SAND2015-6559PE

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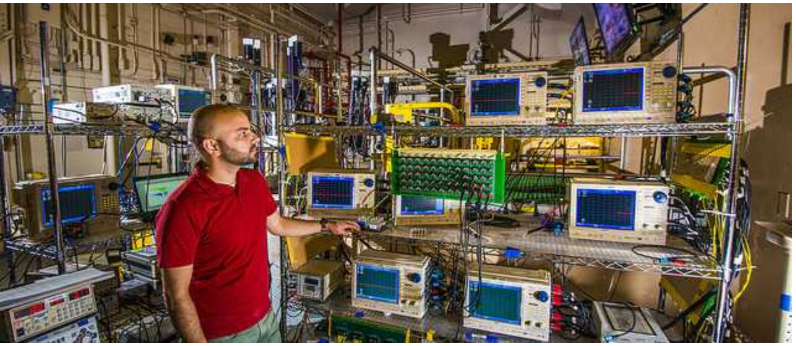
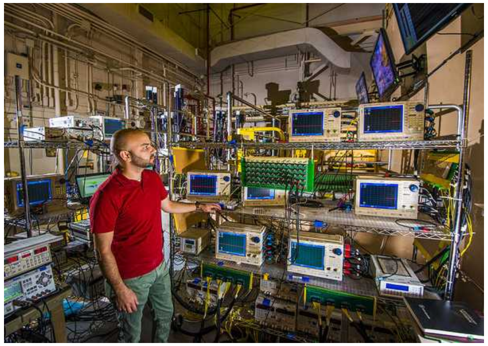
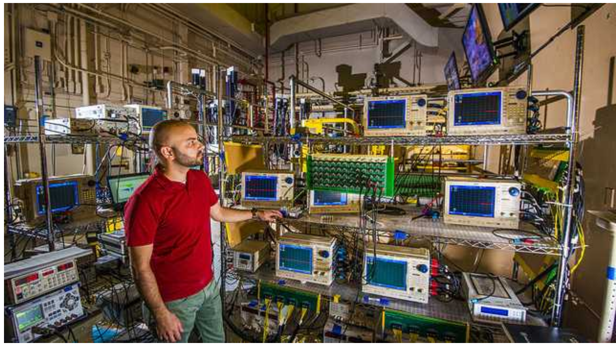




Mysterious Containers, Problems with Many Solutions, and Transport on the Next Generation of Supercomputers

Richard M. Vega
Mentor: Ed Parma
Manager: Ken Reil
Applied Nuclear Technologies, 1384

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Summer 2013

“Any idea what’s in these containers labelled ACPR fuel?”

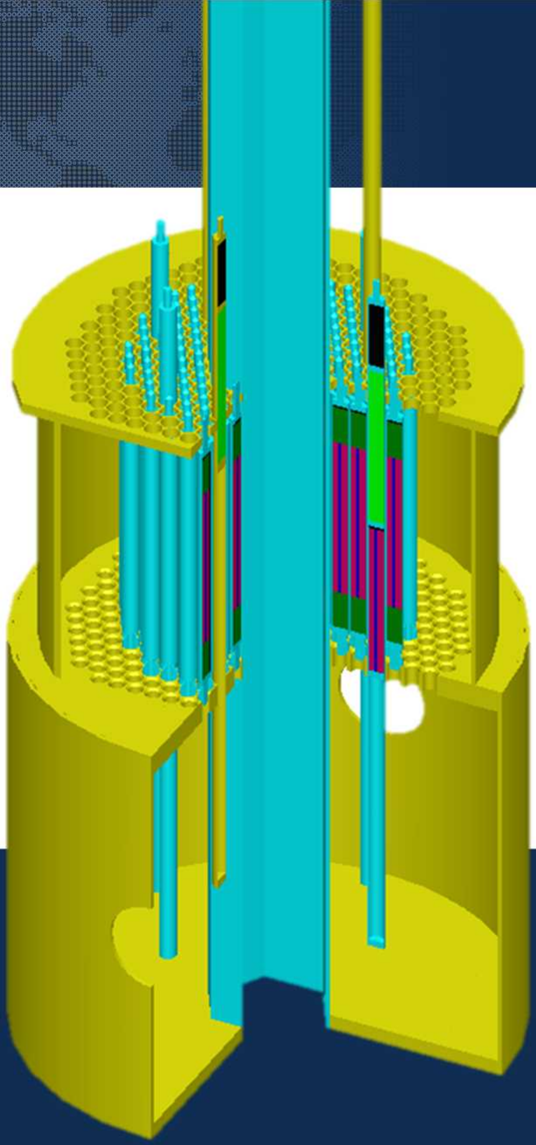
Nuclear Materials Management, 1386

Problem description

Sandia National Laboratories

- Corporate Storage Bunker 37011 was shut down due to a HC3 occurrence in March 2013.
- This sparked interest in what else might be living in this bunker.
- There were several containers in the bunker labeled "ACPR fuel."
  - ACPR, RIP June 1, 1967 – October 1, 1977.
  - Predecessor to ACRR.
- Unknowns about the ACPR fuel in the containers:
  - Pretty much everything.
- My task: to determine HC3 sum of fractions
  - This requires knowledge of the radionuclide inventory.

Problem solution



- Model the reactor and calculate the radionuclide inventory.
- Two models were built
  - TRITON: coupling of KENO-VI to ORIGEN-S
  - Serpent 2 Beta
- The fuel material in the two highest pin powers were tracked separately.
- Isotope inventories tracked: ^{241}Am, ^{242m}Am, ^{243}Am, ^{242}Cm, ^{245}Cm, ^{137}Cs, ^{154}Eu, ^{3}H, ^{166m}Ho, ^{85}Kr, ^{59}Ni, ^{237}Np, ^{233}Pa, ^{147}Pm, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{151}Sm, ^{90}Sr, ^{99}Tc, ^{228}Th, ^{230}Th, ^{234}U, ^{236}U, and ^{90}Y.

Assumptions and conditions

- Validity of the steady state approximation to pulse power.
- Determination of the steady state power level without the energy release logs.
  - One case for each pulse height representing four pulses per day.
  - One case to match the SAR statement of burnup: “Through the year 1972, the ACPR had accumulated a total of only 13.2 MWd of operation.”

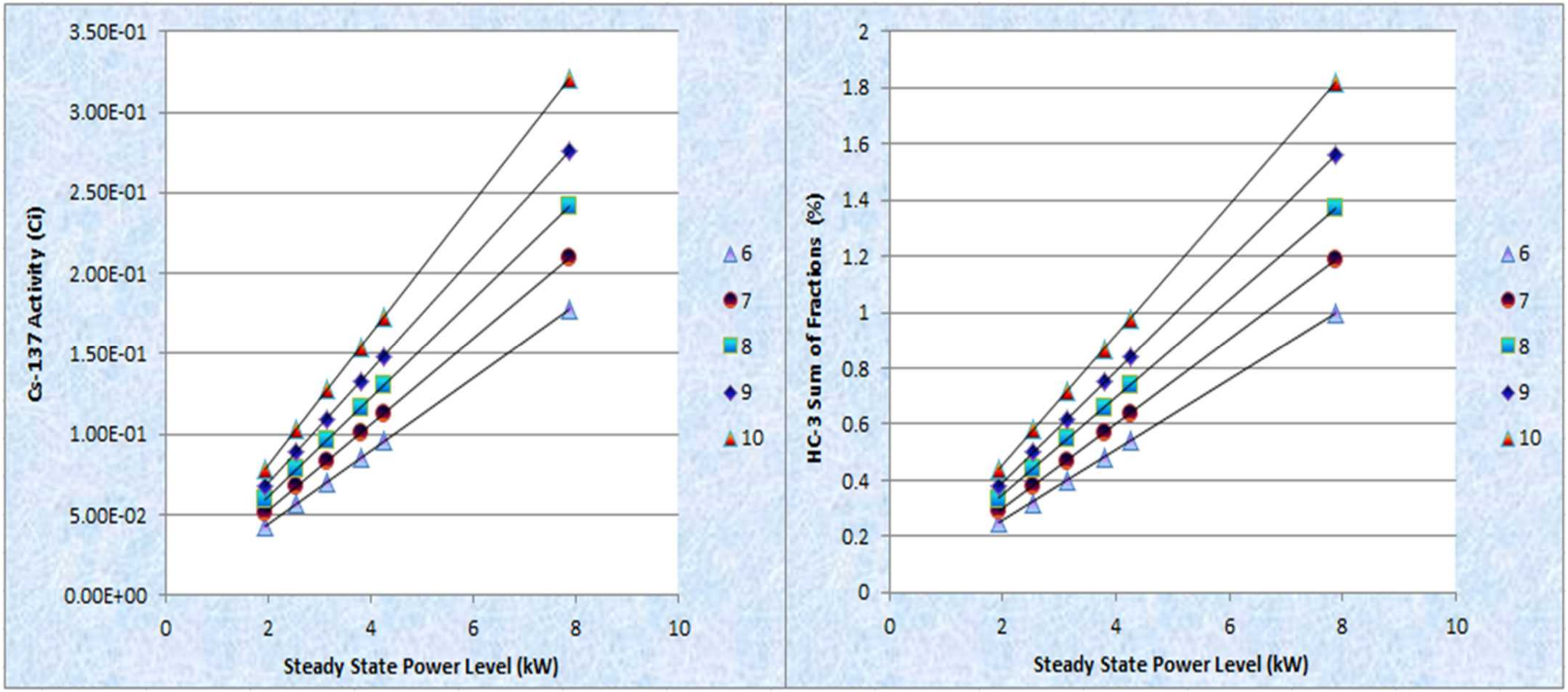
Reactivity ($)	FWHM (msec)	Maximum Measured Temperature (°C)	Energy Release (MJ)
2.50	10.6	435	42
3.00	8.0	518	55
3.50	6.3	602	68
4.00	5.3	678	82
4.42	4.6	737	92

