The emperor has no clothes: the truth about nuclear data for fission modeling

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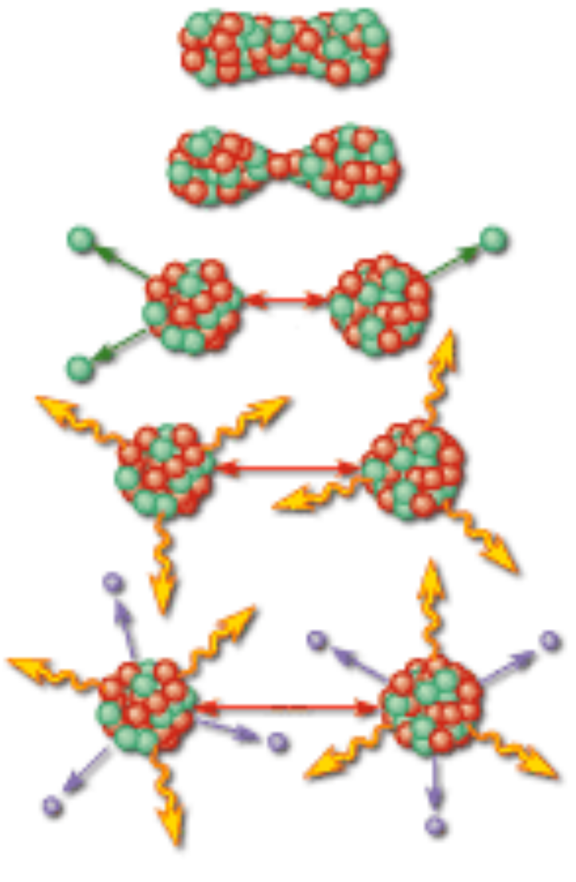
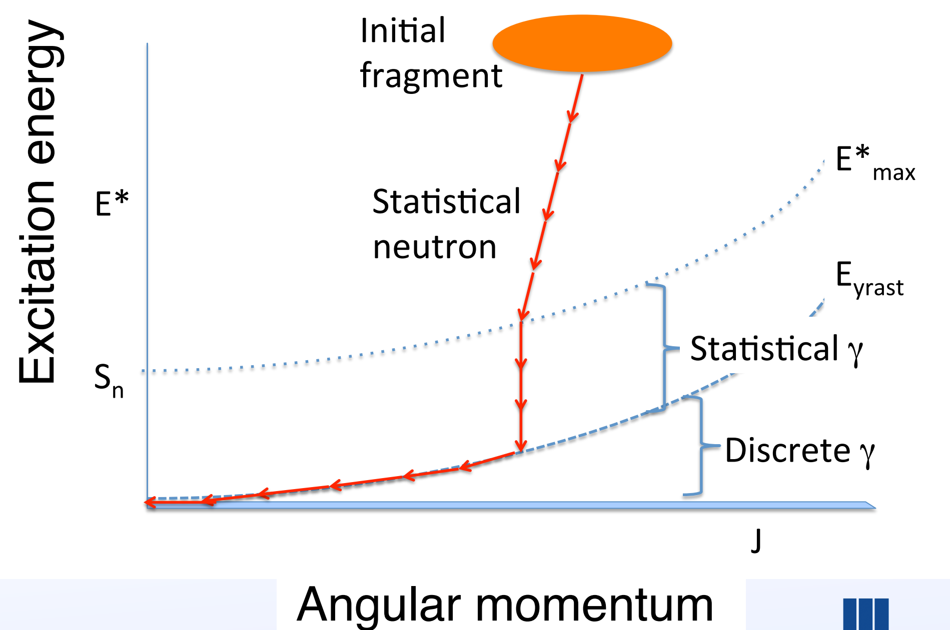
Modeling fission requires lots of data

- Left: Encyclopedia Brittanica's schematic rendition of fission
- Right: Schematic view of fragment de-excitation and decay
- Looks simple, right? Requires an amazing amount of nuclear data: some of it easy – masses; some not – everything else





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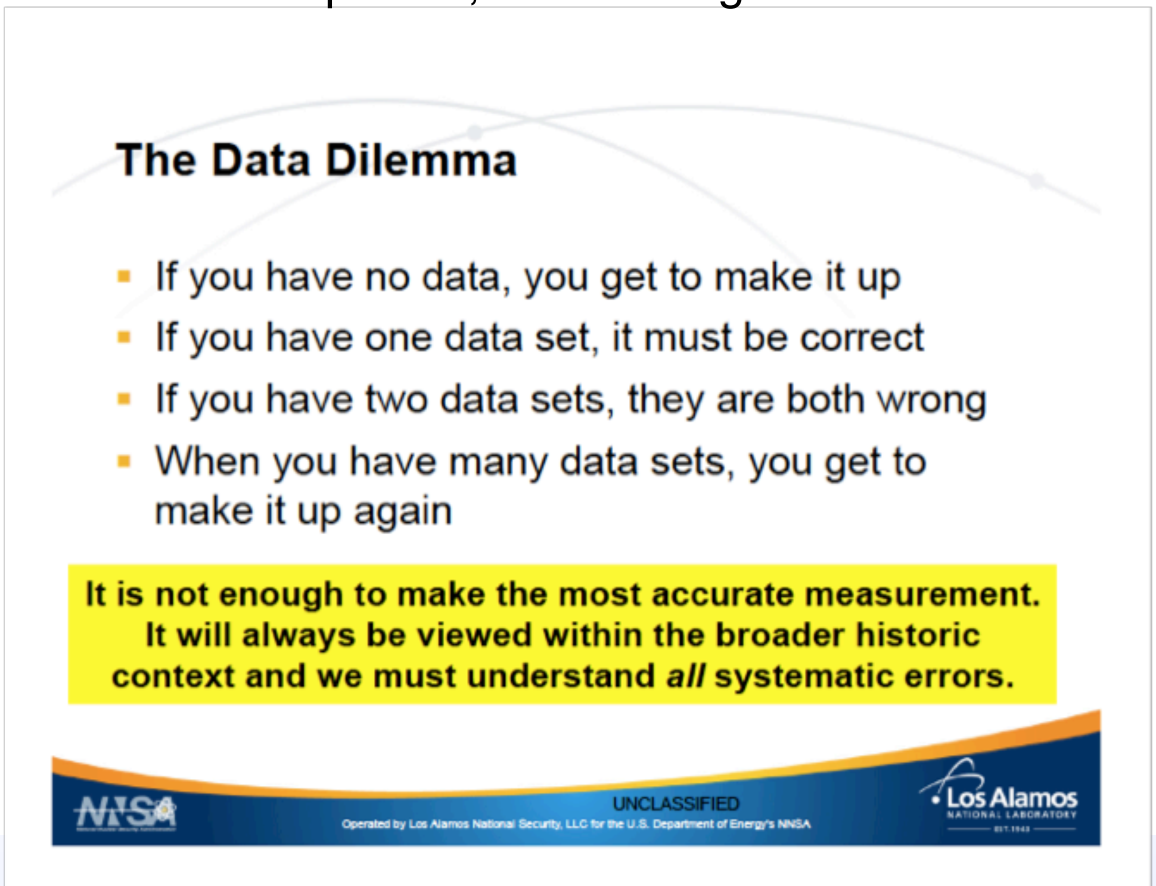
The applications/data types discussed in this talk are two-fold

