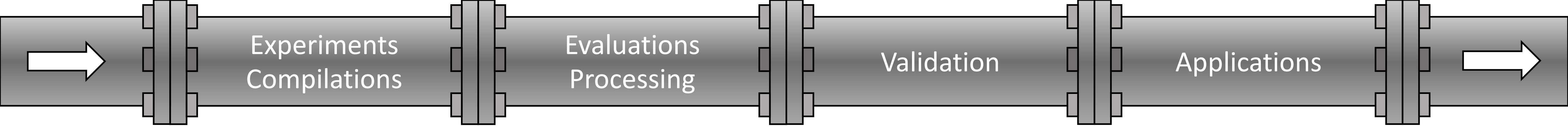
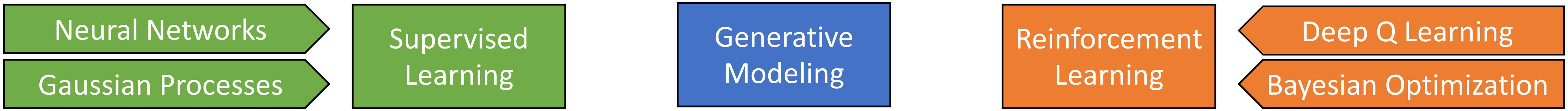
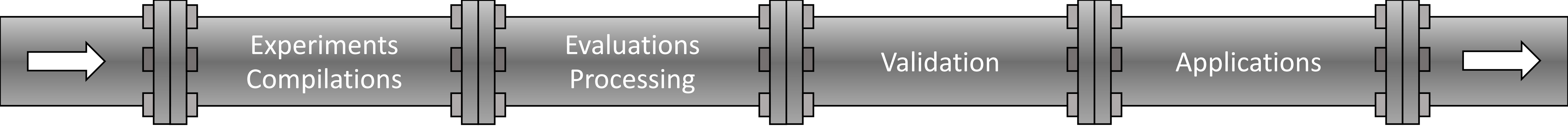


AI/ML for Nuclear Data

Part I: Prepared remarks

Part II: Open discussion





AI/ML for Nuclear Data

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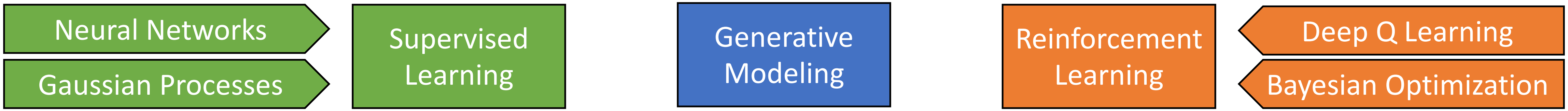
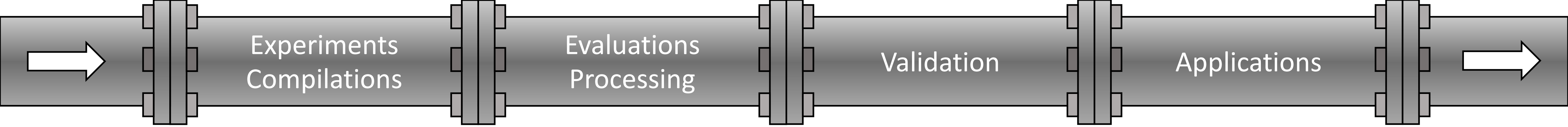
Closing Plenary	Guannan Zhang			Questions / Discussion

Break

Part II: Moderated Discussion

Discussion Lead	Kyle Wendt
Moderated Discussion	All
Summary	Session Organizers





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Neural Networks

Gaussian Processes

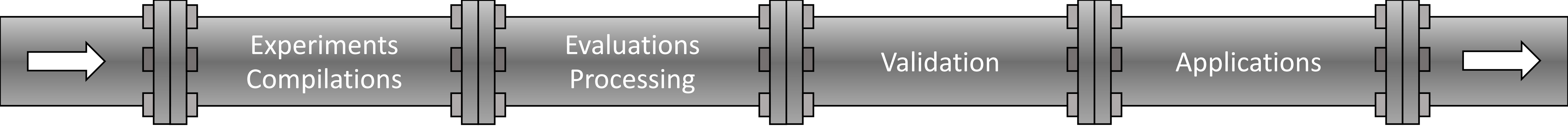
Supervised Learning

Generative Modeling

Reinforcement Learning

Deep Q Learning

Bayesian Optimization



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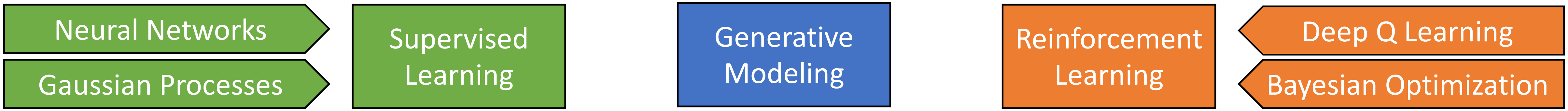
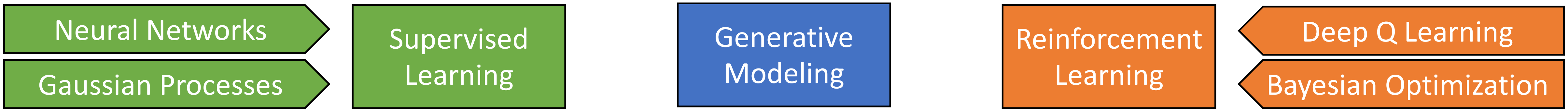
What is artificial intelligence (AI) and machine learning (ML)?

- AI: methods of using computers to learn, reason, and carry out tasks that are generally considered to require human intelligence
  - Play games, identify objects in images, design experiments, etc.
- ML: methods of learning patterns in systems and making predictions using data without explicit human direction
  - Types of Learning:
    - Supervised Learning
    - Unsupervised Learning
    - Reinforcement Learning
- Both of these definitions are very fluid:
  - The boundaries of what is AI and ML in science and industry vary
  - No concrete expert consensus on definition



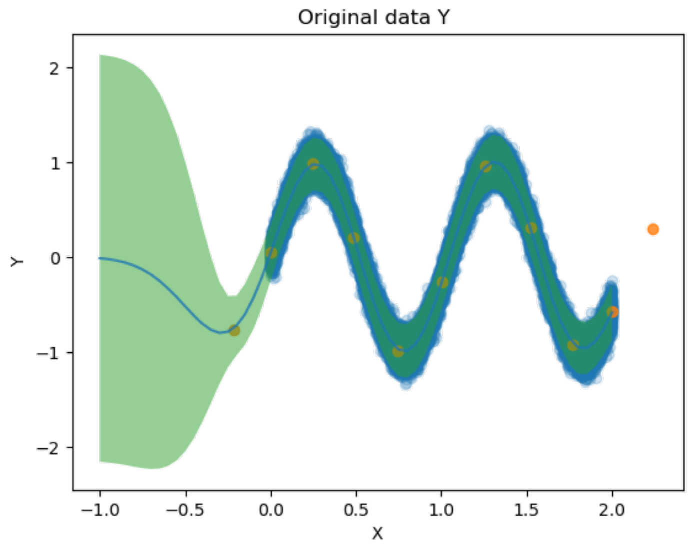
Supervised, Unsupervised and Reinforcement Learning

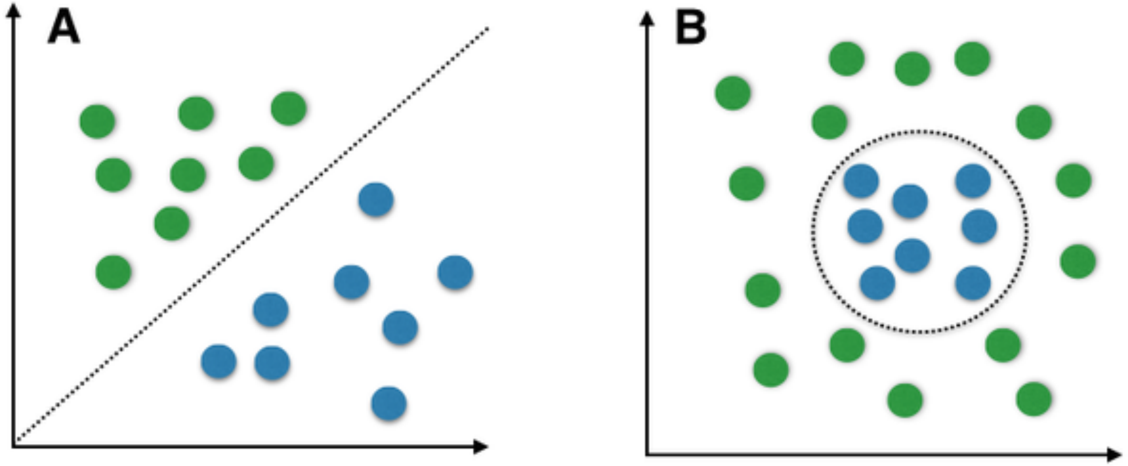
- Do you have a collection of data with labels/values and have interest in predicting the label/value for data outside of this set?
  - Yes: **Supervised**
    - Predicting cross section as a function of energy
    - Classifying an observed particle as a neutron or gamma in scintillator
  - No: **Unsupervised**
    - Grouping together time series values that look similar to find abnormal behavior
    - Learning distribution of images to generate realistic synthetics
  - No, but can take actions, collect data, and update based on feedback: **Reinforcement**
    - Learning to policy for playing Go or StarCraft by playing many games and learning what works.



Two Main Forms of Supervised Learning

- Regression:
  - Predicting a continuous-valued output as a function of a set of input *features*
    - One use is supervised learning to build *emulators* of expensive computer models
- Classification:
  - Predicting qualitative class label as a function of a set of input *features*





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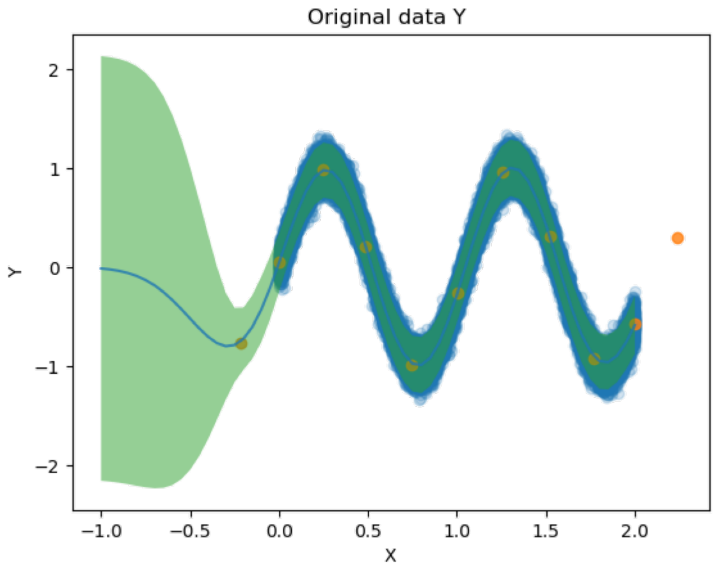
Common Supervised Learning Methods

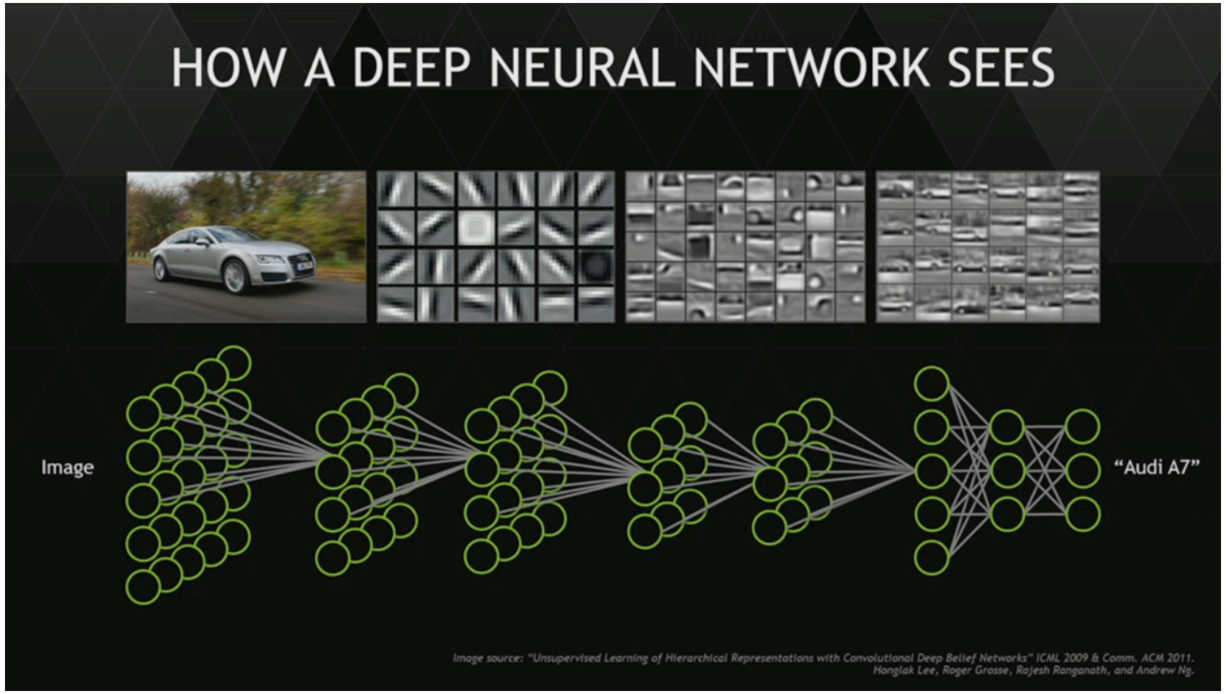
- Deep Neural Networks
  - More on the next slide
- Gaussian Processes
  - Bayesian prior on a function space
    - Defined through mean and covariance functions
    - Function space defined by covariance function
      - Can allow for infinite basis regression and quantification of uncertainty in predictions
  - Flexible and accurate for small to medium data problems
    - Uncertainty most valuable for small data problems
- Random Forests
  - Ensemble method
  - Flexible, fast, and accurate for medium to large data problems



Neural Networks | Gaussian Processes | Supervised Learning | Generative Modeling | Reinforcement Learning | Deep Q Learning | Bayesian Optimization

What are Deep Neural Networks?

- Complex tool for (mostly) supervised learning
- Great for:
  - HIGH dimensional input spaces
  - HUGE amounts of data
- Ideally learning structure in the inputs that can then be used to predict the output
  - Hierarchical, automatic feature learning
- Stack of linear combinations of previous layer, fed through non-linear transfer function
  - The structure of the layers is critical to application



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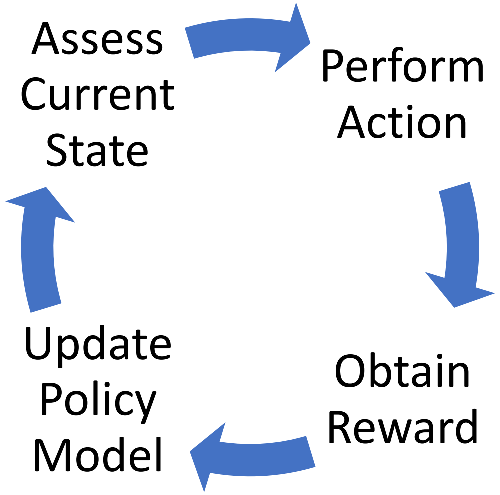
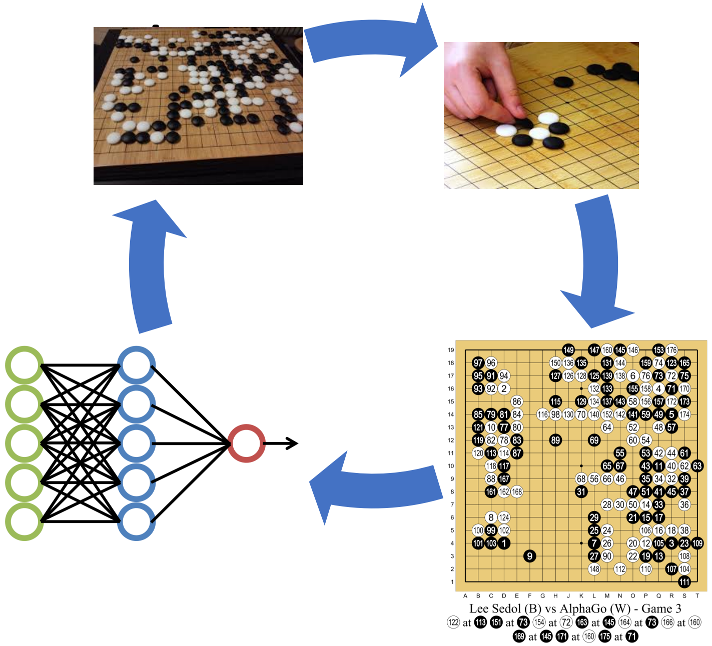
Reinforcement Learning (RL)

- Utilizing ML to learn through trial and error
  - RL agent is able to take actions, receive feedback, and use ML to attempt to learn an optimal policy for decision-making
- Current successes in iterative games like Go and StarCraft
  - But more broadly can think of action as “propose experimental design”, etc.





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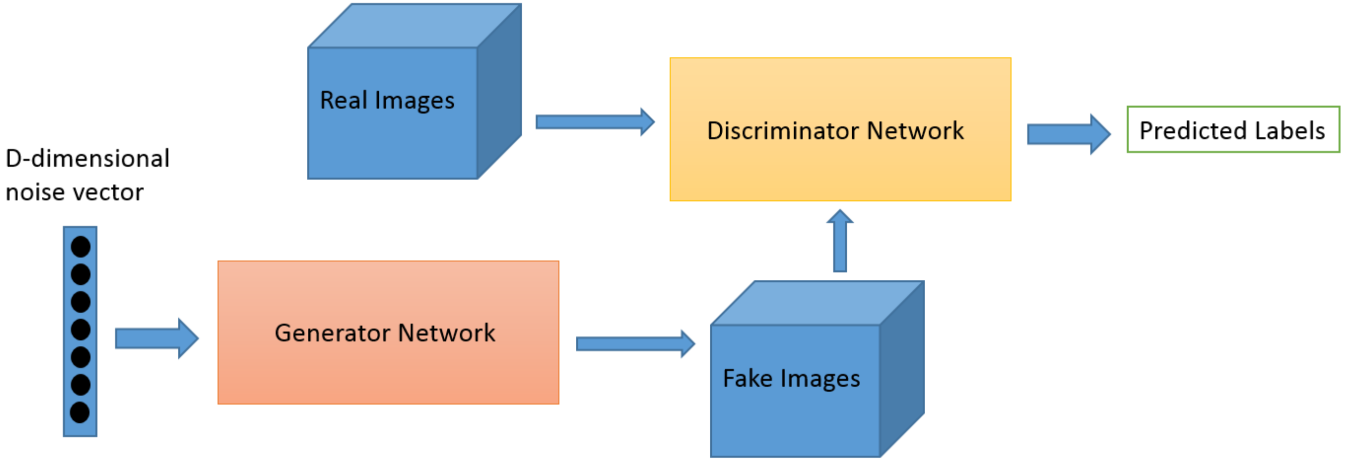
Generative Modeling

- Method for generating ‘realistic’ synthetic data
- One approach is Generative Adversarial Networks (GAN)
  - Build model to *generate* random synthetic data
  - Train a model to *discriminate* between real and generated data
  - Iteratively improve generator to fool discriminator and improve discriminator
- Popular for synthetic image generation, but new applications are being aggressively investigated



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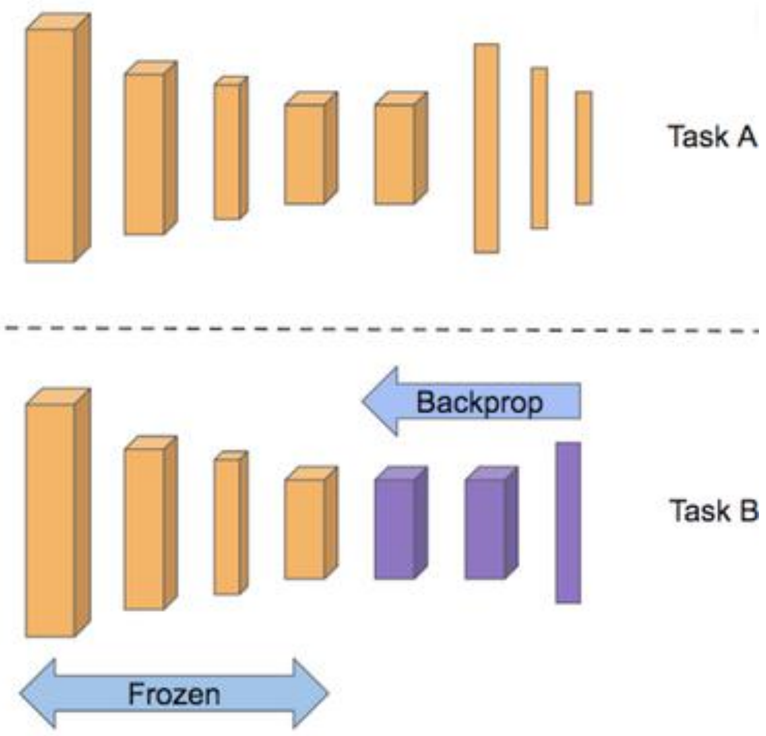
Transfer Learning

- Utilizing ML models trained on one application or data set, either in part or in whole, for use in another task
- Current work largely focused on fixing part of a neural network trained on one large set of data
  - The used with a task for which less data exists or the cost of training the full network would be prohibitive
- Takes advantage of intrinsic feature learning in early layers



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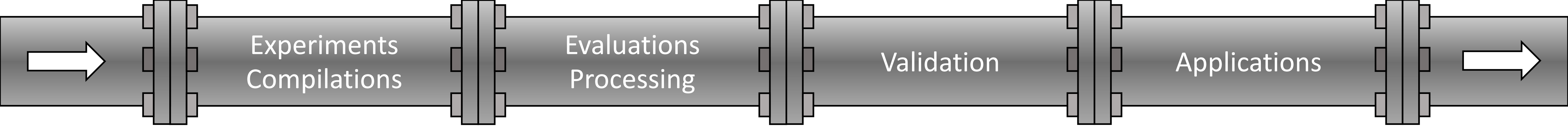
ML Interpretability

- Understanding what drives the prediction/decisions made by ML models is critical for building trust in their use and can lead to insight for physics problems
- Underlying prediction/decision models is some quantitative function
  - Assessment of how dependent predictions are on the input features can communicate importance
  - Local and global importance, individualized or holistic
- Close relation to sensitivity analysis in applied math and statistics



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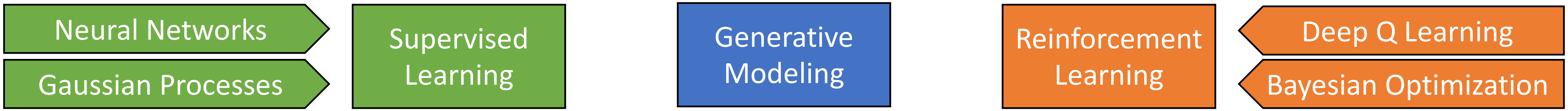

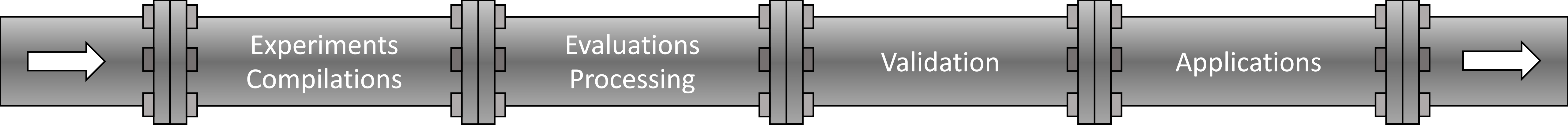

Nuclear Data Pipeline to AI/ML Methods

Vladimir Sobes
University of Tennessee

Neural Networks
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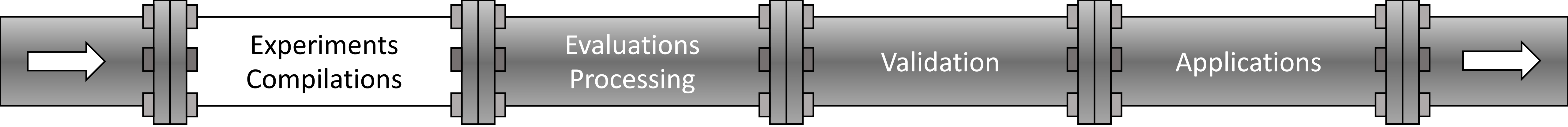

Compilation of Data

Experimental Measurements

PHYSICAL REVIEW C **95**, 064605 (2017)

Neutron scattering cross section measurements for ^{56}Fe

A. P. D. Ramirez,[1,*] J. R. Vanhoy,[2] S. F. Hicks,[3] M. T. McEllistrem,[1] E. E. Peters,[1] S. Mukhopadhyay,[1] T. D. Harrison,[2] T. J. Howard,[3] D. T. Jackson,[3] P. D. Lenzen,[3] T. D. Nguyen,[3] R. L. Pecha,[3] B. G. Rice,[2] B. K. Thompson,[2] and S. W. Yates[1]
[1]Departments of Chemistry and Physics & Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA
[2]Department of Physics, U.S. Naval Academy, Annapolis, Maryland 21402, USA
[3]Department of Physics, University of Dallas, Irving, Texas 75062, USA

(Received 25 January 2017; revised manuscript received 2 May 2017; published 9 June 2017)

Elastic and inelastic differential cross sections for neutron scattering from ^{56}Fe have been measured for several incident energies from 1.30 to 7.96 MeV at the University of Kentucky Accelerator Laboratory. Scattered neutrons were detected using a C_6D_6 liquid scintillation detector using pulse-shape discrimination and time-of-flight techniques. The deduced cross sections have been compared with previously reported data, predictions from evaluation databases ENDF, JENDL, and JEFF, and theoretical calculations performed using different optical model potentials using the TALYS and EMPIRE nuclear reaction codes. The coupled-channel calculations based on the vibrational and soft-rotor models are found to describe the experimental (n,n_0) and (n,n_1) cross sections well.

