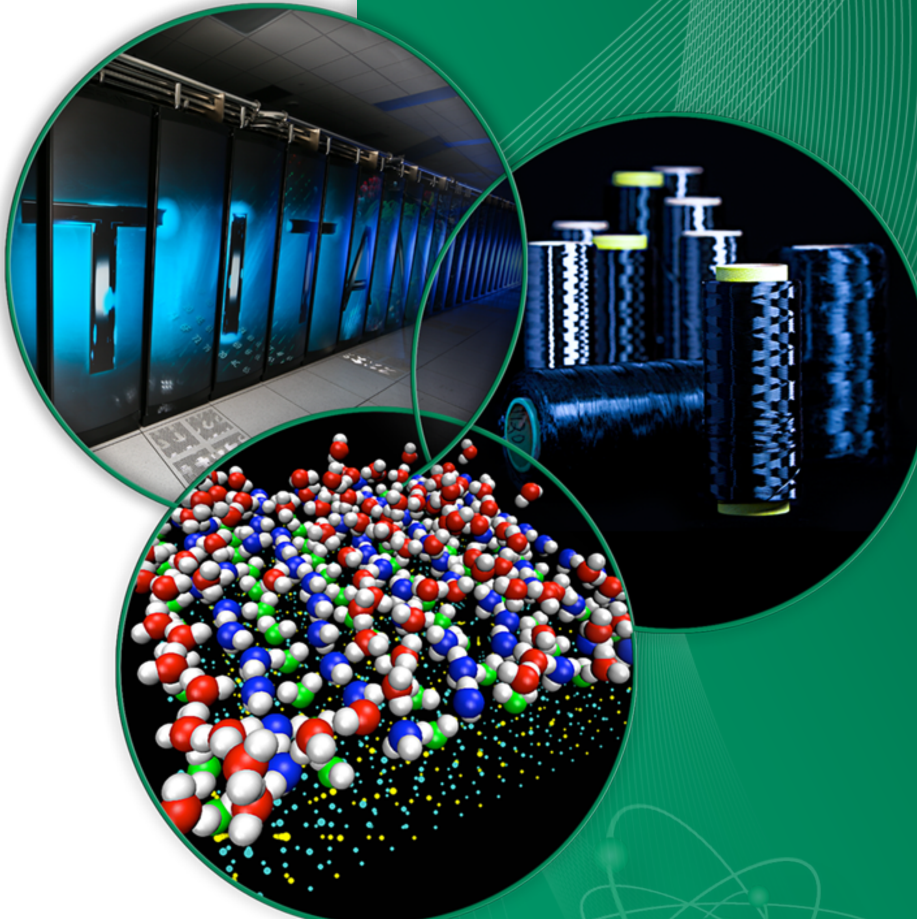
Integral Benchmark Experiments in the Inverse Sensitivity/ Uncertainty Computations



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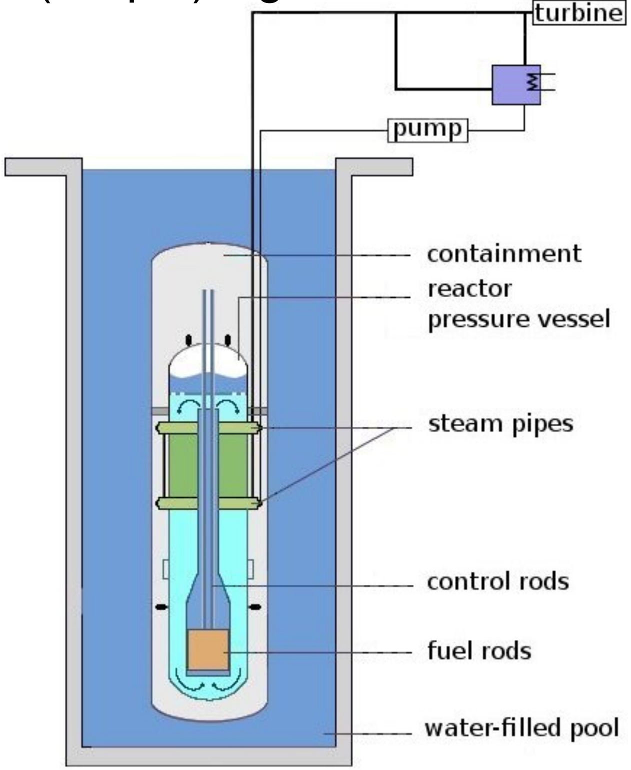
Inverse Sensitivity Uncertainty (IS/U) Intro

- Definition: Determine target accuracies of nuclear data needed to model applications within prescribed tolerances.
- Why? Nuclear data measurements are expensive
  - between $ ~400,000 and ~1,000,000
- ⇒ Measurements must be carefully chosen and prioritized
  - They are application-dependent (e.g. which nuclear reactor design?)
  - Presently guided by expert opinion
- A poorly designed experiment may miss the mark
  - Example: a generic burnup credit cask benchmark experiment

