Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

The Nuclear Data Pipeline

David Brown

National Nuclear Data Center,

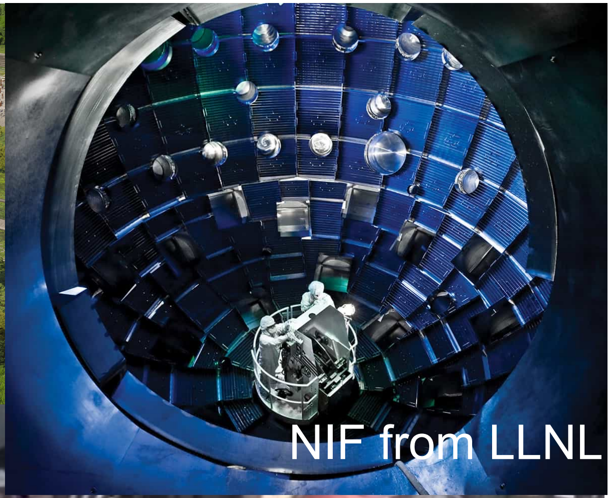
Brookhaven National Laboratory

@BrookhavenLab

26 Feb 2024

WANDA 2024

Modern nuclear applications require detailed and complex modeling



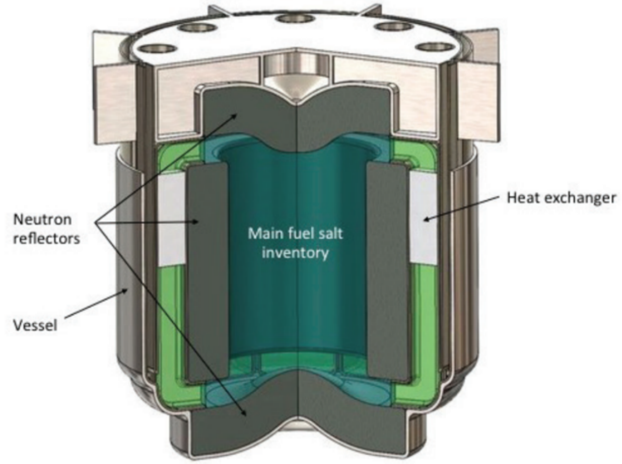
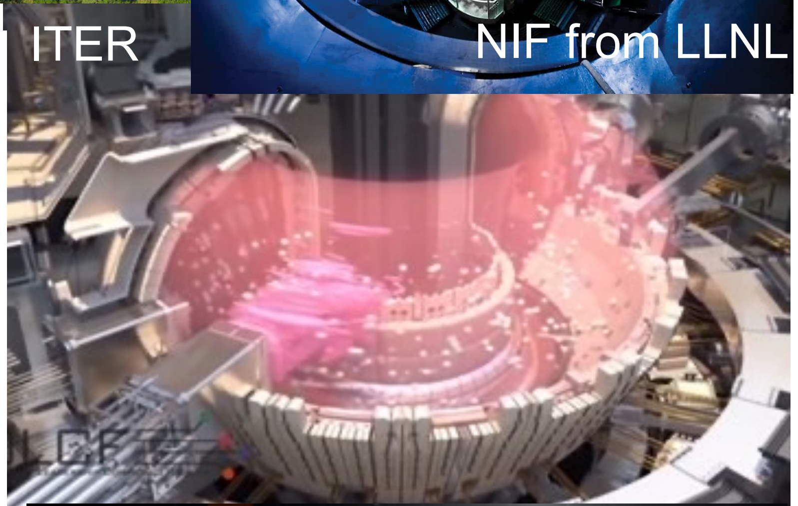
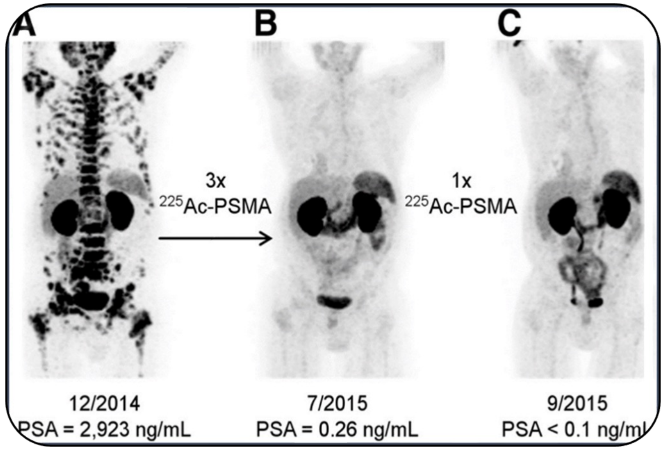
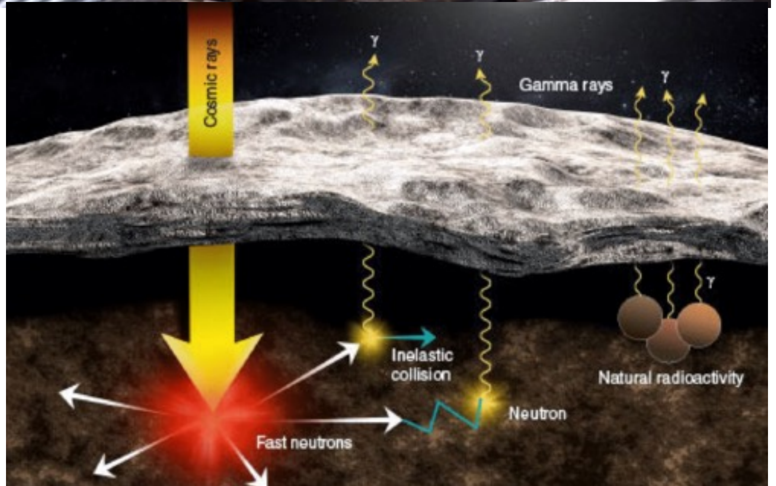


Figure 8. Exemplary molten salt fast reactor model (Terrapower 2020).

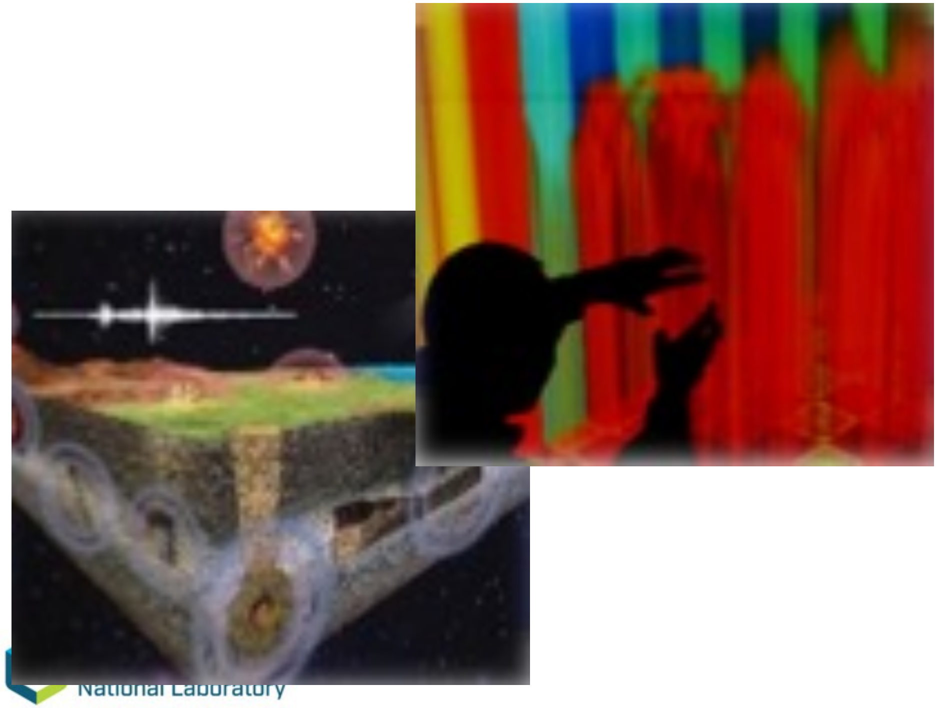




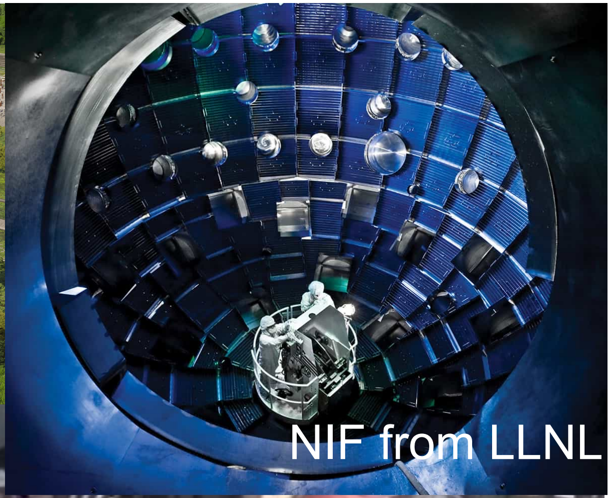
Ethan Balkin's WANDA 2024 talk

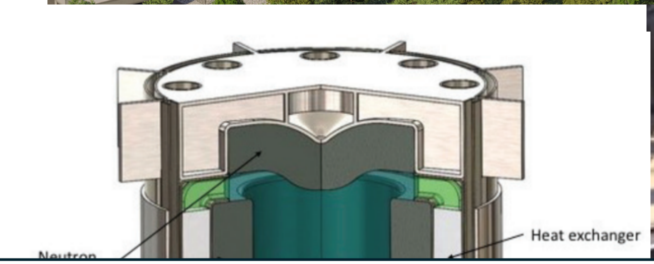


Veronica Chen in https://str.llnl.gov/2019- 05/burks (2019)



Modern nuclear applications require detailed and complex modeling





MCNP6

PHITS
Particle and Heavy Ion Transport code System

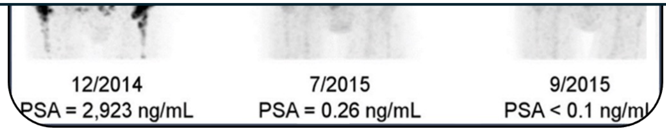
GEANT4
A SIMULATION TOOLKIT

scale
Nuclear Systems Modeling & Simulation

GENIE 2000
Applications Software

OpenMC

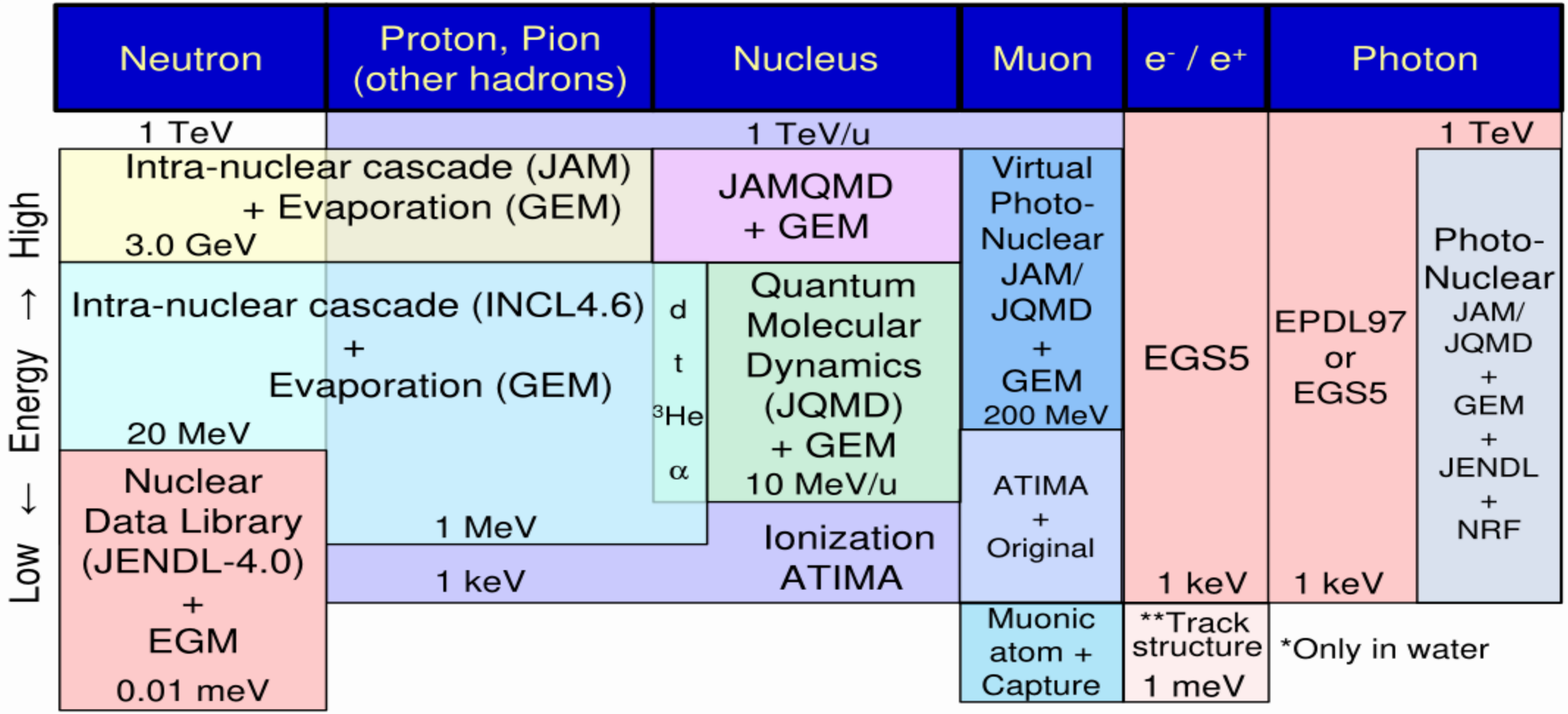
FLUKA



Ethan Balkin's WANDA 2024 talk

Veronica Chen in https://str.llnl.gov/2019- 05/burks (2019)

