Problems in MF-34 Covariances

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Outline

- Limited Availability of mubar data (so far, ~100 isotopes)
  - Only (major) isotopes are O-16, U-235,238, Pu-239
  - Missing: H, D, Be, Li, B, C, N, Al, Fe56, Pu240, … etc.

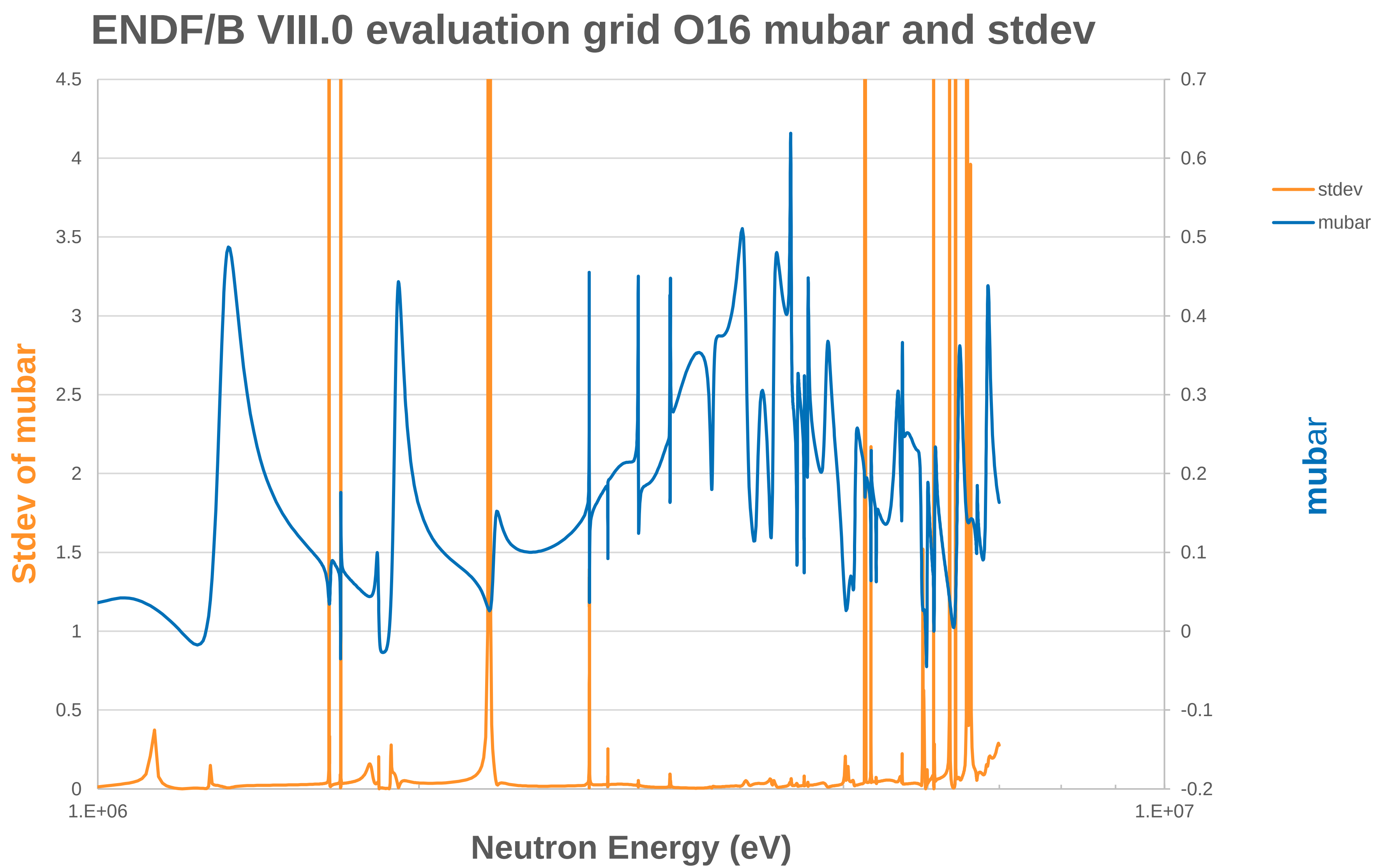
- Physical Limits on absolute mubar covariances < 1.0
  - Future Evaluations should honor this constraint

- Two (*ad hoc*) Proposed Methods for Limiting mubar uncertainty in random sampling
  - Transform to Uniform (Flat) Distribution
  - Transform to truncated Normal Distribution with smaller stdev

