ENDF as a Gaussian Process Regression model and the ENDF Belief Network

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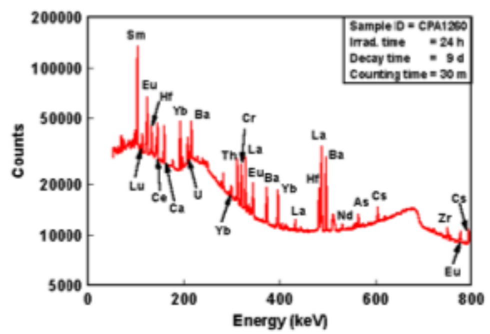
BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

The Nuclear Data Pipeline

Our goal is to get the highest quality data to users

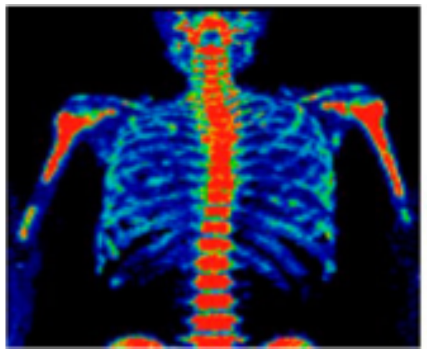
security



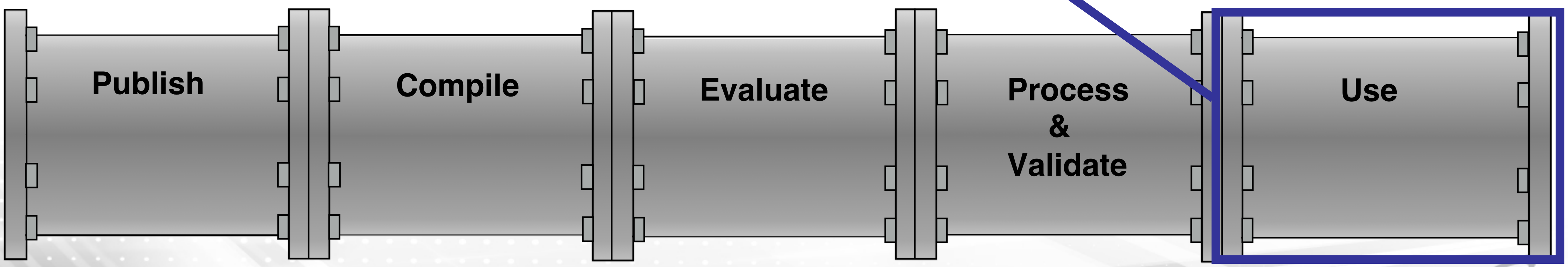
science

FRIB

isotopes

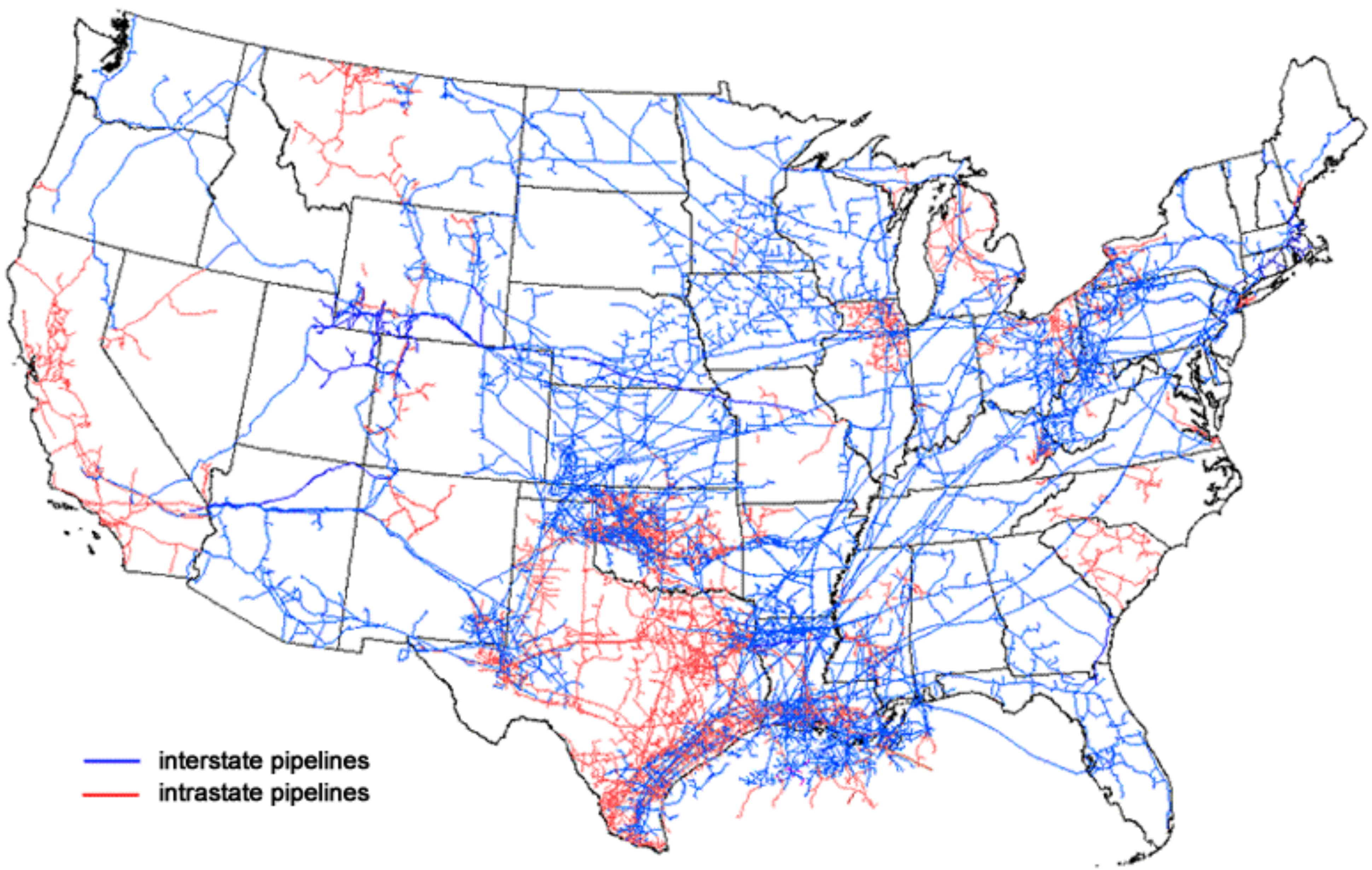


energy



The nuclear data pipeline is more of a network

Map of U.S. interstate and intrastate natural gas pipelines



Source: U.S. Energy Information Administration, *About U.S. Natural Gas Pipelines*