DOI: 10.1103/PhysRevC.95.064605

I. INTRODUCTION

Nuclear data play an important role in modeling future generation nuclear-energy systems [1–3]. Advanced high-temperature nuclear reactors, for example, are being designed for efficient energy generation while addressing safety, waste, and proliferation concerns. Several are under construction for use in the burn-up of heavy element radioisotopes associated with the large waste disposal pools from the operation of conventional energy-producing reactors. Computer models and simulations are used to predict the performance of these reactors under operating conditions, including the effects of severe irradiation on structural properties. These predictions require a vast knowledge of accurate and precise nuclear data, particularly cross sections from neutron-induced reactions.

Iron is one of the primary structural materials in many nuclear energy production systems, making Fe neutron scattering cross sections important input for neutron transport and energy absorption calculations. Elemental iron has four naturally occurring stable isotopes, with 91.75% abundant ^{56}Fe the most significant. In the fast-neutron energy region, the total cross sections for neutron-induced reactions on ^{56}Fe are dominated by elastic and inelastic scattering processes. A number of studies of fast-neutron scattering from ^{56}Fe have been reported [4–12]. Despite these efforts, there are still significant discrepancies among predictions from existing evaluated data libraries, particularly for the inelastic scattering processes [13]. Such discrepancies can be attributed to experimental data that have large or nonexistent uncertainties, lack of information on finite-size sample corrections, or inadequate inelastic scattering data [14]. In addition, sensitivity studies on important reactor quantities, such as criticality, require the reduction of neutron cross section uncertainties on actinides and structural materials to meet the target accuracies for advanced reactor designs [1–3]. Recent high-resolution measurements,

*ap.ramirez@uky.edu

TABLE III. Experimental and calculated angle-integrated cross sections based on spherical (sph), vibrational (vib), and soft-rotor (soft-rot) models for elastic, (n,n_1), (n,n_2), and (n,n_3) neutron scattering on ^{56}Fe. Cross sections are in units of b.

E_n (MeV)	Channel	Expt. (this work)	TALYS (sph)	TALYS (vib)	CC-rot (soft-rot)
4.00	(n,n_0)	2.48(17)	2.21	2.18	2.06
	(n,n_1)	0.455(20)	0.348	0.411	0.413
	(n,n_2)	0.129(8)	0.123	0.123	0.159
	(n,n_3)	0.175(8)	0.154	0.152	0.179
4.50	(n,n_0)	2.41(15)	2.160	2.14	2.098
	(n,n_1)	0.317(17)	0.254	0.311	0.306
	(n,n_2)	0.108(8)	0.091	0.092	0.116
	(n,n_3)	0.125(8)	0.115	0.115	0.131
4.90	(n,n_0)	2.29(15)	2.12	2.10	2.11
	(n,n_1)	0.284(37)	0.199	0.254	0.238
	(n,n_2)	0.100(9)	0.071	0.071	0.083
5.94	(n,n_0)	2.13(21)	2.05	2.03	2.07
	(n,n_1)	0.205(22)	0.129	0.182	0.157
	(n,n_2)	0.064(9)	0.039	0.038	0.047
6.96	(n,n_0)	1.94(13)	1.96	1.94	1.99
	(n,n_1)	0.132(11)	0.098	0.151	0.125
	(n,n_2)	0.030(5)	0.023	0.022	0.031
7.96	(n,n_0)	1.92(13)	1.85	1.83	1.87
	(n,n_1)	0.126(10)	0.081	0.134	0.105

relation reducing significantly the number of optical potential parameters [45]. Here, we adopted the parameters from Ref. [43], which can be retrieved from the reference input parameters library (RIPL-3) [46] with index number 614. The parameters from Ref. [43] are assumed to be valid for iron isotopes with mass numbers between 54 and 58 and incident neutron energies between 1 keV and 250 MeV. These parameters were used as input to the nuclear reaction program EMPIRE [45] to calculate neutron elastic and inelastic cross sections. The calculations include the code OPTMAN [47] which incorporates level-coupling schemes based on a non-axial soft-rotor model to account for the stretching of soft nuclei by rotations.

The comparison between our data and the dispersive coupled-channel calculation based on the soft-rotor model from Ref. [43] at E_n = 6.96 and 7.96 MeV are shown in Fig. 6. A tabulation of the calculated cross sections from different model calculations is given in Table III. Only the data for $E_n \geqslant$ 4 MeV are presented since these cross sections are shown to vary smoothly with bombarding energy according to the ENDF evaluations. All the models were able to describe the elastic cross sections well within 10% for $E_n \geqslant$ 4.90 MeV. The (n,n_1) cross sections obtained from the coupled-channel formalism using the optical potential parameters from Ref. [43] better describe the data than the spherical optical model calculations, although a noticeable underestimation is found for neutron energies 4.90 and 5.94 MeV. For the (n,n_2) and (n,n_3) cross sections, most of the theoretical values are found to be smaller than the experimental ones. The (n,n_2) and (n,n_3) cross sections from TALYS vibrational and spherical model calculations are almost identical as both are calculated using the DWBA.

VI. CONCLUSION

The angular distributions for neutron scattering from ^{56}Fe were measured at 15 incident neutron energies from 1.30 to 7.96 MeV. The neutron scattering cross sections deduced from these data have been compared with values from evaluation databases. Reasonable agreement has been observed for data above 3.5 MeV, although our data tend to be closer to the cross sections from the JEFF library. Our angle-integrated (n,n_1) cross sections, representing the dominant inelastic channel for neutron energies of 5.94 and 7.96 MeV, are slightly higher than those in the evaluations. This result does not support the assertion of Wenner *et al.* [35] that the total inelastic cross section from the ENDF database should be lower by at least 20%.

We have also compared our experimental results with predictions from theoretical calculations using TALYS with default parameters and coupled-channel calculations based on the vibrational model, as well as the EMPIRE nuclear reaction code based on the soft-rotor model with optical model potential parameters from Ref. [43]. In general, the calculations were able to describe the present differential elastic scattering cross sections well, particularly for neutron energies above 4.5 MeV. When the TALYS default were used to calculate the (n,n_1) cross sections through the DWBA method, the predictions significantly underestimated the experimental data for E_n > 3.5 MeV. The TALYS predictions can be improved by employing the coupled-channel vibrational model but with a 64% reduction in the imaginary surface potential depth. Similarly, the EMPIRE calculations based on the soft-rotor model were also found to describe the inelastic cross sections well.

ACKNOWLEDGMENTS

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Belgium, 2005, edited by P. Rullhusen (World Scientific, 2006), pp. 18–31.
G. Palmiotti, M. Salvatores, T. K. Kim, T. A. Tai
Sartori, J. C. Bosq, and J. Tommasi, in Proceed

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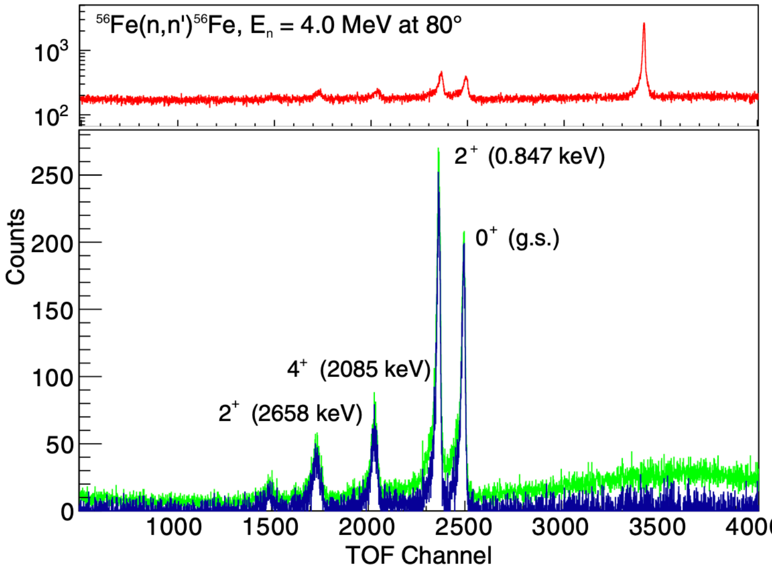

FIG. 1. Typical TOF spectra containing events from the detection of both neutrons and γ rays (red), neutrons only after pulse-shape discrimination (green), and also neutrons only after background subtraction (blue). In the top spectrum, peaks in the middle correspond to events from scattered neutrons while the largest peak on the right corresponds to events from the detection of prompt γ rays.

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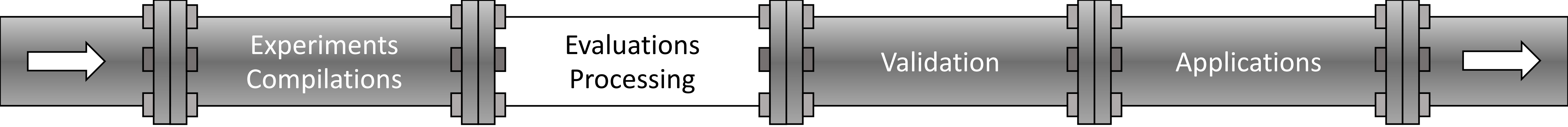
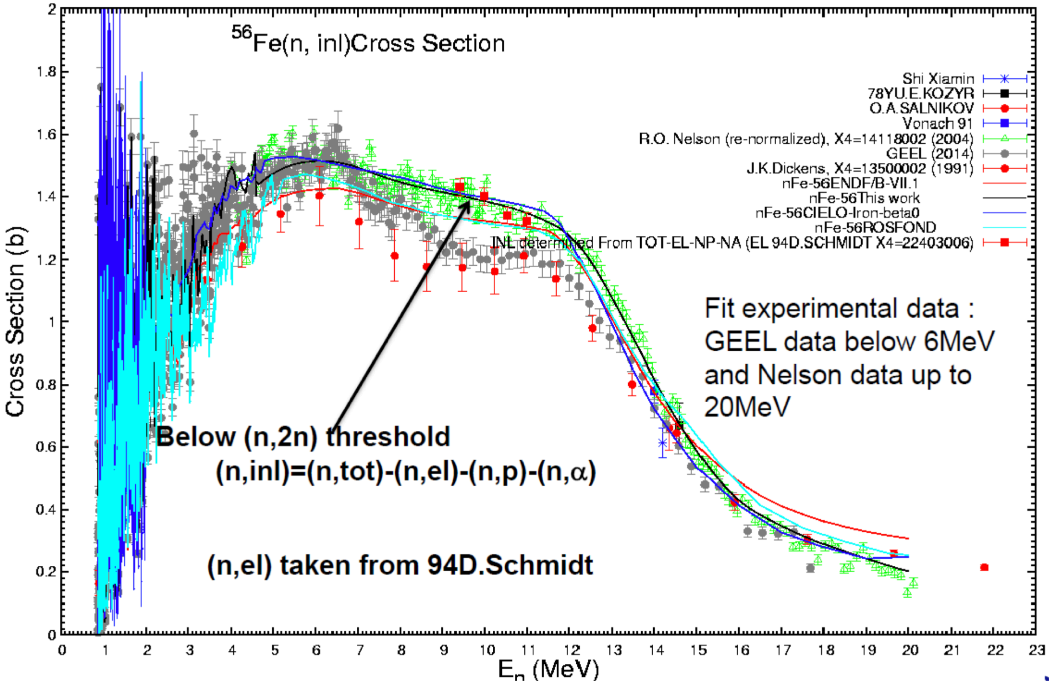
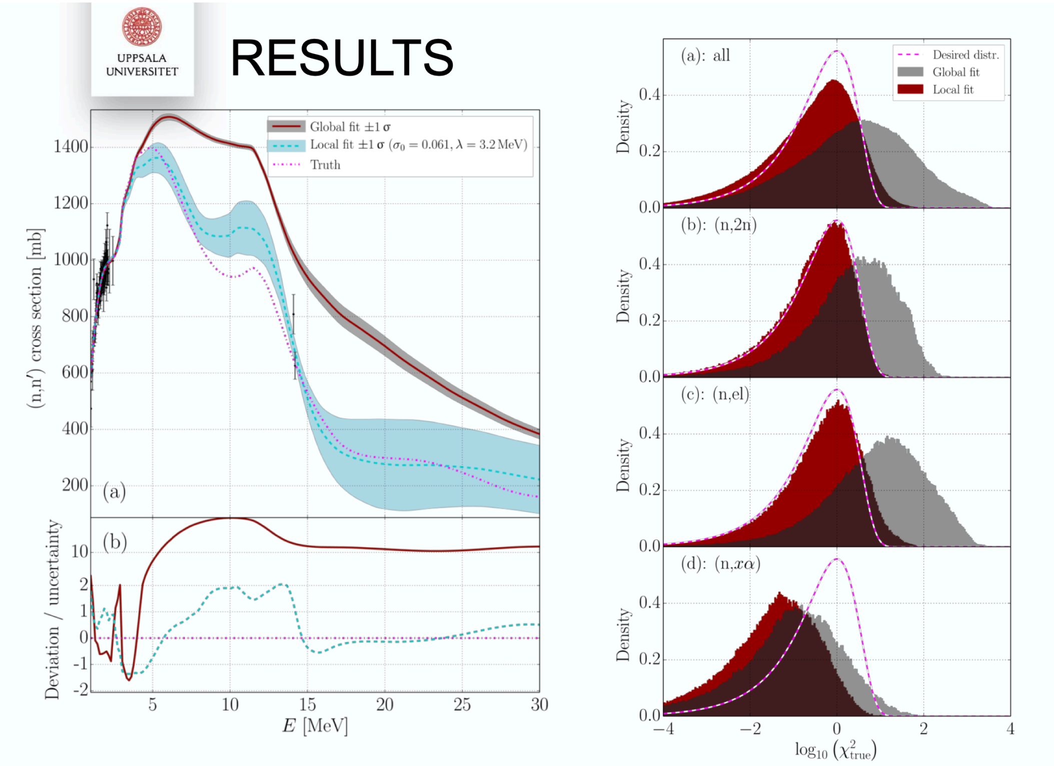


Evaluation of Mean Values

Evaluation of Uncertainty





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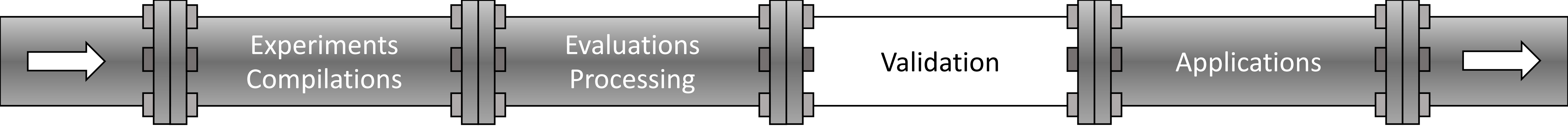
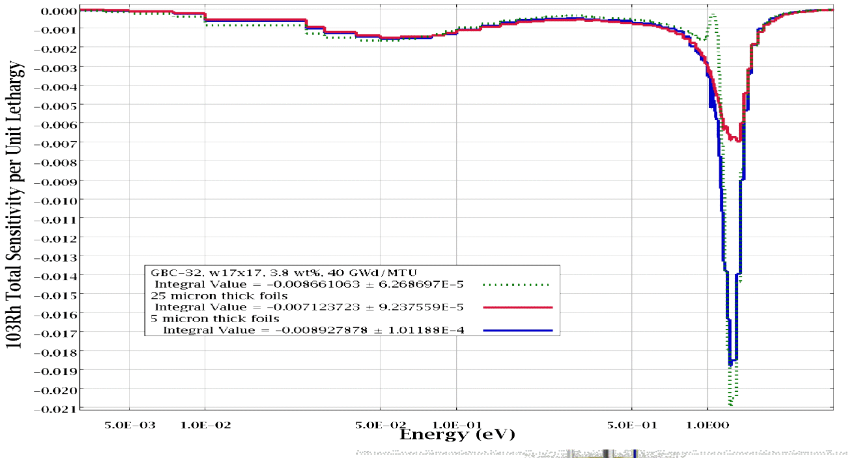
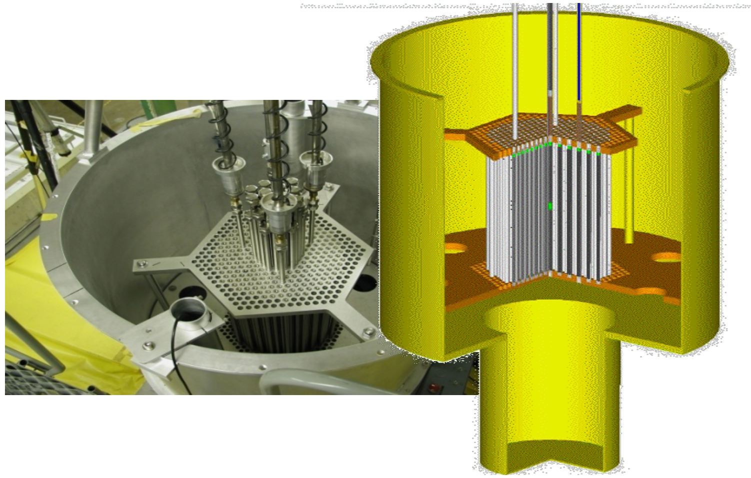
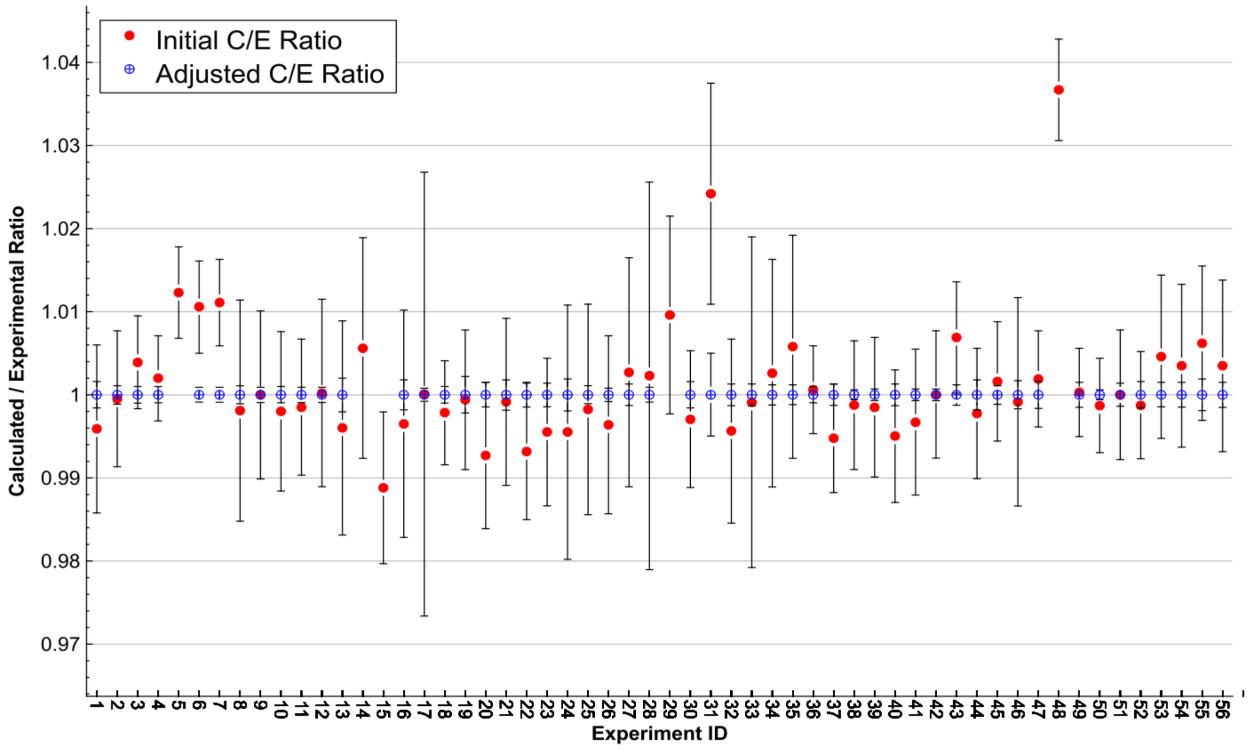


