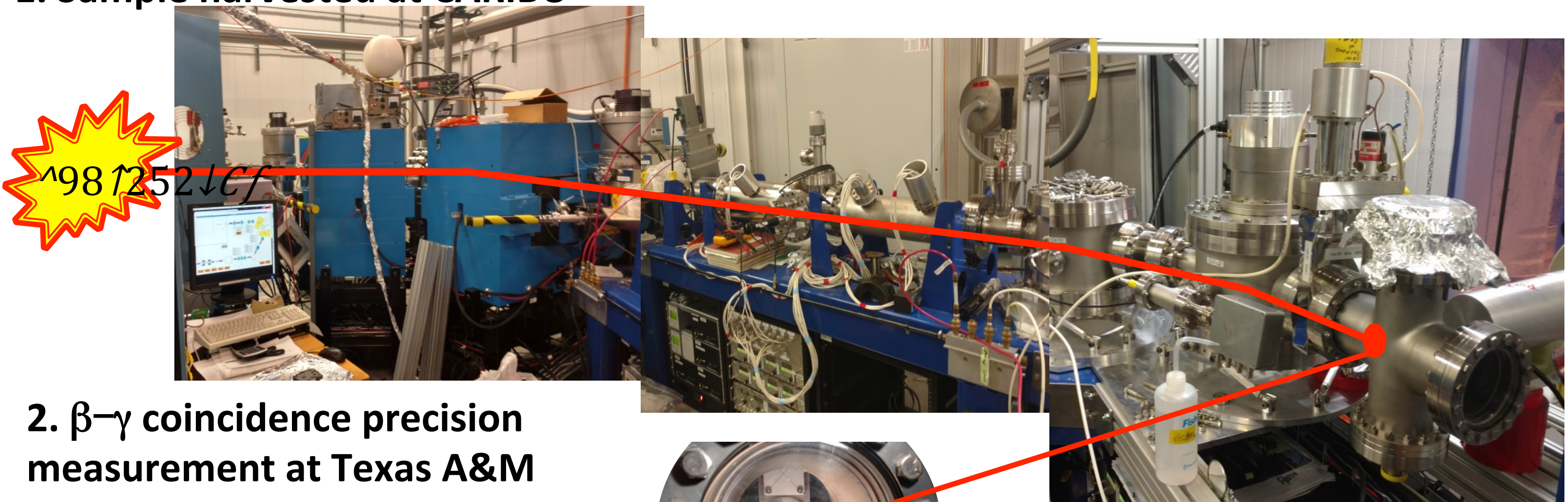
BERKELEY LAB Bringing Science Solutions to the World

TUNL Triangle Universities Nuclear Laboratory

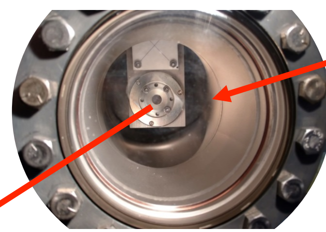
We are developing the RABITTS system at TUNL to measure independent fission product yields next

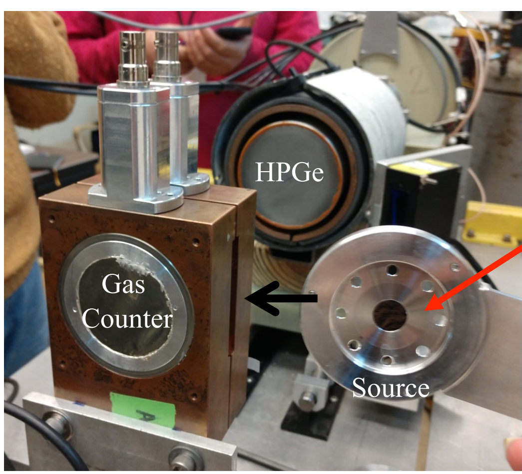
Branching ratios are needed to understand FPY; we can measure them to 1% accuracy

1. Sample harvested at CARIBU



2. β−γ coincidence precision measurement at Texas A&M





$$BR = \frac{N_{\beta\gamma}}{N_{\beta}} \frac{1}{\epsilon_{\gamma}} \frac{\epsilon_{\beta_{tot}}}{\epsilon_{\beta_{\gamma}}}$$

Benchmark result: ^{95}Zr

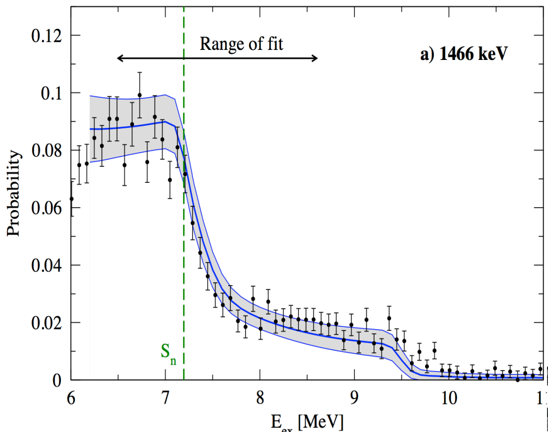
Isotope	E_γ	$I_{\gamma(\text{this work})}$	I_γ
^{95}Zr	724.2 keV	0.4384(25)	0.4427(22)
^{95}Zr	756.7 keV	0.5446(28)	0.5438(22)
Ratio	724.2 keV/756.7 keV	0.805(6)	0.814(4)
^{95}Nb	765.8 keV	0.9978(85)	0.9981(1)

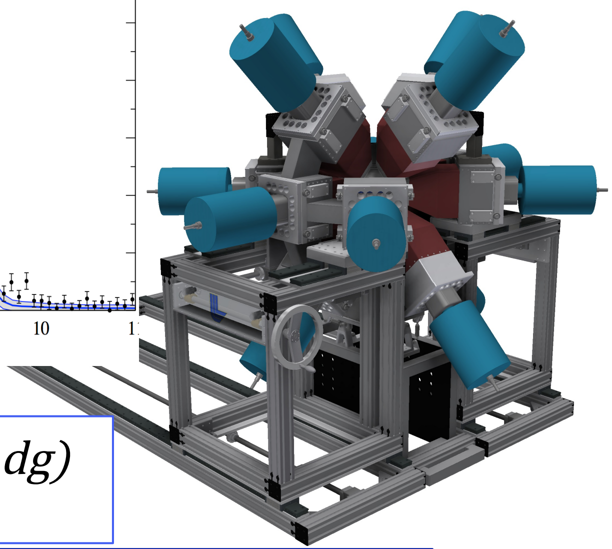
Recent advances in Surrogate measurements are providing new nuclear data for unstable targets