I. Mubar uncertainties from the evaluated ENDF/B data are sometimes too large (e.g., O16)

- Mubar = cosine of the lab elastic scattering angle (P1 only in NJOY)
  = bounded between -1 and 1
  where -1 is backward scattering
  0 is isotropic
  +1 is forward scattering
- The evaluated data is found in MF 4 MT 2 (angular elastic scattering) and MF 34 MT 2 (covariance of angular elastic scattering)
- Our idea is to limit the uncertainty to the physical bounds of mubar in the spirit of PUBS – physical uncertainty bounds

- Use the original O16 evaluation grid (1570x1570) to study this phenomenon, since multi-group collapsing can average out the narrow spikes < 1.0



(Note: the unphysical uncertainty spikes occur at resonance energies – not where mubar = 0.0)

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Some values of the O-16 relative covariance matrix copied from the evaluation (near 1.689320 MeV – the second orange peak on the previous graph)

Relative covariances (257:263,257:263) of (1:1570,1:1570)

7.0437	13.046	30.113	18700	-33.828	-16.44	-10.092
13.046	24.29	56.343	35158	-63.899	-31.2	-19.24
30.113	56.343	131.32	82323	-150.3	-73.716	-45.657
18700	35158	82323	5.184e+07	-95064	-46824	-29122
-33.828	-63.899	-150.3	-95064	175.07	86.583	54.065
-16.44	-31.2	-73.716	-46824	86.583	42.991	26.947
-10.092	-19.24	-45.657	-29122	54.065	26.947	16.953

Mubars (257:263,1) =

-0.01828	-0.0054817	0.011624	0.032618	0.056338	0.081021	0.10471

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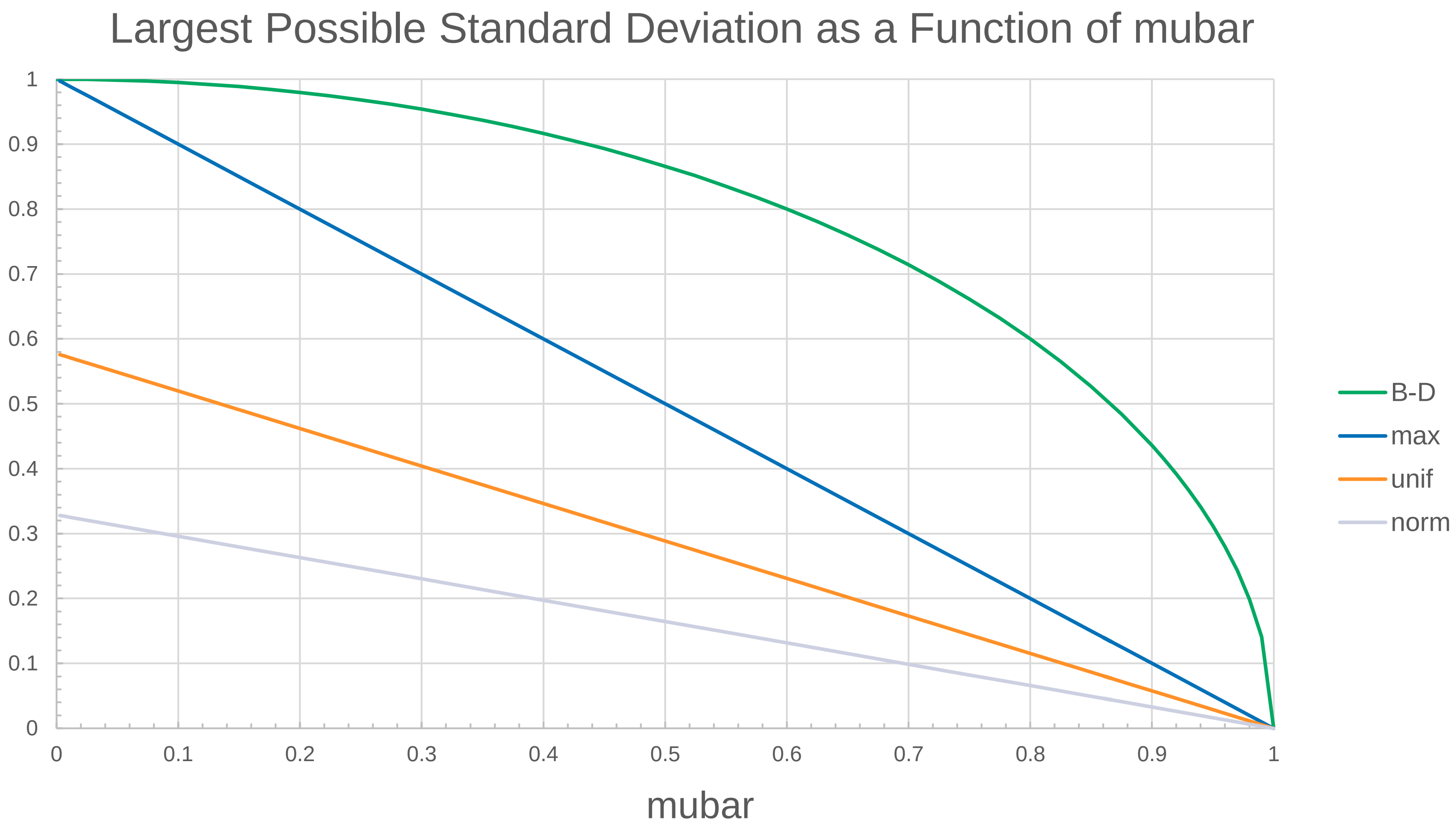
I. Maximum Uncertainty for a Bounded Function