- Energy dependent Q values in the data: how I learned what's swept under the rug
- Fission models:
  - Differences between deterministic and stochastic
  - Data requirements for better fission modeling

The Data Dilemma Indeed

Slide from a talk by Morgan White

As someone who’s ‘made up’ data, I can but agree with all his statements

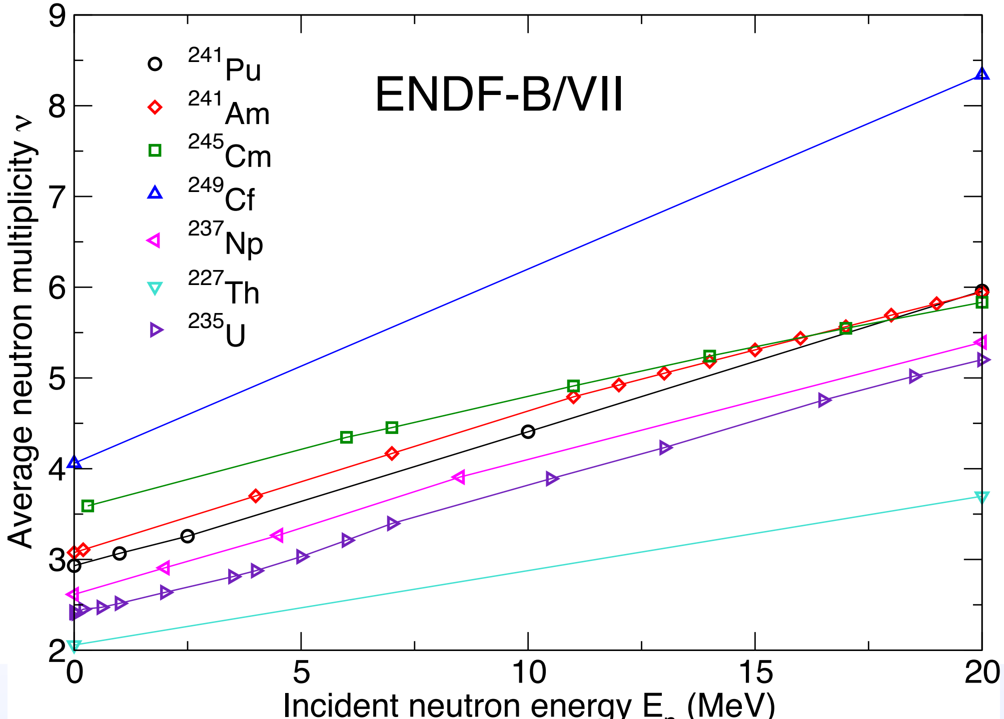


“If you have no data, you get to make it up”

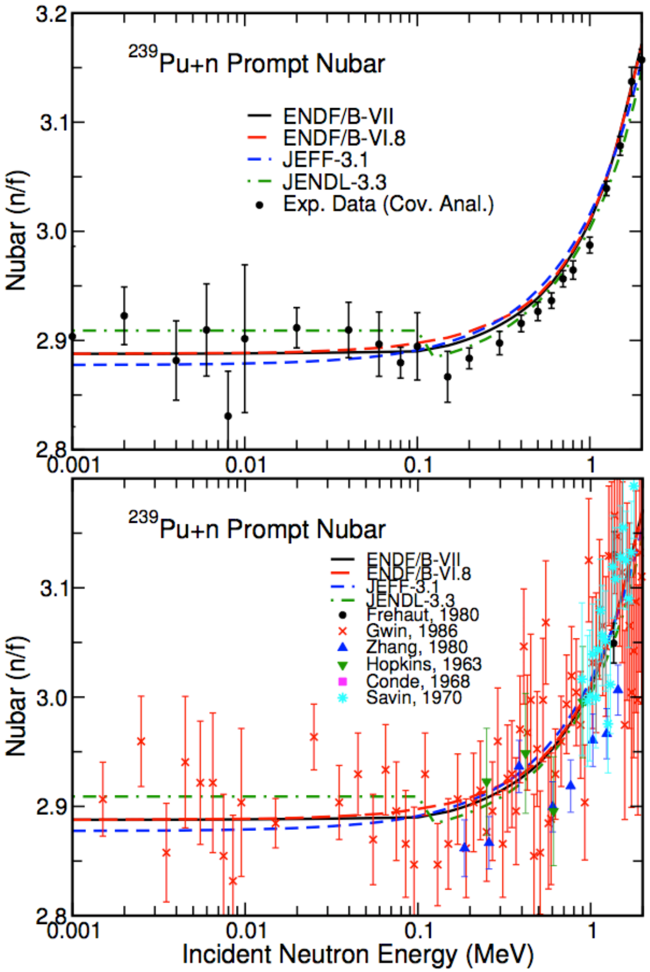
Evaluations of average neutron multiplicity as a function of incident neutron energy

‘Evaluations’ involve compiling data and deciding which are ‘better’; there is also some tweaking going on because the evaluations have to match certain criteria in applications

In some cases where there isn’t ANY data, the evaluations are mainly educated guesses based on models – check out ^{249}Cf and ^{227}Th: with two points, it’s easy to fit a straight line



