MCRT L9: Neutron Transport

• Outline of code for mono-energetic particles, if change particle energy must change cross sections
• Bank locations of fission neutrons for subsequent generations
• Criticality calculations, issues with regular MC neutron generations increasing or dying, method to keep same number of MC particles
Neutron Generations

1\textsuperscript{st} generation
2\textsuperscript{nd} generation
3\textsuperscript{rd} generation
Distance to interaction

- Usual optical depth sampling: \( \tau = -\ln \xi \)

\[
\tau = \int_{0}^{L} n \sigma \, ds
\]

- \( n \) = number density of material
- Total cross section is sum of cross sections for absorption, scattering, and fission: \( \sigma_T = \sigma_A + \sigma_S + \sigma_F \)
- Depending on geometry, determine \( L \) analytically or numerically (e.g., using grid code)
- Uniform density uranium sphere: \( \rho_U \sim 19 \text{ g/cm}^3 \), so \( n_U \sim 4.8 \text{ E}22 \text{ cm}^{-3} \)
- For 1MeV neutrons in U235: \( \sigma_T \sim 5.1 \text{ b}, \sigma_A \sim 0.1 \text{ b}, \sigma_S \sim 4 \text{ b}, \sigma_F \sim 1 \text{ b} \)
- \( L = \tau / (n \sigma_T) \sim 4.1 \tau \text{ cm} \)
Scatter, absorb, or fission?

- Probability of fission \( \frac{\sigma_F}{\sigma_T} \), so use this algorithm to decide whether neutron is scattered, absorbed, or produces fission:

\[
\sigma_T = \sigma_A + \sigma_S + \sigma_F \\
\text{ran} = \xi \\
\text{if (ran .lt. } \frac{\sigma_A}{\sigma_T} \text{) then} \\
\quad \text{neutron absorbed} \\
\text{elseif(ran .lt. } \frac{\sigma_A + \sigma_S}{\sigma_T} \text{) then} \\
\quad \text{neutron scattered} \\
\text{else} \\
\quad \text{fission event} \\
\text{endif}
\]
Scatter, absorb, or fission?

• Scatter: assume isotropic scattering as with photon scattering simulation, so new directions for neutron are:

\[
\begin{align*}
\theta &= \cos^{-1}(2\xi - 1) \\
\phi &= 2\pi \xi \\
n_x &= \sin \theta \cos \phi \\
n_y &= \sin \theta \sin \phi \\
n_z &= \cos \theta
\end{align*}
\]

• Absorb: terminate neutron and start next neutron in the loop
• Fission: decide how many fission neutrons to be emitted and add their locations to the bank
If probabilities of emitting 1, 2, 3,... fission neutrons are $p_1$, $p_2$, $p_3$,... can use this algorithm:

```plaintext
p = p_1 + p_2 + p_3
ran = ξ
if (ran .lt. $p_1/p$) then
  ! add one fission neutron to the bank
  ibank = ibank + 1
  xbank(ibank) = x    ! Same for y and z
elseif(ran .lt. ($p_1+p_2)/p$) then
  ! add two fission neutrons to the bank
  do j=1,2
    ibank = ibank + 1
    xbank(ibank) = x    ! Same for y and z
  end do
elseif(ran .lt. ($p_1+p_2+p_3)/p$) then
  ! add three fission neutrons to the bank
  do j=1,3
    ibank = ibank + 1
    xbank(ibank) = x    ! Same for y and z
  end do
endif
```

$ibank$ is a counter for number of fission neutrons. Set $ibank = 0$ at start of each generation loop over neutrons.