Map of Models Recommended to Use in PHITS

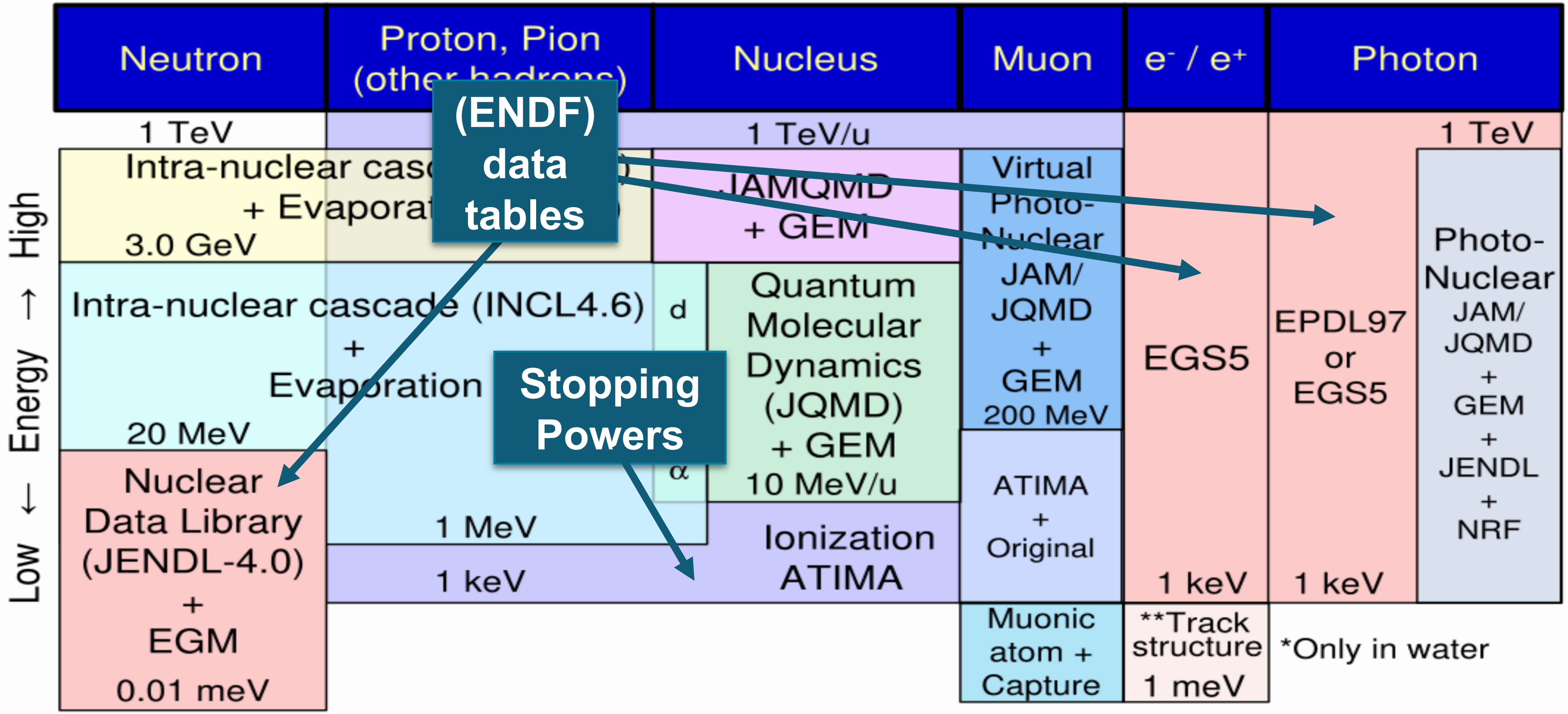


Physics models of PHITS and their switching energies

Switching energies can be changed in input file of PHITS

https://phits.jaea.go.jp/lec/phits-introduction-en.pdf

Map of Models Recommended to Use in PHITS



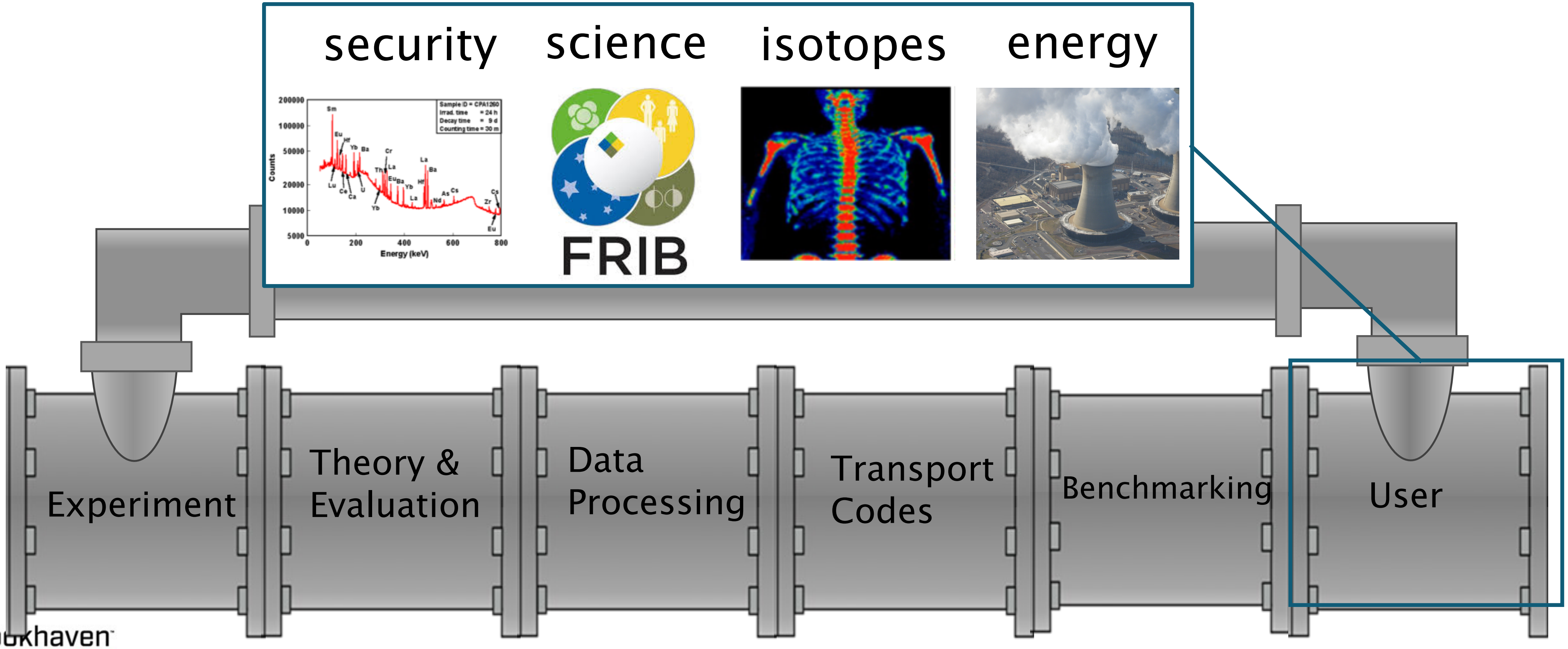
Physics models of PHITS and their switching energies

Switching energies can be changed in input file of PHITS

https://phits.jaea.go.jp/lec/phits-introduction-en.pdf

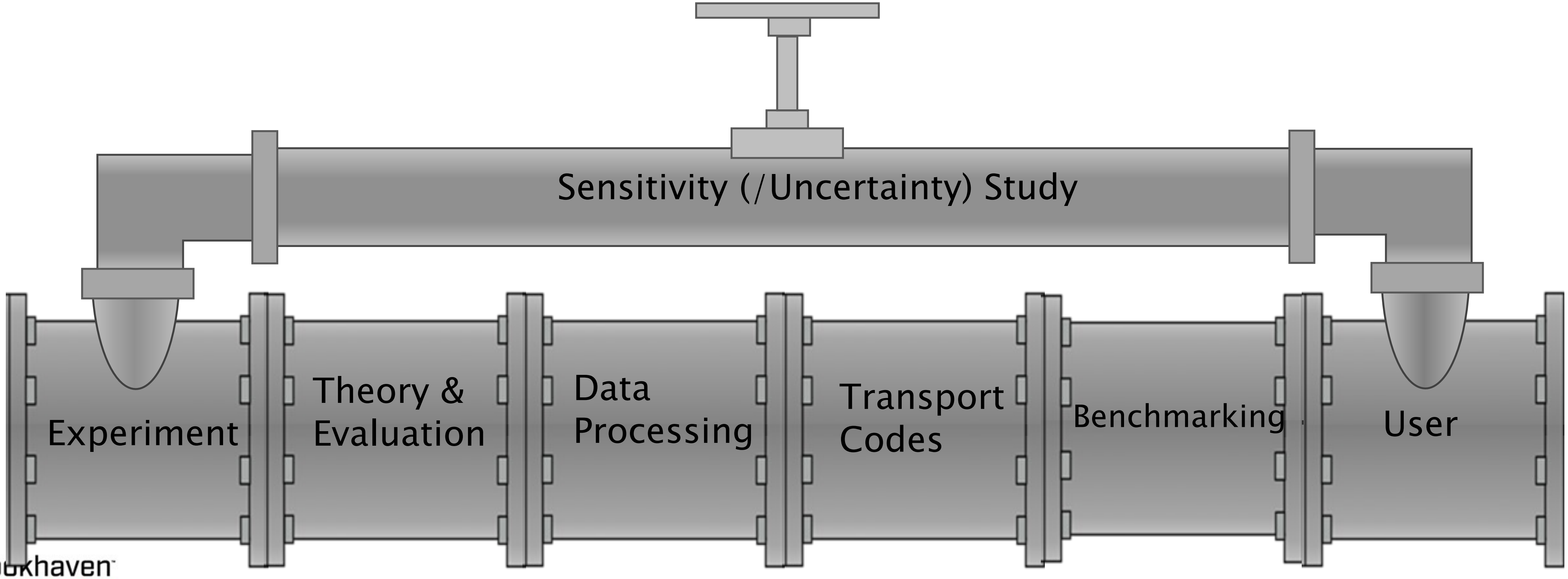
The Nuclear Data Pipeline

Our goal is to get the highest quality data to users



The Nuclear Data Pipeline

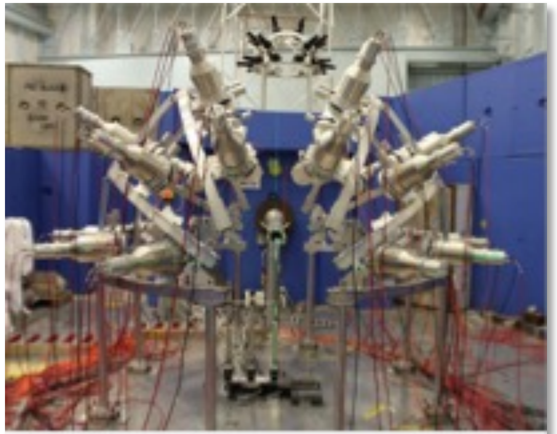
Uncertainties are needed so users can properly inform priorities



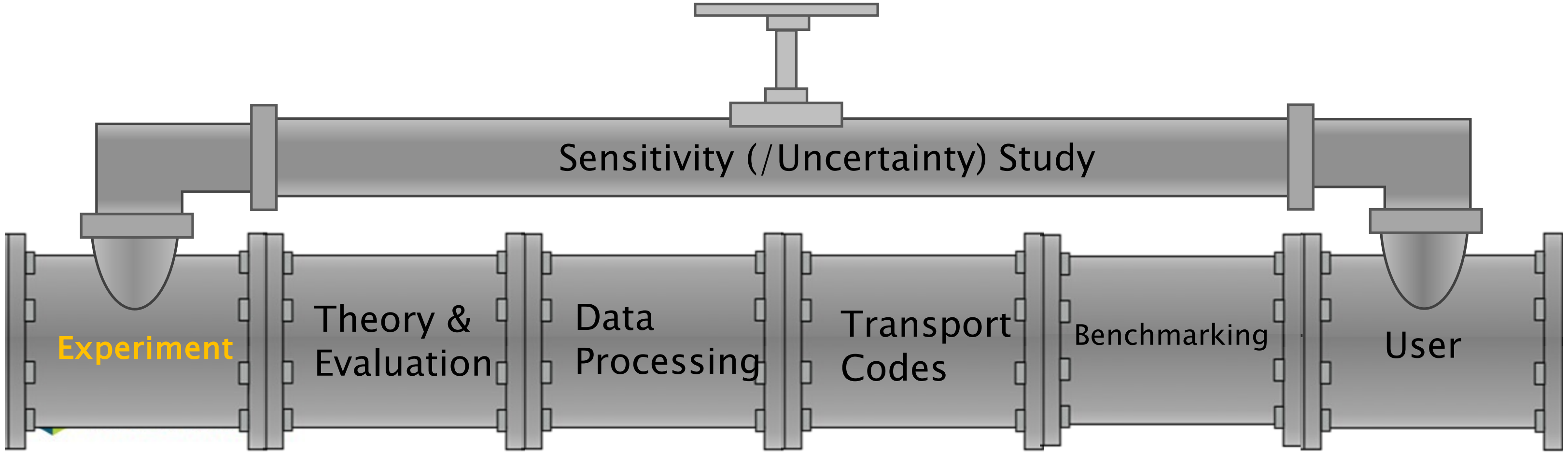
Why do we need experiment?

- We do not fully understand the physics
- We can not theoretically calculate Nuclear Data with sufficient accuracy required by applications
  - Experiments constrain the uncertainty of evaluated data
  - Test the accuracy of evaluated files and codes physics

AMANDA Li-Glass detector array at RPI



Chi-Nu EJ-309 Detector array at LANL



Slide based on Y. Danon's WANDA 2020 Pipeline Talk

Why do we need experiment?

Differential experiments, examples:

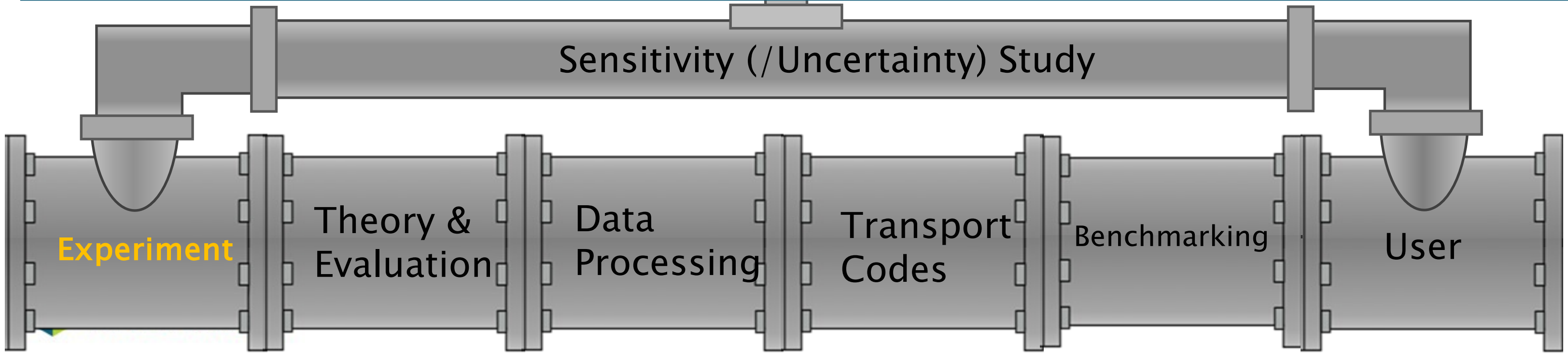
- Neutron cross section as a function of neutron energy
- Neutron capture cascades gamma spectrum
- Fission fragment yields
- Quasi-differential experiments

Validation experiments, examples:

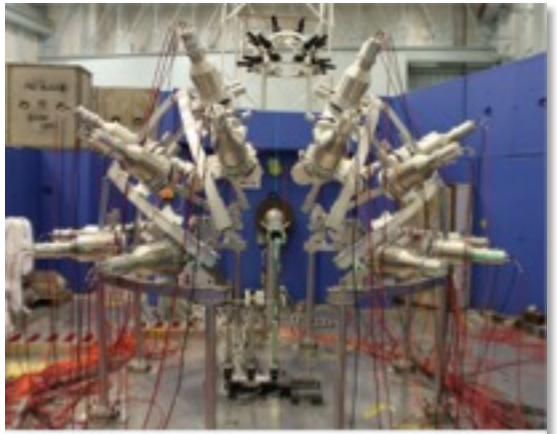
- Criticality experiments (benchmarks)
- Integral shielding measurements
- Quasi-differential experiments