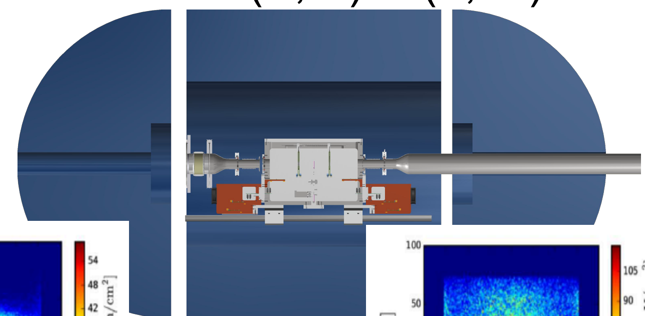
Hyperion:
(p,d)->(n,γ)

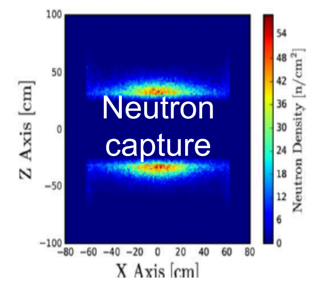
All data collected at Texas A&M cyclotron

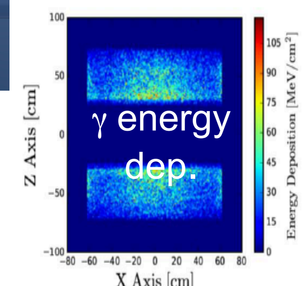
NeutronStars:
(α,α') ->(n,xn)



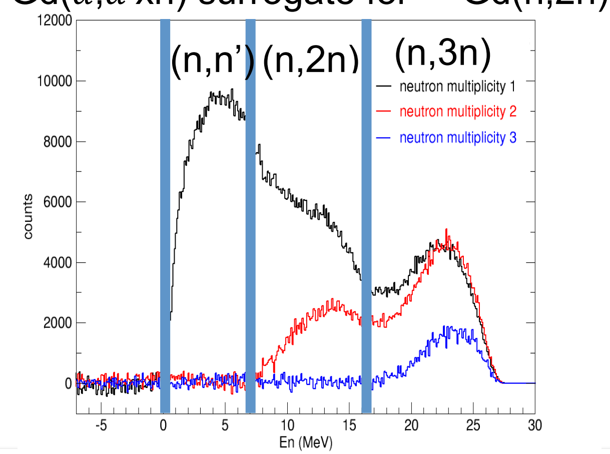








^{156}Gd(α,α'xn) surrogate for ^{155}Gd(n,2n)



$$P_{(p,d\gamma)}(E) = N_{(p,d\gamma)}(E) / \varepsilon_\gamma N_{(p,d)}(E)$$

A Surrogate experiment gives

$$P_{(p,d\gamma)}(E) = \sum_{J,\pi} F_{(p,d)}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

Unstable target cross section:

$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+target}^{CN}(E,J,\pi) \cdot G^{CN}_{\gamma}(E,J,\pi)$$

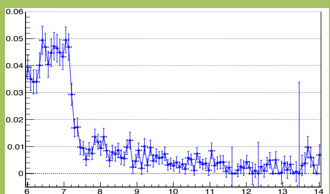
LLNL supports a wide range of theory efforts, which support nuclear data development and Evaluation

Theory Areas	Codes	Approach/Formalism	Used for
Nuclear Structure	BIGSTICK*	Shell model	Properties of light & medium nuclei
	HFBTHO/ HFODD	Density functional theory	Properties of medium & heavy nuclei
Light-ion reactions	FUSION	Ab Initio/RGM	Cross section predictions for light nuclei
	HYRMA*	R-Matrix	Fitting resonance cross sections
Reactions	FRESCO*	Coupled-Channels Reactions	Predicting/fitting direct reactions, support for HF and Surrogate calculations
	YAHFC*	Hauser-Feshbach Theory	Predicting/fitting statistical reactions
Surrogate reactions	CNXS	Generalized Multistep Reactions	Cross sections for short-lived isotopes from indirect data & theory
Fission	FELIX	Microscopic Fission theory	Predict fission product yields
	FREYA	(Semi-)Phenomenological	Prompt fission neutron spectrum

*not discussed further in this presentation

Surrogate reactions: Combining theory & experiment to determine unmeasureable cross sections

Surrogate reaction experiments



Compound-nucleus decay observables

CNXS* Code Framework

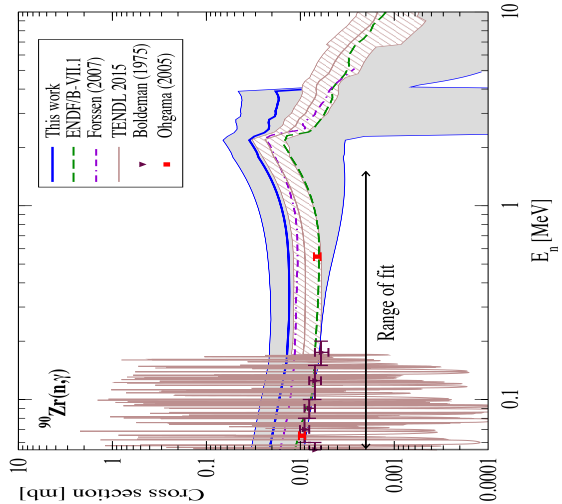
Compound-nucleus formation mechanism
- *Transfer reactions*
- *Inelastic scattering*