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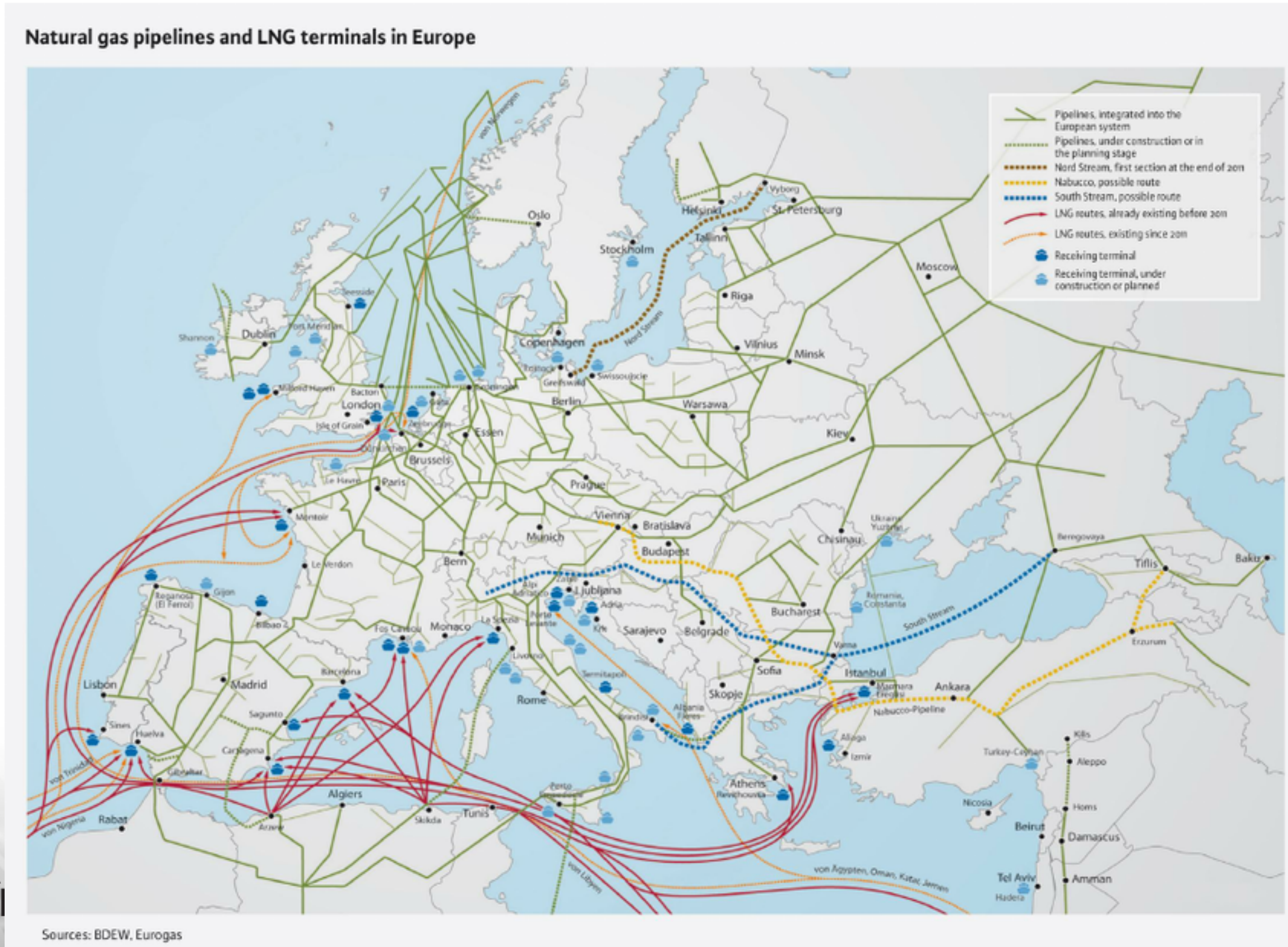
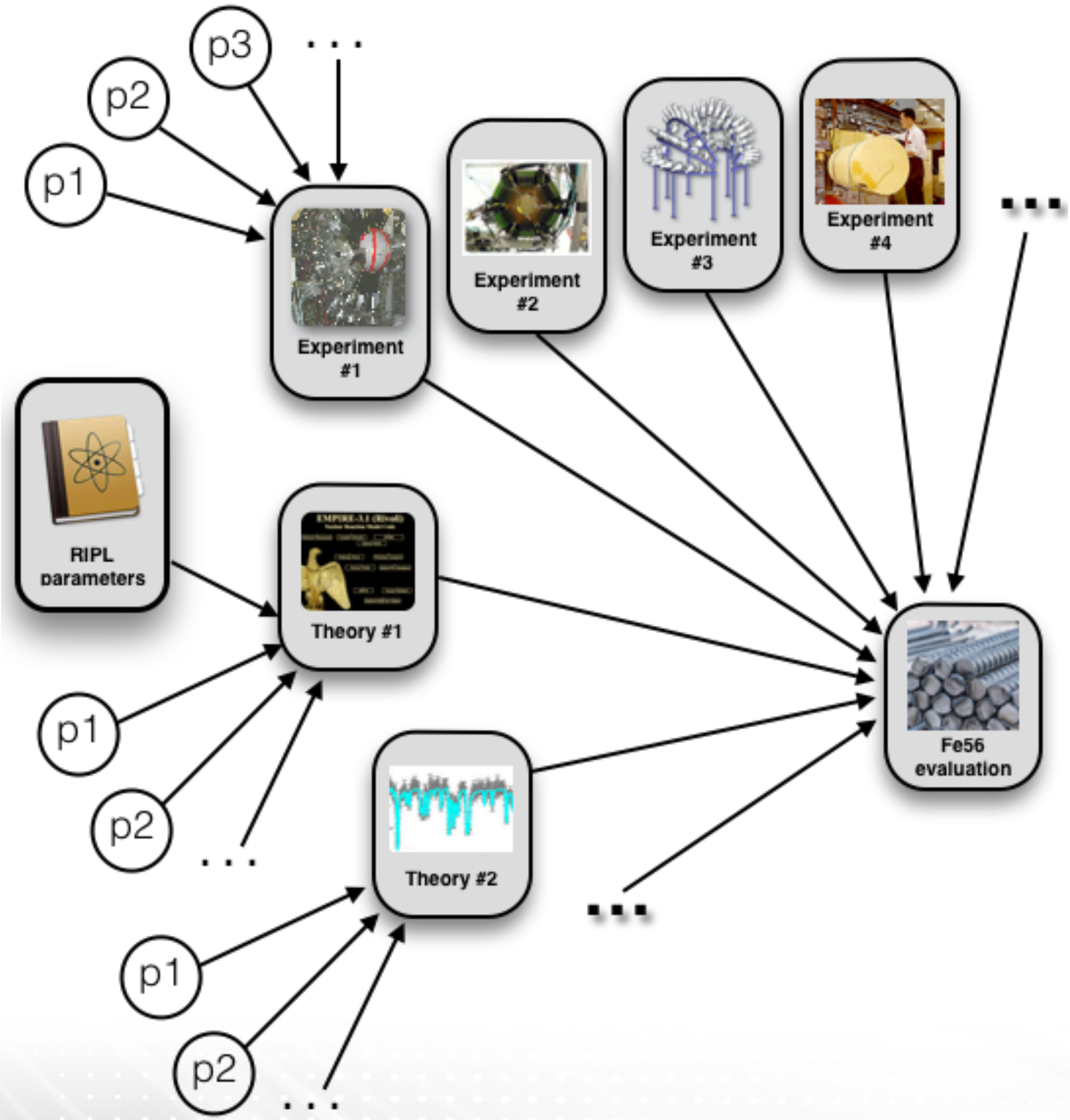
The nuclear data pipeline is more of a network





An ENDF evaluation *aims* to be a Gaussian Process Regression (GPR) model built from the Bayesian Network of relevant experiments & theory models

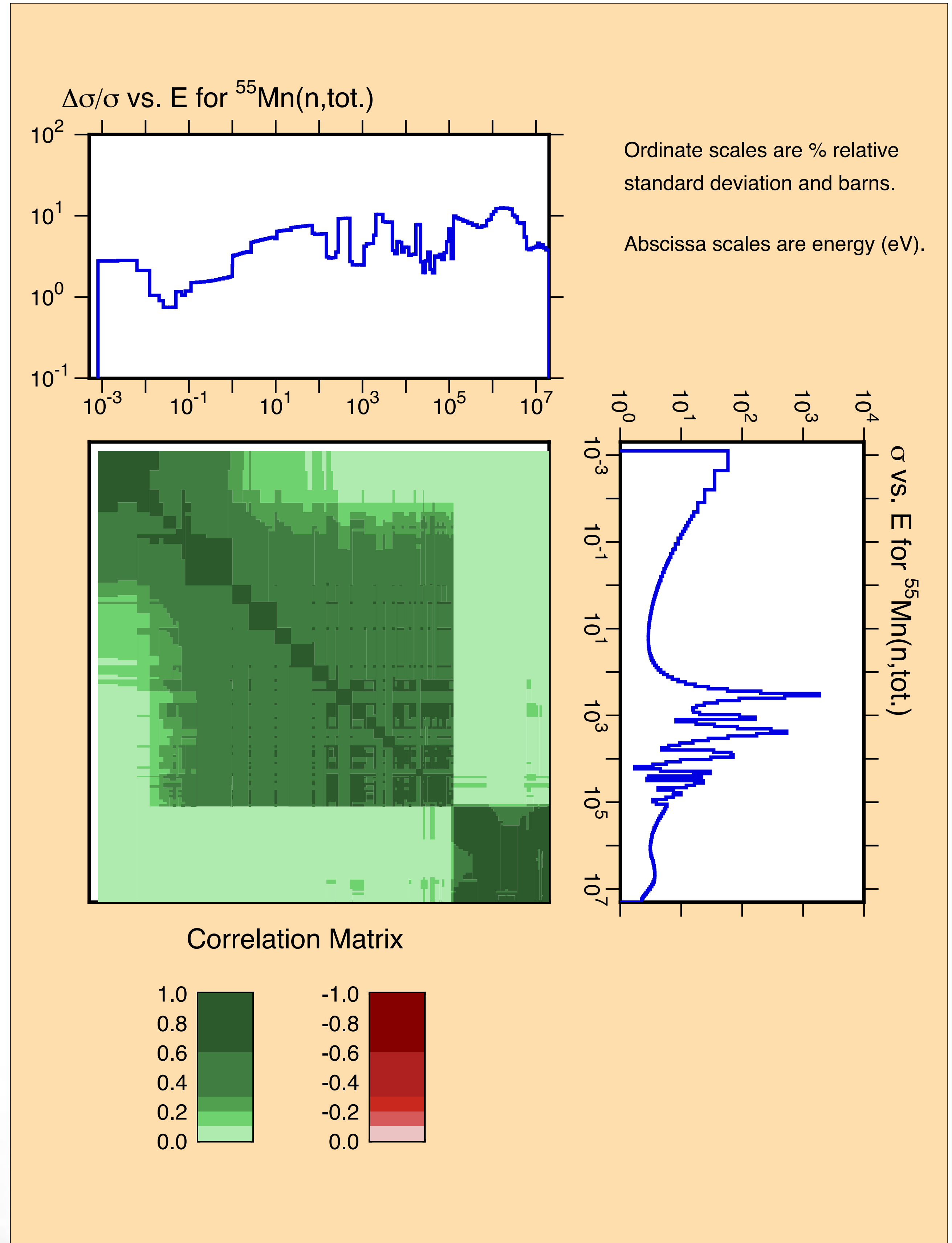
The assumed ENDF GPR model

- For a given reaction *rxn*, every emitted particle *p*, store

$$\sigma_{rxn}(E)$$

$$P_{rxn,p}(E',\mu\,|\,E)$$

- both as linear interpolatable functions
- and, the covariance matrices for each (what that means is a different question…)



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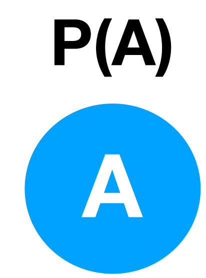
The Nuclear Data Belief Network

A belief network is a DAG that encodes probabilities

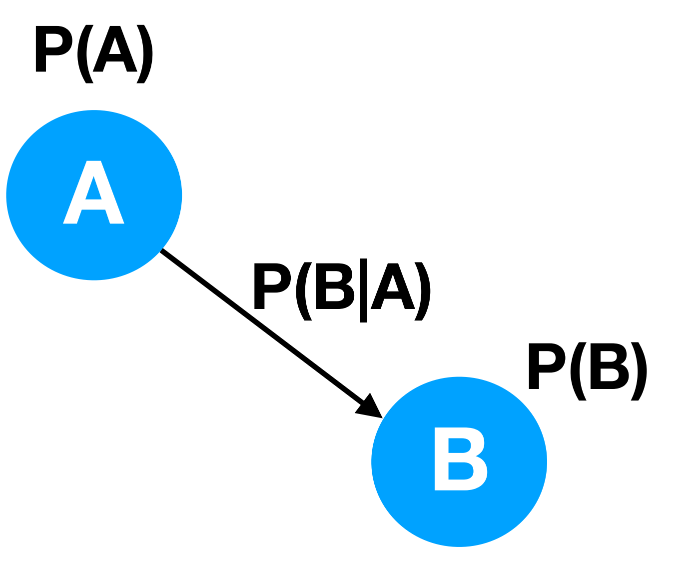
- ***Belief* is the unconditional probability associated with a node, P(A)**



