Nuclear Theory Tools for Fuel Cycle R&D

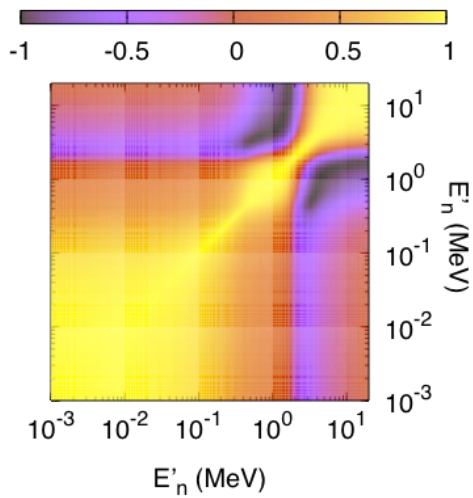
[1]P.Talou, [1]T.Kawano, [1]A.C.Kahler, [1]G.M.Hale, [1]S.Holloway, [1]J.E.Lynn, [1]P.G.Young, [1,2]O.Bouland, [1,3]M.Rising

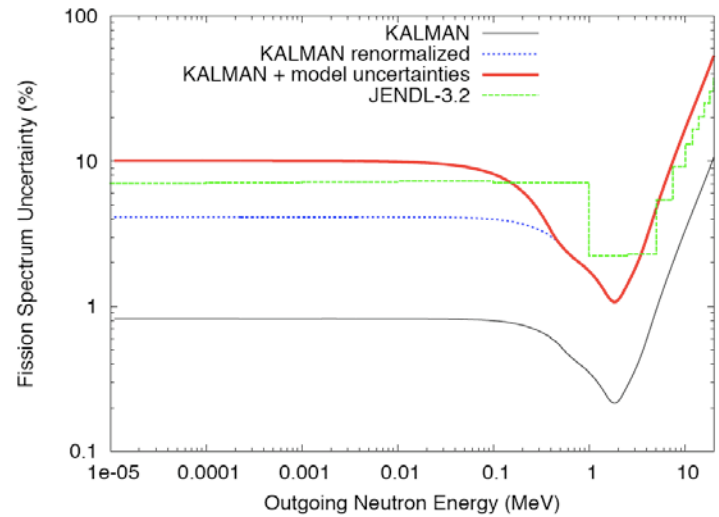
[1]Los Alamos National Laboratory
[2]CEA-Cadarache, France
[3]University of New Mexico

Major Recent Accomplishments (1/3)

- **Uncertainty Quantification of Prompt Fission Neutron Spectrum (PFNS)**
  - Significant efforts on Methods & Codes
    - Modern PFNS code, implementing Madland-Nix model equations.
    - Suite of Fortran 95 modules and Perl scripts to perform a complete evaluation and uncertainty quantification of PFNS

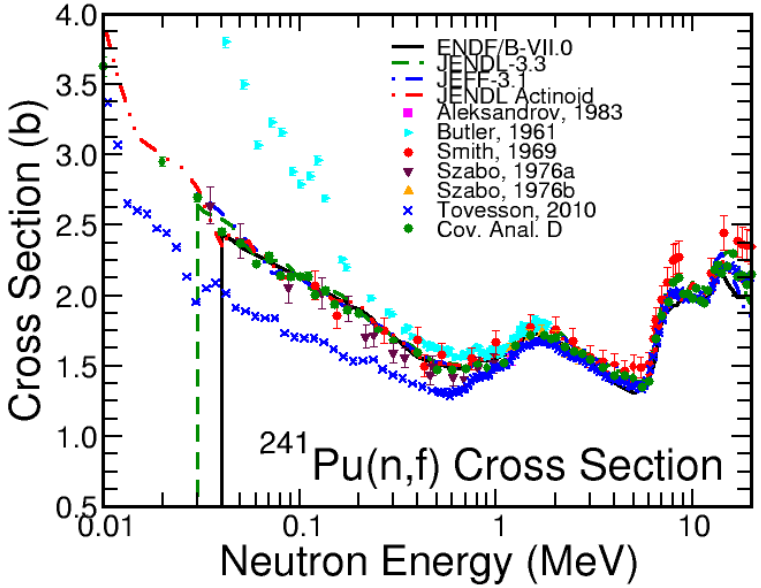
- Application to n(0.5 MeV)+^{239}Pu and ^{240}Pu
  - Included in AFCI-1.3 covariance library
  - ^{239}Pu: publication accepted in Nucl. Sci. Eng (2010)