Auxiliary calcs
- *Nuclear structure*
- *Interactions*

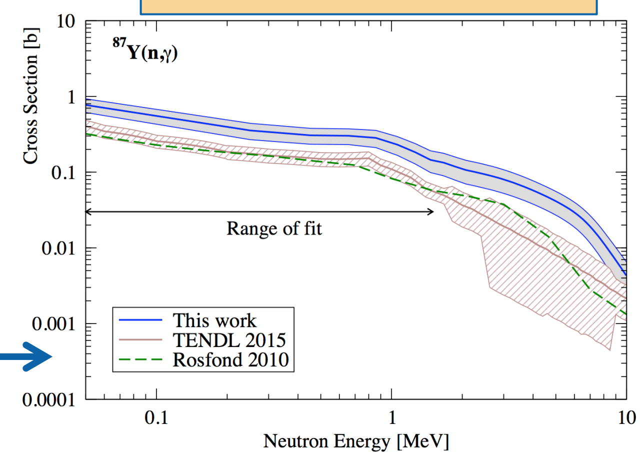
Bayesian Parameter Fit
- *Run CN decay model w/ sample parameters*
- *Compare calculated & experimental observable*
- *Determine best fit*
- *Calculate desired cross section w/uncertainty*

Modified compound-reaction code

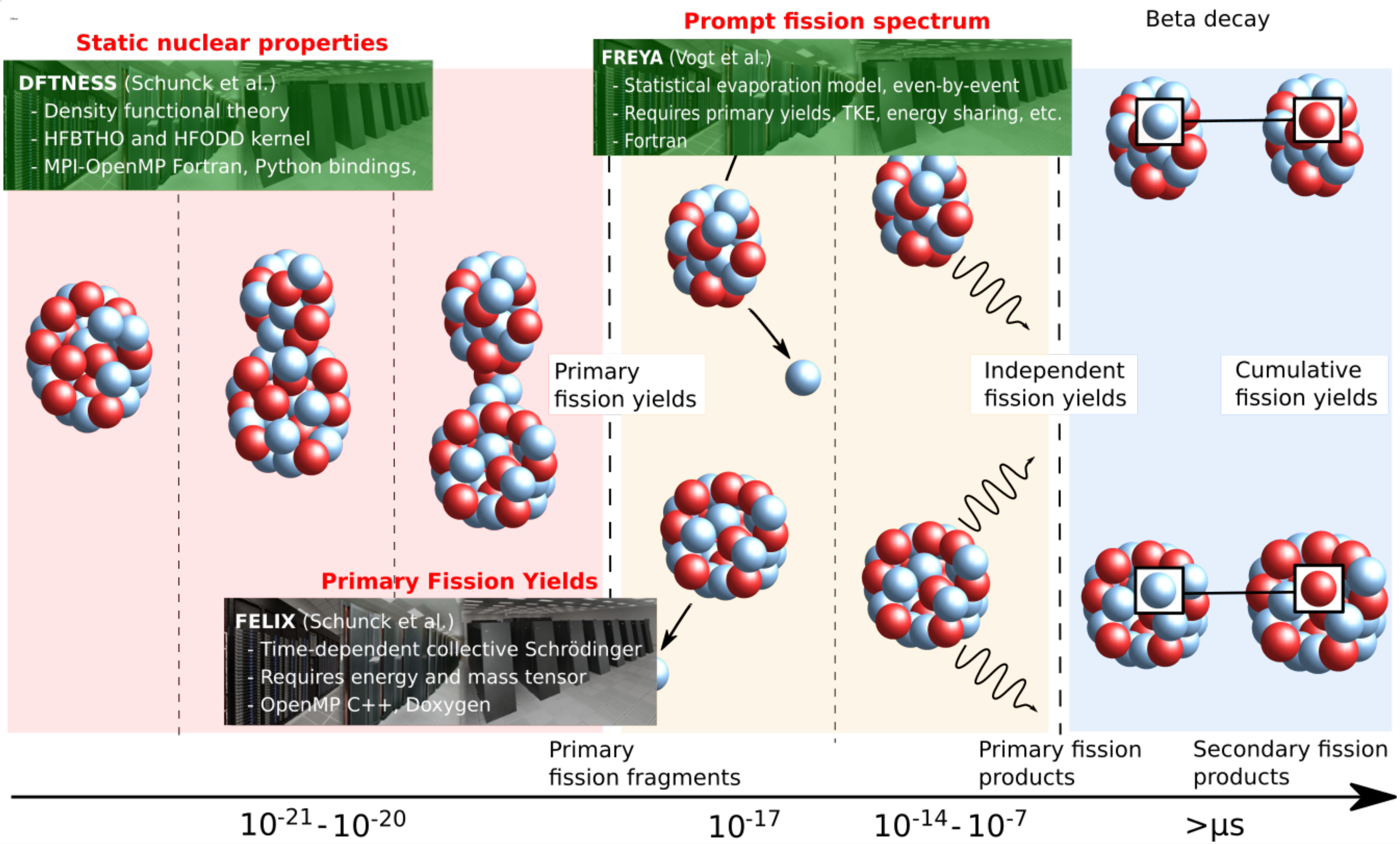
Proof-of-principle



New result for unknown

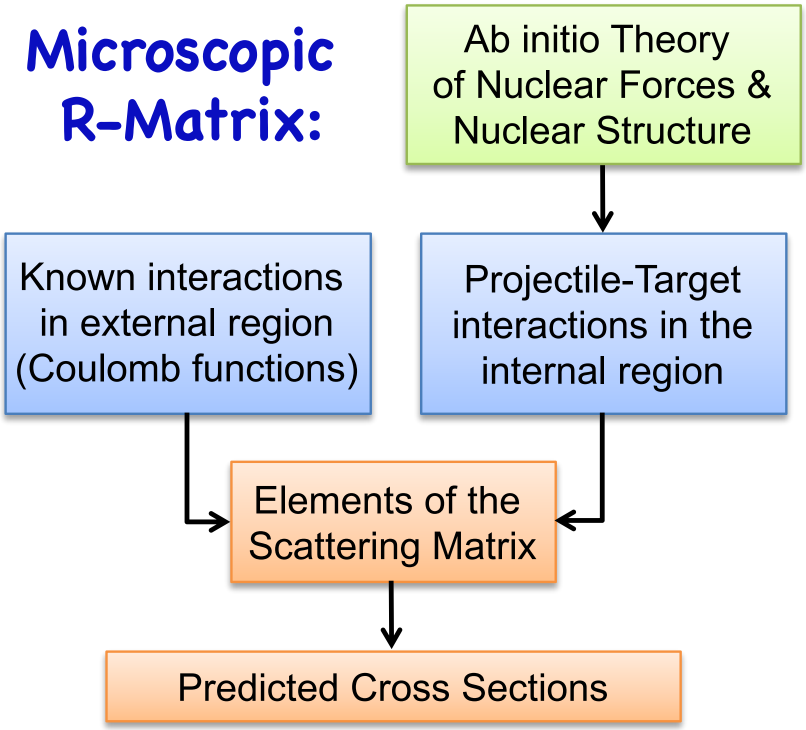