Experiment Design





Nuclear Data Validation



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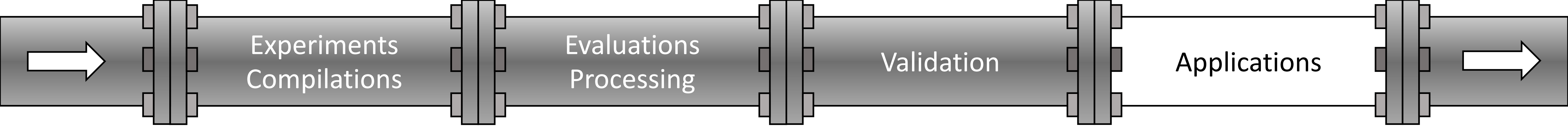
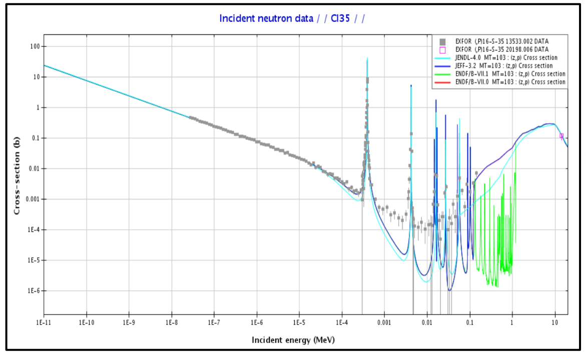
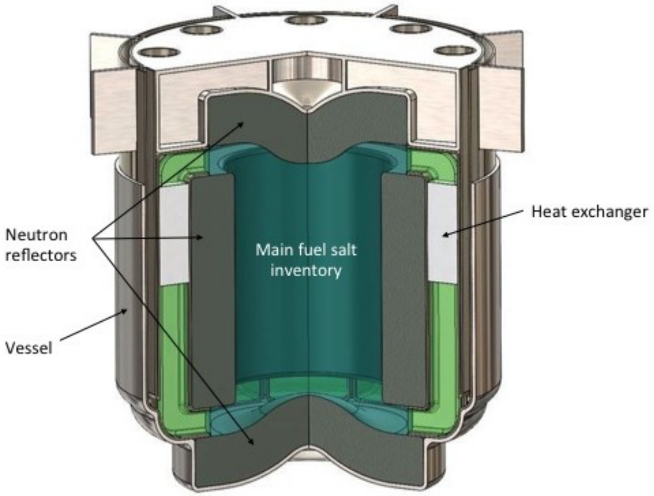


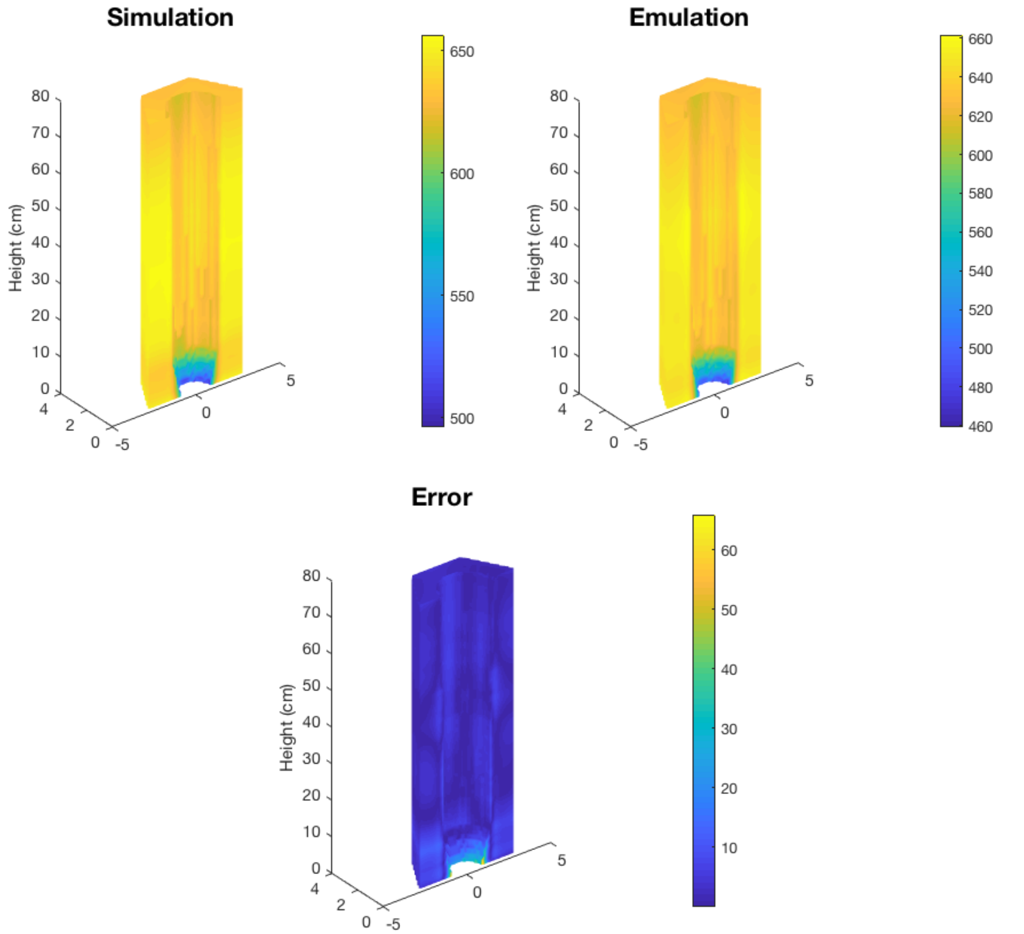
Nuclear Data Impact on Application





A change in absorption cross section of ^{35}Cl resulted in 2000 pcm change in BOL k_{eff}

Surrogates in Applications Modeling



Neural Networks

Gaussian Processes

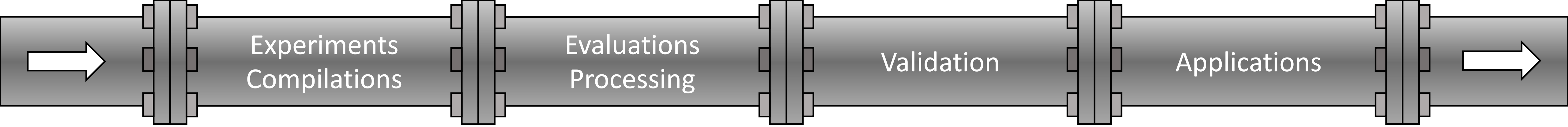
Supervised Learning

Generative Modeling

Reinforcement Learning

Deep Q Learning

Bayesian Optimization



AI/ML for Nuclear Data

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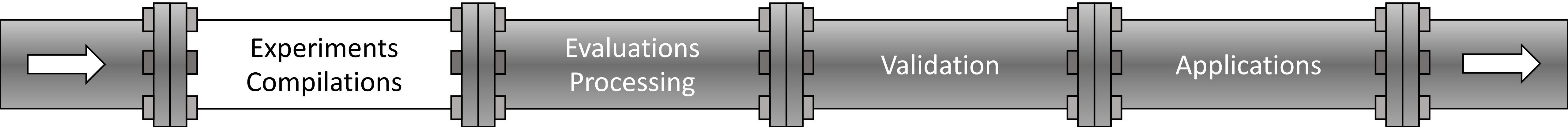
Nuclear data application area

- Incomplete or incorrect data can lead to very precise and very inaccurate predictions

https://projects.fivethirtyeight.com/2016-election-forecast/



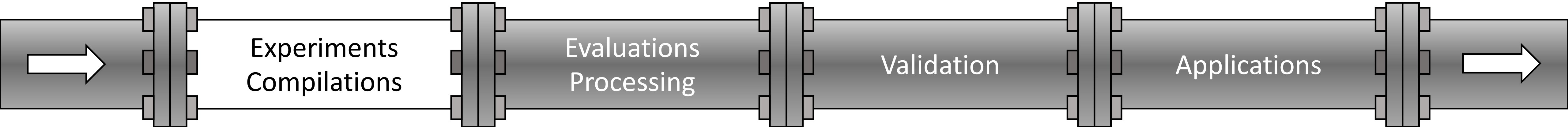
Nuclear data application area

- Machine learning is dependent on standardized data that is quality-verified and well-characterized

"EXFOR is a **compilation of the author's original published experimental data**.

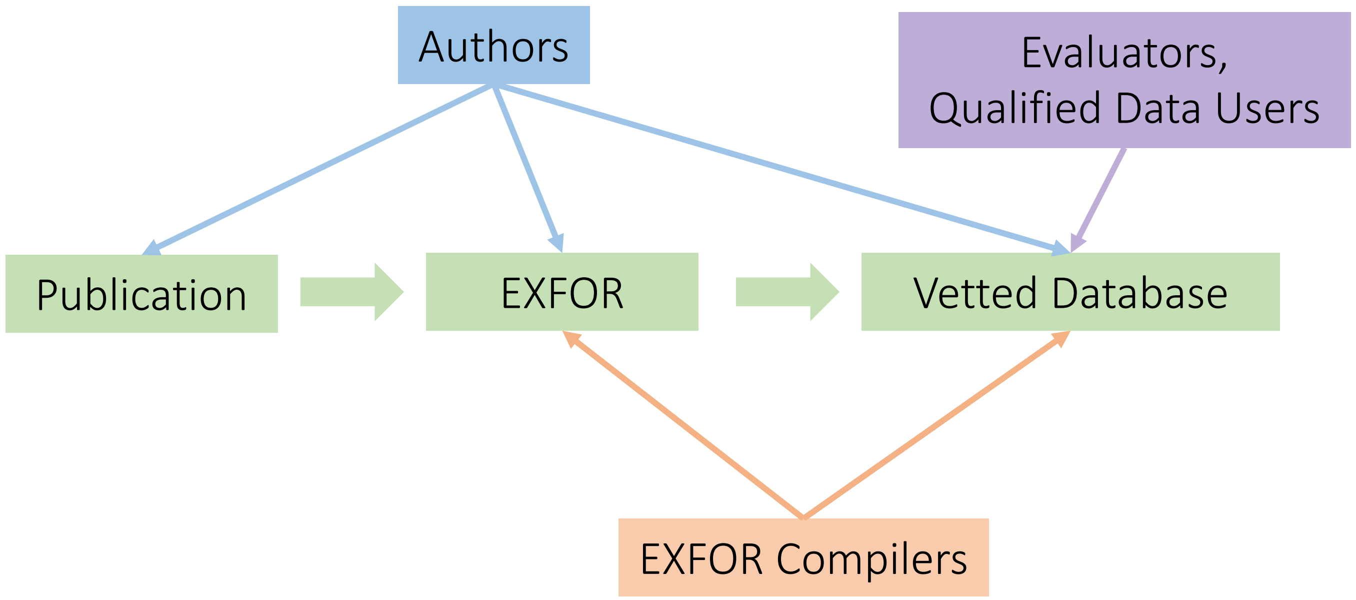
While the format allows the inclusion of data renormalized to up-to-date standard values… this task is normally left to data evaluators…"

– Principles of EXFOR

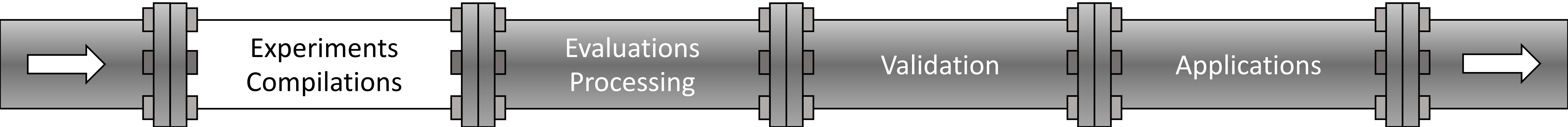


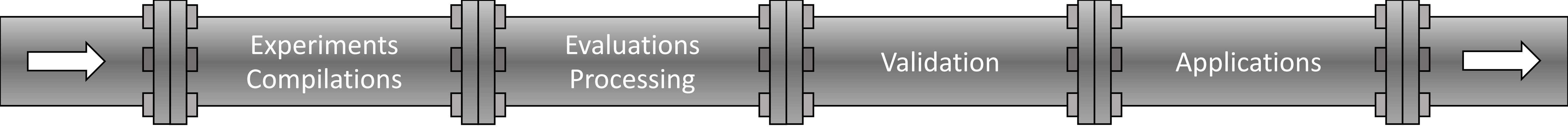
Future

- A new database is needed, parallel to (or included within) EXFOR for **vetted, standardized, and possibly adjusted** data sets



- Standardization is especially important, for both formats and uncertainties
- This work is already done by evaluators for evaluations and should be done for current ML projects using EXFOR
- Natural language processing and currently available ML data verification software can be utilized for large scale checks





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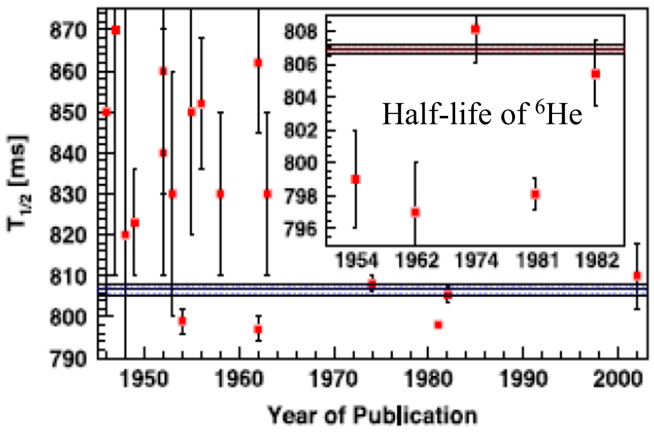
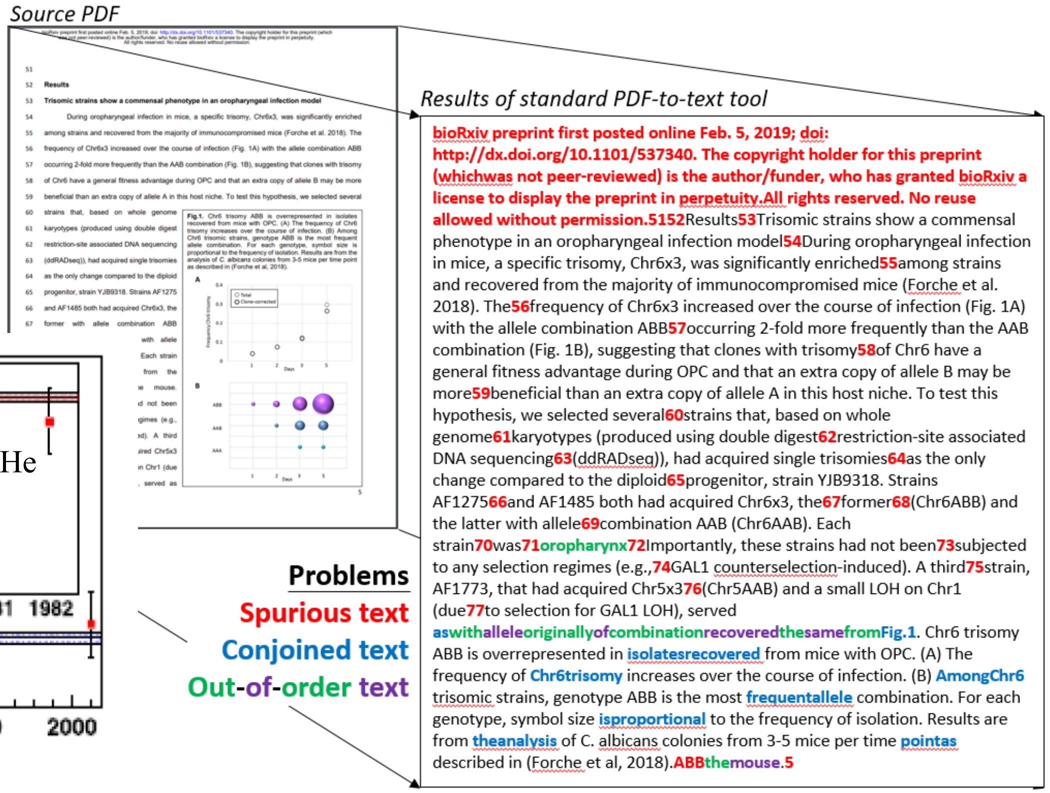
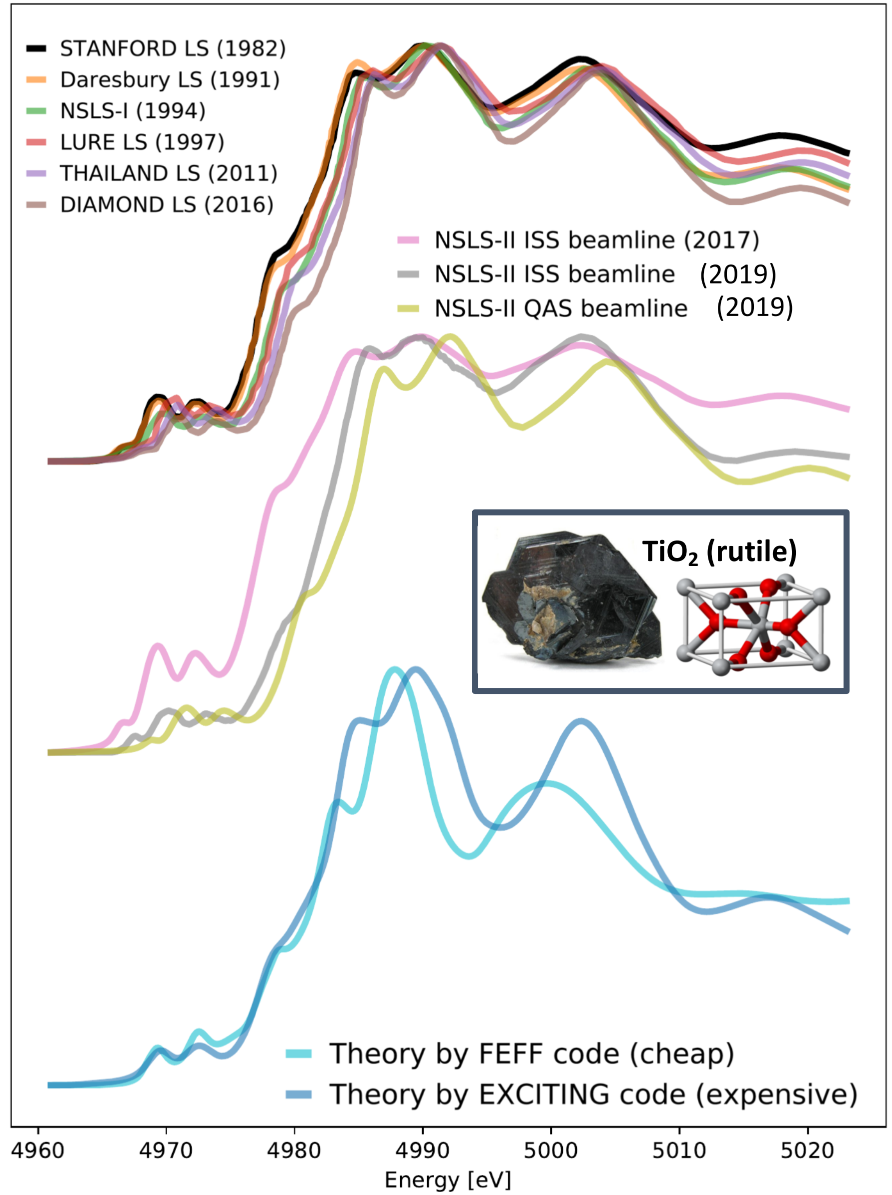
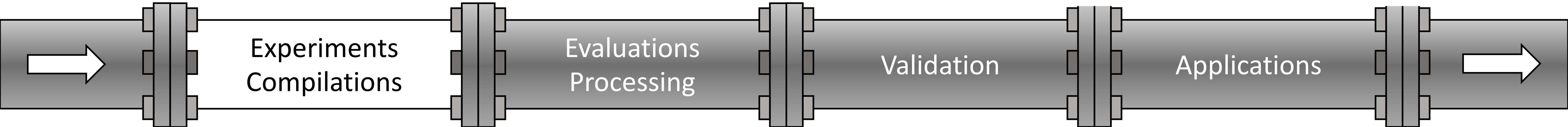
Nuclear data application area

- Diverse quality in experiments and simulations
- Collection errors in processing pipeline



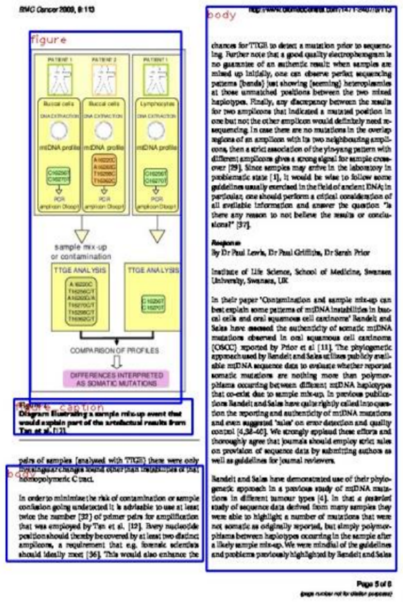


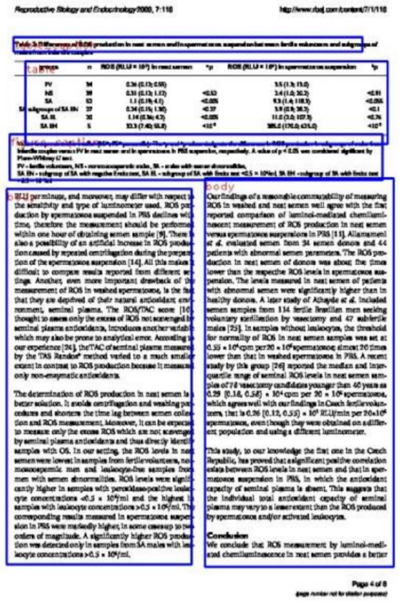


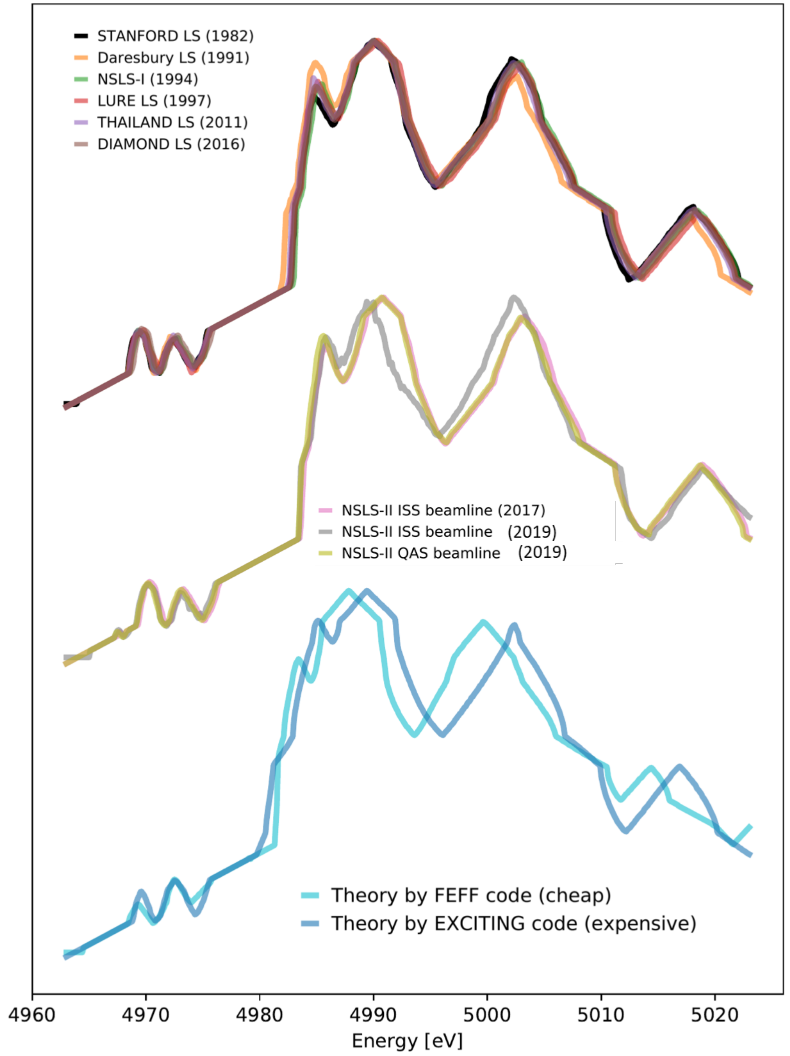


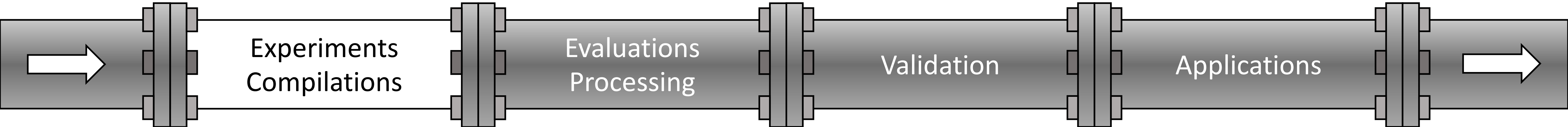
Nuclear data application area

- Adopted non-parametric transformation and alignments
- Visual layout analysis to suppress PDF processing



