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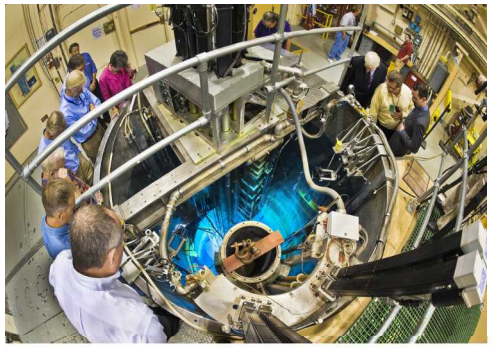
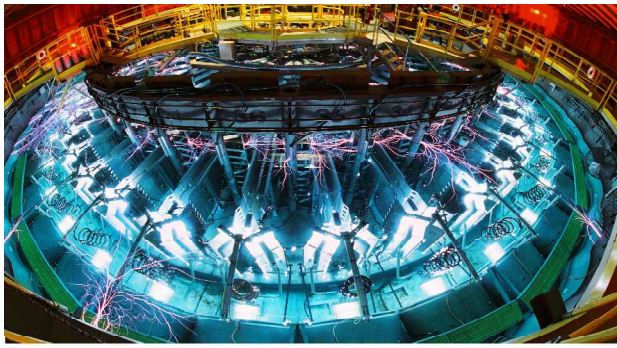

# Development of a Genetic Algorithm for Neutron Energy Spectrum Adjustment

Richard Vega and Edward Parma

8/13/14

TA-V LEADING NUCLEAR TECHNOLOGIES

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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# Motivation for spectrum adjustment

- High energy resolution measurement of a neutron energy spectrum is extremely difficult
- Monte Carlo neutron transport codes are typically used to calculate them
  - MCNP
  - Serpent
  - SCALE
- Statistical errors can be made vanishingly small, but modelling errors are often impossible to eliminate
- Higher accuracy in the spectrum leads to higher accuracy of radiation damage parameters

  - Fe DPA
  - Si Kerma
  - GaAs damage

  - Fluence > $E_0$
  - Fluence < $E_0$
  - $^{32}$S(n,p)$^{32}$P reaction rate

# What is spectrum adjustment?

- The adjustment of a spectrum produced by a transport code so that it is more consistent with experimental data
- What experimental data?
  - Neutron activation analysis
  - Bonner sphere detector response
  - Other integral quantities
- Complication: there are typically around 50 integral quantities and hundreds of energy groups
  - Each integral quantity is an equation:

$$I = \int \sigma \phi dE \approx \sum_{i=1}^{n} \sigma_i \phi_i \Delta E_i$$

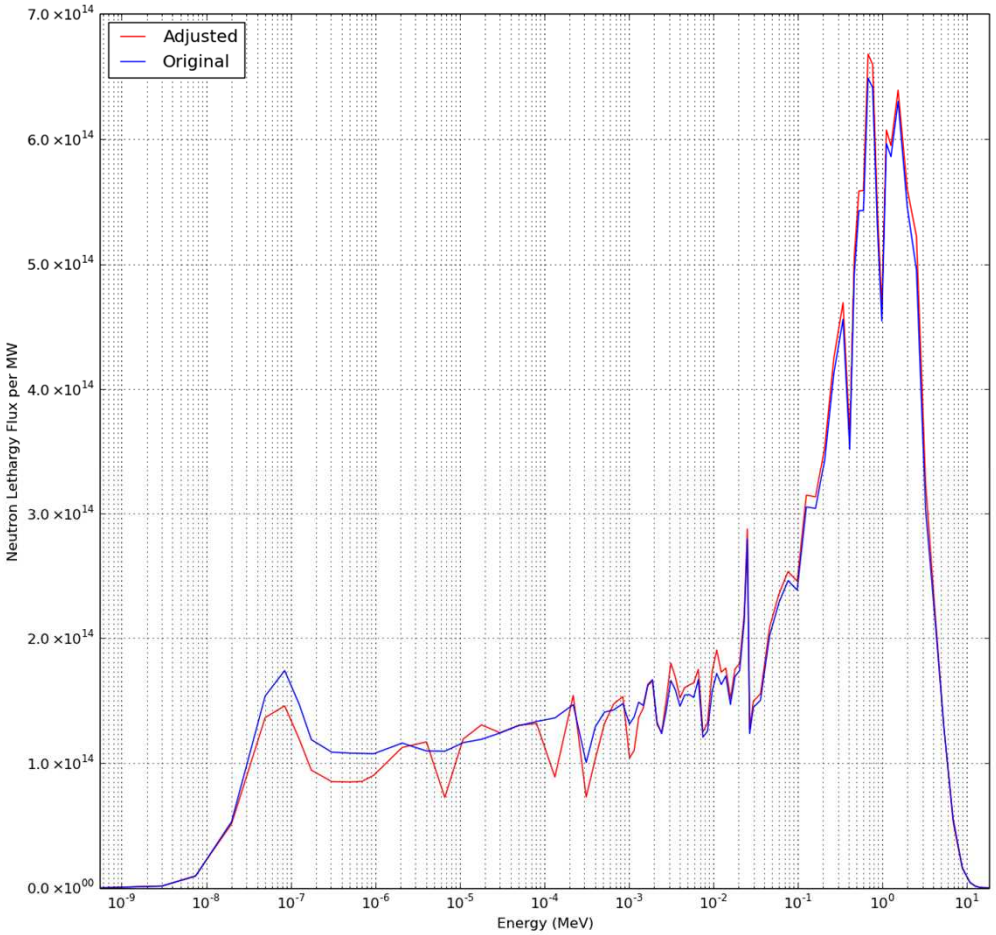
  - The flux in each energy group is a variable


# How has this been done in the past?

- There are a plethora of codes to chose from, each with its own method:
  - SAND-II: iterative perturbation method
  - STAY'SL: least squares fitting
  - LSL-M2: logarithmic least squares fitting
  - MAXED: maximum entropy optimization
  - FORIST: constrained least squares fitting
  - FLYSPEC: differentiation of the recoil proton energy distribution
  - GRAVEL: modified SAND-II iterative method
  - And many, many more …
- With so many options, we made the only rational decision
  - We wrote our own!

# So if there are so many codes, why introduce another?

- Spikes in the trial spectrum are evidence of cross section resonances, but new spikes after adjustment have no valid explanation
- Post-adjustment smoothing may remove peaks that are actually there
- As the resolution of the trial spectrum increases, so does the variance in the adjusted spectrum
- These characteristics are not unique to LSL-M2