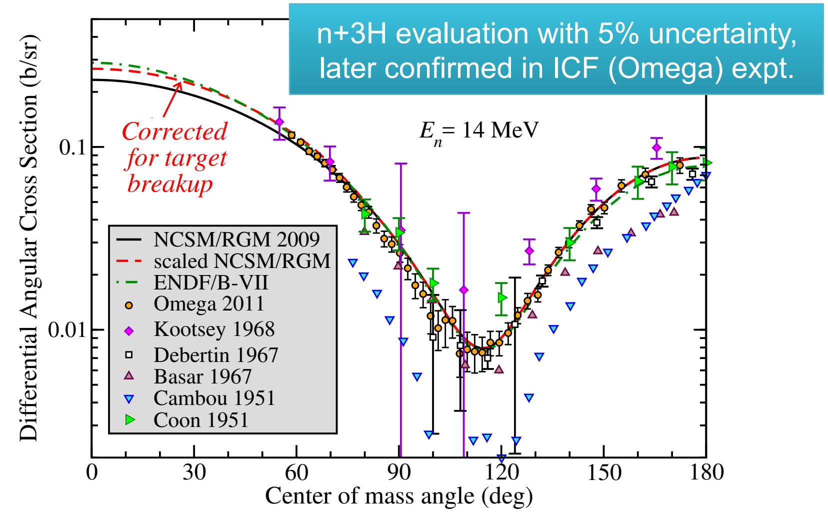
Microscopic Fission Theory is part of an integrated modeling effort to understand fission better

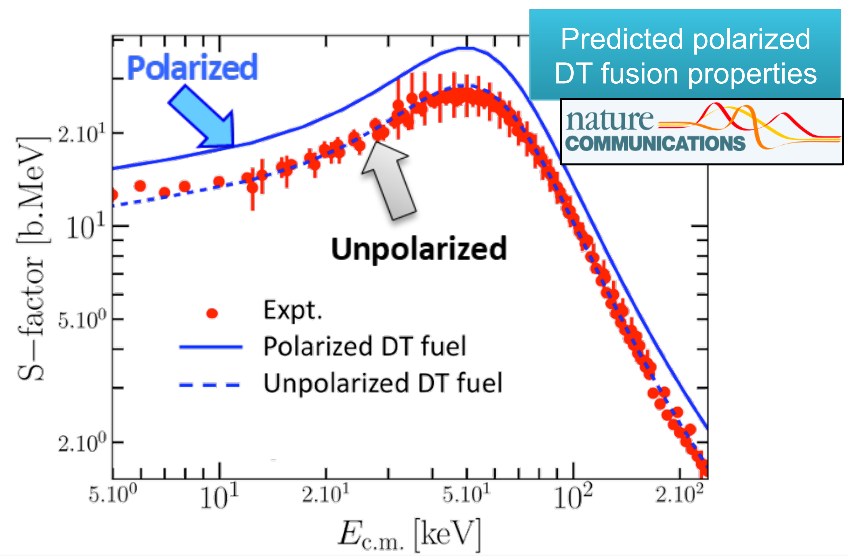


Light-ion reactions can be predicted from scratch using the microscopic version of R-matrix theory

Microscopic R-Matrix:







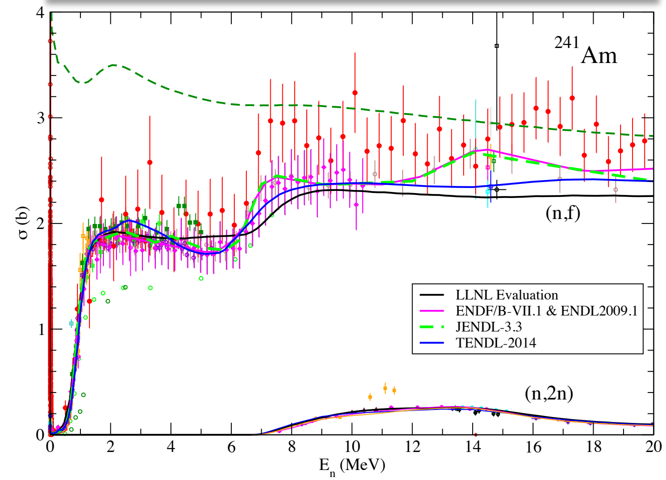
Suite of Codes: **FUSION** (MPI/OpenMP)

- Collab. TRIUMF, I2PN3
- >500 Mcpu-hrs/past 3 years
- UNIQUE to LLNL/TRIUMF/I2PN3 collab.