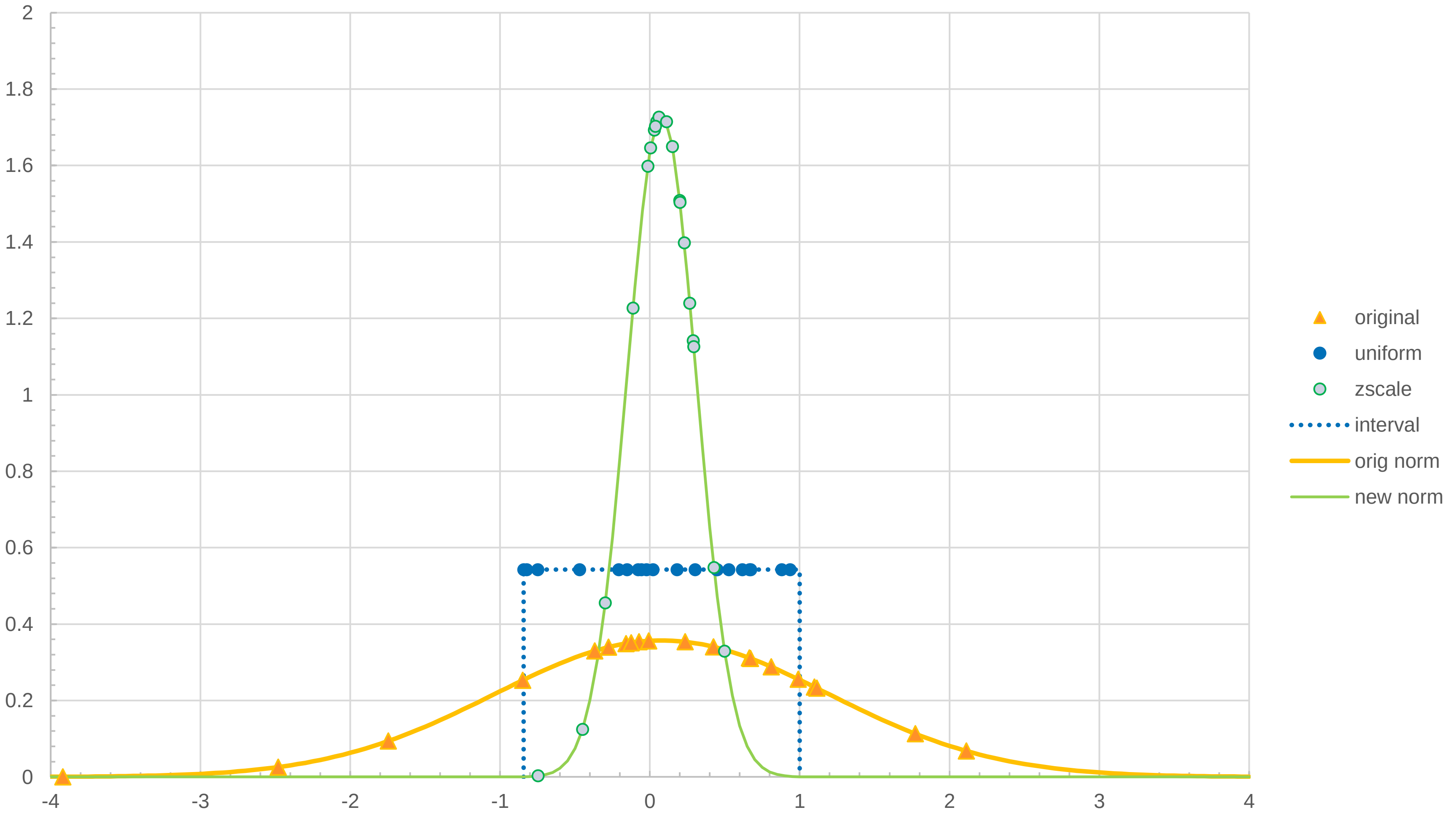
- Consider mubar: (cosine of the lab elastic scattering angle)
  - P_1/P_0 elastic scattering
  - Its possible values are bounded between -1 and +1
- So, What is the maximum possible uncertainty for mubar?
  - In general, it is 1.00 (either for the variance or for the stdev)
    - *Put ½ of the sampled points at -1.0, the other ½ at 1.0*
  - For a uniform (i.e., flat) distribution, it is even less:
    - Maximum variance = 1/3 = 0.3333333…
    - Maximum stdev = 1/sqrt(3) = 0.57735027…
  - For a truncated normal distribution, it is even less, depending on the truncation (*how many sigma's are included*)
  - For forward peaked scattering, it is even less …
    - Especially if the sampled points are symmetric about mubar
    - Bhatia-Davis inequality gives value for asymmetric distributions
- Out of 1570 values in O16, 15 diag. values have stdev > 1.0