Facilities at many National Labs and universities

Archived in EXFOR
https://www-nds.iaea.org/exfor/



AMANDA Li-Glass detector array at RPI

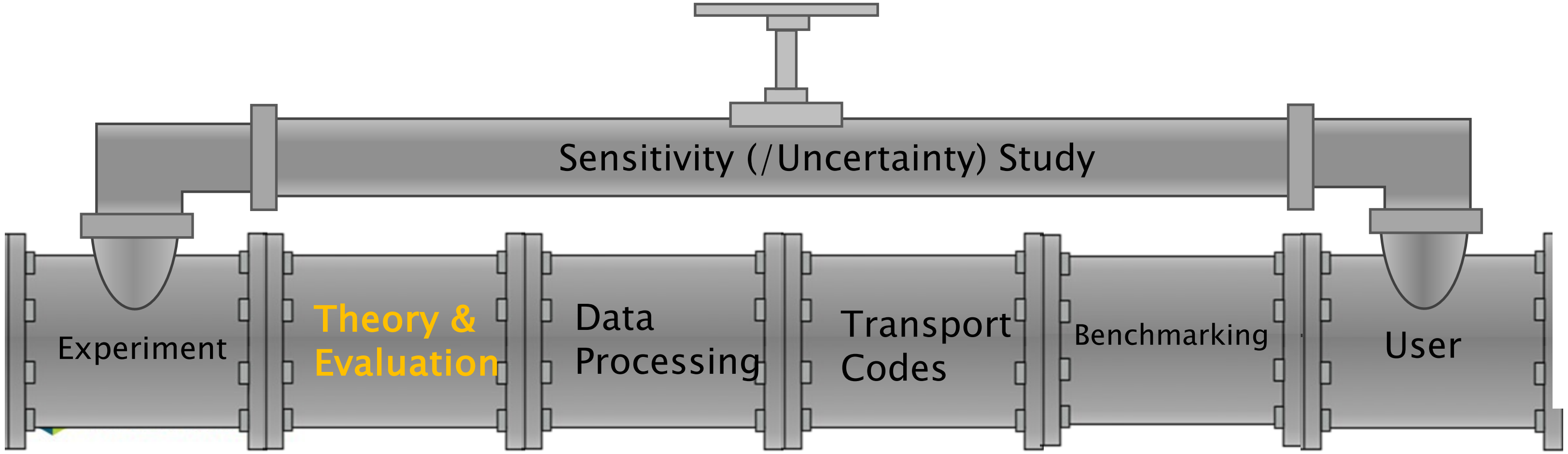


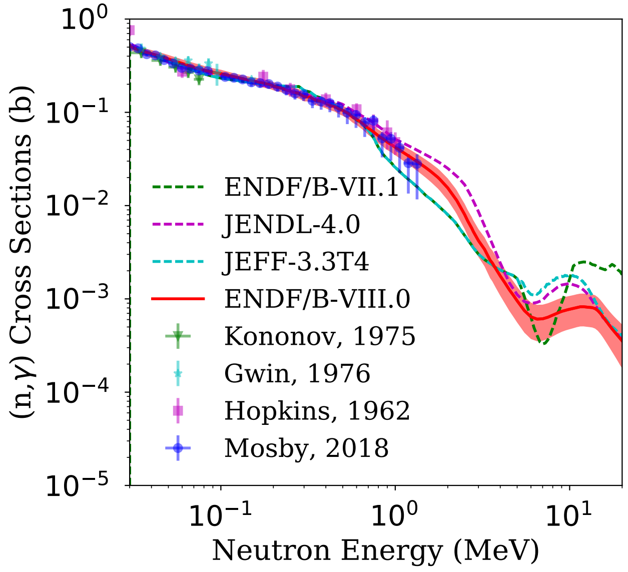
Chi-Nu EJ-309 Detector array at LANL

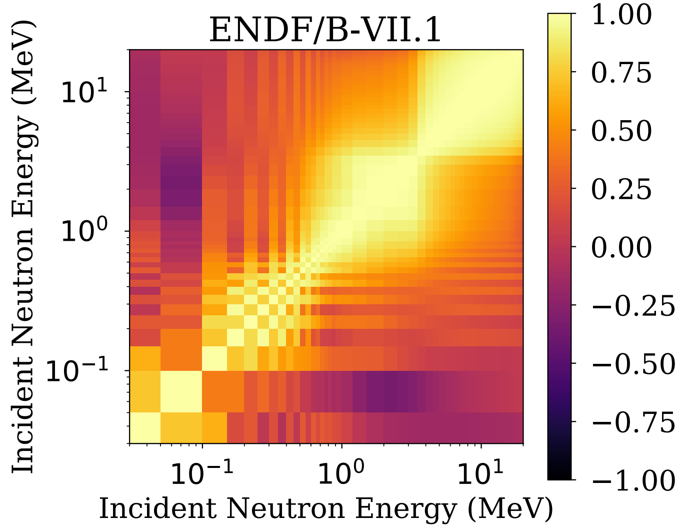
Slide based on Y. Danon's WANDA 2020 Pipeline Talk

Theory + Experiment + Statistics = Evaluation

- Experiments rarely cover all that users want
- Nuclear Theory is needed!
  - Complete data files for users
  - Make predictions/extrapolate (beyond calibration)
    - Provide estimates of uncertainties & correlations
- Statistics provide the glue
  - "To the best of our knowledge..." (given time, location, resources)
  - Bayesian statistics / Uncertainty Quantification







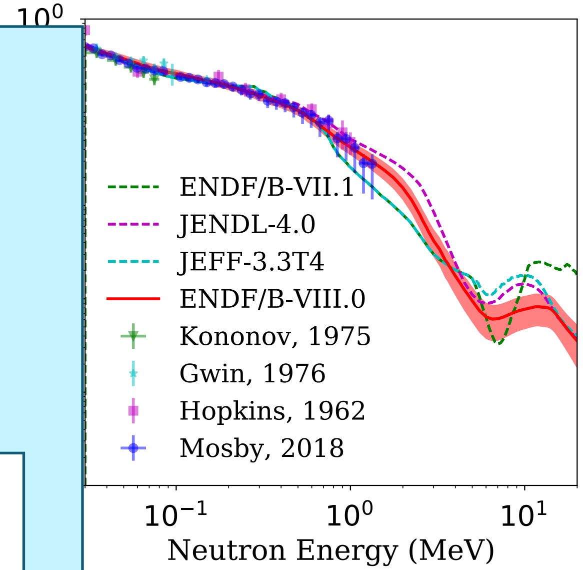
Slide based on P. Talou's WANDA 2020 Pipeline Talk

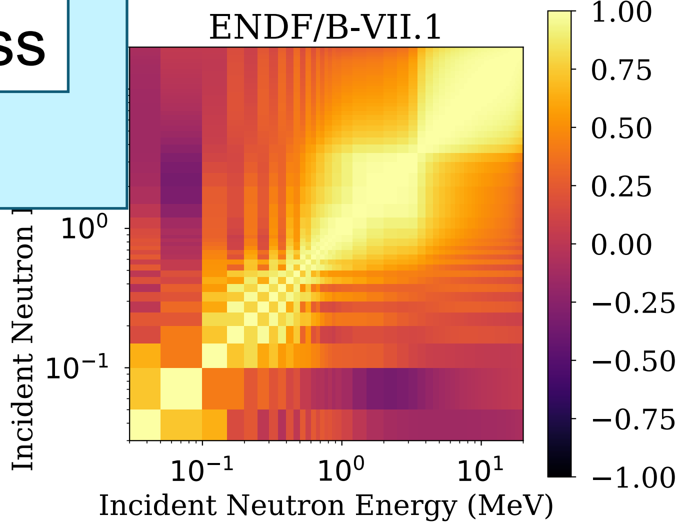
Theory + Experiment + Statistics = Evaluation

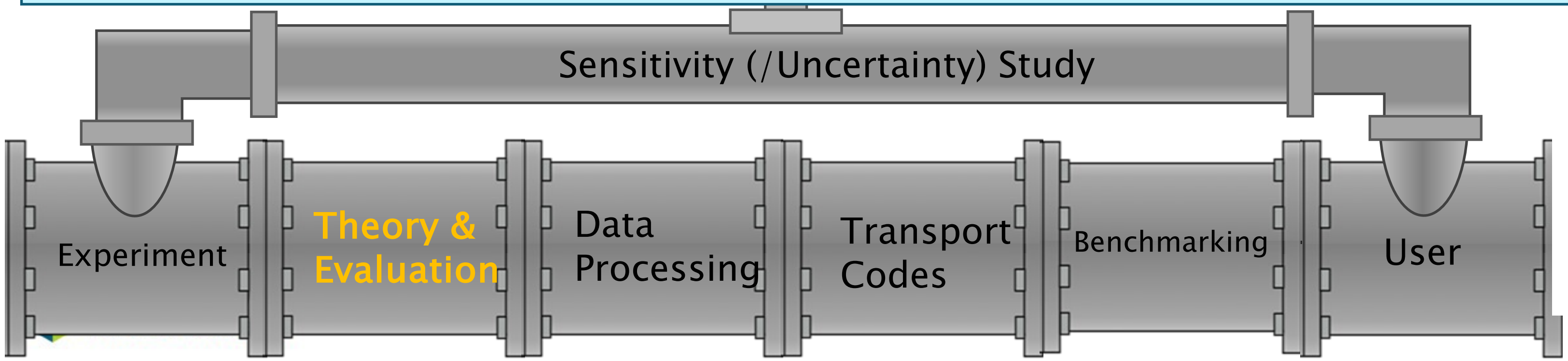
The appropriate theory is problem dependent:
- R-matrix for resonance region
- Optical Model + Hauser-Feshbach for higher energies
- Curve fitting when there is good data
- …

HPC needed in many cases:
- Density functional theory (fission)
- Ab-initio methods
- Uncertainty quantification

AI/ML increasing integrated into evaluation process





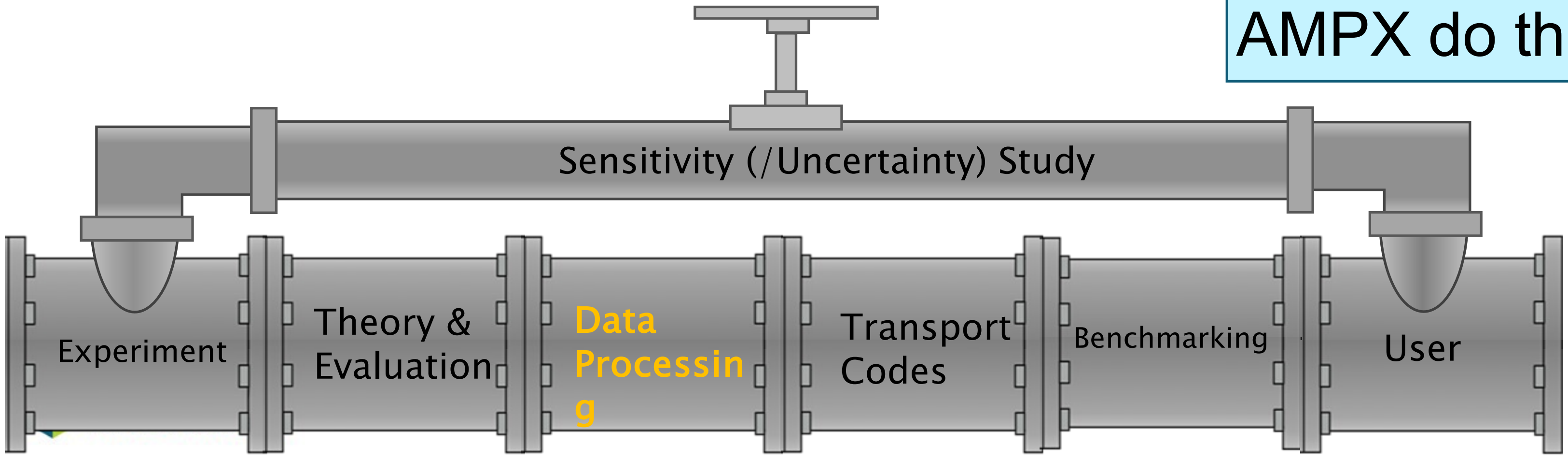


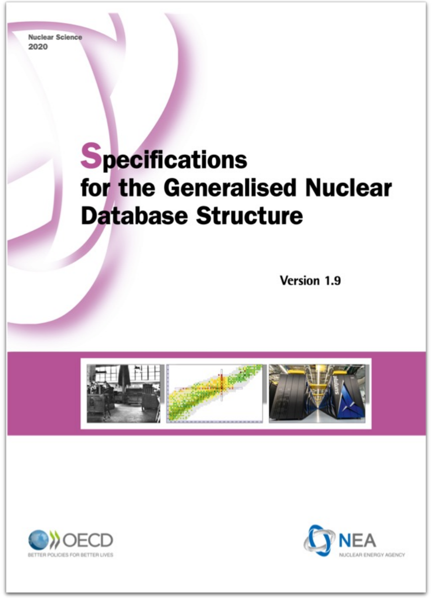
Slide based on P. Talou's WANDA 2020 Pipeline Talk

Data Processing (and formats!)

- ENDF (and soon GNDS) is only an agreed upon intermediate format
  - Evaluations must be translated into a form digestible by downstream codes
  - Requires deep understanding of physics in evaluations and physics as implemented in downstream codes
- Data needed by user may not have a “spot” in existing evaluations or downstream codes
- Underappreciated potential bottleneck

Codes such as NJOY, FUDGE and AMPX do this step



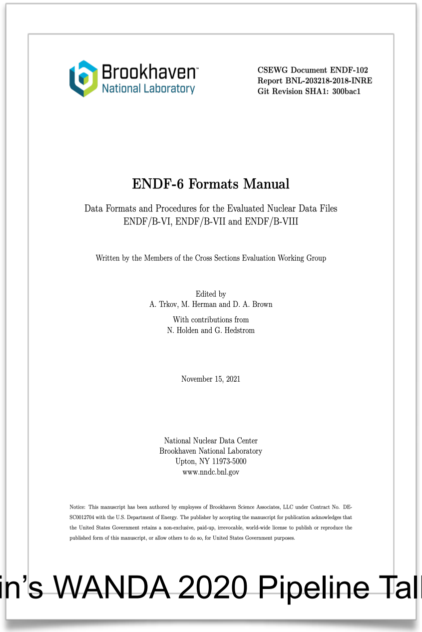

Nuclear Science 2020

Specifications for the Generalised Nuclear Database Structure

Version 1.9

OECD

NEA


Brookhaven National Laboratory

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
Git Revision SHA1: 300bac1

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

With contributions from
N. Holden and G. Hedstrom

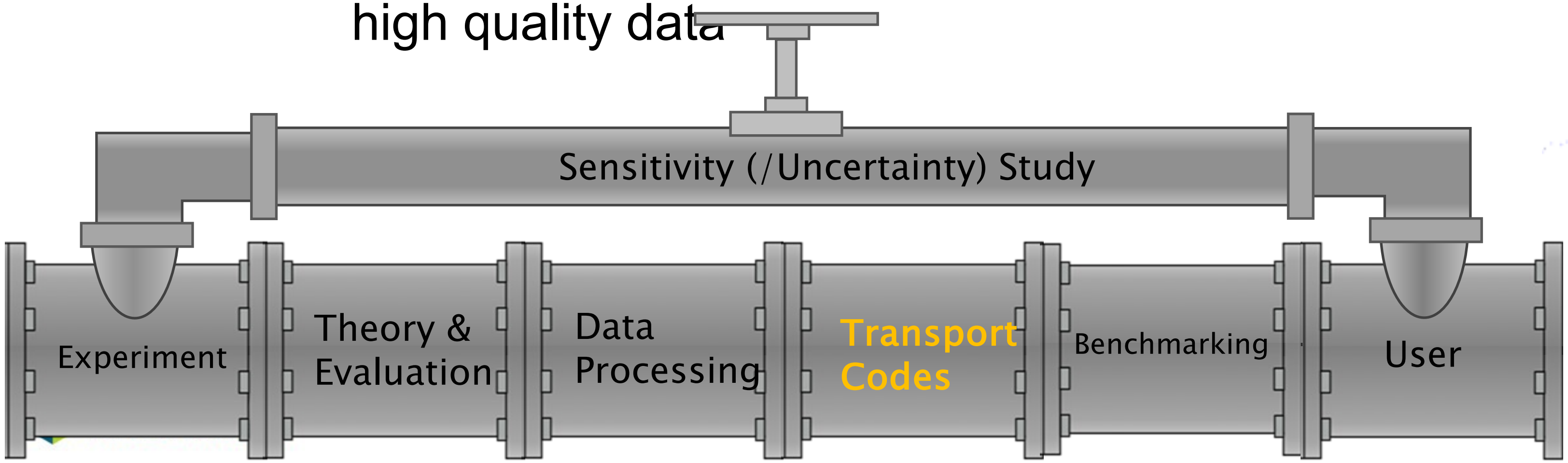
November 15, 2021

National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973-5000
www.nndc.bnl.gov

