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Title: Computational Physics at Los Alamos National Laboratory: Monte Carlo Methods and Code Development for Nuclear Nonproliferation and Safeguards Applications

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NATIONAL LABORATORY
EST. 1943

Delivering science and technology
to protect our nation
and promote world stability

NNSA
National Nuclear Security Administration

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Computational Physics at Los Alamos National Laboratory

Monte Carlo Methods and Code Development for Nuclear Nonproliferation and Safeguards Applications

Oregon State University

Nuclear Engineering Seminar

Michael E. Rising
XCP-3 Group, LANL

March 13, 2017

The role of Los Alamos for the Nation

Office of Science Laboratories

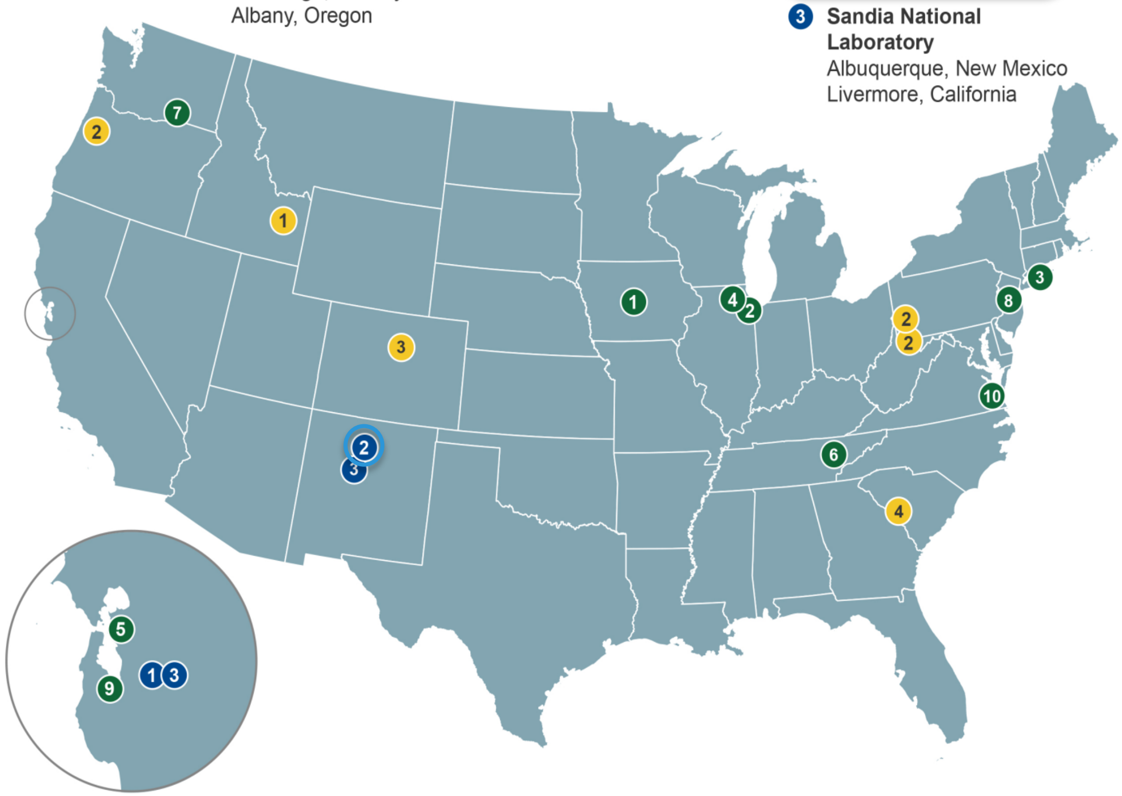
1. **Ames Laboratory**
   Ames, Iowa
2. **Argonne National Laboratory**
   Argonne, Illinois
3. **Brookhaven National Laboratory**
   Upton, New York
4. **Fermi National Accelerator Laboratory**
   Batavia, Illinois
5. **Lawrence Berkeley National Laboratory**
   Berkeley, California
6. **Oak Ridge National Laboratory**
   Oak Ridge, Tennessee
7. **Pacific Northwest National Laboratory**
   Richland, Washington
8. **Princeton Plasma Physics Laboratory**
   Princeton, New Jersey
9. **SLAC National Accelerator Laboratory**
   Menlo Park, California
10. **Thomas Jefferson National Accelerator Facility**
    Newport News, Virginia

Other DOE Laboratories

1. **Idaho National Laboratory**
   Idaho Falls, Idaho
2. **National Energy Technology Laboratory**
   Morgantown, West Virginia
   Pittsburgh, Pennsylvania
   Albany, Oregon
3. **National Renewable Energy Laboratory**
   Golden, Colorado
4. **Savannah River National Laboratory**
   Aiken, South Carolina

NNSA Laboratories

1. **Lawrence Livermore National Laboratory**
   Livermore, California
2. **Los Alamos National Laboratory**
   Los Alamos, New Mexico
3. **Sandia National Laboratory**
   Albuquerque, New Mexico
   Livermore, California



LANL's Mission

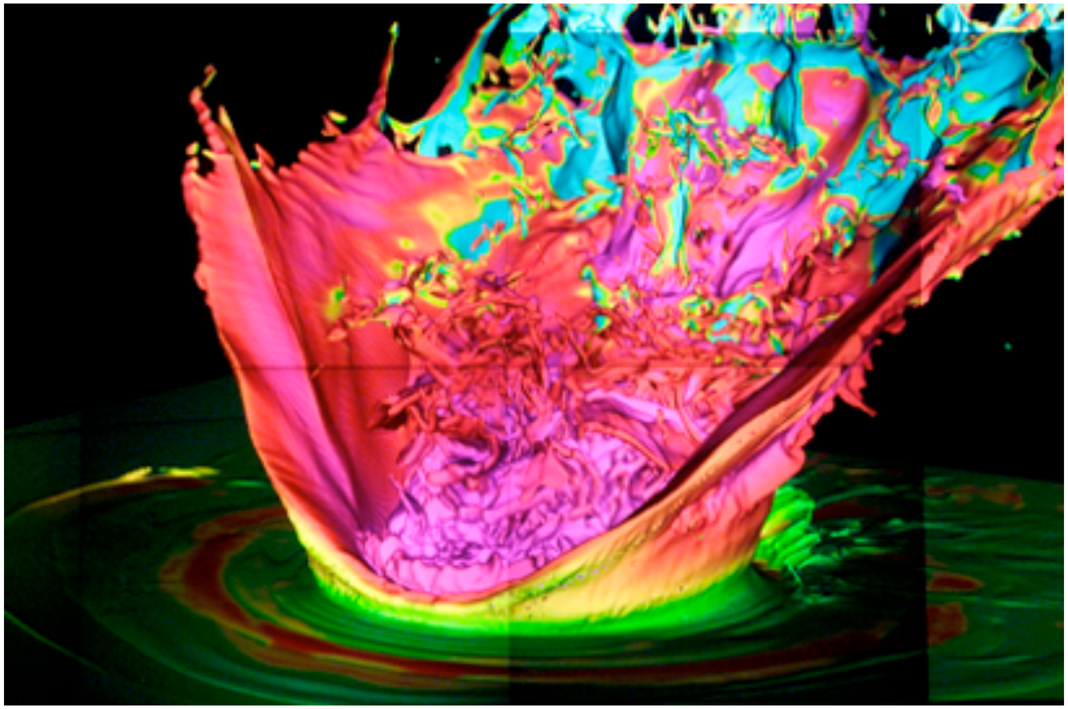
Solve national security challenges through scientific excellence

What does LANL's Computational Physics (XCP) Division Do?

- The X Computational Physics Division (XCP) develops and uses multiphysics simulation codes, as well as underlying physics models and numerical algorithms, to support basic science and applications in national nuclear security.
- We take advantage of some of the world's fastest and most advanced computing platforms running state-of-the-art simulation codes to study a variety of complex physics problems.

Groups within the XCP Division

- XCP-1 Lagrangian Codes
- XCP-2 Eulerian Codes
- XCP-3 Monte Carlo Methods, Codes & Applications
- XCP-4 Methods & Algorithms
- XCP-5 Materials & Physical Data
- XCP-6 Plasma Theory & Applications
- XCP-8 Verification & Analysis



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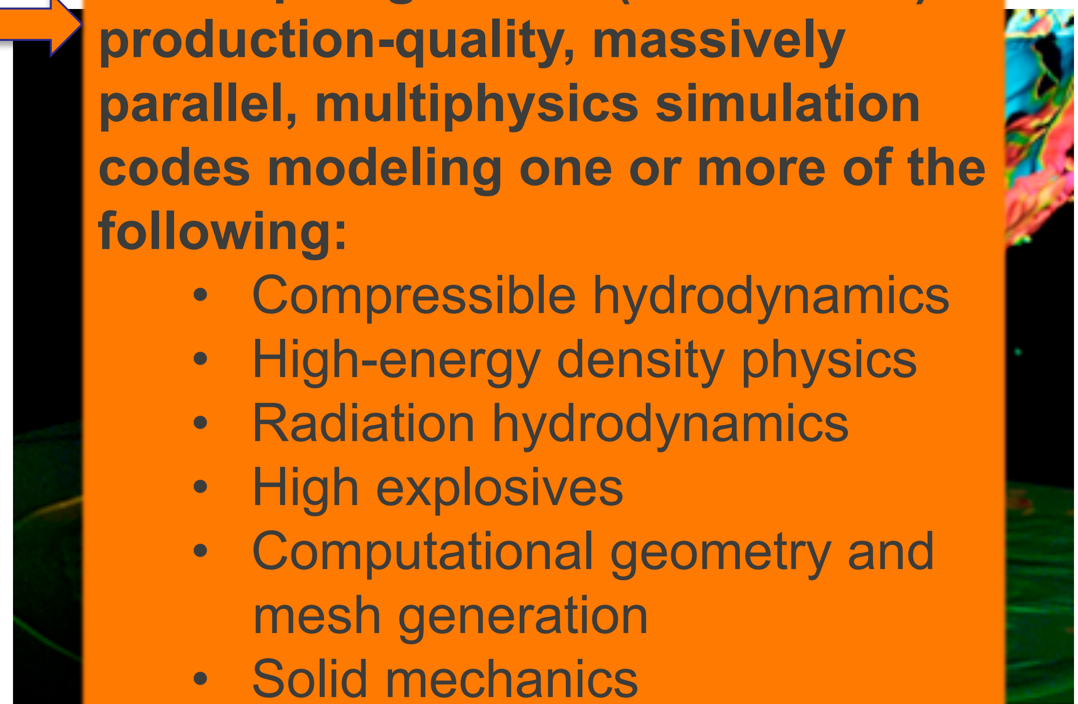

Develop large-scale (~ 1M SLOC) production-quality, massively parallel, multiphysics simulation codes modeling one or more of the following:

- Compressible hydrodynamics
- High-energy density physics
- Radiation hydrodynamics
- High explosives
- Computational geometry and mesh generation
- Solid mechanics
- Turbulent mixing
- Thermonuclear burn physics

