

# Adaptation of GEANT-4 to Criticality Calculations for Nuclear Reactors

*ENSAR2 workshop: GEANT4 in nuclear physics 2018*

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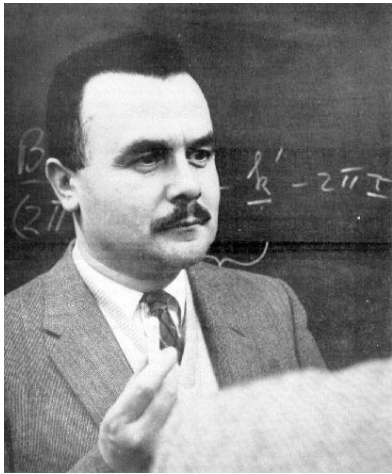
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# The Stage: McMaster

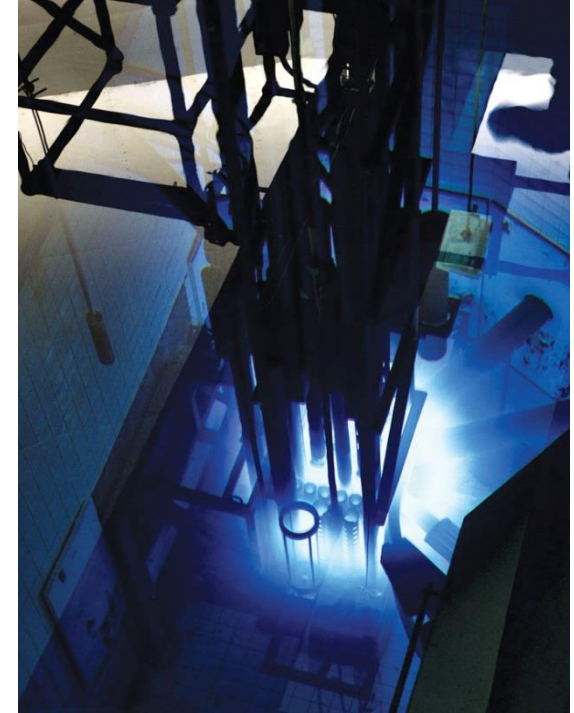
- **McMaster Nuclear Reactor Critical April 1959**  
(First RR at a Commonwealth University) (CERN:1952)
- **Bertram Brockhouse** shared the 1994 Nobel Prize in Physics with American Clifford Shull for developing neutron scattering techniques for studying condensed matter.



**Today:** McMaster Research Funding about \$400M – one of Canada's most research intensive Universities

## **MNR:**

- Intense positron beam
- Small-angle neutron scattering
- Neutron activation analysis
- Neutron radiography



**MNR:** Commercial production of radio-isotopes for medical purposes  
(I-125, Lu-177, Re-186, ...)  
Accelerators (F-18), Hot cells, Sources.

<https://nuclear.mcmaster.ca/>

# Analyzing Nuclear Reactors

- Neutron transport equation describes the behaviour of neutrons in a reactor:

$$\begin{aligned}
 \frac{\partial}{\partial t} n(\mathbf{r}, E, \hat{\Omega}, t) = & \quad \text{Total Absorption} \quad \text{Streaming} \\
 \frac{1}{v} \frac{\partial}{\partial t} \varphi(\mathbf{r}, E, \hat{\Omega}, t) = & - \Sigma_t(\mathbf{r}, E) \varphi(\mathbf{r}, E, \hat{\Omega}, t) - \hat{\Omega} \cdot \nabla \varphi(\mathbf{r}, E, \hat{\Omega}, t) + \\
 & \text{Scattering} \quad + \int_0^\infty dE' \int_{4\pi} d^2 \hat{\Omega}' \Sigma_s(E' \rightarrow E, \Omega' \rightarrow \Omega) \varphi(\mathbf{r}, E', \hat{\Omega}', t) + \\
 & + \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d^2 \hat{\Omega}' \nu(E') \Sigma_f(E') \varphi(\mathbf{r}, E', \hat{\Omega}', t) + \\
 & + s(\mathbf{r}, E, \hat{\Omega}, t) \quad \text{Fission} \quad (1) \\
 & \text{External source}
 \end{aligned}$$

# Steady State

- Traditionally, analysis done in steady state:

$$\frac{\partial}{\partial t} = 0$$

- Concept of criticality:

$$k \equiv \frac{\text{rate of neutron production in reactor}}{\text{rate of neutron loss in reactor}} \equiv \frac{P(t)}{L(t)}. \quad (1)$$

criticality is now given by:

$$k < 1 \quad \text{subcritical} \quad (2)$$

$$k = 1 \quad \text{critical} \quad (3)$$

$$k > 1 \quad \text{supercritical} \quad (4)$$

- Transport equation may be solved numerically.

# Kinetics

- Dynamic changes in the reactor core are usually dealt with by Point Kinetics:
  - Flux shape remains the same.
  - Overall flux (neutron density) changes with time

$$\frac{\partial n(t)}{\partial t} = \frac{(\rho - \beta)}{\Lambda} n(t) + \sum_{i=1}^6 \lambda_i C_i(t)$$

$$\frac{\partial}{\partial t} C_i(t) = -\lambda_i C_i(t) + \frac{\beta_i}{\Lambda} n(t), \quad i = 1 \dots 6$$

$\beta$ : delayed fraction  
 $\rho$ : reactivity ( $1 - 1/k$ )  
 $\lambda$ : decay constant  
 $\Lambda$ : neutron generation time

- Reactors only work because of delayed neutrons!