Slide based on J. Conlin’s WANDA 2020 Pipeline Talk

Transport codes

- Transport codes:
  - Numerically solve the linear Boltzmann Transport Eq.
  - Deterministic (S_N,P_N) & Stochastic (Monte Carlo)
- Calculations tend to be relatively expensive, driving codes to HPC and emerging architectures
- Transport code developers:
  - Often the first customer of nuclear data
  - Often develop a strong interest in nuclear data
  - Develop a deep understanding about need for high quality data



PHITS Particle and Heavy Ion Transport code System

OpenMC

MCNP6

scale Nuclear Systems Modeling & Simulation

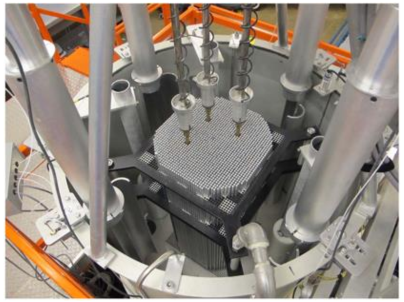
GEANT4 A SIMULATION TOOLKIT

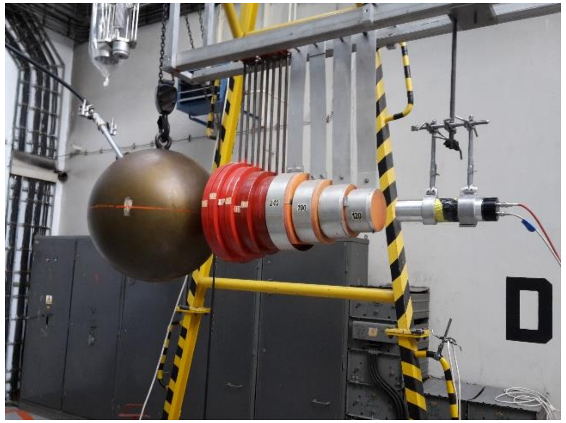
FLUKA

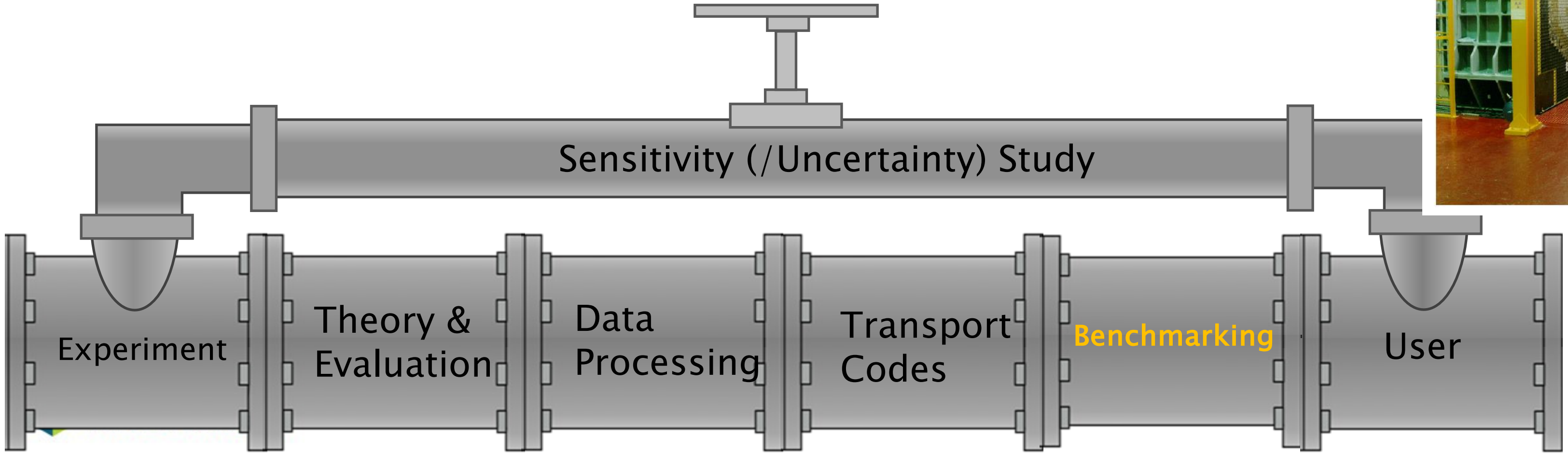
Slide based on T. Bailey's WANDA 2020 Pipeline Talk

Benchmarking

- Do you trust this Byzantine process?
- You shouldn't!
- Validation that analytical method adequately represents reality for a given application.
- Integrated test of
  - Evaluated nuclear data
  - Nuclear data processing codes
  - Transport codes



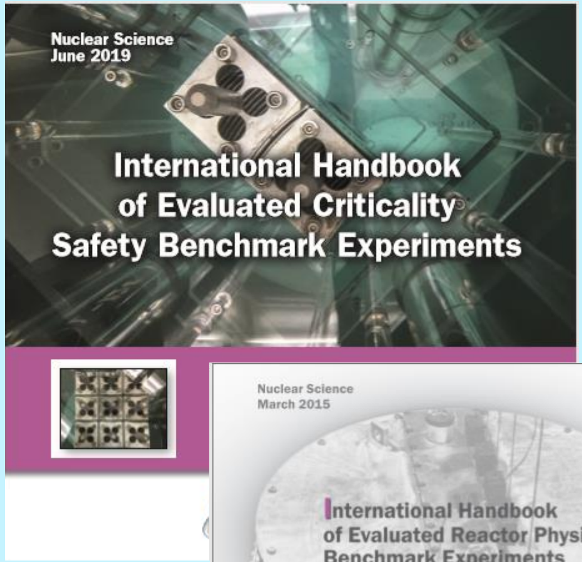


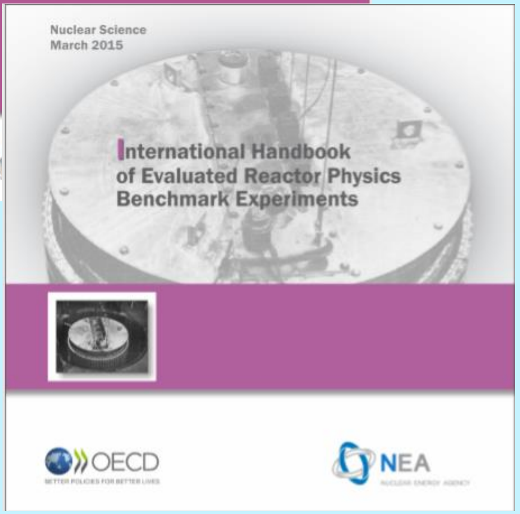


Slide based on M. Zerkle's WANDA 2020 Pipeline Talk

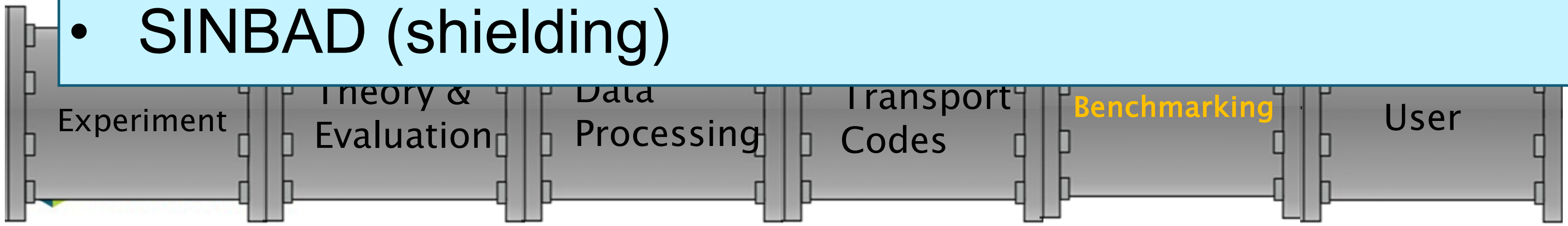
Benchmarking

Basic data for benchmark development
- Critical assemblies
- Subcritical assemblies
- Engineering mockup critical assemblies
- Reactor startup exp.
- Reactor operation data
- Shielding experiments



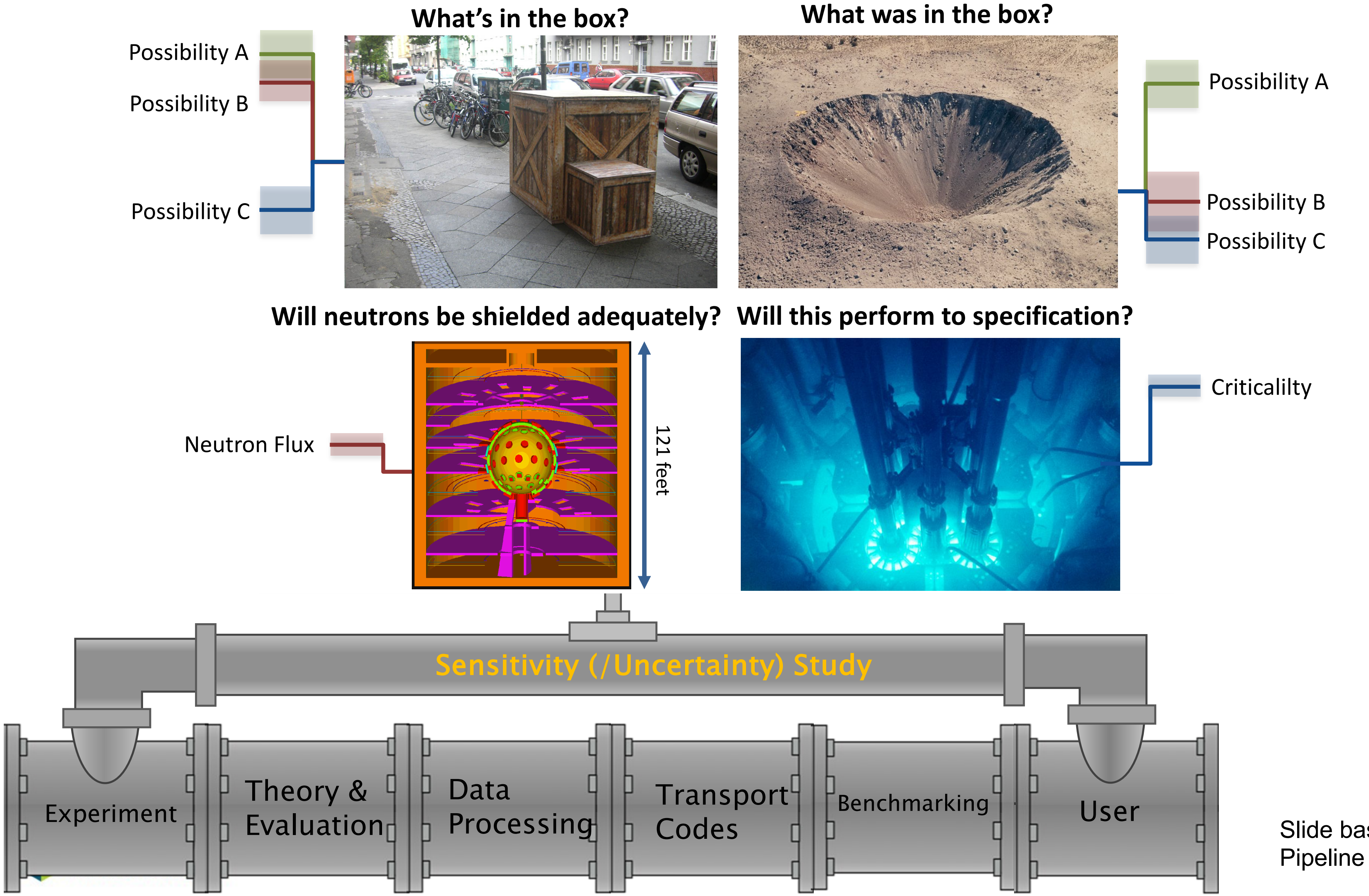


Well characterized experiments in established handbooks:
- ICSBEP (criticality safety)
- IRPhEP (reactor physics)
- SINBAD (shielding)



Slide based on M. Zerkle's WANDA 2020 Pipeline Talk

Uncertainty Quantification/Sensitivities



Uncertainty Quantification helps inform decision makers, and identifies sources of uncertainty that could be reduced.

Slide based on R. Casperson's WANDA 2020 Pipeline Talk

Uncertainty Quantification/Sensitivities

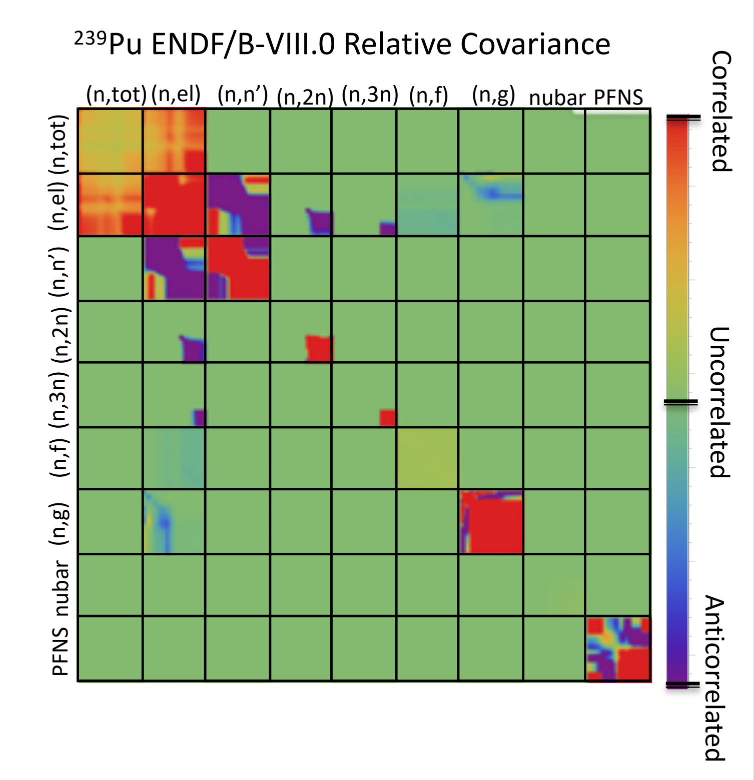
What's in the box? **What was in the box?**

Forms of Uncertainty Propagation

- UQ involves propagation of uncertainties through models of interest, and analysis of output distributions.
- Sensitivity studies useful as an intermediate step.
- Inverse UQ using experimental output data is relevant to some applications, and can produce constrained input distributions.

Best method to define required experiment.

