Lawrence Livermore National Laboratory

# Covariance Applications at LLNL

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# LLNL focus on UQ:

- LLNL is developing new tools for large-scale UQ studies
  - '... goal is a UQ computational "pipeline" that is self-adapting and self-guiding. It incorporates all data—assumptions, inputs, known errors, ... and approximations inherent in the physics and mathematics of the model itself.' (from [1])

- Key technical areas
  - (Curse of Dimensionality) Research in non-intrusive techniques: dimension reduction, adaptive sample refinement, advanced response models, etc.
  - (UQ Pipeline) Workflow management with self-guiding, self-adaptation, data analysis and visualization
  - (Error Estimation) Discretization error estimation in multi-physics and multi-scale algorithms and codes

# Role of Nuclear Data in UQ studies:

- Nuclear data and covariances are needed as input to the 'UQ Pipeline'. Initial effort:
  - Covariance data now available in the ENDL library (before 2009, no covariance information in ENDL)!
  - 'Kiwi' was created as an interface for applying these covariances

- Some remaining obstacles:
  - Currently, data handling is inflexible and very inefficient when applied to UQ studies
  - Only handling simplest covariances right now

# Nuclear data uncertainties and Kiwi:

- Kiwi, an interface to nuclear data and covariances
  - Uses covariance info when varying cross sections
  - Enables processing new variations for Monte Carlo and deterministic codes
  - Result is a new library with varied data (a 'realization' of the nuclear data)

# Overview of Kiwi:

- From absolute covariance matrix M and a requested variation vector V (given in σ), produce the actual variation R:

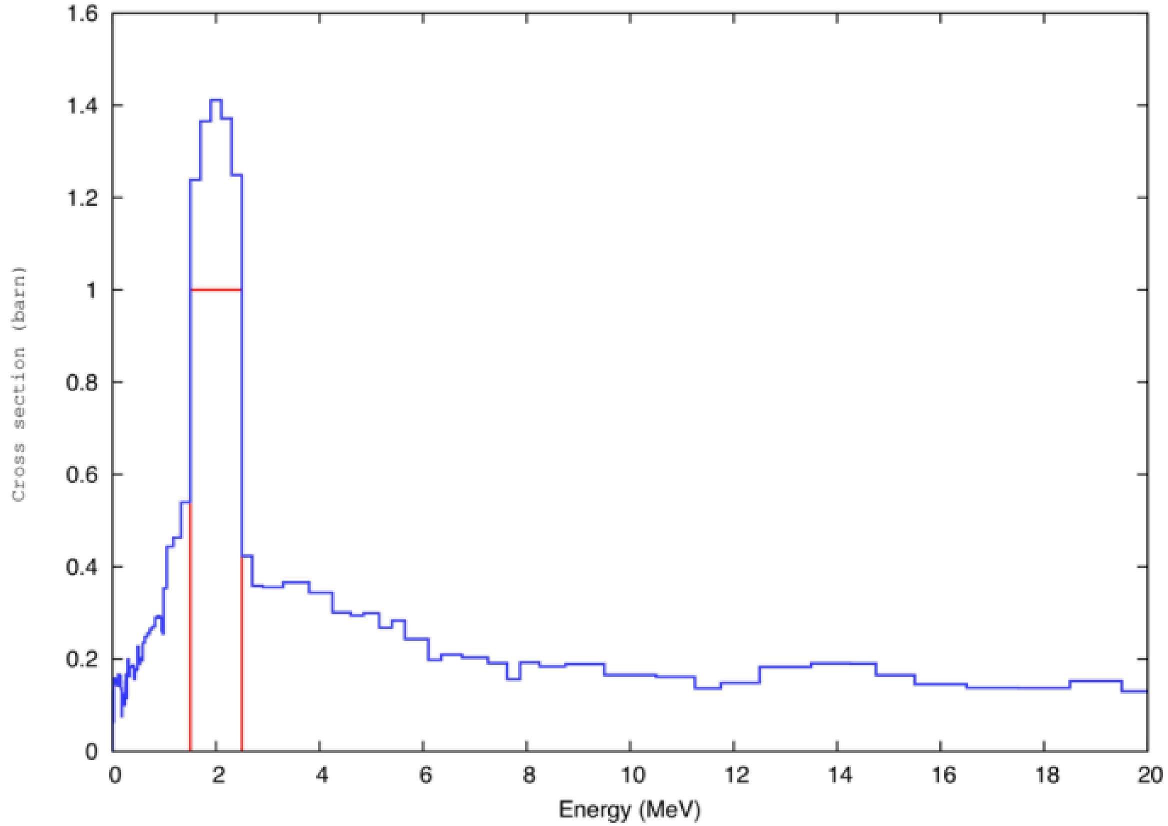
$$R_i = \sum_j \eta_j \Lambda_{j,i}$$

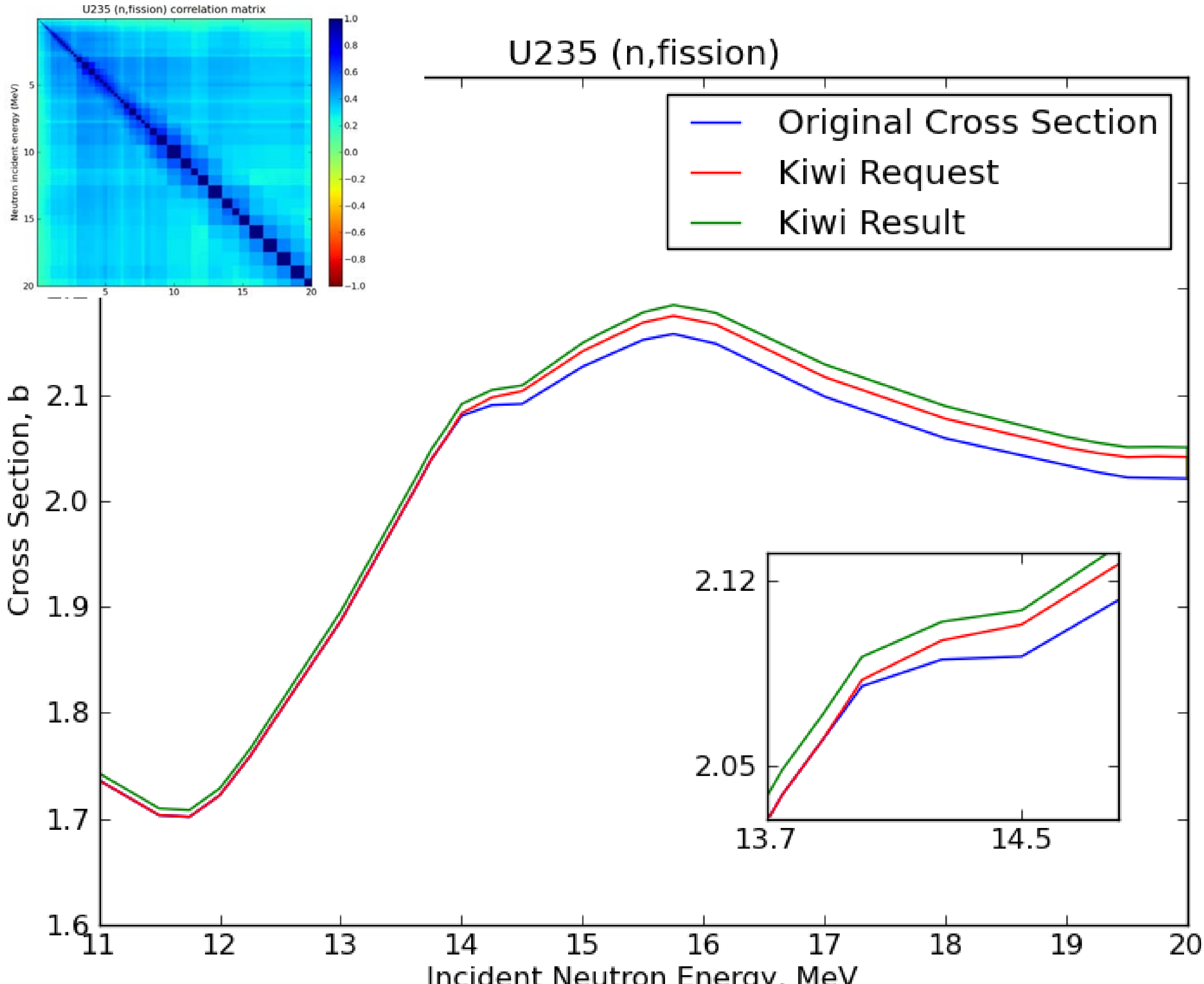
$$\eta_j = \sqrt{\lambda_j}(V \cdot \Lambda_j)$$