Applications

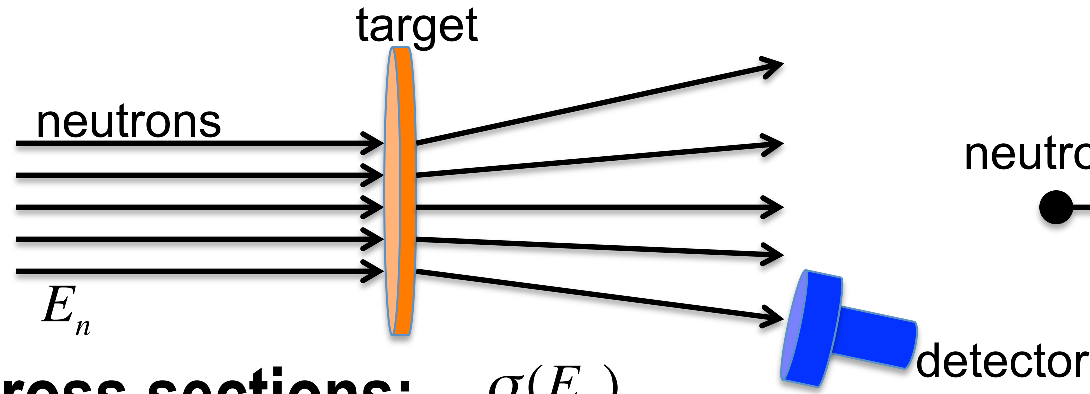
- Light Water Reactors
- Fast neutron reactors
- Spent Nuclear Fuel
  - Reprocessing
  - Transport
  - Disposal
- Generally: Complex systems
  - Difficult to build or prototype
  - Burden on modeling
    - Uncertainties are important
  - Application modeling uses:
    - Differential data
    - Integral data

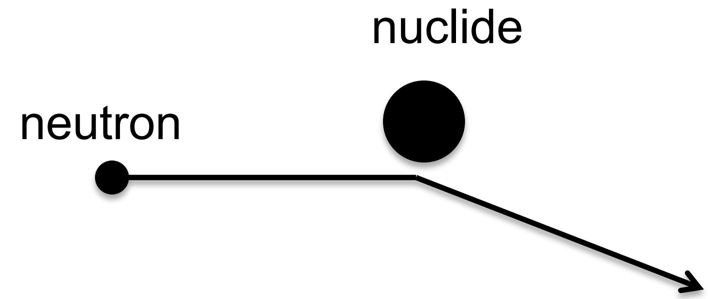
A (simple) Light Water Reactor



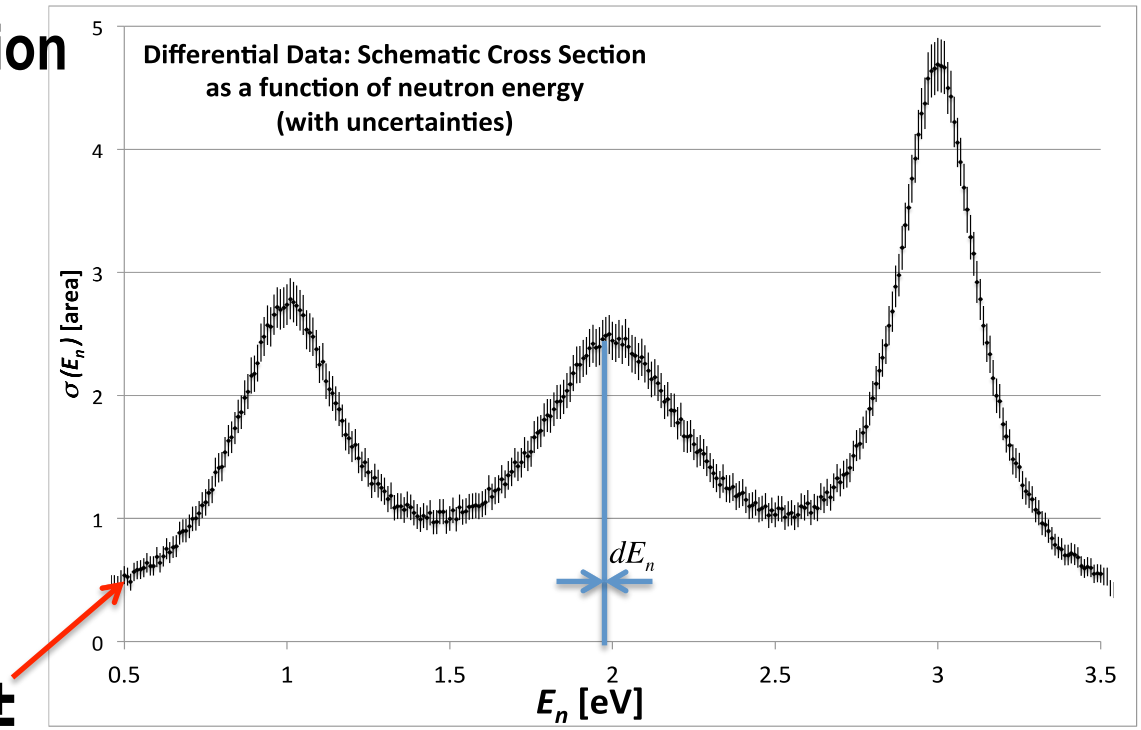
- **Responses:**
  - **Neutron multiplication factor, cycle length, power distribution, reaction rate ratio, material worth, radiation dose, etc.**

Differential Data ("microscopic")





- **Cross sections:** $\sigma(E_n)$
  - **Scattering, capture, fission**
    - **per nuclide**
  - **Measured for each incoming energy** E_n
    - $\Longrightarrow$ **differential**
  - **Cost: ~$400 K**
    - **Data acquisition**
    - **Data evaluation**
  - **Includes uncertainties; ±**
  - **Used for neutron transport**