Bounding Case	Steady State Power Level (kW)
Four 42 MJ pulses per day	1.944
Four 55 MJ pulses per day	2.546
Four 68 MJ pulses per day	3.148
Four 82 MJ pulses per day	3.796
Four 92 MJ pulses per day	4.259
SAR statement of burnup	7.885

HC3 sum of fractions (assuming 10 years of irradiation)

Nuclide	HC3 Threshold (Ci)	Case 1 (Ci)	Fraction	Case 2 (Ci)	Fraction	Case 3 (Ci)	Fraction	Case 4 (Ci)	Fraction	Case 5 (Ci)	Fraction	Case 6 (Ci)	Fraction
Am-241	2.890E+00	3.060E-08	1.059E-08	7.839E-08	2.713E-08	1.676E-07	5.800E-08	3.250E-07	1.124E-07	4.996E-07	1.729E-07	3.165E-06	1.095E-06
Am-242m	3.220E+00	6.243E-13	1.939E-13	2.228E-12	6.920E-13	6.349E-12	1.972E-12	1.579E-11	4.904E-12	2.851E-11	8.855E-12	3.321E-10	1.031E-10
Am-243	2.920E+00	3.737E-16	1.280E-16	6.612E-16	2.264E-16	1.513E-15	5.180E-16	3.941E-15	1.350E-15	7.533E-15	2.580E-15	1.581E-13	5.414E-14
Cm-242	2.350E+01	5.149E-13	2.191E-14	1.837E-12	7.816E-14	5.231E-12	2.226E-13	1.302E-11	5.539E-13	2.351E-11	1.000E-12	2.738E-10	1.165E-11
Cm-245	2.820E+00	3.866E-23	1.371E-23	6.980E-23	2.475E-23	1.197E-22	4.246E-23	2.255E-22	7.997E-23	3.746E-22	1.328E-22	1.429E-20	5.067E-21
Cs-137	6.040E+01	7.867E-02	1.302E-03	1.033E-01	1.710E-03	1.277E-01	2.115E-03	1.544E-01	2.556E-03	1.733E-01	2.868E-03	3.210E-01	5.314E-03
Eu-154	2.250E+02	4.110E-07	1.827E-09	7.051E-07	3.134E-09	1.078E-06	4.790E-09	1.570E-06	6.979E-09	1.974E-06	8.774E-09	6.780E-06	3.014E-08
H-3	1.660E+04	8.008E-05	4.824E-09	1.051E-04	6.334E-09	1.301E-04	7.838E-09	1.574E-04	9.480E-09	1.767E-04	1.064E-08	3.281E-04	1.977E-08
Ho-166m	1.020E+02	1.518E-13	1.488E-15	2.204E-13	2.160E-15	3.015E-13	2.956E-15	4.039E-13	3.960E-15	4.882E-13	4.787E-15	1.282E-12	1.256E-14
Kr-85	3.330E+04	2.399E-03	7.205E-08	3.149E-03	9.455E-08	3.894E-03	1.169E-07	4.706E-03	1.413E-07	5.282E-03	1.586E-07	9.784E-03	2.938E-07
Np-237	5.360E+00	1.206E-08	2.251E-09	1.632E-08	3.044E-09	2.060E-08	3.843E-09	2.564E-08	4.784E-09	2.928E-08	5.462E-09	5.918E-08	1.104E-08
Pa-233	2.980E+03	1.206E-08	4.048E-12	1.632E-08	5.476E-12	2.060E-08	6.913E-12	2.564E-08	8.605E-12	2.928E-08	9.825E-12	5.918E-08	1.986E-11
Pm-147	2.400E+03	2.050E-05	8.541E-09	2.687E-05	1.120E-08	3.324E-05	1.385E-08	4.020E-05	1.675E-08	4.510E-05	1.879E-08	8.357E-05	3.482E-08
Pu-238	2.620E+00	7.376E-08	2.815E-08	1.342E-07	5.120E-08	2.165E-07	8.265E-08	3.396E-07	1.296E-07	4.443E-07	1.696E-07	1.630E-06	6.222E-07
Pu-239	2.400E+00	5.906E-04	2.461E-04	7.945E-04	3.310E-04	1.002E-03	4.175E-04	1.233E-03	5.137E-04	1.403E-03	5.846E-04	2.592E-03	1.080E-03
Pu-240	2.400E+00	1.836E-06	7.652E-07	3.538E-06	1.474E-06	6.027E-06	2.511E-06	9.576E-06	3.990E-06	1.286E-05	5.359E-06	4.388E-05	1.828E-05
Pu-241	1.320E+02	1.740E-07	1.318E-09	4.463E-07	3.381E-09	9.537E-07	7.225E-09	1.848E-06	1.400E-08	2.843E-06	2.154E-08	1.801E-05	1.364E-07
Pu-242	2.560E+00	1.185E-14	4.631E-15	4.165E-14	1.627E-14	1.154E-13	4.507E-14	2.811E-13	1.098E-13	4.965E-13	1.939E-13	5.843E-12	2.282E-12
Sm-151	3.040E+03	3.333E-03	1.096E-06	4.365E-03	1.436E-06	5.384E-03	1.771E-06	6.490E-03	2.135E-06	7.271E-03	2.392E-06	1.325E-02	4.358E-06
Sr-90	2.590E+01	7.345E-02	2.836E-03	9.643E-02	3.723E-03	1.193E-01	4.604E-03	1.442E-01	5.566E-03	1.618E-01	6.246E-03	2.996E-01	1.157E-02
Tc-99	7.610E+02	2.951E-05	3.877E-08	3.873E-05	5.089E-08	4.792E-05	6.297E-08	5.792E-05	7.611E-08	6.498E-05	8.539E-08	1.204E-04	1.582E-07
Th-228	2.890E+00	5.016E-09	1.736E-09	7.137E-09	2.470E-09	9.710E-09	3.360E-09	1.273E-08	4.403E-09	1.522E-08	5.265E-09	2.815E-08	9.740E-09
Th-230	2.844E+00	9.369E-12	3.294E-12	1.177E-11	4.140E-12	1.414E-11	4.971E-12	1.680E-11	5.908E-12	1.870E-11	6.575E-12	3.275E-11	1.151E-11
U-234	1.320E+01	2.879E-08	2.181E-09	3.511E-08	2.660E-09	4.133E-08	3.131E-09	4.831E-08	3.660E-09	5.333E-08	4.040E-09	9.027E-08	6.839E-09
U-235	1.460E+01	1.154E-04	7.902E-06	1.153E-04	7.900E-06	1.153E-04	7.897E-06	1.152E-04	7.891E-06	1.152E-04	7.889E-06	1.149E-04	7.867E-06
U-236	1.430E+01	8.584E-07	6.003E-08	1.134E-06	7.928E-08	1.410E-06	9.862E-08	1.713E-06	1.198E-07	1.928E-06	1.348E-07	3.570E-06	2.496E-07
U-238	1.540E+01	7.192E-05	4.670E-06	7.192E-05	4.670E-06	7.192E-05	4.670E-06	7.192E-05	4.670E-06	7.192E-05	4.670E-06	7.188E-05	4.668E-06
Y-90	1.767E+03	7.349E-02	4.159E-05	9.647E-02	5.460E-05	1.193E-01	6.752E-05	1.442E-01	8.161E-05	1.618E-01	9.158E-05	2.996E-01	1.696E-04
Ni-63*	5.240E+03	2.235E-03	4.266E-07	2.980E-03	5.687E-07	3.740E-03	7.137E-07	4.573E-03	8.726E-07	5.180E-03	9.886E-07	9.576E-03	1.828E-06
Fe-55*	2.410E+03	7.957E-06	3.302E-09	1.058E-05	4.392E-09	1.333E-05	5.531E-09	1.626E-05	6.748E-09	1.844E-05	7.651E-09	3.406E-05	1.413E-08
Co-60*	2.900E+02	2.693E-07	9.285E-10	3.533E-07	1.218E-09	4.451E-07	1.535E-09	5.361E-07	1.849E-09	6.059E-07	2.089E-09	1.123E-06	3.873E-09
Ni-59*	1.270E+04	2.411E-05	1.899E-09	3.215E-05	2.531E-09	4.035E-05	3.177E-09	4.929E-05	3.881E-09	5.588E-05	4.400E-09	1.033E-04	8.130E-09
Sum of fractions			0.44%		0.58%		0.72%		0.87%		0.98%		1.82%

