Better Data for Better Models

Evolving Needs For Nuclear Data Adjustment

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This presentation will attempt to convince you

(1) Improvements in modelling and simulation require new data.

(2) Our modelling and simulation capabilities have recently improved enough to require rethinking the data needed.

(3) The international collaborations and data that form the backbone of modern validation will require significant effort to support robust adjusted nuclear data libraries, for a wide range of applications.

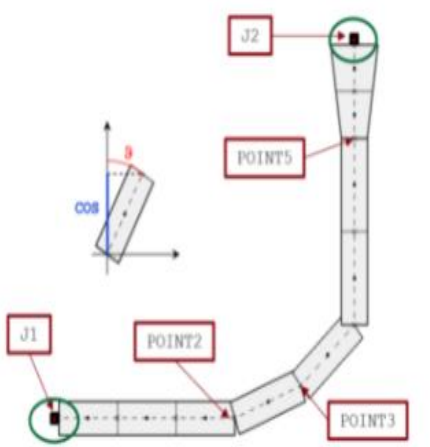
Other presentations will provide more details on the history of adjustment, and current flaws in methods. Based on the excellent speakers, I trust they will cover the issues thoroughly!

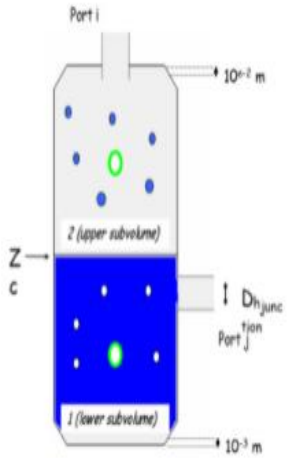
My set of near term recommendations can be found in the final slide of '**Past, Present, and Future Benchmark Efforts for Nuclear Data Validation**', **WANDA 2021.**

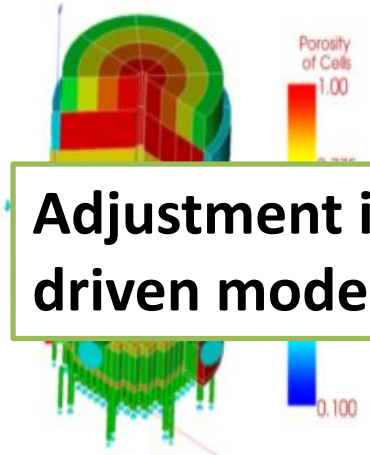
Improvements in modelling and simulation require new data.

Fluid mechanics: Increased computing power and methods improvements have made computational fluid dynamics feasible. The increased computational resolution makes it possible to use TBs of data in resources such as digital videos of fluid flow, to validate of these models/methods.

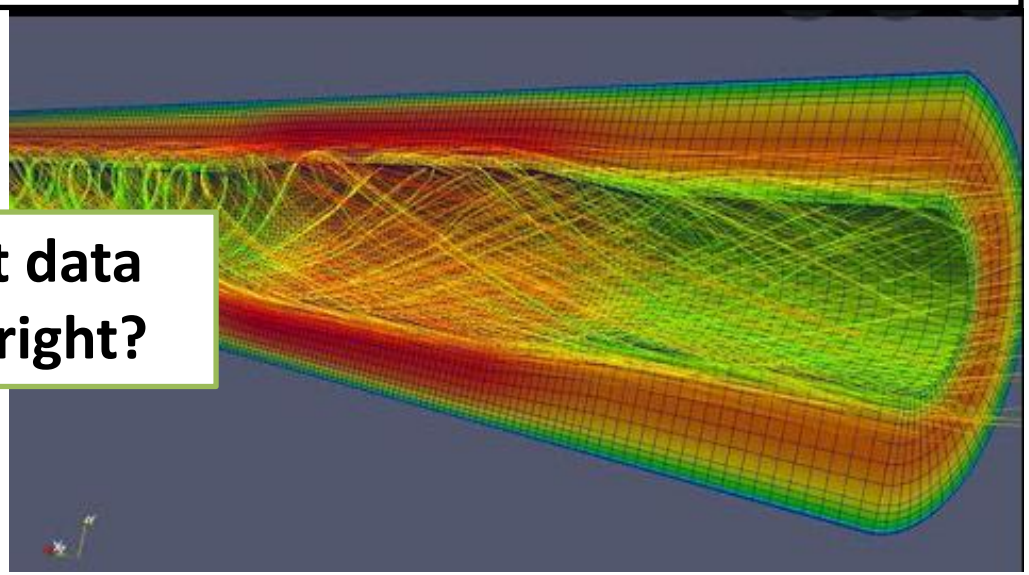
'Fluid mechanics has been traditionally concerned with big data. For decades it has used ML to understand, predict, optimize, and control flows. Currently, ML capabilities are advancing at an incredible rate, and fluid mechanics is beginning to tap into the full potential of these powerful methods.'
'Data-driven modeling may be a potent alternative in revisiting existing empirical laws in fluid mechanics.'
https://www.annualreviews.org/doi/pdf/10.1146/annurev-fluid-010719-060214







Adjustment is just data driven modelling right?