I. Physical Limits on mubar Uncertainty (further constraints due to forward scattering)



III. The Transformation of Random Normal Points to Uniform (Flat) Points or to zscaled Normal Points

(*Note: the areas under the curves are ~= 1.00*)



III. Changing a Set of Random Normal Samples to Random Uniform Samples

- Use a CDF Function
  - The original correlated normal samples go from -∞ to +∞
  - The resultant uniform samples go from 0.0 to 1.0

- Scale the range (0 to 1) of the uniform samples to the desired range, e.g.,
  - -1.0 to 1.0 for mubar = 0.0
  - (-1.0 + 2*mubar) to 1.0 for positive mubars
  - -1.0 to (2*mubar + 1.0) for negative mubars
  - Height of the uniform curve determined by the area under the curve = 1 normalization

- How about the **linear** correlations that were built into the correlated random normal samples?
  - Surprisingly, they are (almost) preserved -- because the rank ordering of points is preserved
    - **Rank** correlation **is** preserved
    - **Linear** correlation is (**almost**) preserved
  - This near preservation of linear correlation is the basis of copula methods of random sampling
  - Related to the NORTA method of sampling (NORmal To Anything)
  - See lesson 7 of my tutorial guide about random sampling
  - Iterative improvement of the final linear correlations is often possible

III. Another Method of Transforming Normal Random samples that have Unphysically Large Uncertainties

- Use a "**ZSCALE**"-like transformation and force a normal distribution of random samples to be contained in a subset of the -1.0 to 1.0 interval
- Only changes the variance and the standard deviation – to pretty small values
  - (1.0 – mubar) / (either 3 sigma or 4 sigma …)
- Several sigma's must be included on either side of mubar within the interval
- Preserves mubar, rank correlation, and also linear correlation

- Of course, a normal distribution is infinite in extent, but it is very rare to have random samples beyond 3 or 4 sigma's away from the mean. Therefore, for this ad hoc fix, we will force all the random sampled points inside the interval.

III 2 Methods of Enforcing Limits on the MF 34 Uncertainty (when the mubar uncertainties are too large)

Uniform (Flat) Distribution Samples

- "Symmetric" about mubar
- Preserves value of mubar
- Allows **larger** mubars
  - Absolute Stdev < 1/sqrt(3)
- Preserves rank correlation
- Approximately preserves linear correlation
  - *Iterative improvement of linear correlation is often possible*

- Involves "CDF" functions to transform from normal samples (-∞ to +∞) to uniform (0 to +1)

Truncated Normal Distribution Samples

- "Symmetric" about mubar
- Preserves value of mubar
- Mubars limited to **smaller** values
  - Absolute Stdev < 1/3 or 1/4
- Preserves rank correlation
- Preserves linear correlation

- Involves "ZSCORE" functions to squeeze 3 or 4 standard deviations into a sub-interval of -1 to 1

Summary

- More MF 34 data is needed
- Some MF 34 mubar covariances in ENDF/B VIII.0 are **too large**

- Mubar uncertainties (absolute) are physically limited to be < 1.0
  - Hopefully, future nuclear data evaluations will honor this constraint

- Proposed 2 reasonable (albeit, ***ad hoc***) workarounds to limit the mubar uncertainties in correlated random sample generation.
  - Mubar and Rank Correlation are preserved and Linear Correlation is approximately preserved by the **uniform** (flat) method.
  - For smaller values of mubar, the zscale-like approach (**truncated normal distribution**) also preserves Linear Correlation.