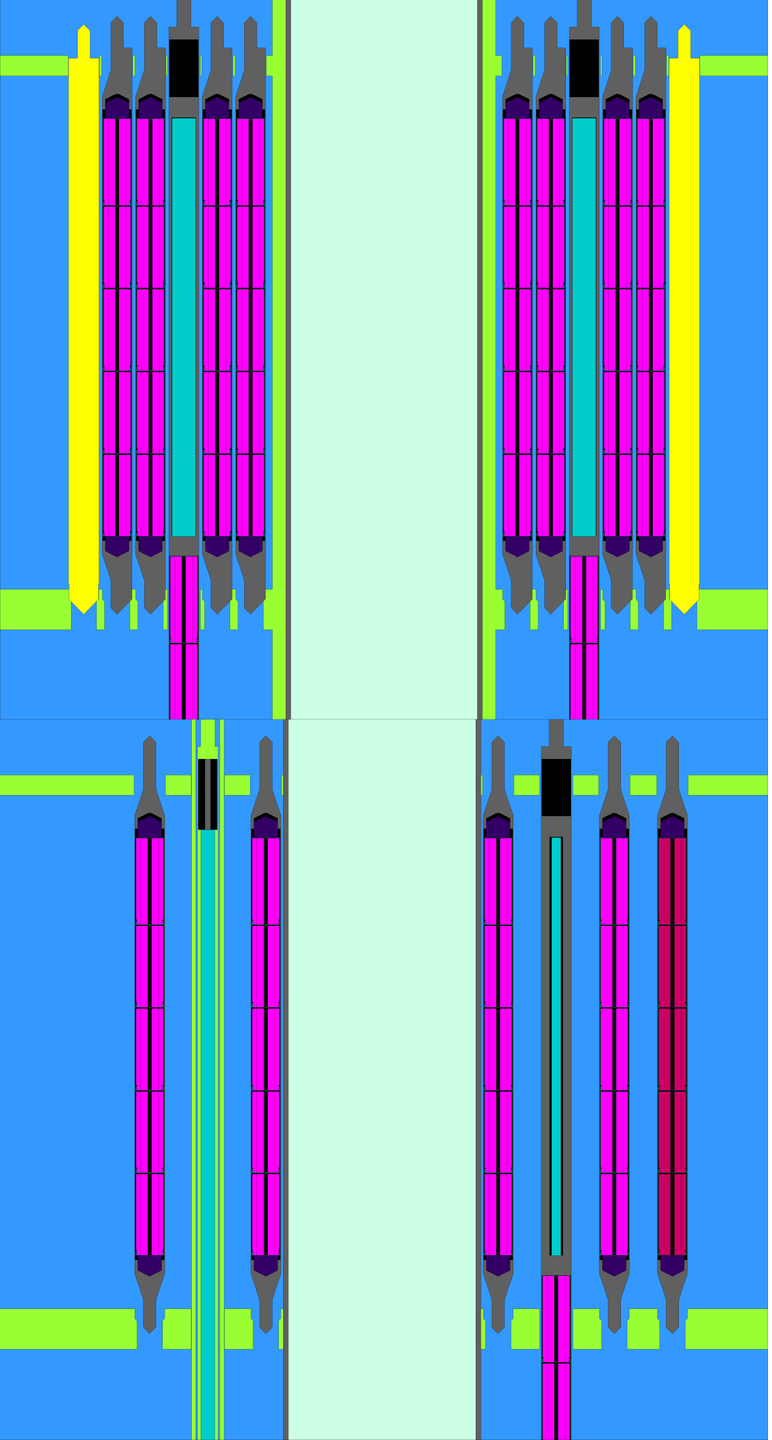
Worst case scenario vs. reality

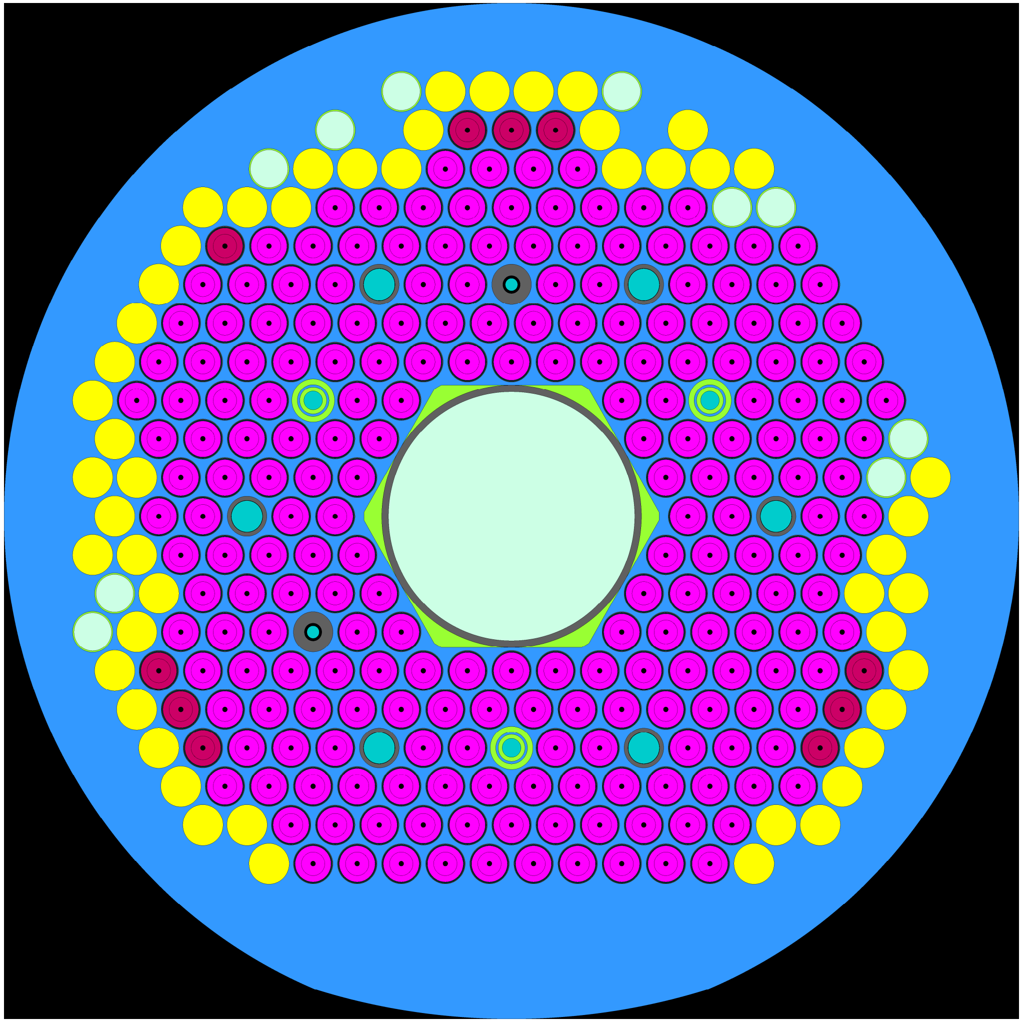


Answer to the original question

- If the container does indeed contain ACPR irradiated fuel, the HC3 sum of fractions should be less than 2%.
- This is a worst case scenario.
- It is likely to be less.
- A more accurate estimate could be determined from the ^{137}Cs activity.

Also while in 1386…





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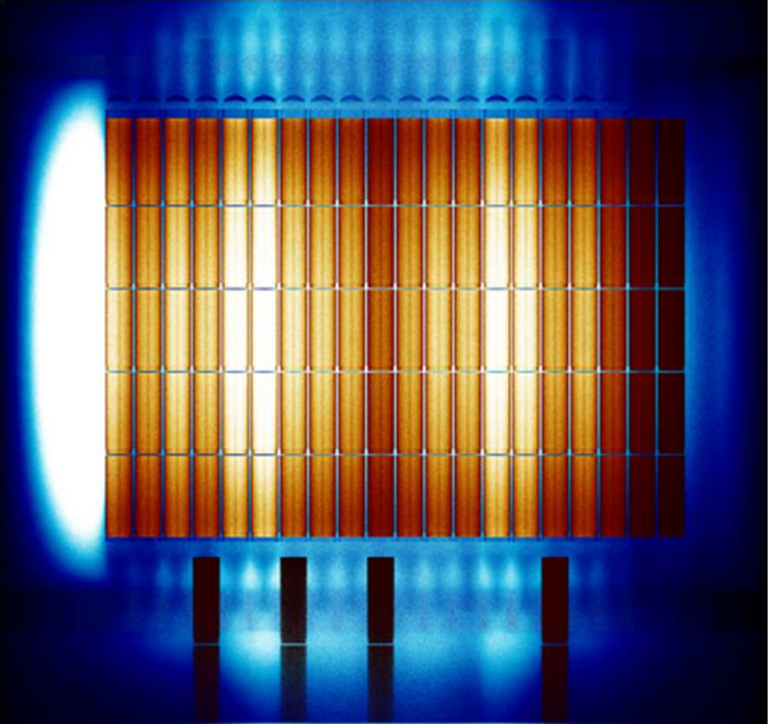