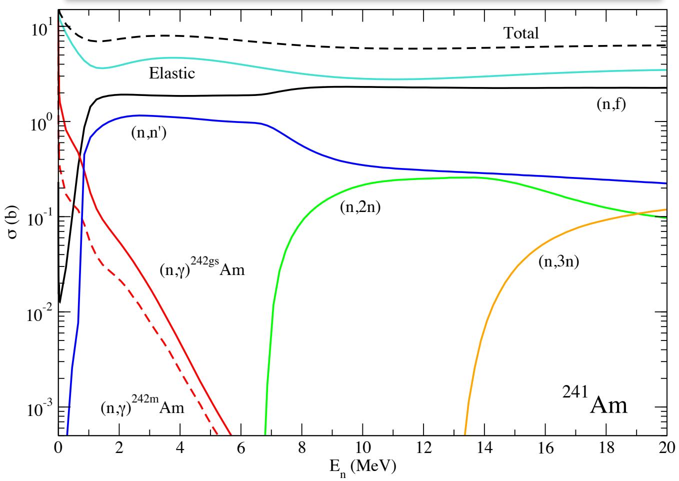
Evaluation utilizes theory and measurement to arrive at nuclear data "best values"

- Evaluation is an international collaboration
- An experiment does not an evaluation make
  - Conflicting data
  - Not everything is measured
    - There are many channels; spectra; angular distributions; correlations
- Modeling augments experiments to provide a full evaluation
  - Arbiter between conflicting data
  - Fills in gaps where data doesn't exist
  - Provides understanding of correlations between channels
- LLNL is in a phase of increasing demand for Evaluation

Modeling guides ^{241}Am(n,f) and ^{241}Am(n,2n)



Modeling completes ^{241}Am(n,X) evaluation



LLNL has led the development of the Generalized Nuclear Data Structure (GNDS)

- Because we share data, we need to agree on a common format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               format="1.9" projectileFrame="lab">
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        <XYs1d label="recon"> ... </XYs1d>
      </crossSection>
      <outputChannel genre="twoBody">
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            <distribution> ... </distribution>
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        </products>
      </outputChannel>
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    ...
  </reactions>
</reactionSuite>
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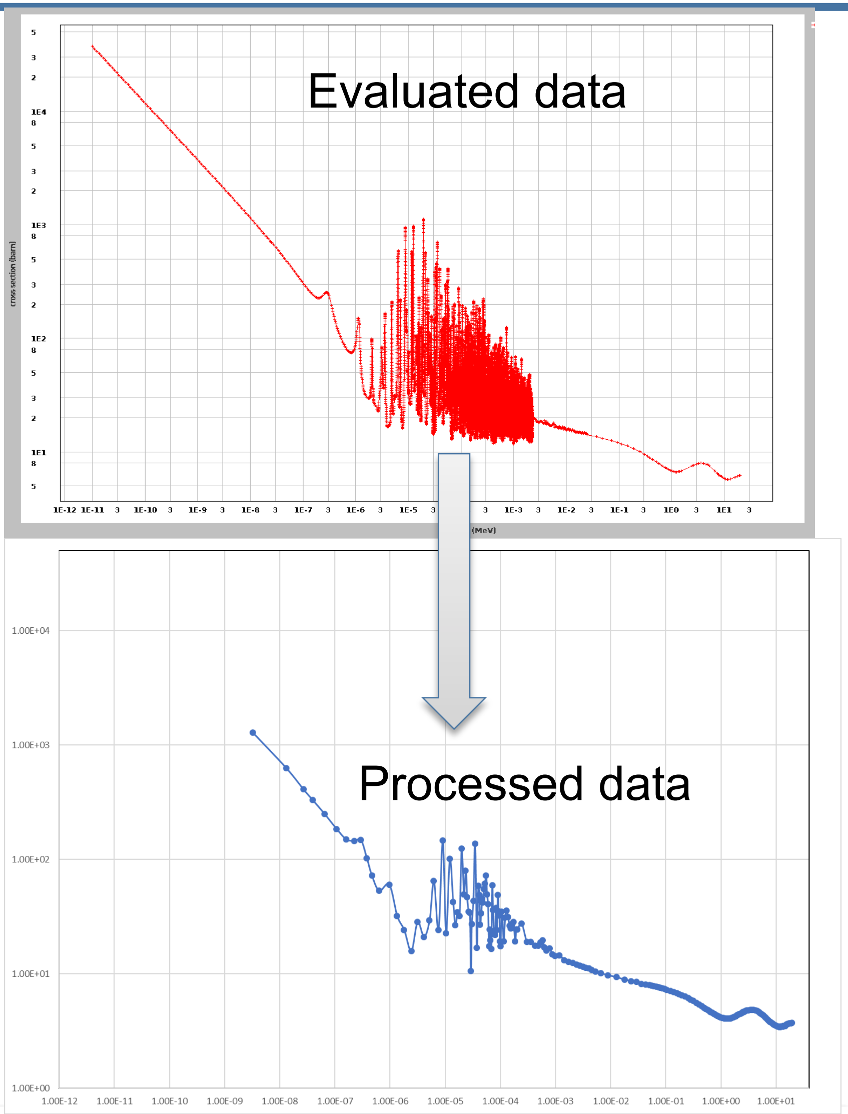
- GNDS will replace ENDF6 and ENDL
- Adoption is starting to happen

ENDF/B-VIII.0 library was released in the old ENDF6 and GNDS formats

Processing software delivers nuclear data libraries to the simulation codes

- Processing turns evaluated data into something simulation codes can use
  - Interpolates and/or averages the data
- Processing adds important physics
  - Doppler Broadening of cross sections
  - Thermal upscatter physics
- FUDGE: LLNL's complete processing code
  - Neutron, gamma, charged particle data
  - First code to support GNDS
  - Only two other processing codes are supported in the US: AMPX (ORNL) and NJOY (LANL)