$\lambda$ and $\Lambda$ are eigenvalues and vectors of M

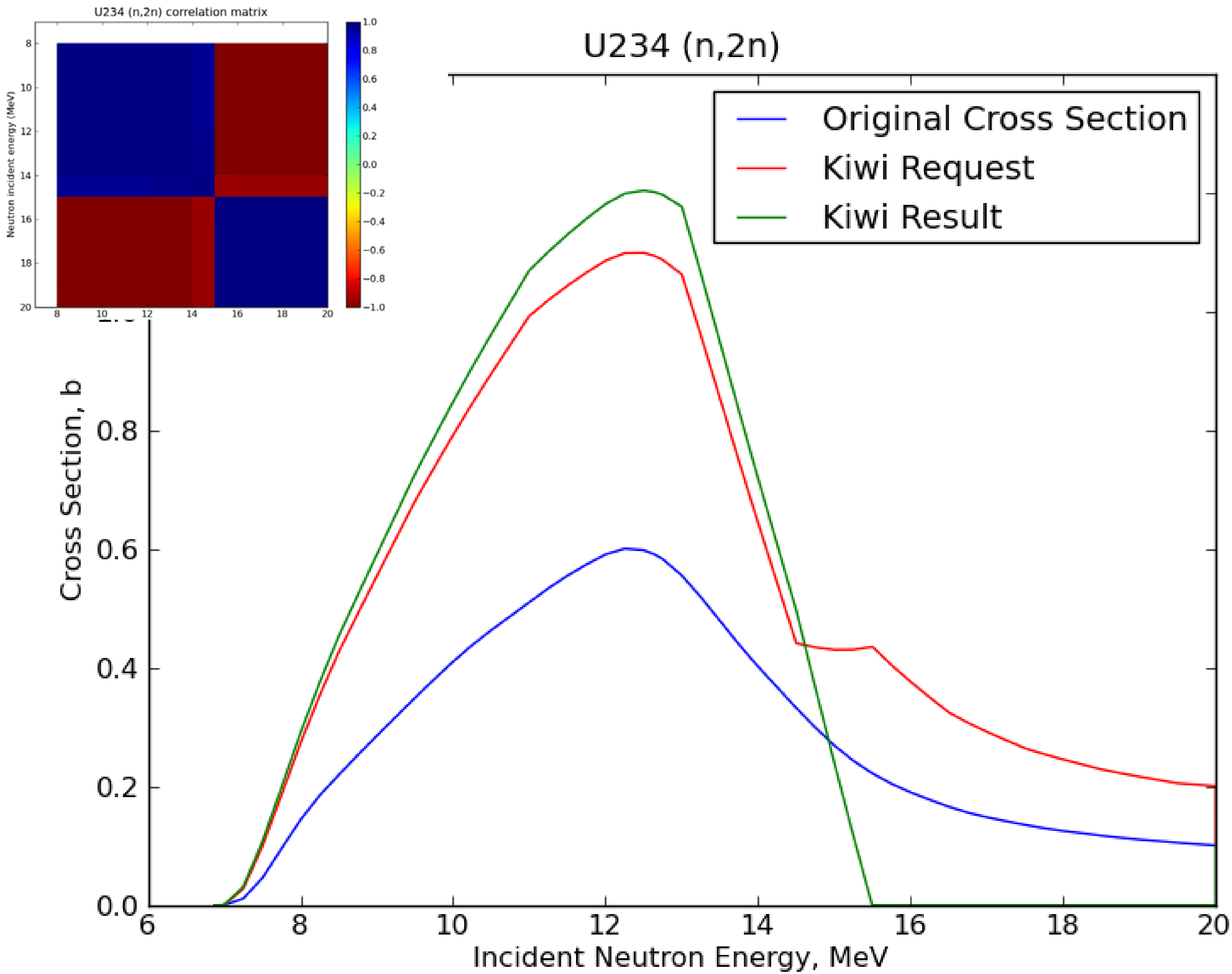
# Using Kiwi:

- User requests a variation (in barn or sigma)
- Kiwi gives back closest variation, respecting covariances





U235 (n,fission) correlation matrix
Neutron incident energy (MeV)
U235 (n,fission)
Original Cross Section
Kiwi Request
Kiwi Result
Cross Section, b
Incident Neutron Energy, MeV
2.12
2.05
13.7
14.5



U234 (n,2n) correlation matrix
Neutron incident energy (MeV)
U234 (n,2n)
Original Cross Section
Kiwi Request
Kiwi Result
Cross Section, b
Incident Neutron Energy, MeV

# Lesson from Kiwi:

- Kiwi is very sensitive to off-diagonal components of the matrix!
  - QA code ‘unCor’ doesn’t do enough to check off-diagonal parts. Perhaps a warning should be issued whenever strong anti-correlations are present in (cross section) covariance matrix?