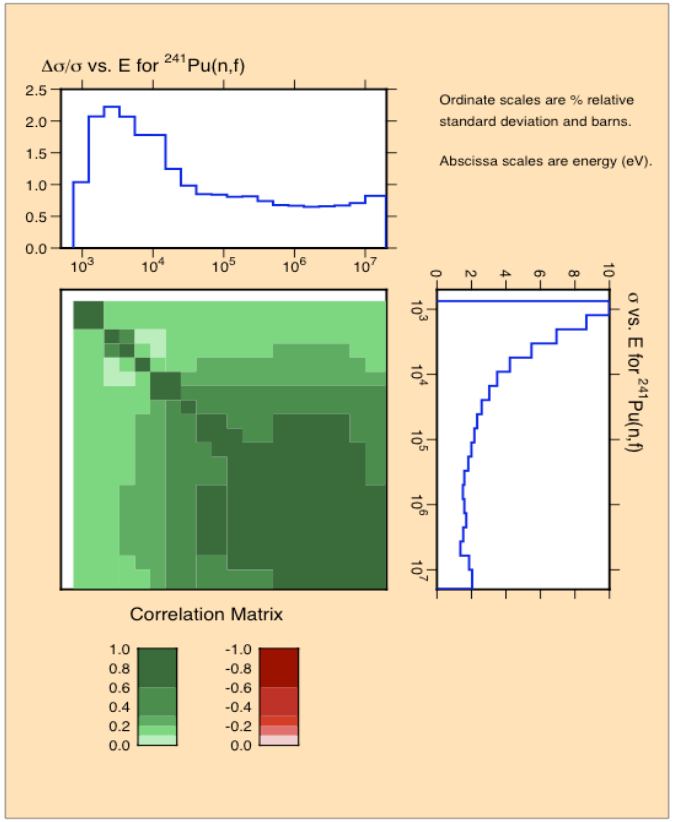




Major Recent Accomplishments (2/3)

- **^{241}Pu (n,f) Cross Section Uncertainties**
  - New LANSCE data
    - Large discrepancies with bulk of data below 1 MeV
    - Difficult to handle consistently with other data sets

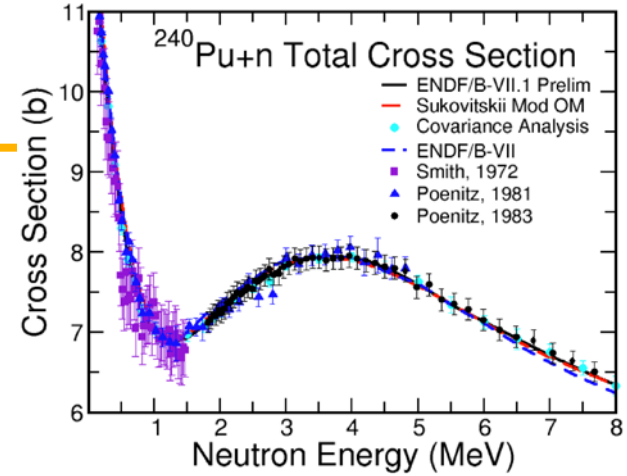




ENDF-formatted covariance file delivered to BNL in April 2010.

Major Recent Accomplishments (3/3)

- **n+^{240}Pu new evaluation including UQ**
  - New coupled-channels calculation using recently developed Soukhovitsky optical potential
  - New GNASH reaction calculations
  - Covariance matrix evaluations for all major reaction cross-sections, and prompt fission neutron spectrum and neutron multiplicity.



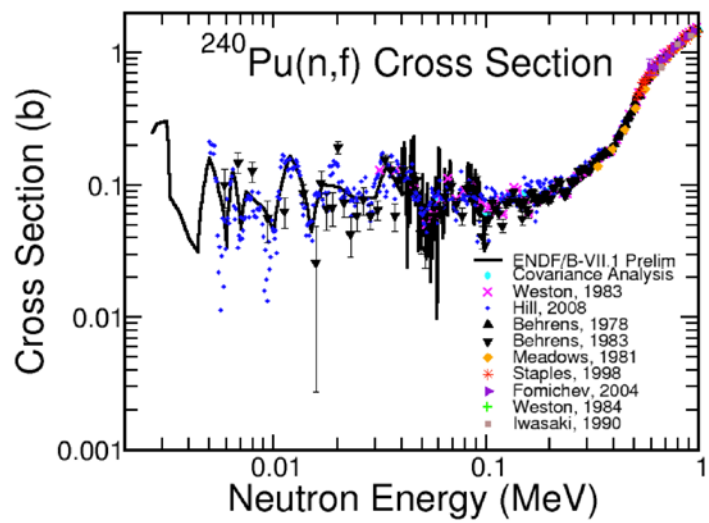
LA-UR-09-08071

TECHNICAL REPORT ON
N+^{240}PU EVALUATION AND UNCERTAINTY QUANTIFICATION

P.Talou, P.G.Young, T.Kawano, A.C.Kahler and M.B.Chadwick

T-2, Nuclear Physics Group,
Theoretical Division, Los Alamos National Laboratory

Sep. 23, 2009



Ongoing Work

- **Working with BNL toward AFCI-2.0 covariance library**
  - n+^{238}Pu evaluation + covariance
  - Covariance work on Americium isotopes
  - Light elements: ^{16}O, ^{4}He
  - Review of AFCI-1.3 library → lingering questions on ^{235}U capture and ^{239}Pu $<\nu>$
- **Develop PFNS UQ tools for a large set of actinides**
  (w/ A.Prinja*, M.Rising* (PhD student), University of New Mexico)
- **Simultaneous evaluation of (χ,ν) and incident-energy dependent PFNS covariance + inclusion of $<\nu>(E_{inc})$ in evaluation**
- **Advanced fission cross-section modeling**
  (w/ O.Bouland, CEA, France & W.Nazarewicz* et al., UTK)
- **Advanced modeling of PFNS (Monte Carlo)**
  (w/ Y.Danon*, B.Becker* (postdoc), RPI)