- Replace existing evaluation with hypothetical experiment? ✗
- Trust existing evaluation and identify constraints that most impact applications? ?
- Work with evaluator? ✓



at

Slide based on R. Casperson's WANDA 2020 Pipeline Talk

US Nuclear Data Program is the custodian of most nuclear data needed for applications

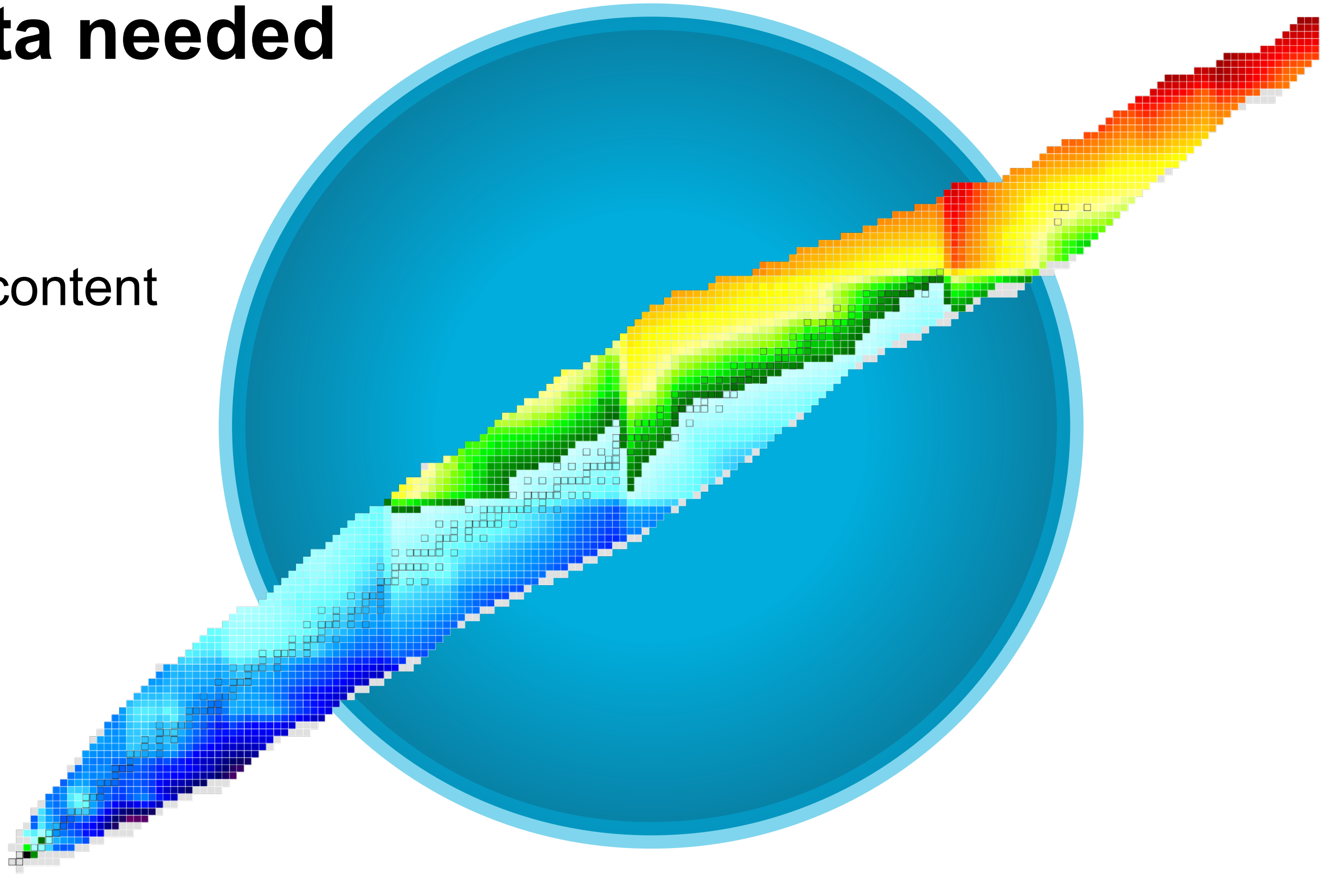
Nuclear Science References (NSR)
Nuclear physics articles indexed according to content

EXFOR
Compiled nuclear reaction data

XUNDL
Compiled nuclear structure and decay data

ENSDF
Recommended nuclear structure and decay data

ENDF
Recommended particle transport and decay data, with a strong emphasis on neutron-induced reaction data



NNDC website: www.nndc.bnl.gov

Brookhaven National Laboratory

The Cross Section Evaluation Working Group produces ENDF/B library

- **Formed 1966 & Chaired by BNL**
- **Currently ~200 members of the collaboration from 25 institutions**
  - US programs, industry and international partners
  - If you see something in the library, at some point a sponsor somewhere wanted it
- **All steps of nuclear data pipeline coordinated through CSEWG**
- **Depending on what needs done, getting required data in library can be major effort**

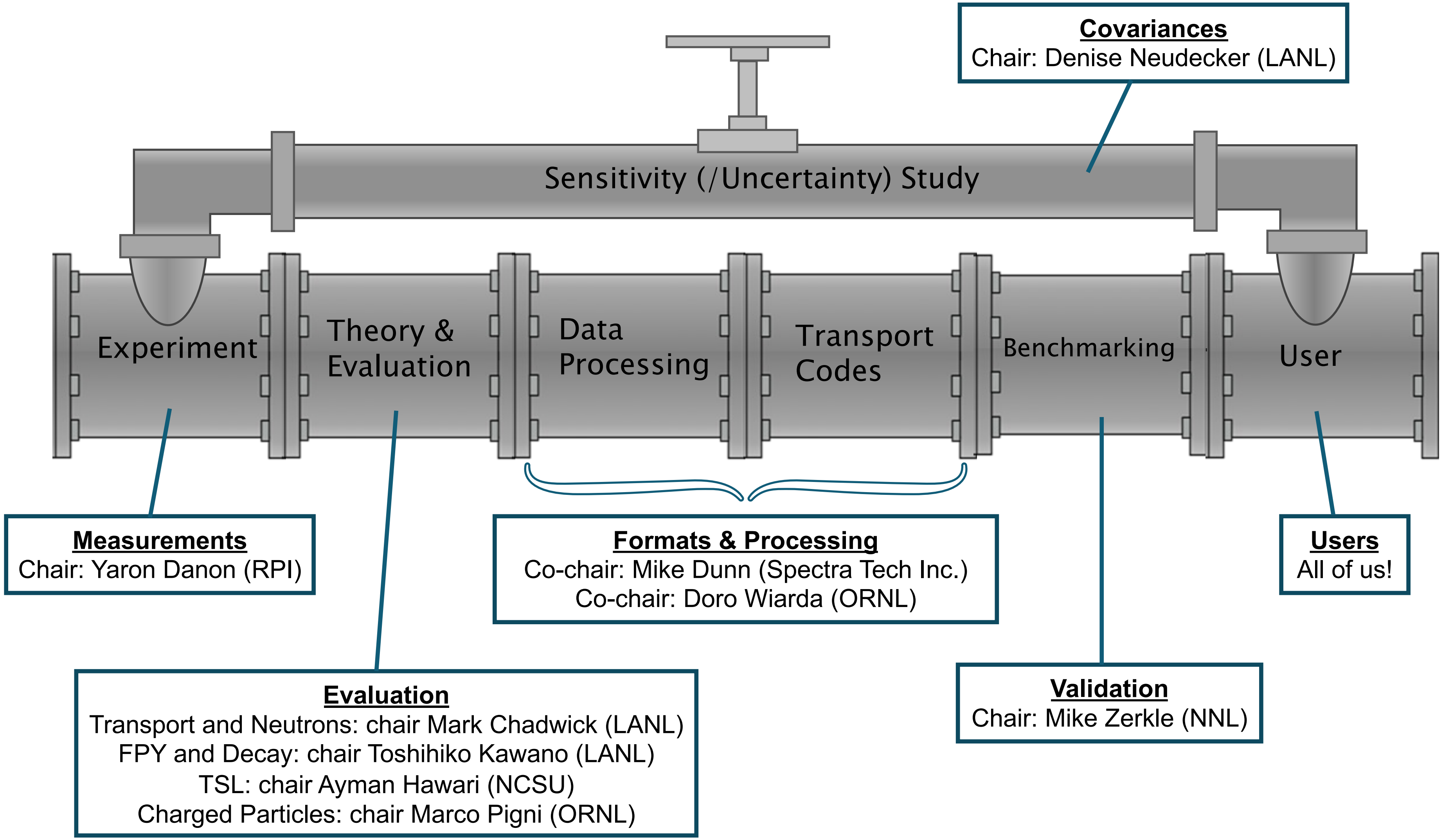
We are always open to new users and collaborators

CSEWG collaboration meeting in November 2022: our first in-person meeting since the pandemic started!

All steps of nuclear data pipeline are coordinated through CSEWG

Chair:
David Brown (BNL)
dbrown@bnl.gov

Library Manager:
Gustavo Nobre (BNL)
gnobre@bnl.gov



Brookhaven National Laboratory

Summarizing

- **CSEWG and ENDF:**
  - Welcomes collaboration in and out of US (but inside is easier)
  - Long tradition of quality/continuous improvement
  - Conservative, driven by experiment when possible
  - Golden Rule (whoever has the gold makes the rules)
- **USNDP and NNDC are a resource for many other data products**

A Gallery of Nuclear Data Pipelines

David Brown

National Nuclear Data Center,

Brookhaven National Laboratory

26 Feb 2024

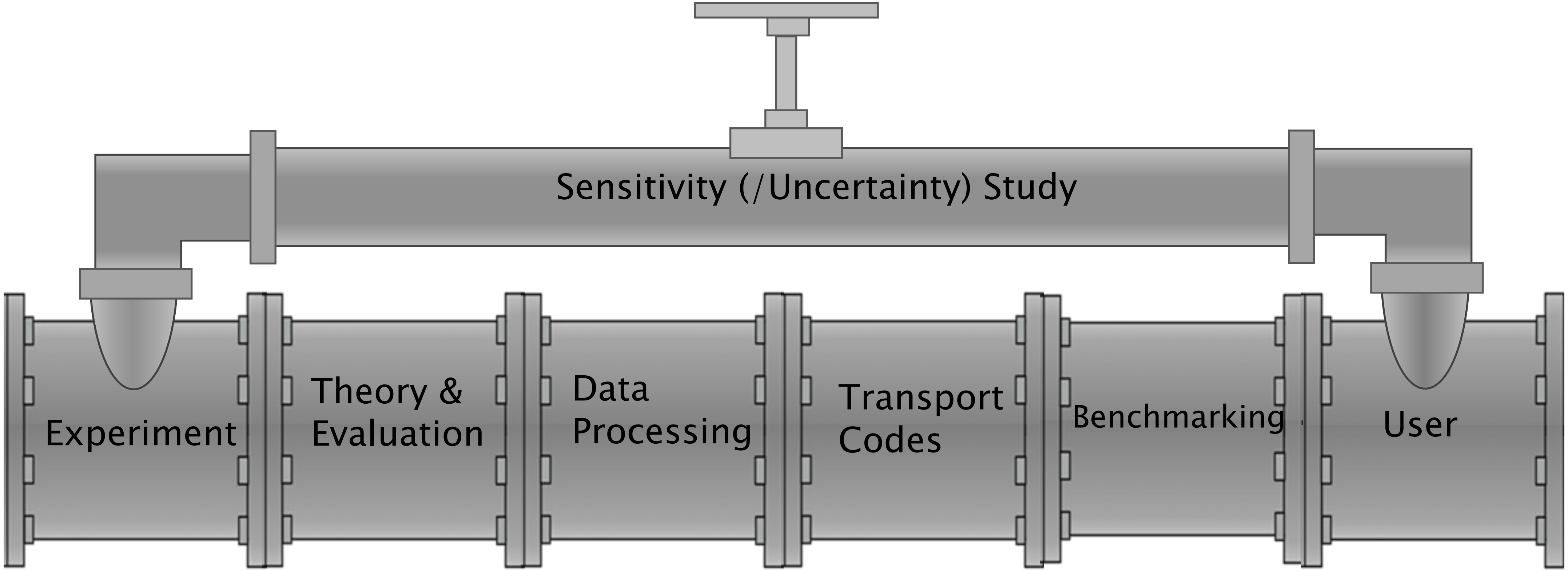
WANDA 2024

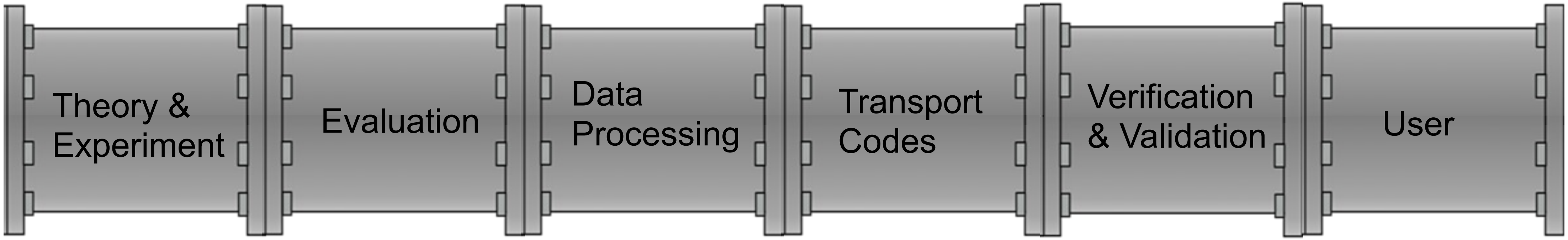
Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

@BrookhavenLab

The pipeline is, of course, a metaphor and the contents depend on what message one is trying to convey





Main points:

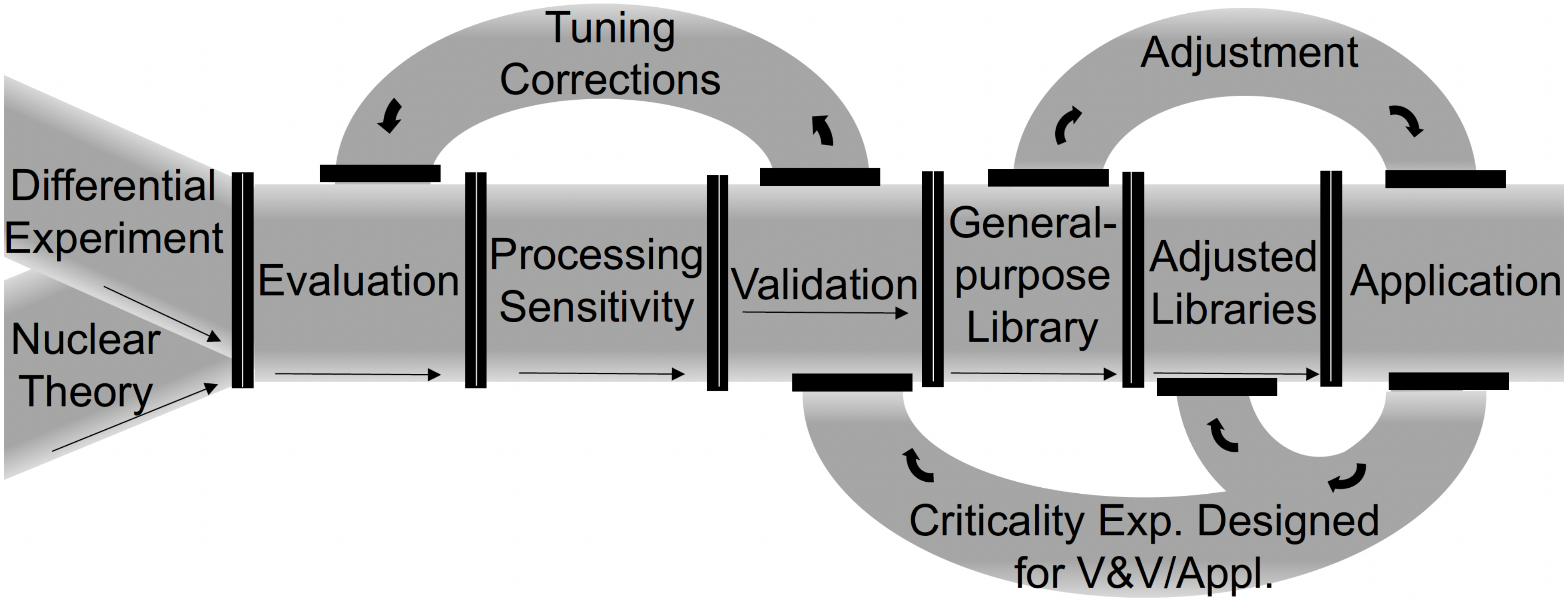
- There are a few important, high-level steps
- Theory and experiment are co-equal

Main points:

- There are a few important, high-level steps
- The creator of the graphic was an experimentalist

PHYSICAL REVIEW RESEARCH 4, 021001 (2022)