At end of the loop over the current neutron generation, the value of $ibank$ is the number of fission neutrons produced. Can then compute $k_{eff} = ibank / N$, where $N$ = number of neutrons emitted in the current generation.
Neutron Transport & Criticality: Analog Monte Carlo

- Loop over initial generation of neutrons – either from a point or some guess of the final distribution, or uniformly throughout the medium
- Counter for how many neutrons go into the bank – $i_{bank}$
- $k_{eff} = \frac{i_{bank}(\text{generation } i)}{i_{bank}(\text{generation } i-1)}$
- Loop over multiple generations of neutrons until exceed space you have allocated in the bank or bank is emptied (population dies out)
- In each generation, loop over all the neutrons in the bank, i.e., emit all neutrons in the bank for each generation
Launch 5 neutrons:
1 scatters and escapes
1 is absorbed (produces $\gamma$-ray)
3 produce fissions
3 fission sites produce a total of 7 neutrons
Add locations to the bank
\[ k_{\text{eff}} = \frac{7}{5} \]
2\textsuperscript{nd} generation: emit the 7 neutrons from the bank
2\textsuperscript{nd} generation: emit the 7 neutrons
1 escapes without interacting
2 are absorbed
1 scatters and escapes
3 produce fissions (after scattering)
3 fission sites produce 9 neutrons for 3\textsuperscript{rd} generation
\(k_{\text{eff}} = \frac{9}{7}\)
Track the 3rd generation neutrons…
Make the position bank 2D arrays: \( x_{\text{bank}}(n_{\text{bank}}, 2) \), \( y_{\text{bank}}(n_{\text{bank}}, 2) \), \( z_{\text{bank}}(n_{\text{bank}}, 2) \), where \( n_{\text{bank}} = \) a large number (say one million)

First generation, store the locations of fission neutrons at \( x_{\text{bank}}(i_{\text{bank}}, 1) = x \), recall we increment the counter \( i_{\text{bank}} \) and at end of the generation \( i_{\text{bank}} \) is the total number of fission neutrons produced

Second generation, emit \( i \)-th neutron from \( x_{\text{bank}}(i,1) \), store fissions in \( x_{\text{bank}}(i_{\text{bank}}, 2) \)

Third generation, emit \( i \)-th neutron from \( x_{\text{bank}}(i,2) \), store fissions in \( x_{\text{bank}}(i_{\text{bank}}, 1) \)

Need an algorithm so that the second index of the bank arrays for storing locations of fission neutrons cycles from 1 to 2 depending whether the generation is odd or even:

When emitting \( i \)-th neutron for generation “gen”, use source locations \( x_{\text{bank}}(i,\text{current}) \)

When banking neutrons produced in generation “gen”, store the locations in \( x_{\text{bank}}(i_{\text{bank}},\text{next}) \)

\[
\text{if}(\text{mod}(\text{gen},2) = \text{eq}.0) \text{ then} \\
\quad \text{current} = 1 \\
\quad \text{next} = 2 \\
\text{else} \\
\quad \text{current} = 2 \\
\quad \text{next} = 1 \\
\text{endif}
\]
Critical Mass of Uranium Sphere

\[ M_{\text{super}} \]

\[ M_{\text{crit}} \]

\[ M_{\text{sub}} \]
Alternative criticality calculation

- Criticality calculations, issues with number of neutrons in *analog* or *regular* MC generations increasing or dying out
- Algorithm to prevent runaway increase or decrease of number of particles being tracked – emit N Monte Carlo neutrons at every generation
- Emit N neutrons in first generation, bank the locations of fission neutrons as before
- Emit N neutrons in the 2\textsuperscript{nd} generation – take the locations to be either the first N from the bank (if N < nbank) or take all neutrons in the bank and then take those from the start of the bank until have N for the 2\textsuperscript{nd} generation
- Randomly sample from the “relaxed” distribution of neutrons – just take the first N from the bank (they are produced randomly anyway) if generate more than N. If generate less than N, then cycle through the bank multiple times until have N.
Emit 10 neutrons from centre of sphere
They produce 16 fission neutrons for second generation
\[ k_{\text{eff}} = \frac{16}{10} \]
Have an increasing population of neutrons
Choose the first ten neutrons in the bank as source for 2nd generation
Choose the first ten neutrons in the bank as source for 2\textsuperscript{nd} generation
Emit 10 neutrons in 2\textsuperscript{nd} generation
They produce 18 fission neutrons for 3\textsuperscript{rd} generation
\( k_{\text{eff}} = \frac{18}{10} \)
Have an increasing population of neutrons
Choose the first ten neutrons in the bank as source for 3\textsuperscript{nd} generation
Choose the first ten neutrons in the bank as source for 3\textsuperscript{rd} generation
• In reality there are more than \( N \) neutrons in a real life situation, so our \( N \) Monte Carlo neutrons are a statistical sampling of the actual number of neutrons
• Neutron histories are all randomly generated, so it is ok to choose source locations from the bank as described above
• \( k_{eff} \) is then always \( ibank/N \) from generation to generation, where \( ibank \) is updated as in analog simulation for banking neutron locations
Just in case you think you’re doing something new...