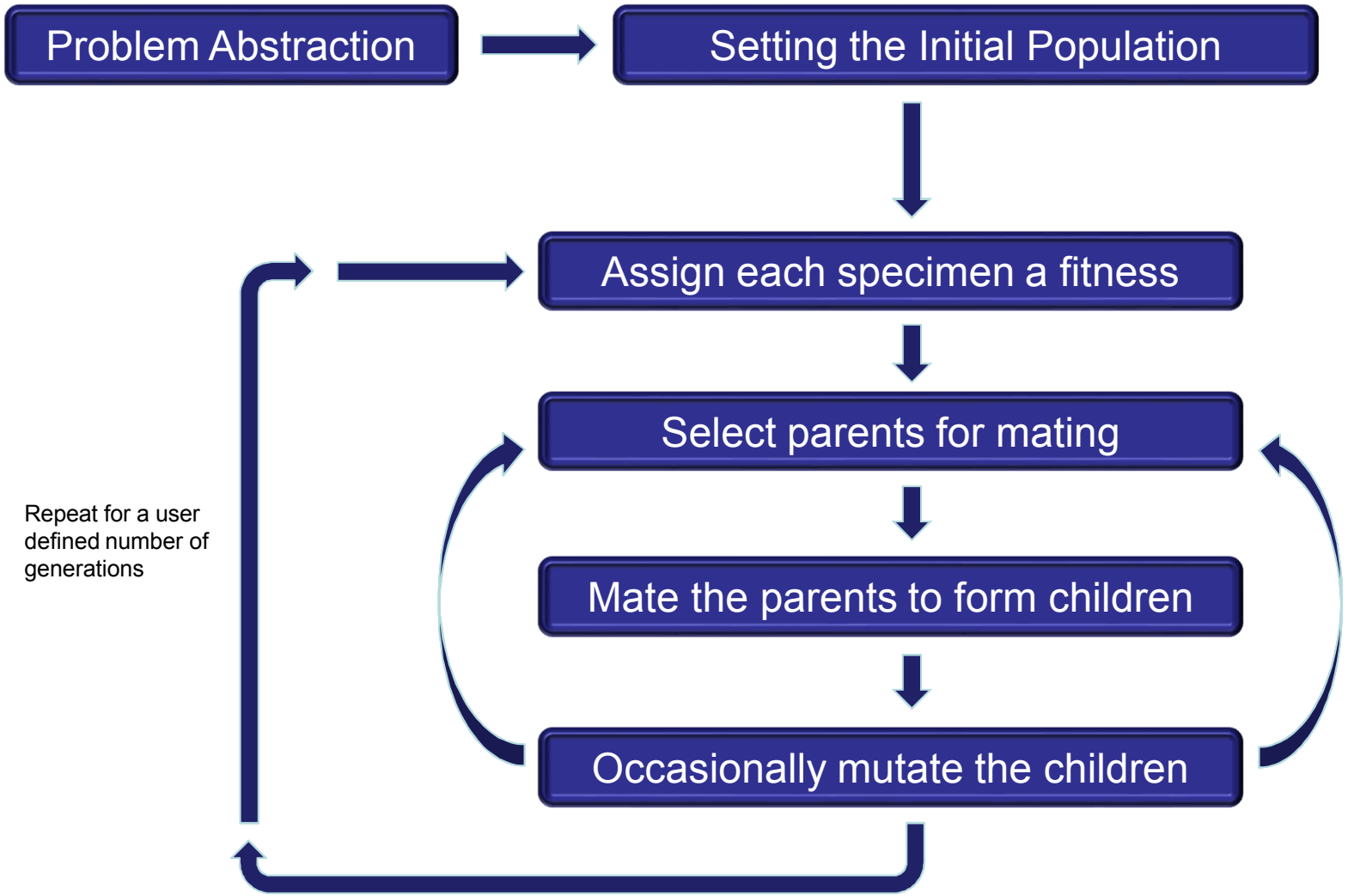
# The goal:

- To create an adjustment method that preserves trial spectrum features without introducing new features
- In addition, the proposed method should produce a spectrum which predicts the observed data reasonably well, and at least as well as the adjusted spectra of other codes
- The integrity of the method should be as independent of input trial spectrum resolution as possible

# The genetic algorithm

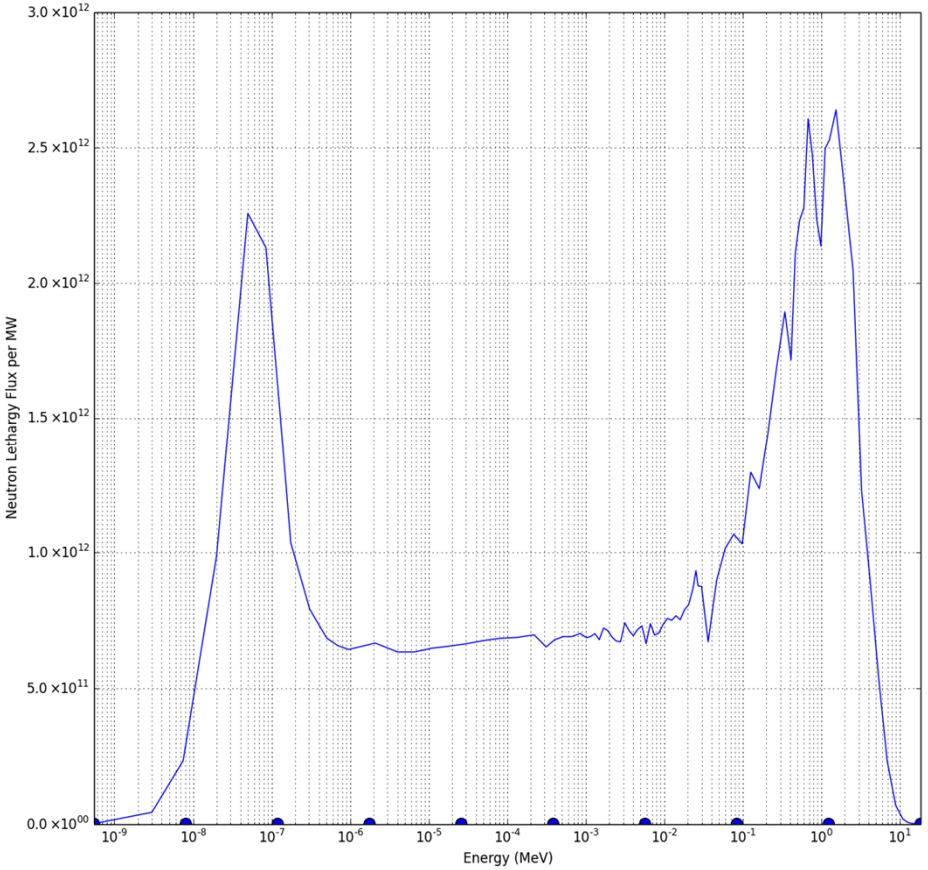
- What is it?
  - An optimization method
  - Designed to mimic natural selection
  - Excellent for optimization problems of low complexity (where a single metric can easily define the quality of the solution)
    - Travelling salesman problem
    - Number partitioning problem
    - Antenna design
- Why did we choose it?
  - Introduced to it in physics undergrad
  - It's application to engineering has not been thoroughly explored