Integral Data Potentially Used for Adjustment: International Data Sources

Parameter	Benchmarks	Database Software	Uncertainties	Issues
K-effective	Yes (ICSBEP) ~5000	DICE/API	Well Quantified	**Missing shared uncertainty**
Reactivity Effects	Yes (IRPhE) ~200	IDAT	Quantified	**Missing sensitivity, input models**
Spectral Characteristics	Yes(IRPhE) ~250	IDAT	Quantified	**Missing sensitivity, input models**
Reaction Rate Distributions	Yes(IRPhE) ~100	IDAT	Quantified	**Missing sensitivity, input models**
Kinetics Parameters	Yes(IRPhE) ~10	IDAT	Quantified	**Missing sensitivity, input models**
Subcritical Measurements	Yes	DICE	Quantified	**Missing sensitivity, input models**
Count Data (semi integral)	No (with exceptions)	No	Experimental	**Transformed into simplified bench. quantity**
Shielding	Documentation (SINBAD) ~100 Experiments	No	Experimental (some in ICSBEP)	**Significant effort required to make benchmark model + BE uncertainty**
PIE Data After Irradiation	SFCOMPO ~750 fuel samples	SFCOMPO2.0	Incomplete	**Significant effort required to make benchmark model + BE uncertainty**
Fuel Performance [Ex. Fission gas release]	Documentation (IFPE) ~1452, only some relevant	DATIF	Incomplete	**Significant effort required to make benchmark model + BE uncertainty**
Station Data	Data internal	Siloed	Experimental	**Lots of data, tough to get**
Proprietary Data	Data internal	Siloed	Varies	**Lots of data, tough to get (**some in IRPhE**)**

The data we have now wasn't designed with 'big data' in mind. Currently data source are underexploited; perhaps in the long run it will also be seen as completely insufficient

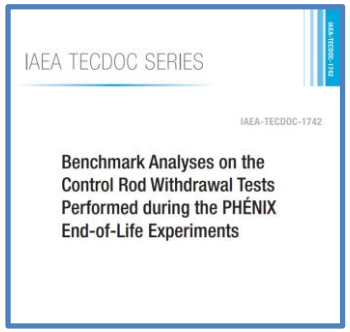
Our modelling and simulation capabilities have recently improved enough to require rethinking the data needed.

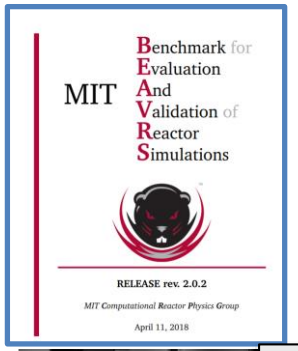
Area	Far Past	Recent Past	Present	Future (2050?)
Sensitivity Data	Deterministic	Monte Carlo (keff) Some Methods gaps	Monte Carlo Few Methods Gaps New parameters feasible	Not Needed? Or only needed for humans? Or to facilitate sharing?
Computational Models (with Feasibility)	Diffusion, Low-Fi	Monte Carlo (keff)	Monte Carlo Time Independent	Monte Carlo Time Dependent
Use of Integral Experiments	In-house	International Sources (Mostly keff) + In-house	International Sources (Mostly keff) + In-house	**See previous slide for starting point**
Nuclear Data	Approximate	Good Untraceable adjustments?	Good Untraceable adjustments?	Good, Prior by theory, then adjusted based on all known data?
Nuclear Data Covariance	Very Limited	Important Covered (quantity) Approximate (Atlas, Modelling) Inconsistent	Nearly Complete (quantity) More Experimental than R.past Inconsistent	Complete. Tested. Data Driven? + Model Driven?
Experimental Data Covariance	Little or None	Sparse	Sparse	Data Driven Probability distributions
Adjustment	Sensitivity based Few Group, Successful Applications (SUPERPHENIX, all SFRs)	Multi-group	Multi-group, ENDF/B file Nuclear Model Parameters	GNDS Nuclear Model Parameters

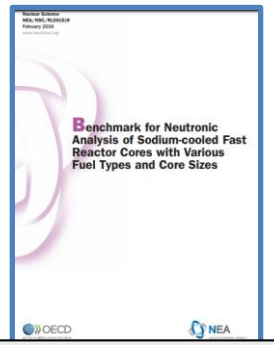
Application Space What Is Needed

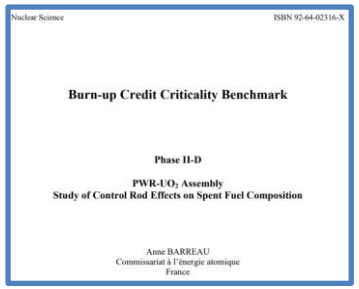
Needs for Industry, design, licensing

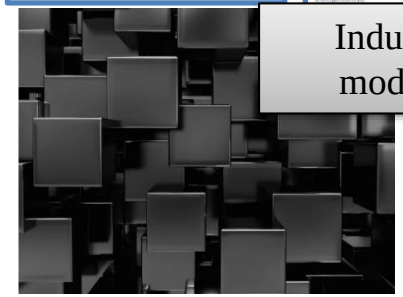
Testing Adjusted Libraries to Predict Applications (collect verification Ex.)