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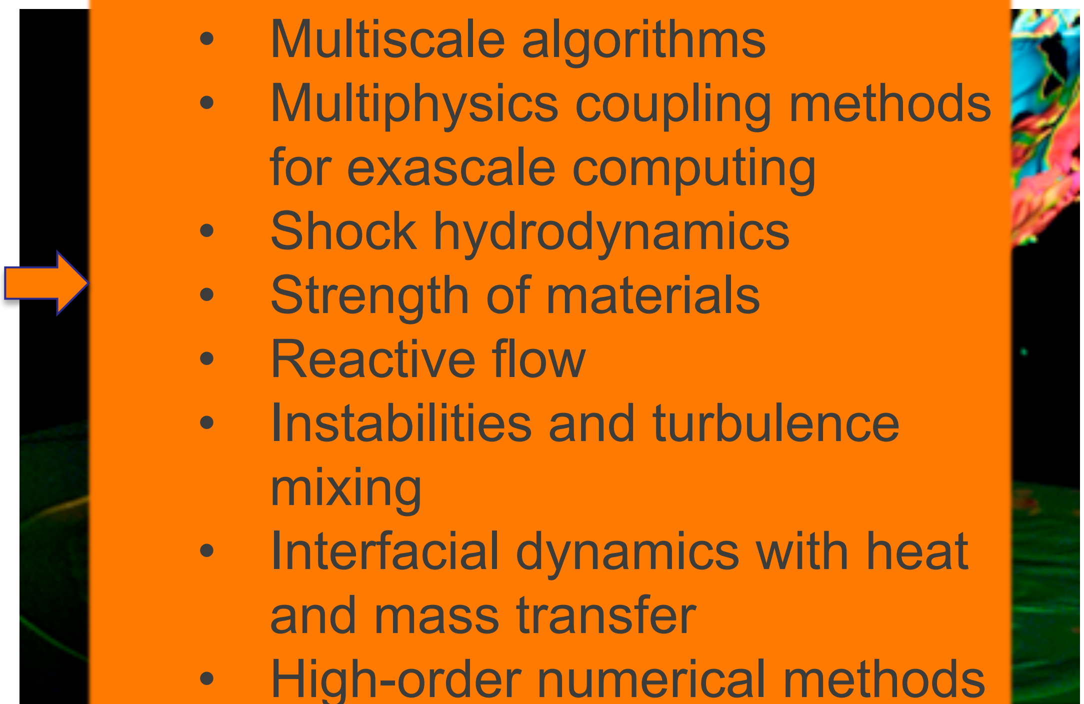

Interest in:

- Multiscale algorithms
- Multiphysics coupling methods for exascale computing
- Shock hydrodynamics
- Strength of materials
- Reactive flow
- Instabilities and turbulence mixing
- Interfacial dynamics with heat and mass transfer
- High-order numerical methods for compressible flow

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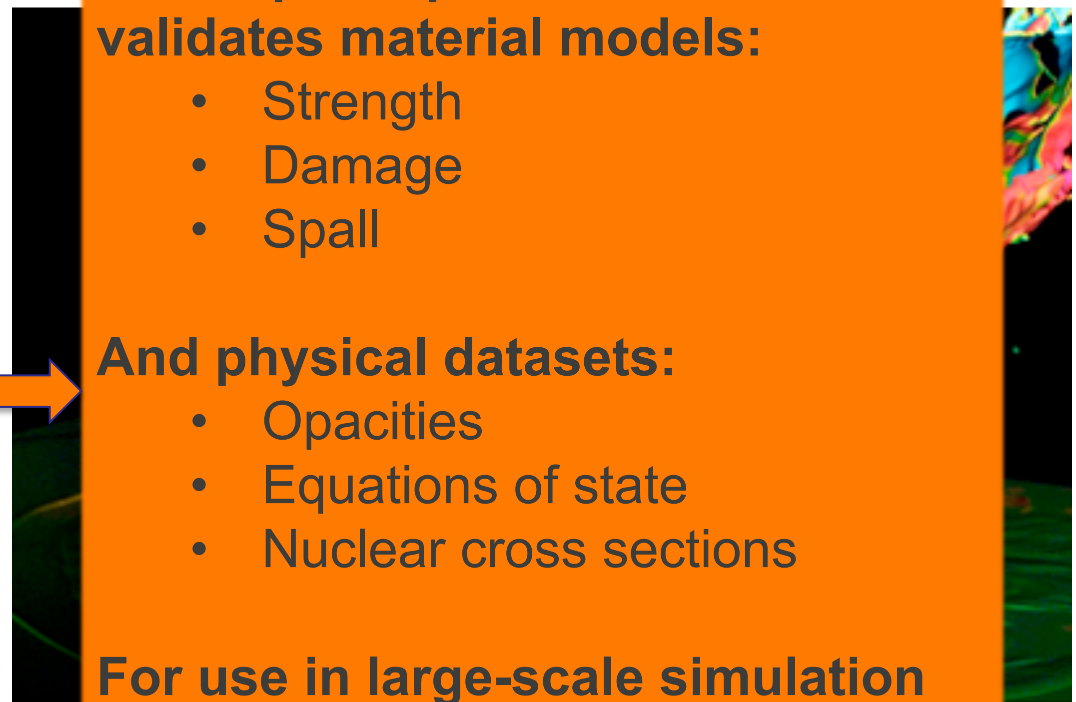


Develops, implements and validates material models:

- Strength
- Damage
- Spall

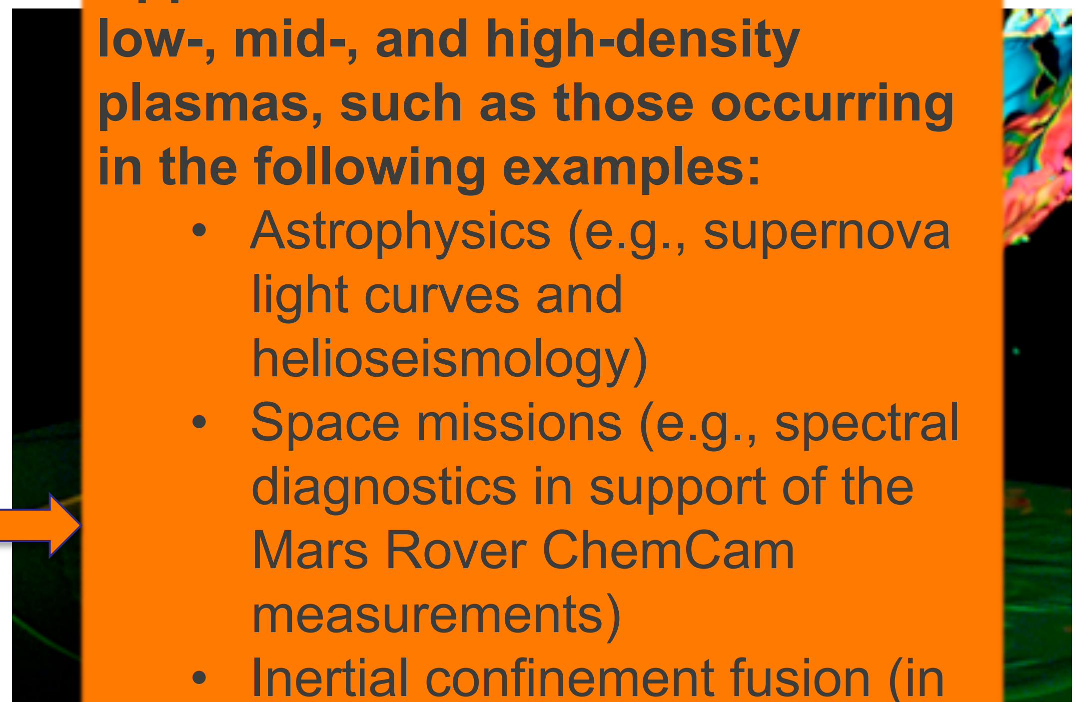
And physical datasets:

- Opacities
- Equations of state
- Nuclear cross sections

For use in large-scale simulation codes

Groups within the XCP Division

- **XCP-1** **Lagrangian Codes**
- **XCP-2** **Eulerian Codes**
- **XCP-3** **Monte Carlo Methods, Codes & Applications**
- **XCP-4** **Methods & Algorithms**
- **XCP-5** **Materials & Physical Data**
- **XCP-6** **Plasma Theory & Applications**
- **XCP-8** **Verification & Analysis**



Applications of interest include low-, mid-, and high-density plasmas, such as those occurring in the following examples:

- Astrophysics (e.g., supernova light curves and helioseismology)
- Space missions (e.g., spectral diagnostics in support of the Mars Rover ChemCam measurements)
- Inertial confinement fusion (in support of Omega and the National Ignition Facility)

Groups within the XCP Division

XCP-1 Lagrangian Codes

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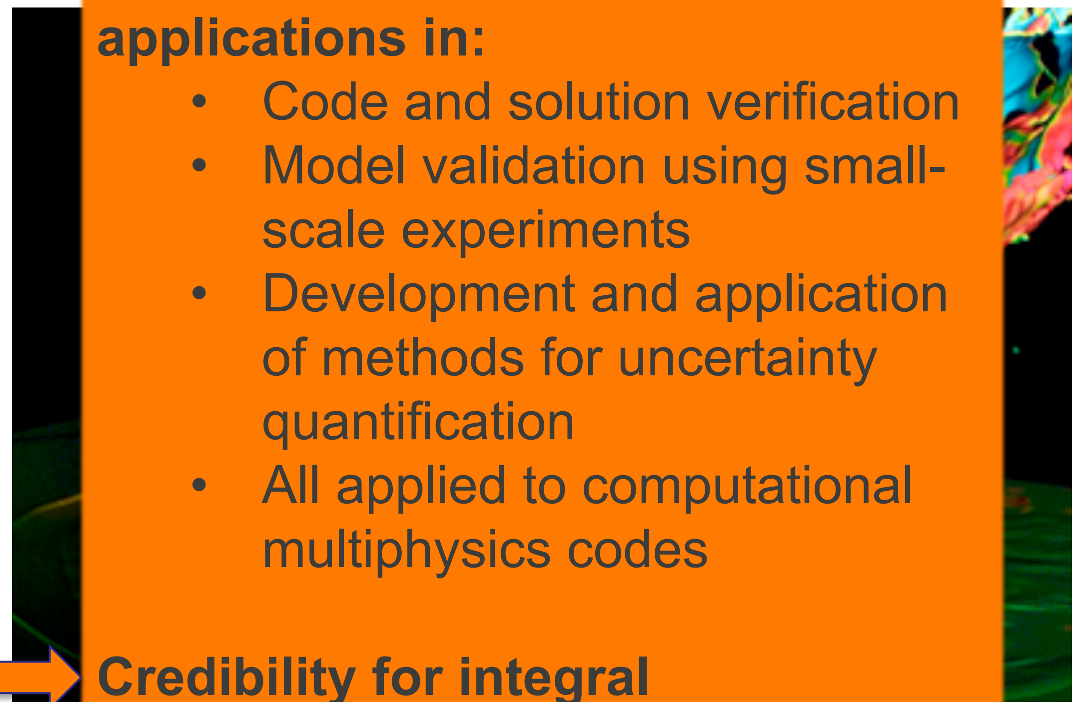

Interested in research and applications in:

- Code and solution verification
- Model validation using small-scale experiments
- Development and application of methods for uncertainty quantification
- All applied to computational multiphysics codes