# The GND hierarchy for nuclear data:

- The goal: make one unified structure for all forms of nuclear data: evaluated, MC, deterministic and experimental
- New data hierarchy must be easily human-readable, and representative of underlying physics
- Define a *structure*, xml is just one implementation

Latest version of GND now available to CSEWG on GForge and on the Green Data Oasis:
https://ndclx4.bnl.gov/gf/project/gnd

ftp gdo-nuclear.ucllnl.org

# Covariances in GND

- ENDF MF31,33,35 already complete
- xml allows more flexible formatting and more possibilities:
  - should we store model-parameter covariances and sensitivities?
  - Eigenvalues/eigenvectors?
  - Monte Carlo realizations?
- The big challenge for GND covariances: linking back to central values!

# <covarianceSuite>:

```
<?xml version="1.0" encoding="UTF-8"?>
<covarianceSuite projectile="n1" target="Pu239" version="gnd version 1.0”>
  <reactionSums>
    <reactionSum id="total" ENDF_MFMT="33,1">...</reactionSum></reactionSums>
  <section id=”... [total nubar]" nativeData="covarianceMatrix">
    <rowData .../>
    <covarianceMatrix>...</covarianceMatrix></section>
  <section id=”... [delayed nubar]" nativeData="covarianceMatrix">
    <rowData .../>
    <covarianceMatrix>...</covarianceMatrix></section>
  ...
</covarianceSuite>
```

- Covariances are stored in a separate file, and use links to associate them to the correct section.
- Each <section> corresponds to one chunk of the ‘full’ covariance matrix:

| | | |
|---|---|---|
| (n,elas) | elastic vs fission | |
| fission vs elastic | (n,f) | … |

# Current status in GND:

```
<section id="n1[multiplicity:'2'] + Mn54 + gamma" nativeData="covarianceMatrix">
  <rowData xlink:type="simple" xlink:href="/reactionSuite/reaction[@label='41']/crossSection" ENDF_MFMT="33,16"/>
  <covarianceMatrix>
    <axes>
      <axis index="0" label="row_energy_bounds" unit="eV" interpolation="linear,flat" length="5">
                  8971600 1.7901e7 2.8371e7 4.4965e7 6e7</axis>
      <axis index="1" label="column_energy_bounds" unit="eV" interpolation="linear,flat"
                  mirror_row_energy_bounds="true"/>
      <axis index="2" label="matrix_elements" unit=""/></axes>
    <matrix dimensions="4,4" type="relative" form="symmetric" precision="6">
      9.009000e-01
      0.000000e+00  2.980270e-02
      0.000000e+00  2.745890e-02  2.757980e-02
      0.000000e+00  2.554860e-02  2.535970e-02  1.231670e-02</matrix></covarianceMatrix></section>
```

- Also translated: ‘summed’ covariances (LB=0), diagonal matrices, rectangular matrices.
- Not currently handled: MF=32, LB=8 and 9, cross-material matrices

# Model parameter covariances

- Benefits: make physical source of correlations more clear. Easy to convert to ‘traditional’ form.
- Also store sensitivity matrix?

```
<modelParameterCovariance type="absolute" form="symmetric">
  <axis index="both" model="EMPIRE" version="3.0.1">
  <!– specify the model, then list parameters. Here using optical-model parameters -->
  <par>UOMPRS</par><par>UOMPRV</par><par>UOMPRW</par></axis>
    <matrix form="symmetric" dimensions=“3,3">
      <row index="0">4.97893459e-5</row>
      <row index="1">1.22425916e-5 7.40552233e-5</row>
      <row index="2">1.97935771e-6 9.30550398e-7 8.70708865e-7</row></matrix>
</modelParameterCovariance>

<!-- sensitivity matrix -->
<sensitivityMatrix type="relative" form="rectangular">
  <axis index="rows" model="EMPIRE" version="3.0.1">
    <par>UOMPRS</par><par>UOMPRV</par><par>UOMPRW</par></axis>
  <axis index="columns" quantity="cross section" units="eV">1.0e-5 ... 20e+7</axis>
  <matrix form="rectangular" dimensions=“3,60"> ... </matrix></sensitivityMatrix>
```

# Conclusions:

- Kiwi is a tool for applying nuclear data covariances in UQ studies
  - Beware of large anti-correlations!
  - Need to support more types of covariance data!

- GND now has initial support for covariances, but still needs to be simpler and more clear

# References

- [1] K. Walter, “Narrowing Uncertainties”, Sci. Tech. Review, August 2010 (https://str.llnl.gov/JulAug10/klein.html)