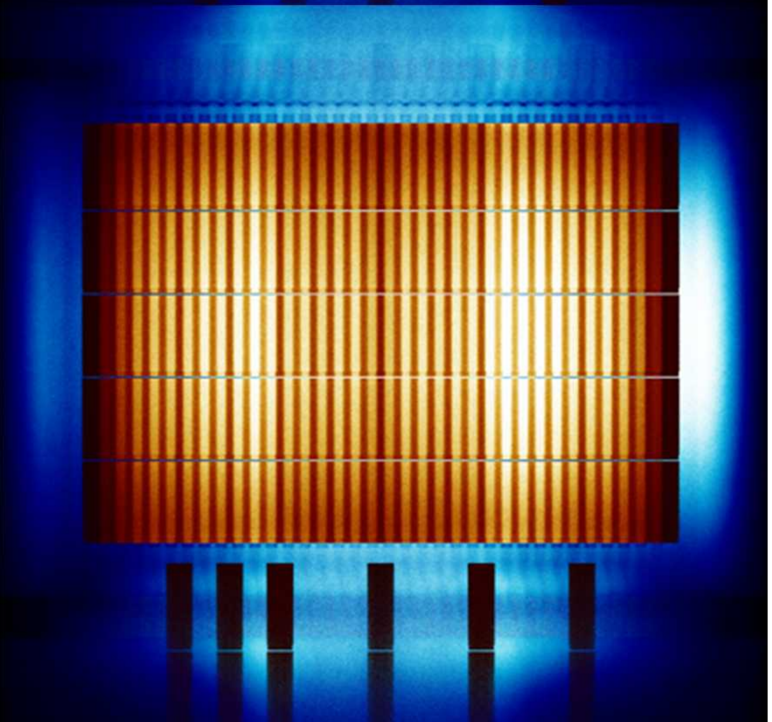

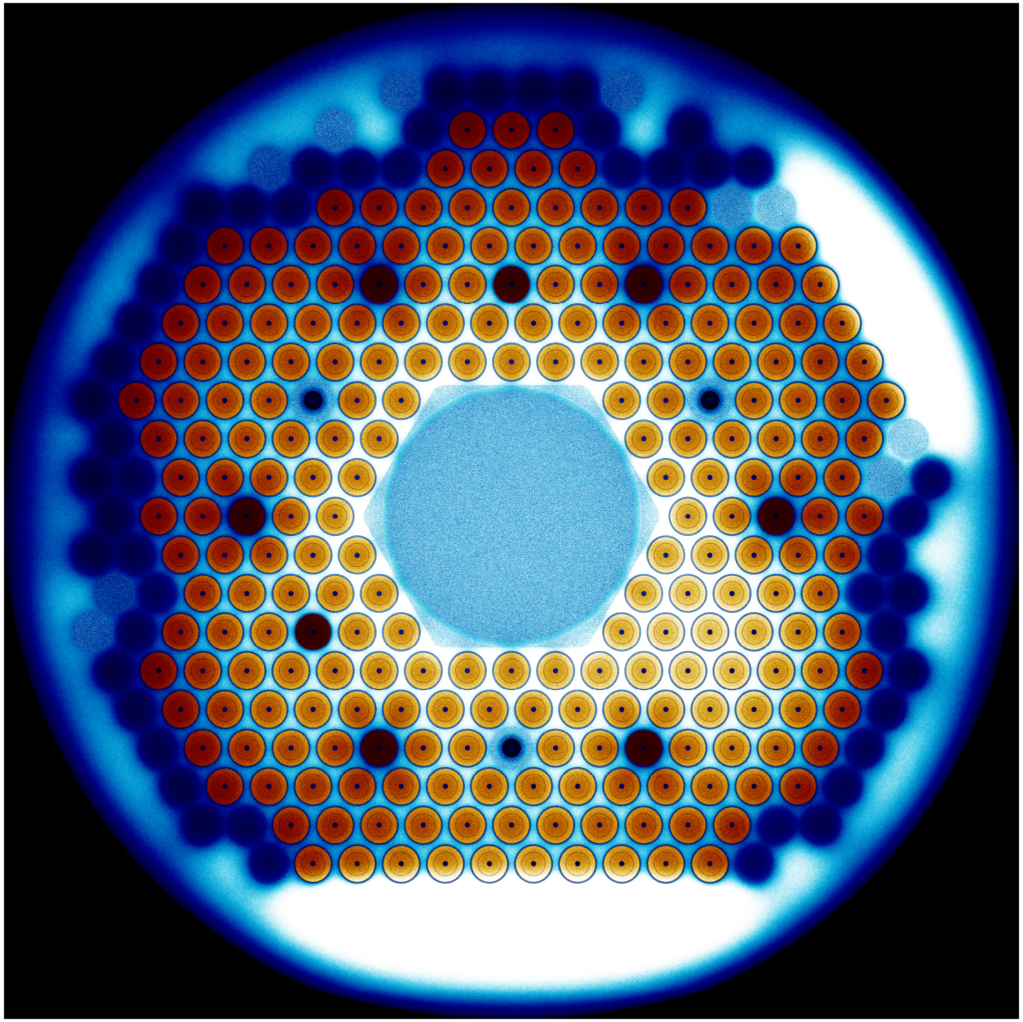

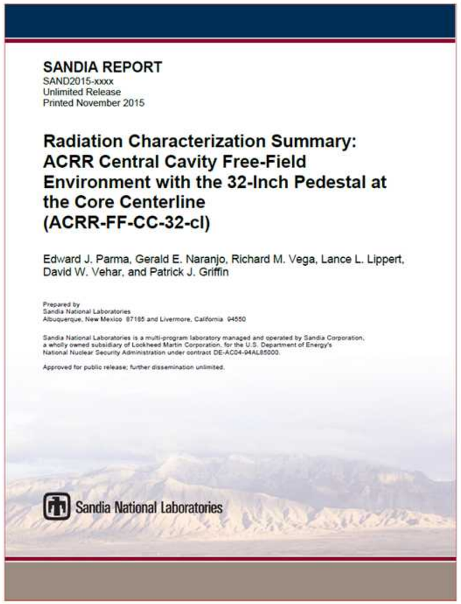
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Radiation Characterization Summary: ACRR Central Cavity Free-Field Environment with the 32-Inch Pedestal at the Core Centerline (ACRR-FF-CC-32-cl)

Edward J. Parma, Gerald E. Naranjo, Richard M. Vega, Lance L. Lippert, David W. Vehar, and Patrick J. Griffin

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Fall 2013 – Summer 2014

"How are your FORTRAN programming skills?"

Applied Nuclear Technologies, 1384

My tasks

- Learn to use LSL-M2.
  - A series of FORTRAN codes automated by a Perl wrapper that reads a text input file.
  - It uses a logarithmic least-squares method to reduce and minimize the uncertainty in the adjusted spectrum.
  - Put my Python skills to use and develop a graphical user interface (GUI) for the input and post-processing.
  - The code is now a series of FORTRAN codes automated by a Perl wrapper that reads a text input file that is created by a Python shell.
- Learn the fine art of spectrum adjustment.
- Learn everything there is to know about reactor dosimetry.
- Perform the neutron spectrum adjustment portion of the ACRR Free-Field characterization.

Spectrum adjustment

- Experimenter's want to know the spectrum with high accuracy to calculate various integral quantities.

$$I = \int_0^\infty \phi(E)R(E)dE$$

- We can calculate the spectrum using MCNP, right?
  - Well, yes…..
  - But how confident are you in the model?
    - Temperatures
    - Densities
    - Approximated geometries
    - Uncertainties in nuclear data
    - Statistical uncertainties
    - Physics models

Spectrum adjustment

- Thus, we acknowledge that the calculated spectrum is close to the actual spectrum, but ultimately incorrect.
- What about measurement of the spectrum?
  - Limited to very low resolution
  - Bonner spheres and other detector methods
    - Limited by the size of the detectors
  - Neutron activation analysis
    - Limited by the number of feasible activation foils available (roughly 30-40)
- Limited to spectrum "unfolding."

Spectrum adjustment

$$I = \int_0^\infty \phi(E) R(E) dE \approx \sum_{i=1}^{n} \phi_i \, R_i \, \Delta E_i$$

Spectrum adjustment

Measured

Variable

Defined

$$I = \int_0^\infty \phi(E) R(E) dE \approx \sum_{i=1}^{n} \phi_i \, R_i \, \Delta E_i$$

Known with some uncertainty

Spectrum adjustment

Measured

Variable

Defined

$$I = \int_0^\infty \phi(E)R(E)dE \approx \sum_{i=1}^{n} \phi_i \, R_i \, \Delta E_i$$