- 0 <= P(A) for all values of A; P(A)<=1 is A discrete
- $\Sigma_A P(A) = 1$
- A can be
  - continuous (cross section at a given energy) or
  - discrete (J) or
  - vector valued (J,Pi or resonance parameters of a resonance)

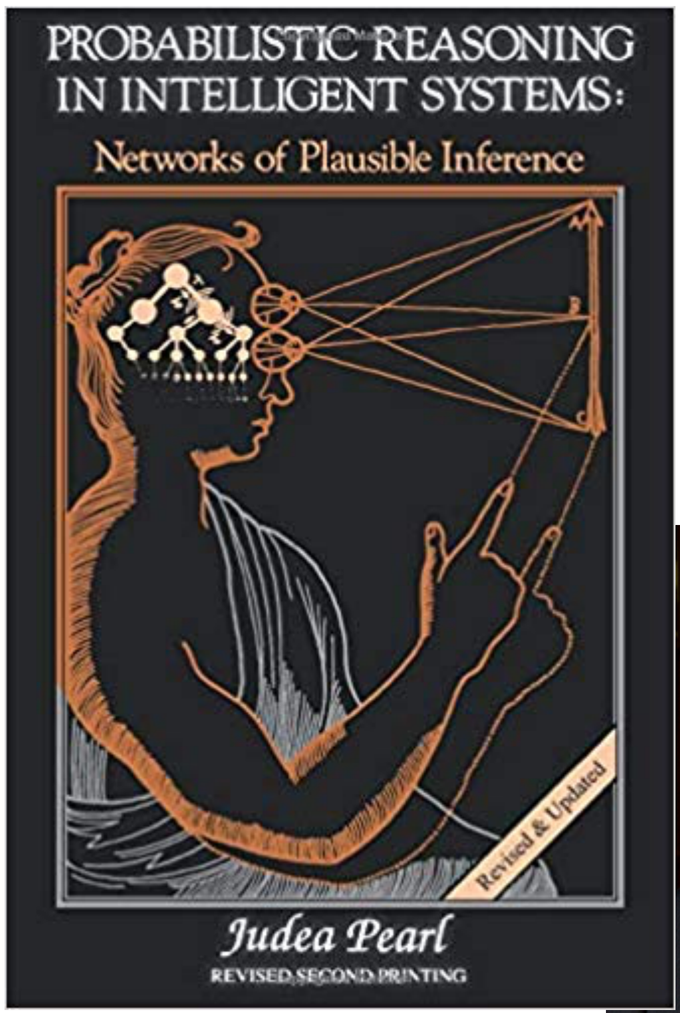
A belief network is a DAG that encodes probabilities

- ***Belief* is the unconditional probability associated with a node, P(A)**
- **The conditional probability P(B|A) is the probability that B observed given A.**
- $0 <= P(B|A) <= 1$
  for all values of B
- $\Sigma_B P(B|A) = 1$

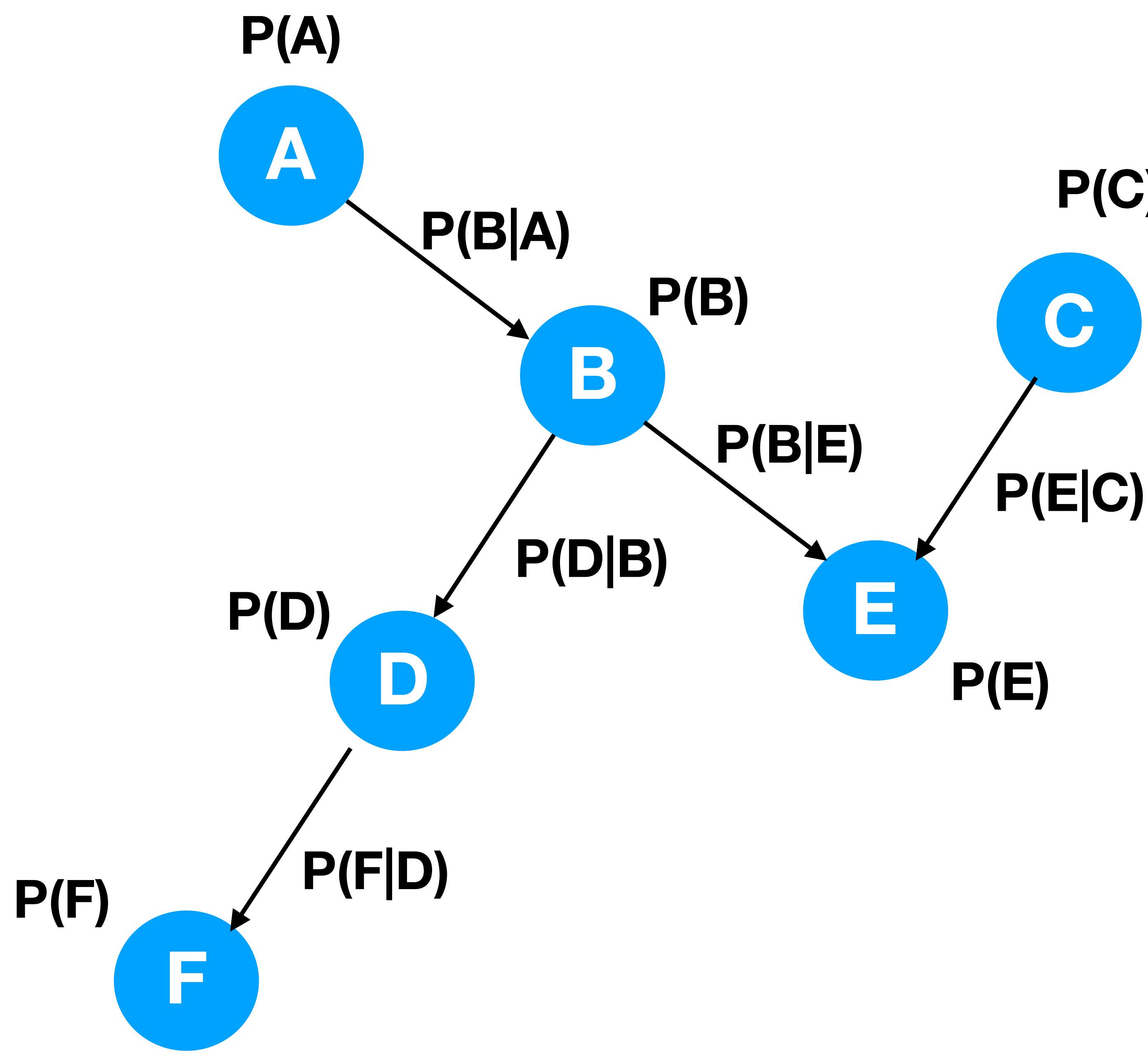


The arrow in the graph tells you “B” depends on “A”

A belief network is a DAG that encodes probabilities



Probabilistic Reasoning in Intelligent Systems, Morgan-Kaufmann, 1988

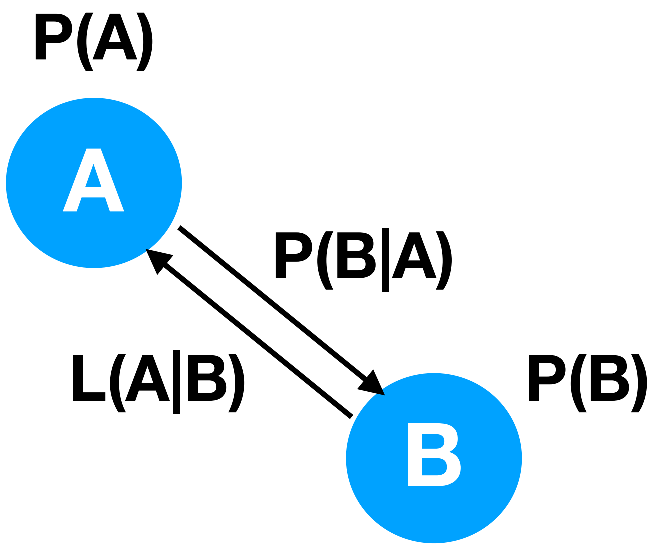


Bayes theorem is a form of message passing along network

- **Forward problems (*prediction*) follow arrows, associated with conditional probabilities, P(A|B)**