Credibility for integral multiphysics calculations

Groups within the XCP Division

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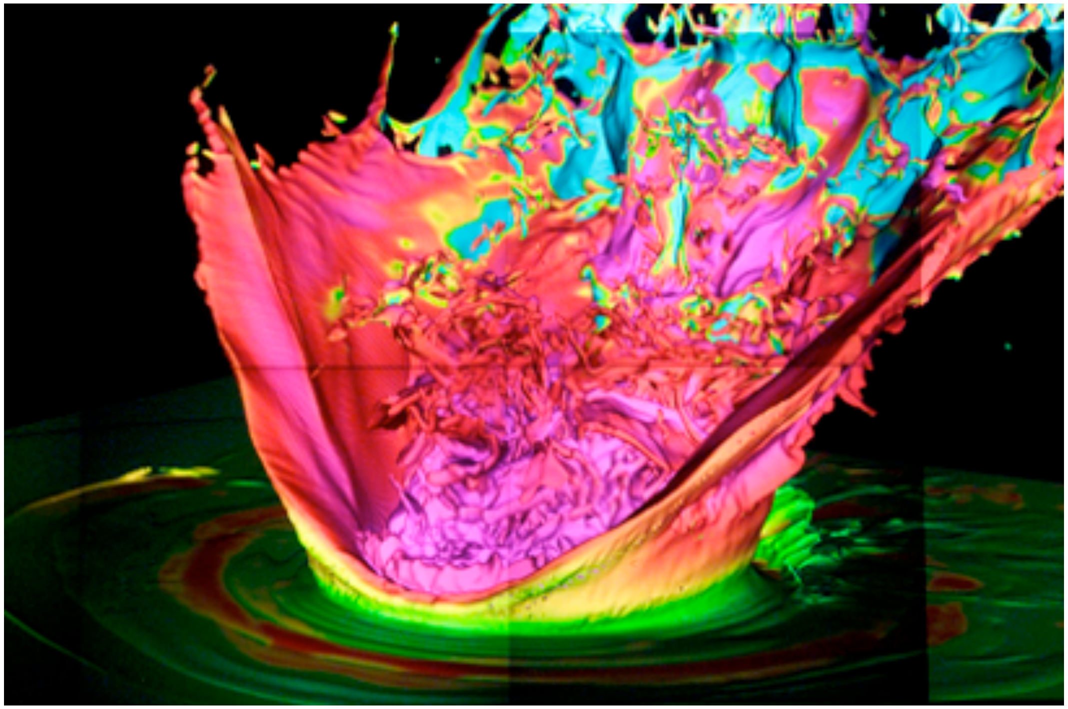
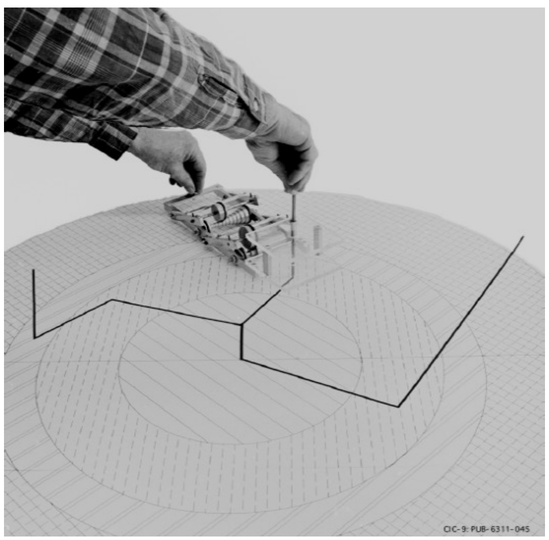


XCP-3: Monte Carlo Methods, Codes & Applications

- **We deliver:**
  - First-principles Monte Carlo methods
  - Production-quality codes
  - Radiation transport-based computational and experimental assessments
- **Our codes:**
  - MCNP
  - MCATK
- **Our applications:**
  - Criticality safety
  - Non-proliferation
  - Nuclear energy
  - Nuclear threat reduction and response
  - Radiation detection and measurement
  - Radiation health protection
  - Stockpile stewardship

LANL’s Long History with Monte Carlo

- **Monte Carlo Method for Radiation Transport Originated at LANL**
  - Stanislaw Ulam, John von Neumann, Robert Richtmyer, and Nicholas Metropolis
  - Early calculations performed on the FERMIAC11 and MANIAC machines
- **Monte Carlo code development and applications have been an important part of LANL efforts since that time**



FERMIAC11 mechanically traced neutron paths

MANIAC computer performed early Monte Carlo calculations

Monte Carlo & MCNP History

ENIAC – 1945

30 tons

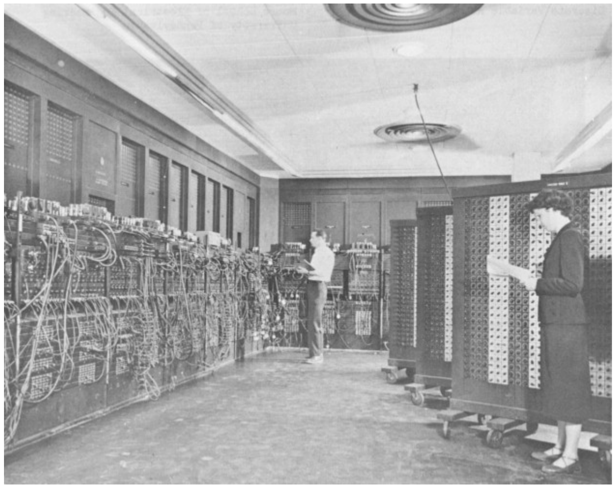
20 ft x 40 ft room

18,000 vacuum tubes

0.1 MHz

20 word memory

patchcords



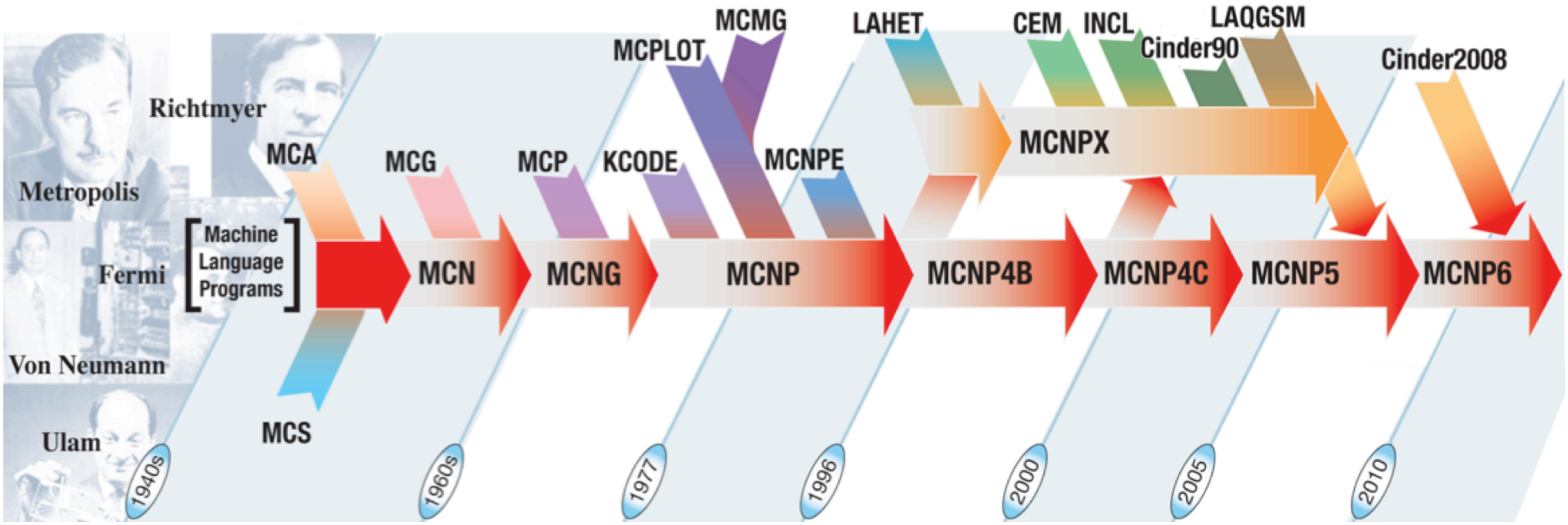
Manhattan Project – 1945...

Discussions on using ENIAC

Ulam suggested using the "method of statistical trials"

Metropolis suggested the name "Monte Carlo"

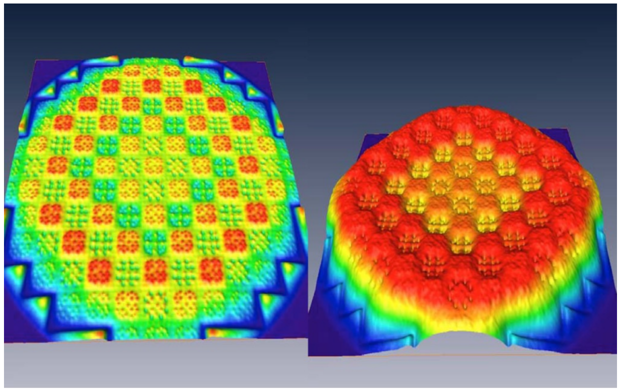
Von Neumann developed the first computer code



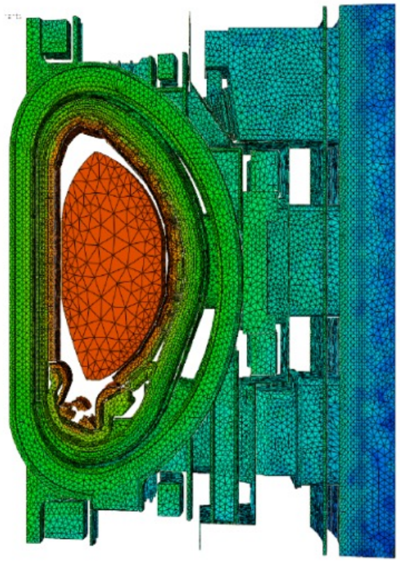
MCNP Capabilities

- **Physics:**
  - Continuous energy particle transport
  - Neutron, photon, electron, and many more particle types
- **Algorithms:**
  - k-eigenvalue calculations
  - Fixed source calculations
- **Recently Implemented Features:**
  - Unstructured mesh transport
  - Electric and magnetic field transport
  - High-energy physics models
  - 33 additional particle types
  - Reactor fuel depletion and burnup
  - Radiation source and detection capabilities
  - Sensitivity and uncertainty analysis for nuclear criticality safety
- **Extensive Variance Reduction**
  - Weight Windows
  - DXTRAN