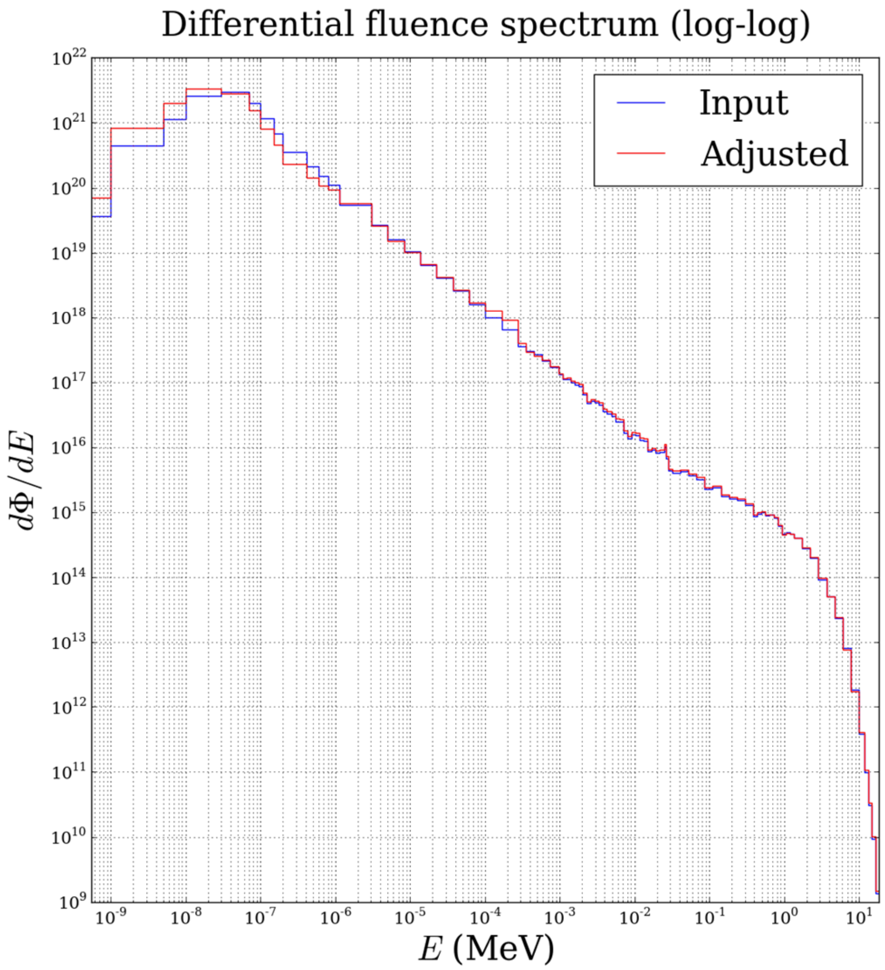
Known with some uncertainty

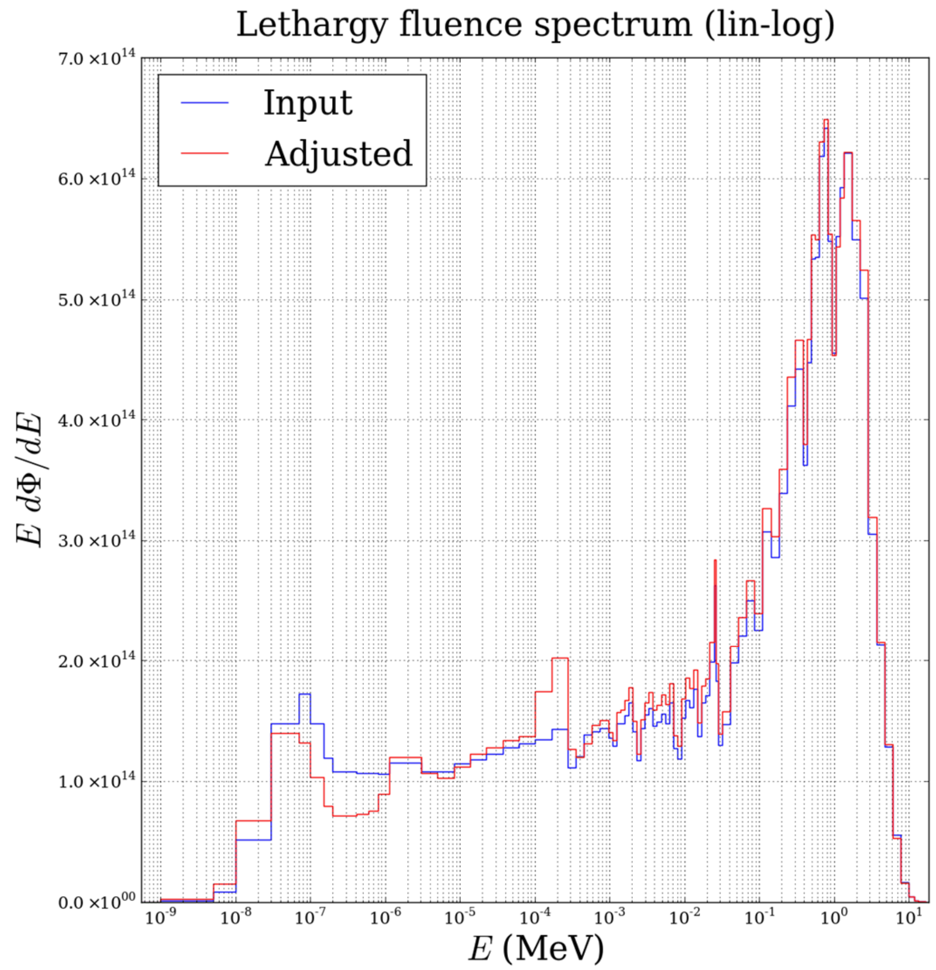
If n is greater than the number of integral quantities, the problem is under-determined, and there are infinitely many solutions.

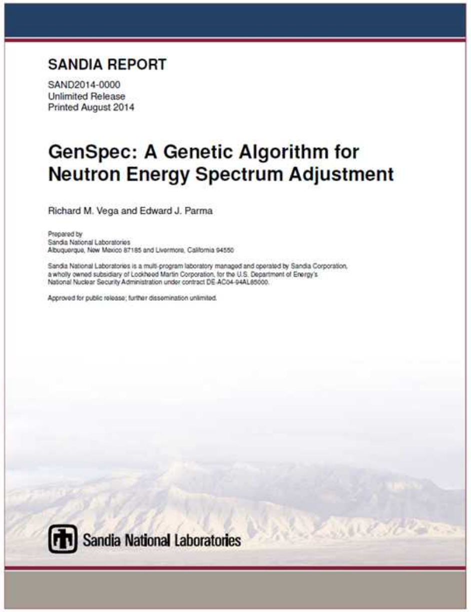
Spectrum adjustment

- This under-determined problem is what we aim to solve in spectrum adjustment.
- In short, we adjust the calculated spectrum to bring it into closer agreement with the experimentally measured integral quantities.
  - Detector responses
  - Activation foils

Free-field adjustment



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GenSpec: A Genetic Algorithm for Neutron Energy Spectrum Adjustment

Richard M. Vega and Edward J. Parma

Prepared by
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Summer 2014 – Summer 2015

"What do you mean you are going to *mate* two spectra?"

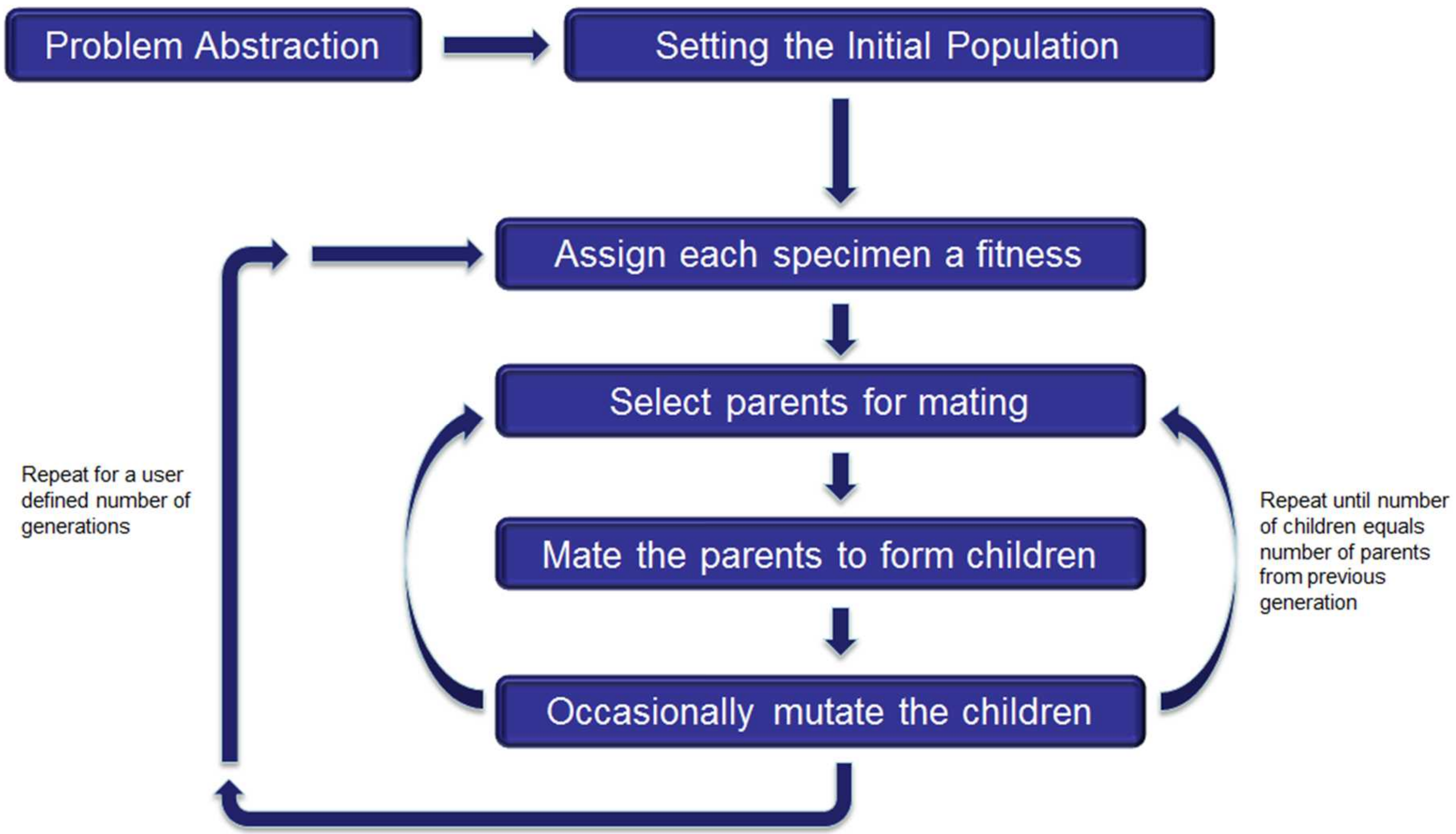
Applied Nuclear Technologies, 1384

Issues with LSL-M2 (and most other methods)

- Artificial spectral shape artefacts.
  - Post adjustment smoothing may remove resonance features from the spectrum.
- Reduction in accuracy for high resolution input spectra.
- Reduction and minimization of uncertainties implies that the *a priori* uncertainties and correlations are known.