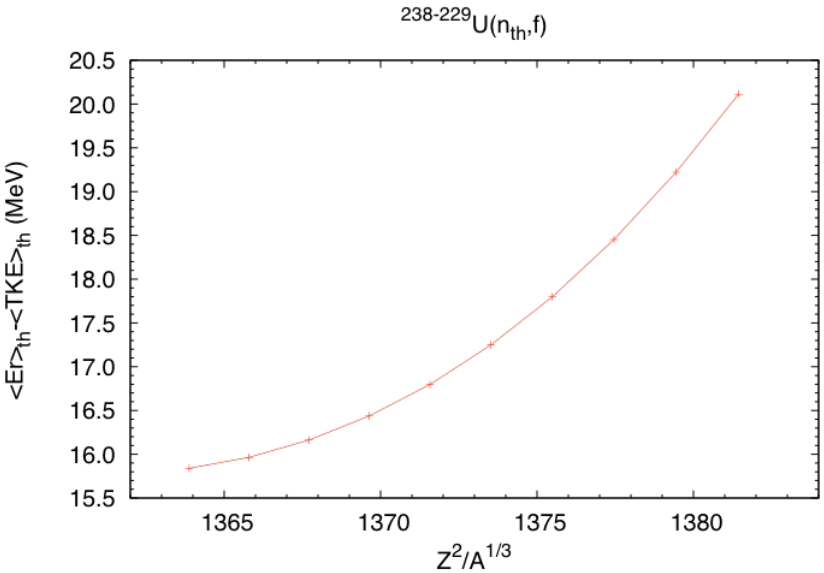
*AFCI-NEUP grant

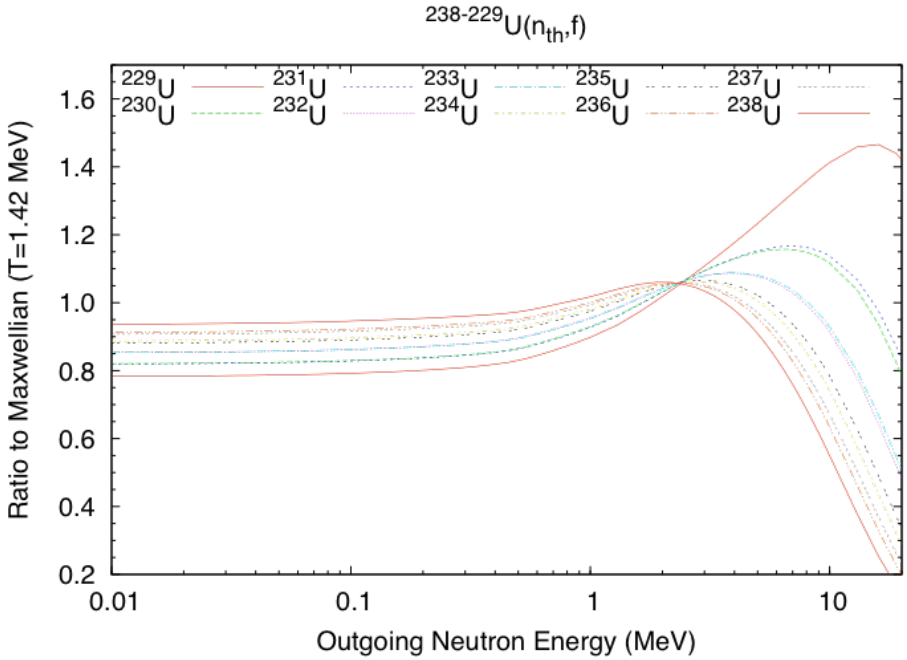
Large-Scale PFNS Uncertainty Quantification

- **Developing methods & codes to perform evaluation + UQ for large set of actinides**
  - Reasons:
    - Many ENDF/B-VII.0 PFNS evaluations are in poor shape
    - Need for covariance matrices
  - Solution:
    - Use Los Alamos model parameters systematics as a starting point
    - Use experimental data sets available from the EXFOR database
    - Perform Bayesian statistics to obtain posterior evaluations and covariances
- **Where do we stand?**
  - Full suite of Fortran 95 codes and Perl scripts being developed → from raw data and prior parameters to ENDF-formatted files
  - Use of Tudora systematics [A.Tudora, Annals Nuclear Energy 36 (2009) 72]
  - In progress: Application to all U and Pu isotopes

Systematics for Uranium Isotopes

$\langle E_r \rangle - \langle TKE_{th} \rangle = f(Z^2/A^{1/3})$





Simultaneous Evaluation of $(\chi,\nu)_{|Einc}$

- **Use of PFNS and KALMAN codes**
- **PFNS computes both spectrum and multiplicity**
- **KALMAN can also handle both quantities**
- **Use of experimental data sets for both types of data + as a function of incident energy**
  - → large covariance matrix for both χ and ν
  - → Several blocks for different incident energies

In progress

$$R_{ijk} = \frac{\partial \chi_i(E'_j)}{\partial p_{ik}} \times \frac{p^0_{ik}}{\chi^0_i(E'_j)}$$

$$Q_{ik} = \frac{\partial \overline{\nu}_i}{\partial p_{ik}} \times \frac{p^0_{ik}}{\overline{\nu}_i^0}$$

$$\left[\begin{array}{c} \begin{pmatrix} R_{111} & R_{112} & \cdots & R_{11k} \\ R_{121} & R_{122} & \cdots & R_{12k} \\ \cdots & \cdots & \cdots & \cdots \\ R_{1n1} & R_{1n2} & \cdots & R_{1nk} \end{pmatrix} \\ (Q_{11}, Q_{12}, \cdots, Q_{1k}) \end{array}\right] i = 1$$