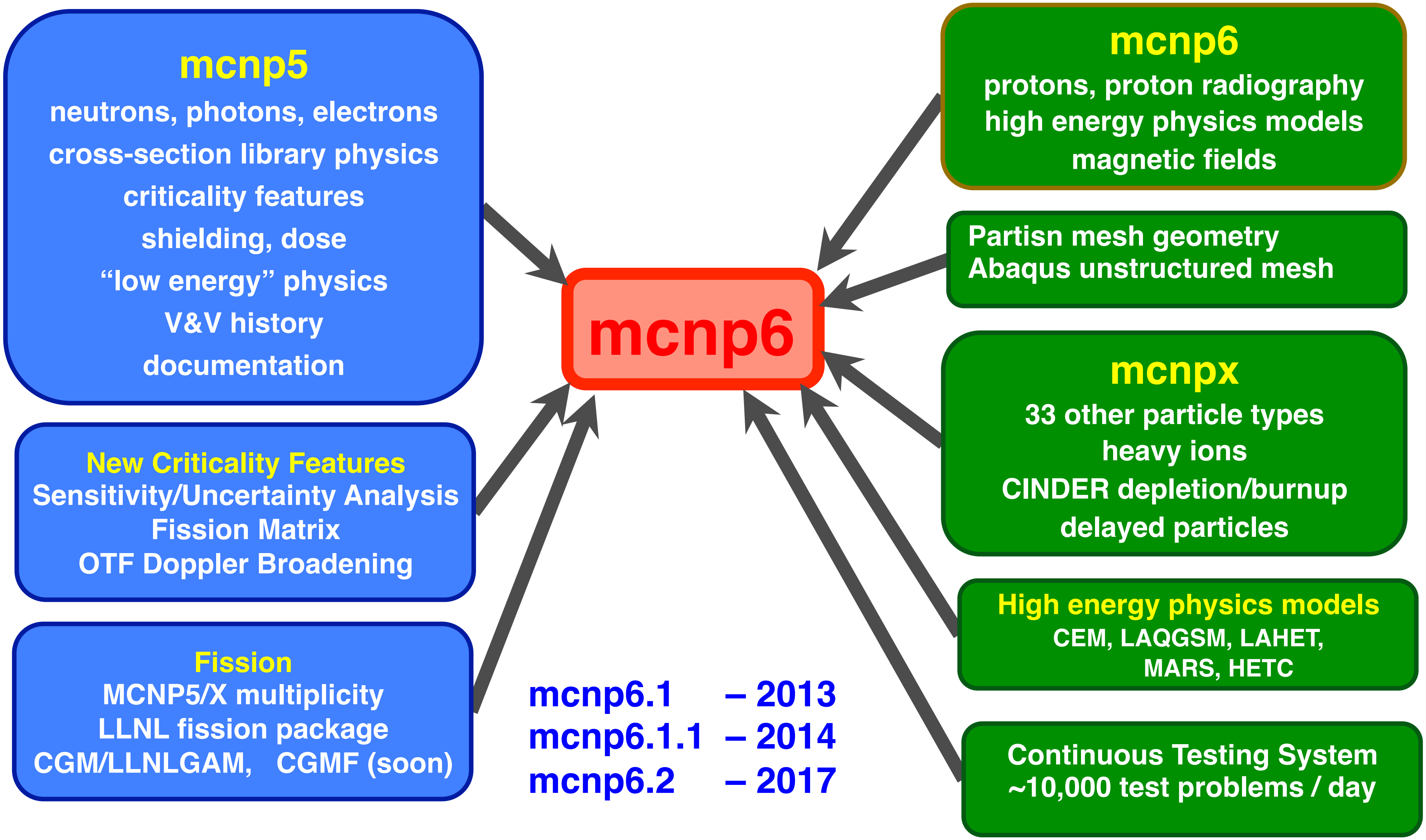
Whole-core Thermal & Total Flux from MCNP5 Analysis (from Luka Snoj, Jozef Stefan Inst.)



ITER Neutron Flux Calculations



From MCNP5 & MCNPX to MCNP6



Monte Carlo Methods and Code Development for Nuclear Nonproliferation and Safeguards Applications

What's new in MCNP6.2 that can be used to solve these kinds of problems?

Background

- **Warhead Measurement Campaign (WMC) meant to passively and actively measure nuclear warheads for treaty verification**
  - New measurements of neutron and photon coincidence data of shielded special nuclear materials (SNM)
  - At the time, the transport simulation tools available were limited in their ability to fully predict WMC-like measurements
  - This was due to the type of nuclear fission data available
  - To address these shortcomings, more detailed behavior of nuclear fission physics was needed
  - Making the transport simulations more predictive in SNM detection applications

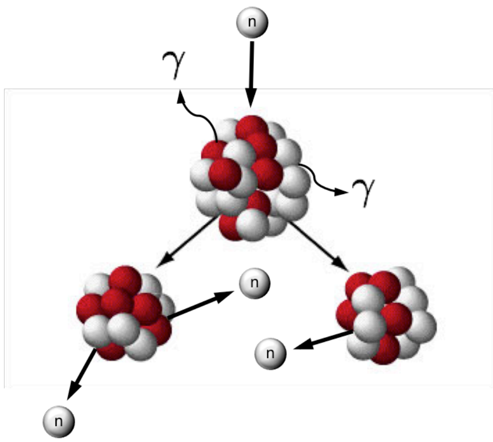
- **Key Issues**
  - Average nuclear data quantities are insufficient
  - Need better ways to compare to experiment

New Fission Multiplicity Models and Post-Processing Tools for MCNP6.2

- **In the release:**
  - CGMF and FREYA fission event generators
  - (M)ISC : MCNP / general intrinsic source constructor
  - MCNPTools : MCNP outputs
- **To be released at a future date:**
  - DRiFT : Detector Response Function Toolkit
- **Presented at workshop at 2016 ANS ANNTP Conference in Santa Fe, NM (look on website under technical references and workshops)**
  - LA-UR-16-27559 : MCNP6 basics
  - LA-UR-16-27301 : fission multiplicity models
  - LA-UR-16-27265 : ISC and MCNPTools info
  - LA-UR-16-27166 : DRiFT

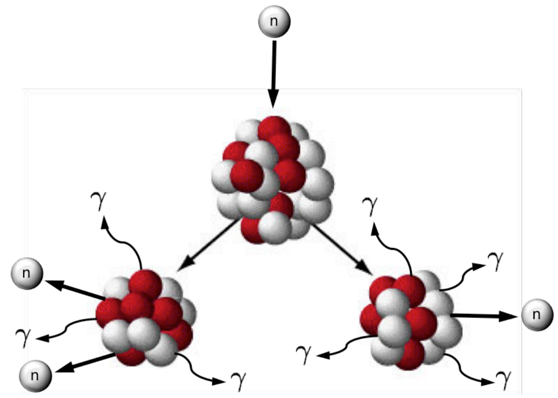
Nuclear Fission Physics

- **MCNP6.1**
  - Average photon production for each collision
  - Average neutron production for each fission
  - Average energy spectra for neutrons and gamma rays
  - Isotropic angular emission
  - No correlations!

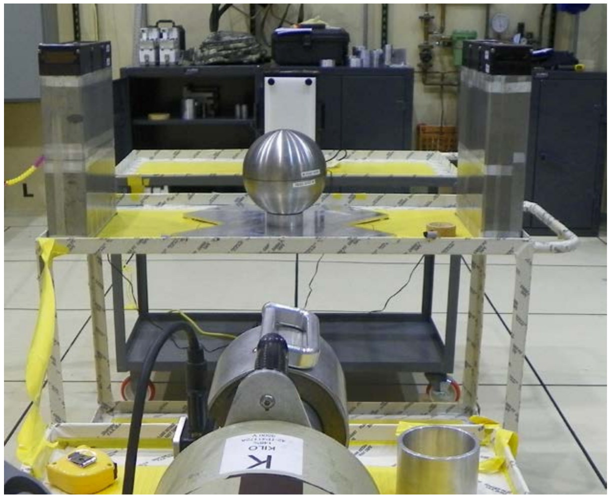


- **Applications**
  - Shielding: current, flux, energy deposition, dose
  - Subcritical / Critical Systems: k_{eff}, flux, reaction rates
  - Reactor Physics: k_{eff}, current, flux, power distributions, burnup
  - Radiation Detection: charge and energy deposition, pulse-height spectra, bulk counting rates

Nuclear Fission Physics



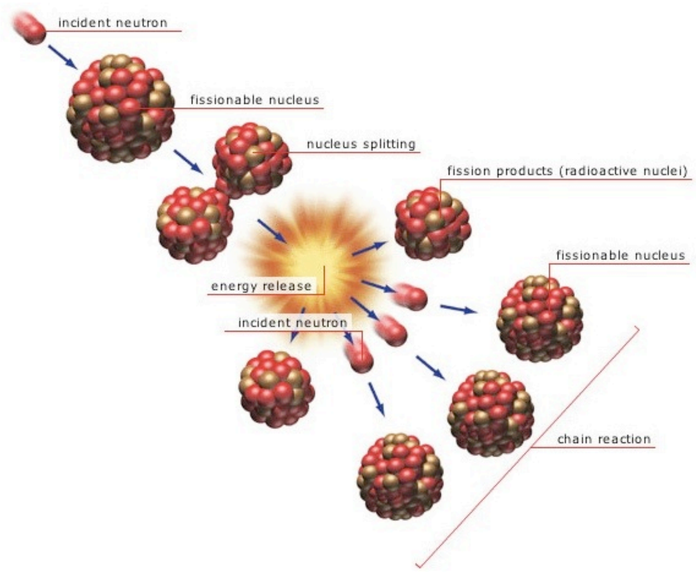
- **MCNP6.2**
  - Multiplicity distribution of gamma rays for each fission
  - Multiplicity distribution of neutrons for each fission
  - Multiplicity dependent energy spectra (energy correlations)
  - Angular emission from fission fragments (angular correlations)
  - Full correlations!
- **Applications**
  - In addition to MCNP6.1 …
  - Subcritical Systems: singles, doubles, etc. counting rates, leakage multiplication, probability of initiation/extinction
  - Reactor Physics: higher-order power distribution fluctuations
  - Radiation Detection: n-n, n-γ, γ-γ time coincidence



New in MCNP6.2

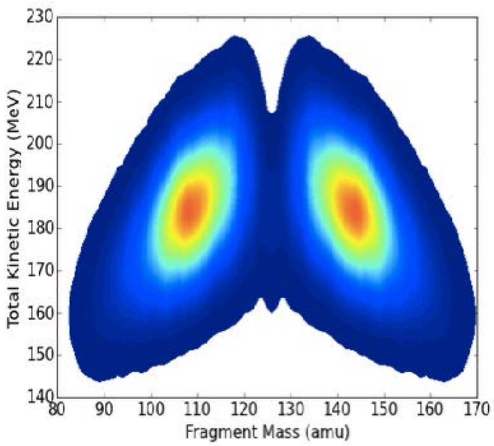
Two new correlated fission event generators (FREYA and CGMF) as well as post processing analysis tools are now available for event-by-event simulations preserving all secondary particle correlations.