# How does it work?



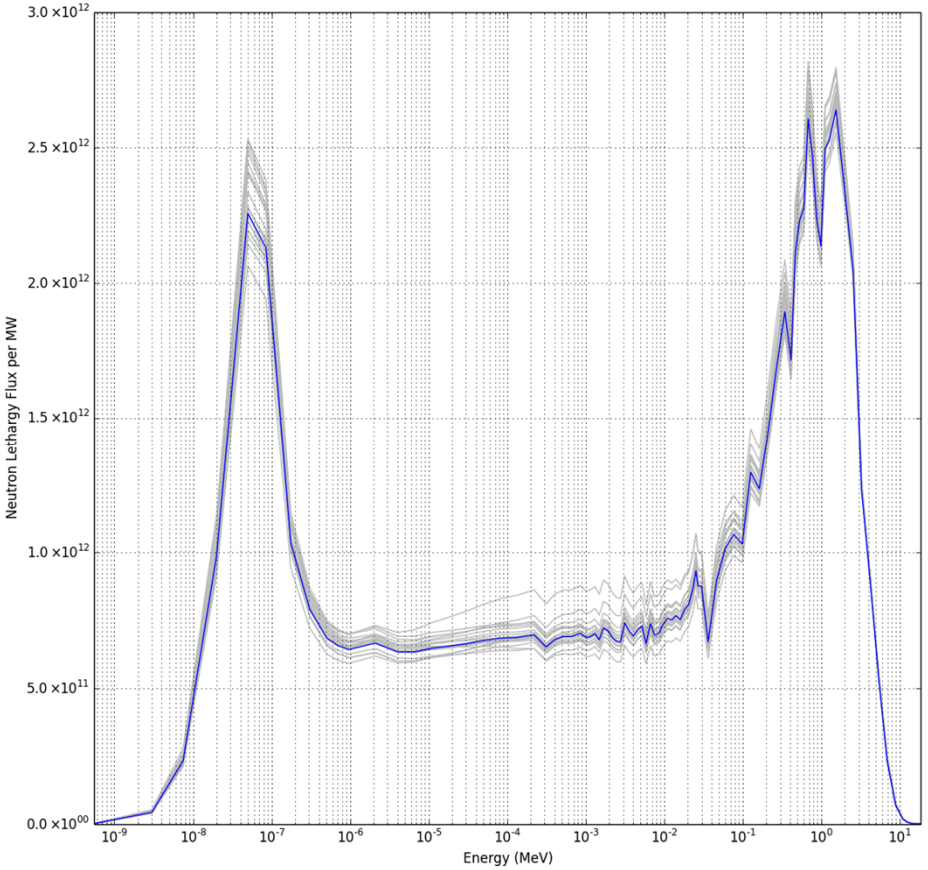
# Abstraction

- Step 1: select the number of gene sites N, to be used
- Step 2: seek the energy domain of the problem (from trial spectrum)
- Step 3: select N points equidistant in log-space covering energy domain
  - These will be referred to as the GENE SITES
- Step 4: each site is assigned a real number (typically close to 1)
  - These numbers will be referred to as the GENES



# Setting the population

- For each specimen:
  - For each gene site:
    - Pull a random Gaussian distributed number ($\mu = 0$, $\sigma = 0.07$)
    - Add it to 1. The result is the value of the gene
  - Perform a polynomial least squares regression through the gene values
    - This polynomial will be referred to as the SHIFT FUNCTION
  - Multiply the flux in each energy group of the trial spectrum with the value of the shift function at the groups midpoint energy
- Repeat this process until the initial population is of the desired size



# Assigning fitness values

- Remember the original goal: we want a spectrum that is consistent with experiment
  - Specifically, we want the activities calculated using the adjusted spectrum and dosimetry cross sections to match well with the measured activities
- The fitness function should be large when the difference between calculation and experiment is small

$$f = C - \sum_{i=1}^{m} \frac{\left| \left\{ \sum_{j=1}^{n} \sigma_{j,i} \phi_j \Delta E_j \right\} - r_i \right|}{r_i}$$

# Parent selection

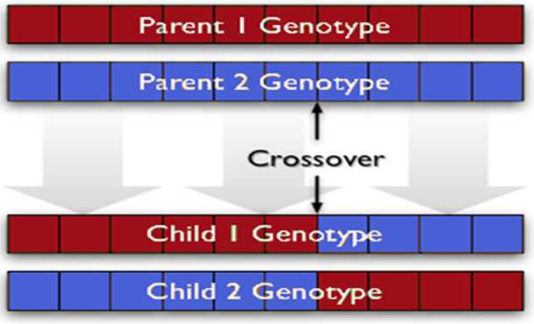
- Proportional selection
  - Specimens with high fitness values have a high probability of being selected for mating
  - Likewise, those with lower fitness values have a low probability of being selected
- Specifically:

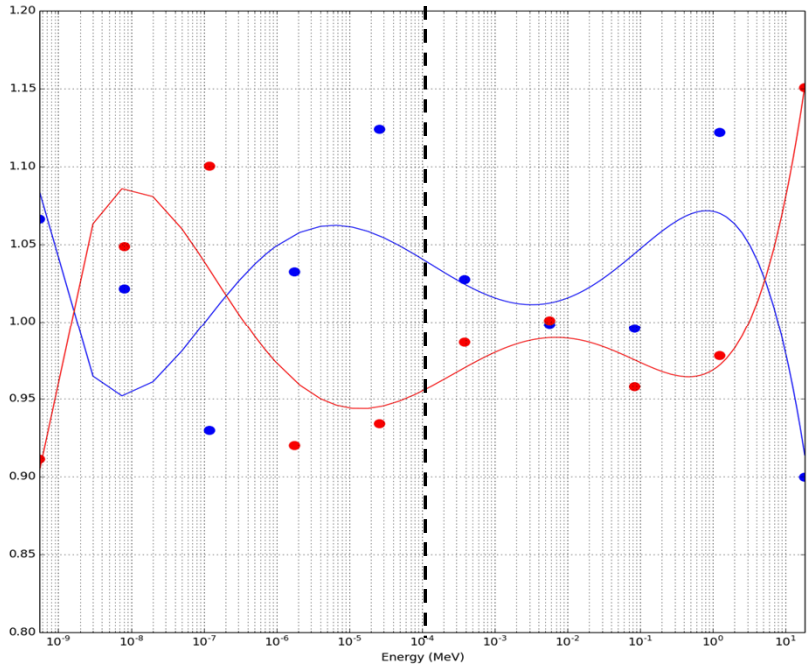
$$P_t = \sum_{i=1}^{S} \{f_i - f_{min}\}$$

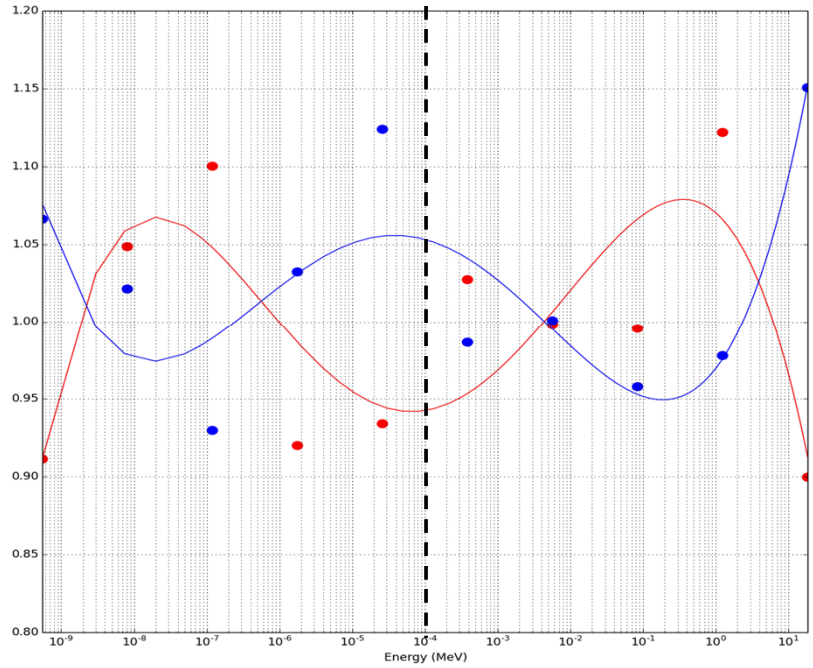
$$P_j = \frac{f_j - f_{min}}{P_t}$$

# Mating

- Crossover: given 2 parents, it will produce 2 children
  - Obviously, other methods exist and we tried many of them.