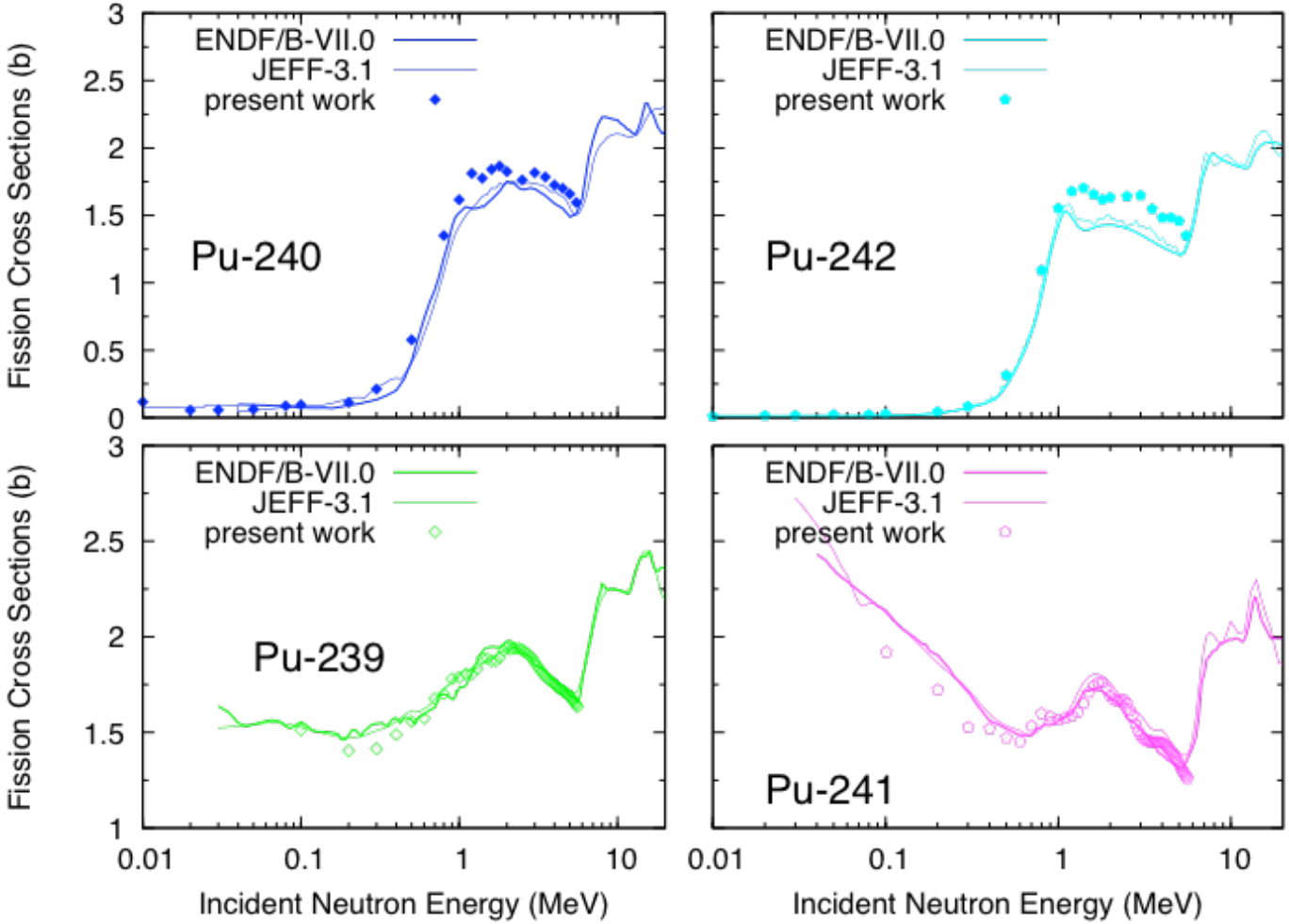
$$\vdots$$

$$\left[\begin{array}{c} \begin{pmatrix} R_{m11} & R_{m12} & \cdots & R_{m1k} \\ R_{m21} & R_{m22} & \cdots & R_{m2k} \\ \cdots & \cdots & \cdots & \cdots \\ R_{mn1} & R_{mn2} & \cdots & R_{mnk} \end{pmatrix} \\ (Q_{m1}, Q_{m2}, \cdots, Q_{mk}) \end{array}\right] i = m$$