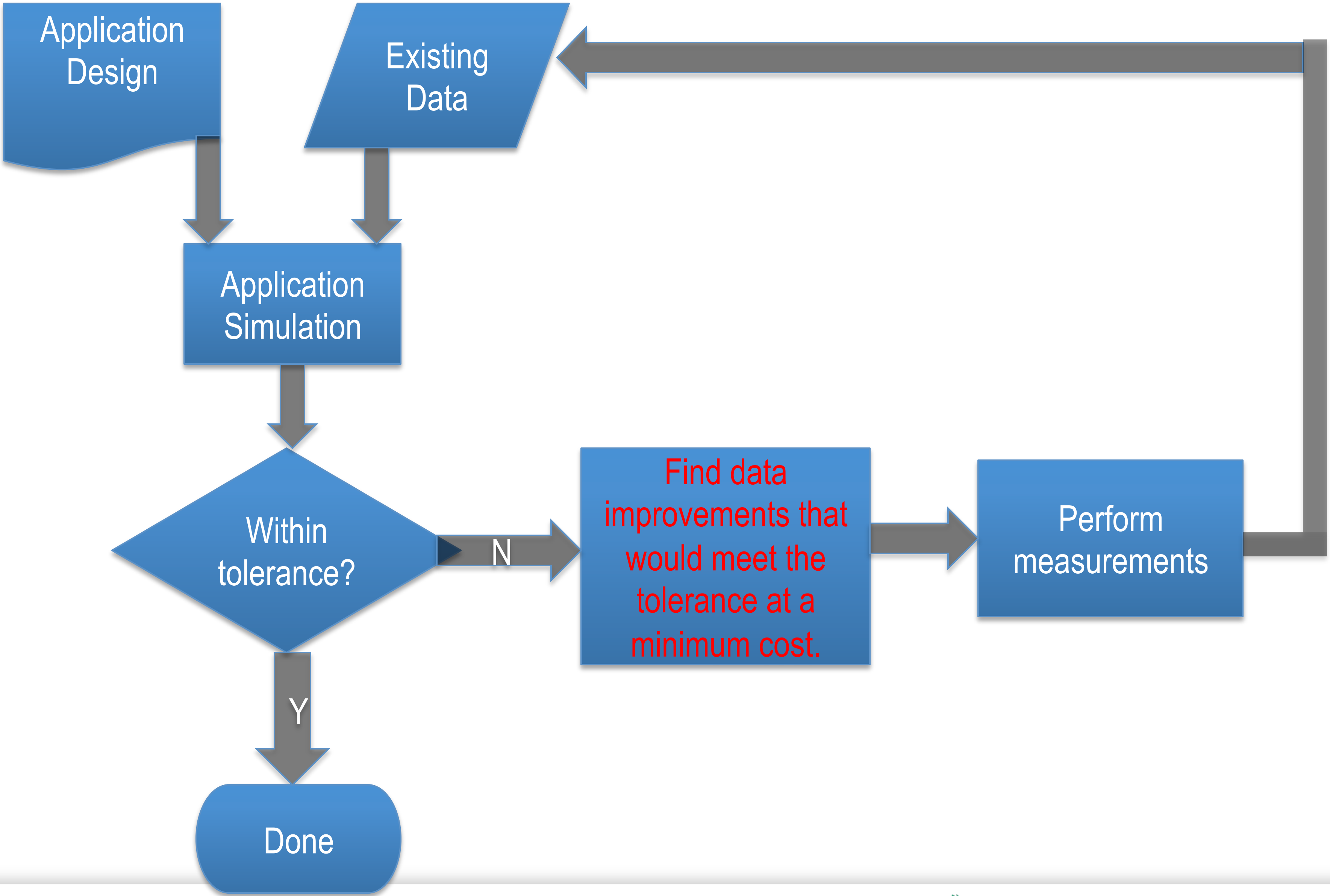


Integral data ("macroscopic")

- Various (sub)critical assemblies
  - Macroscopic objects
    - macroscopic quantities measured
      - E.g. neutron multiplication factor
  - Relatively simple setups
  - Highly accurate measurements
- Provide constraints:
  - Neutron transport simulation using differential cross sections ought to be consistent with measured integral data.
- Very expensive: ~ $ million
  - 1,000's of them measured

LEU-COMP-THERM-001
is used in this work
(photos from IHCSBE 2008)

Inverse S/U Use Case



Inverse S/U: Definitions

- A nuclear application design specifies maximum allowed uncertainties on performance parameters ("responses")
  - e.g. the multiplicity factor and its tolerance

$$R \pm \Delta R$$

- Neutron transport using existing cross section uncertainties often leads to an application response uncertainty *greater* than the maximum allowed, i.e.:

$$\sigma_0 \pm \Delta\sigma_0 \Rightarrow R_0 \pm \Delta R_0 \text{ where } \Delta R_0 > \Delta R$$

- Inverse S/U: What set of improved data would lower the response uncertainty below the specified tolerance?
  - While minimizing the cost of data measurements (to be defined).

$$\sigma' \pm \Delta\sigma' \Rightarrow R' \pm \Delta R' \leq \Delta R \text{ for } \min(\text{cost}[\Delta\sigma'])$$

Inverse S/U Math

- Given a desired responses ± tolerances: $R \pm \Delta R$
- and the existing data ± uncertainties: $\sigma_0 \pm \Delta\sigma_0$
- Minimize the *cost* of acquiring improved data uncertainties that yield a response uncertainty within tolerance:

$$\min\{\mathrm{Cost}[\Delta\sigma]\} \text{ such that}$$

$$S(\Delta\sigma)^2 S^T \leq (\Delta R)^2$$

$$S = \left.\frac{\delta R(x)}{\delta\sigma}\right|_{\sigma=\sigma_0}$$

- This a constrained optimization problem
  – MINCON: open source subroutine is used by MATLAB and DAKOTA