Evaluations: “When you have many data sets, you get to make it up again”



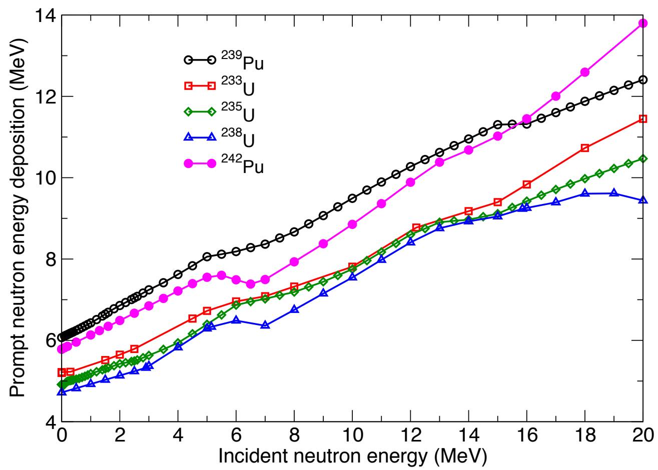
- One of the best known, most measured fission related quantities, the average neutron multiplicity as a function of incident neutron energy – all you need to do is count neutrons
- Bottom plot shows data used to generate the covariance analysis in the upper plot (black points)
- The curves are different evaluations of the black points but are tuned to fit Jezebel k_{eff}
- Almost all curves are above centroids of the evaluated data
- Like that cool change of slope in JENDL-3.3? Whatever it takes to make Jezebel work

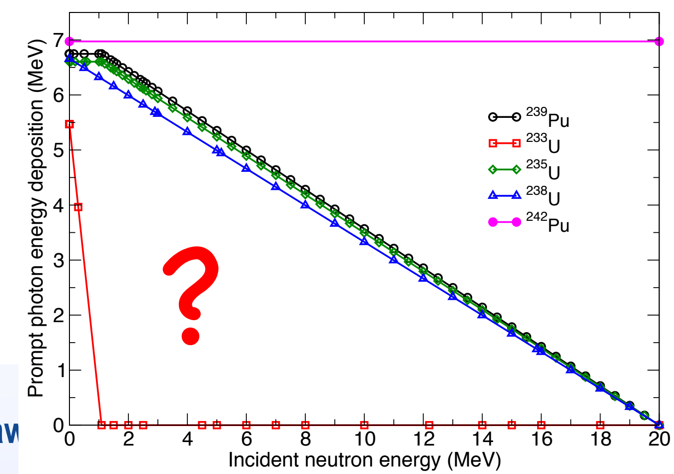
"If you don't like the data, go out and make some of your own" – paraphrase from KFOG

- Early in my career at LLNL, I was asked to look at energy-dependent Q values for fission (MT = 458 in ENDF/B-VII.1 is now built from my systematics)
- I discovered that there is generally 1 value of Q in the data files, independent of energy and whether fission is 1st chance, 2nd chance …
- To build a better Q value is not hard if you are willing to make some bold assumptions and extrapolations, in other words, make some stuff up
- The fission Q, or in other words, the energy release, includes 'easy' stuff like energy deposition by prompt neutrons and photons as well as delayed neutrons and photons
- It also includes the total kinetic energy of fragments, TKE, and delayed emission of electrons (neutrinos are there too in β decay but don't deposit any energy):
  - $ER(E_n) = TKE(E_n) + E_n^p(E_n) + E_\gamma^p(E_n) + E_n^d(E_n) + E_\gamma^d(E_n) + E_\beta(E_n)$
- Seriously, how much of this do you think has been measured for ANY actinide for ALL energies?
- Answer: Almost none of it!
- There is some data on average neutron multiplicity (mostly for the big 3 and a few others) that the neutron energy deposition is based on, some delayed neutron info and TKE measurements vs energy and some systematics on photons, but most of the rest that I had to go on were extrapolations based on models based on systematics, many generated by TALYS
- Is this important? Absolutely! Delayed energy deposition from fission contributes to heat in reactors so you want to know this for modeling your reactor

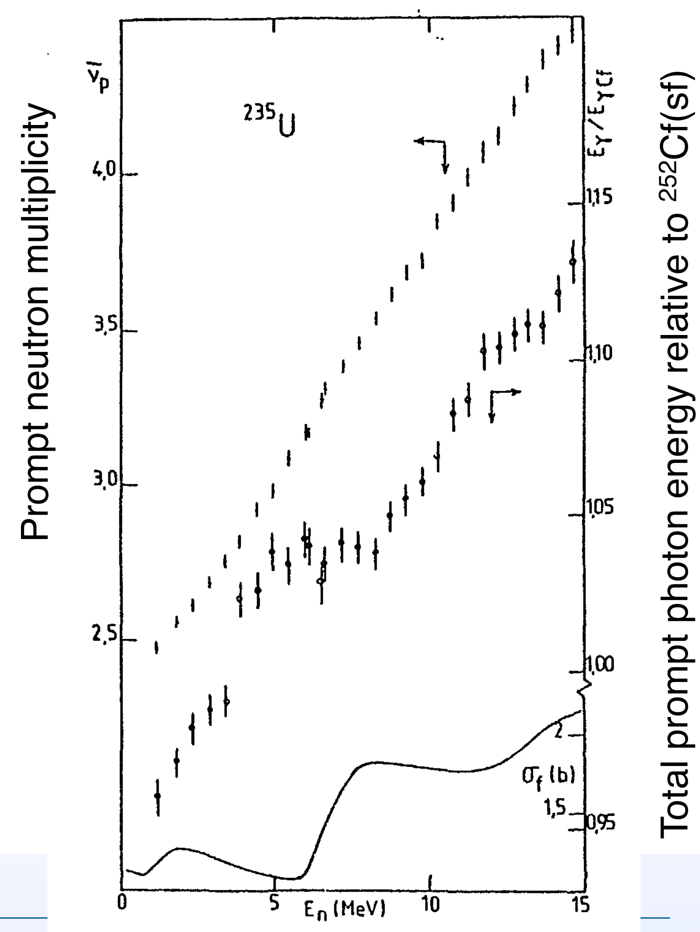
Ask yourself: Does the photon energy deposition make sense?