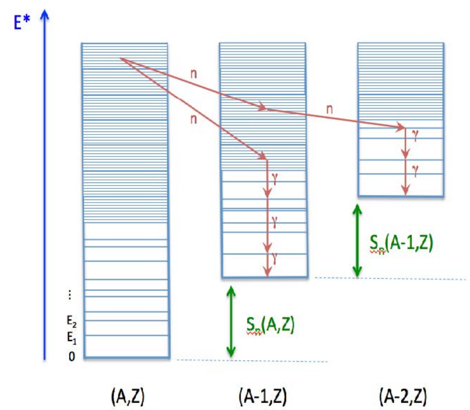
- When a fission event occurs in MCNP, neutrons and gamma rays are generated through a call to FREYA or CGMF
- Kinematics of neutrons and gamma rays emitted returned to MCNP
- Normal secondary particle transport continues throughout simulation



How it Works

- **Both FREYA and CGMF are Monte Carlo codes**
- **Fission fragments are sampled from yields in A, Z and KE**
- **Excited fission fragments are de-excited through particle evaporation**





FREYA (LBNL/LLNL)

- Monte Carlo Weisskopf
- Neutron emitted first…
- Then gamma ray emission
- Very fast simulation

CGMF (LANL)

- Monte Carlo Hauser-Feshbach
- Neutrons and gamma rays compete for emission
- Computationally slow

What was done in FY16
New models integrated

- **LLNL Fission Library 2.0.1**
  - Produces same results from previous version
  - Now includes FREYA 2.0
- **FREYA 2.0**
  - Code and data included
  - Spontaneous fission: ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm, and ^{252}Cf
  - Neutron-induced fission: ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu
- **CGMF 1.0.9**
  - Code and data included (also upgraded CGM)
  - Spontaneous fission: ^{240}Pu, ^{242}Pu, and ^{252}Cf
  - Neutron-induced fission: ^{235}U, ^{238}U, and ^{239}Pu

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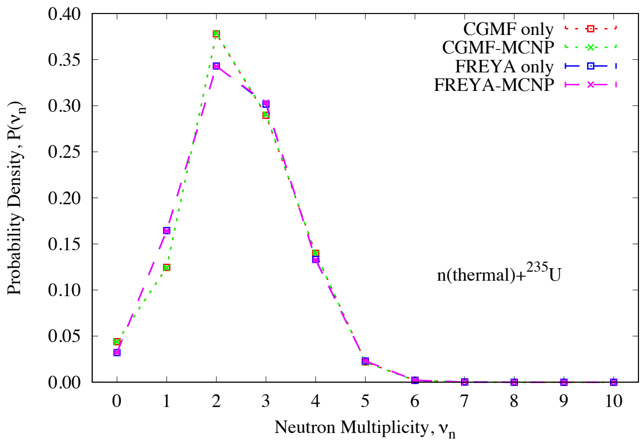
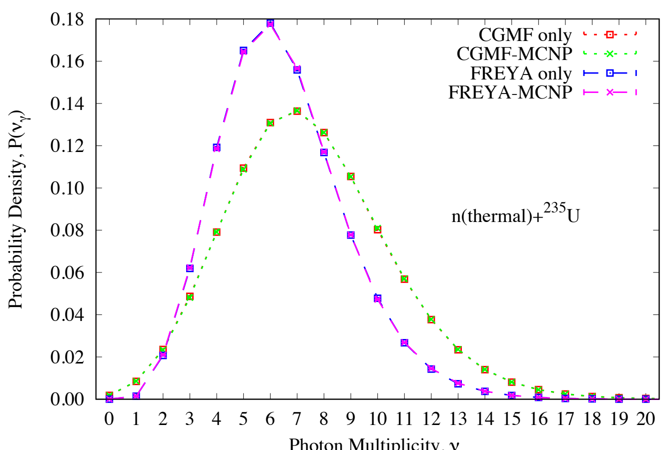
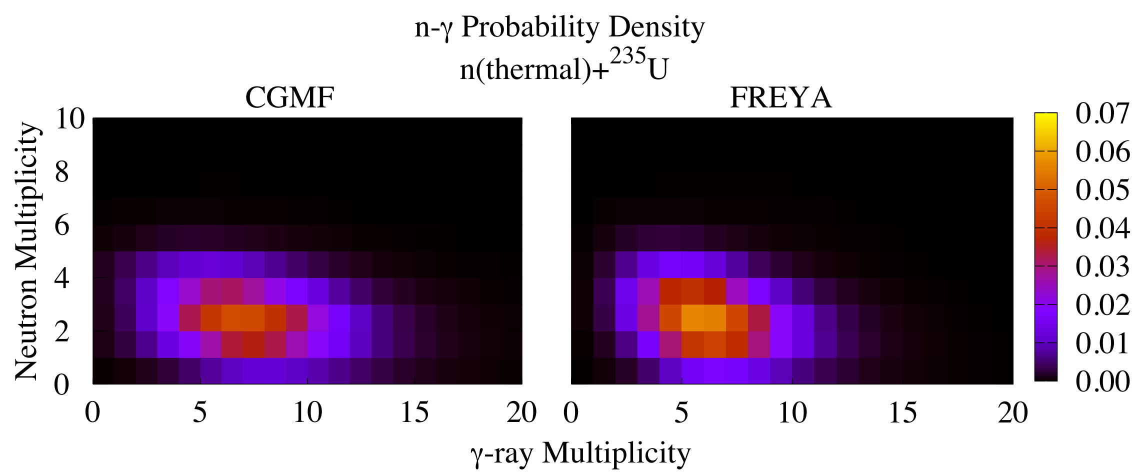
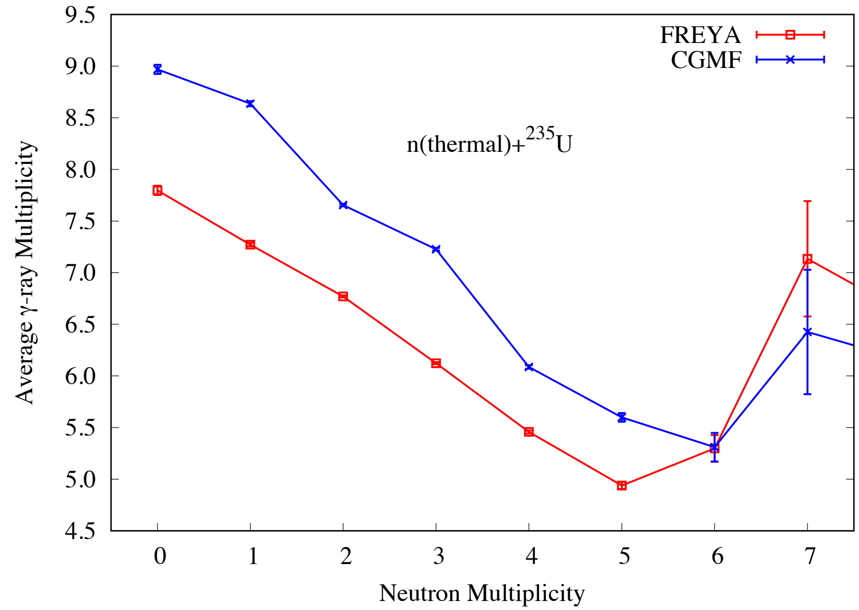
Fission Event Generator Behavior

- **Neutron & gamma-ray multiplicity**



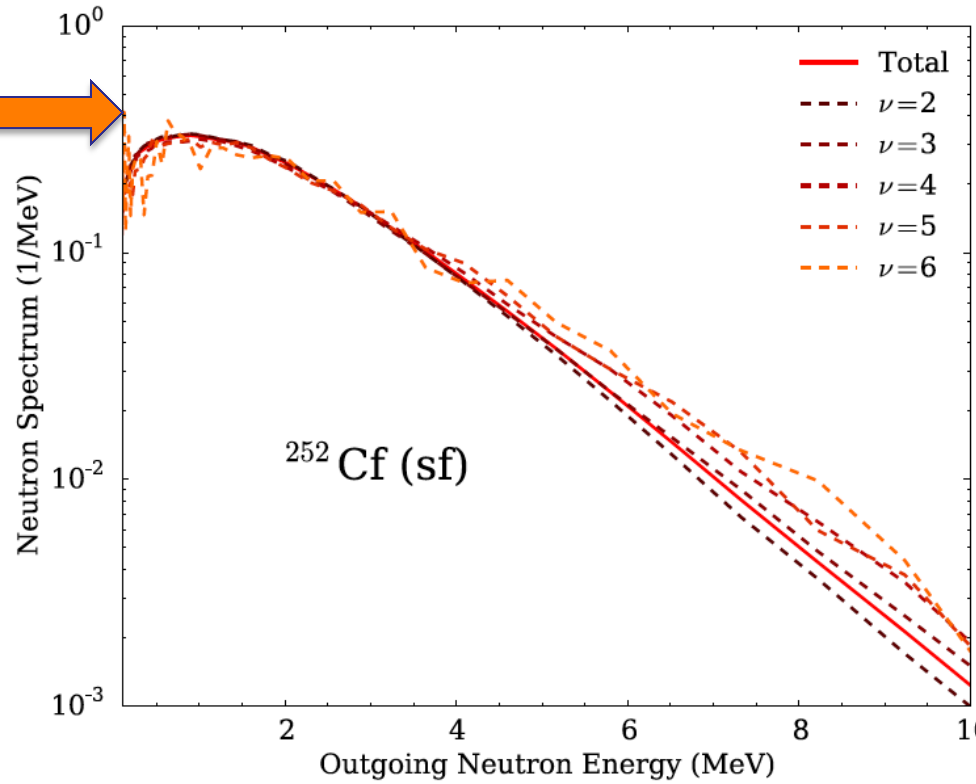


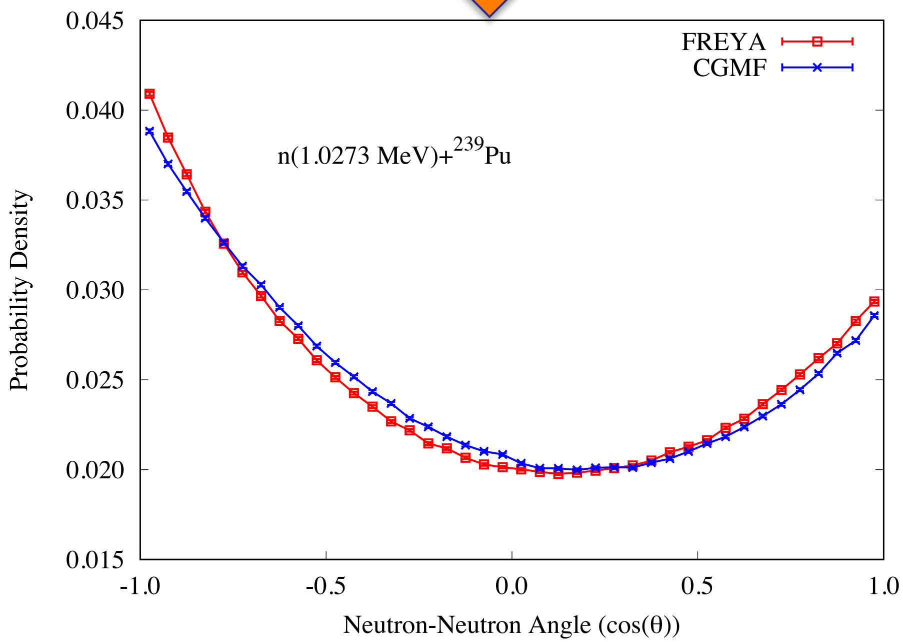




Fission Event Generator Behavior

- **Multiplicity-dependent spectra**
- **Neutron emission angular correlations**





DRiFT – A Detector Response Function Toolkit

- **Accurate detector modeling is a requirement to design systems in many non-proliferation scenarios (e.g. time-coincidence counting)**
  - By determining a Detector's Response Function (DRF) to incident radiation, we can characterize measurements of unknown sources
- **More efficient design processes (cost and time)**
- **Realistic radiation sources may not be available**
- **DRiFT is intended to post-process MCNP output and create realistic detector spectra**
  - Leverages the ability of MCNP to simulate complex radiation sources, materials and geometries
  - DRiFT includes detector physics not present in many radiation transport codes
- **Capabilities currently under development include the simulation of HPGe, He-3 gas, and as will be discussed in this work, <u>scintillator detector physics</u>**

- **Developers: M.T. Andrews, C.R. Bates, E.A. McKigney**

DRiFT – A Detector Response Function Toolkit for MCNP Output

- **Post-processes MCNP output (using MCNPTools), so as new features are added, DRiFT users can readily incorporate them into their simulations**
- **DRiFT detector resolution is reproduced by the variances in signal due to fluctuations in scintillation yields, PMT noise, and quantization error**
- **DRiFT is very fast because it *does not model optical photon transport* however this has a few drawbacks, namely:**
  - Users must input their own optical transport factors (or use default settings which may not be applicable to their particular setting)
  - Effects of optical photon transport on energy resolution are not currently reproduced by DRiFT
- **Scintillator simulations have been recently performed in GEANT4 through the modeling of optical photon transport, they can create PSD plots, however optical photon transport simulations are computationally expensive**