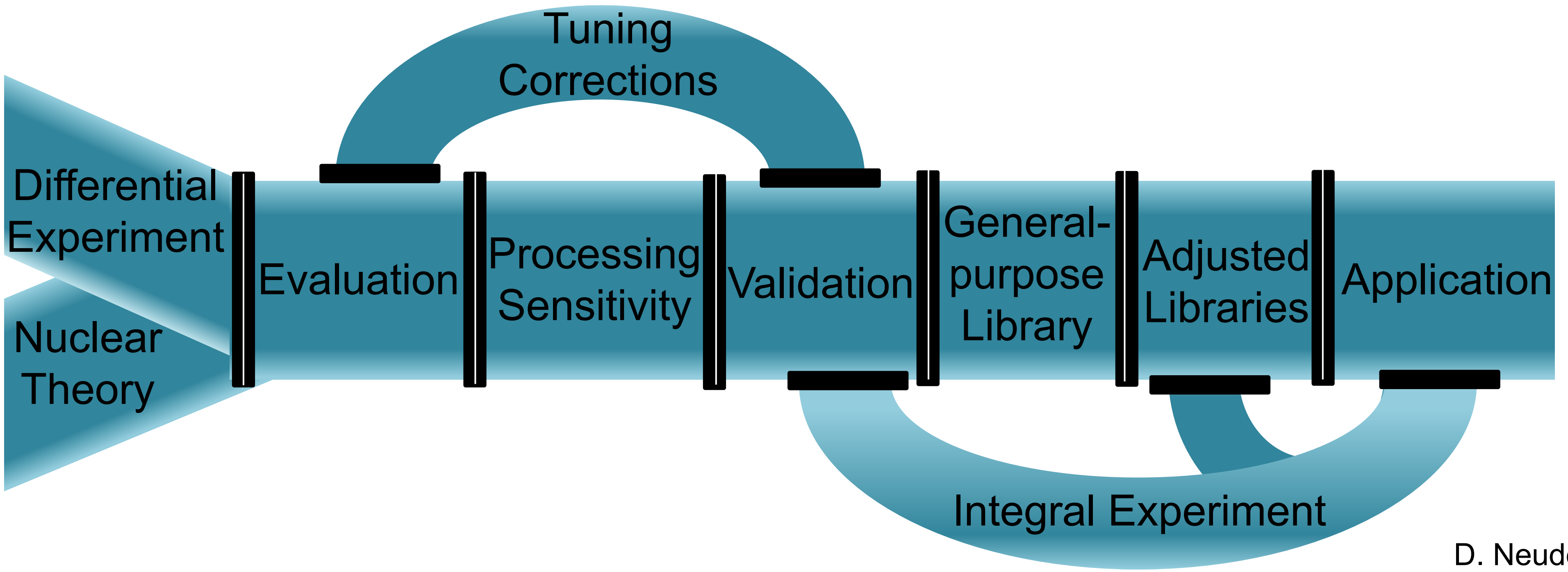
Brookhaven National Laboratory



Main points:

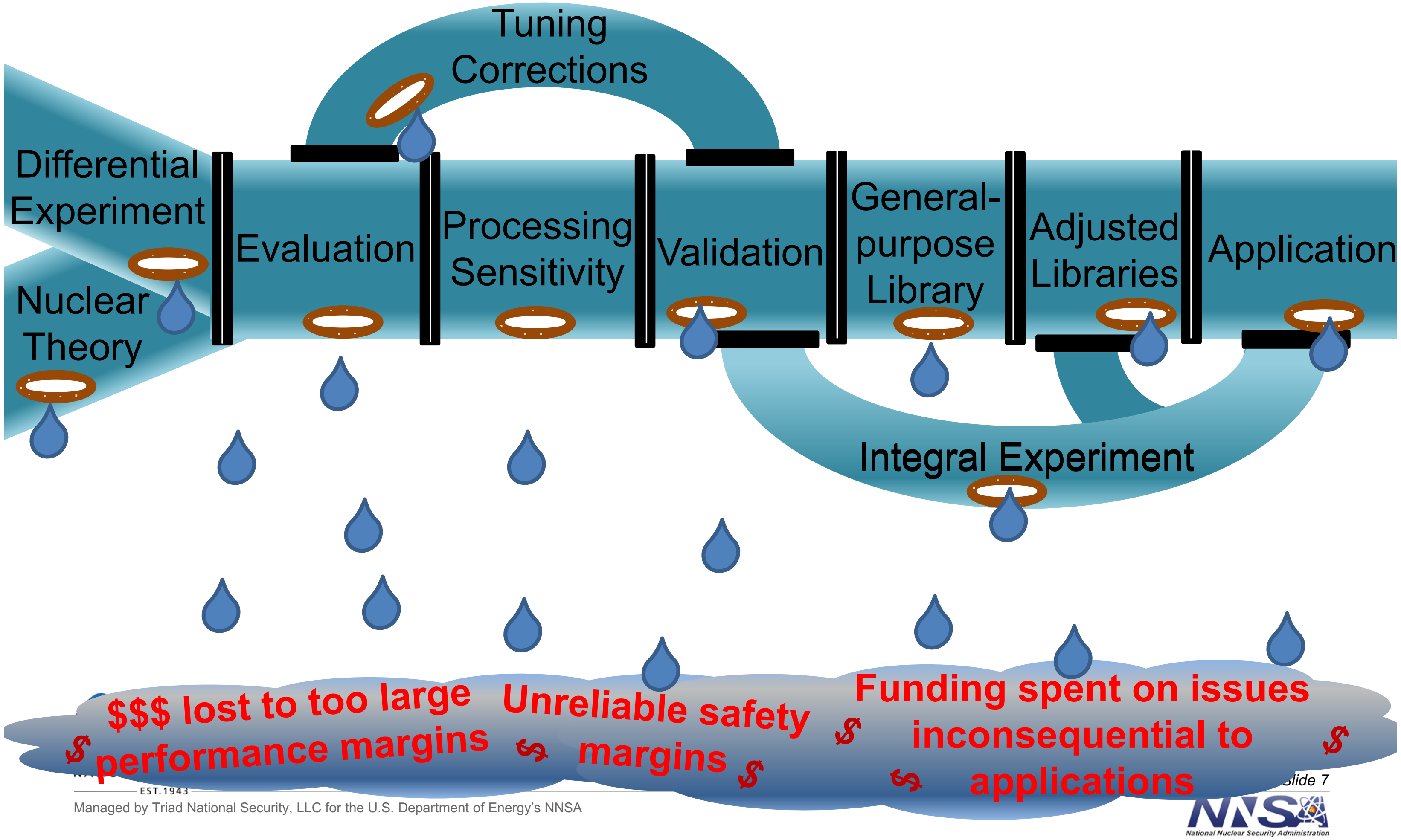
- There are a few important, high-level steps
- There are several feedback loops in the process

D. Neudecker, LA-UR-23-27944



D. Neudecker,
WANDA 2020,
LA-UR-20-216802

Main points:
- There are a few important, high-level steps
- There are several feedback loops in the process
- The pipeline is teal

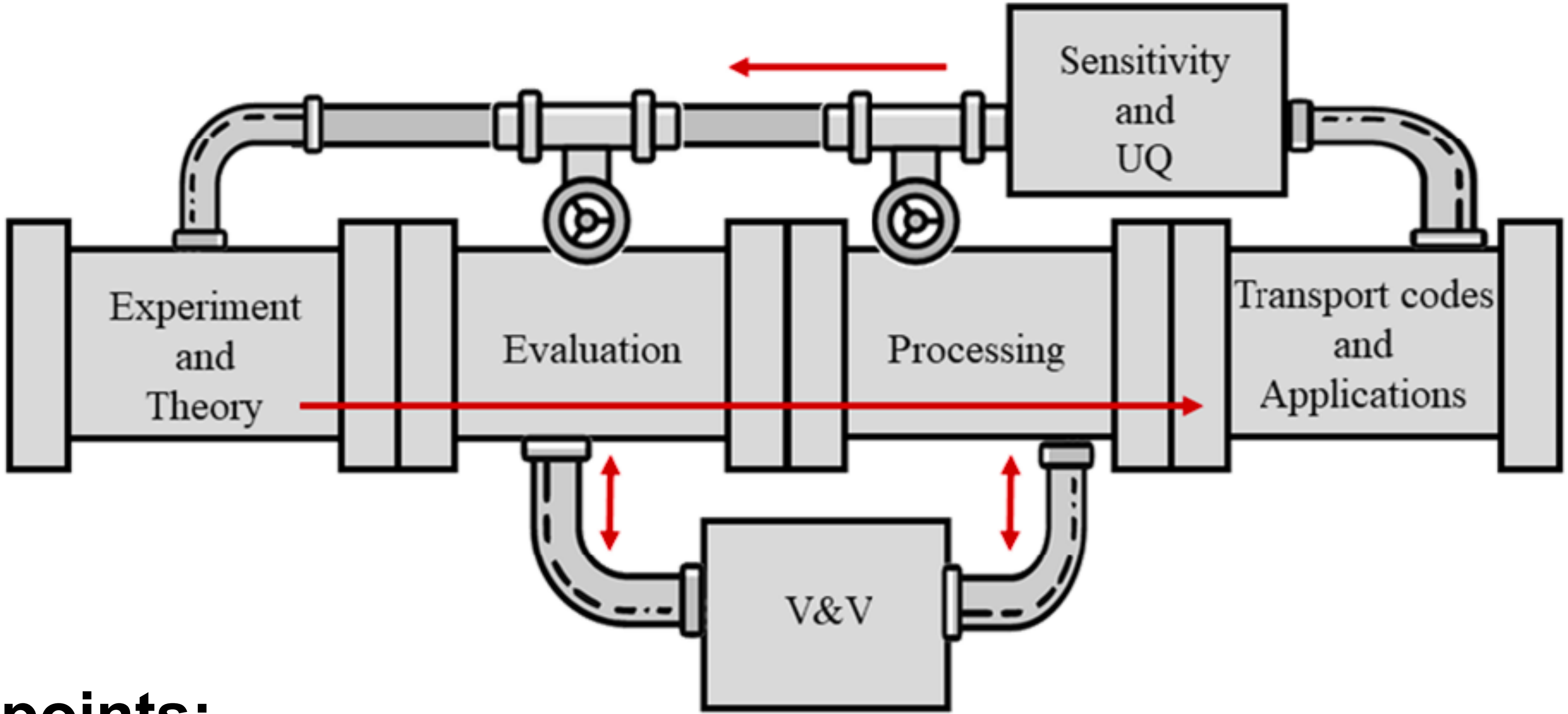


D. Neudecker, WANDA 2020, LA-UR-20-216802

Main points:

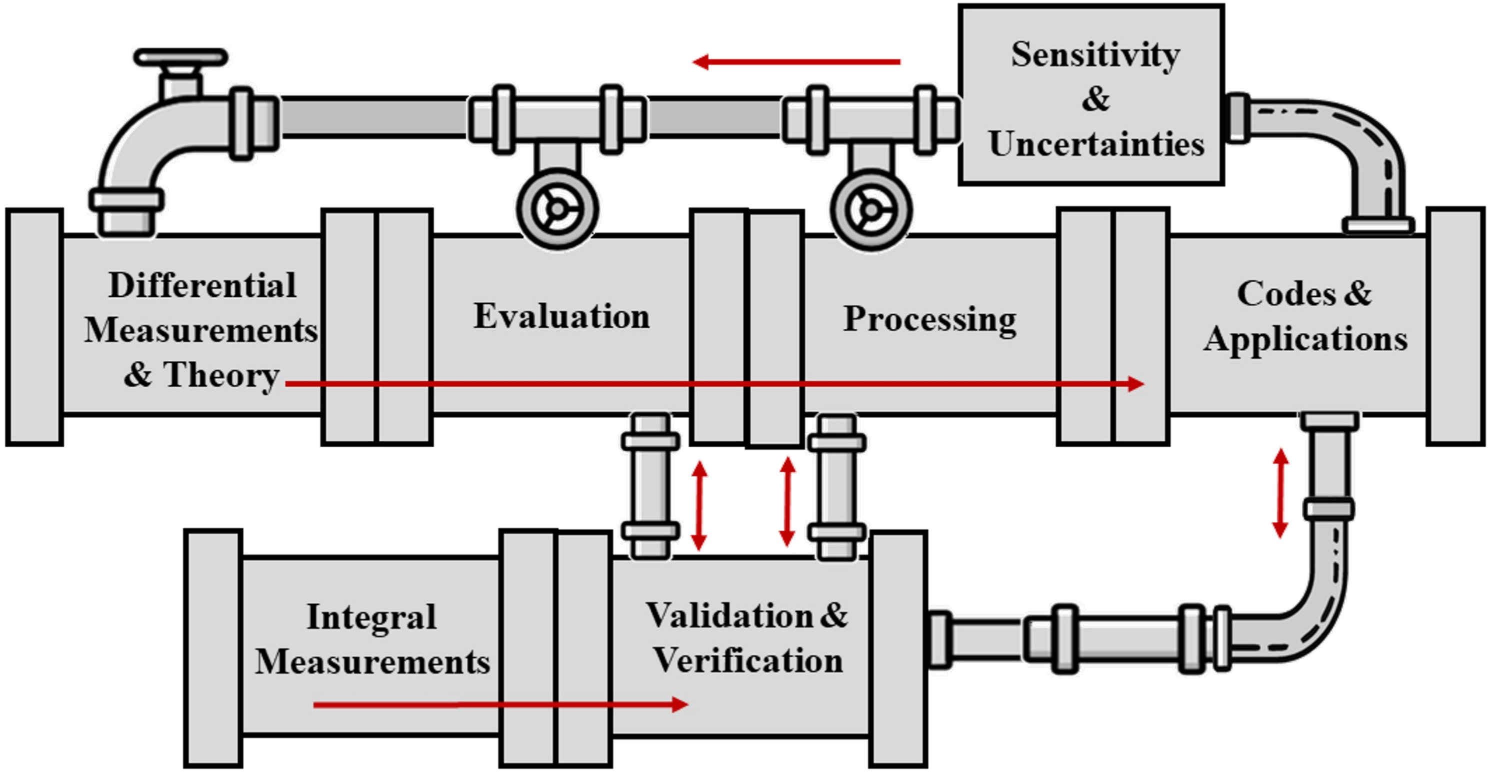
- There are a few important, high-level steps
- There are several feedback loops in the process
- The pipeline is teal and leaky