ENDF/B-VII.1 says that neutron energy deposition goes up with incident energy while prompt photon deposition is flat (for most) or goes down?!
Some things sacrificed to make other things work





Data from Frehaut (IAEA, 1989) shows that neutron multiplicity AND total photon energy relative to ^{252}Cf(sf) increases with incident neutron energy – makes sense



One data set, must be correct; two, they are both wrong

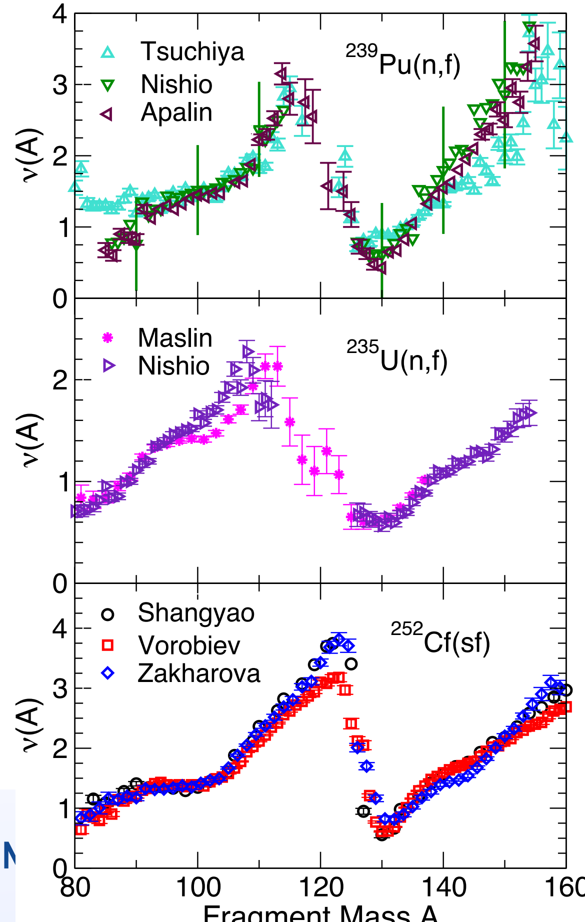
Both $\nu(A)$ and $E_\gamma(A)$ show a sawtooth shape but the slopes of the 'teeth' are not necessarily the same: E_γ for ^{252}Cf(sf) seems to be flatter while N_γ seems to have a stronger A dependence than E_γ for ^{235}U(n,f) while E_γ is more similar to $\nu(A)$, within large uncertainties

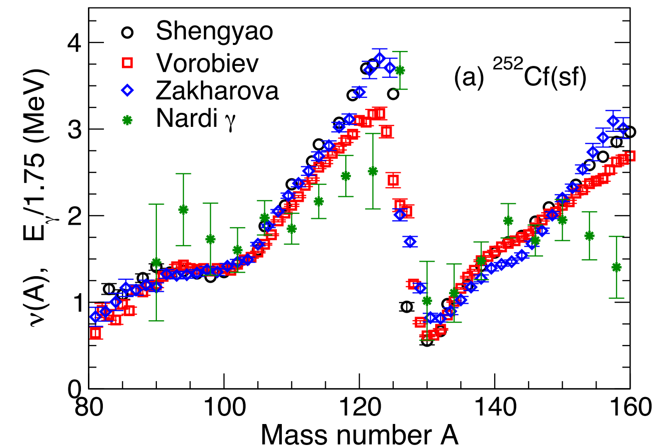
The idea that the photons should follow the neutrons vs. A is based on the mutual increase with E of the Frehaut data and built into some deterministic models

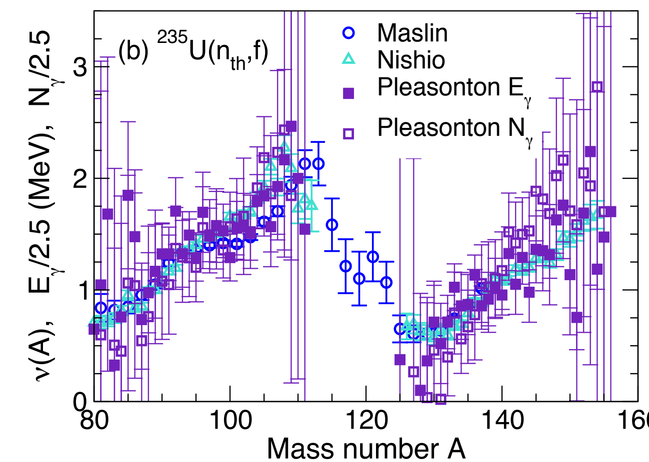
Sawtooth shape of $\nu(A)$ reflects shell structure: A = 132 is doubly-closed shell so hard to excite and thus few neutrons emitted in any case shown

Tooth is 'sharper' for larger A_0

Dependence of shape on neutron energy not well known but some data suggest $\nu(A)$ increases more for heavy fragments







Nature (and computers) abhor a vacuum

- Transport codes want to transport something so if you get an isotope that nothing's known about, you don't want your code to crash, i.e. fictitious data is better than no data at all (maybe…)
- Some examples of fictitious data:
  - Anything to do with multi-chance fission, it's all modeled and the neutron spectra from higher-chance fission is the same as that for the total, Q value is same for 1st, 2nd, 3rd chance fission
  - Prompt photon energy (you saw that), delayed photon energy is worse – in this case files are generally absent but that's OK, it would just be made up anyway
  - My MT = 458 files – I did the best I could but in many cases I made a 'best guess' model of fictitious data