MCNP6.2 Simulations

Scintillator is given a density and atomic ratio corresponding to manufacturer specs:

Detector	Type	H:C Ratio	Density / g cm^{-3}	Scintillation Yield
EJ-301	Liquid	1.212	0.874	12,000 γ/MeVee
EJ-212	Plastic	1.103	1.020	10,000 γ/MeVee

- **MCNP Intrinsic Source Constructor (MISC, CJ Solomon) is used to create source photon spectra**
- **Particle TRACking (PTRAC) card used to record recoil proton's energy, and time as a binary**
  - PTRAC files are post-processed with MCNPTools (CJ Solomon, C.R. Bates)

DRiFT Simulations

- **DRiFT reads an input file containing keywords**
- **DRiFT reads the PTRAC file by calling MCNPTools**

[global]		
Datasource	=	mcnp
Datafile	=	ocf252p
Modeltype	=	event (ptrac)
[Scintillation]		
Detector	=	EJ301
Particle0	=	Proton
Particle1	=	electron
Quenching_data	=	Dekempeener
S_gate	=	22e-9
L_gate	=	90e-9
Sampling_rate	=	500e6
PMTType	=	9821B

DRiFT Simulations – Calculating Photo-electrons

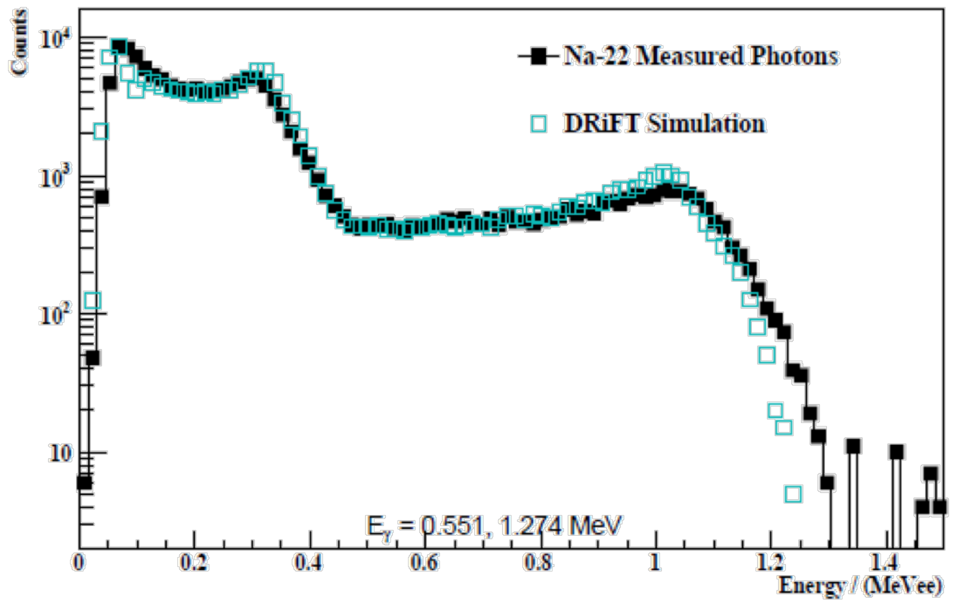
- DRiFT treats each particle separately to properly determine the amplitude and shape of the resulting pulse
- The PTRAC particle's electron equivalent energy (MeVee) is determined for the specific particle type and original energy using quenching data specified in input
- The scintillation yield (12,000 photons/MeVee for EJ-301) is used to determine the mean number of photons produced
- The actual number is sampled from a Poisson distribution

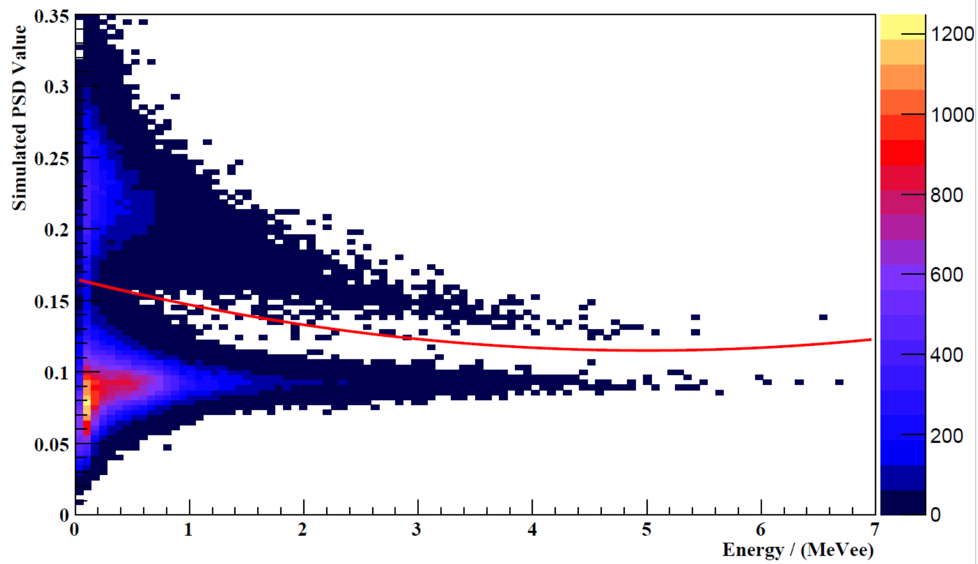
DRiFT Simulations – Simulating Pulse Shape

- Optical photons are distributed in time using pre-defined intensity profiles
- Time interval sizes are matched to the sampling rate of the digitizer
- For histories with more than one recoil, the relative difference in time stamps is used to determine the initiation of their contribution to the overall count
- Optical transport factor and quantum efficiency factors are applied to photons. The remaining number of photons/electrons is sampled from a Poisson distribution
- Noise contributions are included in the calculation of the PMT current

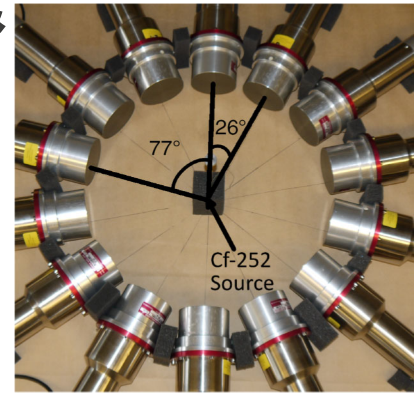
DRiFT Output

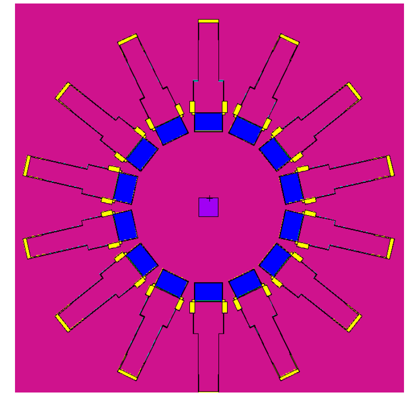
- **An ASCII output file with detected event information**
  - Most common outputs:
    - Detector cell number
    - Pulse height
    - Pulse shape discrimination (PSD) value
    - Time stamp
  - Optional outputs:
    - Source energy
    - Correlated information
- **ROOT files**
  - ROOT trees containing event information
  - ROOT histograms



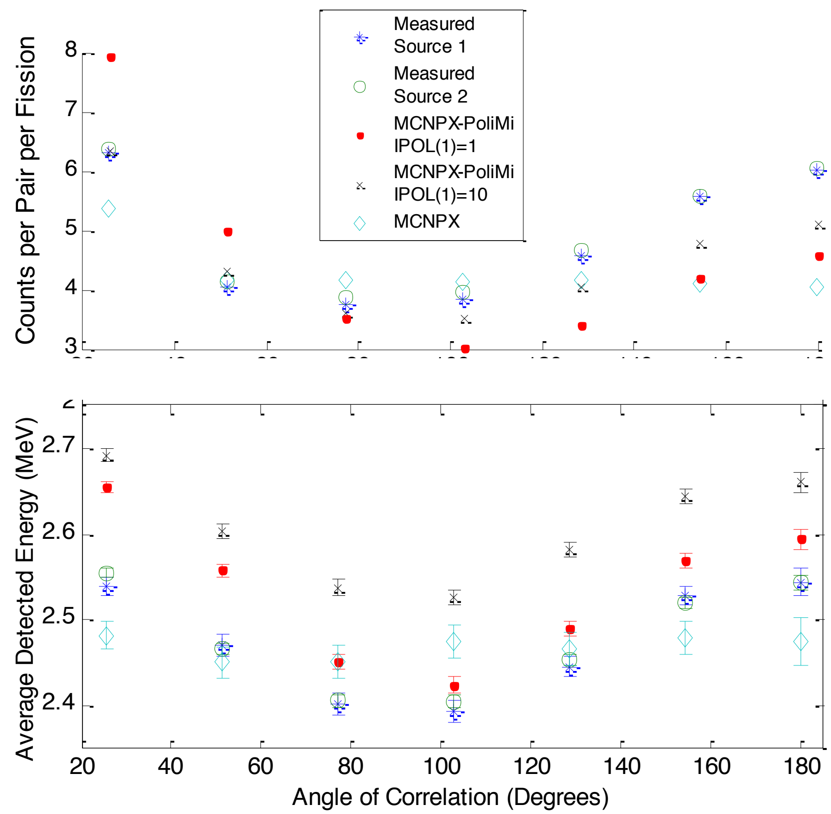


Comparison to Other Codes & Experimental Data

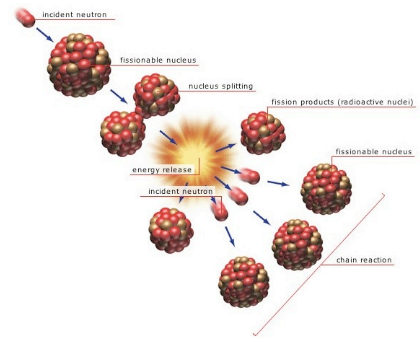




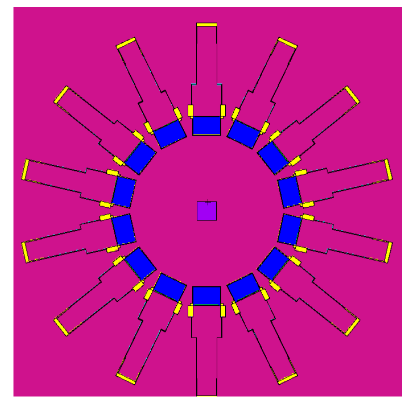
- **University of Michigan differential measurements of angular correlations**
- **Priority is to compare against experimental measurements**
- **Follow-up of 2014 NSE paper by S.A. Pozzi *et al*.**
- **Submitted an abstract to IRRMA X meeting in Chicago, IL, July 9-13**
- **Transport and post-processing code comparisons**
  - MCNP6 / DRiFT
  - MCNP6 / MPPost
  - MCNPX-PoliMi / MPPost
  - MCNPX-PoliMi / DRiFT