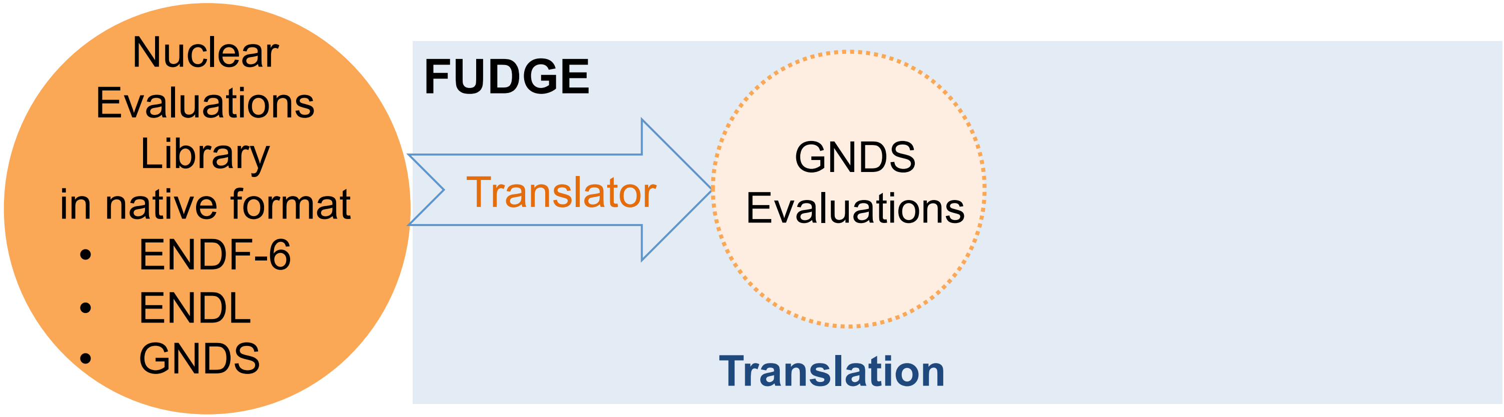


GNDS: from evaluated nuclear data to transport simulations

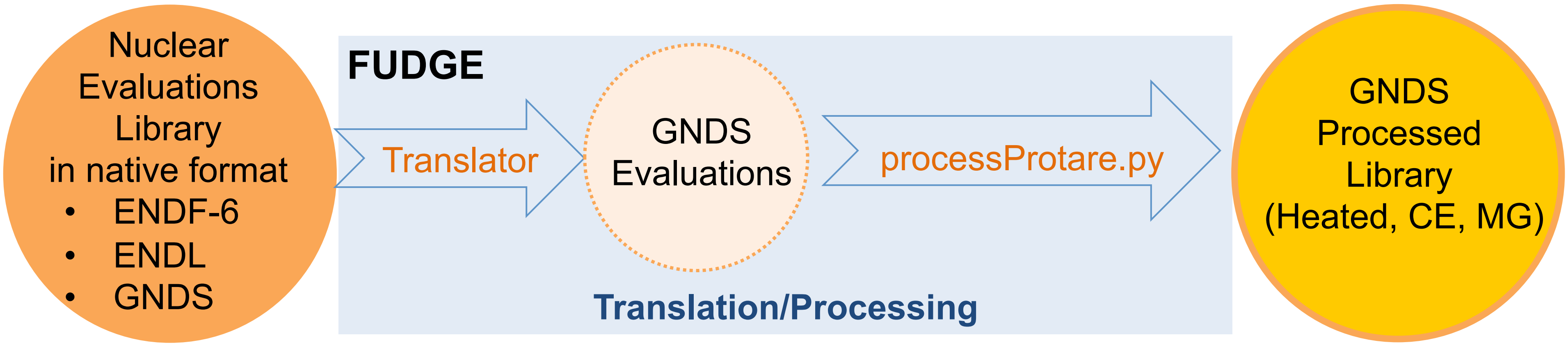
Nuclear Evaluations Library
in native format

- ENDF-6
- ENDL
- GNDS

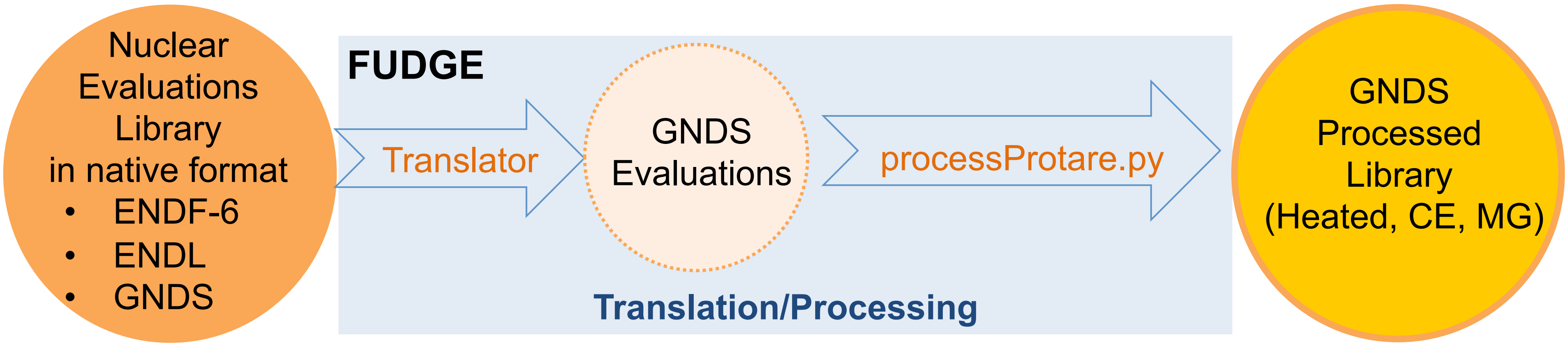
GNDS: from evaluated nuclear data to transport simulations