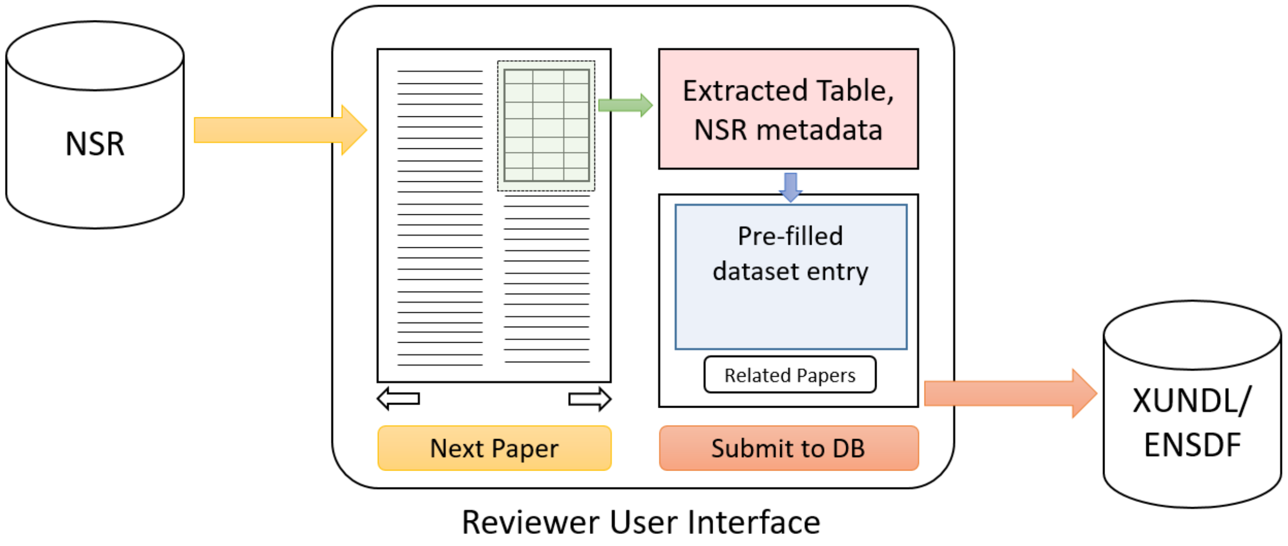




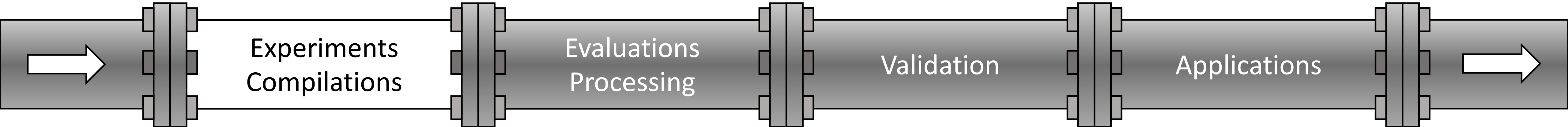


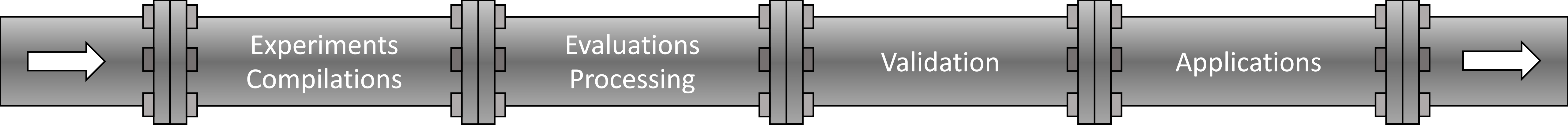
Future

- Batch effect mitigation or removal tools to be used by AI/ML
  - Such tools / algorithms could be AI/ML methods
  - Developed such algorithms for material science and bio-medical domain
- A fully automated NLP pipeline with reviewer user interface



- NLP can not be 100% accuracy and requires human validation
  - Intuitive user interface is required for expert validation
- Automation can significantly reduce manual data extraction burden
  - Table and Figure extraction from PDF





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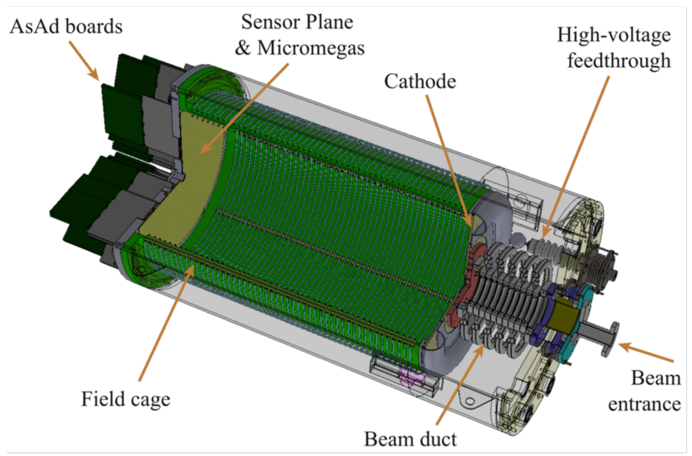
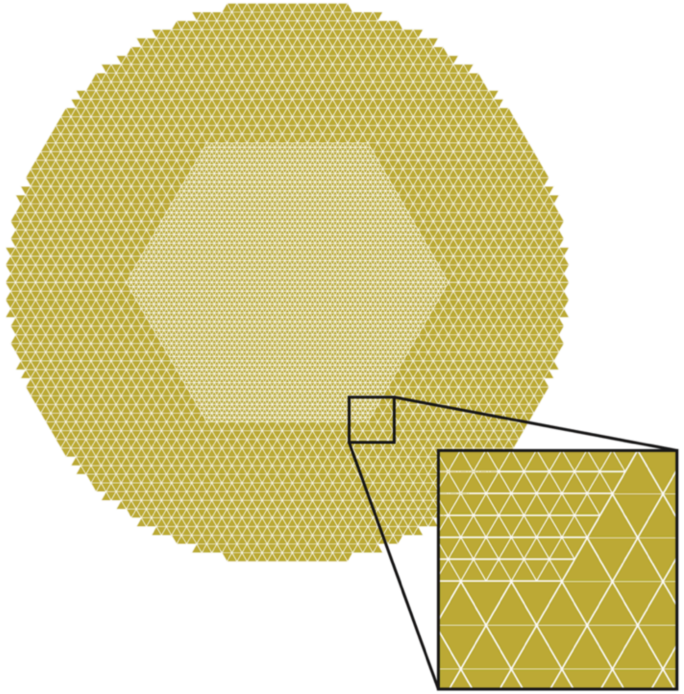
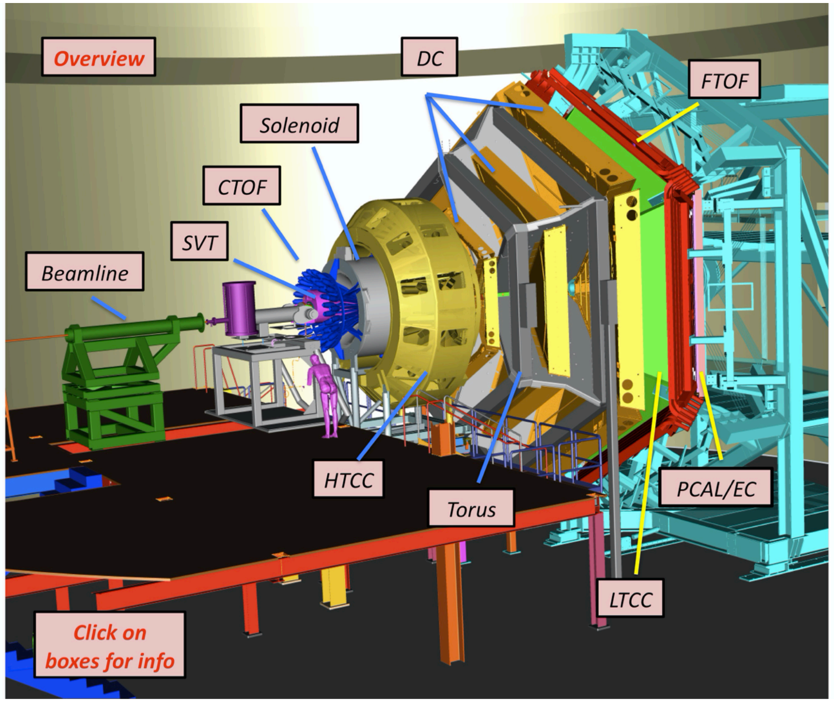
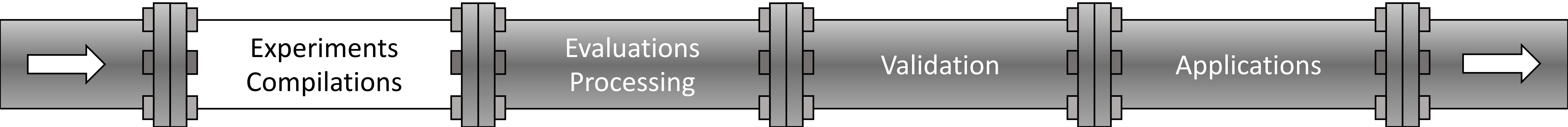
Nuclear data application area

- Fast track selection or event classification in "big data" detectors



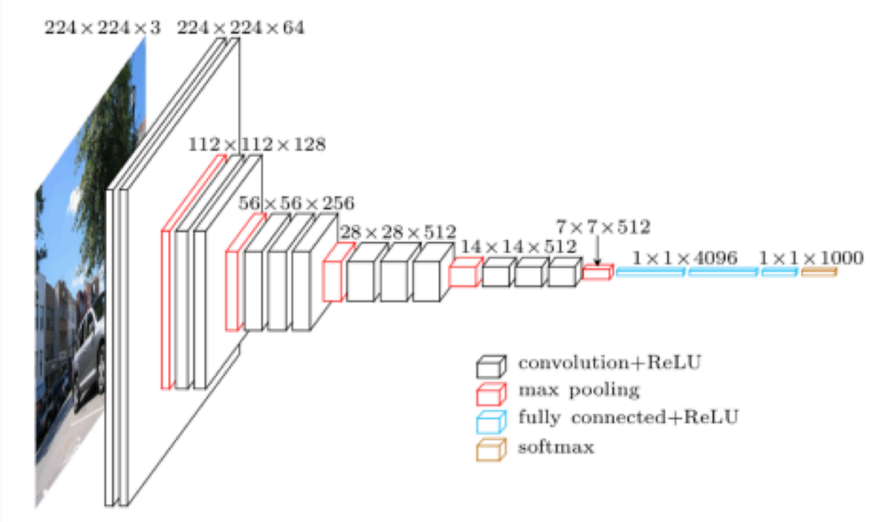






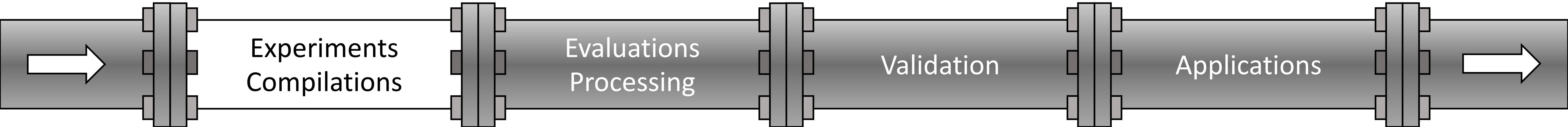
What has been done

- Convolutional Neural Networks



Experiment	Precision	Recall	F1
Experimental → Experimental	0.96	0.90	0.93
Simulated → Simulated	1.00	1.00	1.00
Simulated → Experimental	0.90	0.60	0.72

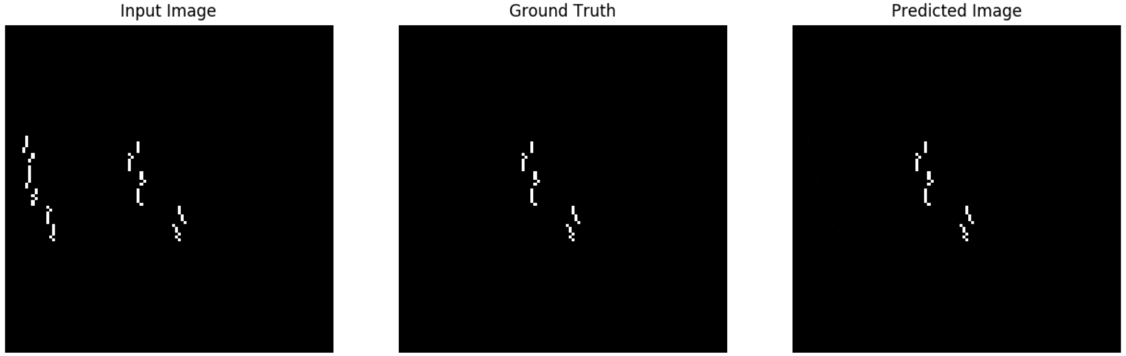
Precision	Recall	F1
0.97	0.93	0.95

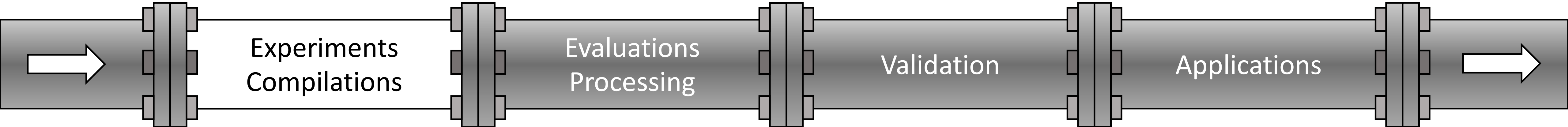


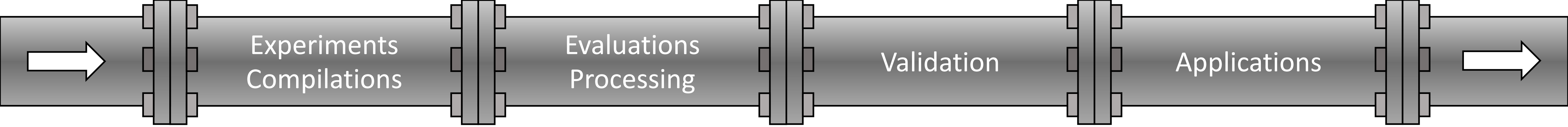
Future

- Current work:
  - cycleGAN
  - Pix2pix

- Can we improve classification using GAN data?
- Can we reproduce these results in 3D to better simulate realistic data?







AI/ML for Nuclear Data

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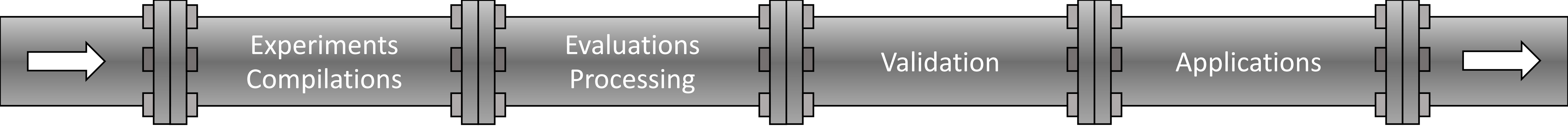

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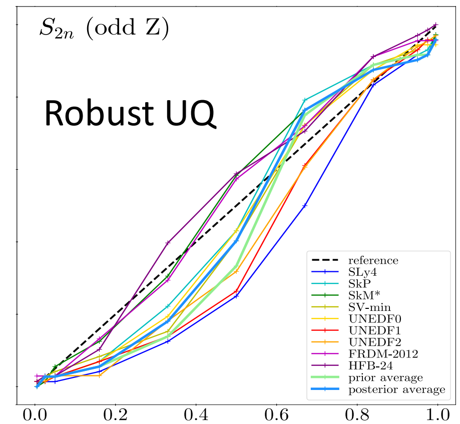
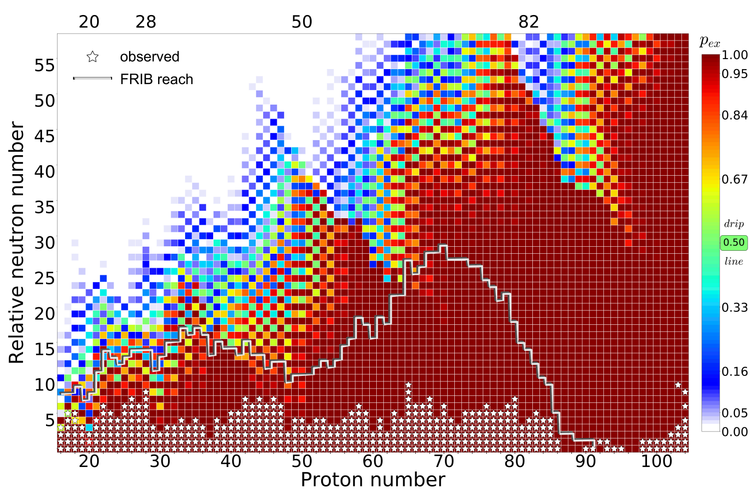
What type of problem can this solve?

→ Robust extrapolation of nuclear observables

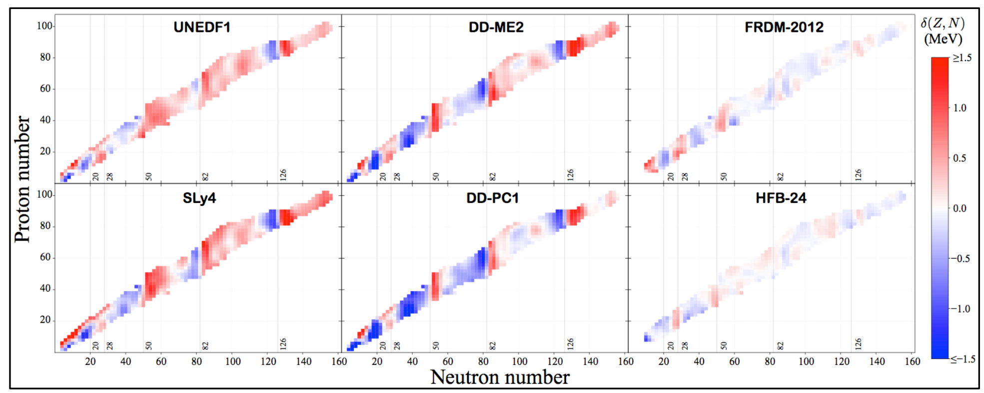


[L. N. et al, Phys. Rev. Lett. 122 (2019)]



Probability of existence of neutron-rich nuclei

[L. N. et al, submitted (2020)]



Evaluation of systematic errors

[L. N. et al, Phys. Rev. C 98 (2018)]

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How does the method work?

- Train Bayesian Gaussian Processes / Neural Network emulators on residuals

$$\delta(Z,N) = S_{2n}^{\text{exp}}(Z,N) - S_{2n}^{\text{th}}(Z,N,\vartheta) \longrightarrow S_{2n}^{\text{est}}(Z,N) = S_{2n}^{\text{th}}(Z,N,\vartheta) + \delta^{\text{em}}(Z,N)$$

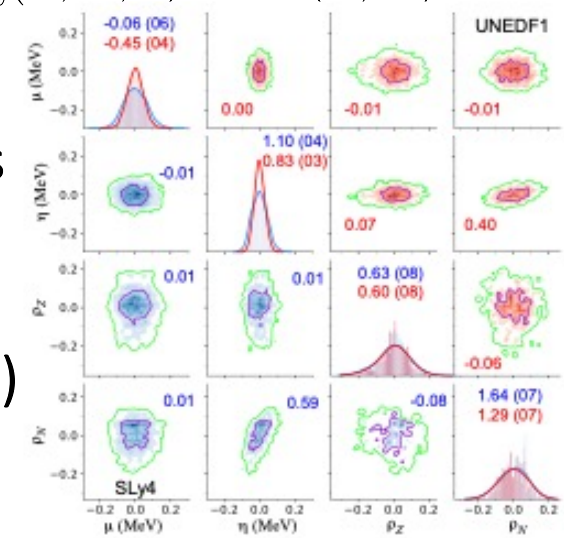
GP outperforms NN

- Sample refined predictions from posterior distributions

$$p(\Theta|y) \propto p(y|\Theta)\boldsymbol{\pi}(\Theta) \longrightarrow p(y^*|y) = \int p(y^*|y,\Theta)p(\Theta|y)d\Theta$$

- Combine models with Bayesian Model Averaging (BMA)

$$p(\mathcal{M}_k|y) = \frac{p(y|\mathcal{M}_k)\pi(\mathcal{M}_k)}{\sum_{\ell=1}^{K} p(y|\mathcal{M}_\ell)\pi(\mathcal{M}_\ell)}$$



[L. N. et al, Phys. Rev. C 101 (2020)]

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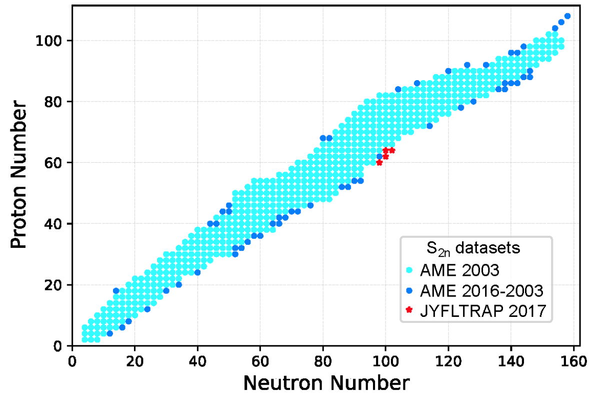
What is needed to use these tools?