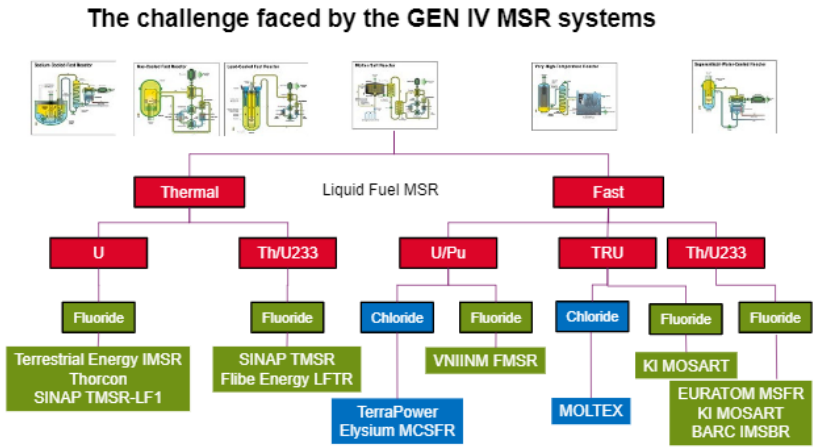






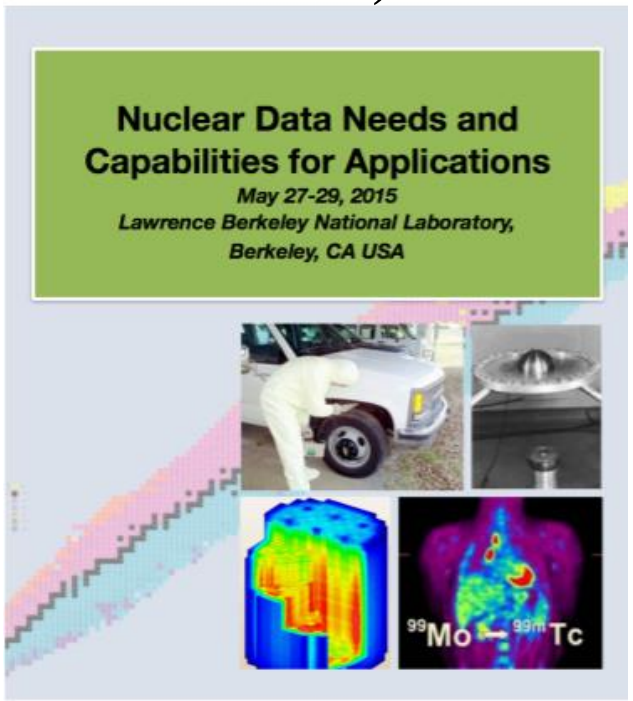
Industry surrogate models/responses

High priority unevaluated measurements (known to be well documented): ZPPR, BFS, Spectral Shift Control Reactor, TAPIRO, spectral characteristics in GODIVA, FLATOP and JEZEBEL.



What accuracy do we need to achieve? (HPRL, SG46)

Justification of the Adjustment Process and Data Used (open science?)



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Final Remarks

- Many fields are looking at data needs to underpin advanced modelling and simulation. Fluid dynamics, fuel performance, thermo-physical models.
- Until recently, most commonly deterministic methods were used for most applications. Low fidelity methods and nuclear data benefited from adjustment, and adjustment was relatively common to support specific applications.
- More applications are adopting high fidelity modelling, generating new data demands. What was sufficient in the past is not always sufficient either today or in the future. The nuclear data evaluation process and uncertainties have evolved and continue to do so.
- **Our international data sources are decent for making adjustments for a narrow range of applications (mostly criticality applications), but they do not cover sufficiently existing reactors, or advanced reactors, or other many other applications. When an adjusted library is used and predictions are tested against high quality experimental data, the results may raise questions regarding the adjustment.**
- **For other applications, it remains possible to do adjustment, but it would take a significant effort to gather and analyse the data (to modern standards!). This incentivises actors to evaluate data 'as needed'. There is a need to capture the accuracy needed (NEA High Priority Request List, WPEC SG46), from all actors.**
- The potential exists to gather 'surrogate models or functions' that encompass most of application space for testing.
- **Big data collection, analysis could lead to adjustment for the general nuclear data library, or perhaps the nuclear models. For experimental data efforts should move towards collecting the underlying experimental data, and making this data widely useable for testing and preparing for the future usage. <u>New collaborations towards this objective?</u>**