Numerical Approach

- We parameterize the uncertainties via the covariance mat. *C*:
  - The diagonal of *C* are the extant diff. cross section σ_0 variances
  - The diagonal of *C'* are the variances $(\Delta\sigma)^2$ to be optimized by the IS/U

$$C'_{ij} = x_i C_{ij} x_j$$

- ***x*'s: parameters varied between 0.0 and 1.0, so that its cost:**

$$\text{cost}[\mathbf{C}'] = \sum_i \frac{w_i}{C'_{ii}} = \sum_i \frac{w_i}{x_i C_{ii} x_i}$$

w_i = 1 for all *i*; for all (44) groups and for all cross sections

- **…is minimized, while the constraint:**

$$\text{diag}[\mathbf{S}_a \mathbf{C}' \mathbf{S}_a^{\mathrm{T}}] \le \text{var}(\mathbf{R})$$

…is satisfied.

Application sensitivity profile. User defined application response variance.

Use of Integral Benchmark Exp's.

- In this work we minimize the Cost(DIFFERENTIAL)
  - We USE the existing INTEGRAL data to inform DIFF. data needs
  - Via the result of the Generalized Linear Least-Squares Method
    - That quantifies the effect of INT. measurement unc's. on DIFF. data unc's.

$$\mathbf{C''} = \mathbf{C'} - \mathbf{C'}\mathbf{S}_b^T\mathbf{D}^{-1}\mathbf{S}_b\mathbf{C'}$$

Because of the minus sign, C' can be larger than before

- **Using C" instead of C' modifies (or eases) the constraint:**

$$\mathrm{diag}[\mathbf{S}_a\mathbf{C''}\mathbf{S}_a^T] \leq \mathrm{var}(\mathbf{R})$$

since the modified constraint uses C" instead of C'

- **A larger C' satisfies this constraint**
  - **A larger C' means larger diff. data unc.' → easier to measure.**
  - **A larger C' → lower cost**
- **Most helpful IBEs have sensitivities similar to the application**

General results

- IS/U results obtained with integral benchmark experiments:
  - Afford larger DIFF. data uncertainties → lower cost of DIFF. data
    - For PWR fuel array overall 6-fold decrease in data cost was achieved.
  - Δk_{eff} = 0.0031 for extant data; we desire Δk_{eff} = 0.001, var(k_{eff})=10^{-6}
  - Leads to the same k_{eff} variance of the PWR fuel array

Table I. Summary of the IS/UQ results

	w/o Benchmark	*w/Benchmark*
Cost (arb.)	53.3	8.6
# iterations	311	186
var(k_{eff})	1.0E-06	1.0E-06

- **Results verified by initiating with different initial values**
- **Neutron multiplication factor, k_{eff}, of a PWR fuel-rods array**
  - **The IBE we use in this work is water-moderated UO_2 fuel rods in 2.032-cm square-pitched arrays (LEU-COMP-THERM-001). This IBE was chosen because of its similarity to the PWR fuel-rods.**

Context for Interpreting the Results

- Diff. data uncertainties are limited by experimental methods
  - Some data already at the present-day limits of exp. precision
  - Uncertainties required by IS/U lower than these may be unrealistic

Table II. Uncertainties of the present-day state-of-the-art measurements for various cross sections

Reaction	*MT*	*Min. Rel. Uncertainty*
Fission	18	0.7%
Capture	102	2%
Neutron yields	452	0.3%
Elastic scattering	2	2%

- **44-group structure energy boundaries**
  - **Groups 1-44 spans $20*10^6$ eV to $1*10^{-5}$ eV**

20.0E6	8.1873E6	6.434E6	4.8E6	3E3	2.479E6
2.354E6	1.85E6	1.4E6	9E5	4E5	1E5
2.5E4	1.7E4	3E3	5.5E2	1E2	3E1
1E1	8.1E0	6E0	4.75E0	3E0	1.77E0
1E0	6.25E-1	4E-1	3.75E-1	3.5E-1	3.25E-1
2.75E-1	2.5E-1	2.25E-1	2E-1	1.5E-1	1E-1
0.7E-2	5E-2	4E-2	3E-2	2.53E-2	1E-2
7.5E-3	3E-3	1E-5			