# Numerical Methods

- Direct solution of the transport equation;
  - Through a variety of techniques.
  - (WIMS, NEWT, DRAGON)
  - Very time consuming, small geometries only (lattice cell)
  - Accurate
- Diffusion calculation;
  - (NESTLE, PARCS, DONJON)
  - Quick, but not always accurate
- Monte Carlo techniques;
  - (MCNP, KENO, SERPENT, OPENMC, SUPERMC)
  - Very accurate, but slow
- Common to all methods: need for **nuclear data libraries**

# Monte Carlo

- Follow neutrons (protons, electrons, gammas) through the geometry (core)
- Submit them to physics:
  - Scattering (elastic, inelastic)
  - Absorption (n,gamma) → energy deposition
  - Fission: creation of new neutrons
- Account for material properties:
  - Density
  - Temperature (Doppler broadening of resonances)
  - Population control (combing)
- Accuracy determined by statistics

# Monte Carlo Codes

- Examples:
  - Standard code is MCNP (developed originally for highly super-critical devices.)
  - KENO (part of the SCALE package)
  - SERPENT (European code)
- Features:
  - Need licence (half of your students can't use half of these codes)
  - Provided as executables only.  
Models are entered by input cards;



# MCNP

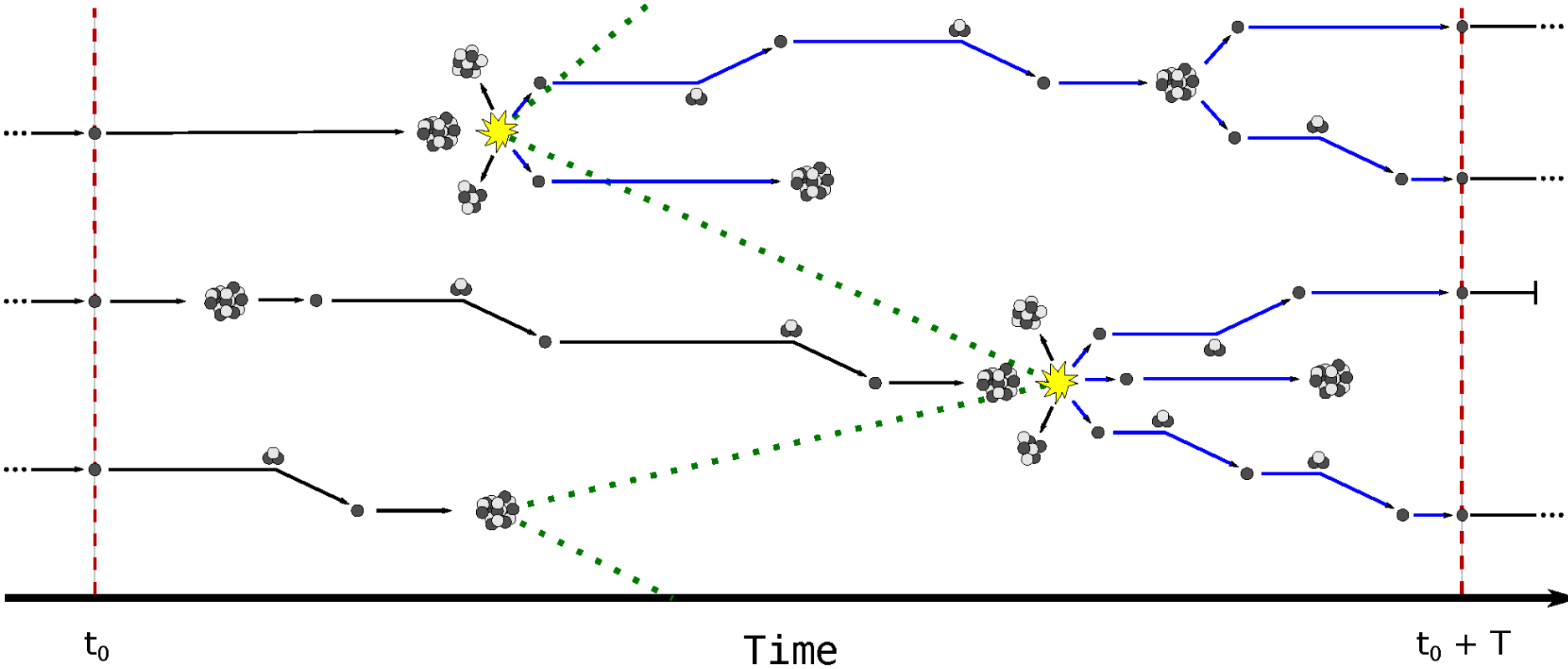
- KCODE calculation:
  1. Start with neutron source distribution  $(r, \nu)$
  2. If absorbed by fissile material, create  $\nu$  new source neutrons as result of fission.
  3. Follow neutrons until all have absorbed
  4. Obtain  $k_{\text{eff}}$  by new/old number of neutrons.
  5. Renormalize source (combing)
  6. Goto 1.
- Variance reduction techniques (weighting)
- Generation-based calculation:  
no concept of time! (shakes)




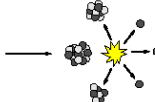





# Geant4 (G4-STORK)

- No licence required
- Hard-code the model
  - Very detailed geometry
  - Allows to change the geometry “on the fly”
  - Allows for temperature change (feedback)
  - On-the-fly Doppler broadening
  - Many physics models
- Simulation accounts for time!
- Population control still needed
- Need to think about  $k_{\text{eff}}$ .