GNDS: from evaluated nuclear data to transport simulations



GNDS: from evaluated nuclear data to transport simulations

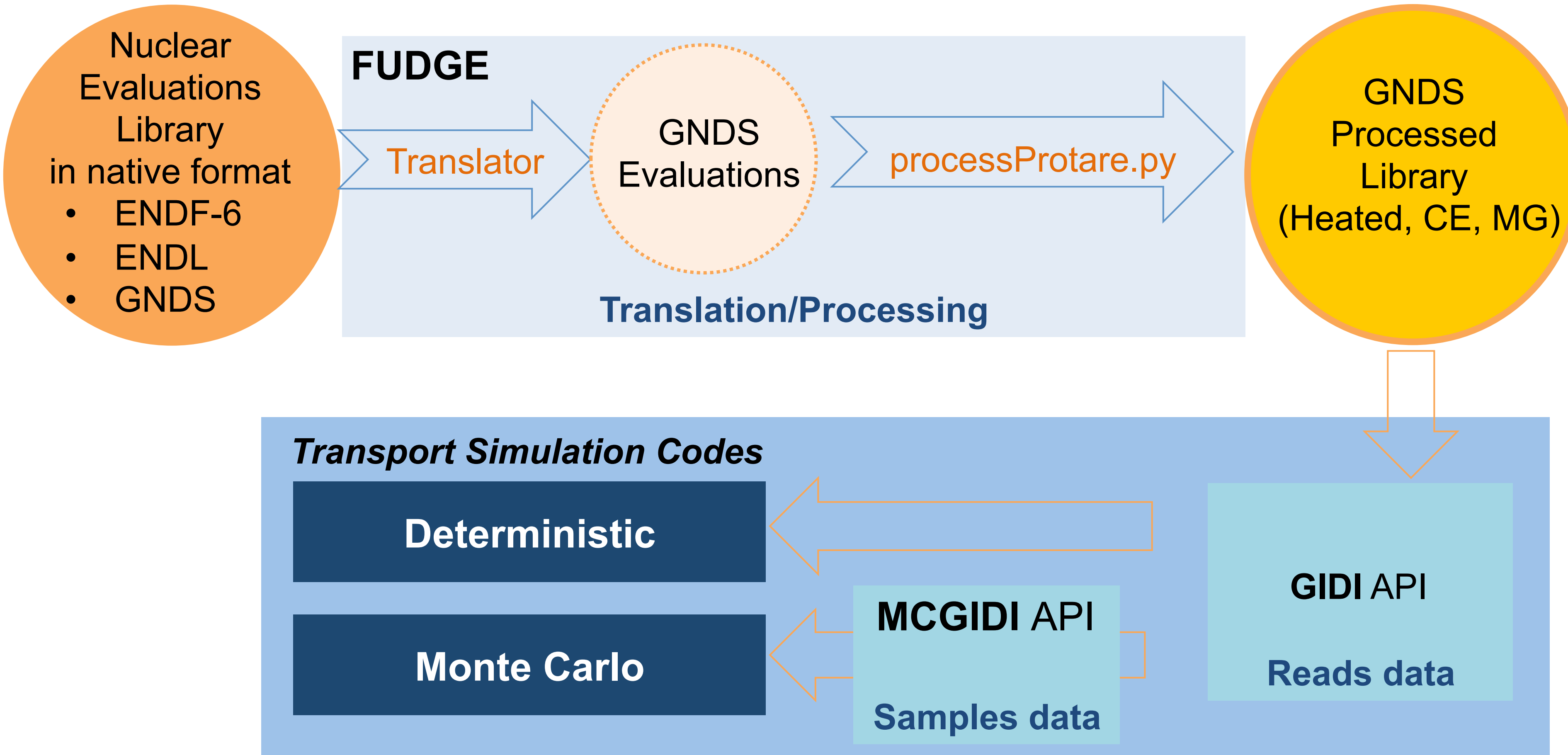


Transport Simulation Codes

Deterministic

Monte Carlo

GNDS: from evaluated nuclear data to transport simulations

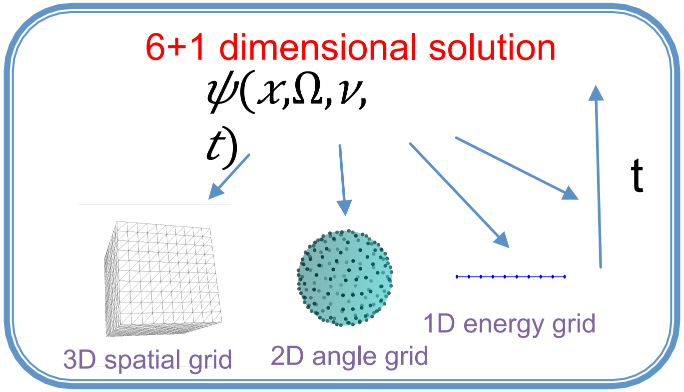


High-quality V&V is important, software bugs masquerade as physics!

The linear Boltzmann equation is the workhorse mathematical model for our simulation codes

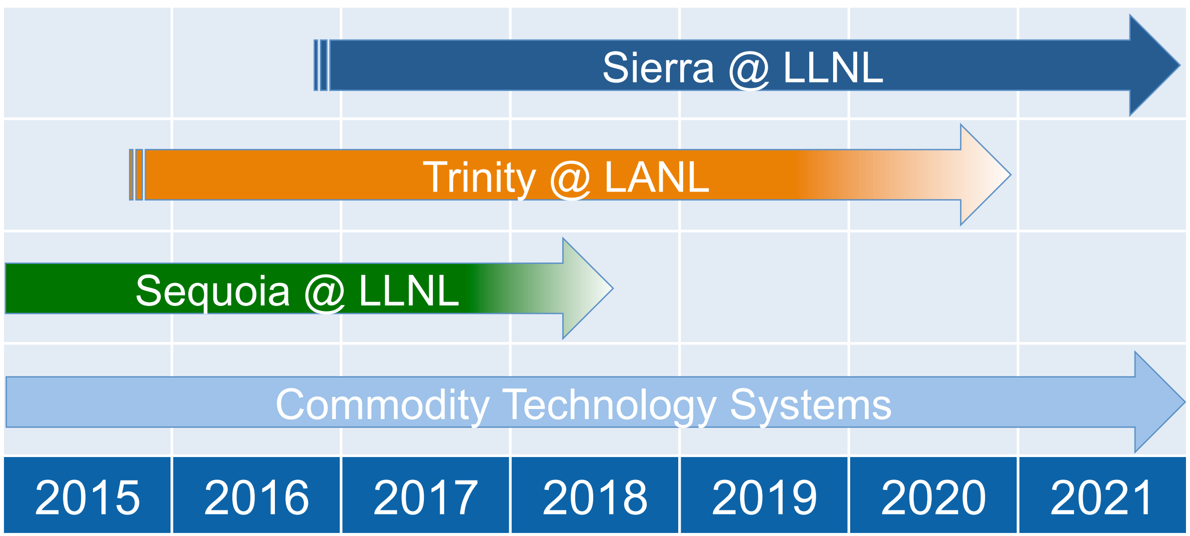
$$\frac{1}{v(E)}\frac{\partial \psi}{\partial t} + \Omega \cdot \nabla \psi + \sigma(r,E)\psi = \int_0^\infty \int_{S^2} \sigma_s(r, \Omega' \cdot \Omega, E' \to E)\, \psi(r,\Omega',E',t)\, d\Omega'\, dE' + \frac{1}{4\pi}\int_0^\infty \nu \sigma_f(r, E' \to E) \int_{S^2} \psi(r,\Omega',E',t)\, d\Omega'\, dE' + q$$