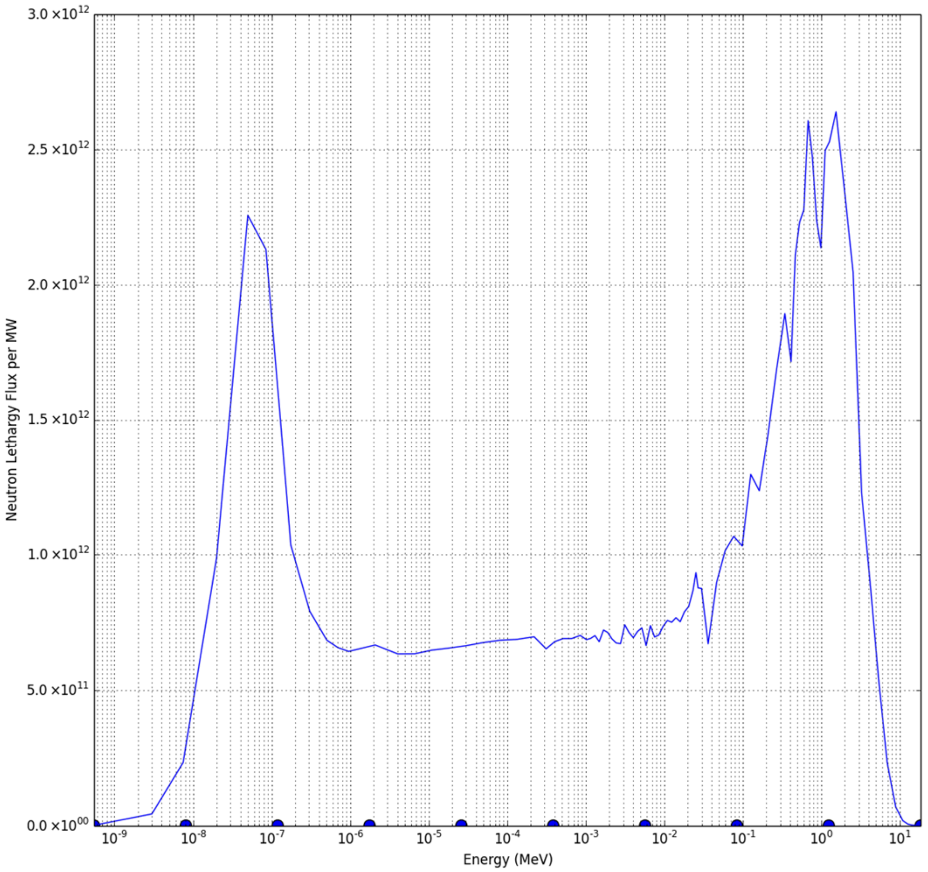
- Solution: use a relative adjustment function for which the smoothness can be controlled, and which is defined at points in energy space that are decoupled from the energy grid structure of the trial spectrum.
  - Then optimize these functions somehow.

Genetic algorithms



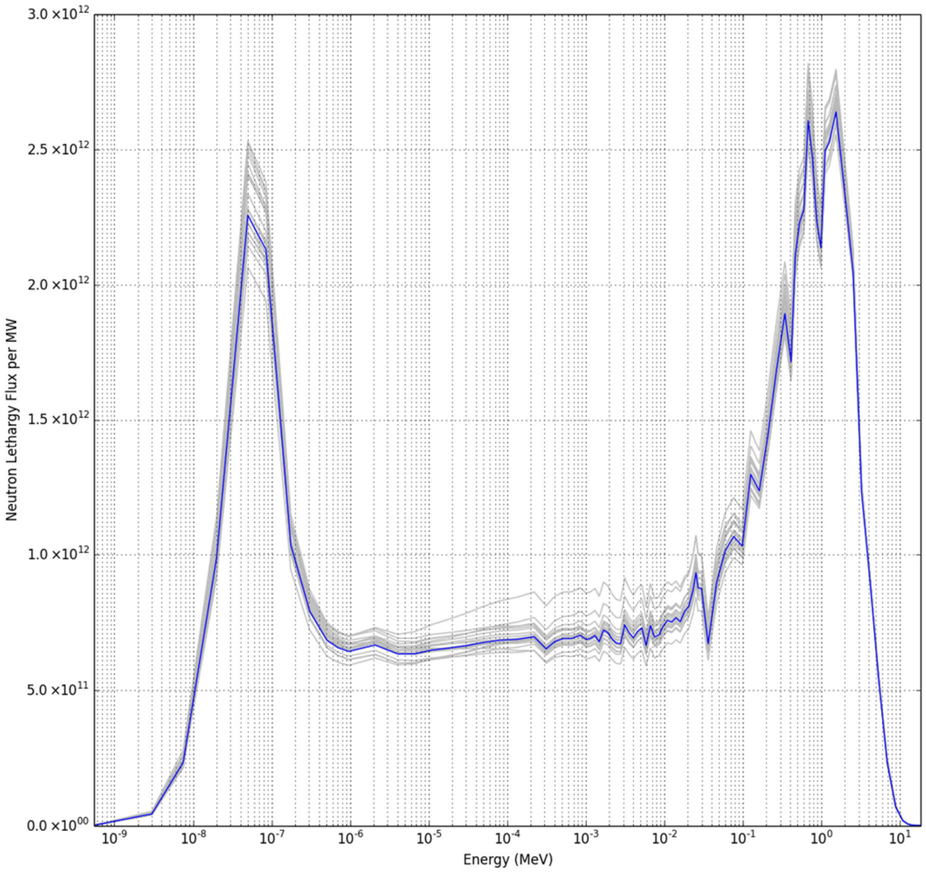
Abstraction

- Step 1: select the number of genes: N.
- Step 2: determine the energy domain
- Step 3: select N points equidistant in log-space: GENE SITES.
- Step 4: each site is assigned a real number (typically close to 1): GENE VALUES.



Setting the population

- For each specimen:
  - For each gene site:
    - Pull a random Gaussian distributed number (μ = 0, σ = 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



Fitness function

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

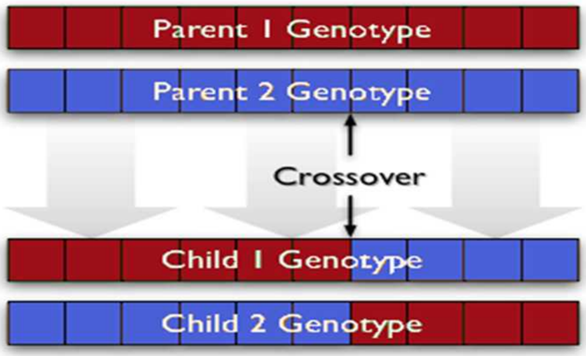
Parent selection

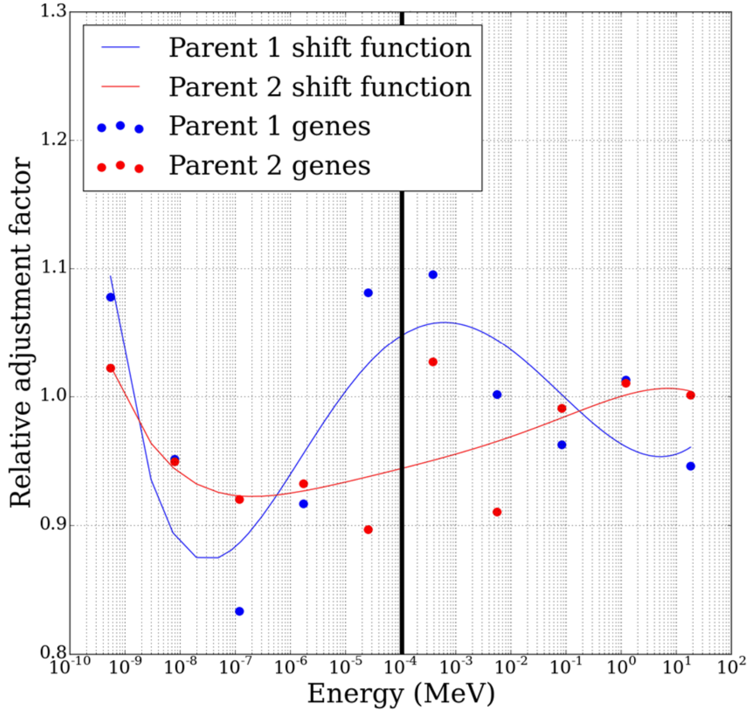
$$P_j = \frac{f_j - f_{min}}{P_t}$$

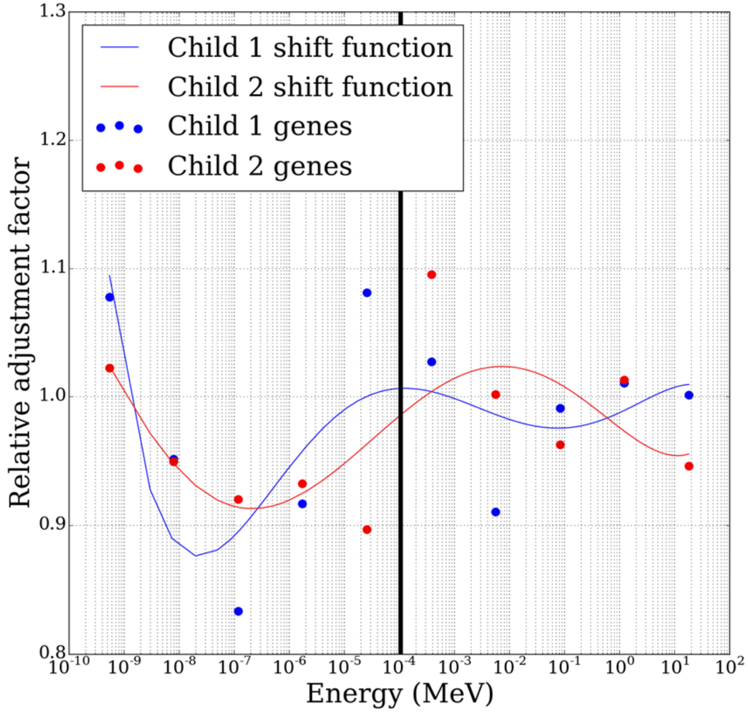
$$P_t = \sum_{i=1}^{s} (f_i - f_{min})$$