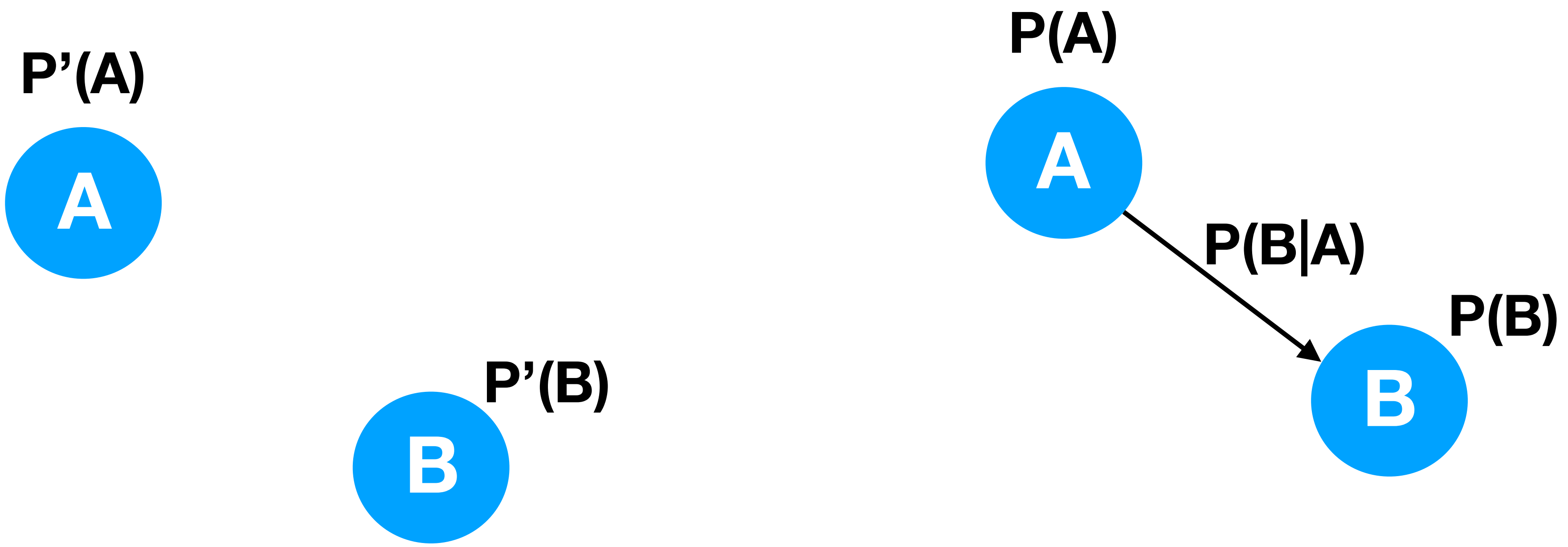
- **Inverse problems (*inference*) run against flow, use likelihood L(A|B) gotten from Bayes' theorem**

- Assimilation is an inverse problem and runs against flow



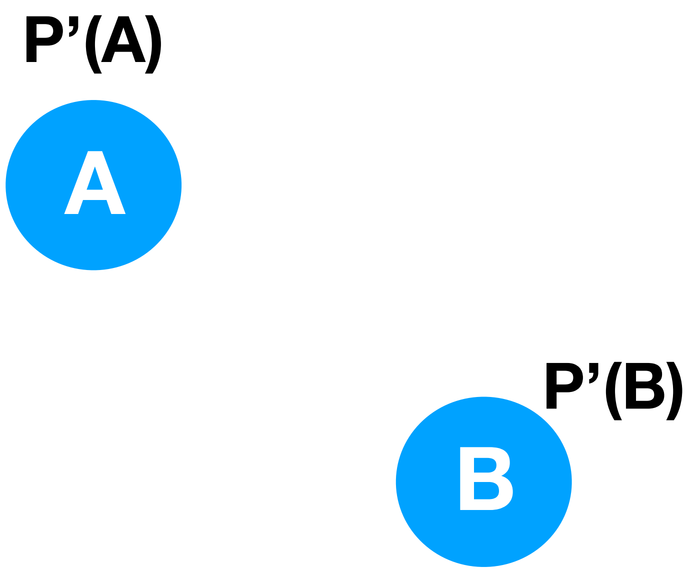
P(A|B) = P(B|A)P(B)/P(A)
= L(A|B)
= likelihood that B explains A

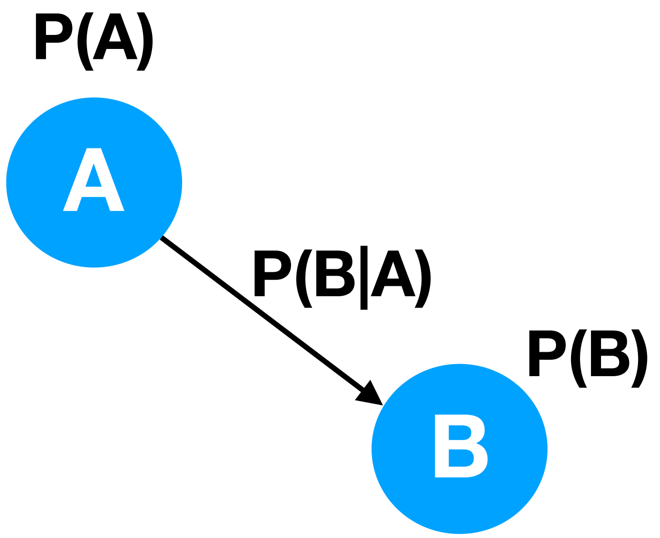
Bayesian update procedure tells us how to update belief as add nodes



Prediction: $P(B) = \Sigma_A \, P(B|A)P'(A)$

Bayesian update procedure tells us how to update belief as add nodes



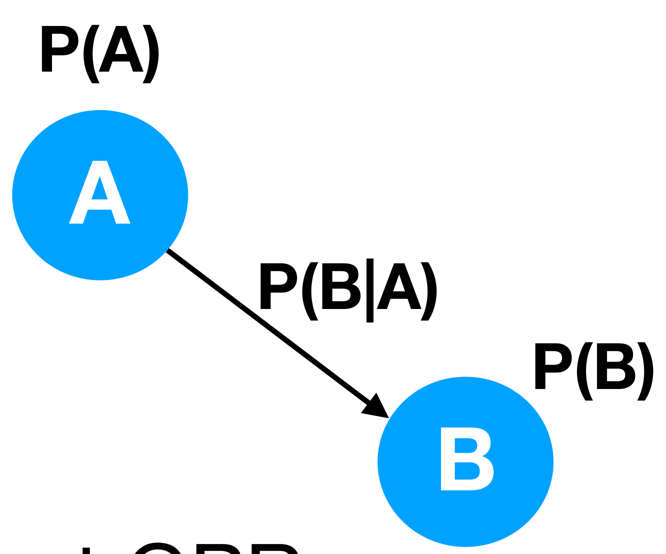


Prediction: $P(B) = \Sigma_A\, P(B|A)P'(A)$

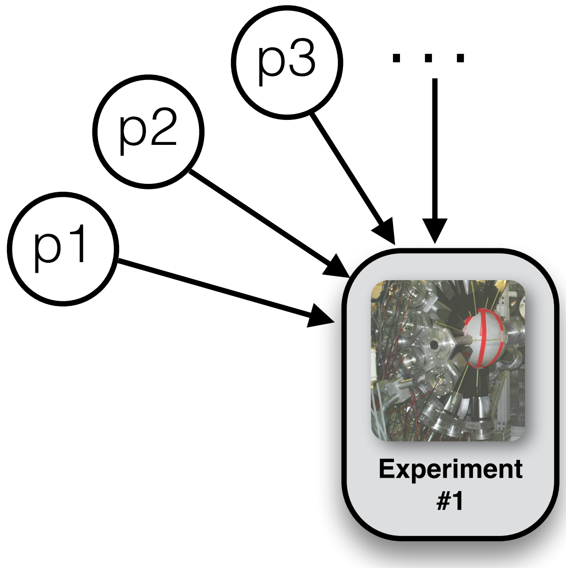
Inference: $P(A) = \Sigma_B\, L(A|B)P'(B)$

A Gaussian process regression (GPR) model assumes all probabilities are Gaussian

- **A GPR is characterized with a set of mean values <A>, <B> and covariance cov(x) where vector x given by x=(A,B)**



  - Least squares fitting is simplest GPR
  - Famous “Sandwich formula” & sensitivity profiles
  - Gaussian process prediction also known as Kriging
- **GPR based updating requires lots of linear algebra, but very GPU friendly & many codes exist**



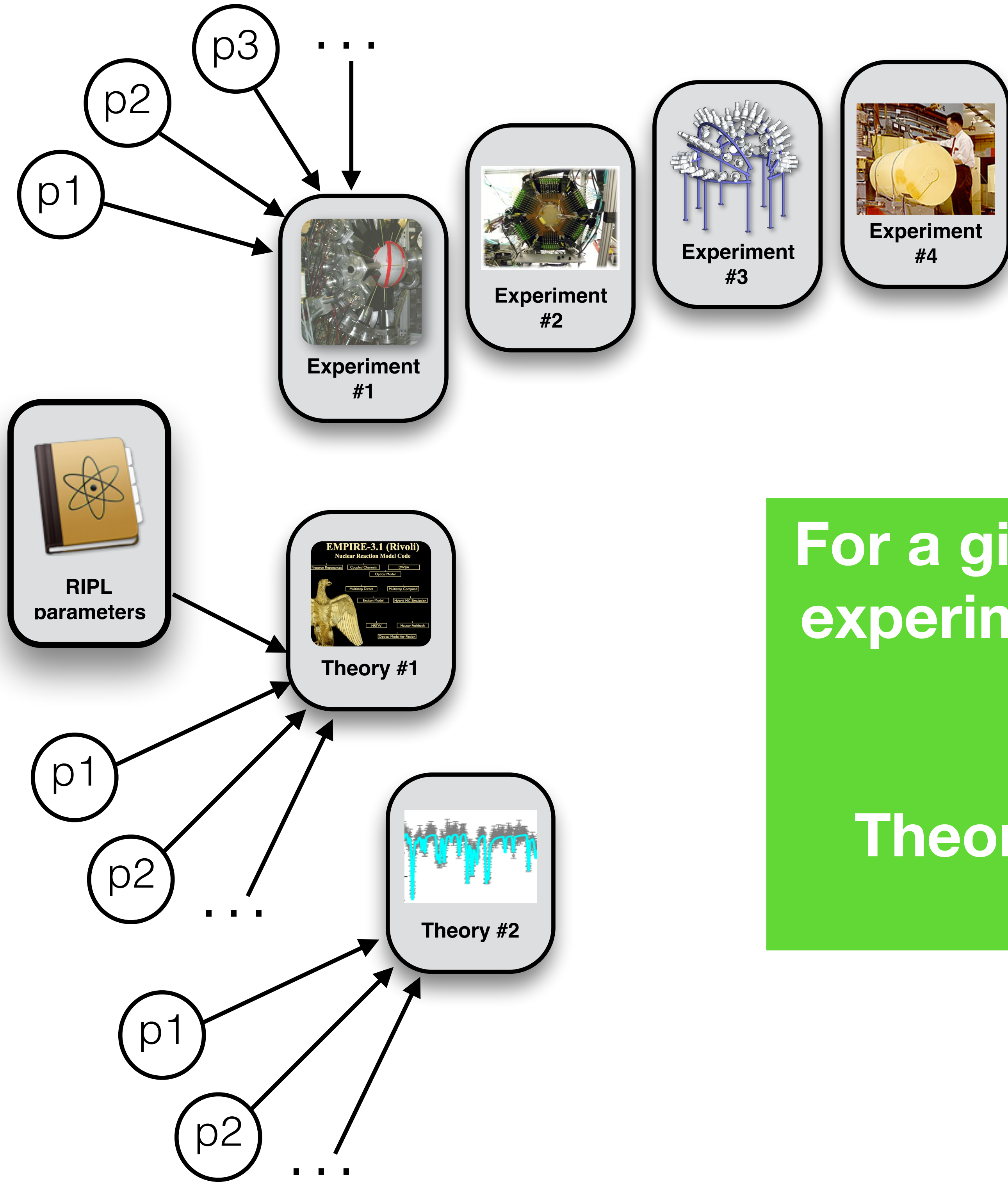
Experiments report a GPR model of say σ(E)

(at least this is what we want to be reported in EXFOR)

This model depends on a lot of parameters:

- **Target thickness**
- **ToF corrections**
- **…**
- **and data itself**

Slide from D. Brown (Nuclear Science and Technology)



For a given observable, there are many experiments, and often several related observables

Theory aims to explain each with a parametric form.