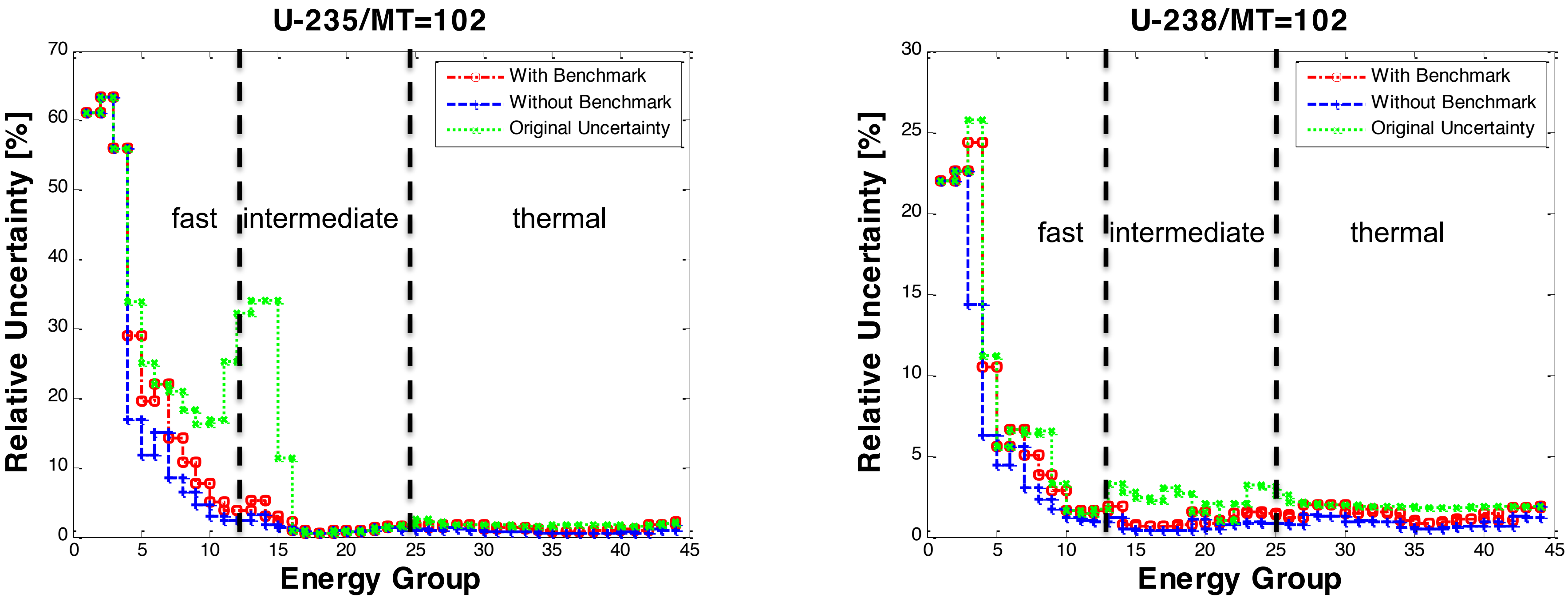
- **The following slides will present DIFF. data uncertainties**
  - **For various cross section as a function of energy group (1-44)**

Context cont'd.

- We use the extant 44-group covariance data (SCALE)
- We compute Sensitivity Data Format files (TSUNAMI)
    - For the application and the integral benchmark experiments
    - Takes into account the implicit self-shielding (B. Khuwaileh's et al. ANS Winter Mtg. '13)
    - Also in 44-group structure
- We use standard subroutine for constrained minimization
  - It uses derivatives of the cost function and the constraint
    - We compute derivatives using analytical expressions
      - This improves performance over the numerical evaluation of derivatives

Inverse S/U Results

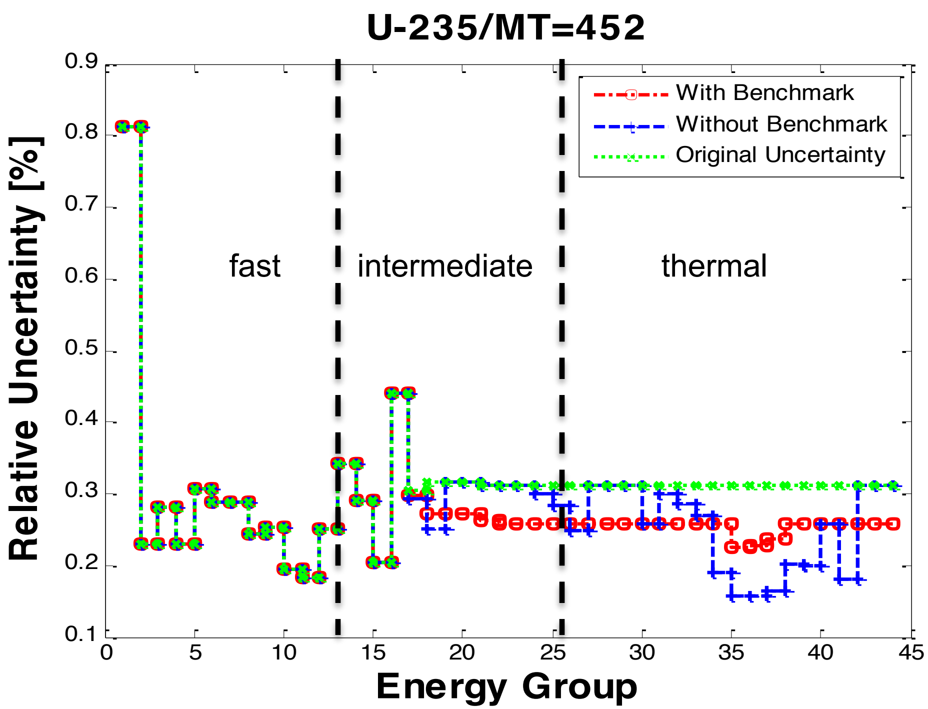
- Required diff. data uncertainties
  - w/ integral benchmarks are not as small as w/o them