Mating

- Crossover: given 2 parents, it will produce 2 children.
- Mutation

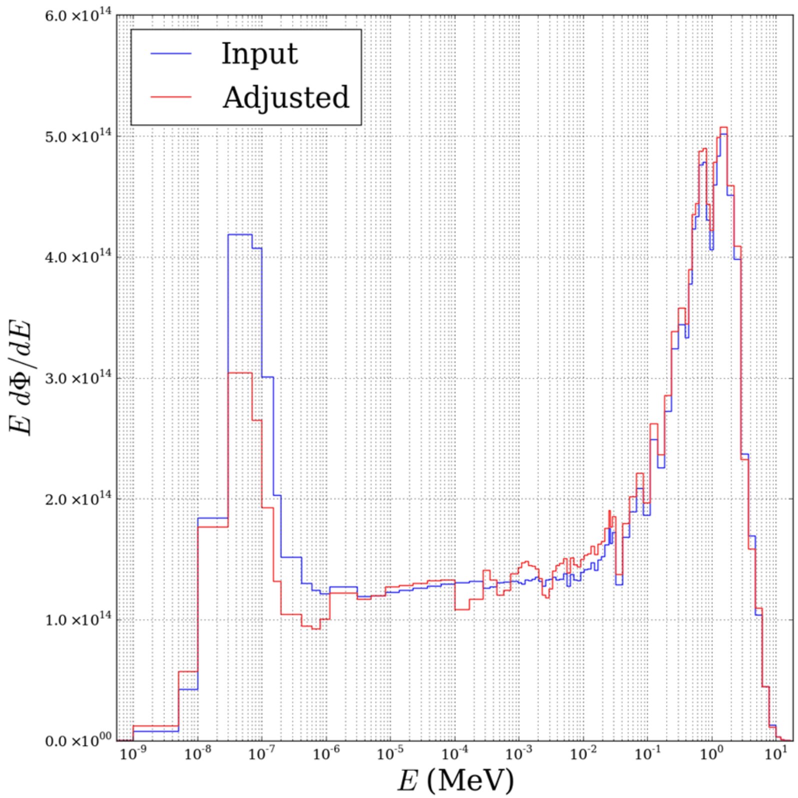




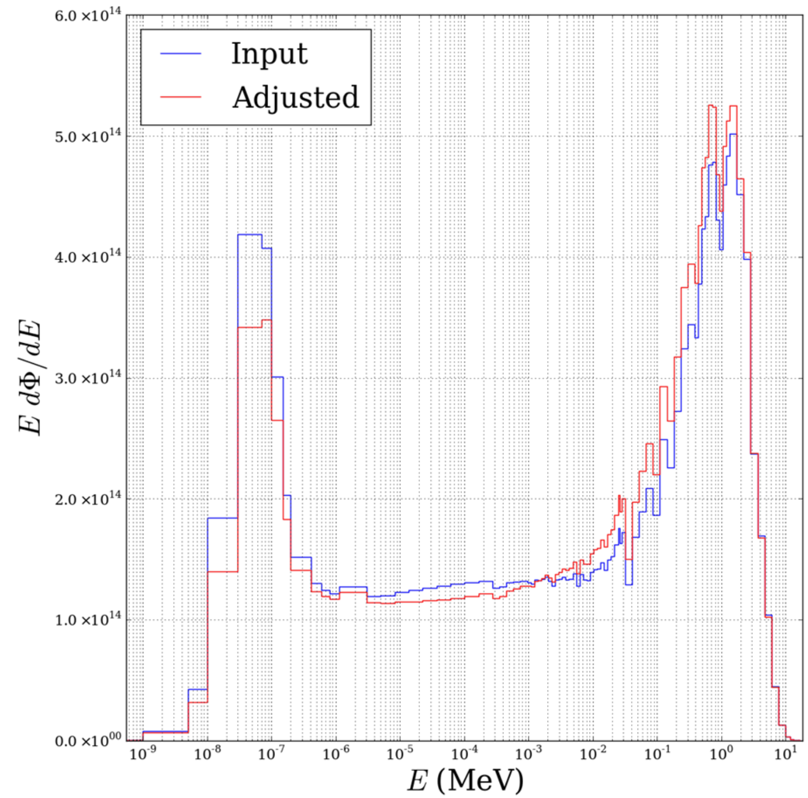


Results (PLG)

LSL-M2

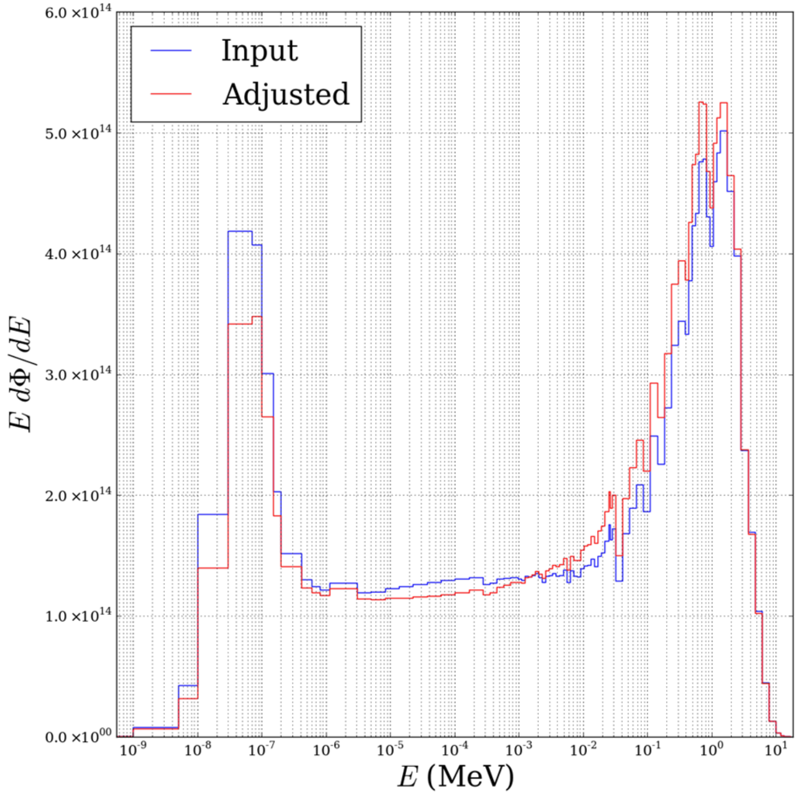


GenSpec

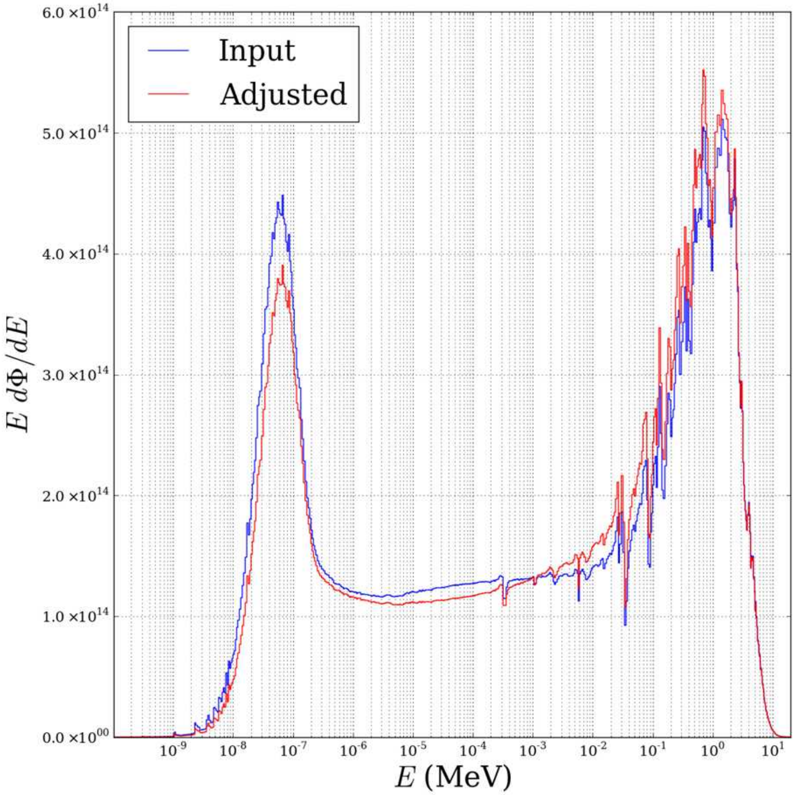


Results (PLG)

89 Groups



640 Groups



Summer 2015 - ??

"If you had to plow a field would you use one Ox or 1,344 chickens?"

Applied Nuclear Technologies, 1384

My current status

- Just finished first year of graduate school at TAMU.
- Just finished first year on the Stewardship Science Graduate Fellowship.
- Dissertation topic: Application of the Linear Discontinuous Finite Element Method to the Slice Balance Approach for Discrete Ordinates Neutral Particle Transport on Unstructured Meshes Using Advanced Computing Architectures.
  - Advanced computing architectures: graphics processing units (GPU's)
- Current collaboration with Sandia:
  - Implementation of dissertation work in the NuGET code for long distance air transport.

Why GPU’s?

Sandia National Laboratories

- Think of a GPU as 1000’s of tiny CPU’s.
  - Ox vs. chickens debate.
- Comparable power consumption.
  - My GPU = 110 W.
  - My CPU = 88 W.
- Limited capabilities.
- Slow global memory access.
- DOE has already invested.