# Show and Tell

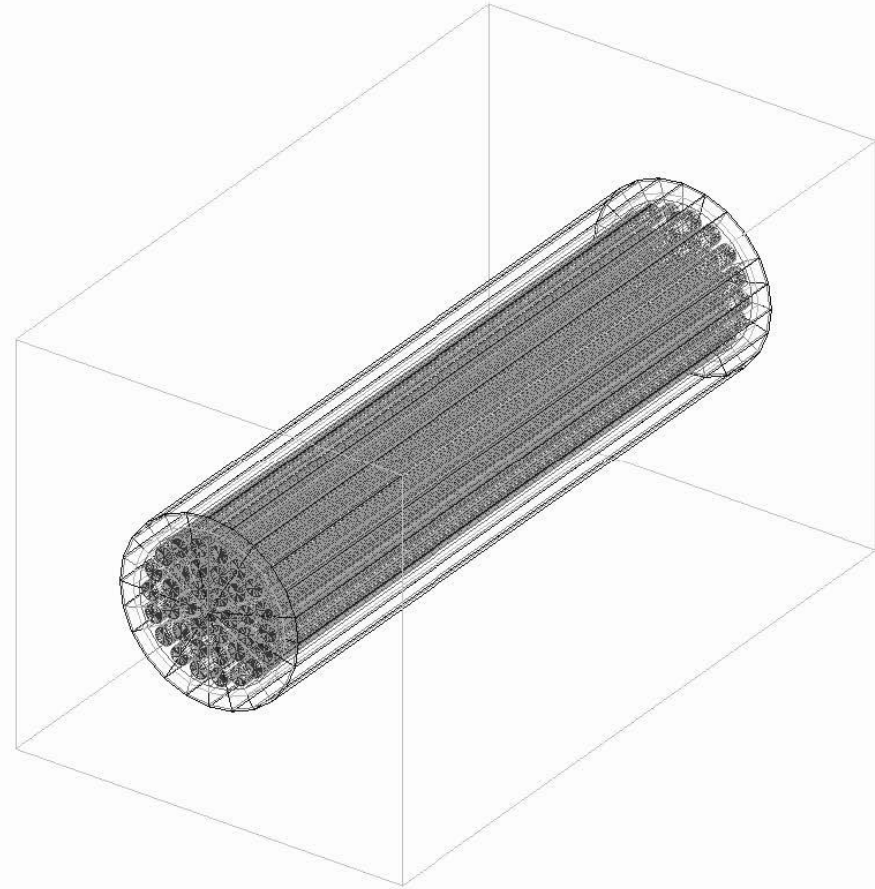
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LEGEND	G4-STORK Run Boundaries	First Fission Generation	Neutron	Fission	Capture	Elastic	Inelastic (n,n')	Inelastic (n,2n)	Terminated by Renormalization
									