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Sandwich Rule Environment versus Direct Propagation of Uncertainties Environment

Sandwich Rule

- Needs sensitivity vectors and covariance matrices – usually in relative form
- If a constraint is needed, it may be applied **either** to the sensitivity vectors **or** to the covariance matrix **or** to both ("*idempotence*")
- Matrix multiplication produces the output variance. (*The only possible indication of a failure would be a negative variance*.)
- WARNING: matrix multiplication works just fine even with an invalid covariance matrix …

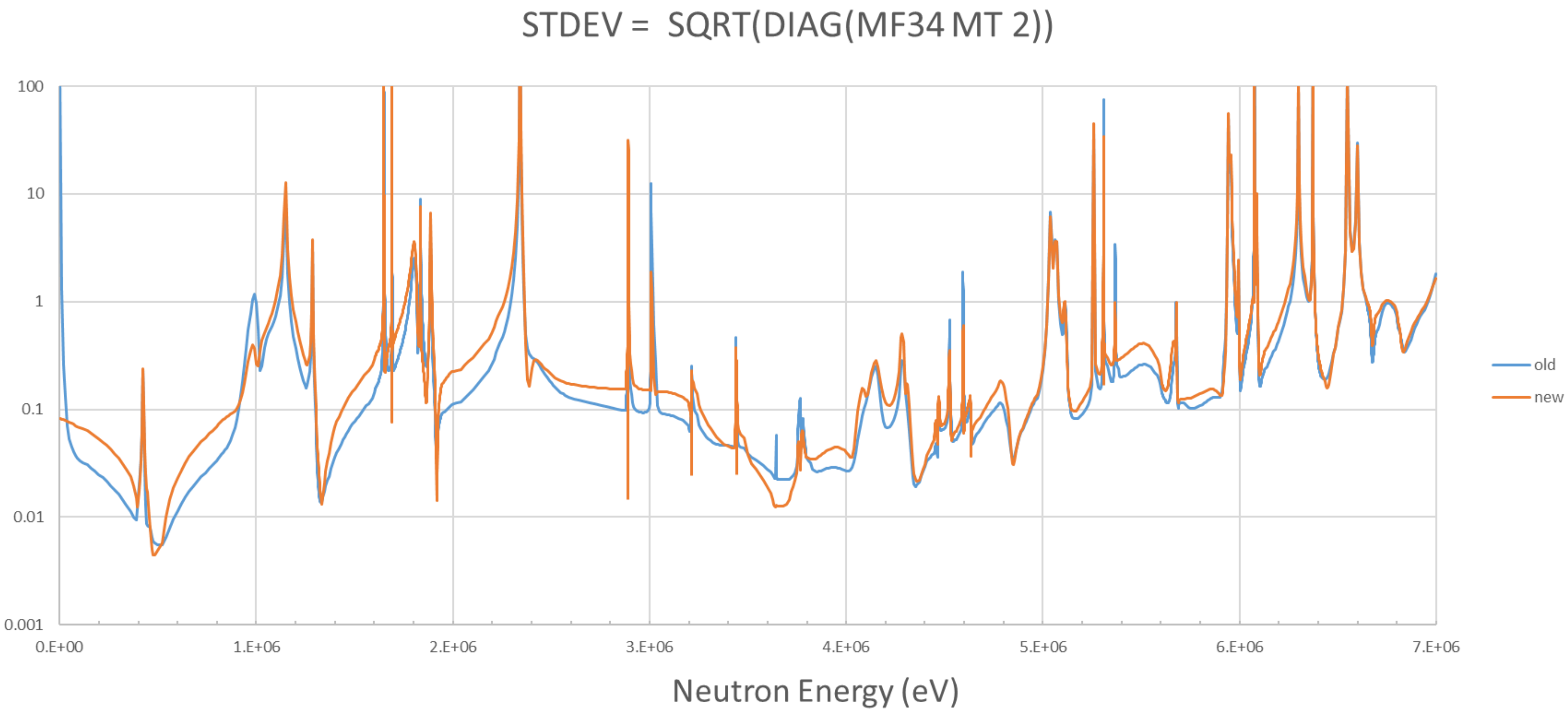
Direct Calculation

- Needs covariance matrices and a "**black box**" code to run repeatedly
- If a constraint is needed, it **must be** applied to the covariance matrix
- Generation of correlated random samples requires (1) no negative eigenvalues and, (*if needed*) (2) constraints in the covariance matrices, and (3) mubar in MF34 MT 2 uncertainties < 1.0.
- Default is multi-variate normal.
- Variance is calculated from selected output quantities from hundreds of "**black box**" code runs

O16 Evaluation file (actual lines)
Notice 825 = o16, mf 34, mt 2

```
1.546682-2  1.609755-2 1.629501-2 1.608465-2 1.548573-2 1.451742-2 82534  2
1.319105-2  1.146638-2 9.143836-3 5.724070-3 5.060936-4-6.600409-3 82534  2
5.184046+7 -9.506366+4-4.682355+4-2.912213+4-1.929689+4-1.289708+4 82534  2
-8.438860+3-5.248424+3-2.944136+3-1.277462+3-7.462962+1 7.895001+2 82534  2
1.405939+3  1.841044+3 2.143233+3 1.946231+3 4.511904+2 2.284212+2 82534  2
```

I. Mubar Uncertainties in LANL O16 data (Evaluation Grid of 1570 intervals)



II. Using mubar as produced by NJOY
(*in the context of the sandwich rule*)

- The NJOY module ERRORR produces mubar for each incoming group (all outgoing groups are lumped together) So, for a 30g transport calculation, NJOY gives 30 values of mubar variance (30g by 1) and a 30x30 covariance matrix