Brookhaven National Laboratory



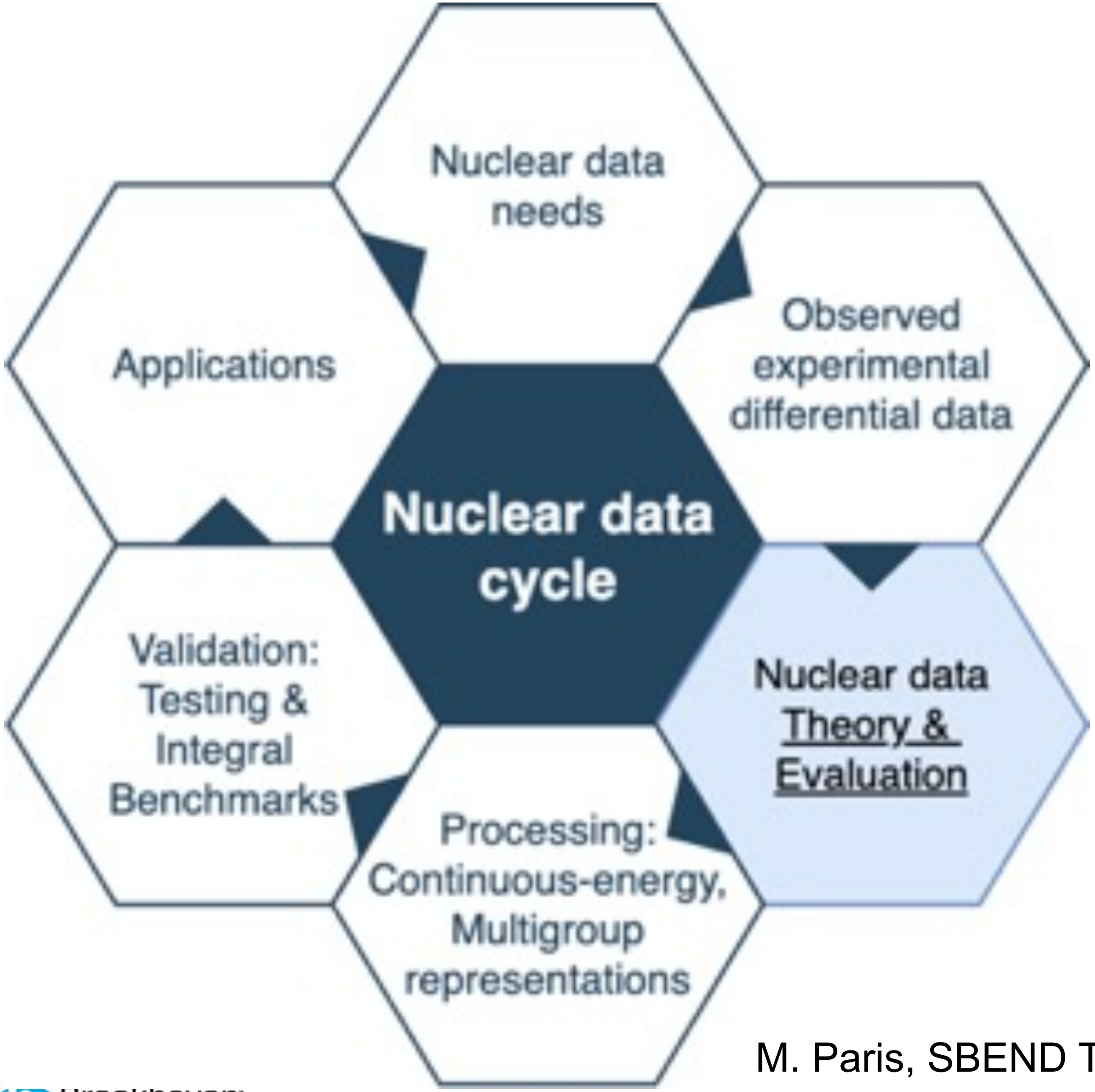
Main points:

- There are a few important, high-level steps
- There are several *more* important feedback loops
- Someone understand pipefitting better than the original creator of the metaphor



Main points:

- There are a few important, high-level steps
- There are *even more* important feedback loops
- I love the steampunk aesthetic



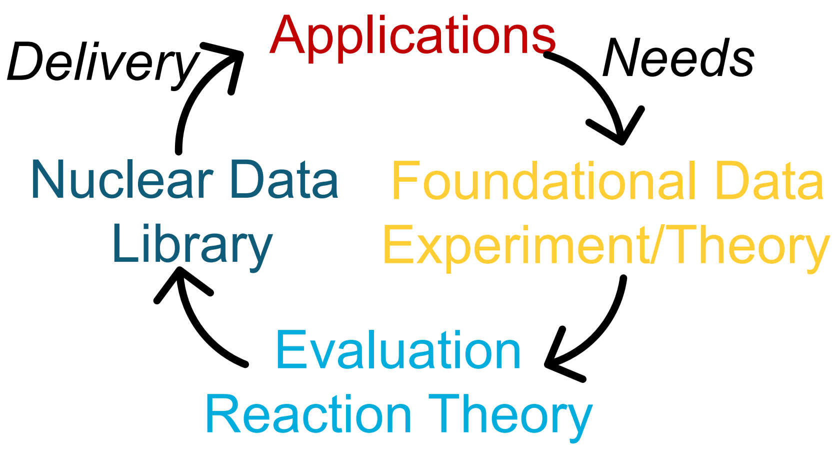
Main points:

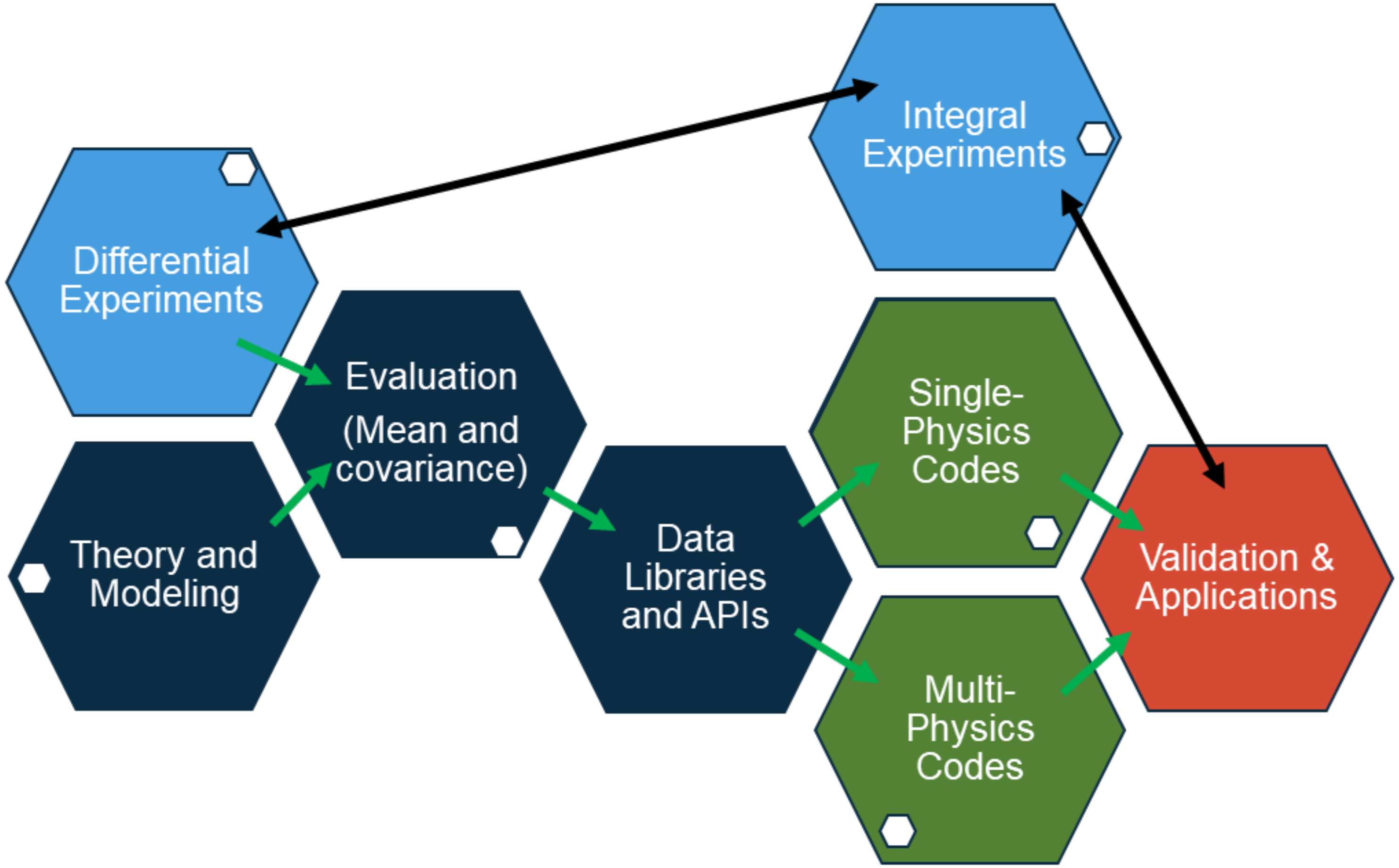
- There are a few important, high-level steps
- The pipeline is more of a cycle of continuous improvement

M. Paris, SBEND Talk, WANDA 2024

Main points:

- There are a few important, high-level steps
- The pipeline is more of a cycle of continuous improvement
- You don't need fancy graphics to make a pipeline

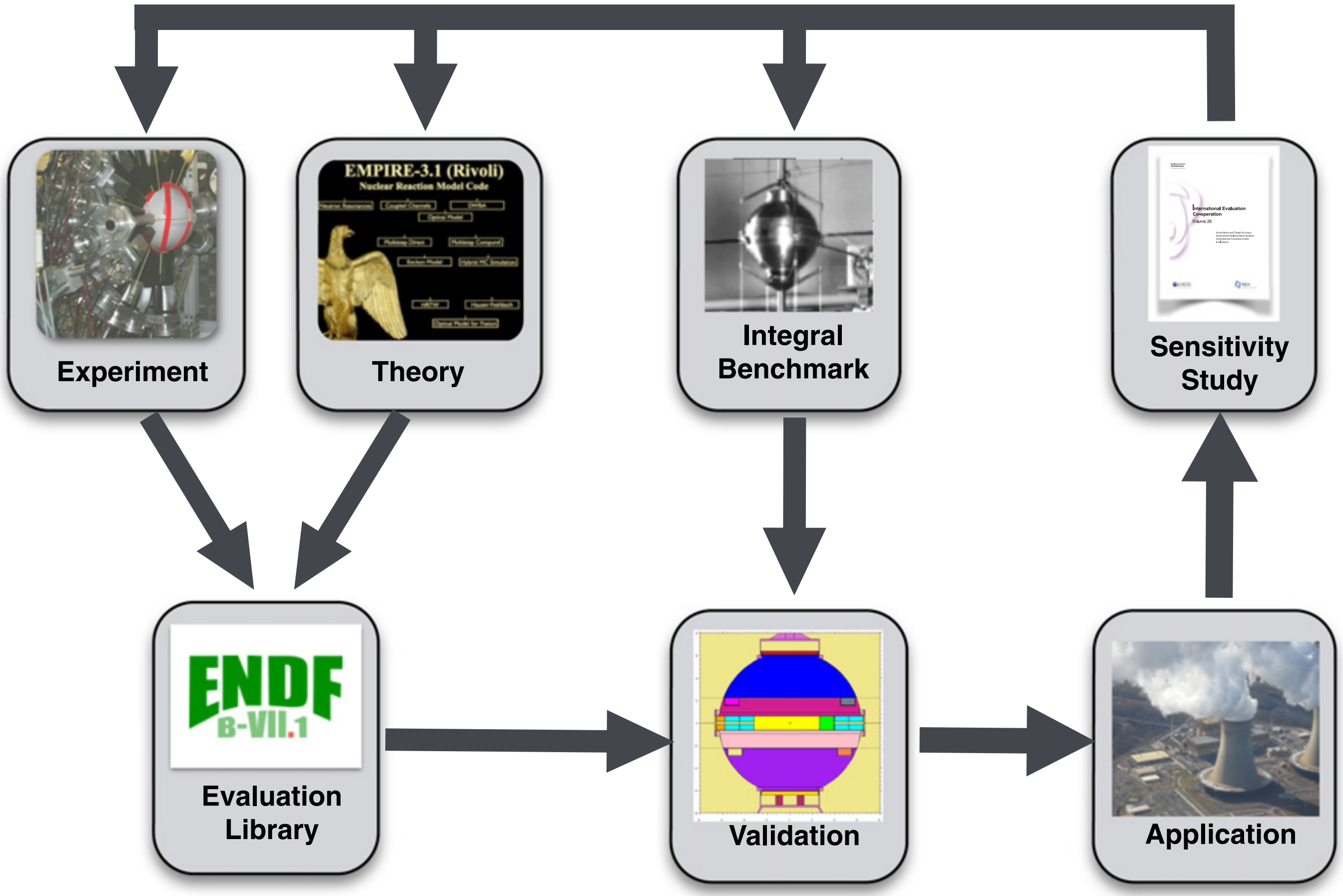




Michael Halfmoon, WANDA 2024

Main points:

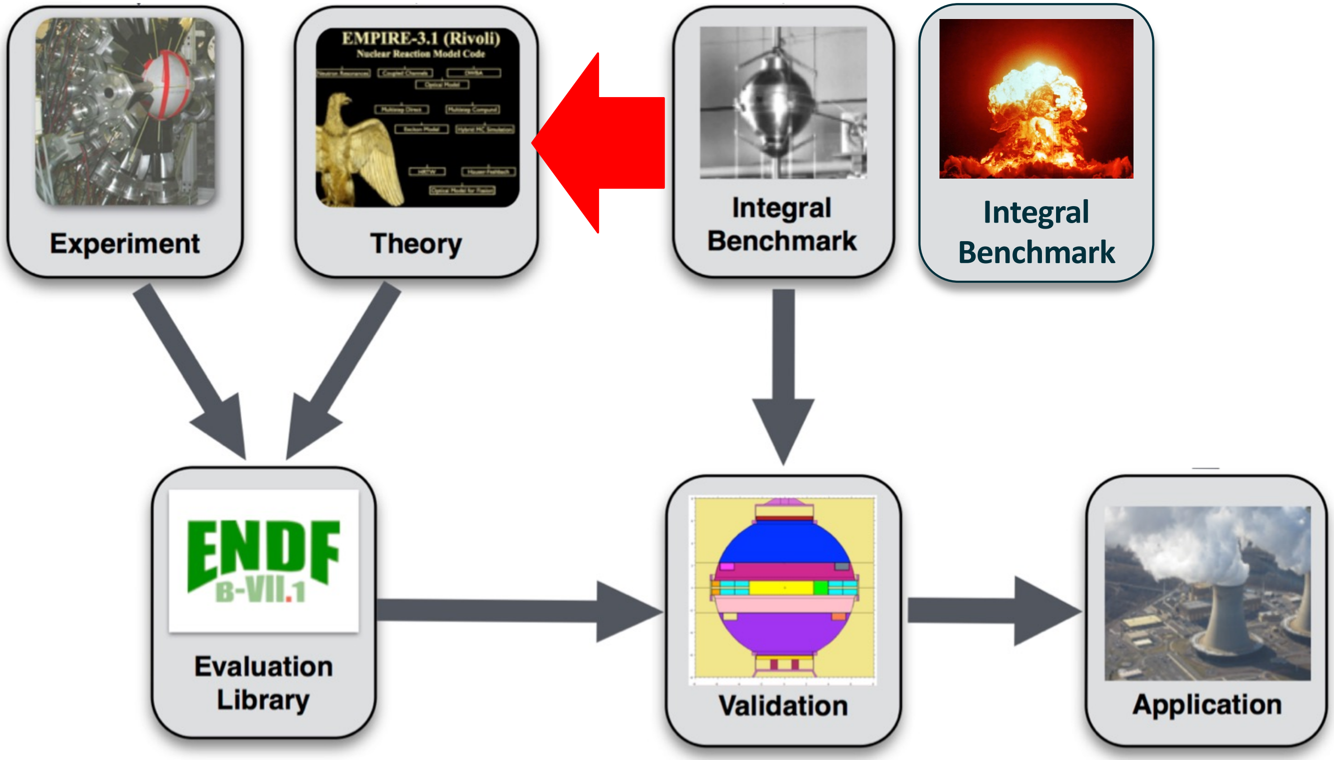
- There are a few important, high-level steps
- There are several important feedback loops
- The pipeline is more of a cycle of continuous improvement
- Hexagons are a popular design choice



J. Phys. G: Nucl. Part. Phys. 42 (2015) 034020

Main points:

- There are a few important, high-level steps
- There are several important feedback loops
- The pipeline is more of a cycle of continuous improvement
- The creator found graphics on the web that looked pretty cool