THE INSTITUTE FOR ADVANCED STUDY

Founded by Mr. Ludwig Bemser and Mrs. P. Foxfield
PRINCETON, NEW JERSEY
School of Mathematics

March 11, 1947

LA AIRMAIL: REGISTERED

Dr. R. Richtmyer
Post Office Box 1665
Santa Fe, New Mexico

Dear Bob:

This is the letter I promised you in the course of our telephone conversation on Friday, March 7th.

I have been thinking a lot about the possibility of using statistical methods to solve neutron diffusion and multiplication problems, in accordance with the principle suggested by Stan Ulam. The more I think about this, the more I become convinced that the idea has great merit. My present conclusions and expectations can be summarized as follows:

1. The statistical approach is very well suited to a digital treatment. I worked out the details of a criticality discussion under the following conditions:

   - geometry
   - position along the
Just in case you think you’re doing something new…

Dear Bob,

I have been thinking a good deal about the possibility of using statistical methods to solve the neutron diffusion and multiplication problem, in accordance with the principle suggested by Stan Ulam…

If and when the problem of neutron diffusion has been satisfactorily handled… it will be time to investigate the more general case, where hydrodynamics also come into play… I think I know how to set up this problem, too…

John von Neumann had Monte Carlo radiation transport coupled with hydrodynamics all figured out… in 1947!!
Counter proliferation

- Historic concern over proliferation of atomic and thermonuclear weapons
- Enrichment of uranium, breeding of plutonium is expensive and requires extensive infrastructure
- Civilian nuclear energy programmes closely monitored
- Could a bomb be designed and built without live testing: 3D radiation hydrodynamics computer simulations…?
Concerns over last twenty years about research in experimental condensed matter physics, internal confinement fusion research, numerical simulations in astrophysics…
Counter proliferation

- Concerns over last twenty years about university research in experimental condensed matter physics, internal confinement fusion research, numerical simulations in astrophysics…

National Ignition Facility

FLASH Code, University of Chicago
Thermonuclear breakout on a white dwarf
Keeping us safe…

- Thermonuclear weapons simulations need equations of state and behaviour of material properties (opacity) at extreme densities, temperatures, and pressures.

\[ \frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0 \quad \text{Continuity equation} \]

\[ \rho \frac{d\mathbf{v}}{dt} = -\nabla P - \nabla \phi + F_{\text{rad}} \quad \text{Momentum equation} \]

\[ P = f(\rho, T) \quad \text{Equation of state} \]

\[ F_{\text{rad}} = \quad \text{Radiation pressure} \]

- Classified and top secret for elements heavier than gold.
Cosmic Ray Air Showers

- Use similar techniques of generations of particles
- Need probabilities for producing different particles
- Need interaction cross sections to determine distances traveled by particles between interactions
- High energy cosmic ray can generate $10^{12}$ particles
- Can’t follow all $10^{12}$ particles so use techniques to statistically sample particles in the shower: “thin sampling”
Starting from 3D grid code + ideas for banking from neutron code, developed MCRT code for cosmic ray air showers in Jupiter’s atmosphere