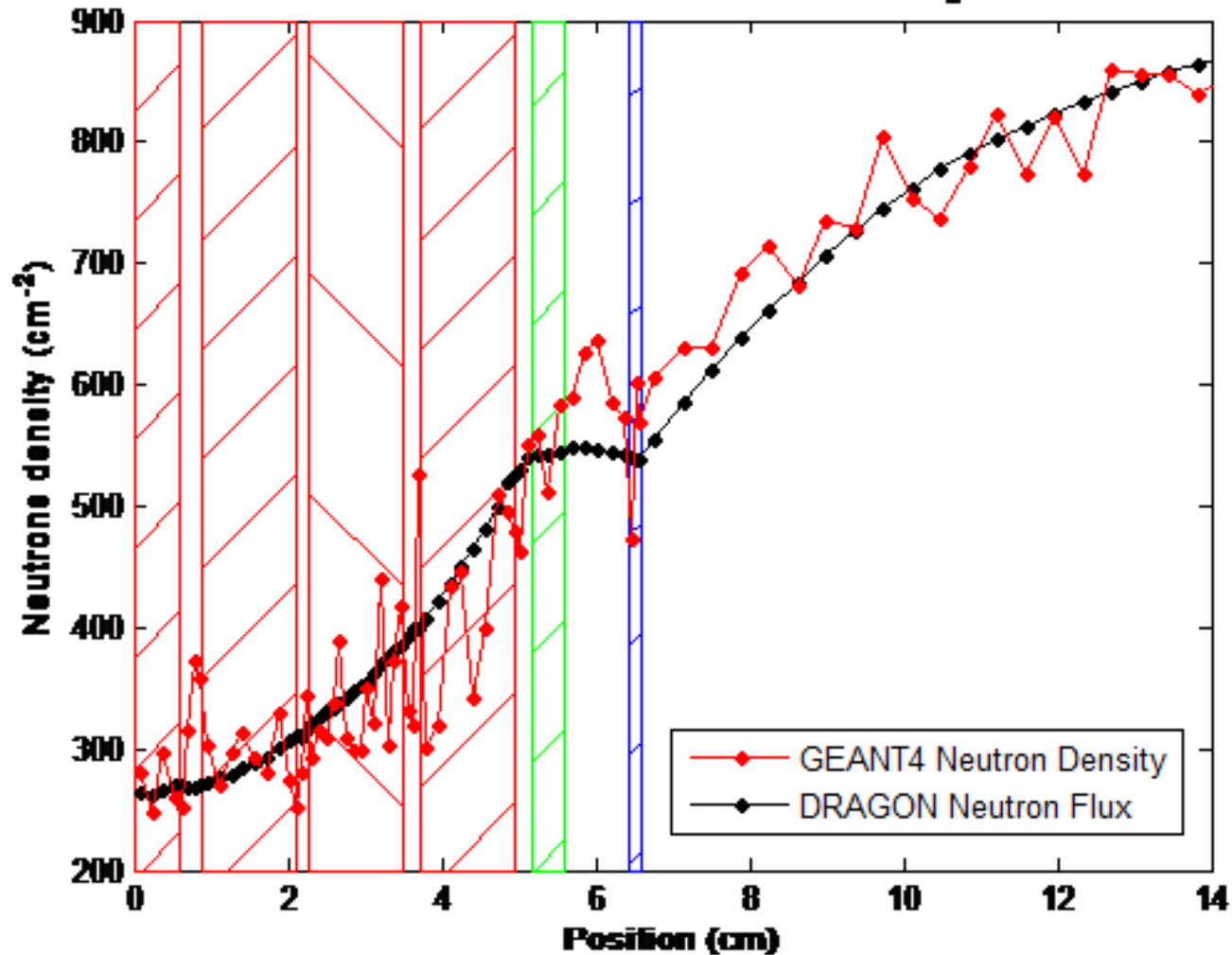
# Benchmarking with Transport Code

- Test of flux distribution
- Use CANDU reactor fuel bundle.
- Fresh fuel (only U in the libraries)



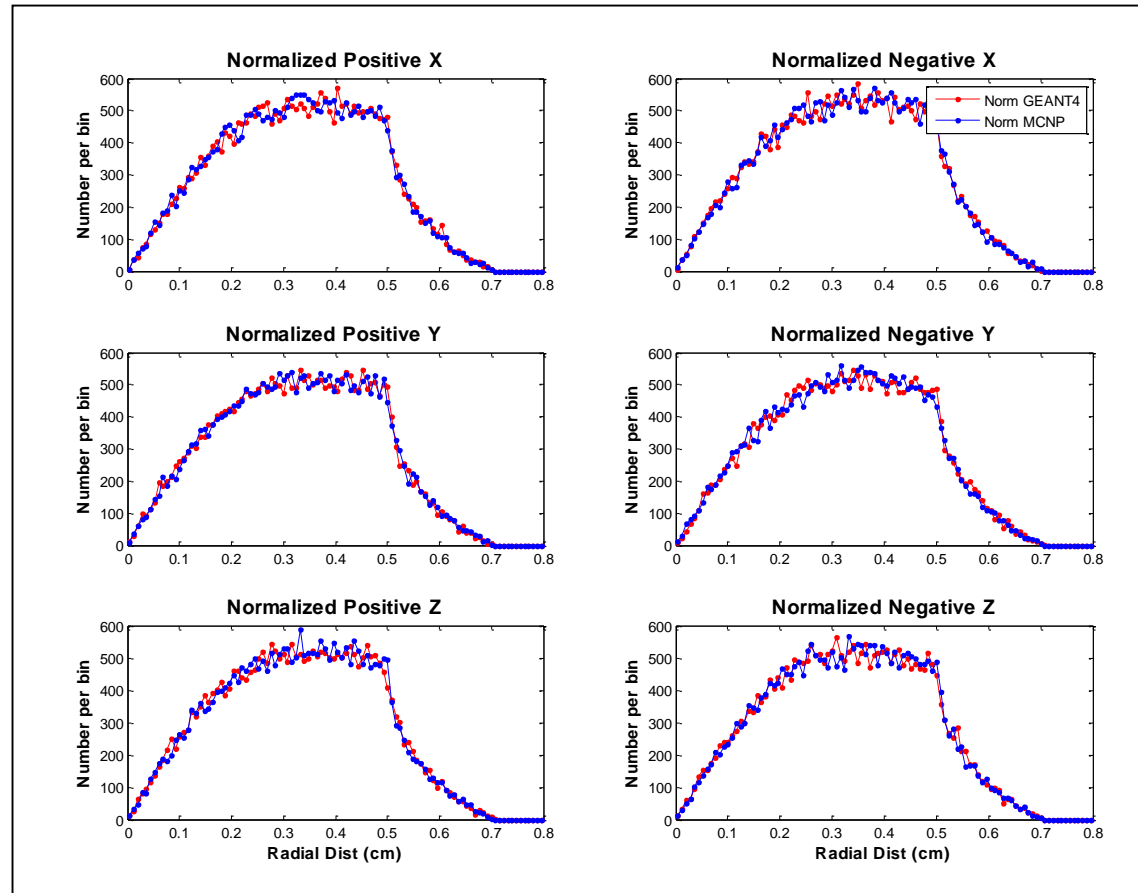
# Compare to DRAGON

**Centerline Neutron Density**



# Simple Comparison to MCNP

- Mono-chromatic beam on a U-235 slab.
- Beam  $E = 0.0253$  eV



$k_{\text{eff}}$

True multiplication constant

$$k_{\text{dyn}} = \frac{R_{\text{prod}}}{R_{\text{lost}}} = \frac{\Delta N_{\text{prod}} / \Delta T}{\Delta N_{\text{lost}} / \Delta T} = \frac{\bar{N}_{\text{prod}}}{\bar{N}_{\text{lost}}}$$