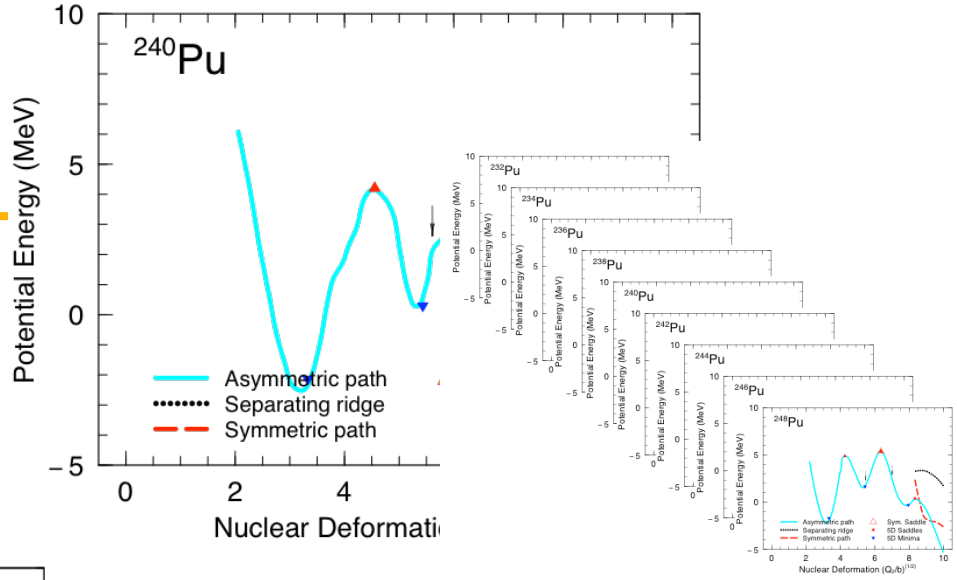
Advanced Fission Cross-Section Modeling

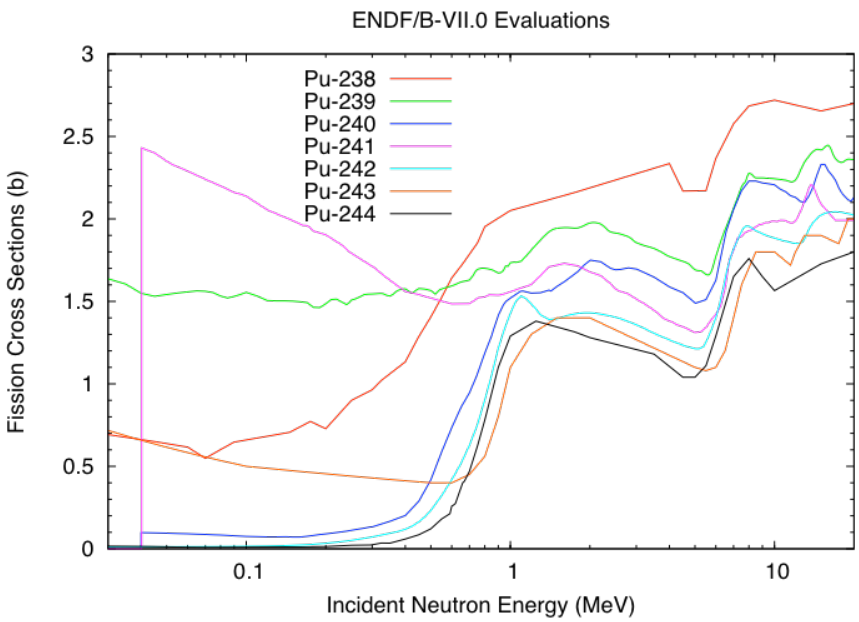
- **R-matrix formalism applied to nuclear fission**
  "The double-humped fission barrier"
  S.Bjørnholm, J.E.Lynn. Rev. Mod. Phys., vol. 52, No. 4, 725-931 (1980).
- **We are developing a modern version of the AVXSF code by J.E.Lynn, to be coupled with modern LANL nuclear reaction codes**
- **Toward robust and predictive fission cross-section capabilities**
  - Using modern calculations of fission paths (e.g., FRLDM, HFB)
  - Combinatorial calculations of level densities
  - Individual transition states at saddle points obtained from both theory and experiment (e.g., (d,pf) transfer reactions)
- **First application to Pu isotopes**