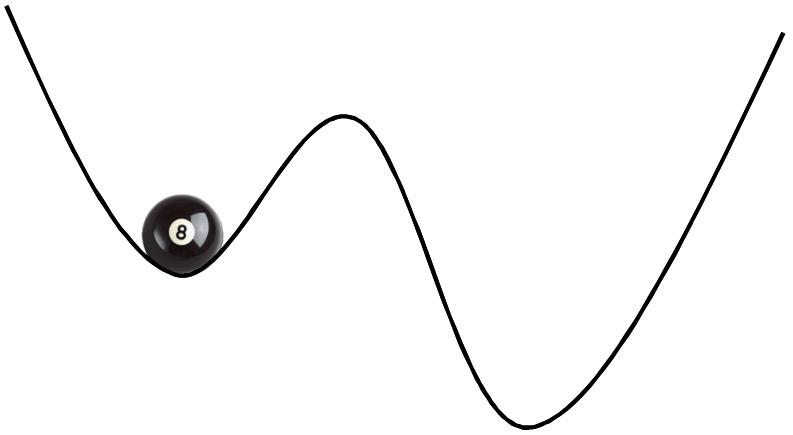


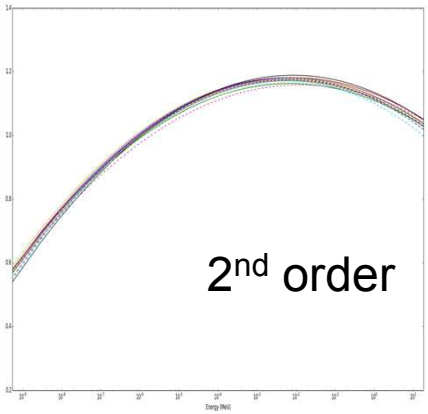



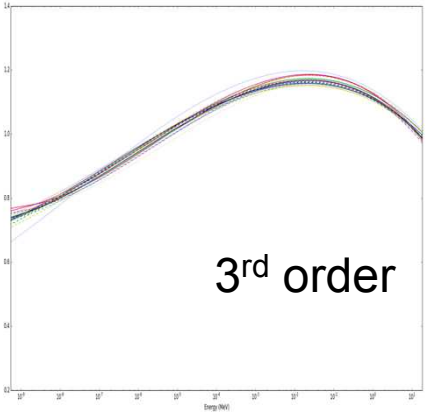
# Mutation

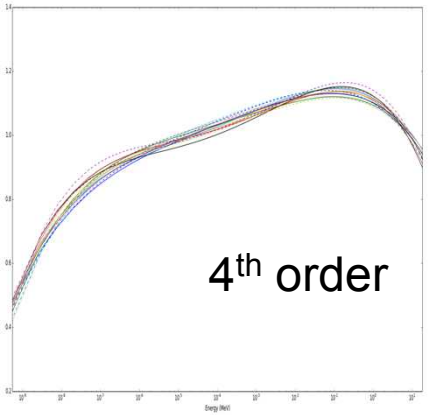
- Gene-wise mutation:
  - As each child receives each of it's genes from it's parents, each gene has a set probability of being selected for mating
  - Gene Mutation in this case is simply adding another random Gaussian distributed number ($\mu = 0, \sigma = 0.02$) to the inherited gene value
- Why do we need mutation?
  - It is common for genetic algorithms to converge upon a solution with a high fitness, but not the absolute highest fitness possible
  - Mutation ensures that the entire solution space is being explored