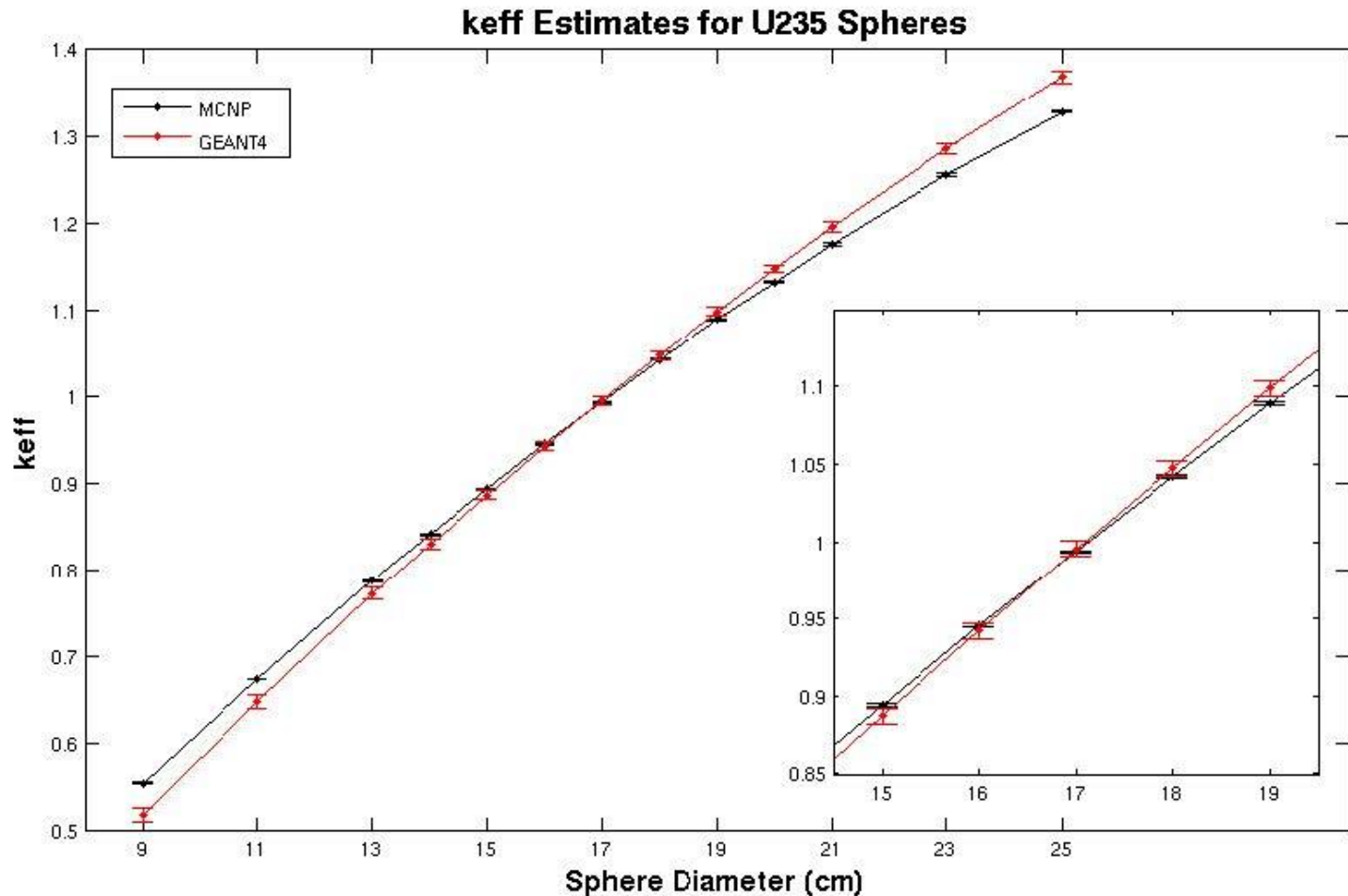
Whereas the generational  $k$  is given by

$$k_{\text{gen}} = \frac{N(\text{generation } i + 1)}{N(\text{generation } i)}$$

They are identical for  $k = 1$ .