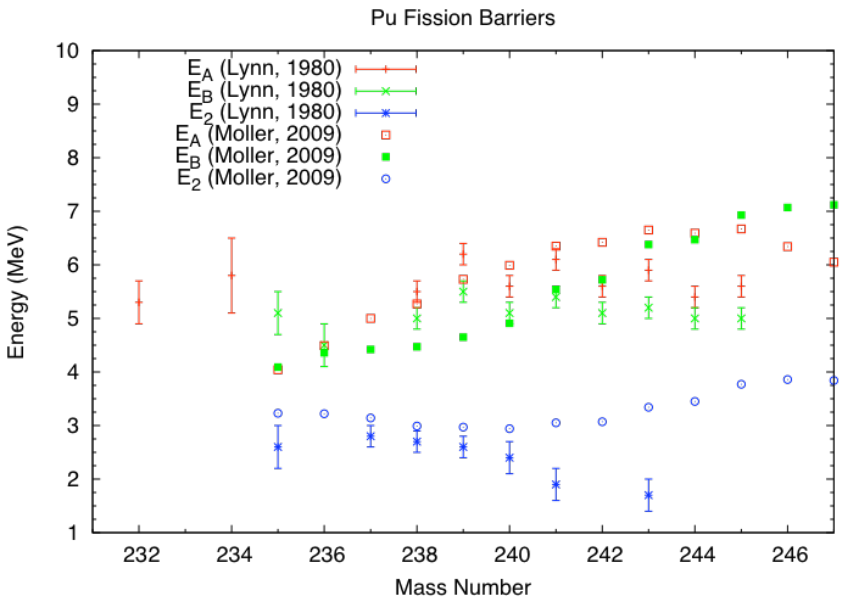
Suite of Pu isotopes



Suite of Pu isotopes



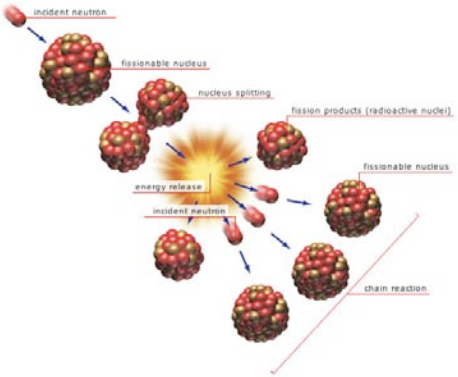




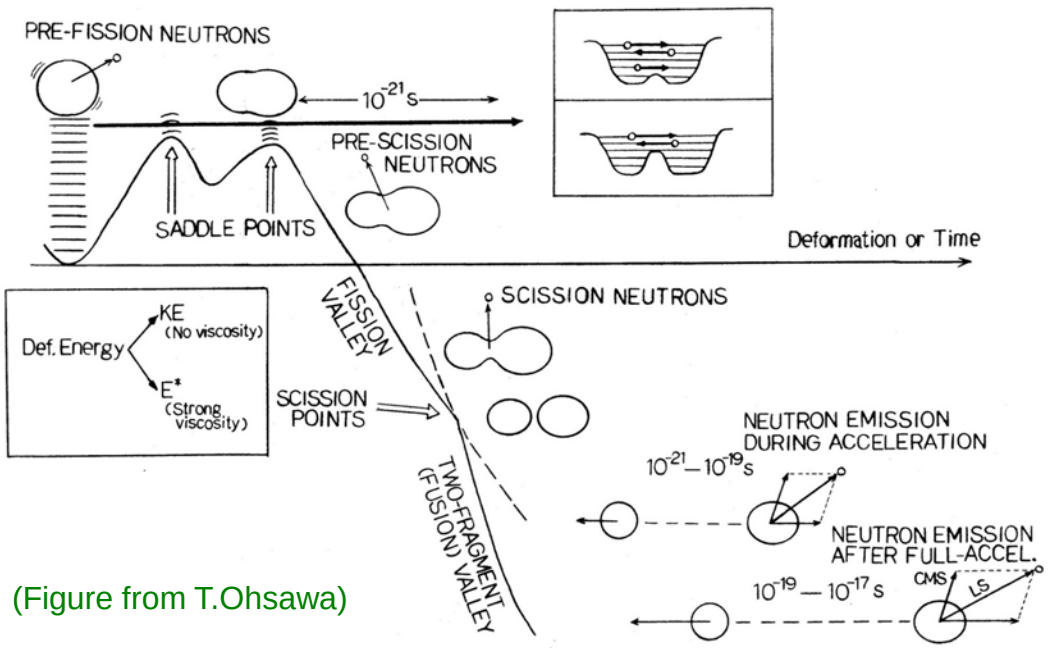
Monte Carlo Simulation of Fission Fragment Evaporation – PFNS and more!

- **Madland-Nix or Los Alamos model:**
  - Average over entire fission fragment distributions **and** neutron cascades
  - Several important assumptions regarding what happens near scission
  - Main advantage: very few tunable parameters!
  - Main disadvantage: computes averages only:
    - Average neutron multiplicity $<\nu>$
    - Average neutron spectra $<\chi>(E_{in},E_{out})$
- **From the prediction of a few average quantities (χ,ν) to detailed exclusive quantities: P(ν), $\chi_{(\nu=1,2,...)}$, n-n correlations, …**
  - → Monte Carlo simulation of the de-excitation of the primary fission fragments
- **Much more physics**
  - → to be used in advanced transport simulations

Prompt Fission Neutron Physics



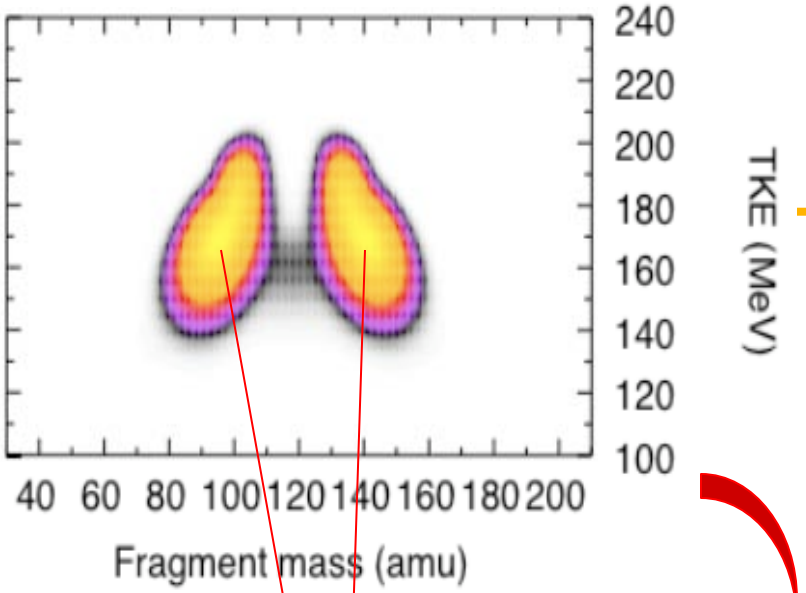
- **Excited primary fission fragments Y(A,Z,KE,U,J,π)**
- ***Prompt* decay by neutron and γ-ray evaporation**
- **Then can further β-decay, and emit *β-delayed* neutrons and gammas**