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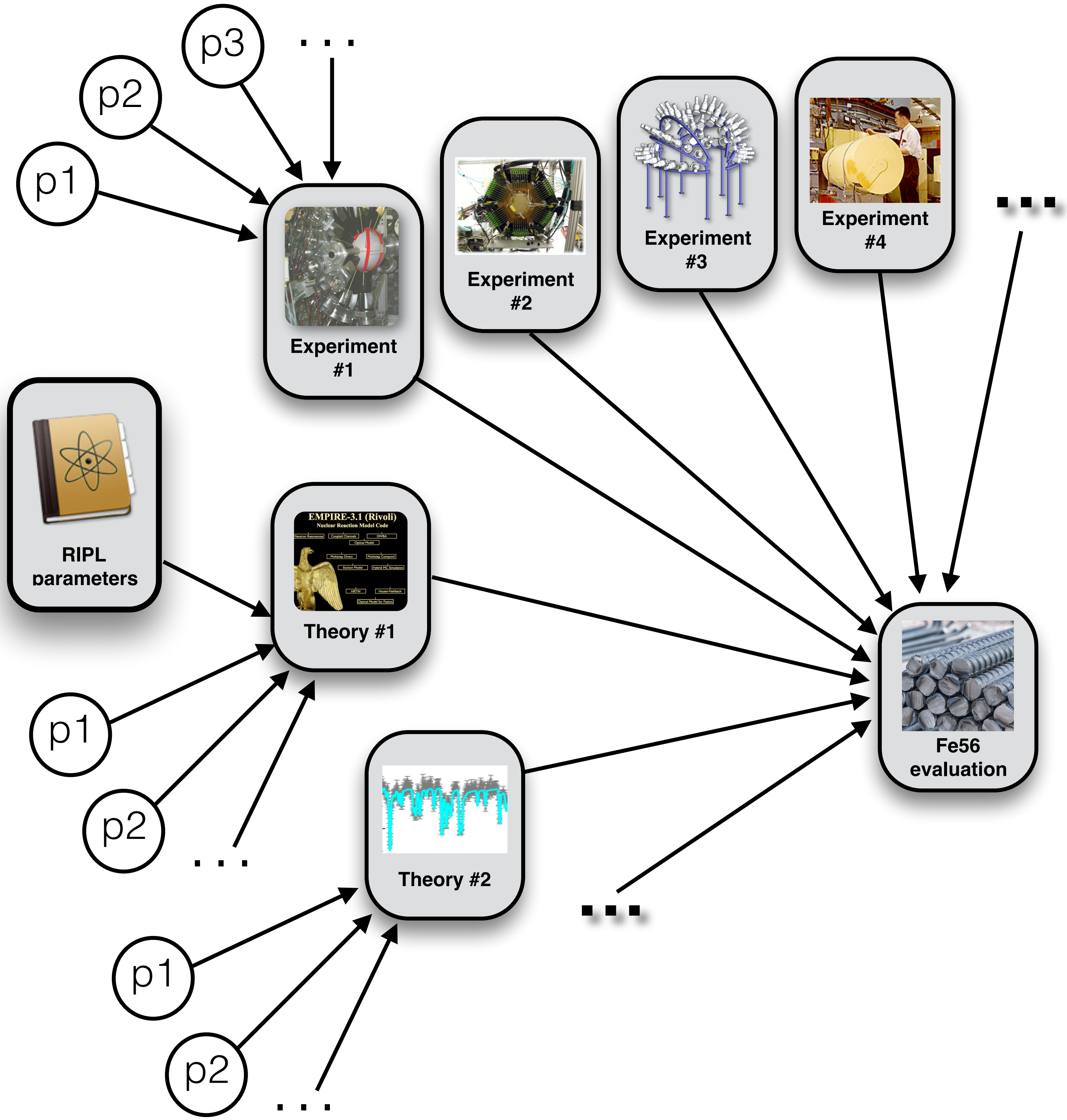

An evaluation is supposed to be a GPR model of observables required by a class of applications

Mean values & covariances determined by using theory as regression model of data

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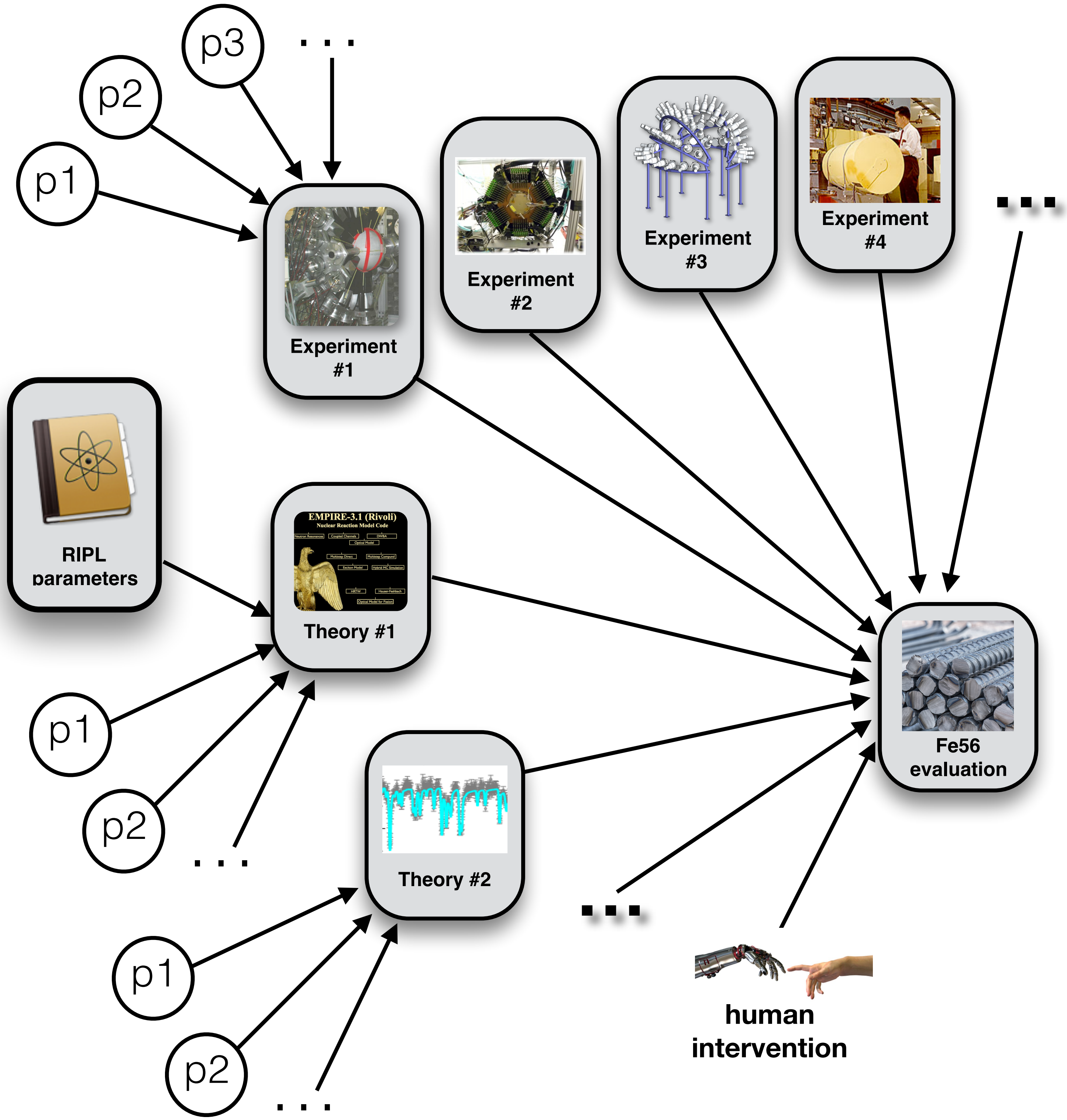

An evaluation is supposed to be a GPR model of observables required by a class of applications

Mean values & covariances determined by using theory as regression model of data

Humans are needed:

- **model misfit**
- **discrepant data**

Humans introduce bias and are not “automatable"