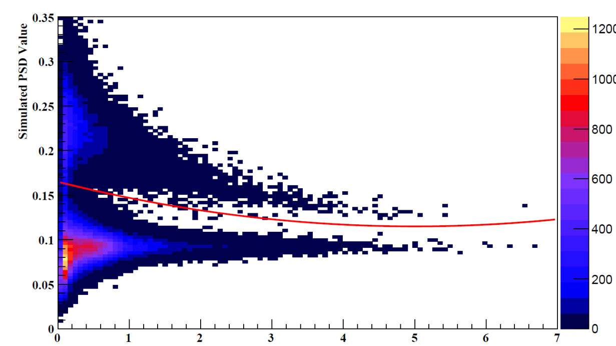
Putting It All Together



- ✓ **Can simulate spontaneous fission source for ^{252}Cf using FREYA and CGMF fission event generator models in MCNP**

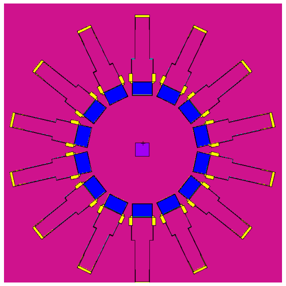


- ✓ **Can model the complex geometry of the detector array in MCNP and gather particle collision information inside each detector**

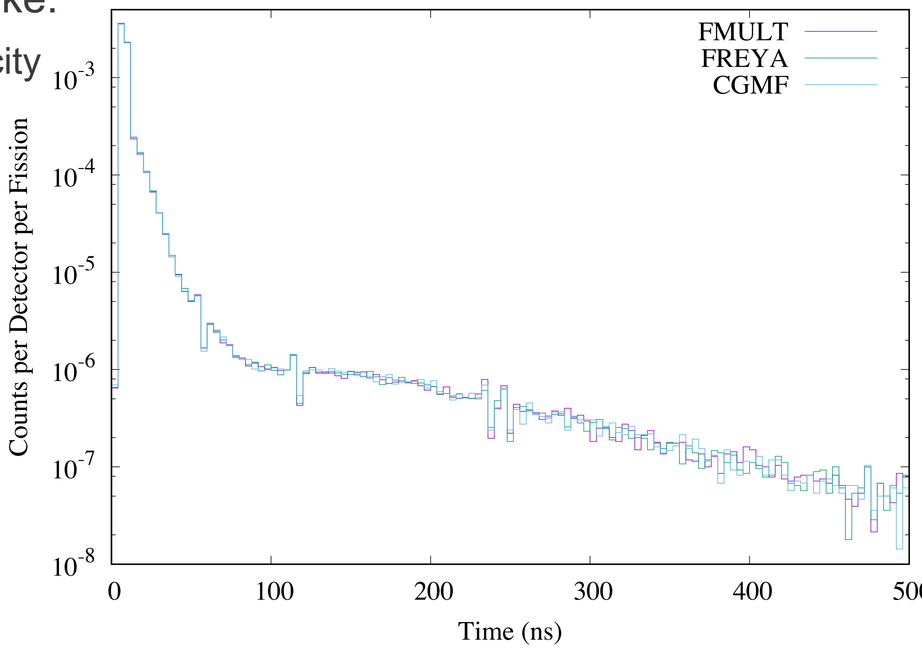


- ✓ **Can post-process the output to get the detector responses and compare directly to the experimental data (rather than unfolding the measured to data to compare with the simulation)**

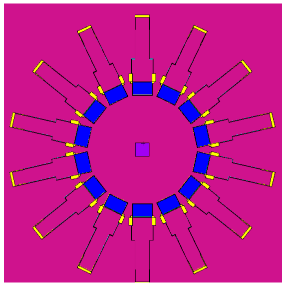
Preliminary MCNP6.2 & DRiFT Results (1)



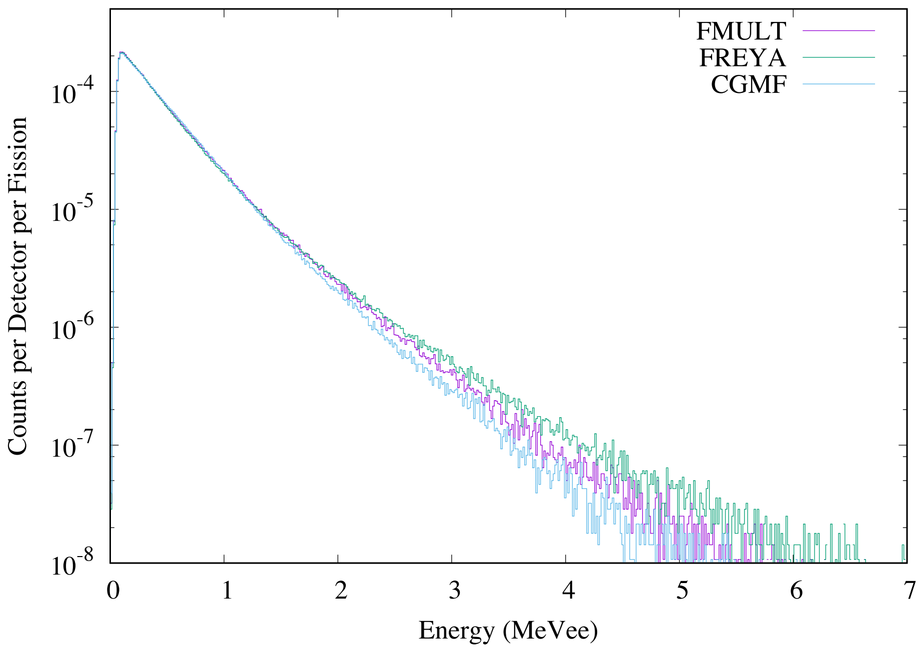
- **Still need to obtain experimental data**
- **Current comparisons between fission multiplicity models**
  - Neutron-only simulation for now
- **FMULT input card**
  - Option in MCNP with some flexibility
  - Can select fission emission parameters like:
    - Multiplicity distribution and average multiplicity
    - Energy spectrum (Watt parameters)
  - No gamma rays
  - No angular distributions
- **First, we can look at the time-stamp distribution for each model**
  - No pulse height threshold set

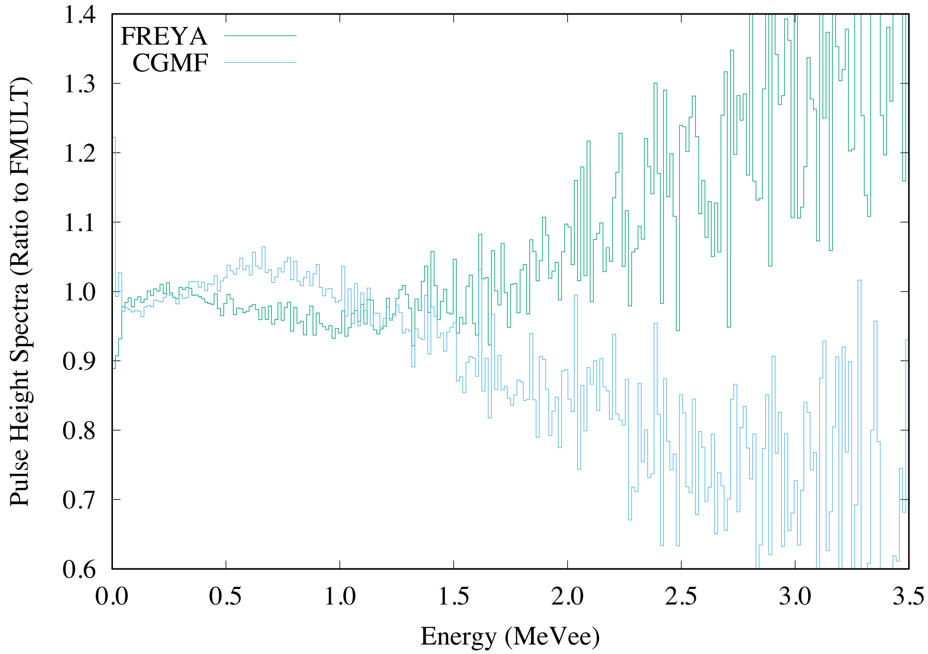


Preliminary MCNP6.2 & DRiFT Results (2)



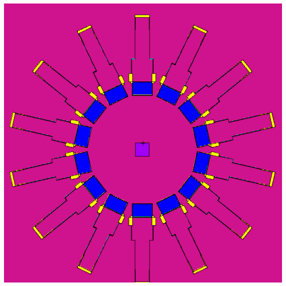
- **Pulse height distributions**



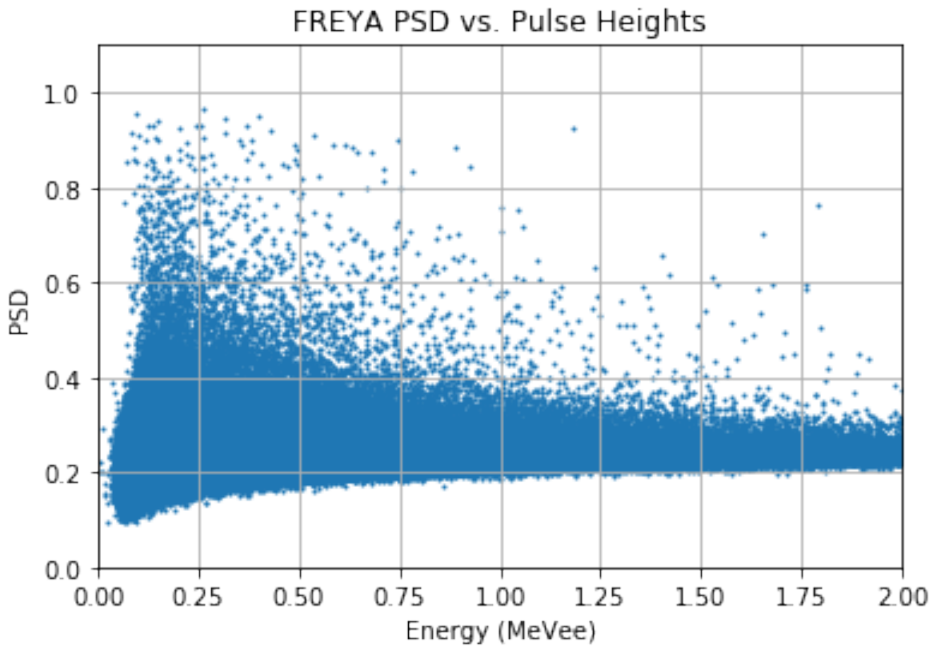


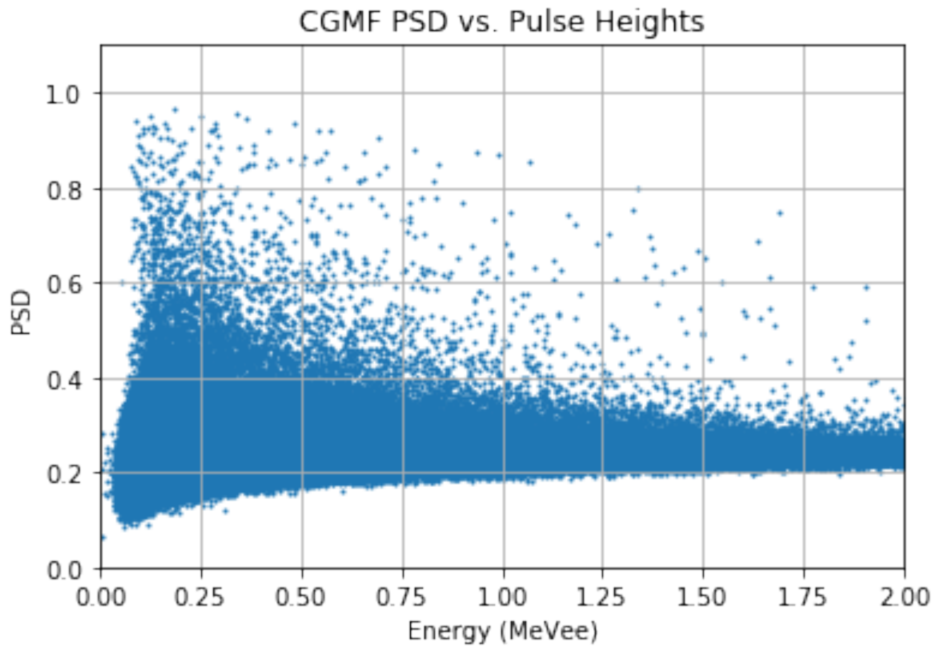
- **Large differences in high energy tail of pulse height distributions**
  - Likely due to differences in the fission energy spectra in the models