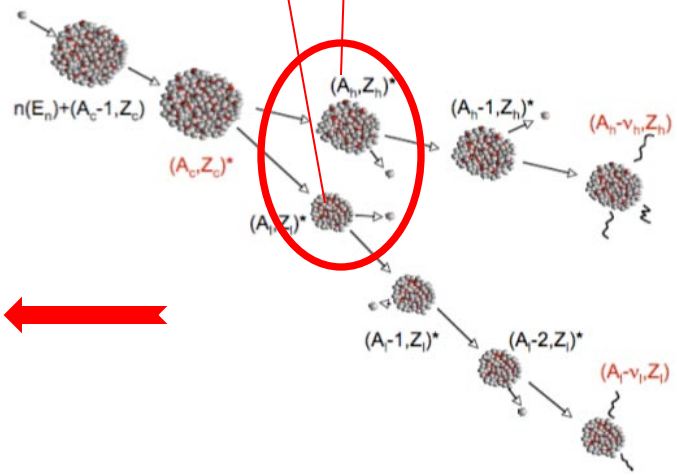
(Figure from T.Ohsawa)

- **Several stages:**
- **Pre-scission** (compound nucleus)
- **Scission** (neck break-up)
- **During acceleration**
- **After full-acceleration**

Monte Carlo Hauser-Feshbach Simulations



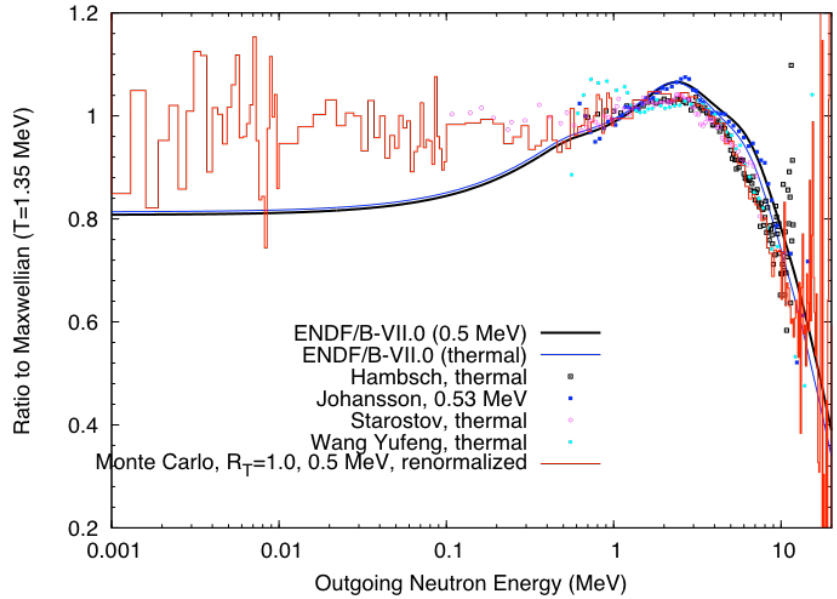
1. **Sample from Y(A,Z,TKE) distribution**
2. **Infer E^*_{tot} and $\langle J_{tot}\rangle$, and partition between the two fragments**
3. **Infer temperatures T_l and T_h → $R_T=T_l/T_h$**
4. **Apply Hauser-Feshbach equations**



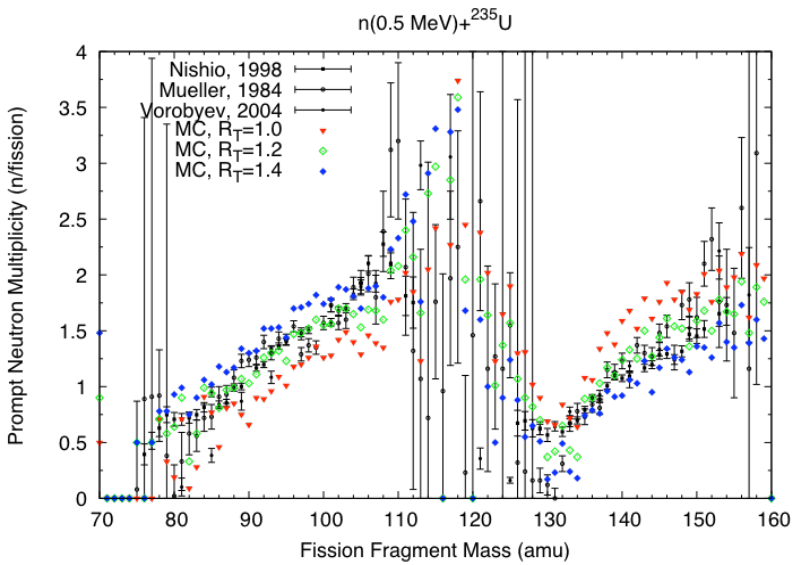
$\langle\chi\rangle(E)$, $\langle\nu\rangle$, $P(\nu)$, $\chi(E)_{|\nu}$, n-n correlations, etc.