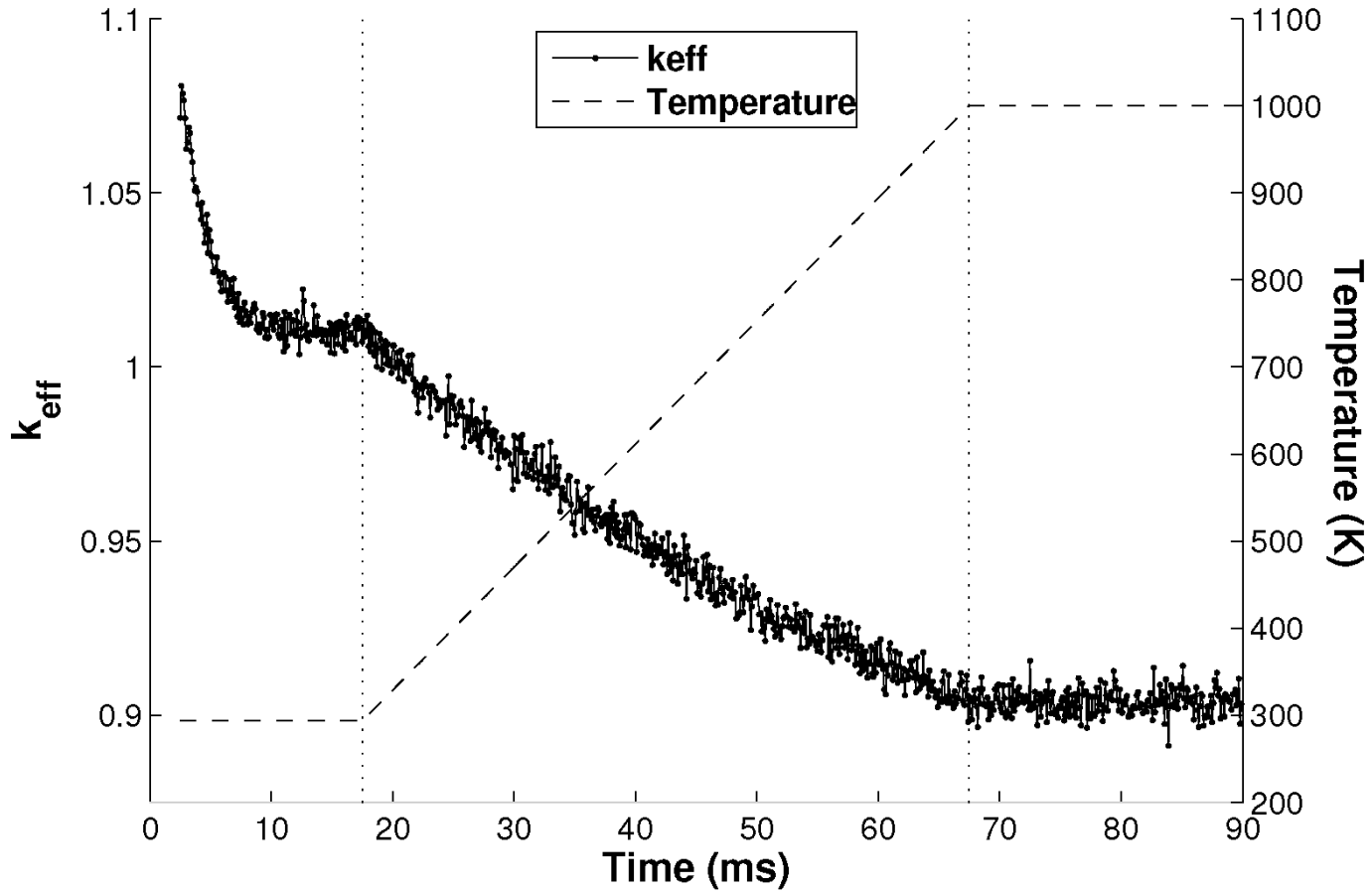
$$k_{\text{eff}}$$

- Converged source (Shannon Entropy)