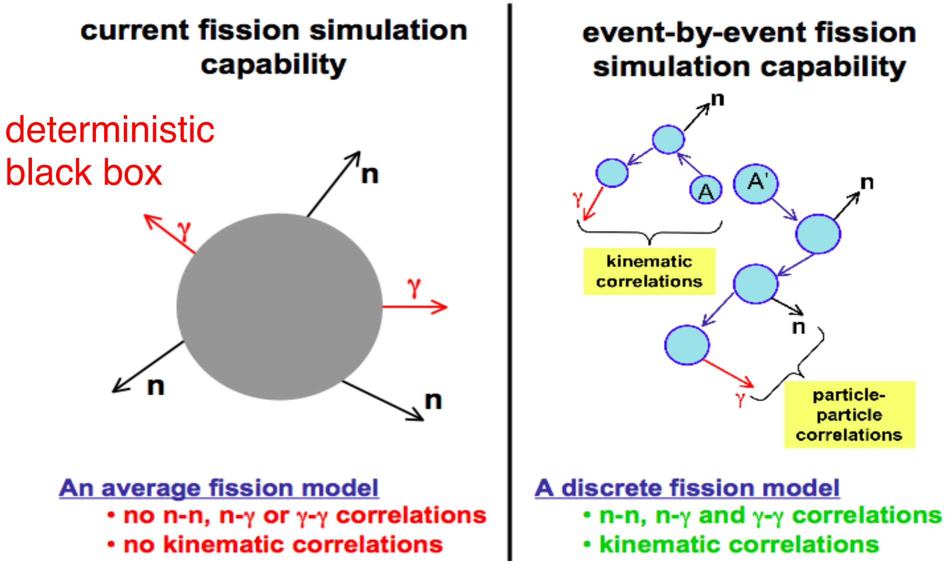
Beyond the average Q value: fission models

- Three things have been very important for application codes: the average neutron multiplicity, the prompt fission neutron spectrum (PFNS), and the fission cross section. Other observables are often ignored, energy and momentum are not conserved, and the same spectrum is sampled for all neutrons emitted in an event.
- Having come from high energy nuclear physics where single events with thousands of particles can be successfully simulated while conserving energy and momentum, finding this out was an unpleasant surprise
- The average multiplicity as a function of incident neutron energy is evaluated and tabulated in databases. For some isotopes it is very well known (claimed to be known better than 0.1%) and regarded as sacrosanct. For others, it's not known at all. (See previous slides.)
- The PFNS is also an evaluated quantity with evaluations based on the "Los Alamos" model (named for the authors from LANL). Measured uncertainties in certain energy regions can still be large so a great deal of experimental effort has been aimed at reducing these uncertainties. (Hint: measuring neutron energies accurately is REALLY hard)

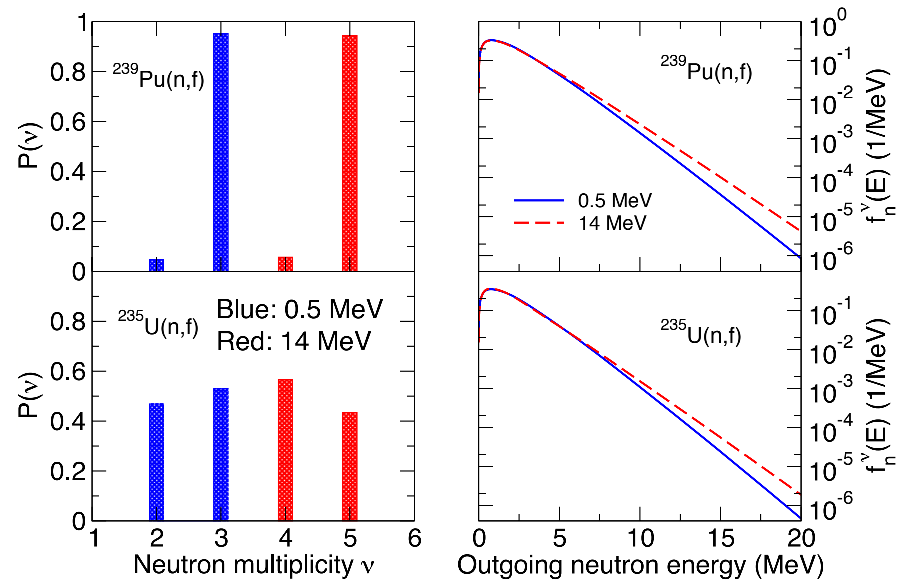
Los Alamos model (Madland & Nix, 1982)

- This deterministic approach, based on an 'average' fission event, has been the 'gold standard' in PFNS evaluations since it was first developed.
- It assumes that the light and heavy fragments are the 'average' ones, those that are the most probable. It also assumes an average value of the separation energy, S_n, based on the identities of the most probable fragments.
- They also make assumptions about the average fission Q value and the average total kinetic energy, TKE, to obtain the average total excitation energy. The average neutron multiplicity is then $\langle\nu\rangle = (\langle E^*\rangle - \langle E_\gamma\rangle)/(\langle S_n\rangle + \langle E\rangle)$ since the average energy emitted by photons is subtracted.
- The Weisskopf-Ewing spectral shape, $dN/dE \sim E \exp(-E/T_{max})$, is used with T_{max} the maximum temperature of the daughter nucleus, obtained for E = 0, giving an average neutron kinetic energy of $\langle E\rangle = 2T_{max}$
- The average neutron spectrum is obtained from this spectral shape folded with a triangular temperature distribution, $P(T) = 2T/(T_{max})^2$ for $T \leq T_{max}$; 0 for $T > T_{max}$; the average neutron spectrum is then $\int_0^{T_{\max}} \frac{dN}{dE} P(T) dT = \frac{2E}{T_{\max}^2} \int_0^{T_{\max}} \exp(-E/T) \frac{dT}{T}$ with an average energy of $\langle E\rangle = (4/3)T_{max}$
- Many variants of this model exist but all provide smooth PFNS for all incident energies

What part of ‘energy and momentum are conserved’ do you not understand?