- However, sensitivity codes like SENSMG and MCNP “ksen” and Sn codes like Partisn generate or use each outgoing group value separately (the P_ℓ elastic scattering matrices are 30g by 30g)
- For the “sandwich rule”: use a sum of the relative sensitivity coefficients from the outgoing terms of the groupwise elastic P_1 sensitivity with the relative covariance matrix (30g by 30g) produced by NJOY and ERRORR (*thanks to Jeff Favorite for this as yet unpublished result*)
- For Jezebel, this produced a mubar uncertainty of 156 pcm – very comparable with other CIELO uncertainties due to fission, capture, PFNS, etc.

II. Allocating P_1 Elastic Scattering from mubar

- As given by NJOY, mubar uncertainty is (groups by 1) – singly differential
- But, the elastic P_1 cross sections are (groups by groups) – doubly differential

- Change all P_1 outscatter cross sections uniformly by mubar ratio for the current inscatter group
  - Allows P_1 sensitivity coefficients to be simply summed over outgoing groups
  - *Not yet published by Jeff Favorite*
  - *(Verified by comparison with central differencing estimation of sensitivities)*

- Change all P_1 outscatter cross sections by proportion of P_0 outscatter cross sections
  - Requires a more complicated weighted sum of P_1 sensitivity coefficients
  - *Not yet published by Jeff Favorite*
  - *(Verified by comparison with central differencing estimation of sensitivities)*

- Other schemes are possible …

III. Basic Properties of Normal and Uniform Distributions (Assume symmetric in range about mu = 0.0)

NORMAL (Standardized)

- Infinite in range
- Normalized to 1.0 under the curve
- Mean is the midpoint
- Variance is the square of the standard deviation
- Skew is 0.0

UNIFORM (Standardized)

- Finite in range
- Normalized to 1.0 under the curve
- Mean is the midpoint
- Variance is determined by extent of range

  (RHS-LHS)**2 / 12
- Skew is 0.0

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III. Comparisons of Standardized Curves

moment	*zeroth*	*first*	*second*	*third*	*fourth*
	area under the curve	mean	variance	skew	kurtosis
normal	1	0	1	0	3
uniform	1	0	1	0	-1.2