- A set of experimental data
  - Divided into training and testing set
  - Bayesian models are meaningful even with little data



[L. N. et al, Phys. Rev. C 98 (2018)]

- A set of theoretical calculations for models of interest

- Computing cores for Monte-Carlo simulations

  → conditional distributions of GP on large dataset require $O(n)$ matrix inversions

  → ~ 50 cores x 1 week per model

Neural Networks | Gaussian Processes | Supervised Learning | Generative Modeling | Reinforcement Learning | Deep Q Learning | Bayesian Optimization

Experiments Compilations → Evaluations Processing → Validation → Applications

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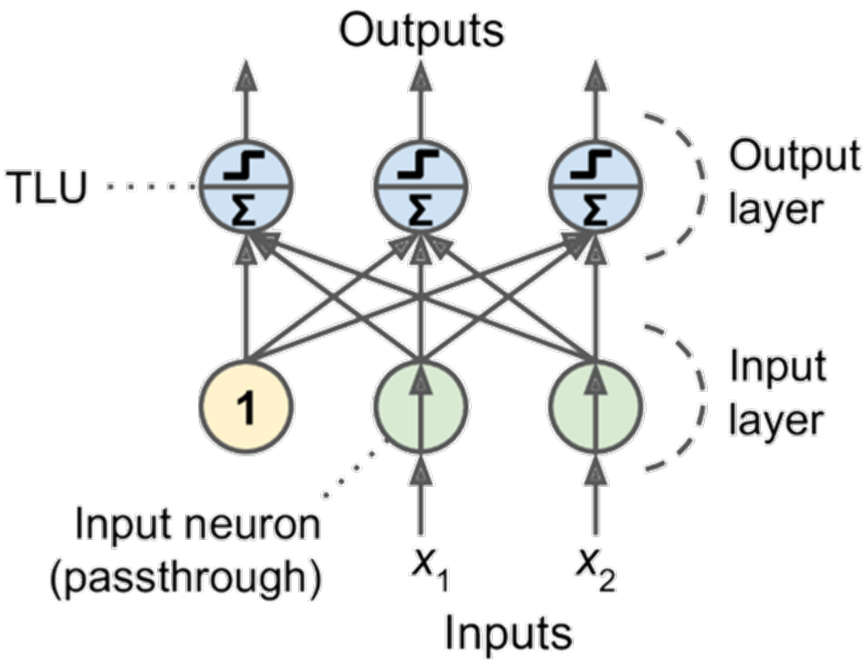
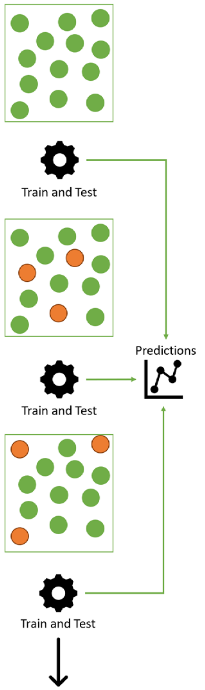
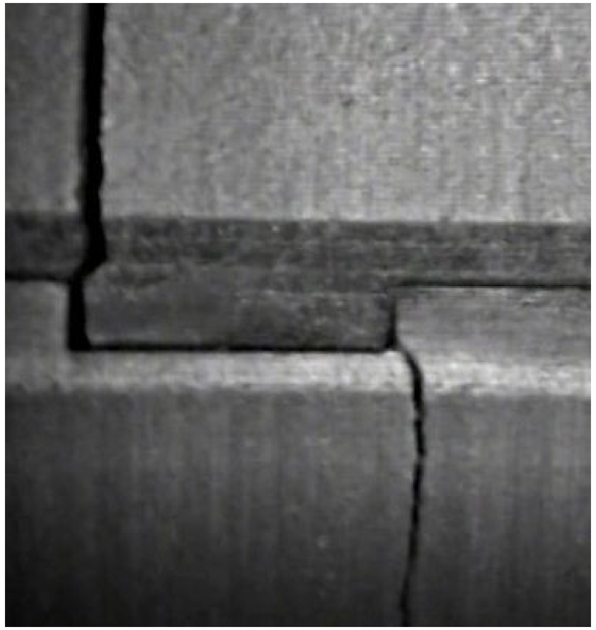
What type of problems can this solve? – DNN and GB

- MLPs **compute the gradient** with respect to every model parameter (coefficients) and it is used to **perform a Gradient Descent step.**
- **GBM** trains many weak learners to create a strong learner (**ensemble method**).



Aurelien Geron, 2019





Neural Networks, GB

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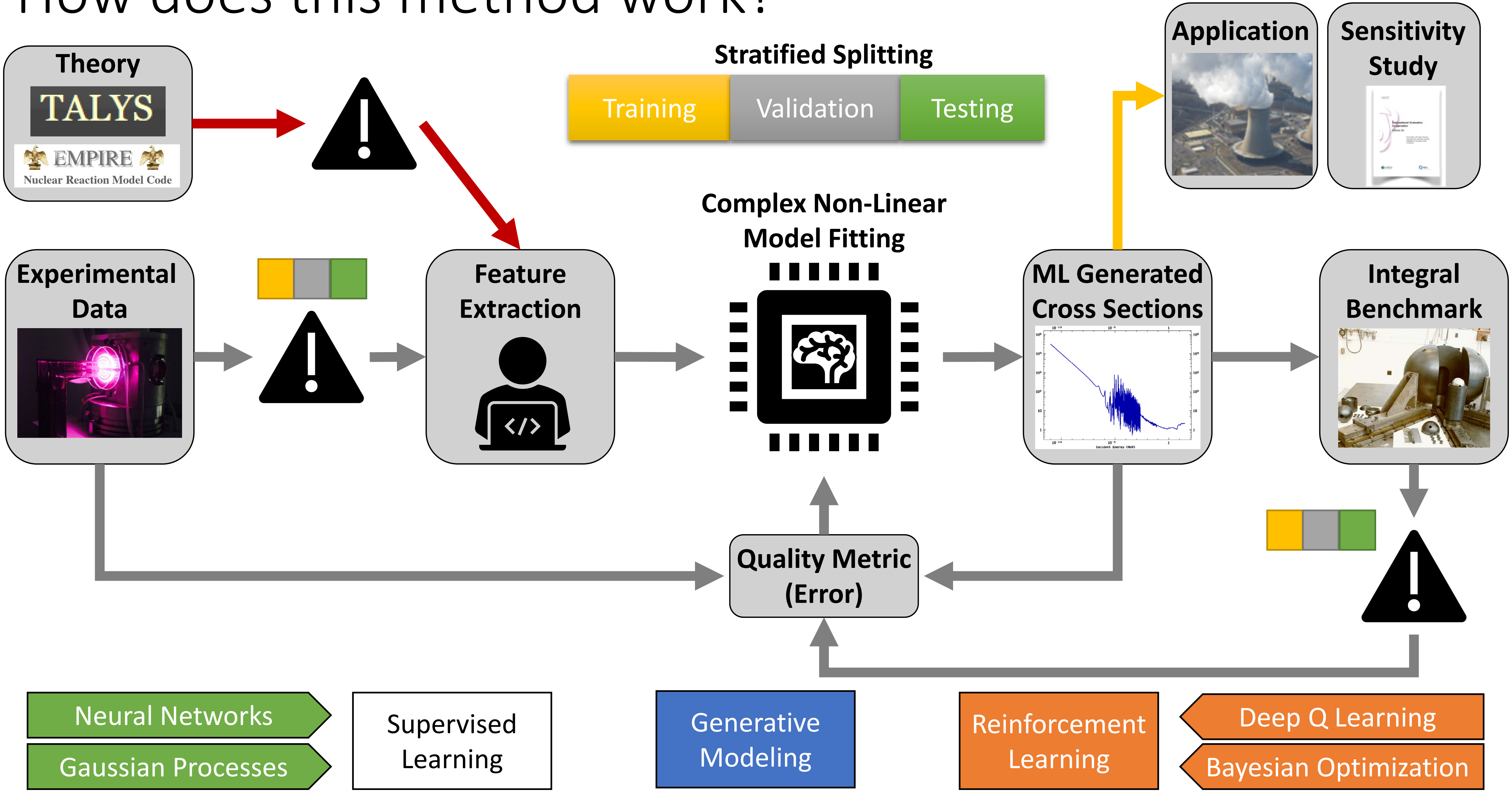
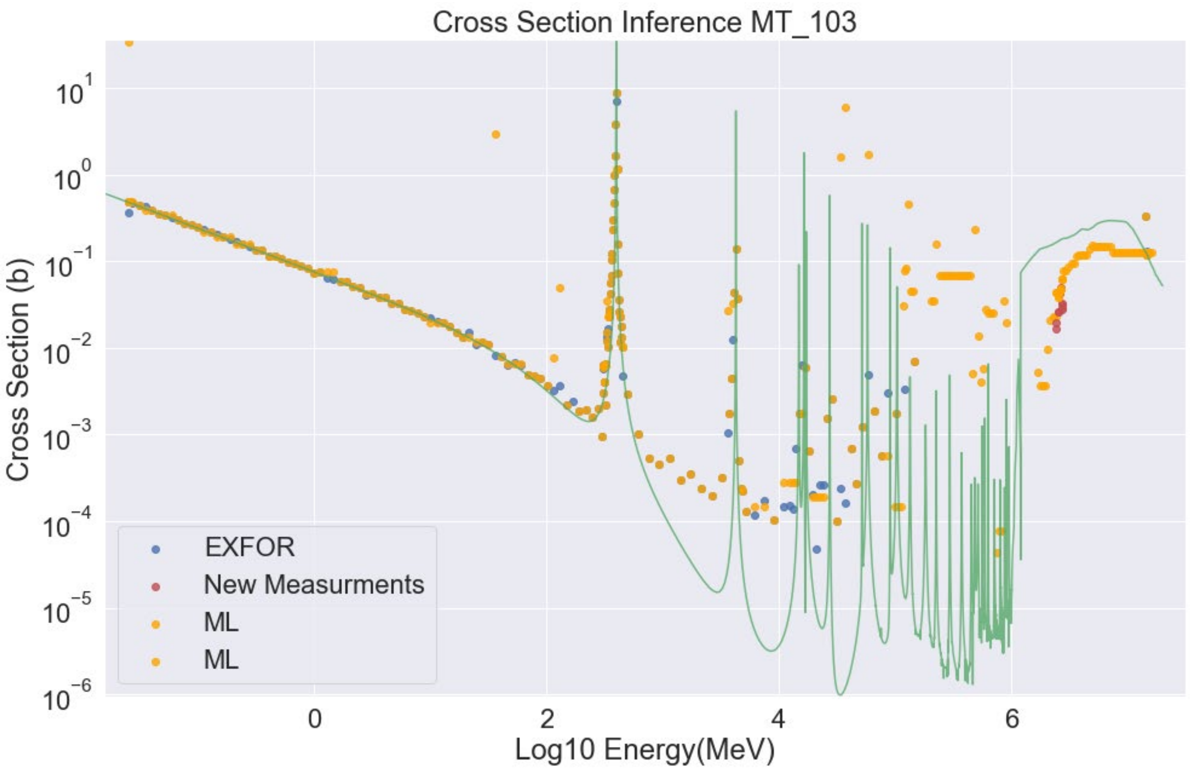
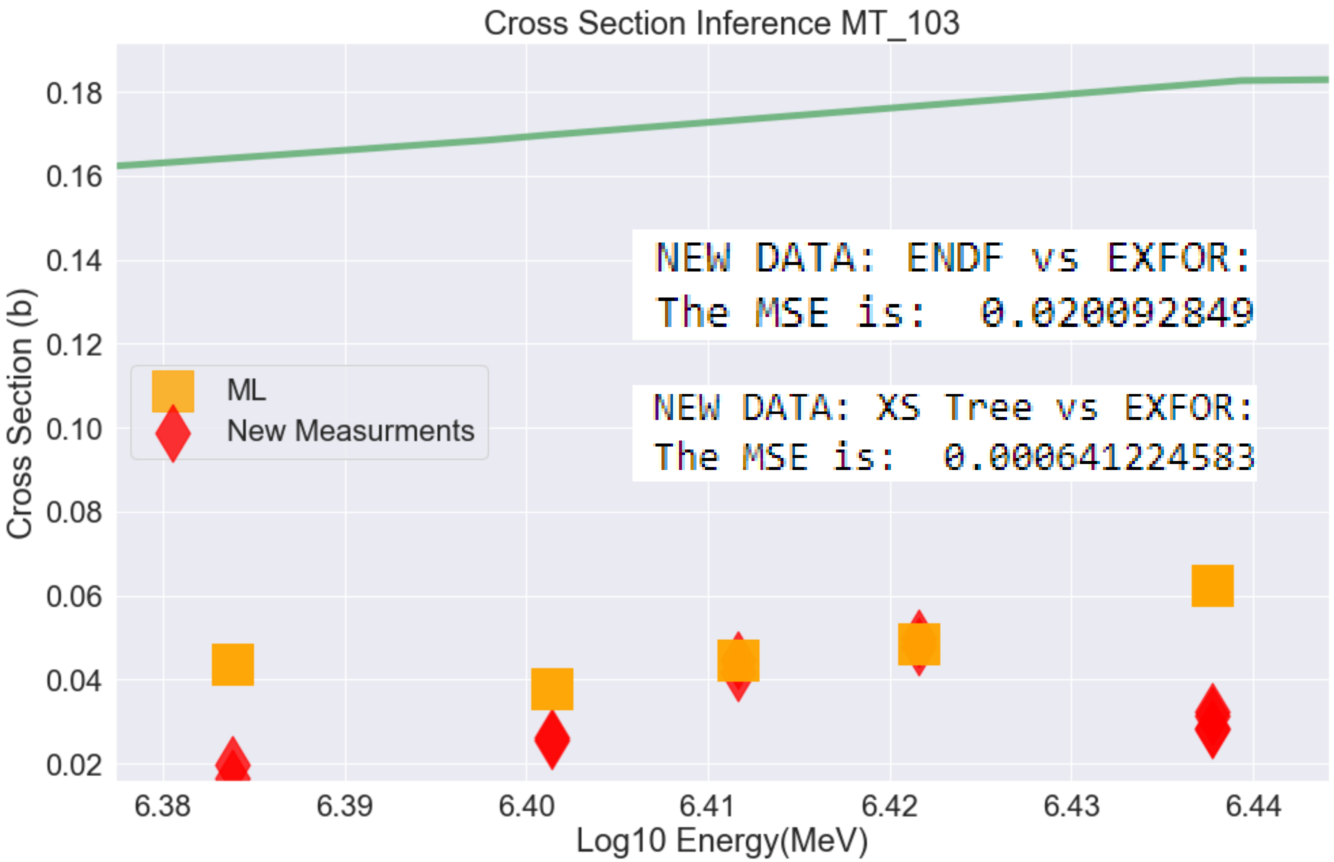
How does this method work?



What is needed to use these tools? – Representative Data!

- Measurements of other isotopes in the same reaction channel and energy range enable a GBM ML model to make better predictions than traditional evaluation tools.





GBM

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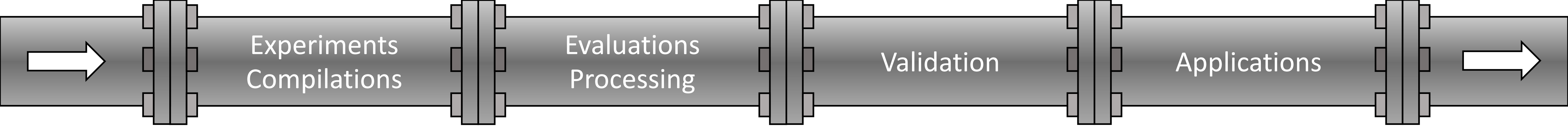

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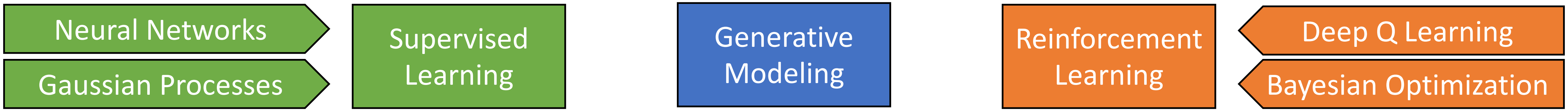

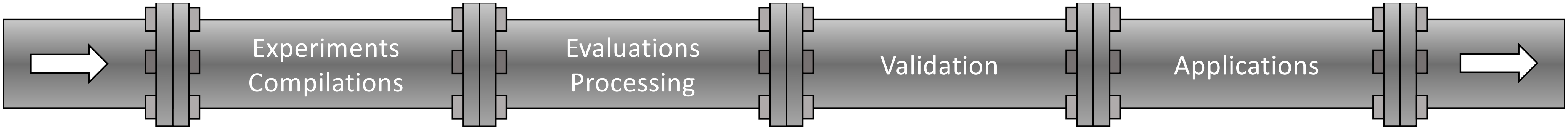

AI/ML for Nuclear Data

Building robust science-based evaluations and establishing guidance for next-generation reaction theories

Jutta Escher
escher1@llnl.gov

Workshop for Applied Nuclear Data Activities
George Washington University
March 3-5, 2020
Washington, D.C.

Lawrence Livermore National Laboratory
LLNL-PRES-xxxxxx
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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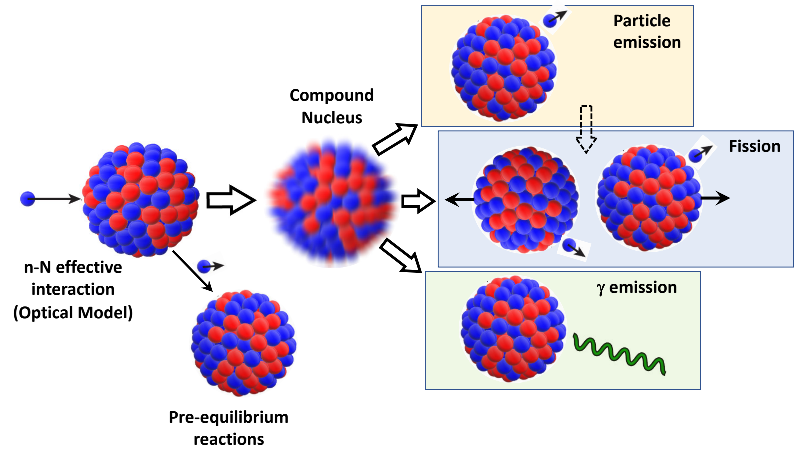
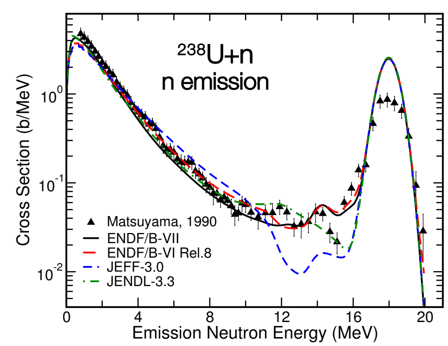
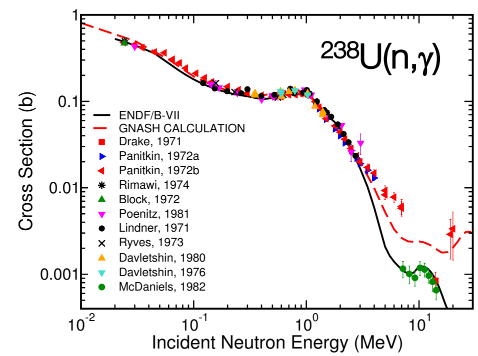
Nuclear data application area

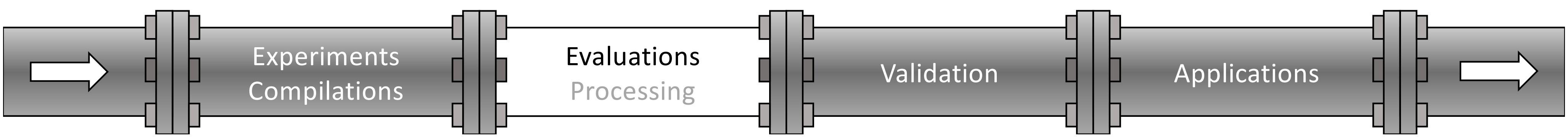
Evaluated and predicted cross sections are critical to national security, energy and astrophysics applications

- Reaction data must be evaluated for use in applications
  - Central tool: Extended Hauser-Feshbach reaction framework
  - Uses diverse mix of structure & reaction models
- Challenges for reaction evaluations
  - Correlated reaction channels
  - Correlations across isotopes
  - No optimal combination of models
  - No model uncertainties
  - Need to sample models and large parameter spaces
  - Data do not give unique constraints to disentangle inputs
- Additional challenges for predictions
  - Lack of constraints
  - Extrapolation of models







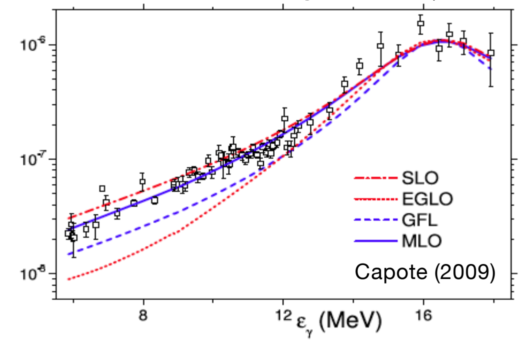


What has been done

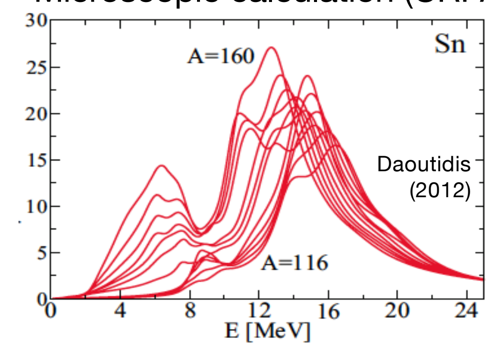
Significant progress in recent years, but work remains to be done

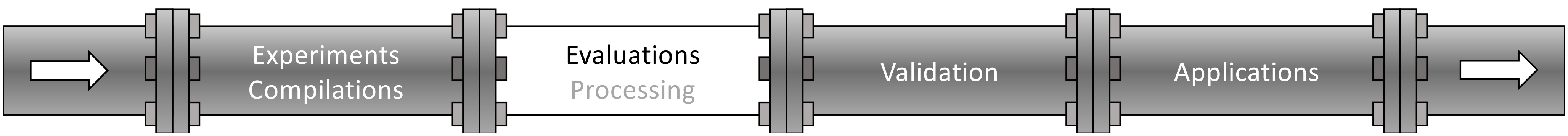
- Significant progress in improving reaction framework
  - Nuclear structure: phenomenological models complemented by microscopic theories (e.g. E1 strength, level densities)
  - Reaction mechanisms are being revisited (e.g. pre-equilibrium)
  - Limited use of AI/ML tools so far
- Significant progress in quantifying uncertainties
  - From fitting visually to minimizing χ^2 to Bayesian approaches
  - Importance of covariances is recognized
  - Use of AI/ML techniques just starting
- Predictions - extrapolations are problematic
  - Models are extrapolated to regions where they have not been validated
  - ML techniques useful for improving microscopic theories (e.g. mass models)

Phenomenological E1 γSF



Microscopic calculation (CRPA)