Average fission model in frequently used simulation codes like **MCNP**:



- In ‘average’ models, fission is a black box, neutron and gamma energies sampled from same average distribution, regardless of multiplicity and energy carried away by each emitted particle; fluctuations and correlations cannot be addressed
- **Monte Carlo models** generate complete fission events: energy & momentum of neutrons, photons, and products in each individual fission event; correlations are automatically included

- Traditionally, neutron multiplicity sampled between nearest values to get correct average value
- All neutrons sampled from same spectral shape, independent of multiplicity

Building a better mousetrap: making a fission event generator

Event-by-event modeling is efficient framework for incorporating fluctuations and correlations

Goal(s): *Fast* generation of (large) samples of complete fission events

Complete fission event: Full kinematic information on all final particles

Two product nuclei: $Z_H, A_H, \boldsymbol{P}_H$ and $Z_L, A_L, \boldsymbol{P}_L$

ν neutrons: $\{ \boldsymbol{p}_n \}$, $n = 1,\ldots,\nu$

N_γ photons: $\{ \boldsymbol{p}_m \}$, $m = 1,\ldots,N_\gamma$

Advantage of having *samples* of complete events:

Straightforward to extract *any* observable,
including fluctuations and correlations,
and to take account of cuts & acceptances

Advantage of *fast* event generation:

Can be incorporated into transport codes

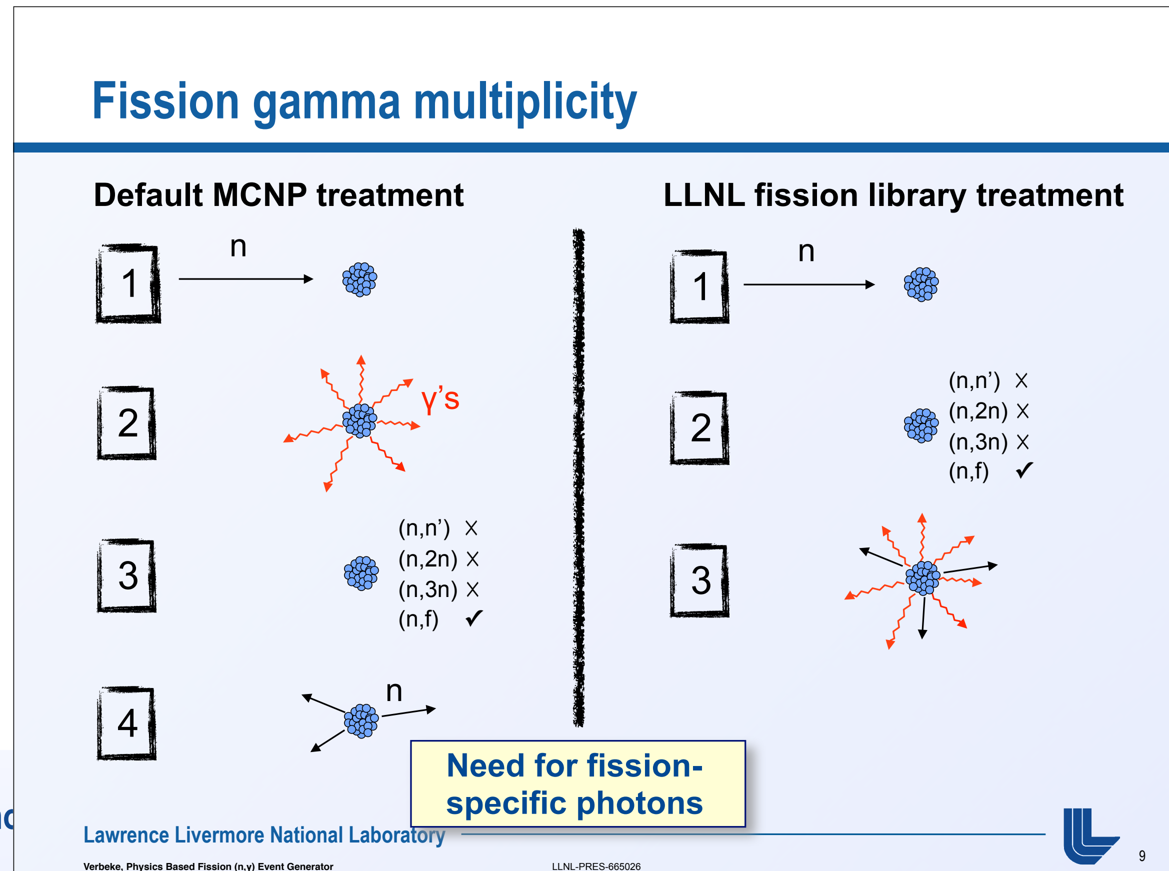
Available MC fission codes include CGMF (LANL), FIFRELIN (CEA), FREYA (LLNL & LBNL), GEF (KHS)

Just because you have a model doesn't mean that the physics is correct… sometimes the cart is in front of the horse

From a talk by Jerome Verbeke (LLNL)

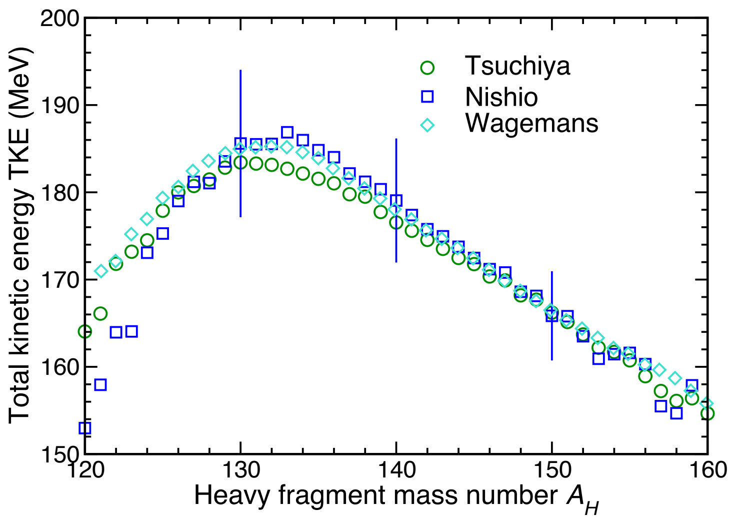
MCNP currently emits photons before it knows what reaction occurred

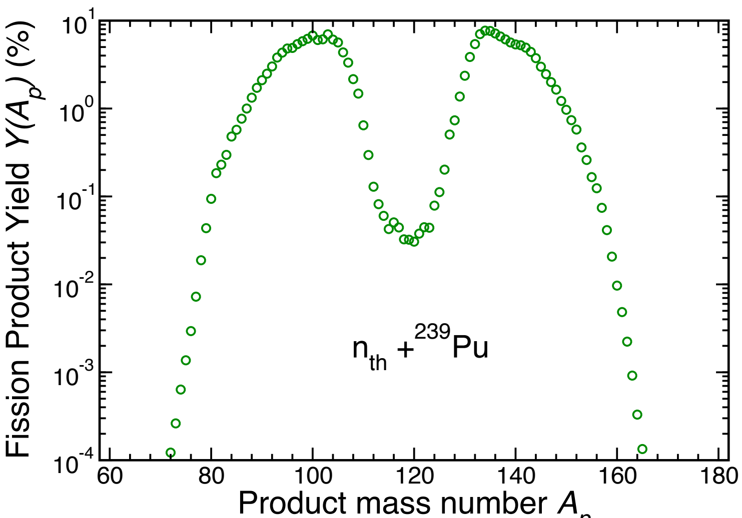
This behavior is incompatible with fission event generators, being worked on