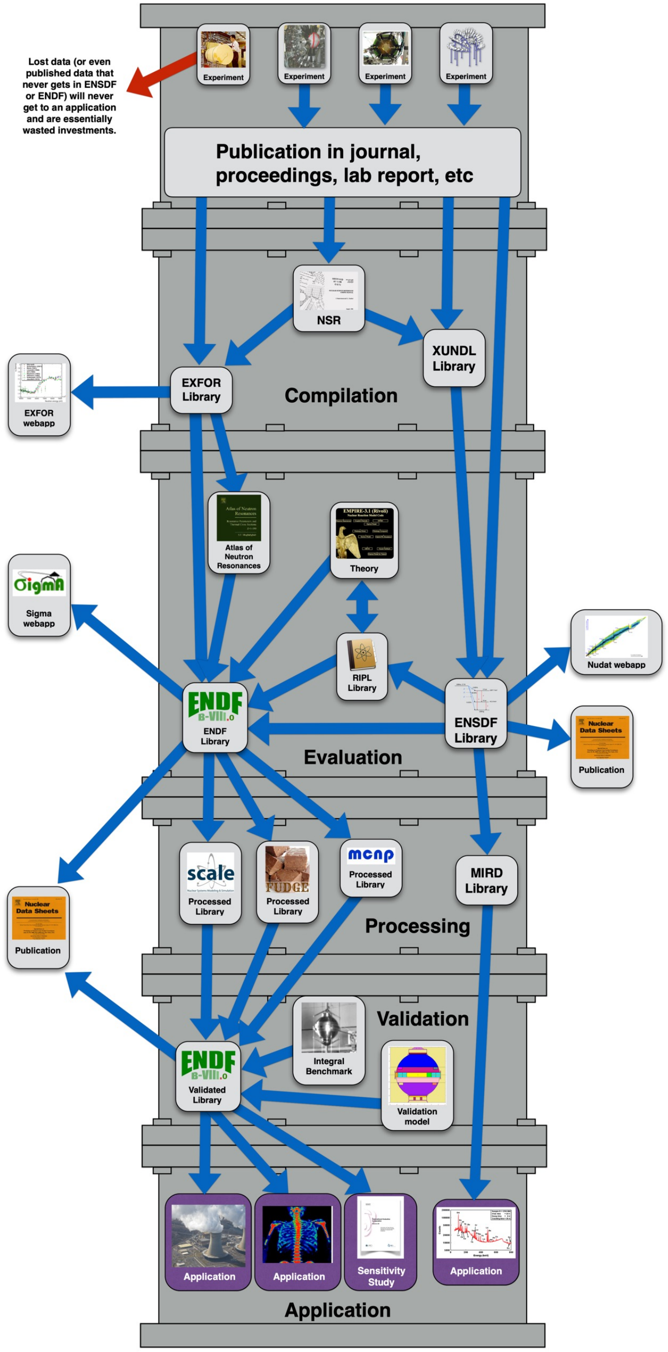


L. Bernstein, WANDA 2023

Main points:

- There are a few important, high-level steps
- There are several important feedback loops
- The pipeline is more of a cycle of continuous improvement
- We need to have a discussion about derivative work

Brookhaven National Laboratory



Data starts here.

It can take years to plan and execute an experiment. Then it can take another year to publish.

That's just the beginning…

***Compilation*: collect unevaluated data together**
- **NSR:** Bibliographic data collected on an ongoing basis (USNDP project)
- **EXFOR:** Reaction data compiled here within ~6 mos. - 1 yr. (international collaboration)
- **XUNDL:** Structure data compiled here within 1 week to a few months (USNDP project)

***Evaluation*: combine all available information into one set of recommended values & covariance**
- **ENDF:** Reaction evaluations can take anywhere from ~1 month ("easy isotope") to ~3 years ("hard isotope" e.g. ^{238}U, ^{235}U, ^{239}Pu, ^{56}Fe, …). Prioritization and funding is done on a per-program level. If no one funds it, it doesn't get done. (CSEWG collaboration, includes USNDP, DP, NCSP, many others)
- **ENSDF:** Structure evaluations typically take a few months to a year; all nuclei are re-evaluated on a ~7 year cycle. The process can be sped up with additional funding. (USNDP project)
- **Other libraries:**
  - **RIPL**: inputs for models (IAEA)
  - **Atlas**: neutron resonances (NNDC)

***Processing:* prepare data for use in an application code**
In US, there are 3 main processing codes, each tied to specific application codes:
- **NJOY (LANL):** serves MCNP
- **AMPX (ORNL):** serves SCALE
- **FUDGE (LLNL):** serves LLNL codes

Additionally, **MIRD library** used in medical physics. Processing is done on an ad-hoc basis so can take ~6 mo. - 1yr. to get results.

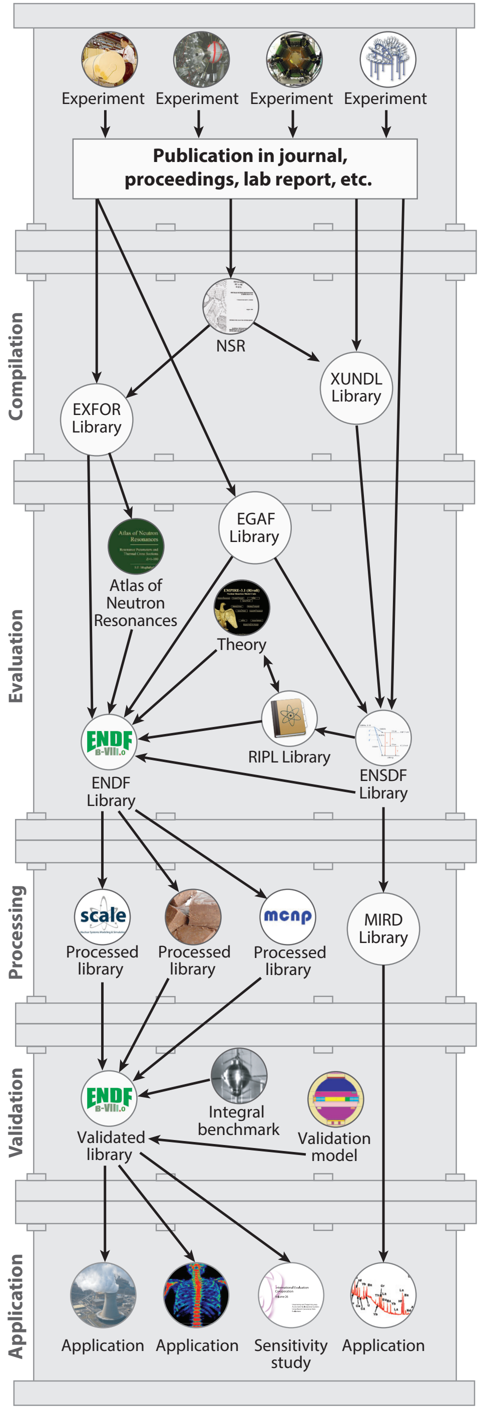
***Validation:* test data in simulation of a non-trivial but well understood nuclear system**
There are several sources of high quality benchmark data:
- **ICSBEP:** Criticality safety (NEA coordinated, large NCSP investment)
- **IRPhEP:** Reactor physics (NEA coordinated, large US investment)
- **SINBAD:** Shielding (NEA coordinated)

Testing done on ad-hoc basis so results may not be available for ~6 mos. - 1 yr.

Main points:

- There are a few important, high-level steps
- Each step really is many smaller steps
  - Each step is carefully defined in small print
  - Each step has a notional timeline
- The orientation is vertical, much like pipelines in the sanitation industry*

* note: users are at the receiving end of the metaphor



Main points:

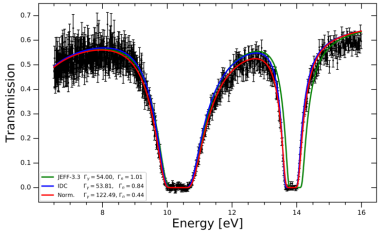
- There are a few important, high-level steps
- Each step really is many smaller steps
- The orientation is vertical, much like pipelines in the sanitation industry
- The publisher did not like the small print

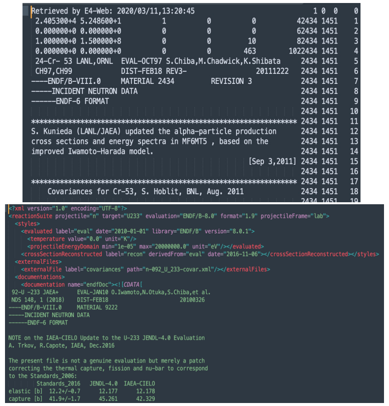
Annu. Rev. Nucl. Part. Sci. 2019.69:109-136.

Motivation

Differential Measurements	Data Evaluations	Evaluated Nuclear Data Files (ENDF)	Nuclear Data Processing	Validation / Applications

SAMMY





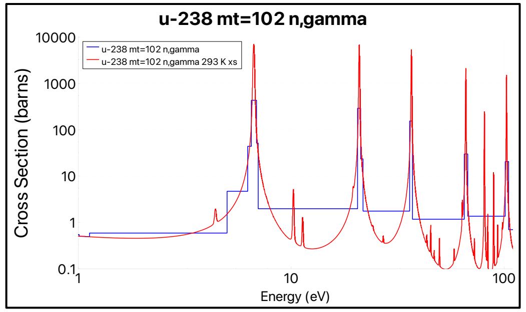
```
Retrieved by E4-Web: 2020/03/11,13:20:45                           1 0  0     0
 2.405300+4 5.248600+1          1          0          0        42434 1451    1
 0.000000+0 0.000000+0          0          0          0        62434 1451    2
 1.000000+0 1.500000+8          0          0         10        82434 1451    3
 0.000000+0 0.000000+0          0          0        463      1022434 1451    4
 24-Cr- 53 LANL,ORNL  EVAL-OCT97 S.Chiba,M.Chadwick,K.Shibata      2434 1451    5
 CH97,CH99            DIST-FEB18 REV3-                  20111222   2434 1451    6
----ENDF/B-VIII.0     MATERIAL 2434         REVISION 3             2434 1451    7
-----INCIDENT NEUTRON DATA                                         2434 1451    8
------ENDF-6 FORMAT                                                2434 1451    9
                                                                   2434 1451   10
****************************************************************** 2434 1451   11
S. Kunieda (LANL/JAEA) updated the alpha-particle production      2434 1451   12
cross sections and energy spectra in MF6MT5 , based on the        2434 1451   13
improved Iwamoto-Harada model.                                     2434 1451   14
                                                   [Sep 3,2011] 2434 1451   15
                                                                   2434 1451   16
****************************************************************** 2434 1451   17
    Covariances for Cr-53, S. Hoblit, BNL, Aug. 2011               2434 1451   18
```

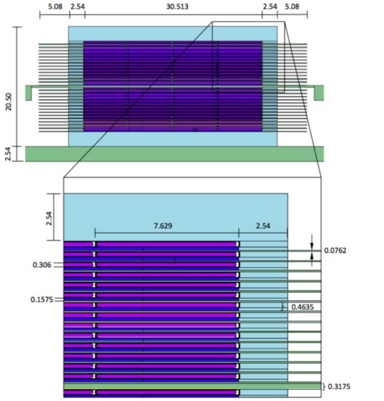
```
<?xml version="1.0" encoding="UTF-8"?>
<reactionSuite projectile="n" target="U233" evaluation="ENDF/B-8.0" format="1.9" projectileFrame="lab">
  <styles>
    <evaluated label="eval" date="2010-01-01" library="ENDF/B" version="8.0.1">
      <temperature value="0.0" unit="K"/>
      <projectileEnergyDomain min="1e-05" max="20000000.0" unit="eV"/></evaluated>
    <crossSectionReconstructed label="recon" derivedFrom="eval" date="2016-11-06"></crossSectionReconstructed></styles>
  <externalFiles>
    <externalFile label="covariances" path="n-092_U_233-covar.xml"/></externalFiles>
  <documentations>
    <documentation name="endfDoc"><![CDATA[
 92-U -233 JAEA+      EVAL-JAN10 O.Iwamoto,N.Otuka,S.Chiba,et al.
 NDS 148, 1 (2018)    DIST-FEB18                      20100326
----ENDF/B-VIII.0     MATERIAL 9222
-----INCIDENT NEUTRON DATA
------ENDF-6 FORMAT

NOTE on the IAEA-CIELO Update to the U-233 JENDL-4.0 Evaluation
A. Trkov, R.Capote, IAEA, Dec.2016

The present file is not a genuine evaluation but merely a patch
correcting the thermal capture, fission and nu-bar to correspond
to the Standards_2006:
          Standards_2016   JENDL-4.0  IAEA-CIELO
elastic [b]  12.2+/-0.7      12.177      12.178
capture [b]  41.9+/-1.7      45.261      42.329
```


AMPX





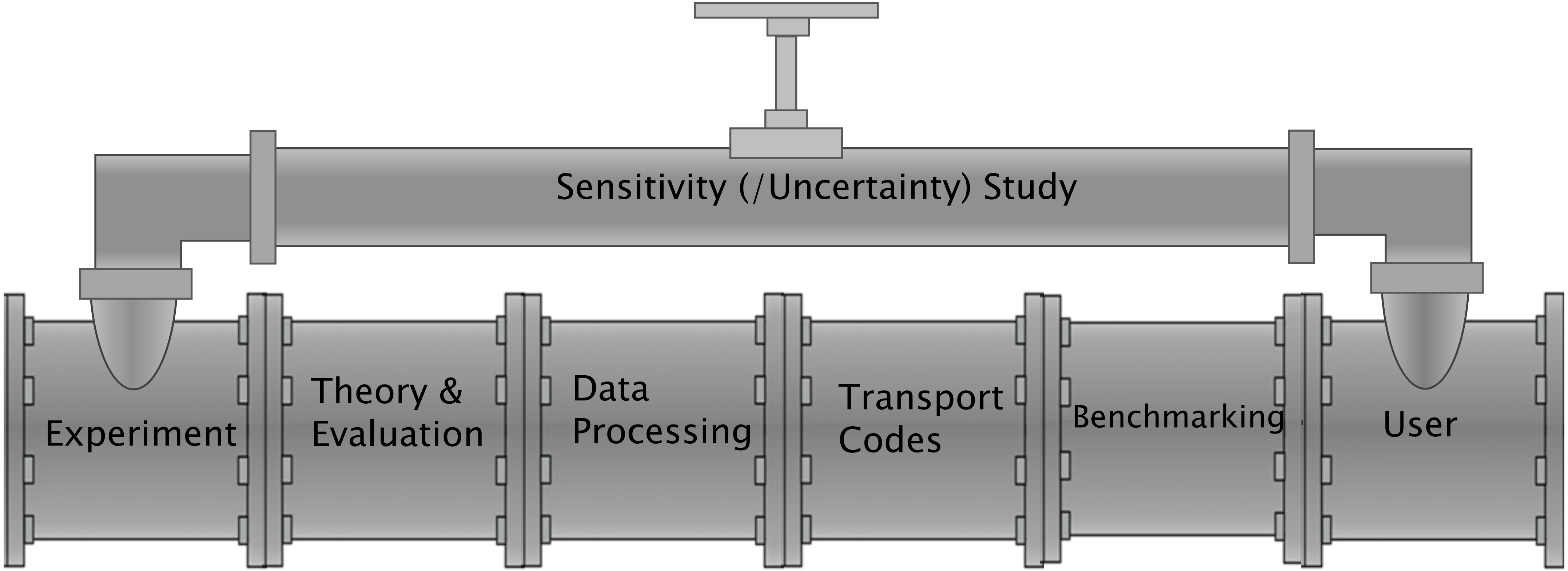
M Percher, C., et al. *Thermal Epithermal eXperiments (TEX): test bed assemblies for efficient generation of integral benchmarks*. No. LLNL-CONF-776306. Lawrence Livermore National Lab.(LLNL), Livermore, CA (United States), 2019.

Foundation

Main points:

- There are a few important, high-level steps
- You don't need a pipeline to convey the information in the metaphor

Brookhaven National Laboratory



Main points:

- There are a few important, high-level steps
- S/U studies are by far the most important feedback loop
- We built the whole talk around this graphic last year and I didn't want to remake the slides