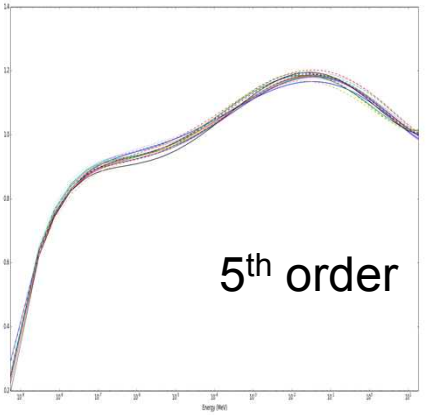


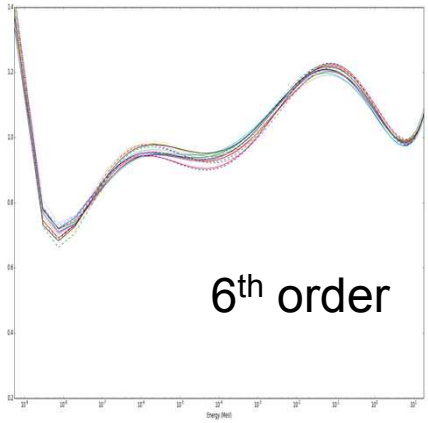
# Results: effect of polynomial order

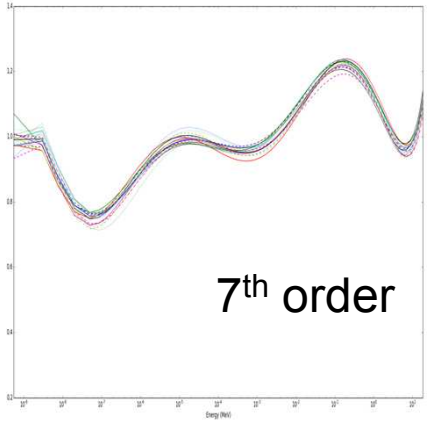


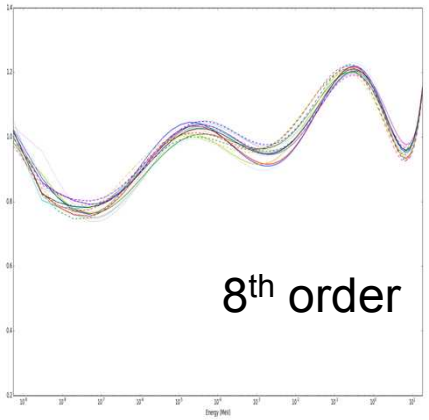



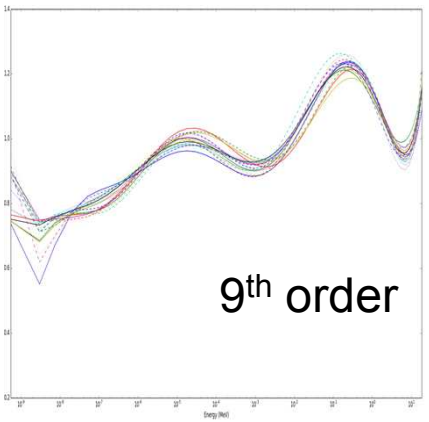



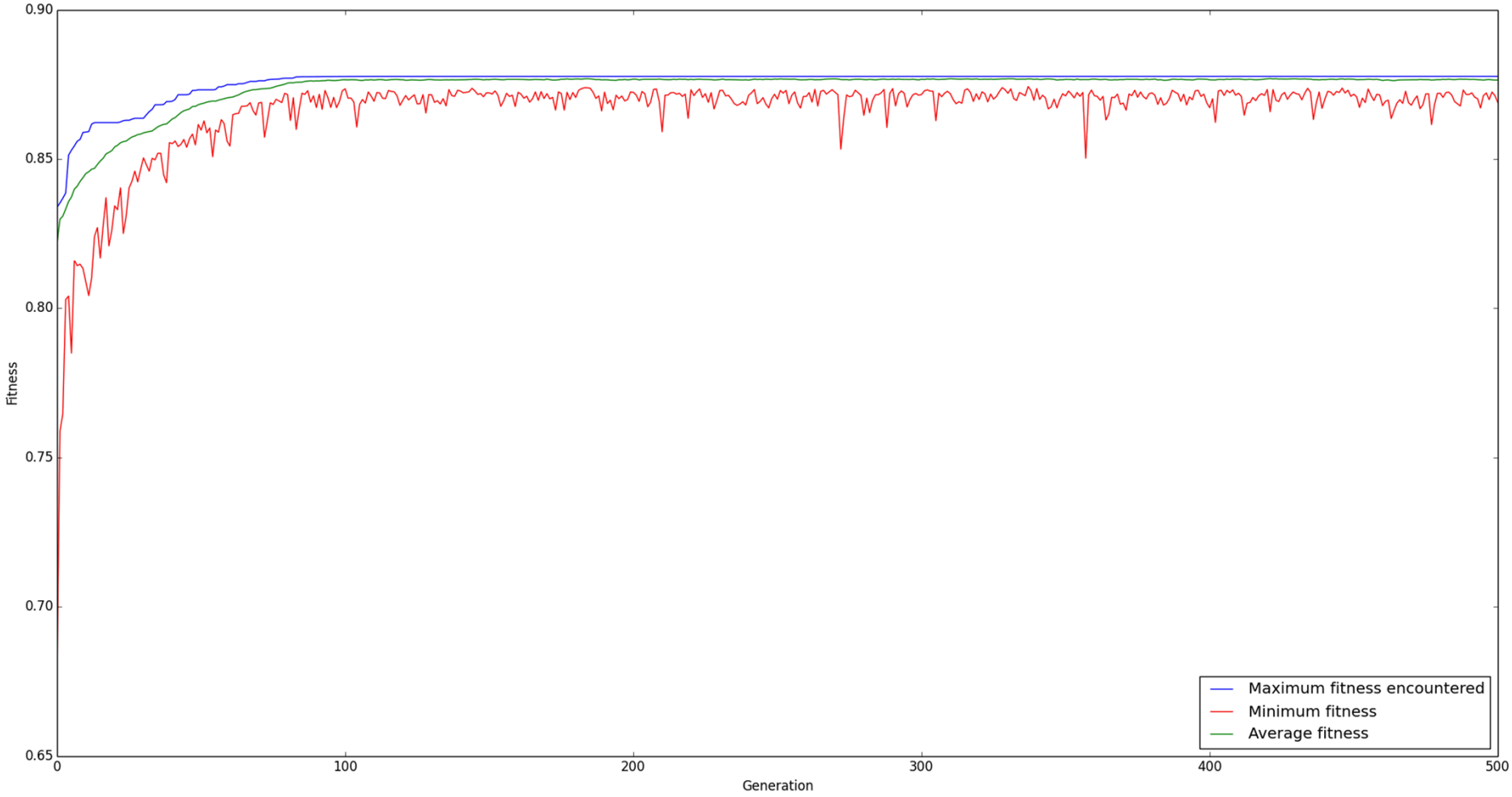



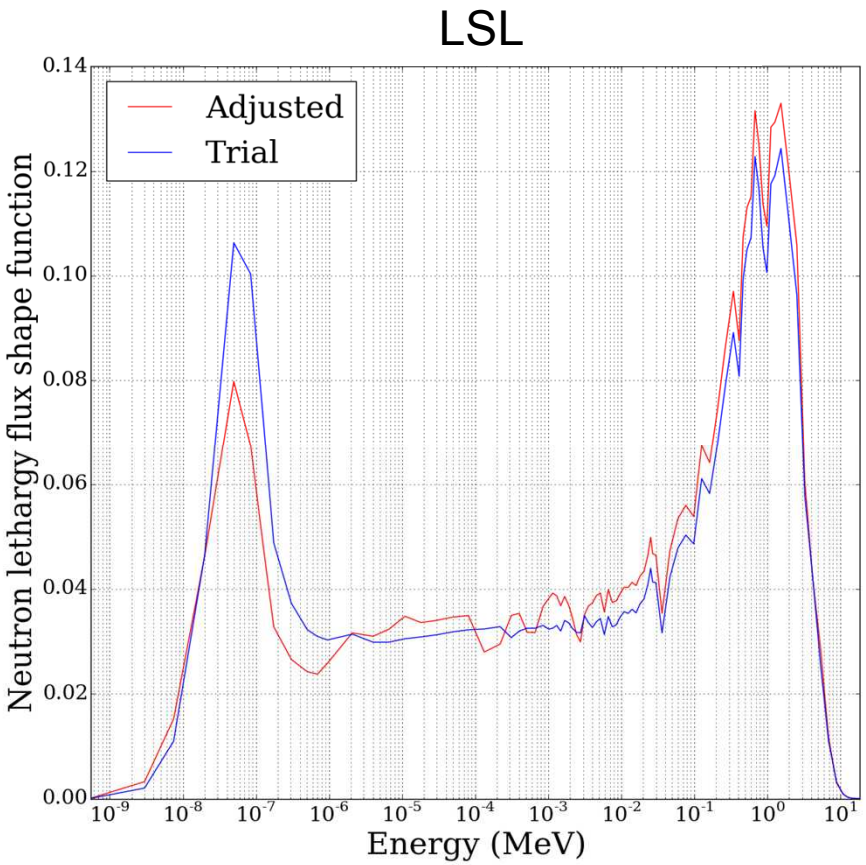



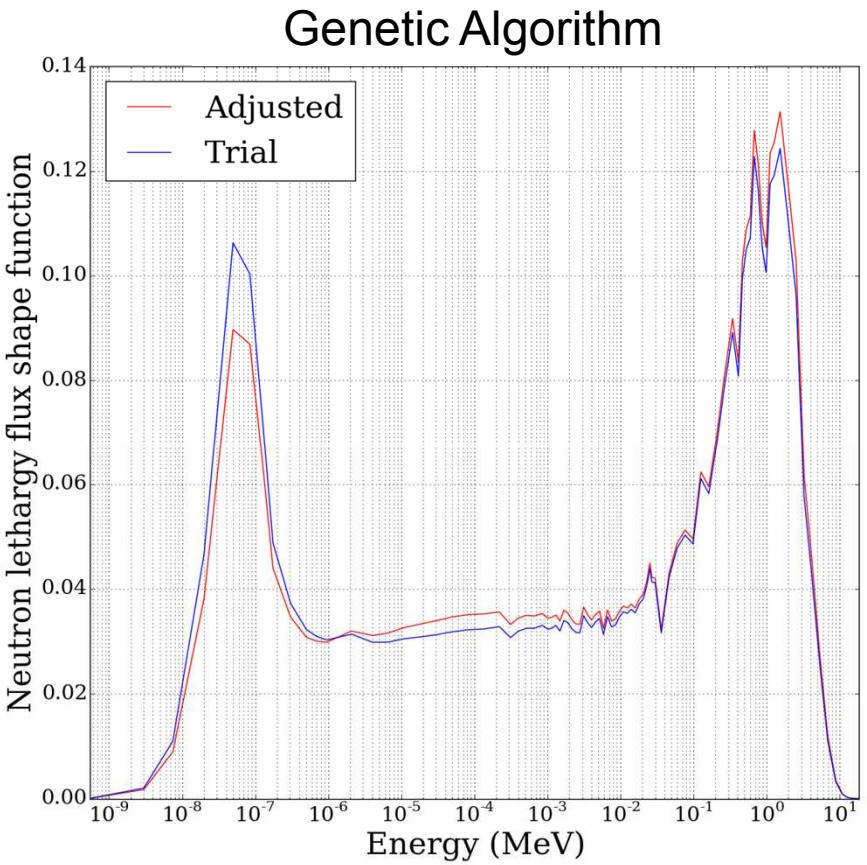



# Results: convergence speed

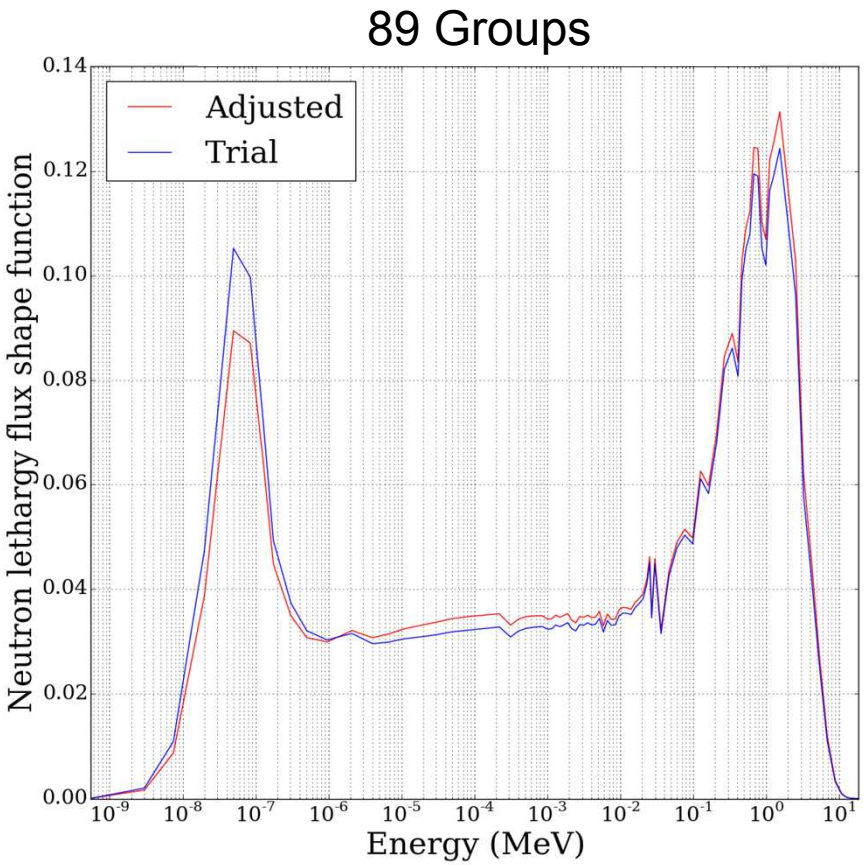


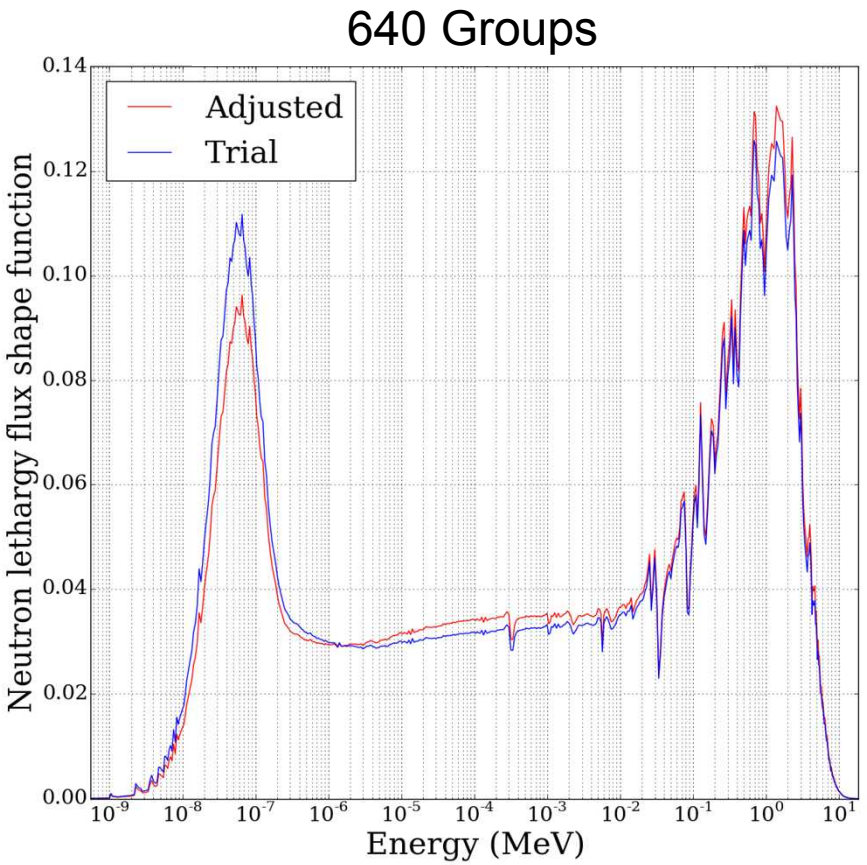
# Results: PLG final adjustment



# Results: Resolution dependence



# Results: experimental consistency

| Foil identification | LSL | Genetic | Measured | LSL % diff | Genetic % diff |
|---|---|---|---|---|---|
| al27a#-ml3x-bahl | 3.736E-13 | 3.768E-13 | 3.774E-13 | 1.008% | 0.171% |
| au197g#-dil3-bahl | 2.439E-07 | 2.386E-07 | 2.404E-07 | 1.467% | 0.756% |
| au197g#-dil3-cdhl | 1.803E-07 | 1.777E-07 | 1.788E-07 | 0.841% | 0.630% |
| co59g#-mil2-bahl | 2.797E-08 | 2.720E-08 | 2.724E-08 | 2.694% | 0.140% |
| co59g#-mil2-cdhl | 5.391E-09 | 5.591E-09 | 5.329E-09 | 1.165% | 4.918% |
| co59p#-mil2-cdhl | 8.216E-13 | 8.014E-13 | 8.157E-13 | 0.723% | 1.753% |
| co592#-mil2-cdhl | 1.128E-13 | 1.112E-13 | 1.117E-13 | 0.989% | 0.425% |
| cu63a#-mil5-bahl | 3.014E-13 | 2.933E-13 | 3.596E-13 | 16.182% | 18.426% |
| cu63g#-mil5-bahl | 3.310E-09 | 3.220E-09 | 3.305E-09 | 0.162% | 2.577% |
| cu63g#-mil5-cdhl | 5.135E-10 | 5.490E-10 | 4.975E-10 | 3.216% | 10.353% |
| fe54p#-mil5-bahl | 5.032E-11 | 5.024E-11 | 4.970E-11 | 1.249% | 1.089% |
| fe56p#-mil5-bahl | 6.122E-13 | 5.970E-13 | 6.200E-13 | 1.255% | 3.714% |
| fe58g#-mil5-bahl | 9.783E-10 | 9.375E-10 | 9.335E-10 | 4.804% | 0.426% |
| fe58g#-mil5-cdhl | 1.548E-10 | 1.512E-10 | 1.493E-10 | 3.667% | 1.304% |