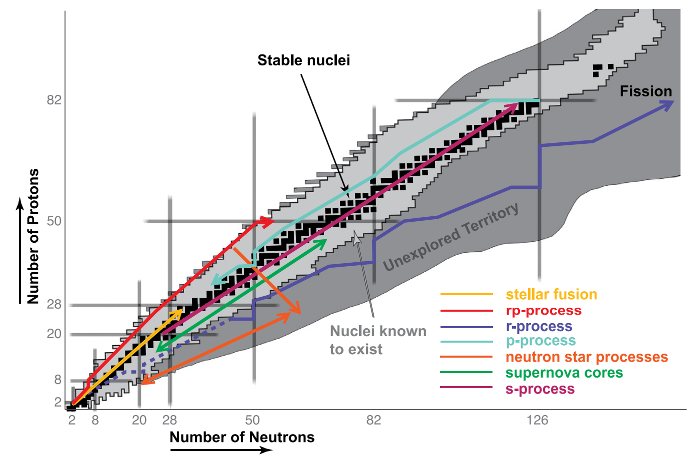


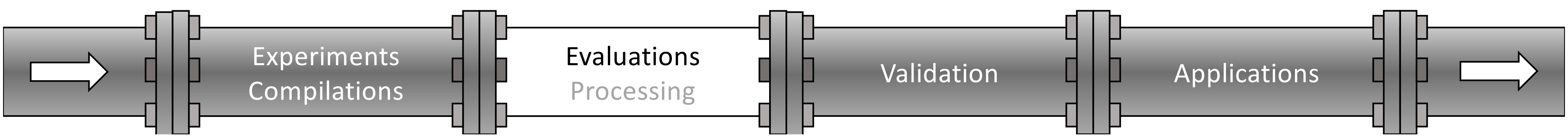
Future

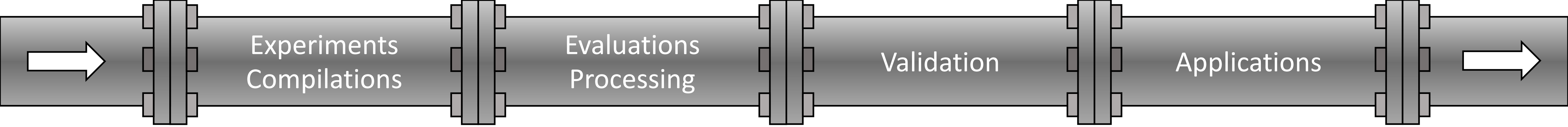
Vision: Building robust science-based evaluations and establishing guidance for next-generation reaction theories

- Develop evaluation tools to handle complex connections between models and their relations to observables
  - Allow for optimization across multiple reaction channels and sets of isotopes
  - Utilize direct and indirect data, plus theoretical constraints
  - Implement modular structure to allow for replacing outdated nuclear models
- Provide guidance to nuclear theory
  - Critically examine physics models and identify shortcomings
  - Assign uncertainties to models
- Identify experiments to most effectively constrain theory

Reaction calculations for astrophysics require extrapolations







AI/ML for Nuclear Data

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Gaussian Processes

Supervised Learning

Generative Modeling

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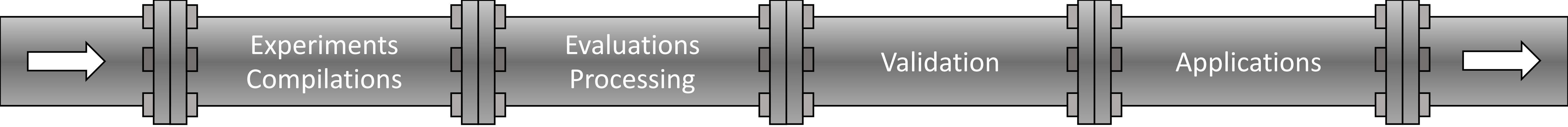
Deep Q Learning

Bayesian Optimization



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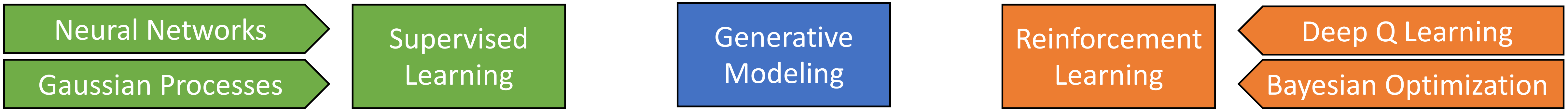
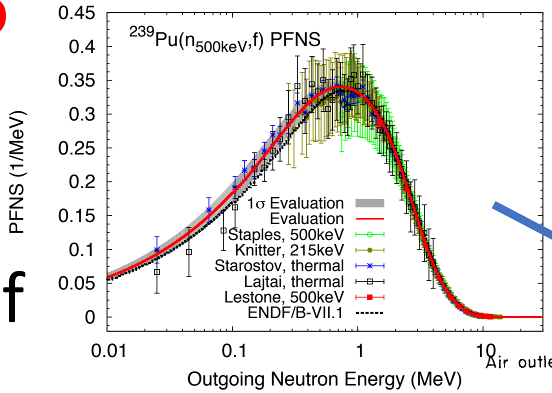


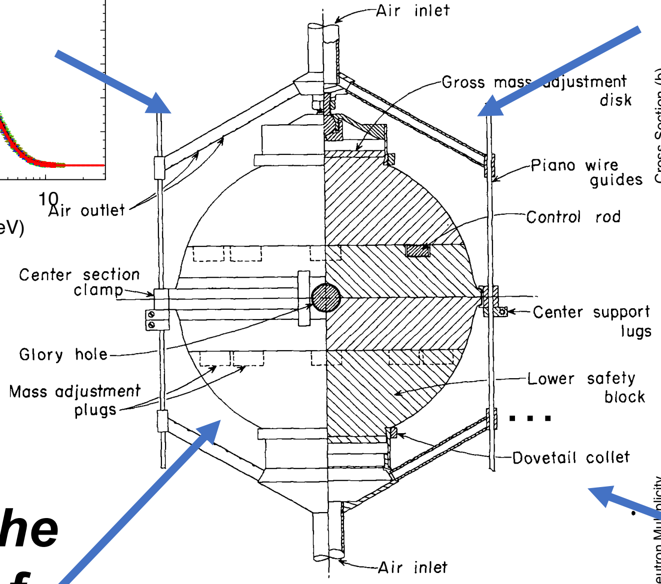
Nuclear data application area

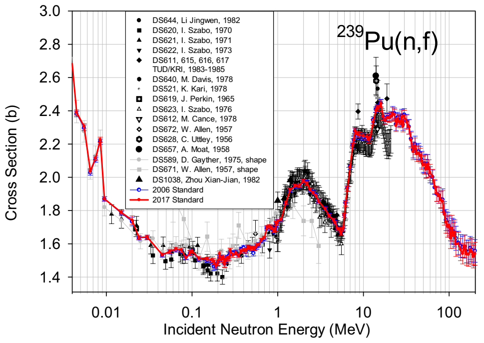
- **Nuclear data validation relies on expert judgment to identify where are errors in nuclear data** responsible for a difference in simulated versus experimental values of validation measurements.
- **1000s of nuclear data are used to simulate 1(!) validation experimental value. A human brain cannot keep track of all these inter-dependencies.**

Prompt Fiss. Neutr. Spectr.

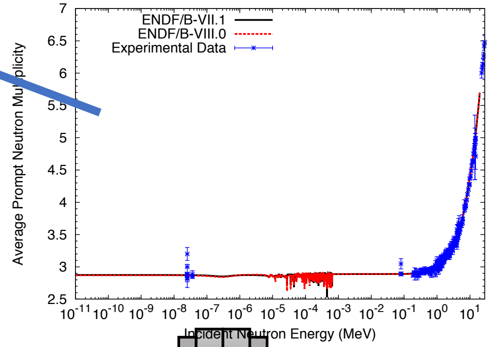


Av. Prompt Neutr. Multiplicity





Fission Cross-section



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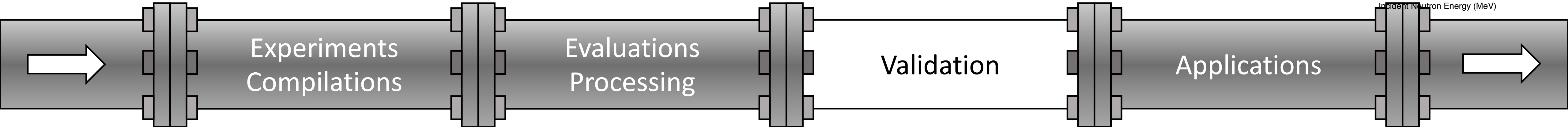
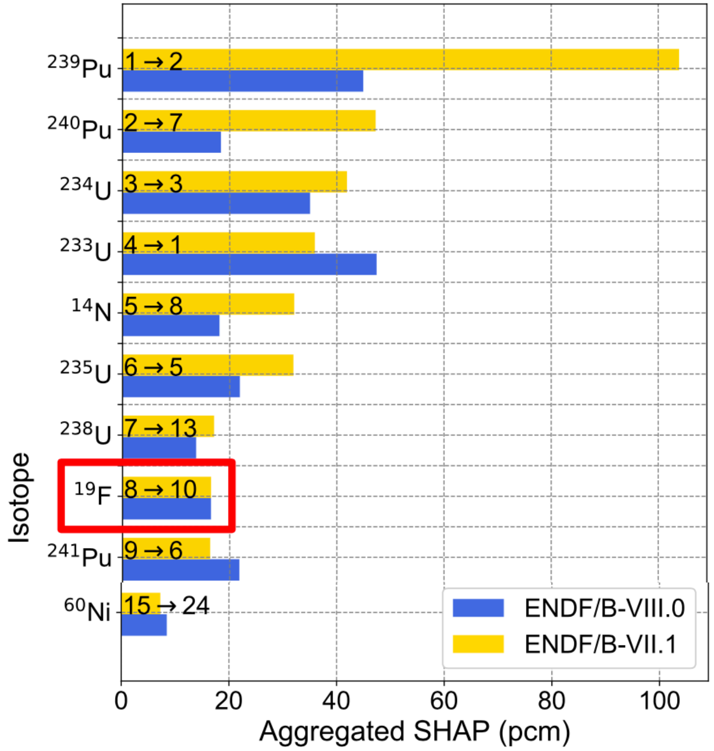
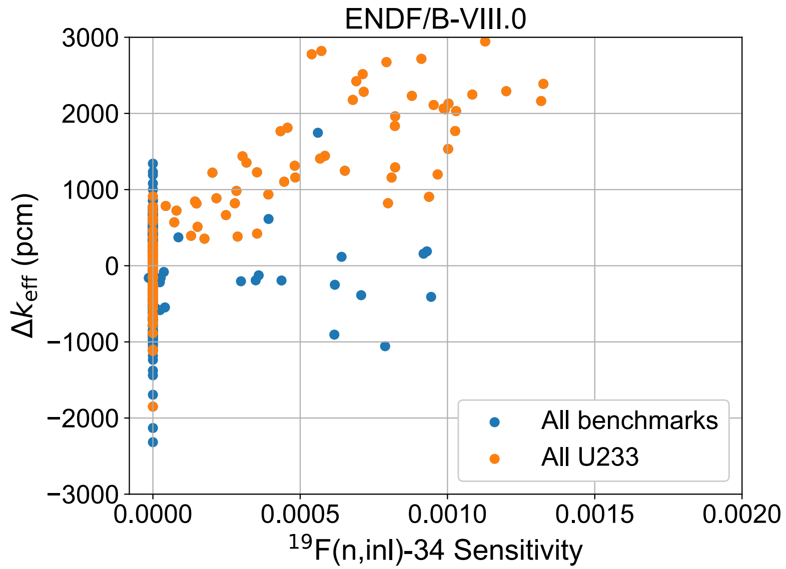
Simulating the criticality of Jezebel takes 100s of nuclear data

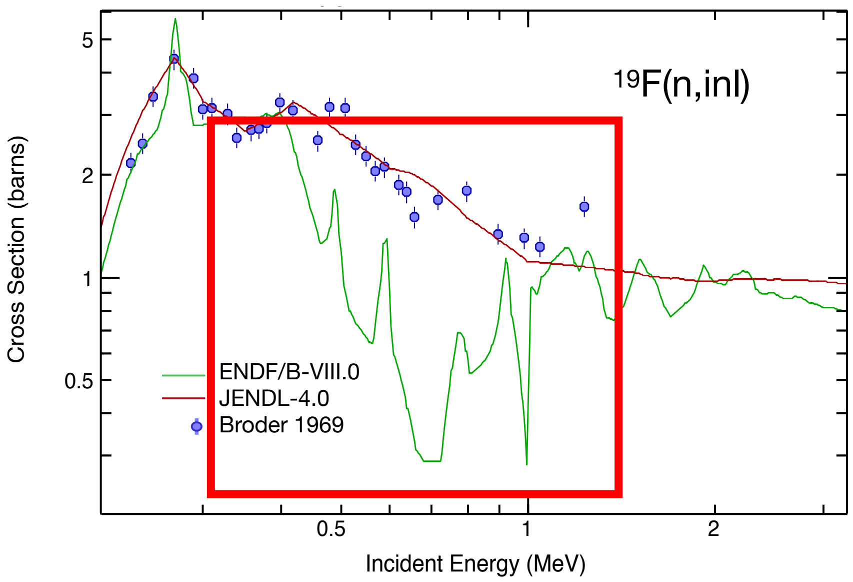


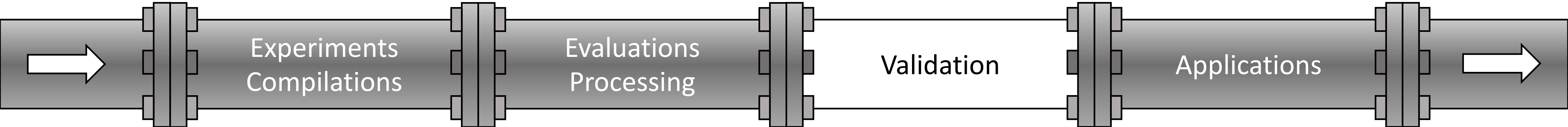
What has been done

Random forests were used successfully to augment expert knowledge in pin-pointing errors in nuclear data and benchmark experiments leading to bias in simulating criticality benchmarks; E.g.: ML found $^{19}F(n,inl)$ issue missed by experts





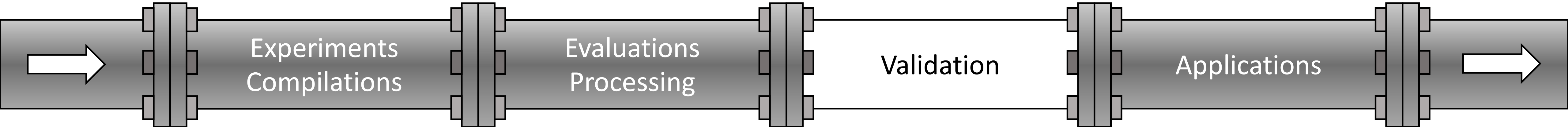


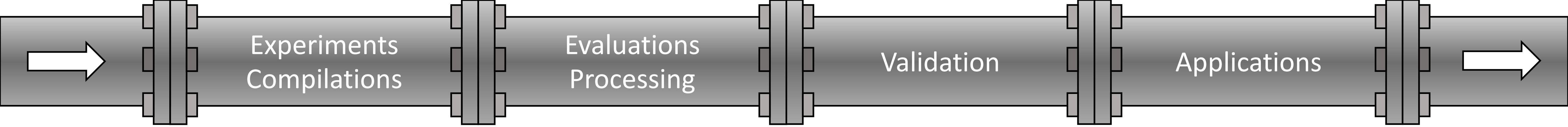


Future

These ML techniques can be used for and enhance already now nuclear data validation. For more effective future use, one needs to address the major obstacle that **several combinations of nuclear data lead to the same simulated criticality value -> no unique answer which nuclear data should be improved.** We can resolve this in the future by:

- Using importance assessment metrics better suited for correlated input,
- Using comprehensive set of validation experiments: requires *sensitivity tools* to link nuclear data and simulations, *benchmark quality validation experiments beyond criticality* and *ML algorithms able to handle those*.





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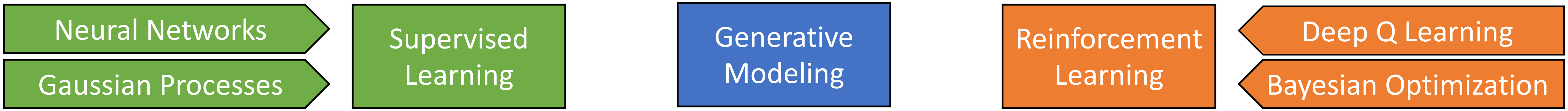
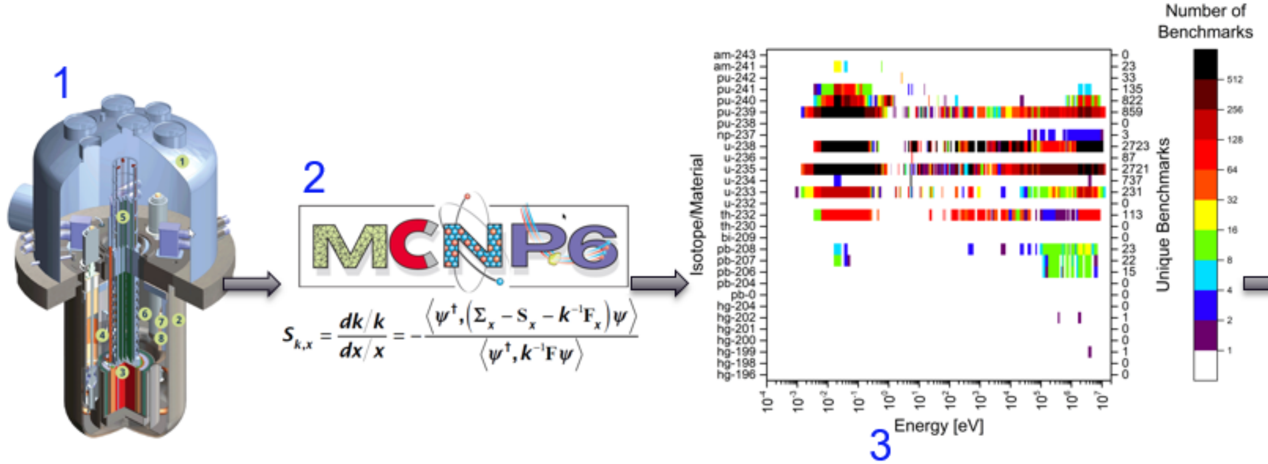


Nuclear data application area

- Develop and refine advanced tools and a build a framework that enables optimized design of new benchmark experiments for validation of predictive simulations.
  - What is the "ideal critical experiment" to support a given application?

LDRD Reserve ARCHIMEDES



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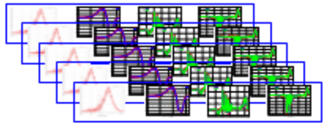
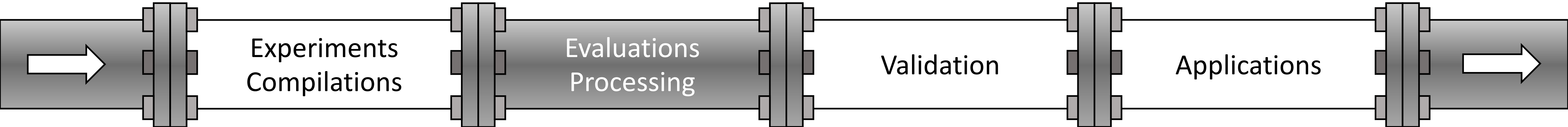


Catalog of Whisper sensitivity profiles for 1100+ experiments

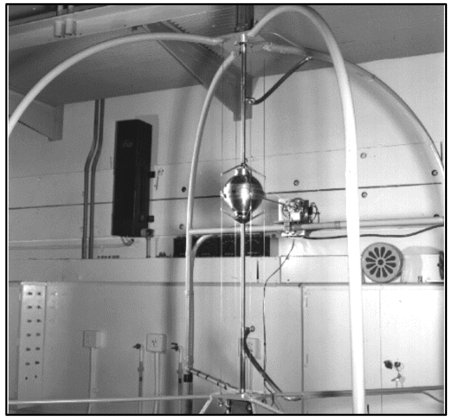
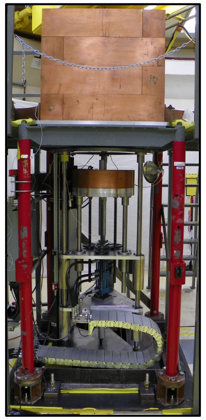
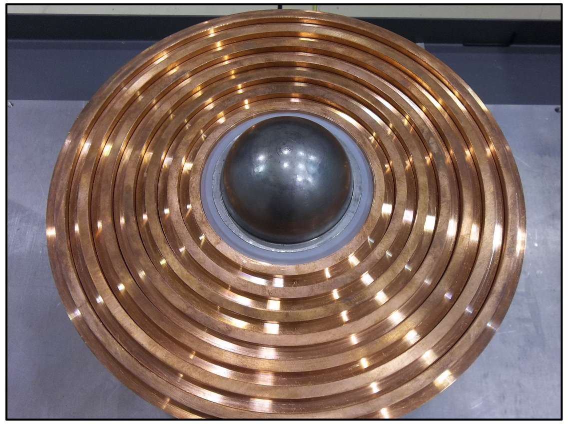
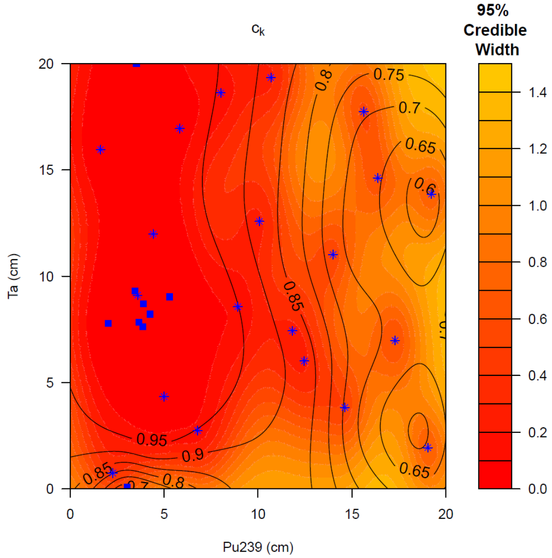
4

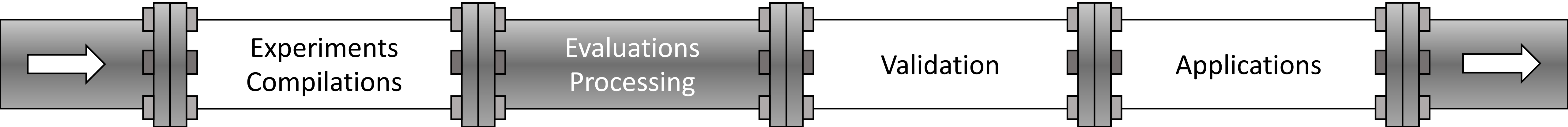
1: **Generate model** (Monte Carlo or deterministic) of application for radiation transport simulations.
2: Perform cross-section **sensitivity simulations**.
3: Perform a **gap analysis** to investigate if similar benchmarks exist.
4: Perform **optimization** to design new experiments that are more sensitive to the application than existing benchmarks.



What has been done

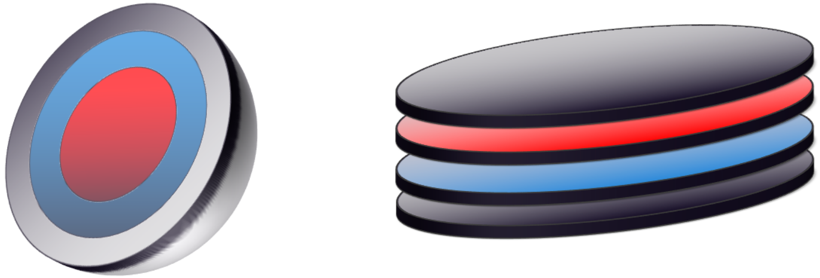
- Critical experiment design history:
  - Initially only expert-judgement was used (1940s).
  - Simulations (largely Monte Carlo) were used to aid in experiment design (1950s-2000s)
  - Cross-section sensitivities introduced in SCALE and MCNP (2000s)
  - Now AI/ML is being utilized in critical experiment design:
    - LLNL OPTIMUS
    - LANL Bayesian optimization
    - ARCHIMEDES uses Gaussian process optimization



Future

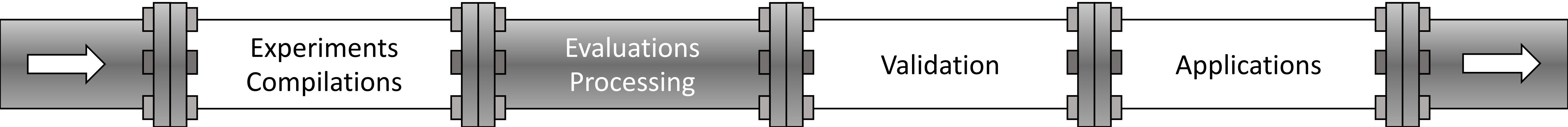
- EUCLID (Experiments Underpinned by Computational Learning for Improvements in nuclear Data) aims to utilize advancements from ARCHIMEDES and the Nuclear Data Machine Learning projects.
- Optimization includes several parameters (not just c_k).
- Focus is not a single experiment/measurement but how to combine multiple configurations and methods to maximize nuclear data impact.