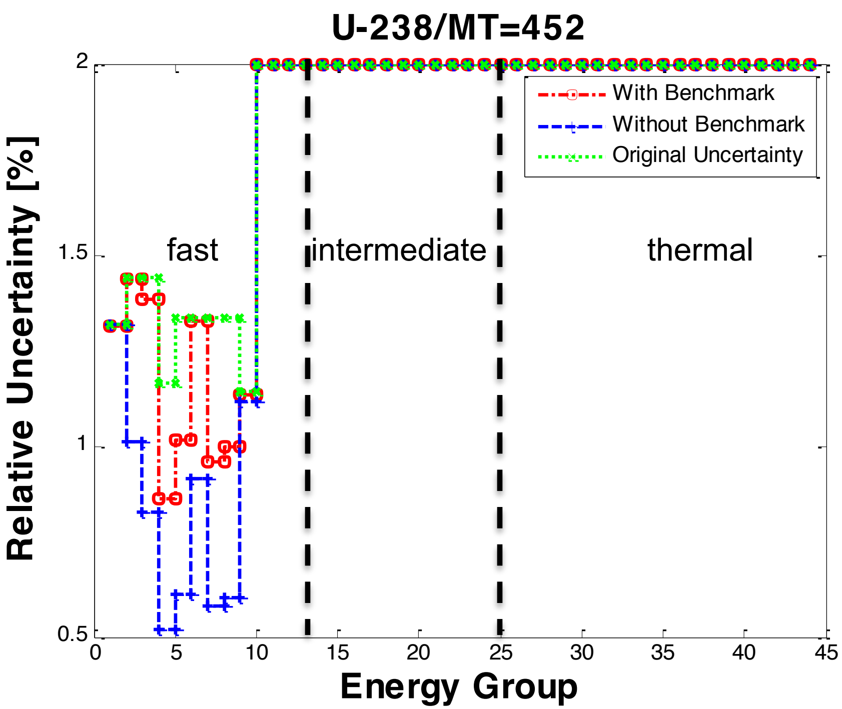


Required relative uncertainties (benchmark vs. no benchmark) for neutron capture cross section (i.e. MT=102) on U-235 (left) and on U-238 (right). The plots show that inclusion of a benchmark affords less stringent uncertainties. Such uncertainties are more realistically achievable, especially when the extant uncertainties are already near or below the high-precision uncertainties listed in Table II. This happens here in groups 15-44.

Inverse S/U Results cont'd.

- Neutron yield: average number of fission neutrons, "ν-bar"





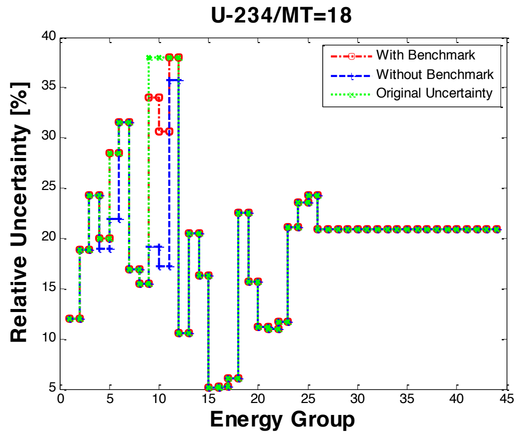
For U-235 neutron yield (MT=452) extant uncertainties (green) are already near (or smaller than) the ENDF guidance value of 0.3%. Here too, the IS/U with integral benchmark experiment (IBE) (red) require uncertainties that are not as small as those w/o IBEs (blue).

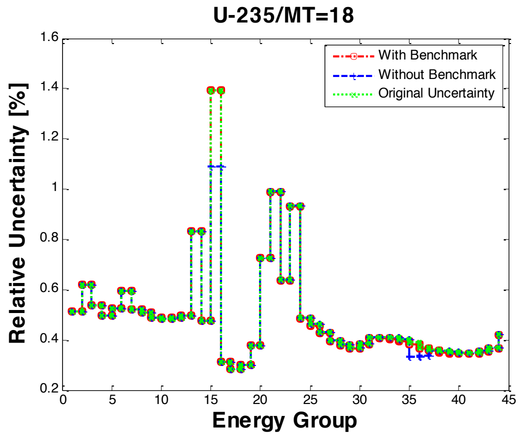
Summary and Outlook:

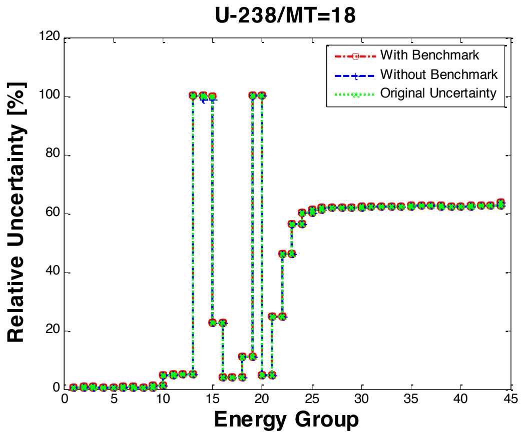
- A new application of the Inverse Senstivity/Uncertainty to
  - cost-optimized prioritization of nuclear data measurements
  - Demonstrated the benefit of using integral benchmarks in the IS/U
    - w/o IBE DIFF. data uncertainties may be unachievable, and vice versa.
- Outlook
  - Formalism sufficiently general to minimize the TOTAL cost of data
    - Of differential data, and integral benchmark experiments (IBEs), simultaneously
    - It may be extended to optimize and design IBEs
- IS/U capability can be used for various nuclear fuel cycle applications

IS/U Results: Fission

- The IS/U uncertainties for fission are somewhat affected
  - For fission too IBEs allow greater uncertainty