| in115n#-mil5-bahl | 1.545E-10 | 1.564E-10 | 1.651E-10 | 6.434% | 5.274% |
| mg24p#-mil5-bahl | 8.013E-13 | 8.042E-13 | 7.661E-13 | 4.592% | 4.973% |
| mn55g#-mil2-cdhl | 1.490E-09 | 1.436E-09 | 1.487E-09 | 0.209% | 3.400% |
| mn552#-mil2-bahl | 1.168E-13 | 1.151E-13 | 1.375E-13 | 15.045% | 16.271% |
| mo98g#-mil5-bahl | 8.740E-10 | 8.642E-10 | 8.667E-10 | 0.842% | 0.284% |
| mo98g#-mil5-cdhl | 7.940E-10 | 7.881E-10 | 7.982E-10 | 0.528% | 1.271% |
| na23g#-pelt-bahl | 3.242E-10 | 3.155E-10 | 3.057E-10 | 6.064% | 3.219% |
| na23g#-pelt-cdhl | 3.358E-11 | 3.547E-11 | 3.245E-11 | 3.469% | 9.305% |
| nb932#-mil5-bahl | 2.438E-13 | 2.435E-13 | 2.411E-13 | 1.124% | 0.976% |
| ni58p#-milx-bahl ** | 6.879E-11 | 6.879E-11 | 6.879E-11 | 0.000% | 0.000% |
| ni582#-milx-cdhl | 2.293E-15 | 2.332E-15 | 2.152E-15 | 6.569% | 8.382% |
| ni60p#-milx-cdhl | 1.228E-12 | 1.189E-12 | 1.254E-12 | 2.040% | 5.168% |
| rmldu#-rmld-fiss | 2.250E-10 | 2.281E-10 | 2.194E-10 | 2.546% | 3.958% |
| rmleu#-rmle-fiss | 2.463E-09 | 2.495E-09 | 2.573E-09 | 4.257% | 3.040% |
| rmlpu#-rmlp-fiss | 2.796E-09 | 2.803E-09 | 2.570E-09 | 8.776% | 9.072% |
| s32cf#-void-bare | 5.845E-02 | 5.886E-02 | 5.437E-02 | 7.501% | 8.262% |
| sc45g#-mil5-bahl | 1.802E-08 | 1.730E-08 | 1.731E-08 | 4.087% | 0.057% |
| sc45g#-mil5-cdhl | 1.295E-09 | 1.314E-09 | 1.352E-09 | 4.208% | 2.791% |
| ti46p#-milx-bahl | 6.700E-12 | 6.509E-12 | 6.400E-12 | 4.684% | 1.698% |
| ti47p#-milx-bahl | 1.237E-11 | 1.243E-11 | 1.265E-11 | 2.188% | 1.723% |
| ti48p#-milx-bahl | 1.639E-13 | 1.628E-13 | 1.625E-13 | 0.839% | 0.183% |
| zn64p#-milx-bahl | 2.403E-11 | 2.408E-11 | 2.451E-11 | 1.940% | 1.735% |
| zr902#-milx-bahl | 5.670E-14 | 5.689E-14 | 5.748E-14 | 1.353% | 1.023% |