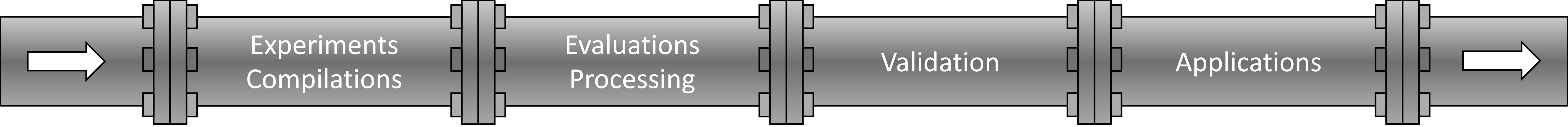


Spherical and cylindrical geometries.

$$\eta = (g, m_1, d_1, m_2, d_2, \dots) \longrightarrow S_\eta \longrightarrow c_k$$

$$c_k(A,B) = \frac{\vec{S}_A \bar{C}_{xx} \vec{S}_B^T}{\sqrt{\vec{S}_A \bar{C}_{xx} \vec{S}_A^T} \cdot \sqrt{\vec{S}_B \bar{C}_{xx} \vec{S}_B^T}}$$





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Gaussian Processes
Supervised Learning
Generative Modeling
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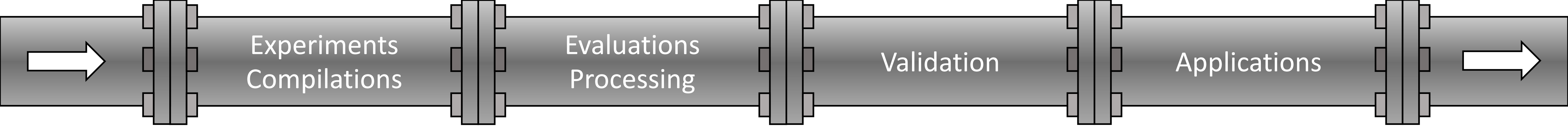
Deep Q Learning
Bayesian Optimization



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What type of problem can this solve?

- Framework: nuclear density functional theory (DFT) for fission
- Ingredients needed to compute fission fragment distributions
  - Potential energy surfaces (PES) in some collective space
  - Time-dependent dynamics (classical or quantum)
- Depend on energy density functional – calibrated on experimental data
- Propagate uncertainties from energy functional to fission fragment distributions
  - Start with building emulator of 1D fission paths from ground-state to scission
  - Build posterior by conditioning on values of "experimental" barriers

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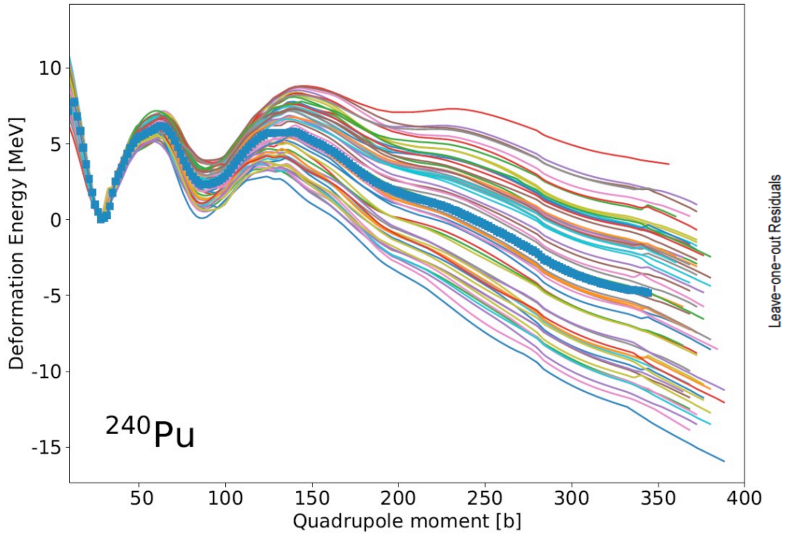
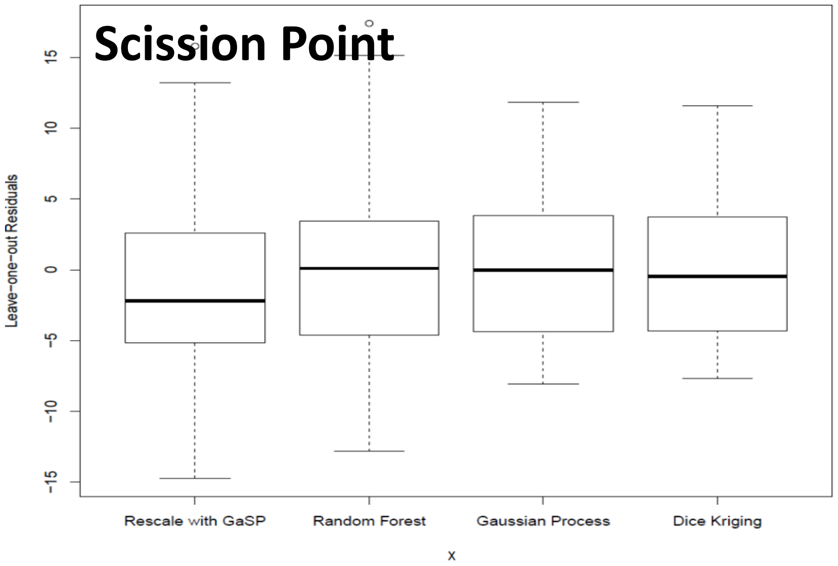
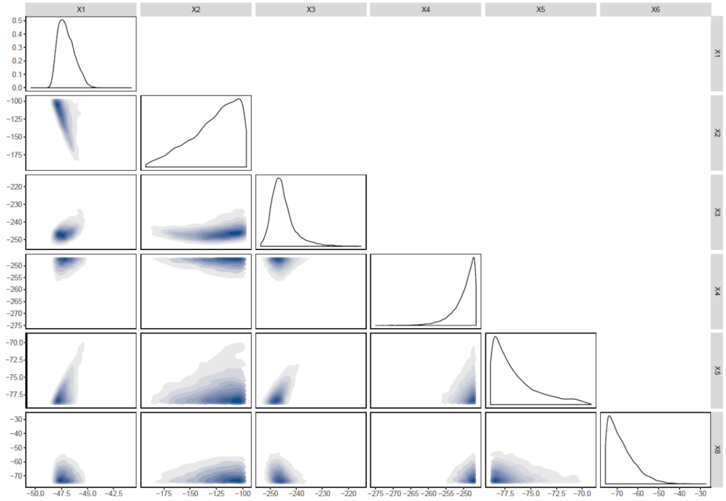
How does the method work?







Training
Perform DFT calculations of fission path from ground-state to scission

Emulator
Build local emulator with Gaussian processes

Posterior
Compute posterior distribution of EDF parameters based on fission barriers

Neural Networks

Gaussian Processes

Supervised Learning

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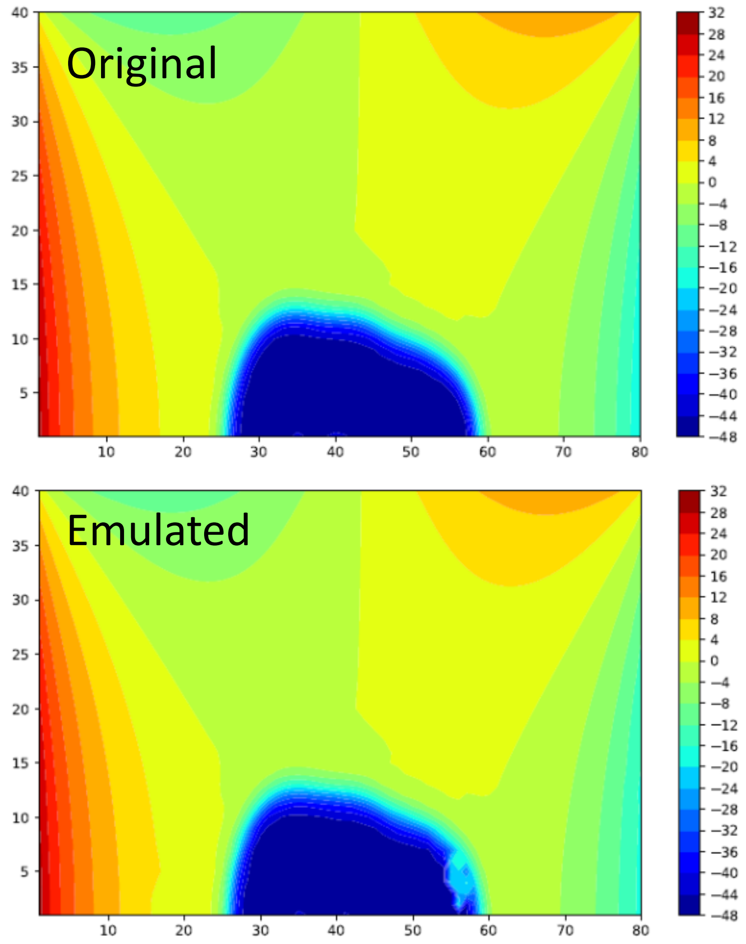
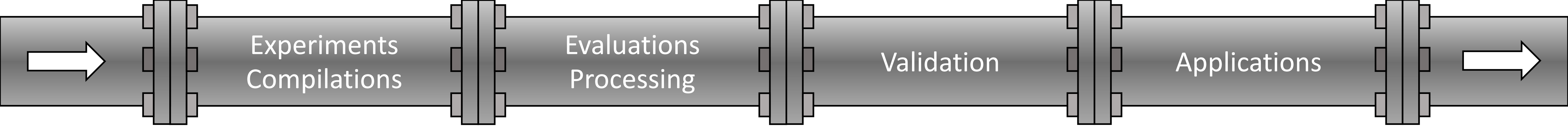
What is needed to use these tools?

- Supervised learning for theoretical models
  - Data is set of theoretical calculations
  - Computationally expensive (hours on supercomputers)
- Outlook
  - Expand concept to values of mean field on spatial lattice
  - High-precision irrelevant: use emulator as starting point to speed up calculations of large potential energy surfaces



Neural Networks | Gaussian Processes | Supervised Learning | Generative Modeling | Reinforcement Learning | Deep Q Learning | Bayesian Optimization



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What type of problem can this solve?

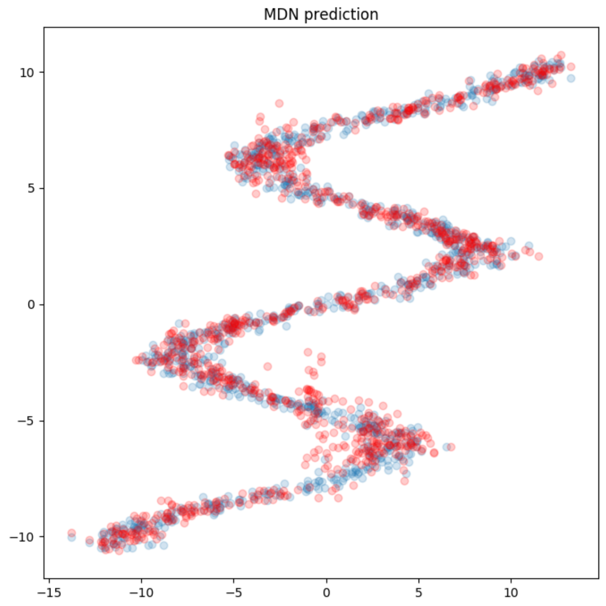
Mixture Density Network (MDN)

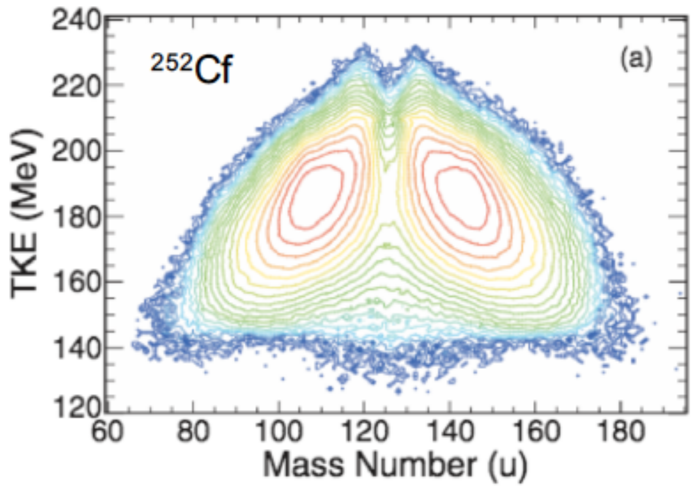
Can describe probabilistic data/observables

Used in cases where the input to output mapping is not one-to-one (e.g. systems where a single input can have multiple outputs – applications to synthesizing speech, financial risk analysis, etc.)

We have been exploring the MDN to emulate fission observables (fission yields)

C.M. Bishop, Neural Computing Research Group Report NCRG/94/004 (1994)





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How does the method work?

$$f(\mathbf{x}) = \alpha_1 \mathcal{N}(\mu_1, \sigma_1) + \alpha_2 \mathcal{N}(\mu_2, \sigma_2) + \ldots + \alpha_n \mathcal{N}(\mu_n, \sigma_n)$$

Standard neural network

Input → output

$$y = f(x)$$

In the Mixture Density Network, neural network learns the Gaussian variables instead of the mapping between x and y directly

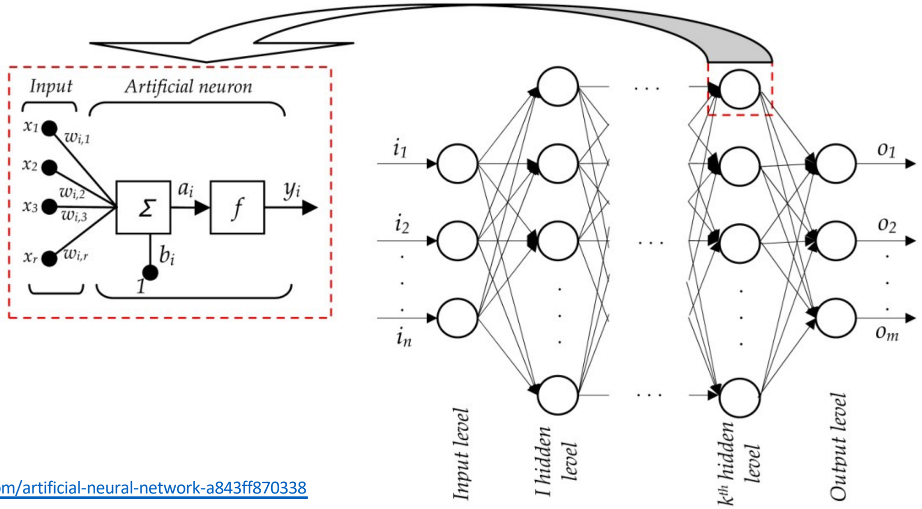
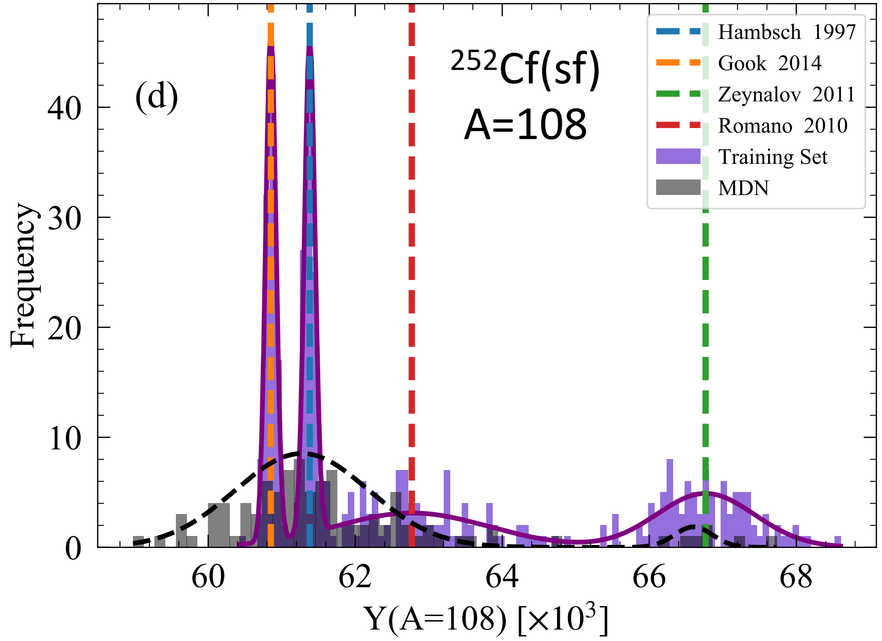


Figure: https://hackernoon.com/artificial-neural-network-a843ff870338



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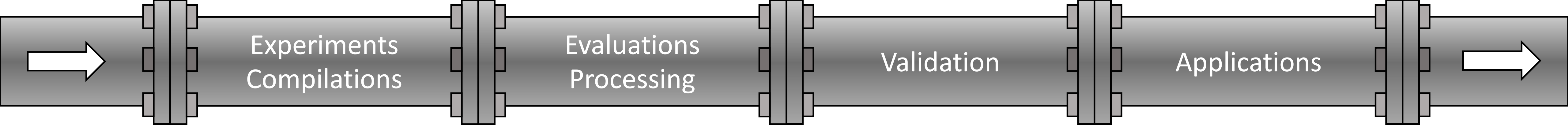
What is needed to use these tools?

- Data are needed with uncertainties
  - Any type of data where the underlying distribution is believed to be or can be described as a probability distribution (e.g. experimental data where the errors are taken to be Gaussian)
  - Multi-dimensional input and output can be handled
  - Correlations between data points and uncertainties can be included
- Discrepant data sets do not have to be removed
- Noisy data can be included in the training



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Moderated Discussion	All			
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Gaussian Processes

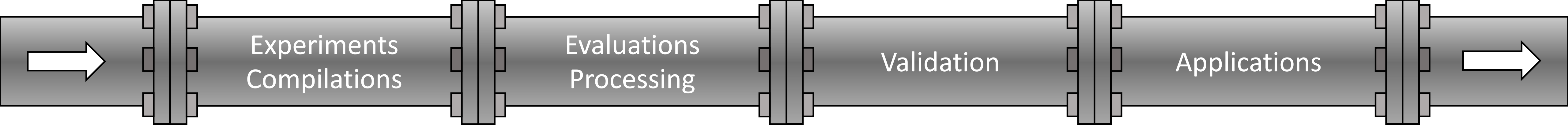
Supervised Learning

Generative Modeling

Reinforcement Learning

Deep Q Learning

Bayesian Optimization



AI/ML for Nuclear Data

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Additional AI/ML Perspectives for Nuclear Data

Optimization algorithms for AI/ML

- Classical algorithms, e.g., stochastic gradient descent, Bayesian optimization, evolution strategy, trust region methods, show weakness in training complex AI/ML models.
  - ➢ SGD does not work in large-batch training due to the loss of Stochasicity.
  - ➢ Reinforcement learning cannot use automatic differentiation (AD), so gradient-free (black-box) optimization algorithms are needed.
  - ➢ Besides AD, most algorithms do not work well in very high-dimensional spaces.
- Heuristics used in ML/AI training significantly prohibits reproducibility, such that a lot of “new” ML/AI models/methods can not be verified.

Additional AI/ML Perspectives for Nuclear Data

Optimization algorithms for AI/ML

- Training ML/AI with physical constraints
  - Most existing ML/AI training algorithms are non-constraint optimization, but ML/AI problems related to nuclear data may require either hard or soft constraints.
  - Soft constraints could be handled by adding regularization terms to the loss function, but hard constraints are generally difficult to handle.
- Generalization gap
  - Since the loss function only involves training data, the global optimum of the loss function may not be a good choice for your ML/AI model.
  - If the training data can fully represent the entire population, global optimum is the best. Otherwise, a local minimum with small curvature is preferred.

Additional AI/ML Perspectives for Nuclear Data

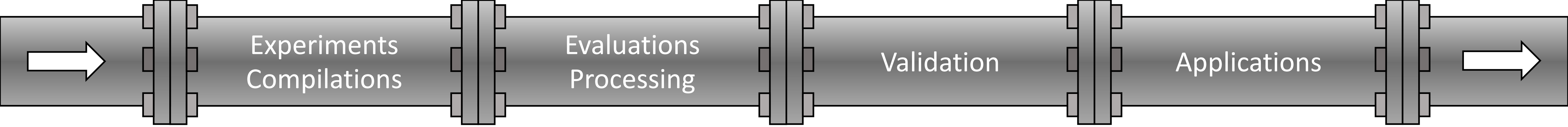
Surrogate modeling

- Dimensionality reduction (DR) in both input and output spaces.
  - ➢ Nuclear simulators are usually very time-consuming, so it is unaffordable to generate large amount of training data.
  - ➢ Reducing the input and output dimensions can significantly improve the accuracy of surrogates using limited amount of data.
  - ➢ Linear DR methods: active subspaces, inverse regression, Nonlinear DR: reversible NNs
- Multi-fidelity surrogates
  - ➢ Use low-fidelity nuclear simulators to generate a lot of training data and use high-fidelity simulators to improve the accuracy in predictions.

Additional AI/ML Perspectives for Nuclear Data

Stability and Robustness of AI/ML prediction

- Stability means the sensitivity of ML model output with respect to small perturbations of inputs
  - ➢ Deep NNs may have stability issue when viewing them as dynamical systems, i.e. ODEs
  - ➢ Possible strategies include implicit neural networks, reversible networks
- Robustness means the ML can alleviate the influence of adversarial attacks
  - ➢ Intentionally or non-intentionally generated or crafted data to hurt the predictability of deep neural networks, e.g., mis-classification.