$\psi(r, \Omega, E, t)$ = neutron angular flux
r = (x, y, z) point in physical space
E, E' = energies (in MeV)
Ω, Ω' = directions, points on unit sphere
$q(r, \Omega, E, t)$ = external source
$v(E)$ = neutron speed, energy dependent
$\sigma(r,E)$ = total cross section (all reactions added up)
σ_s = scattering cross section/distribution
σ_f = fission cross section/distribution
ν = Average neutrons per fission



We develop general particle transport codes that solve the Boltzmann Equation

- Monte Carlo and Deterministic transport options
- High performance computing is a big challenge – transport has fundamental dependencies (remember $\psi(\Omega)$)

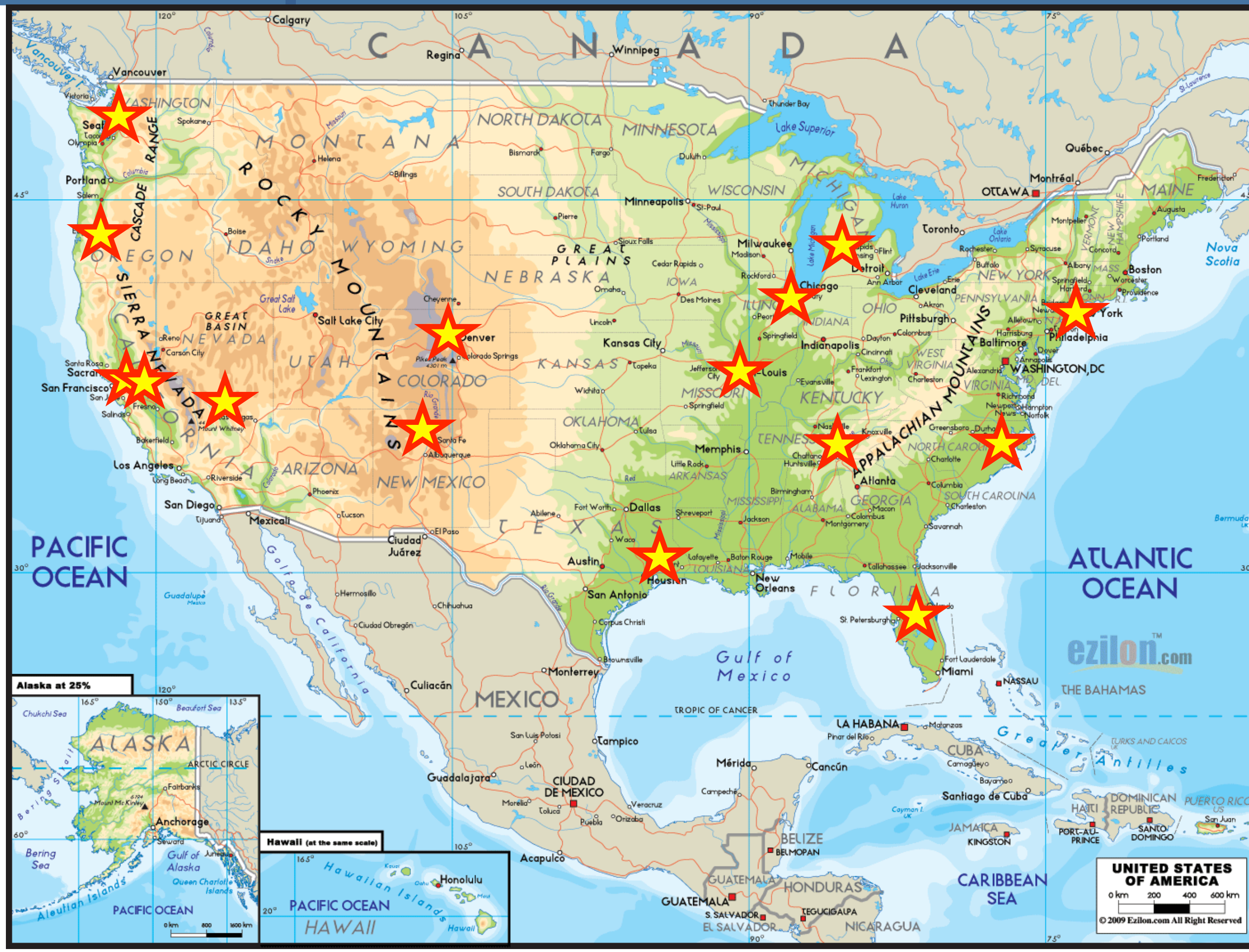


- Sierra: IBM Power + Nvidia Volta GPU
- Trinity: Intel Xeon Haswell + Intel Xeon Phi Knights Landing MIC
- Sequoia: IBM PowerPC
- Commodity: Intel Xeon

Heterogeneity

Nuclear Data uncertainty is becoming our biggest source of error. HPC allows us to run big enough calculations to overcome numerical error.

LLNL’s Nuclear Science capability is a truly national enterprise



- We have collaborators and use facilities across the United States
- We really appreciate our strong collaboration with Texas A&M

We are hiring in the field of Nuclear Science: careers.llnl.gov

- Over 1000 summer students in 2016, in all disciplines/programs
- Lawrence Scholar Program
- LLNL/TAMU Engineering Fellowship
- 229 postdocs in 2016
- 6 Lawrence Fellows
- Full time staff positions

My contact information: bailey42@llnl.gov

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