# Time Evolution





# Validation with Reactor

- SLOWPOKE

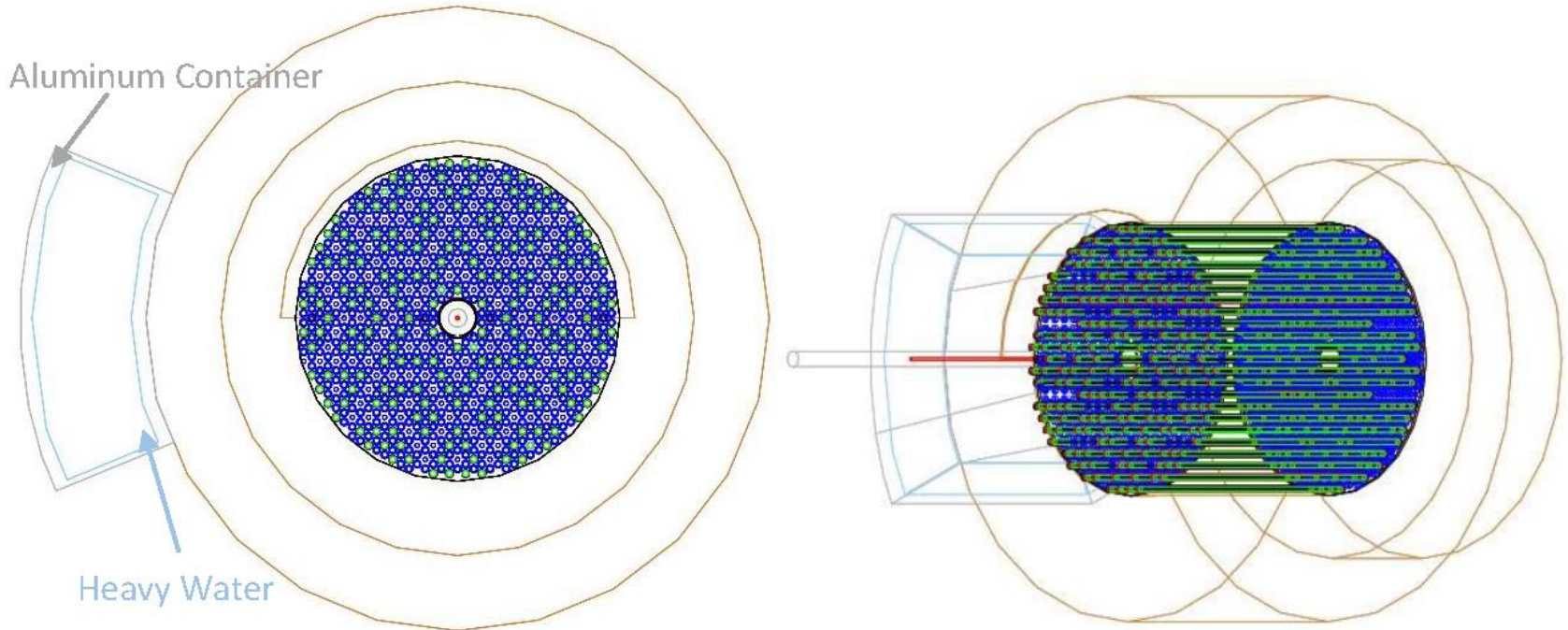
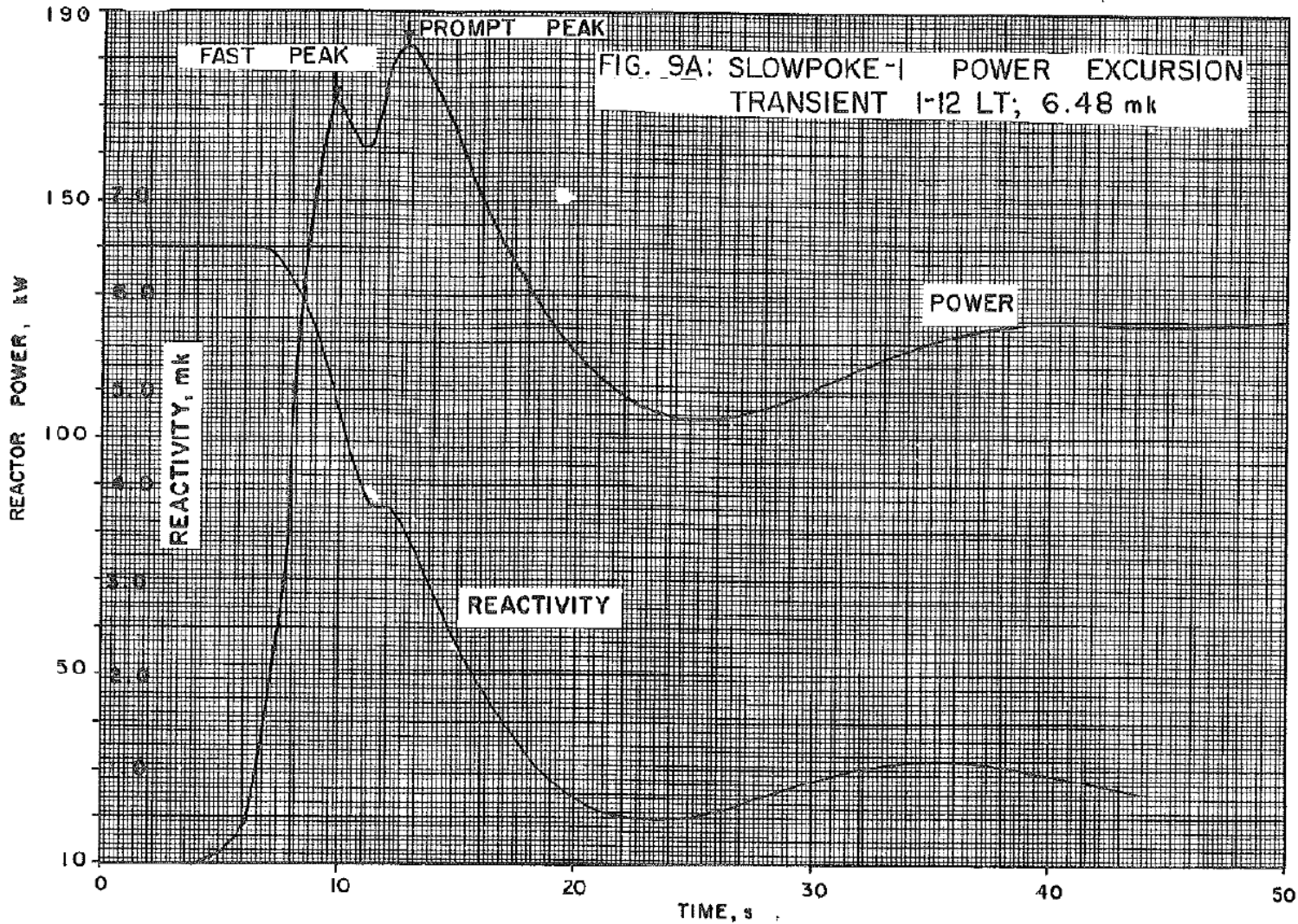