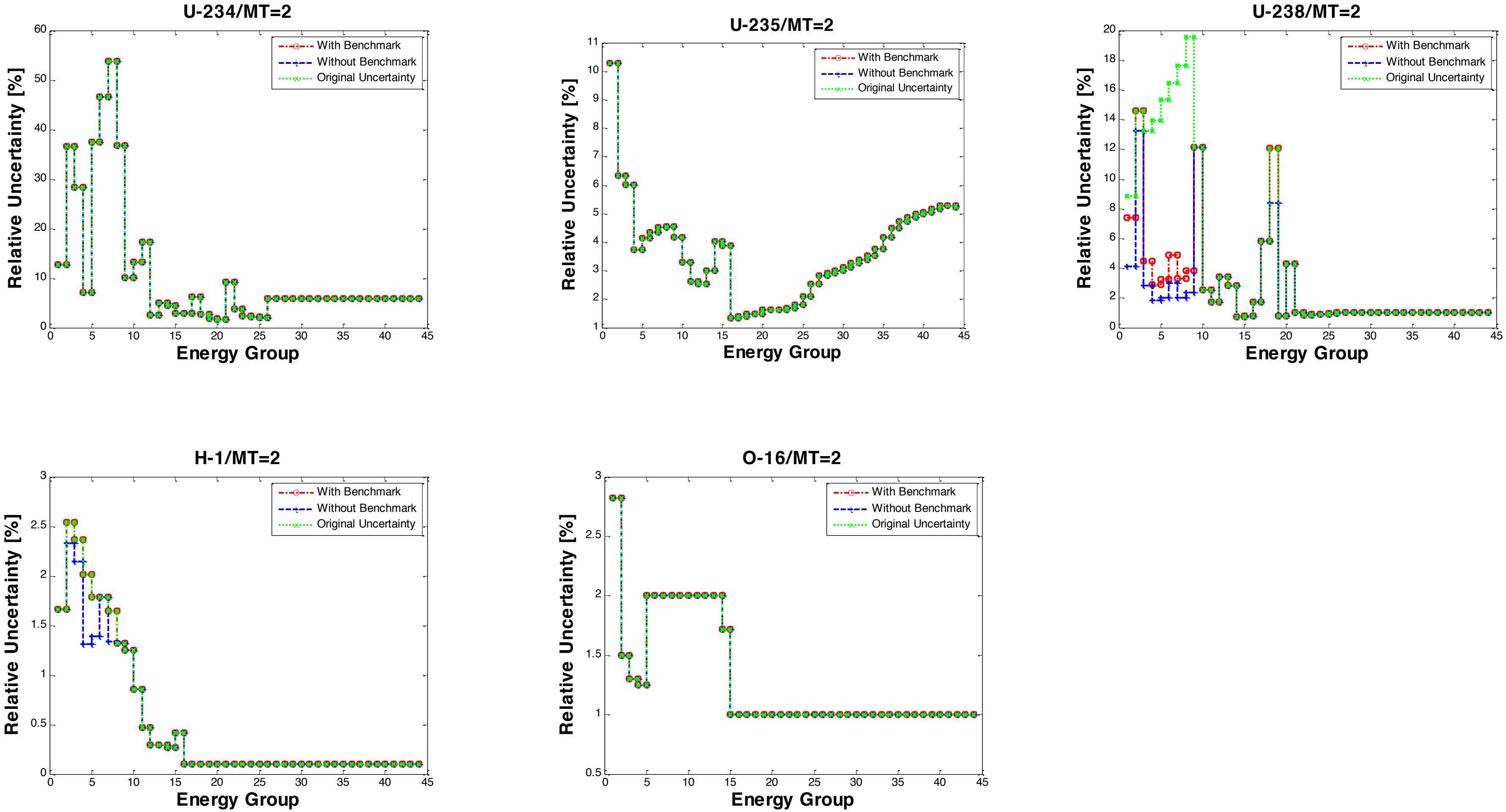






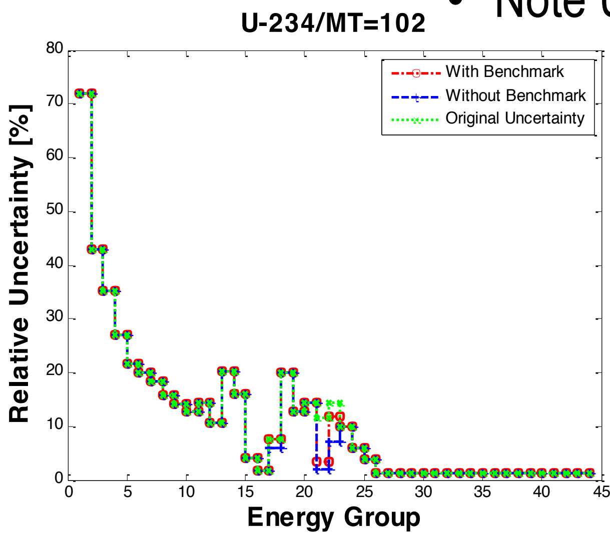
IS/U Results: Elastic

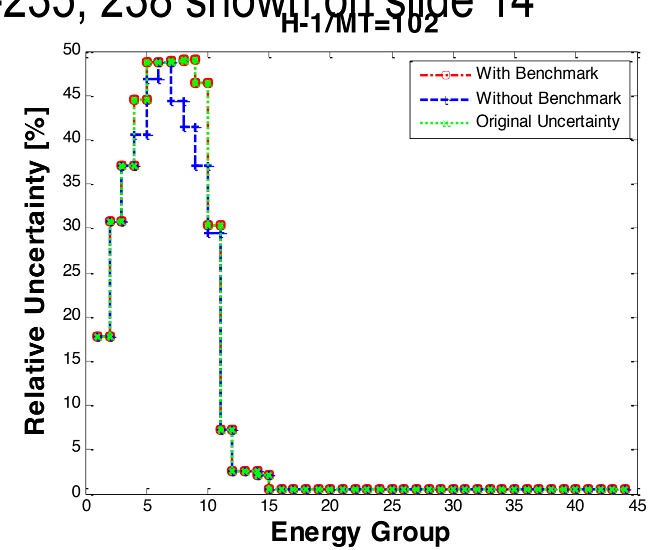
- Only high energy groups of U-238 affected
  - There too IS/U uncertainties are slightly larger when IBE used