Preliminary MCNP6.2 & DRiFT Results (3)



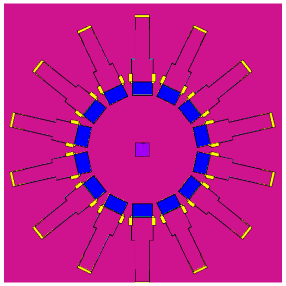
- **Pulse shape discrimination**



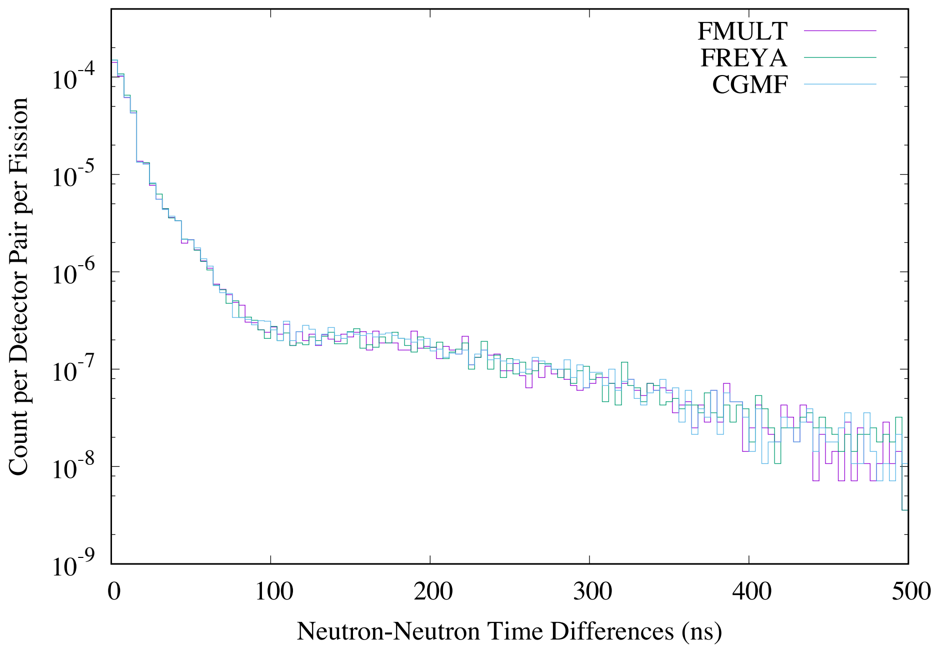


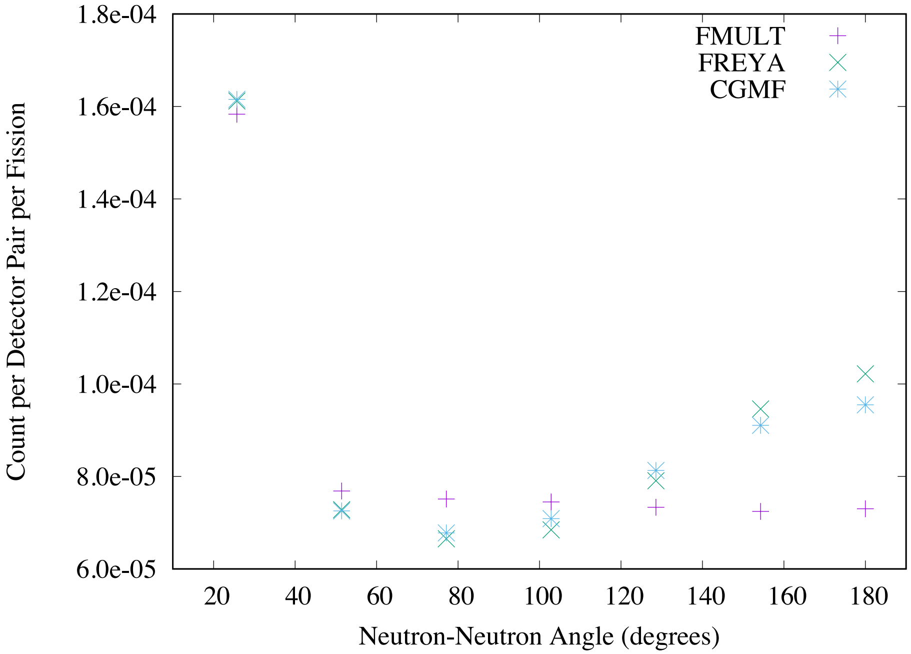
- **Not much difference here, still need to account for gamma rays**
  - PSD will be used to separate gamma rays from neutrons in the liquid scintillators

Preliminary MCNP6.2 & DRiFT Results (4)



- **Correlated counts**

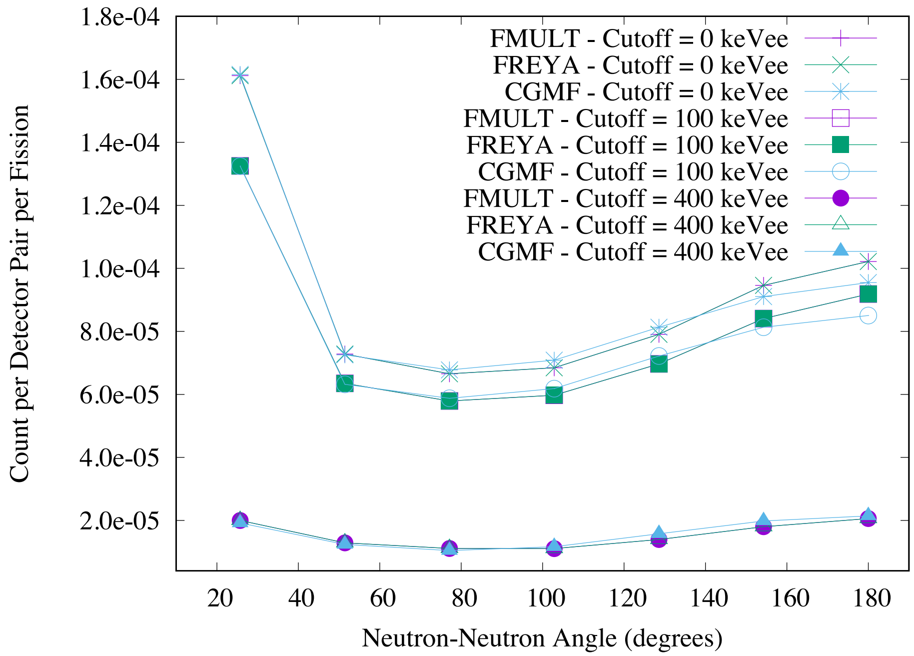




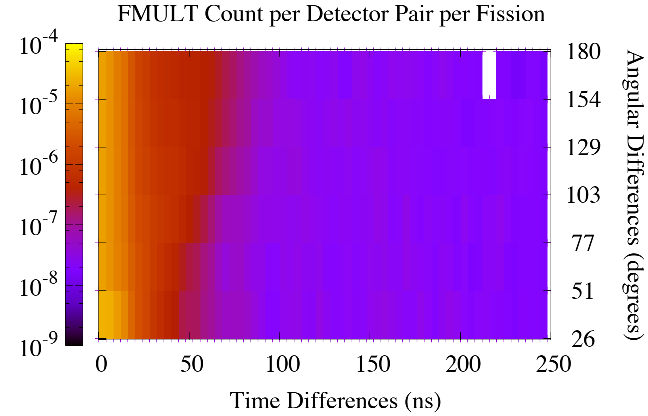
- **Time-stamp differences are small**
- **Angular differences are significant!**
  - Lots of cross-talk between detectors at small angles

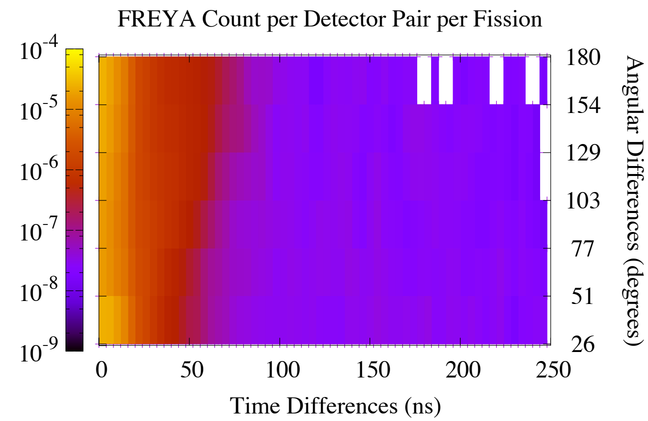
Preliminary MCNP6.2 & DRiFT Results (5)

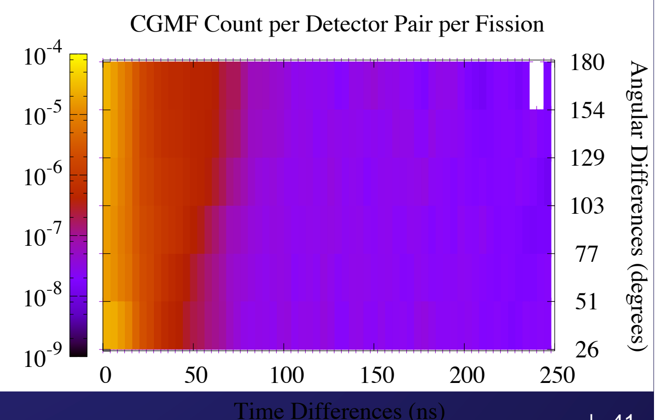
- **Correlated counts**



- **Changing pulse height thresholds changes:**
  - Overall count rates
  - Removes some of the cross-talk effect
- **Time stamp differences change w.r.t angle**







Conclusions

Impact

- **Excellent collaboration with LBNL/LLNL researchers and University of Michigan professors and students under NA-22 venture project**
- **Improved results when compared to experiment for some complex coincident/ multiplicity measurements**
- **New capabilities in MCNP6.2 and post-processing tools available now to users in many application areas**

Future Work

- **Improvements to FREYA and CGMF**
  - More isotopes/energies and photofission
  - Time-dependent gamma-ray emission
- **MCNP6 improvements to algorithms, list-mode output and parallel computing capabilities**
- **Validation – more simulation vs. experiment**

Thank you!

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