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Theory & Evaluation

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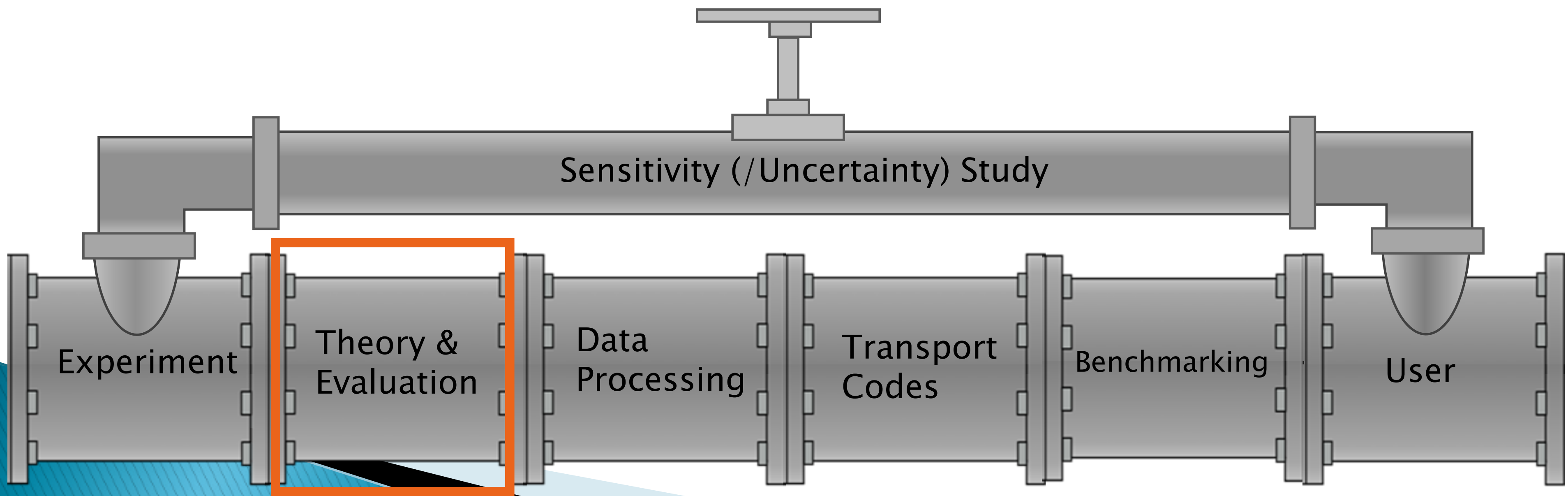
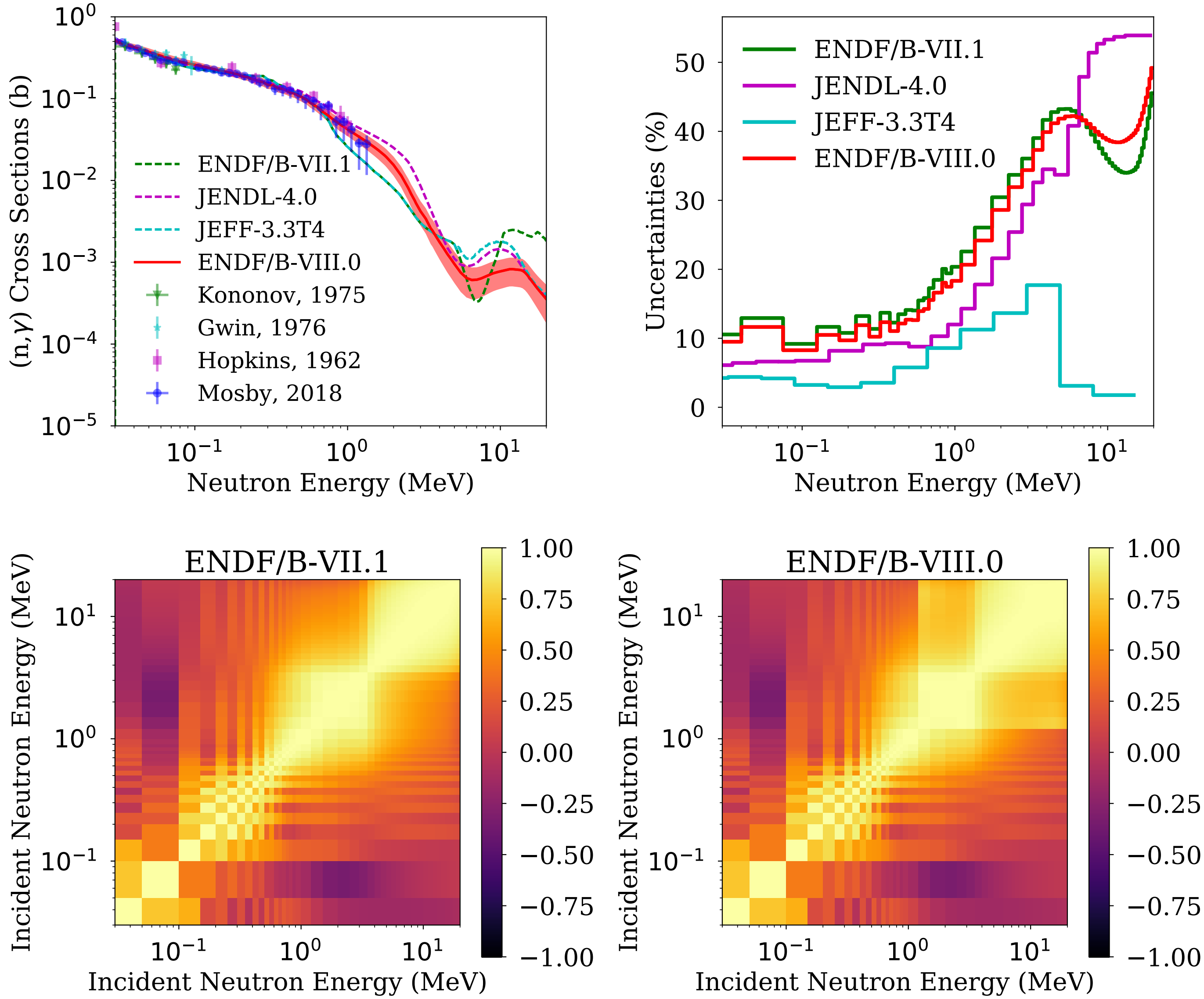
Theory & Evaluation