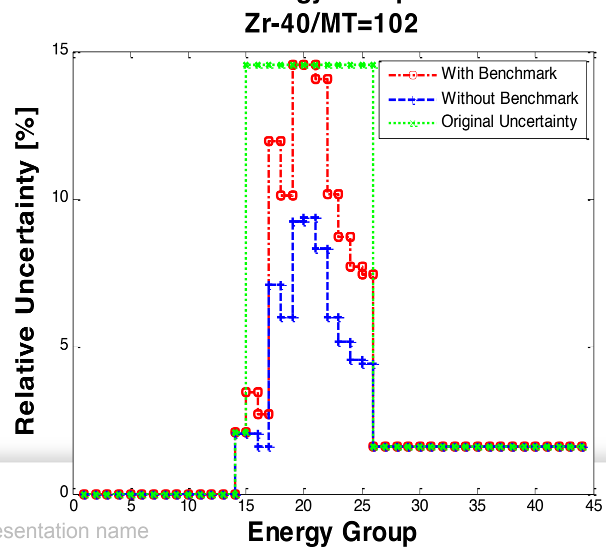


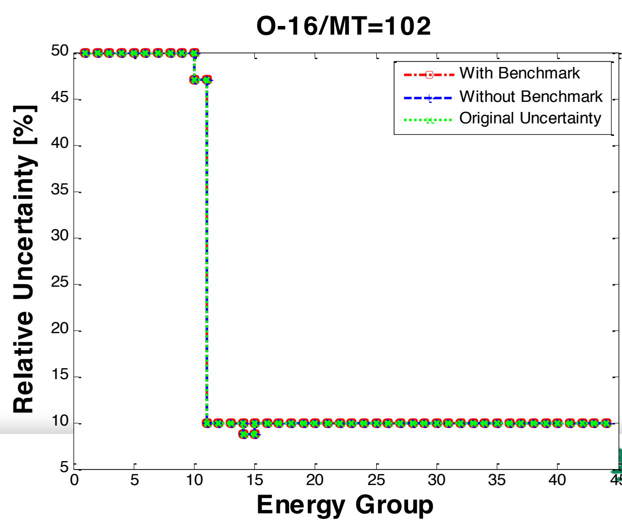
IS/U Results: Capture

- Large effect for Zr-40; small for U-234, H-1; none for O-16
  - Using IBEs allows uncertainties larger than w/o IBEs.
    - Note U-235, 238 shown on slide 14









IS/U Generalization to Integral Data

- The formalism can be used to minimize the total cost
  - Total Cost(DATA) = Cost(DIFFERENTIAL) + Cost(INTEGRAL)
    - Generally Cost (INT.) << Cost(DIFF.)
    - Depends on whether an IBE experiment is still available to be re-measured at a higher precision
- It may be used to design or optimize INT. benchmark exp's.
  - By e.g. maximizing the similarity of sensitivity profiles of INT. benchmark exp. to that of the nuclear application considered.

Application to Integral Benchmark Exp.

- a generic burnup credit cask model
  - In retrospect, a thinner foil of Rh-103 was needed to make it more sensitive to Rh-103 cross section

Figure 4. View of the Critical Assembly in the Reactor Room.

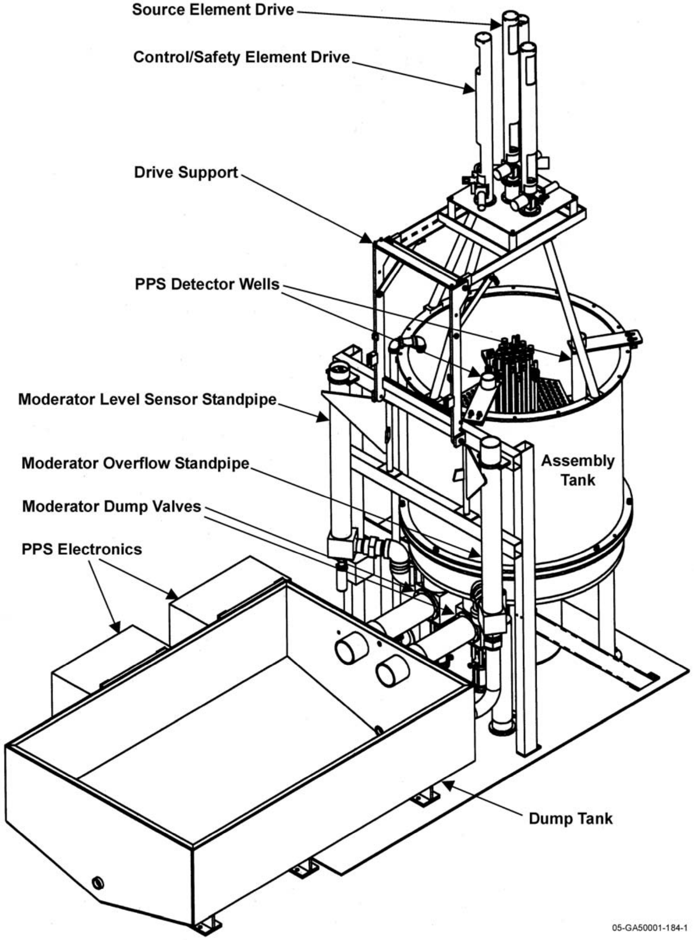


Figure 1. Overall Concept of the Critical Assembly.