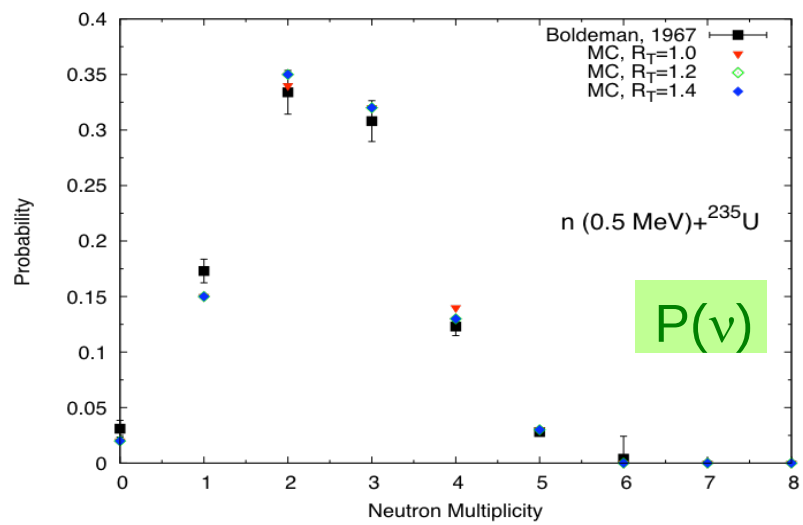
Application to n+^{235}U

- **Using experimental primary fission fragment yields $Y_{exp}(A,KE)$**
  [F.-J.Hambsch, private communication]



<ν>(A)

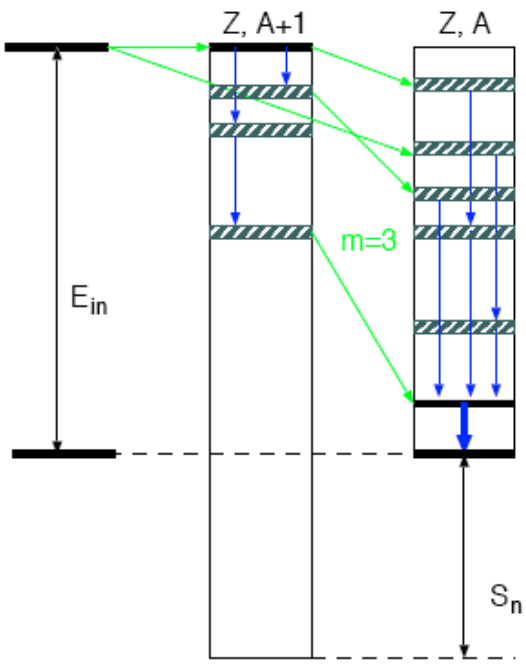


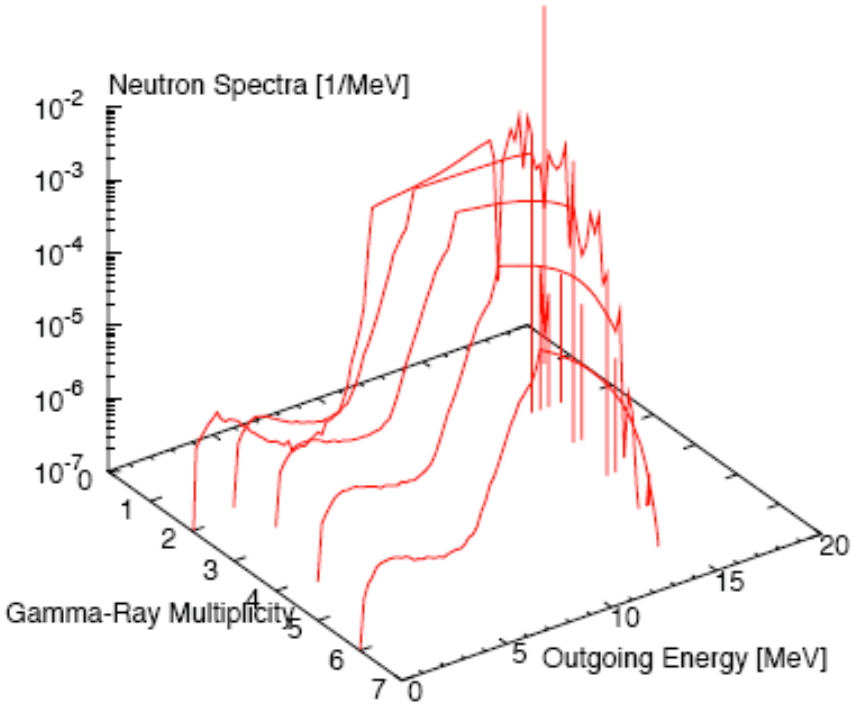


P(ν)

Prompt Fission Gamma Rays…
Monte Carlo Hauser-Feshbach Simulations

- **Towards a fully Monte Carlo Hauser-Feschbach solution**
- **New code being developed in our group** → *to be applied to this problem*
- Example: n(20 MeV)+^{56}Fe gated on 0^+-2^+ E2 transition





Plans for FY11

- Continue work with BNL on AFCI-x.y covariance libraries
- Completely revamp ENDF/B-VII library for (χ,ν) evaluations and UQ
- Work with LANSCE experimentalists to produce meaningful experimental covariance matrices for $\sigma_{(n,f)}$ (F.Tovesson et al.) and (χ,ν) (R.C.Haight et al.)
- Complete work on Pu isotopes (238-244) fission cross-sections with R-matrix formalism
- Continue collaborations under AFCI-NEUP grants
- CINDER?