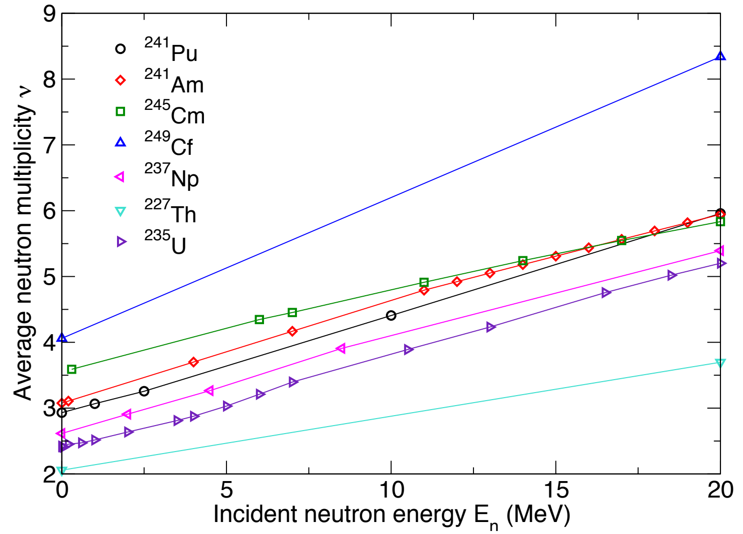
Monte Carlo fission models require inputs about fragment yields, kinetic energies, and neutron multiplicities

Input data: Y(A), TKE(A)

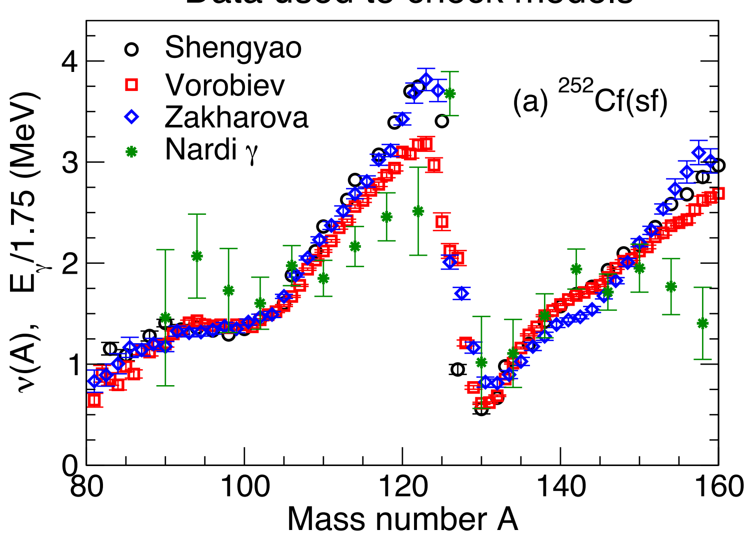




Data one fits to: neutron multiplicity



Data used to check models



Fission data are often insufficient for comprehensive (MC) modeling of fission process

- Fission experiments have most often focused on measuring only a single type of observable, *e.g*. the fragment mass and/or charge or the number and/or energy of prompt neutrons or prompt photons (fission TPC will measure cross sections, not fragment distributions; chi-Nu measures neutron spectra, not fragments; SPIDER measures fragments)
- Such inclusive data provides only limited guidance for fission modeling, in contrast to more exclusive data, *e.g*. prompt neutrons and/or prompt photons together with the fragment mass and/or charge
- Fission experiments largely focus on just a few cases for applications, such as ^{239}Pu, ^{235,238}U or ^{252}Cf(sf)
- Some (n,f) data, such as $Y(A_f)$, $TKE(A_H)$ and $\nu(A_f)$, have been measured only at low (or thermal only) incident energies, new experiments may improve range for $Y(A_f)$ and $TKE(A_H)$ but not simultaneously $\nu(A_f)$, $E_\gamma(A_f)$
- Limited range of isotopes, observables, and energies that have been measured means that models have be built on systematics
- My ideal would be the 'mother of all fission experiments' where the fragments, the prompt neutrons and the prompt photons are all measured in the same setup at the same time for a range of actinides and energies from thermal up to > 20 MeV
- Deterministic models used in many codes have similar drawbacks but require fewer data

FREYA (Fission Reaction Event Yield Algorithm) known and available

- FREYA developed in collaboration with J. Randrup (LBNL); neutron-transport code integration by J. Verbeke (LLNL)
- FREYA journal publications: Phys. Rev. C **80** (2009) 024601, 044611; **84** (2011) 044621; **85** (2012) 024608; **87** (2013) 044602; **89** (2014) 044601; **90** (2014) 064623; Comp. Phys. Comm. **191** (2015) 178
- User manual LLNL-TM-654899, code release LLNL-CODE-636753; in addition to MCNP release, **FREYA1.0** is also available in TRIPOLI4.9 and Geant4
- FIFRELIN and CGMF also published and documented although not as available at this point (FREYA and CGMF are in development for MCNP6 through NA22)