Preliminary study

- 3-D Cartesian cubic domain (32 × 32 × 32).
  - LDFEM.
- Variable number of angles.
  - Discrete ordinates.
- Variable number of energy groups.
  - Standard multigroup.
- CPU used: single core of an Intel i7=4700HQ.
- GPU used: NVIDIA GTX 870M

Total number of cores	1344
Core clock rate (MHz)	941
Memory (GB)	3
Memory bandwidth (GB/s)	120
Processing power (GFLOPS)	2599
Number of compute units	7

Preliminary results

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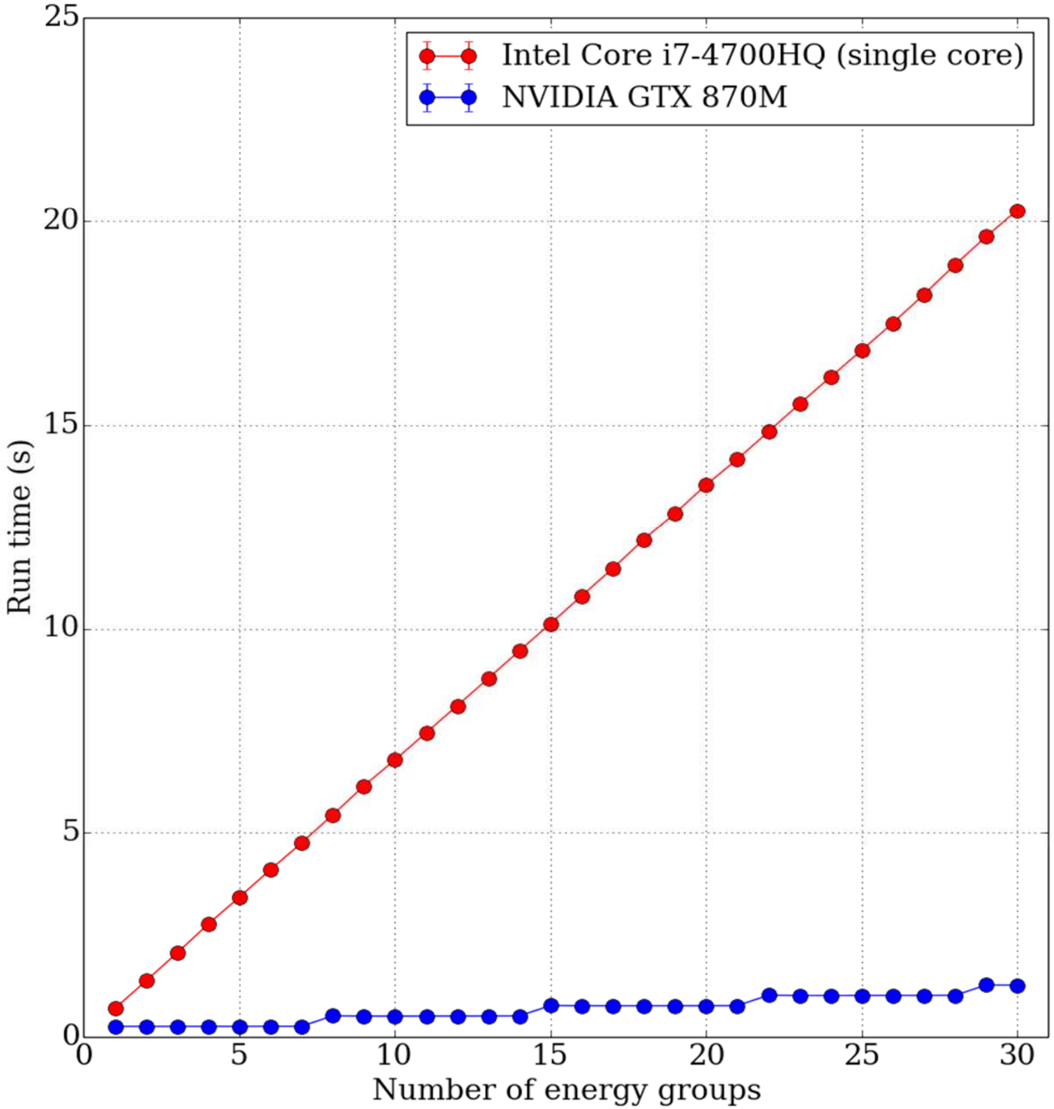


Number of energy groups n	S_n/S_1
7	6.925989
14	6.949351
21	6.972942
28	6.981601
35	6.973584
42	6.976728
49	6.979962

Preliminary results

No local memory usage, double precision

Angles	50	500	1,000	3,000
Send time	0.000777	0.003936	0.006429	0.017100
Sweep time	0.124067	1.236908	2.473309	7.417332
Receive time	0.001008	0.000498	0.000275	0.000259
Total time	0.125852	1.241343	2.480014	7.434691
Sequential time	0.342542	3.456955	6.865171	20.43647
Speedup	2.721778	2.784852	2.768199	2.748798
TOTAL SPEEDUP $\approx 2.75 \times 7 = 19.25$				

Preliminary results

With local memory usage, double precision

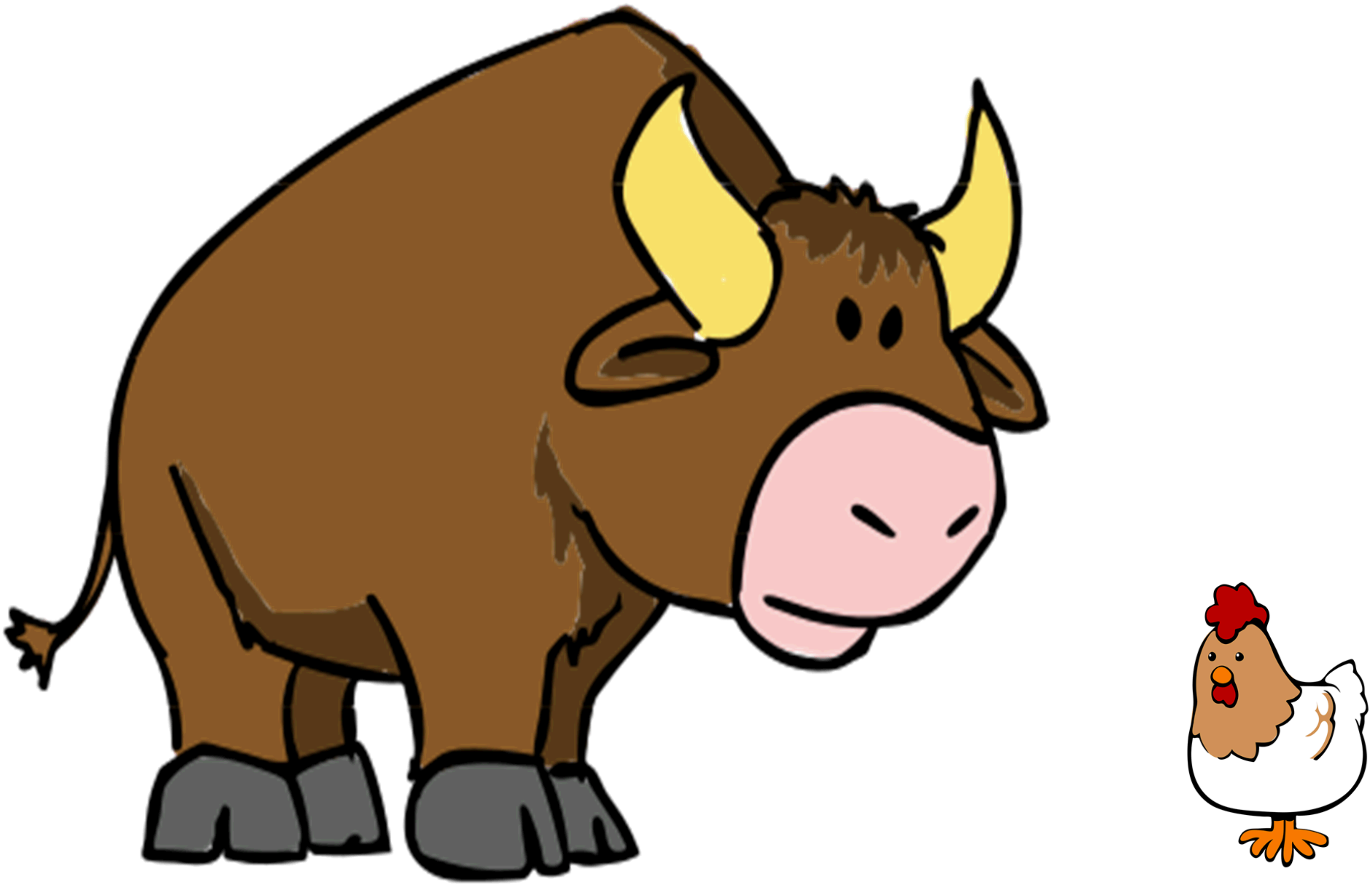
Angles	50	500	1,000	3,000
Send time	0.000773	0.003916	0.006524	0.017086
Sweep time	0.108265	1.072916	2.147477	6.437213
Receive time	0.000932	0.000550	0.000240	0.000502
Total time	0.109970	1.077383	2.154241	6.454801
Sequential time	0.342542	3.456955	6.865171	20.43646
Speedup	3.114858	3.208660	3.186816	3.166088
TOTAL SPEEDUP $\approx 3.15 \times 7 = 22.05$				

Preliminary results

With local memory usage, single precision

Angles	50	500	1,000	3,000
Send time	0.000378	0.002304	0.003647	0.009334
Sweep time	0.073435	0.729614	1.463238	4.388410
Receive time	0.000849	0.000975	0.000610	0.000516
Total time	0.074661	0.732893	1.467495	4.398260
Sequential time	0.336183	3.377517	6.703176	19.98432
Speedup	4.502774	4.608471	4.567768	4.543688
TOTAL SPEEDUP $\approx 4.55 \times 7 = 31.50$				

Have I answered the question?



Have I answered the question?

A better, less funny question…

- How do you utilize the entire machine?
  - Multi-physics?
  - Staggered high-order low-order methods?
  - Scheduling?

And finally, is Sandia right for you?

- Great work environment.
- Very well managed.
- Not in the middle of nowhere (…. INL, LANL).
- But also not in a over-crowded city (… ANL).
- Not an insanely high cost of living (… LLNL).
- There’s a lot of interesting work to be done.
- Flexibility.
- Training opportunities.
- Year-round opportunities.
- Travel opportunities (conferences).
- Lots of cool toys (White).

Questions?