Figure 10 Reactor with added  $D_2O$  thermal column (On the left is a top view and on the right is a 45 degree view)

# Transient



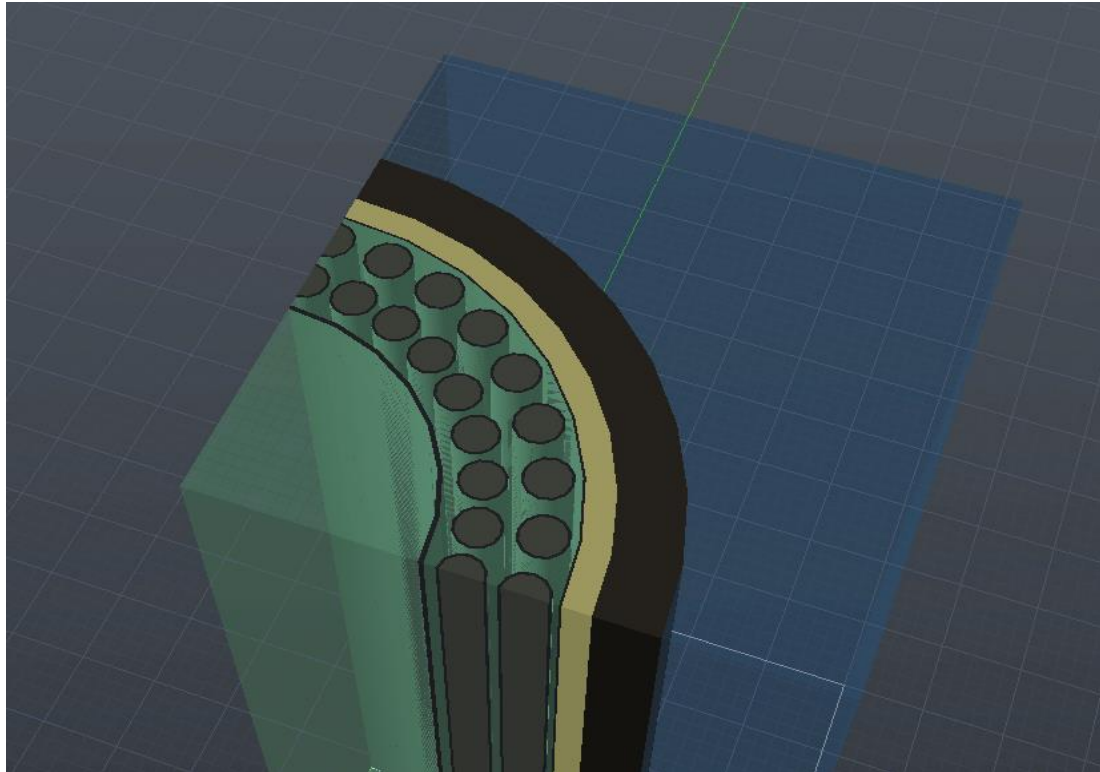
# Delayed Neutrons

- From delayed precursors (fission products)
- Do not identify precursors, rather combine them in groups
- Establish equilibrium concentration
- Determine decay time.
- Need to do population control as well



# Detailed Benchmark with MCNP

- Case: Super-critical water reactor
- Crucial parameter: coolant void reactivity



# G4-STORK-MCNP for SCWR

## MCNP6.1 Settings:

- Same as G4-STORK
- Using thermal scattering
- Using implicit absorption
- Using unresolved resonance regime model

$K_{inf}$ Cases	Fully Cooled	Void Inner Coolant	Void Outer Coolant	Void all Coolant	CVR (mk)
G4STORK	$1.253 \pm 0.003$	$1.206 \pm 0.001$	$1.258 \pm 0.003$	$1.215 \pm 0.002$	$-25.0 \pm 1.1$
MCNP6.1	$1.286 \pm 0.0001$	$1.249 \pm 0.0003$	$1.298 \pm 0.0003$	$1.266 \pm 0.0002$	$-12.09 \pm 0.07$

# Apples-to-Apples

$K_{inf}$ Cases	Fully Cooled	Void inner Coolant	Void Outer Coolant	Void all Coolant	CVR (mk)
G4-STORK	1.2978±0.0007	1.2499±0.0007	1.3057±0.0008	1.2639±0.0006	-20.7±0.61
MCNP 6.1	1.2979±0.0002	1.2562±0.0003	1.3085±0.0002	1.2708±0.0002	-16.4±0.17

- The generational criticality method has been implemented in G4-STORK;
- in MCNP
  - the thermal scattering data,
  - unresolved resonance, and
  - implicit capture models were turned off.

# Summary

- GEANT4 can be used to simulate “neutron-multiplying systems”
- Well-suited for transient calculations
- Very much limited by speed.
- **Requests:**
  - General speed-up of the code, but especially
  - Improve on-the-fly Doppler algorithm
  - Provide the tool to create G4NDL