# Recap

- Pros
  - The method guarantees an adjustment which preserves trial spectrum features without introducing unrealistic ones 
  - The calculated activities match experimental data at least as well as LSL-M2 
  - The method seems to be resolution independent 
- Cons
  - Data means nothing without error bars, and the method does not have any way to inherently handle uncertainty quantification (LSL-M2 does) 
  - Users of other spectrum adjustment methods would say that an accurate representation of the variance in the output spectrum is what determines the quality of adjustment, and not simply the agreement with a limited experimental data set 

# A closer look at LSL-M2

- A brief look at the method
  - Takes an underdetermined problem and makes it an over-determined problem
  - Method guarantees to minimize the variance in the adjusted quantities
  - One catch: all input parameters are adjusted, not only the spectrum
- In the universal language:

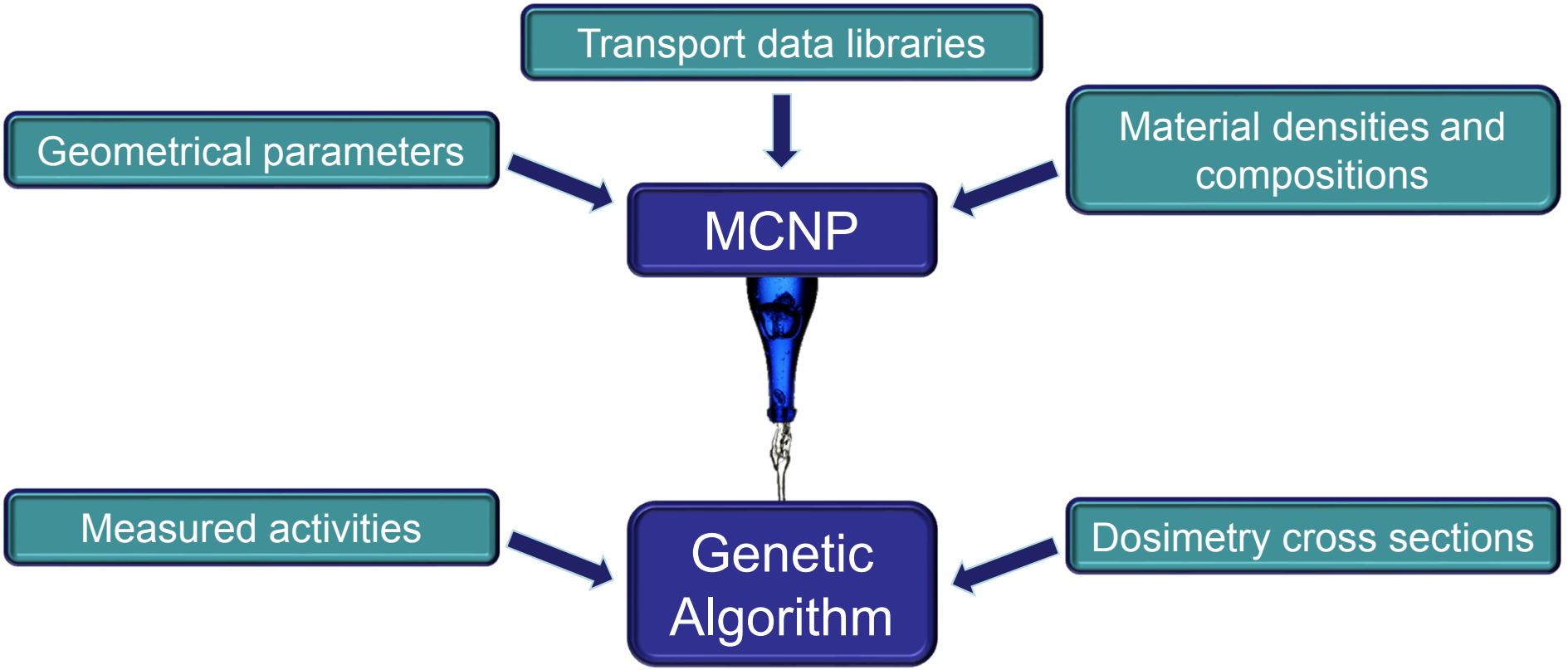
$$\chi^2 = (\phi_0 - \phi)^T [\mathrm{cov}(\phi_0)]^{-1} (\phi_0 - \phi) + (\sigma_0 - \sigma)^T [\mathrm{cov}(\sigma_0)]^{-1} (\sigma_0 - \sigma) + (\alpha^m - \alpha)^T [\mathrm{cov}(\alpha^m)]^{-1} (\alpha^m - \alpha)$$

- Where are we getting the covariance matrices from?
  - A detailed uncertainty quantification of the model parameters is the most rigorous method
  - Other estimation techniques exist