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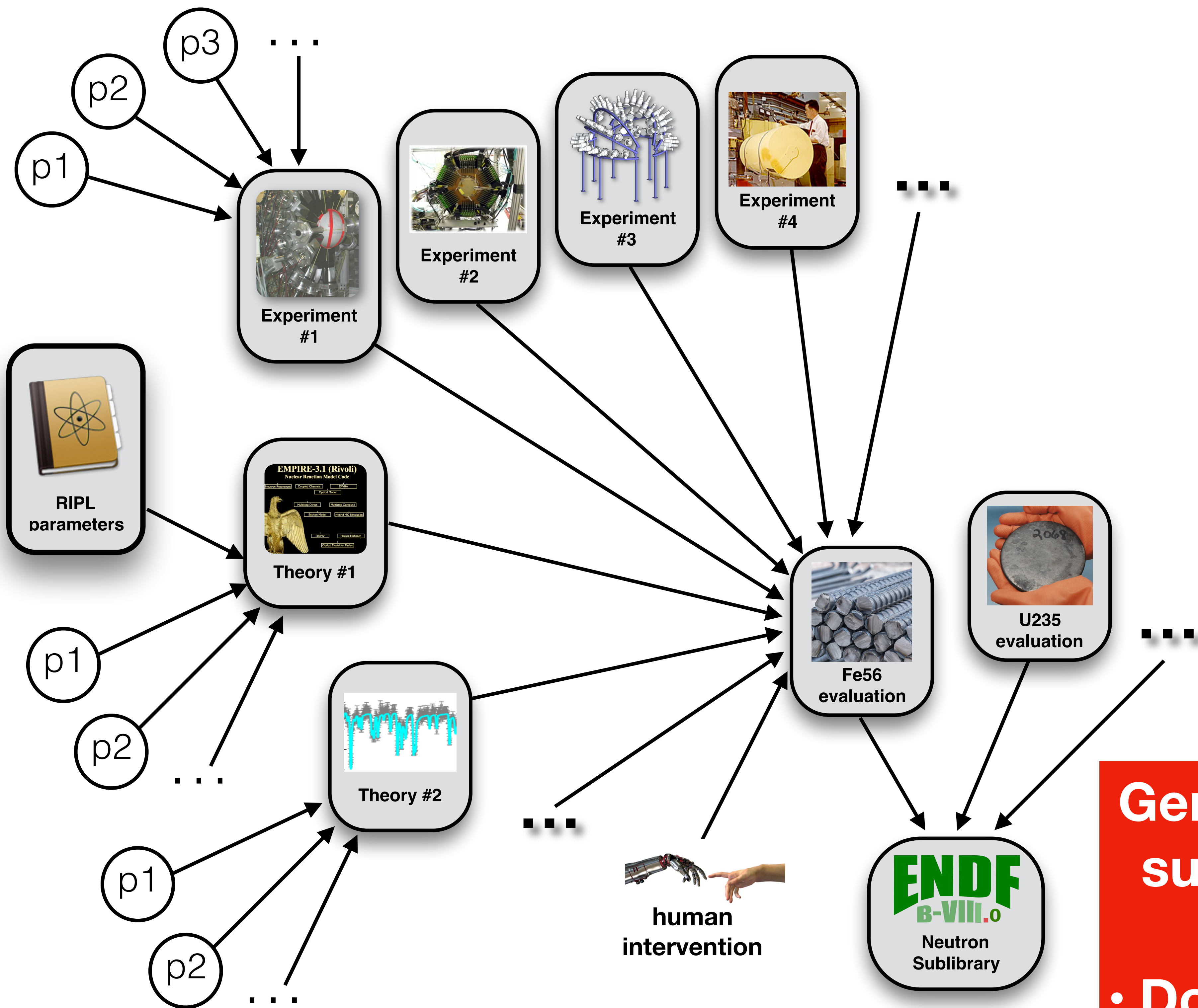

Generating a processed sublibrary can change the GPR too:

- **Doppler broadening**
- **Grouping**

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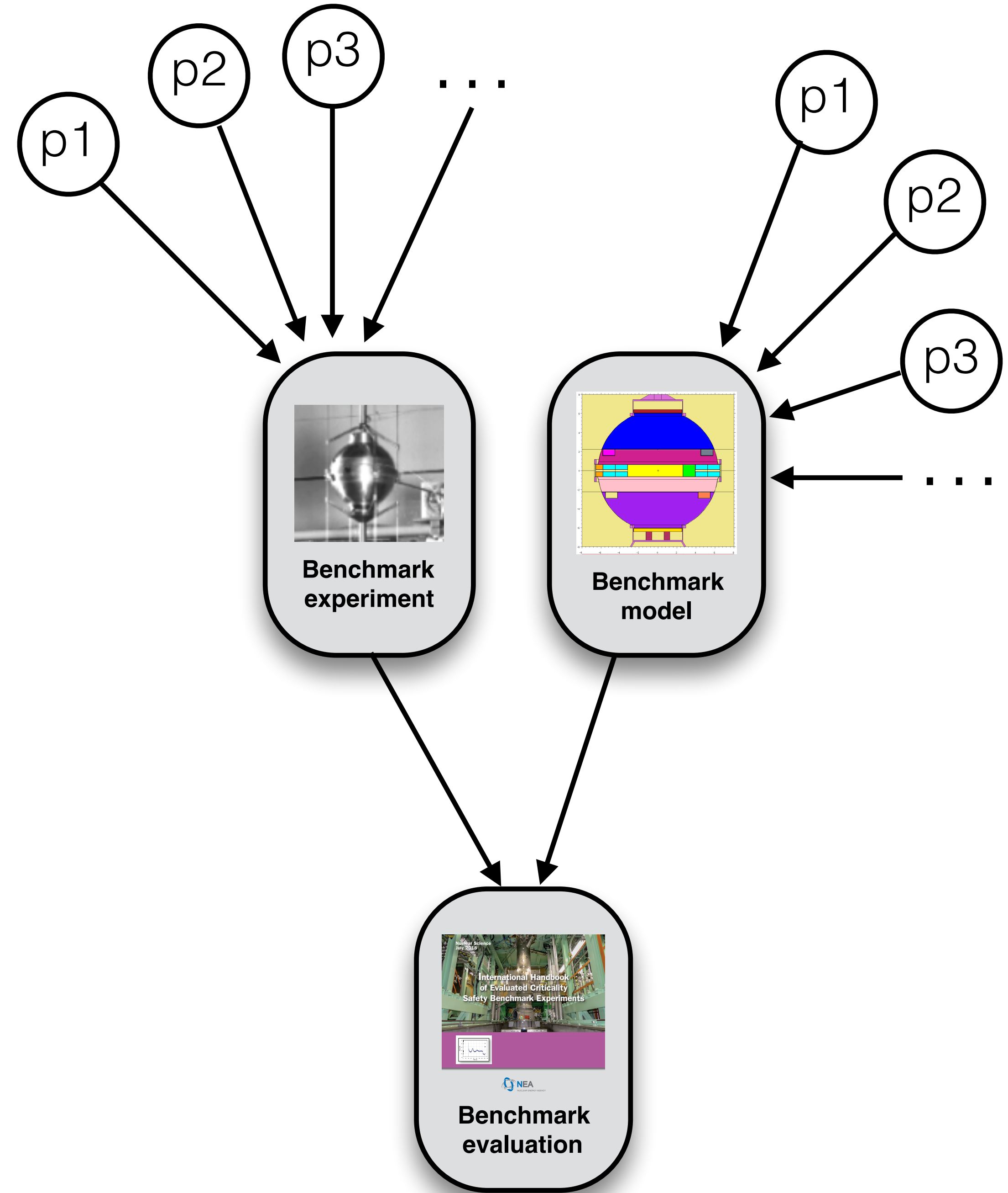
Benchmarks have their own belief network

ICSBEP proves GPR model of fielded experiment and simplified GPR models



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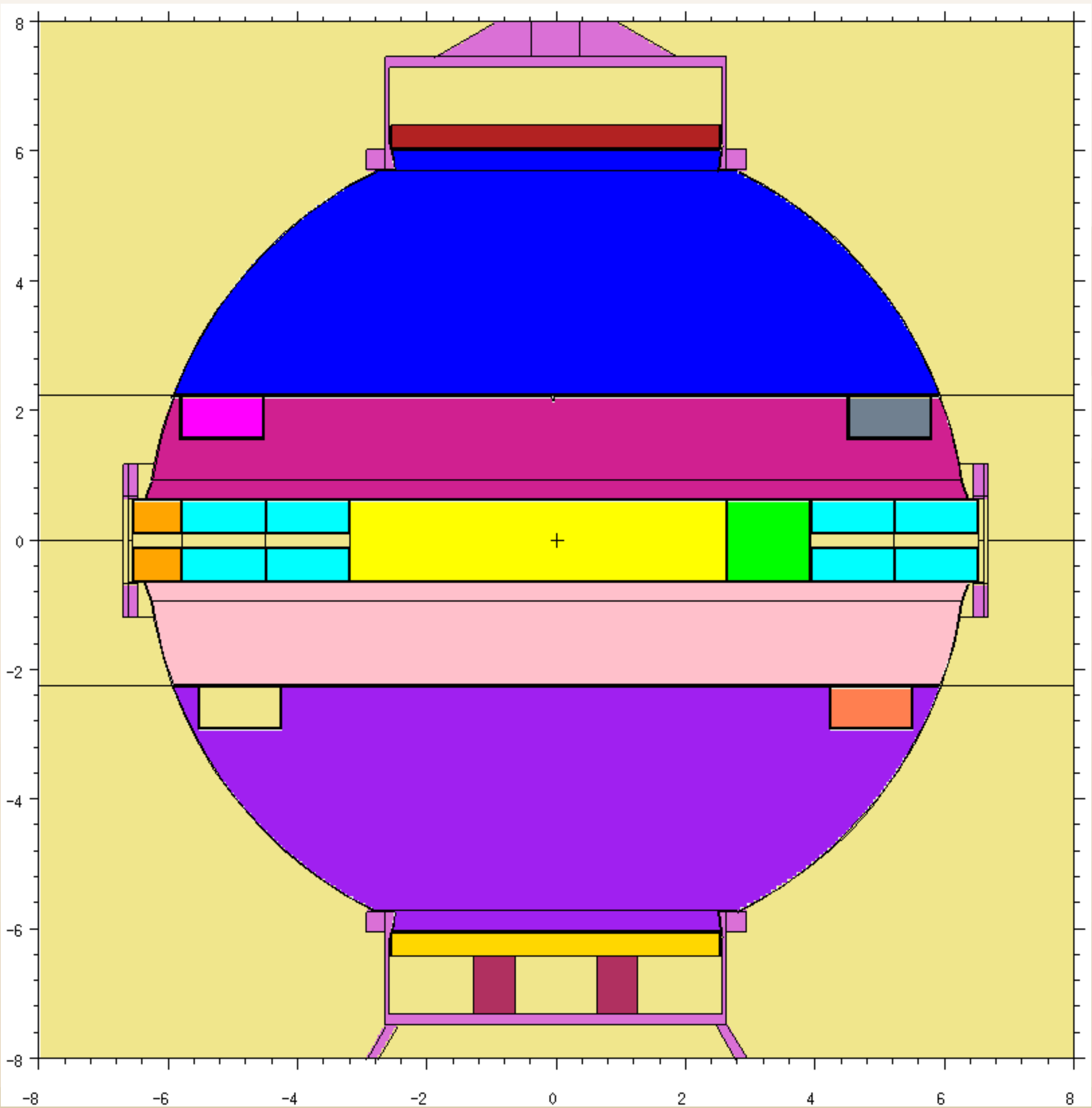
How to model a critical assembly