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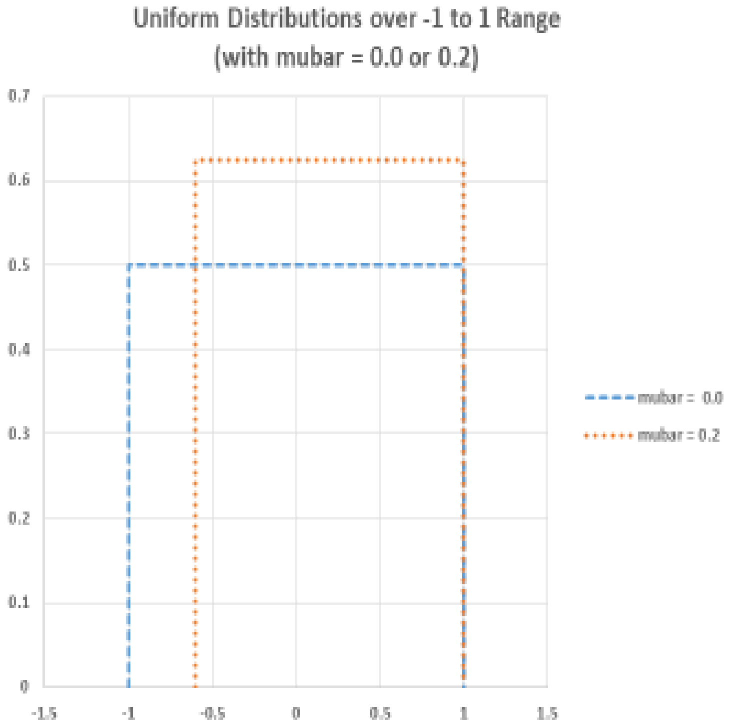
For a function defined between -1 and 1 (Assume symmetry about mubar)



area	1	1
mubar	0	0.2
stdev	0.57735	0.46188
var	0.333333	0.213333
skew	0	0

By changing the normal distribution to a uniform distribution:

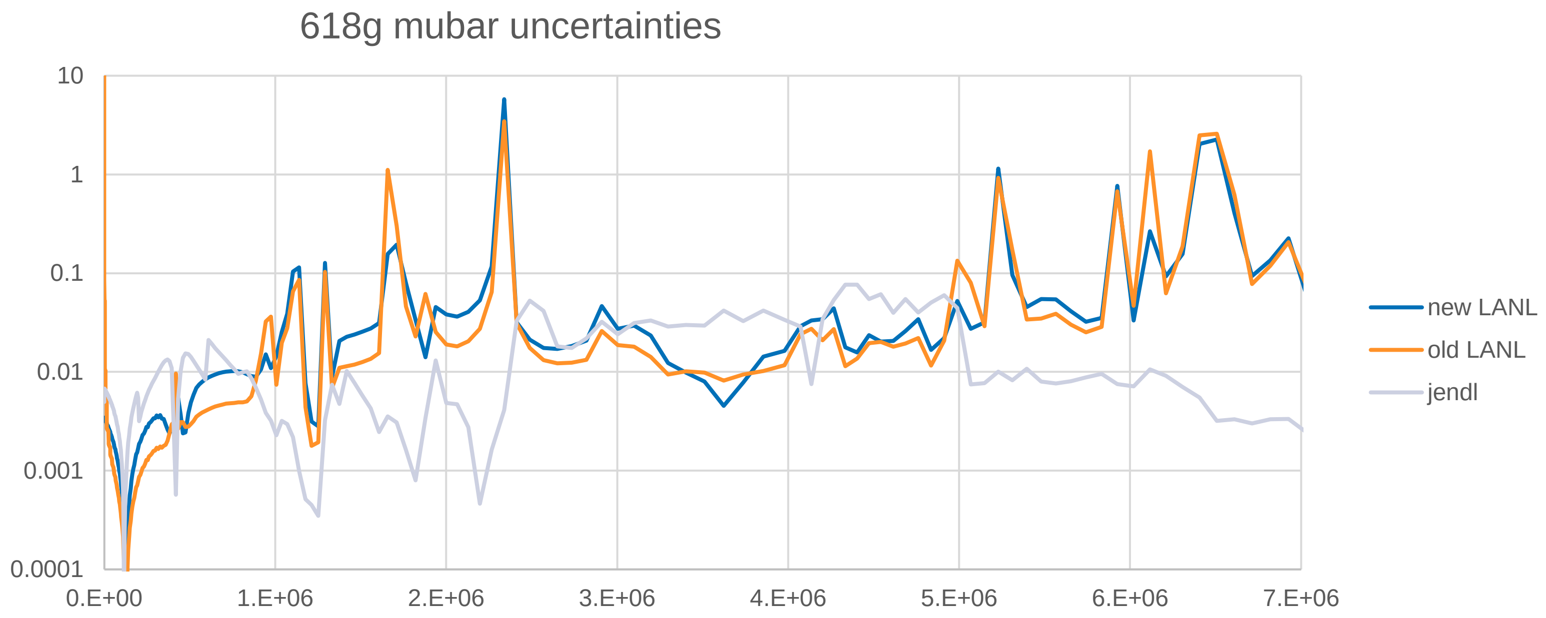
We can enforce a hard limit of 1/sqrt(3) for the standard deviation

(Cf the P_1 scattering in the old multigroup version of KENO.)