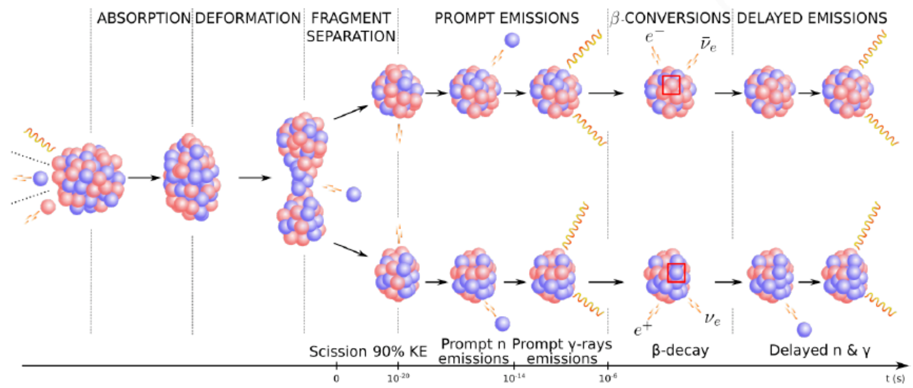
- Nuclear Theory is crucial for the nuclear data evaluation process
  - Need for complete data files to be used in transport codes
  - Theory is needed for predictions (beyond calibration)
  - Provide reasonable estimates of uncertainties and correlations
- Evaluation = Experiments + Theory + Statistics
  - "To the best of our knowledge…" (given time, location, resources)
  - Bayesian statistics / Uncertainty Quantification



Need theory to get complete evaluated data files



Nuclear Theory



- Advances in fundamental nuclear theories
  - Predictions based on more fundamental microscopic theories
  - Ab initio calculations for light nuclei
- Grand Challenges (a selection)
  - Comprehensive, quantitative & predictive theory of **nuclear fission**
  - **Nuclear structure** (level densities, isomeric states, branching ratios), especially for nuclei away from stability
  - Consistent theories/models of **nuclear reaction & nuclear structure**
  - Integration of fundamental nuclear physics codes (microscopic, quantum mechanical, event-by-event) directly into **transport simulations**
  - Development of **machine learning-trained emulators** on fundamental physics codes
- Strengthen University-DOE labs collaborations
  - Lack of a good pipeline of nuclear theory students
  - Links between fundamental and applied research (both ways)
  - Opportunity to use HPC capabilities to tackle problems of common interest

Nuclear Data Evaluations

Combining the best of our knowledge (exp. & theoretical) about nuclear quantities into tabulated data files

- A (necessarily) compromising task
  - Uncertainties and limitations in experimental data
  - Approximations/assumptions of theoretical models
  - Discrepant observations/information
- Historical trend toward a more scientific and rigorous process
  - General use of theoretical models
  - More realistic account of experimental uncertainties
  - Use of rigorous mathematical and statistical tools (Bayes)
  - Better tools to ensure quality assurance and verification of data files

- Still lots of work to be done; some open questions:
  - How to account for model defects?
  - Realistic simulations of experimental setups, their biases and uncertainties
  - Quality control and improvements of the library itself, e.g., GNDS
  - Rigorous derivation of uncertainties and correlations (covariances)
  - "General purpose" and/or "adjusted" libraries
  - Use of ML techniques to better integrate all sources of information (metadata)