“Jezebel”, a bare sphere of ^{239}Pu



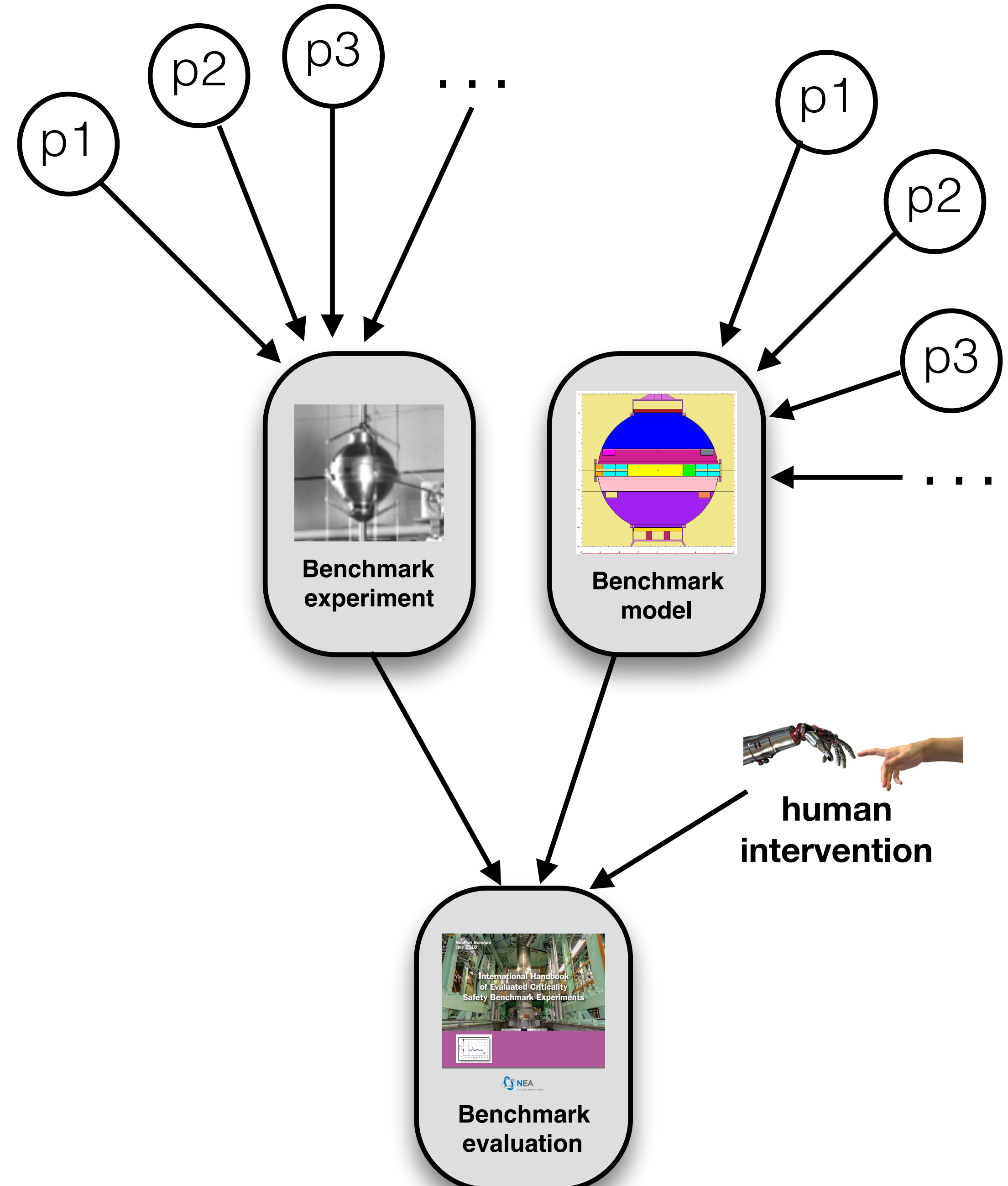
- Geometry of system described in transport code specification
- Requires separate evaluation of blueprints, lab reports, etc.

Benchmarks have their own belief network

ICSBEP proves GPR model of fielded experiment and simplified GPR models

Humans may have intervened too much too:

- **model homogenization**
- **...**



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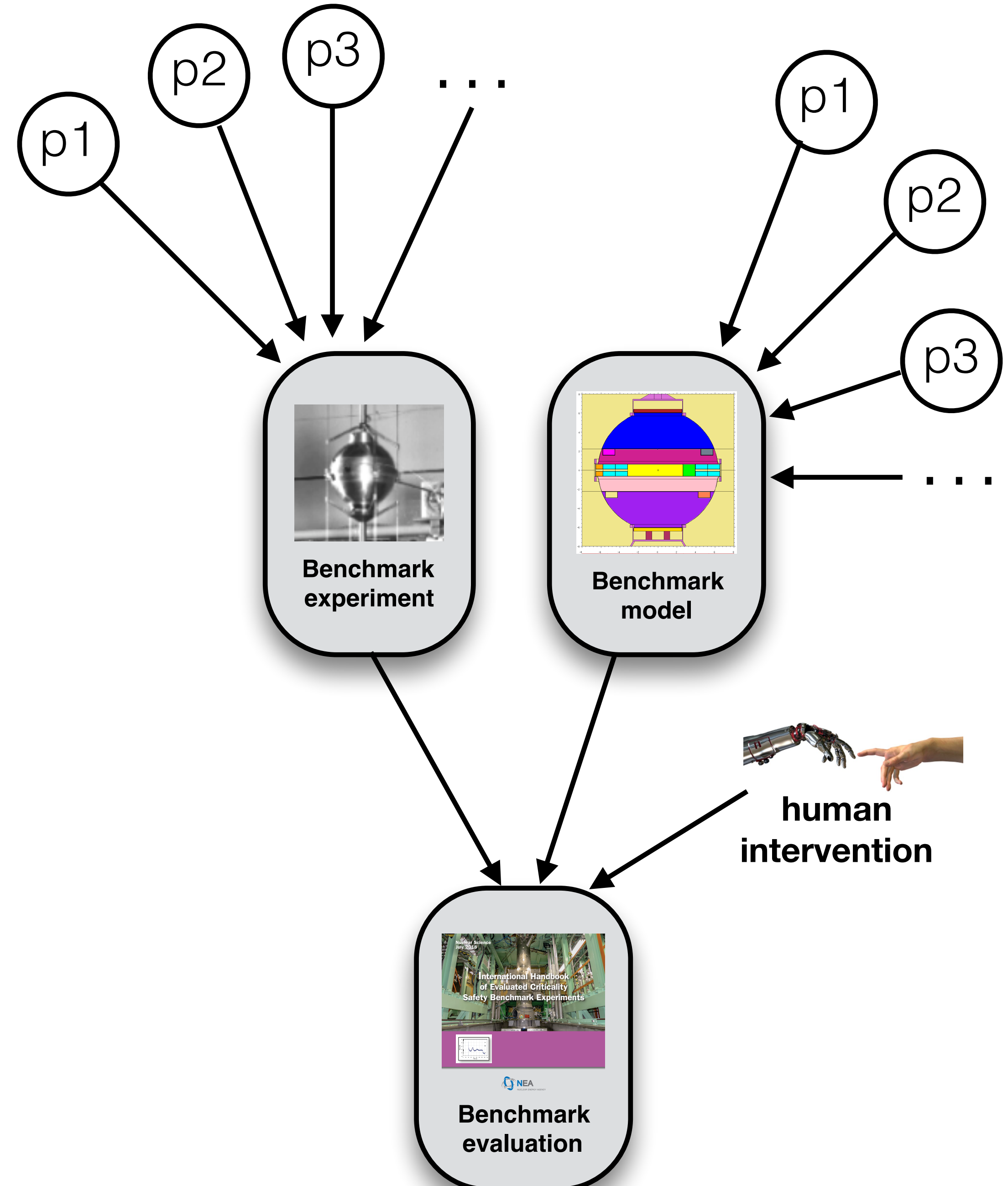
Benchmarks have their own belief network

ICSBEP proves GPR model of fielded experiment and simplified GPR models

Humans may have intervened too much too:

- model homogenization
- ...

Attempts to build trustworthy suite of benchmarks should continue!