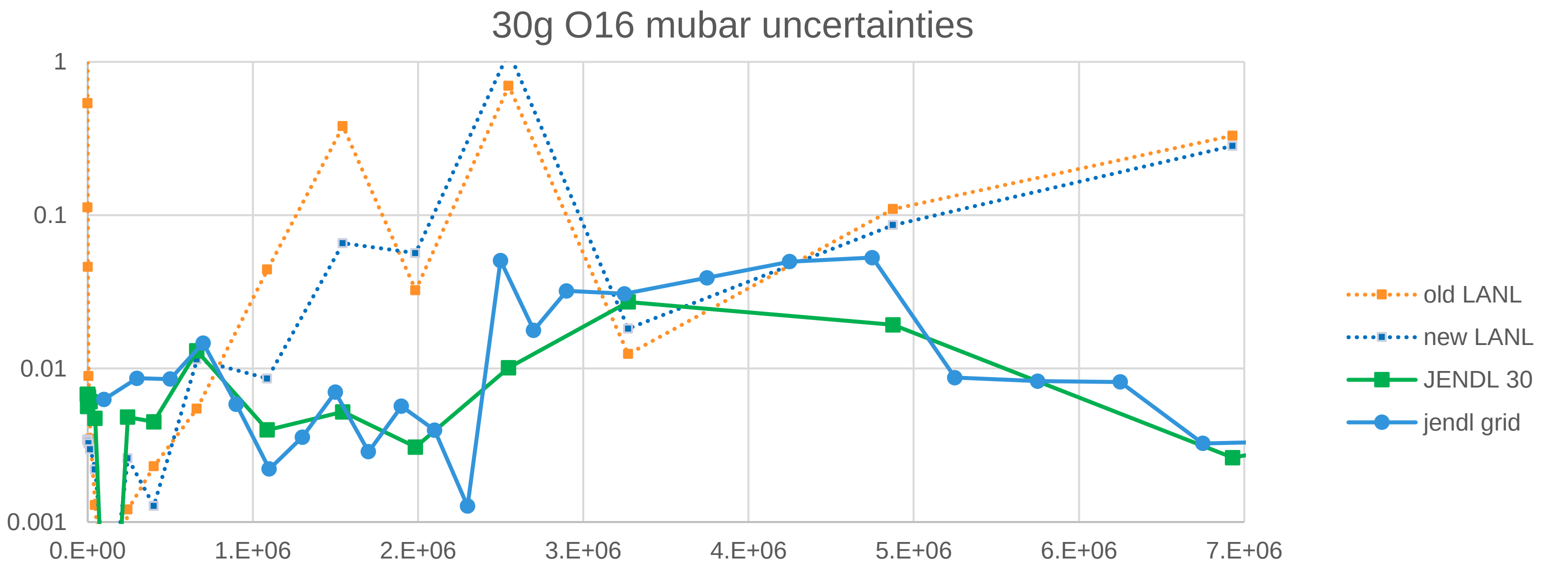
III. Proposed Procedure

- Generate multi-variate normal replica cross sections from covariance matrix produced by NJOY
  - Preserve individual means and standard deviations
  - Preserve original covariance terms (*including the ones that are too big*)
  - Each Group's mubar replicas have Gaussian shapes
- For group mubars (and only for such groups) where the standard deviation is unphysically large
  - Transform Gaussian shape to Uniform distribution (with a CDF function)
  - Preserve the means (by choosing a sub-interval within -1 to 1)
  - Enforces physical limits on the standard deviation (< 1.0/sqrt(3))
  - This procedure (approximately) preserves the **linear** covariances
- Generate 100's, 1000's, or more input NDI tables for Partisn with replica data and run the cases – to accumulate statistics on the outputs like k_{eff}
- Tricky bookkeeping for Sn, since the elastic cross sections are buried inside of the combined Legendre scattering transfer matrix (elastic, inelastic, n2n, n3n, …)

In 618 groups, LANL and JENDL uncertainty data (note: JENDL is lower in the 1-2 MeV range)



In 30 groups, LANL and JENDL data



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