# Expanding the genetic algorithm

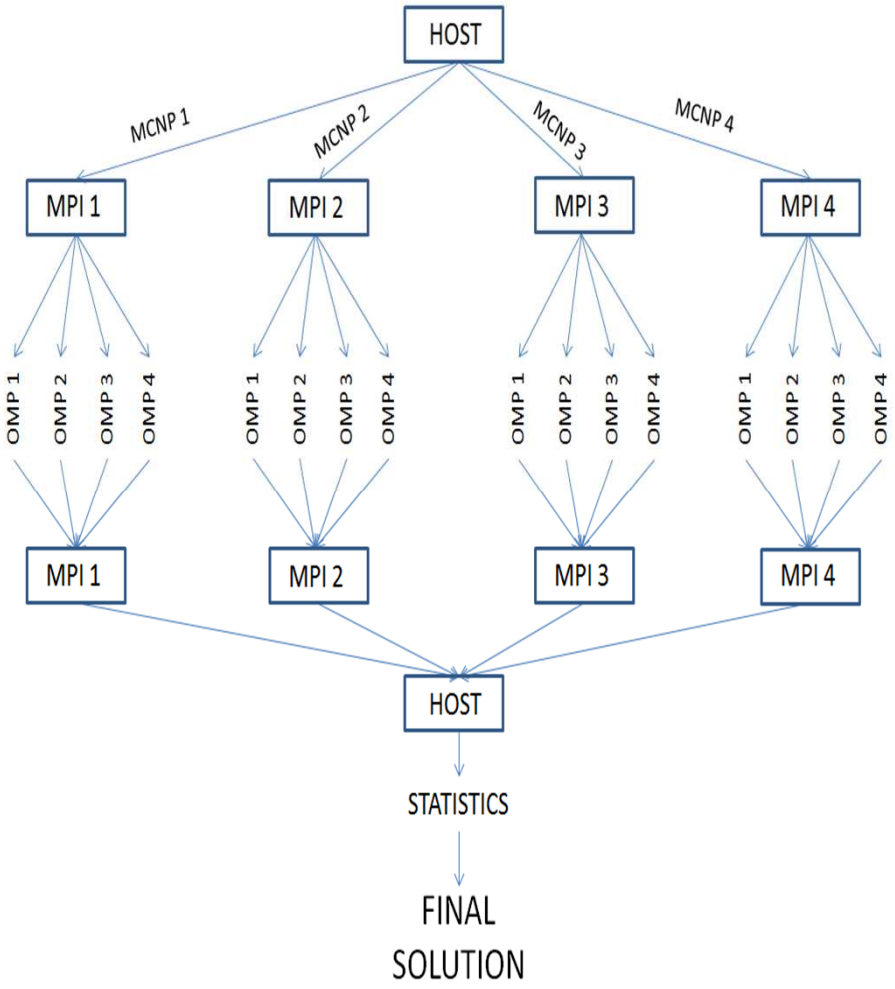
- If we are to include uncertainty quantification into the code, it should be:
  - Rigorous
  - Intrinsic
- What output should we expect?
  - Variance of the flux in each energy group
  - Covariance (or correlation) matrix of the final solution
- Options?
  - Because the method is so abstract, error propagation is much more challenging
  - Leading (and only candidate) at the moment: random sampling
    - Generate many sets of input based on input parameter uncertainties
    - Generate many sets of output
    - Perform the statistics

# Sources of uncertainty



# Parallelization

- Utilizing parallelism: combining MPI and OpenMP
  - Each MPI process will get a MCNP input spectra
  - Each of these processes will be threaded with each thread getting a different set of dosimetry cross sections and activities
- Memory usage?
  - 89 energy groups ≈ 3 MB per process
  - Not really an issue



# Other plans

- Comparison of genetic algorithm to other codes (aside from LSL-M2)
- Adjustment of radiation metrology benchmark fields
- Parametric uncertainty quantification
  - Varying each source of uncertainty individually to see its contribution to the adjusted spectrum's uncertainty
- Verification of covariance matrix estimation techniques using brute force uncertainty quantification

# Conclusions

- The genetic algorithm produces promising, but currently incomplete results
- The method is less likely to produce unrealistic adjustment artefacts
- The method is almost completely independent of trial spectrum resolution

# Acknowledgements


- Ken Reil
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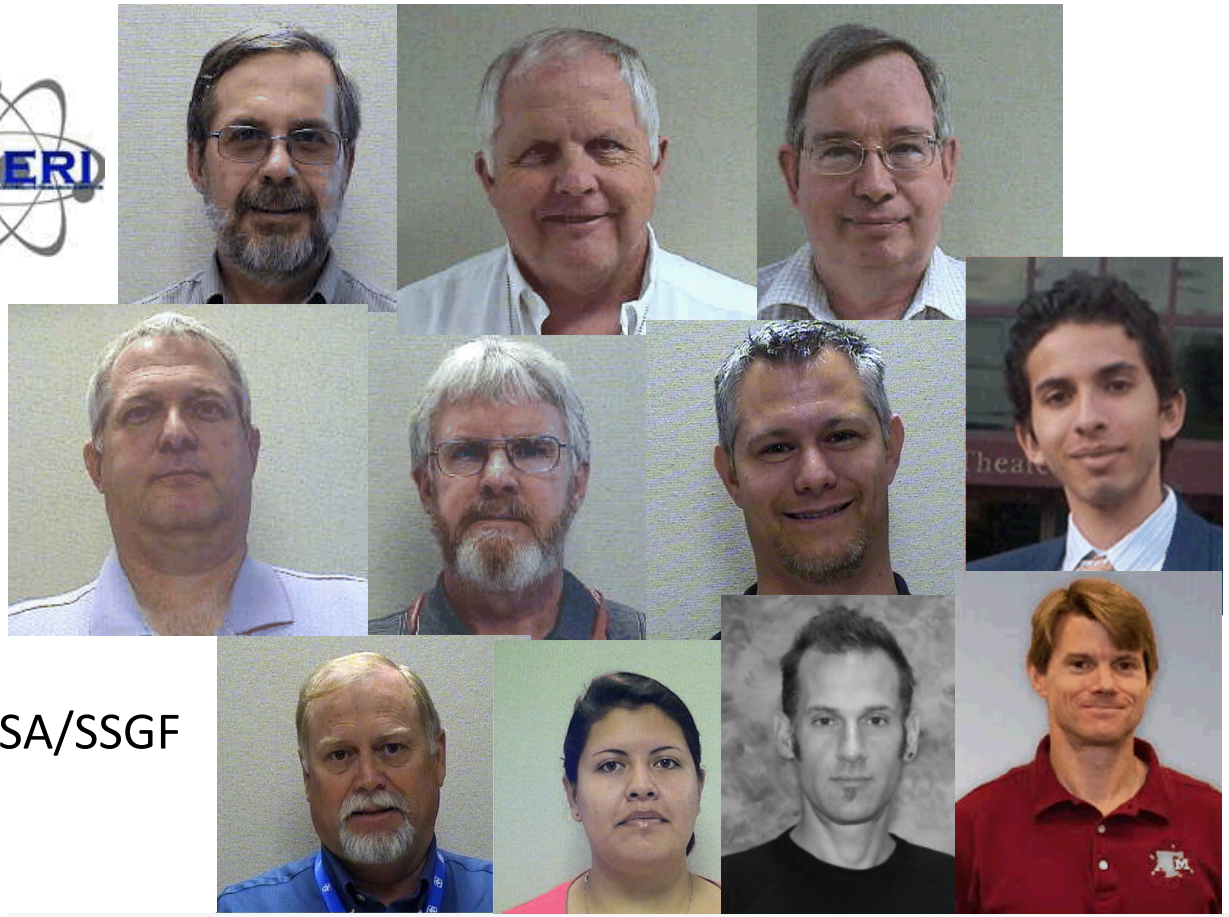
- Danielle Redhouse
- Helmut Katzgraber
- Marvin Adams

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# Questions?