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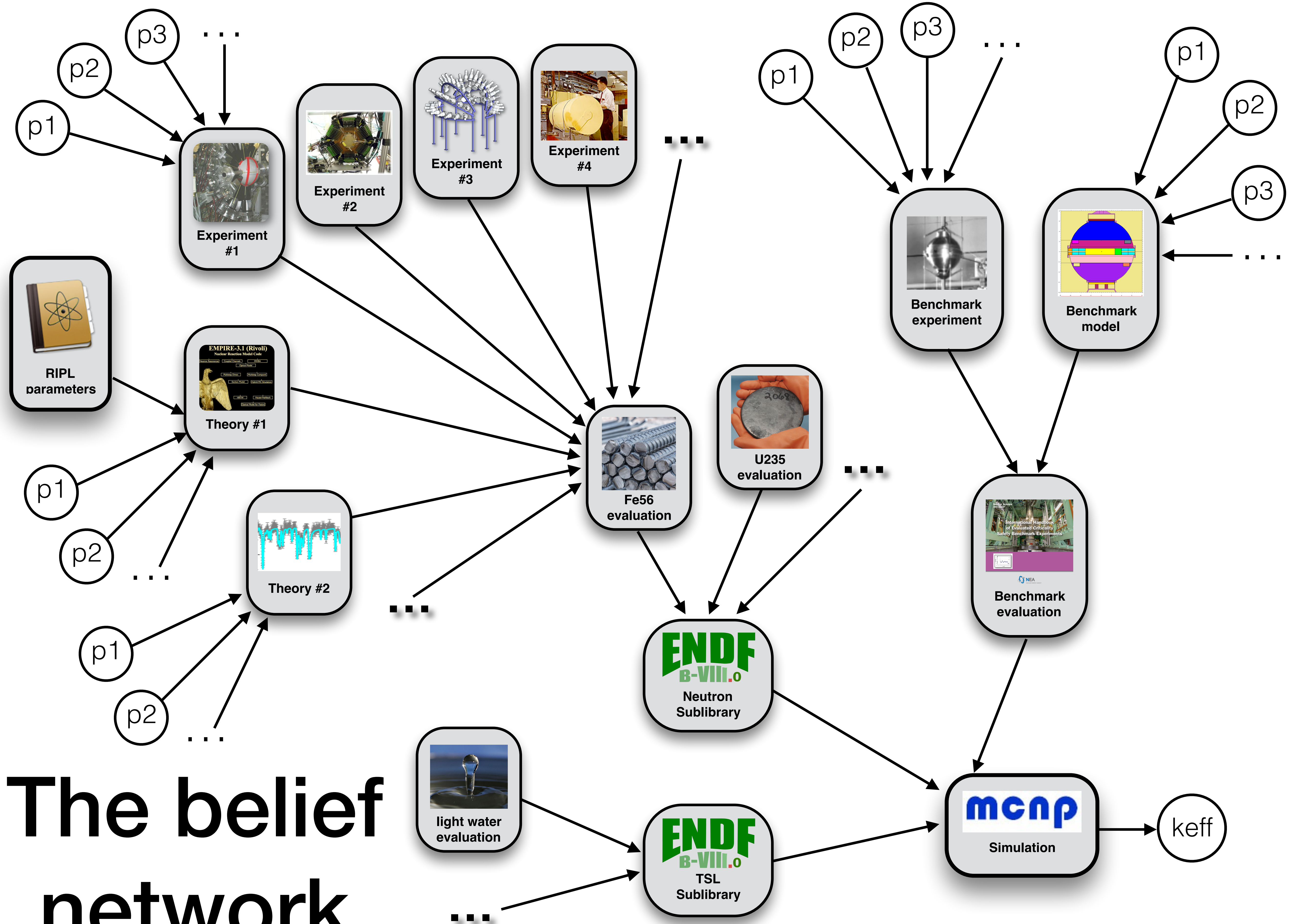

The belief network

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Two WPEC subgroups actively working to automate nuclear data Bayesian Network

Validation of Nuclear Data Libraries (VaNDaL) Project

WPEC subgroup 45 (SG45)

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- SG45 mandate, Co-ordinators: M. White and D. Bernard. Monitor: A. Trkov
- SG45 proposal at the WPEC 2017 meeting, M. White
- SG45 mailing list for questions, comments or to consult archives

Meetings

- NEA, OECD Conference Centre, Paris, France, 14 May 2018
- ND2019, China National Convention Center, Beijing, China, 22 May 2019
- NEA Headquarters, Boulogne-Billancourt, France, 26 June 2019

Contact

For more information, please contact: Michael Fleming

Reproducibility in Nuclear Data Evaluation

WPEC Subgroup 49 (SG49)

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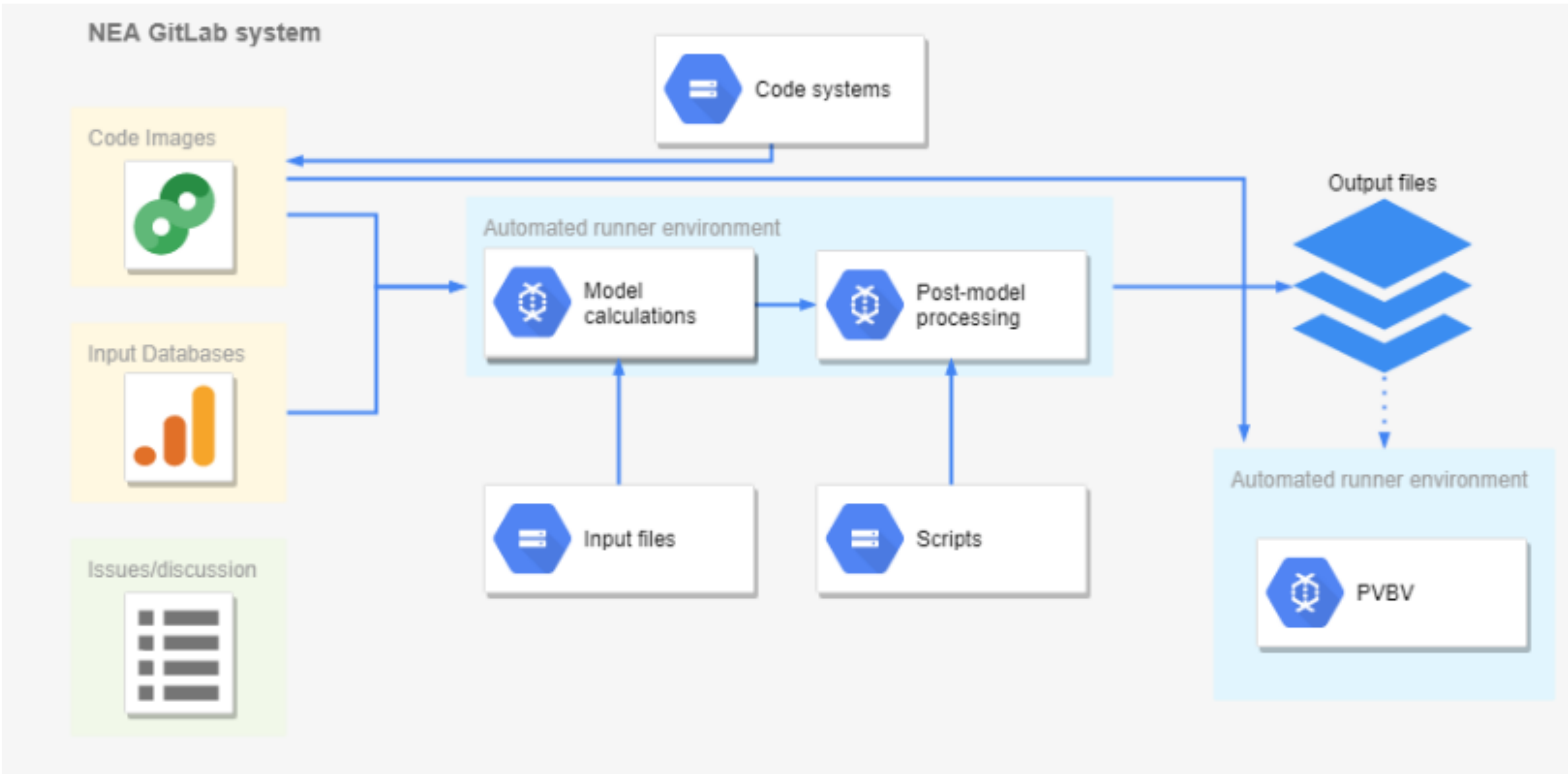
- SG49 Proposal, Co-ordinators: D. Rochman and M. Herman

Meetings

- Workshop, 27 November 2019, NEA Headquarters, Boulogne-Billancourt, France
- Kick-off meeting, May 2020, NEA Headquarters, Boulogne-Billancourt, France

Contact

For more information, please contact: Michael Fleming


NEA GitLab system
Code systems
Code Images
Output files
Automated runner environment
Model calculations
Post-model processing
Input Databases
Input files
Scripts
Automated runner environment
Issues/discussion
PVBV

Containerization can serve multiple purposes

- **Reproducibility** — one container builds one part of the Bayesian network
- **Scalability** — workload can be distributed across labs & continents ("nuclear data cloud")
- **Automation** — Updates can be automatically farmed out to available resources
- **Accuracy** — the full Bayesian network is too big for anyone institution to update (or even hold in memory), with Bayesian message passing the network effectively encodes the full covariance of the GPR

Many technical issues remain

- **Experiment**
  - Experimental data missing covariances or equivalent
  - Experimental data discrepant
- **Theory**
  - Theory models not complete nor entirely predictive
  - Theory models have misfit
- **Processing**
  - Processing distorts evaluation
  - Multiphysics issues in application couple processing step to application
- **Benchmarks**
  - Benchmark models incomplete
  - Benchmark models not trustworthy
- **Overall approach**
  - Belief network too simplistic (many more connections needed!)
  - GPR not applicable in many cases (non-linear parameter response)
  - Dimensions too big for todays computer
  - ENDF regression model too simple, missing physics

Take-away messages

- The consensus nuclear data approach is built off a DAG containing various GPR models of important things (EXFOR, ENDF libraries, ICSBEP benchmarks)
- The nuclear data community is already engaged in hybrid human/machine learning: e.g. assimilation and adjusted libraries
- We are not ready for pure machine learning: we need to get humans out of every step

This could be a VERY fun long term project for the global nuclear data community