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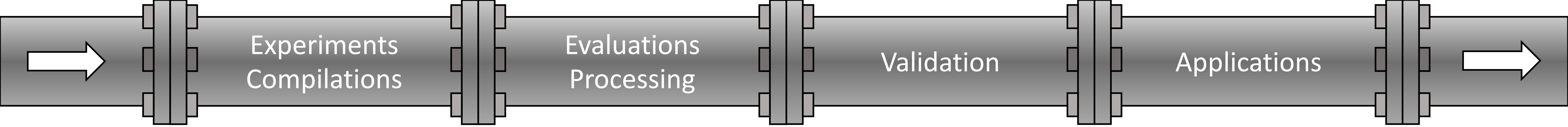

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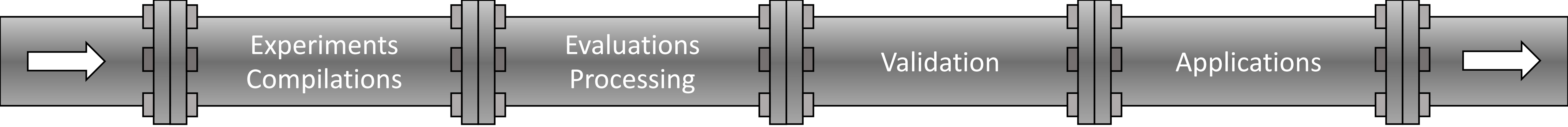

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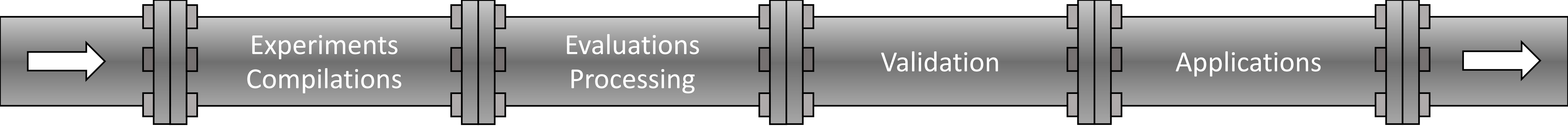

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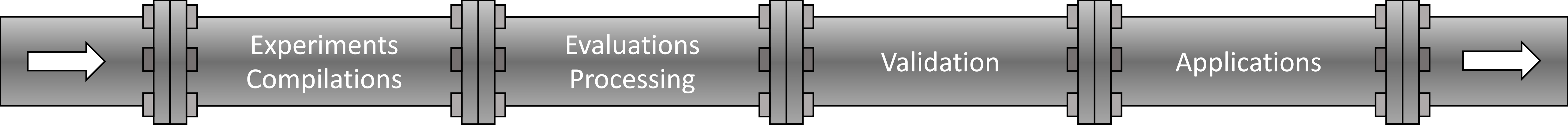
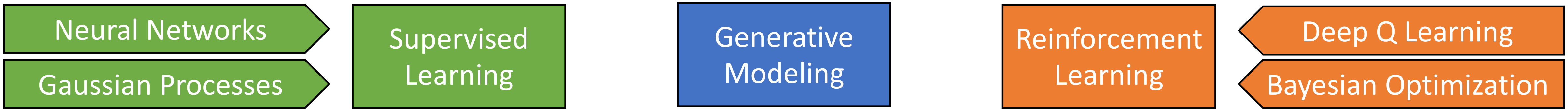
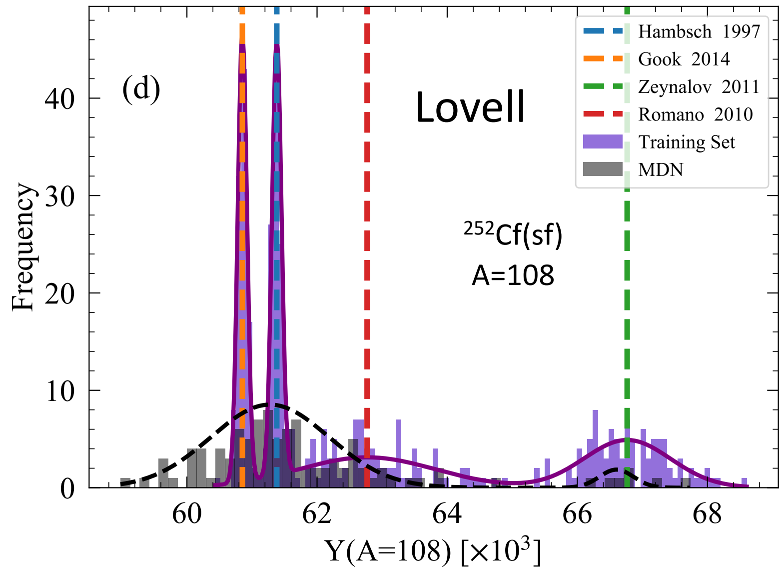
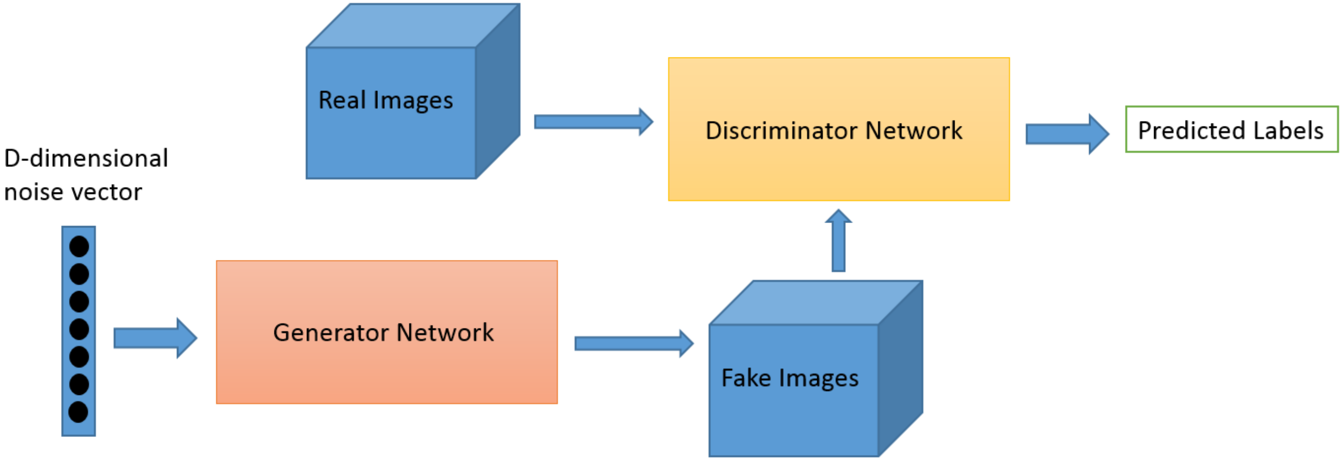


Building a Long-Range AI/ML Vision







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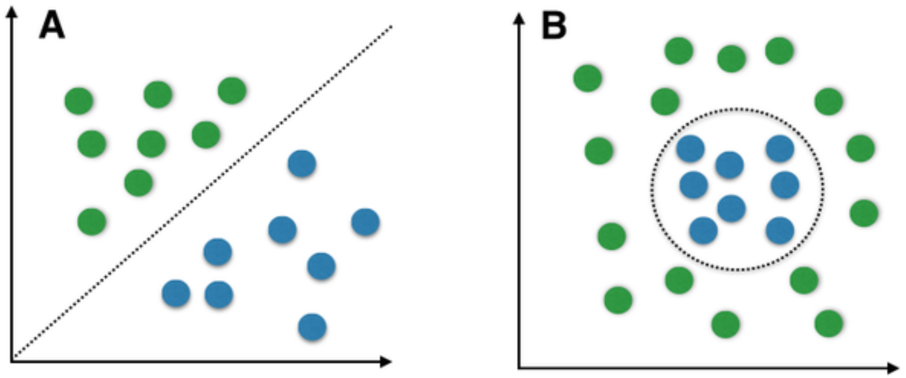

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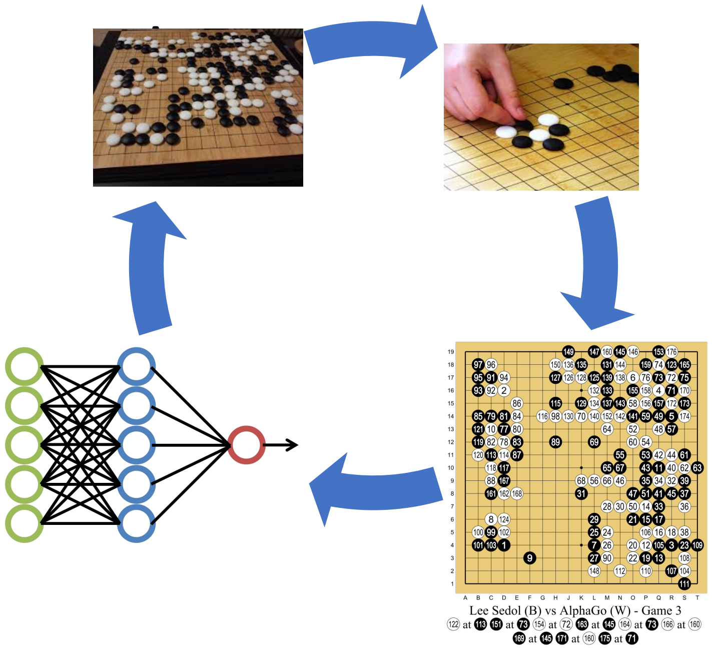

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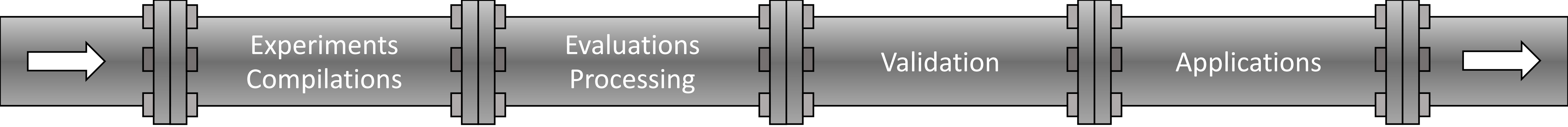
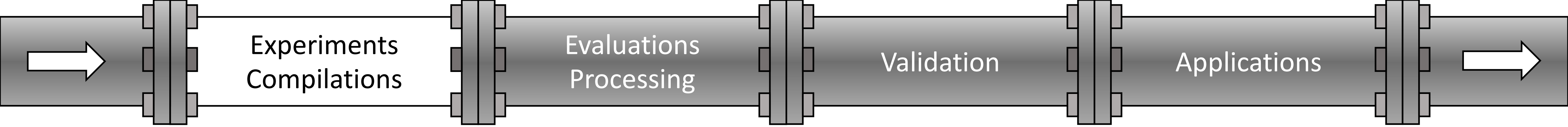


Needed Groundwork

- What common community tools are needed?
- Modernizing/documenting tools
  - Improving ease of access
  - TALYS is a great example.
- Modernizing and open sourcing common codes
- Cleaning up experimental data bases
  - EXFOR

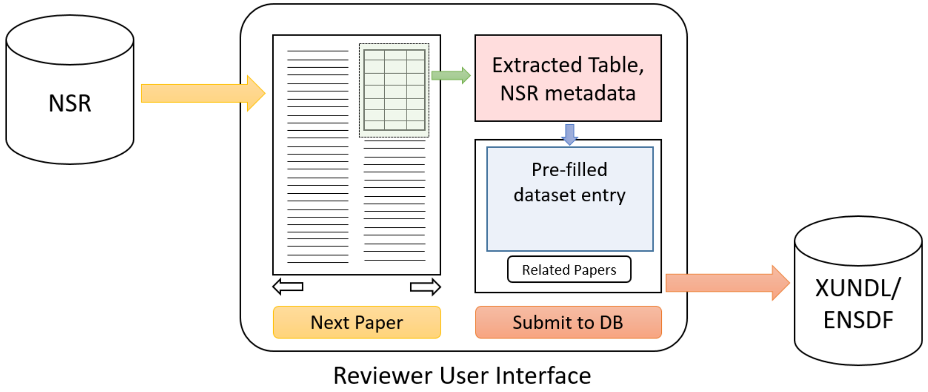
Pitfalls to be avoided

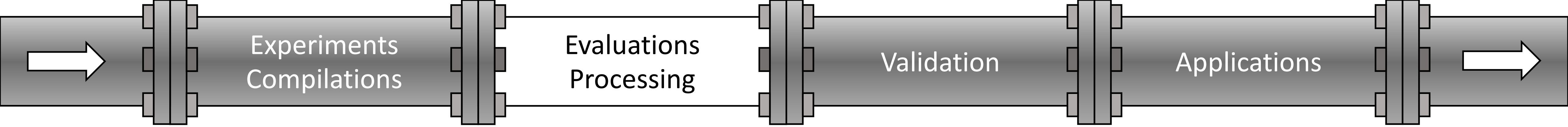
- Need to enforce reproducibility through peer review
  - ML models represented and distributed in a standard format.
- Want to augment missing physics
  - Favor better physics models over more complex ML.



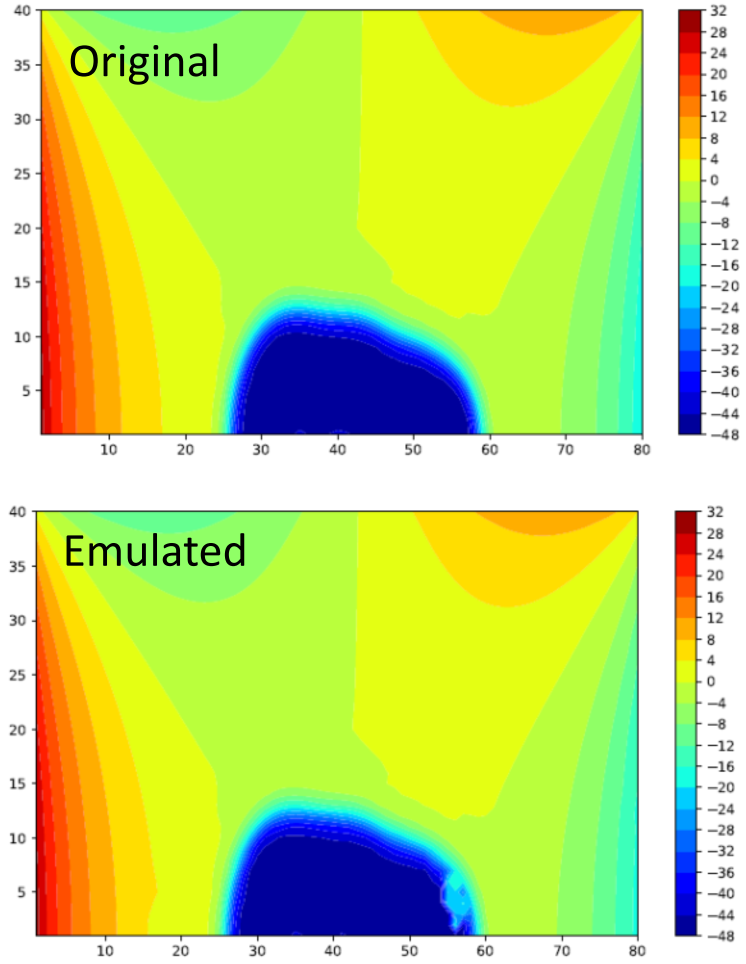
- Can we mitigate human error in compilation?
- Can we use ML to identify/quantify missing systematic errors?
  - Can we "learn" how to correct them?
- Using ML to prioritize new measurements
- Validating old data

Yoo

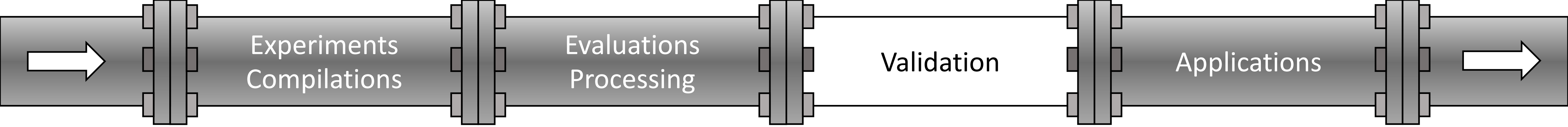




- Emulation of complex and expensive model codes
- Learning model defects
  - Correcting them?
- How can we enhance evaluations with more fundamental but less precise models?
- Can reinforcement learning pick better a sets of models?
- Can we “learn” the intuition behind past evaluations
  - Codification of senior evaluator intuition.
- Can we apply these ideas/tools to structure evaluations

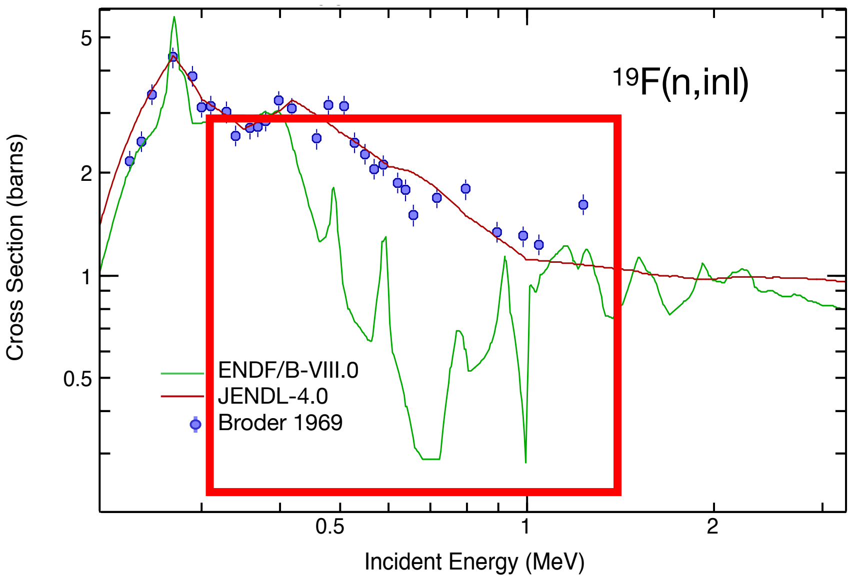


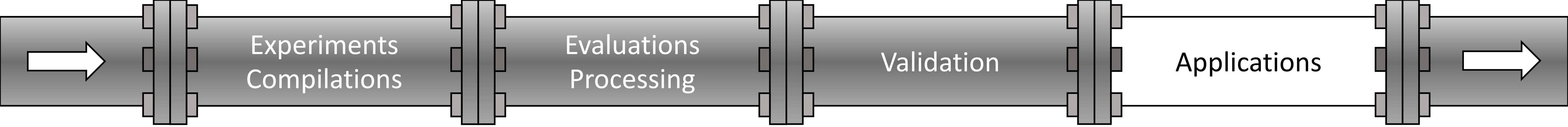
N. Schunk



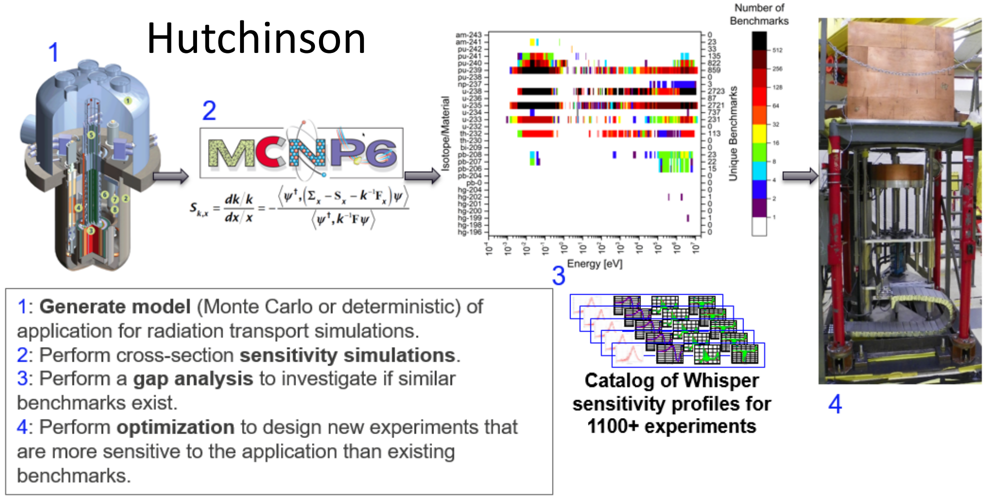
- How can we gauge the correctness of evaluations and models?
  - Does "correctness" have context?
  - What about where there is no data?
    - Very unstable systems
    - r-process
- Can we optimize new experiments to maximize new information gained?
- Can we automatic the consistency checking between models and measure data?

Neudecker



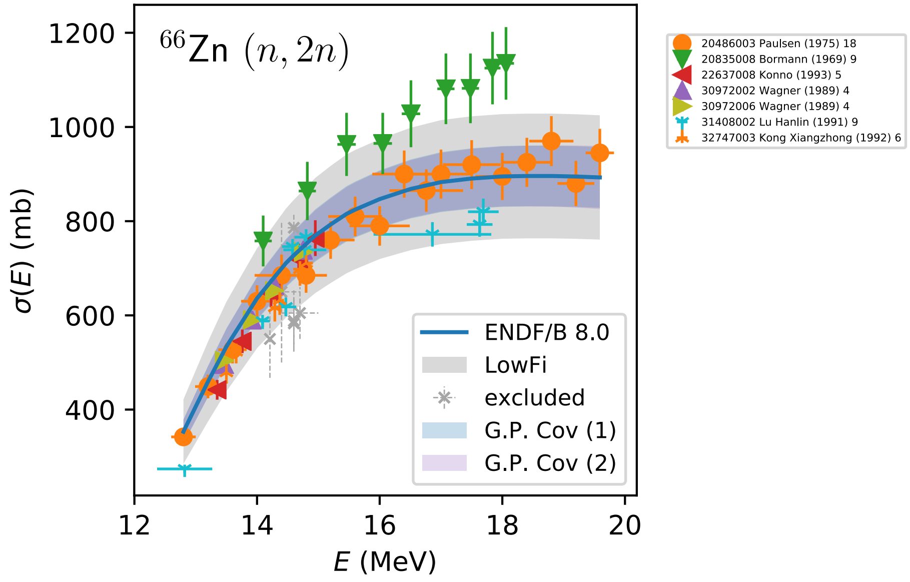


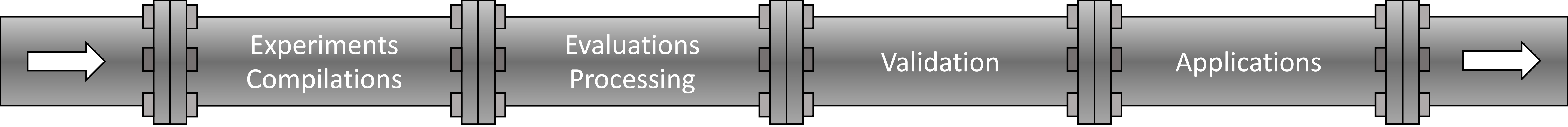
- Connect the (unexpectedly) important features of a reaction to particular application.



- Building application model surrogates for uncertainty propagation.

- How do we fill in gaps of missing information needed by applications





Discussion Time!

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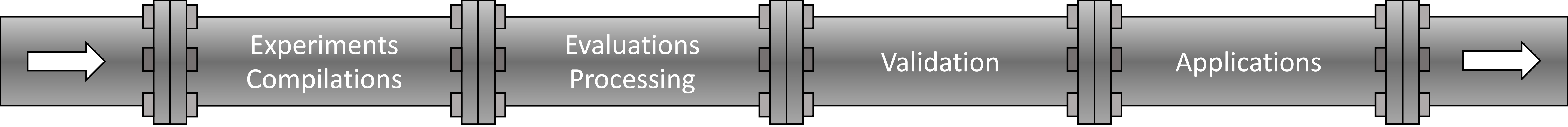

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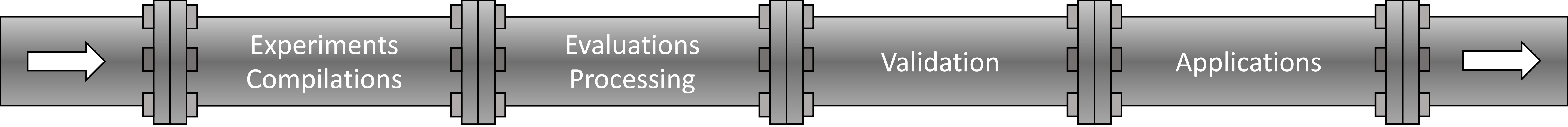

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