External parameters in FREYA which can be adjusted to data

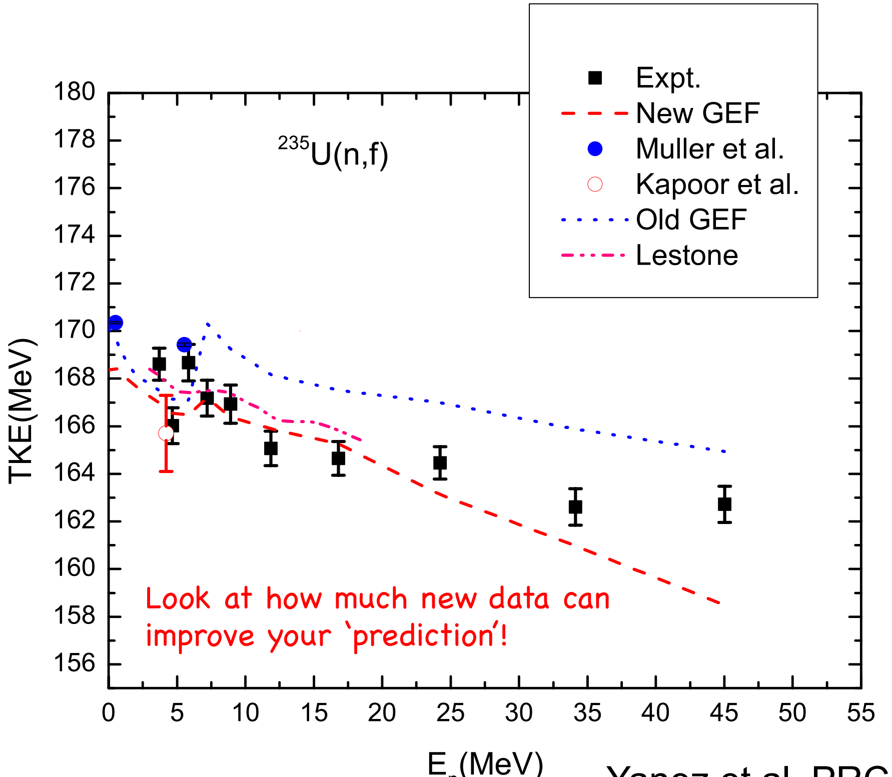
- In addition to isotope-specific inputs such as Y(A) and TKE(A_H), there are also intrinsic parameters such as nuclear masses (Audi and Wapstra for experimentally-measured masses, supplemented by masses calculated by Moller, Nix, Myers and Swiatecki), barrier heights, pairing energies and shell corrections
- There are also external parameters that can be adjusted, either universally or per isotope
  - Shift in total kinetic energy, dTKE, adjusted to give the evaluated average neutron multiplicity
  - Asymptotic level density parameter, e_0, $a_i \sim (A/e_0)[1+ (\delta W_i/U_i)(1 - \exp(-\gamma U_i))]$ where $U_i = E^*_i - \Delta_i$, $\gamma = 0.05$, and the pairing energy, Δ_i, and shell correction, δW_i, are tabulated (if $\delta W_i \sim 0$ or U_i is large so that $1 - \exp(-\gamma U_i) \sim 0$, $a_i \sim A/e_0$)
  - Excitation energy balance between light and heavy fragment, x
  - Width of thermal fluctuation, $\sigma^2(E_f^*) = 2c\underline{E_f}^*T$, c is adjustable (default = 1)
  - Multiplier of scission temperature, c_S, that determines level of nuclear spin
  - Energy where neutron emission ceases and photon emission takes over, $S_n + Q_{min}$
- Almost all models sample input information to fix excitation energy and fit some parameters to other data, maybe not the same as FREYA but idea is the same, result is only as good as available data

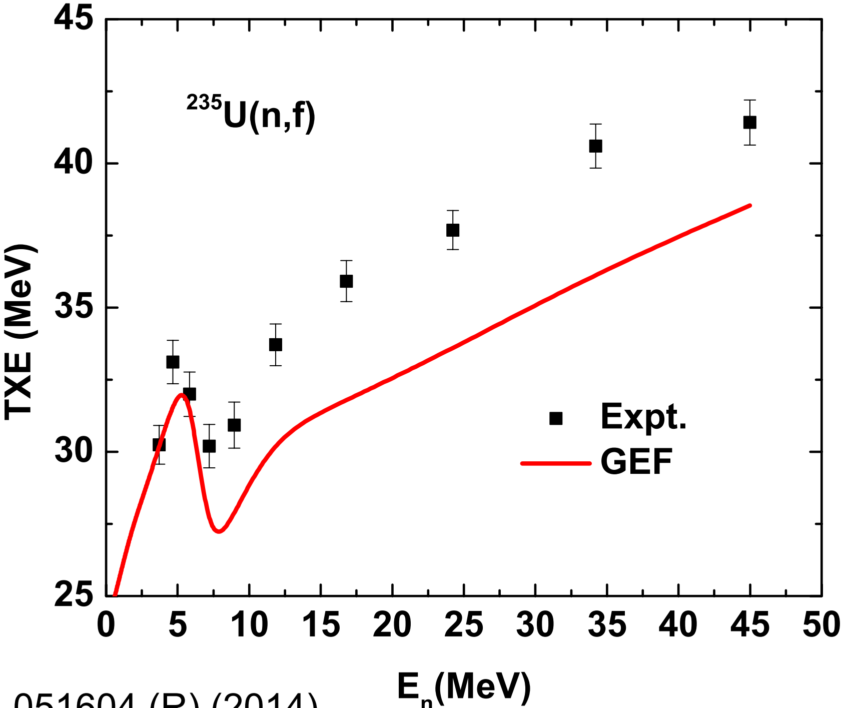
Beware unpublished models: here be dragons

GEF (General Fission Model) is semi-empirical MC, available from a website and described in a 200+ page document, model of energy sharing between fragments published but results with code are not, many parameters in fission barriers, yields, excitation energies, etc., but model of neutron emission is 'statistical'

From Walt Loveland's FIESTA talk: Old GEF is before his data, New GEF is after

I don't have a problem improving a model by adjusting to new data but I think it's important to document changes for users and have a fixed version available to them





Yanez et al. PRC 89, 051604 (R) (2014)

Some final thoughts

- There are lots of holes in the data (not exactly absence because there are numbers there but ignorance means that instead of measurements we have educated guesses)
- Making evaluations based on MC models is hard – I've done it with FREYA and don't find it satisfying – statistics are poor in important regions and some (much) interpolation/extrapolation/fitting is involved
- Can only hope to make progress by having more data:
  - Extending more differential measurements to higher energies to improve models for the big 3
  - Obtaining any data at all for actinides related to the fuel cycle
  - Photofission is of interest for applications but there is almost no data for either input or validation
- Wouldn't hurt to flag the 'made up' data when it gets called so that the user is aware of alligators in the swamp they are entering