UNIVERSITY OF CAMBRIDGE

The Random Ray Method in SCONE (also in OpenMC)

Serpent User Group Meeting 2022

1st September 2022

Paul Cosgrove (pmc55@cam.ac.uk)

Engineering - Energy, Fluid dynamics and Turbo-machinery

Contents

- The Method of Characteristics (MoC)
- The Random Ray Method (TRRM)
- SCONE – and why put MoC in a Monte Carlo code
- Numerical test problems
- Conclusions and future work

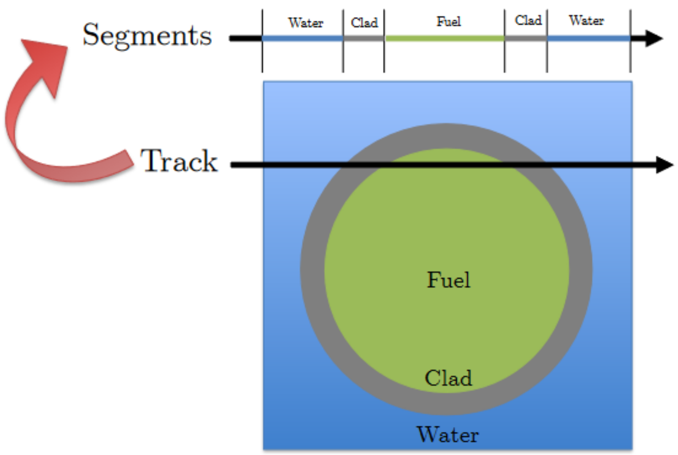
The Method of Characteristics (MoC)

$$\frac{\mathrm{d}}{\mathrm{d}s}\psi_g(s) + \Sigma_{\mathrm{t},g}\psi_g(s) = q_g$$

- The Method of Characteristics (MoC) calculates the change in angular flux along many rays:

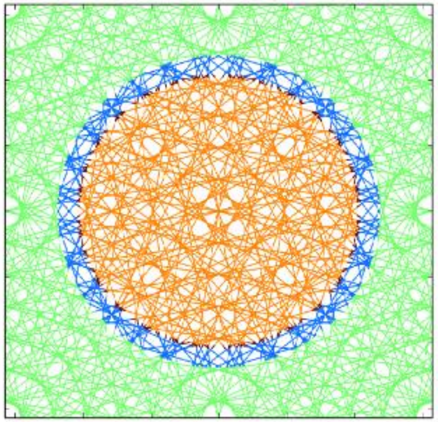
$$\Delta_g = \left(\psi_g(0) - \frac{q_g}{\Sigma_{\mathrm{t},g}}\right)\left(1 - e^{-\Sigma_{\mathrm{t},g}s}\right)$$

$$\psi_g(s) = \psi_g(0) - \Delta_g$$



- This change is used alongside a quadrature to estimate the scalar flux:

$$\phi_g = \sum_t \Delta_g \omega_t + \frac{4\pi q_g}{\Sigma_{\mathrm{t},g}}$$



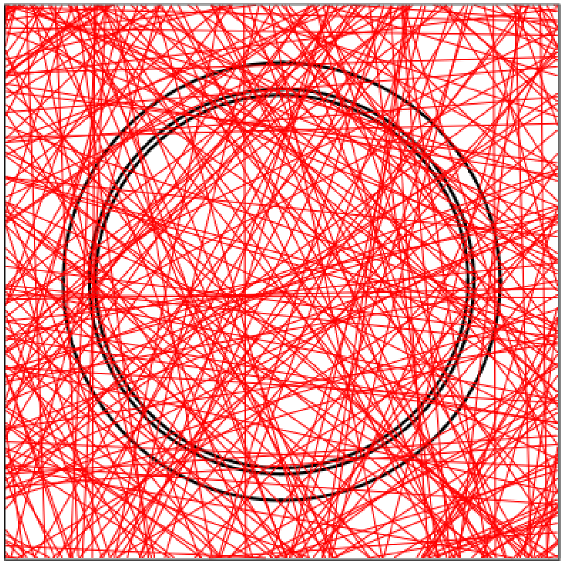
- This quadrature is typically ‘cyclic’, storing angular flux estimates at the boundaries

UNIVERSITY OF CAMBRIDGE

Tramm et al. (2017). “The Random Ray method for neutral particle transport”, J. Comp. Phys.

The Random Ray Method (TRRM)

- Use stochastic set of tracks with position and direction sampled uniformly every sweep
- Boundary fluxes not saved and rays traced OTF → massive memory reduction
- Initial fluxes unknown → obtained with an initial 'dead zone'
- All rays travel the same distance → uniform quadrature
- Stochastic coverage allows coarser track laydown
- Inherently 3D
- Requires active and inactive iterations like MC



UNIVERSITY OF CAMBRIDGE

Tramm et al. (2017). "The Random Ray method for neutral particle transport", J. Comp. Phys.

SCONE – and why put MoC in an MC code?

- Development began in 2017
- Based at Cambridge
- Open-source
- Still relatively early in development, but with a focus on ease of modification/flexibility

Why put TRRM in MC?

- Most complicated aspect of TRRM is geometry routines → these are already present in mature MC codes
- Ray-like objects, stochastic estimators, active/inactive iterations typically present already
- No open-source implementation of TRRM available until now

Implementation details

- Uniquely identifying cells
- Allow ‘particle’ to store MG flux
- Writing the algorithm
- Azimuthally divided pins
- Exponential evaluator
- Distance caching (remember distance to boundary at all CSG universe levels)

Algorithm 1 MOC Power Iteration

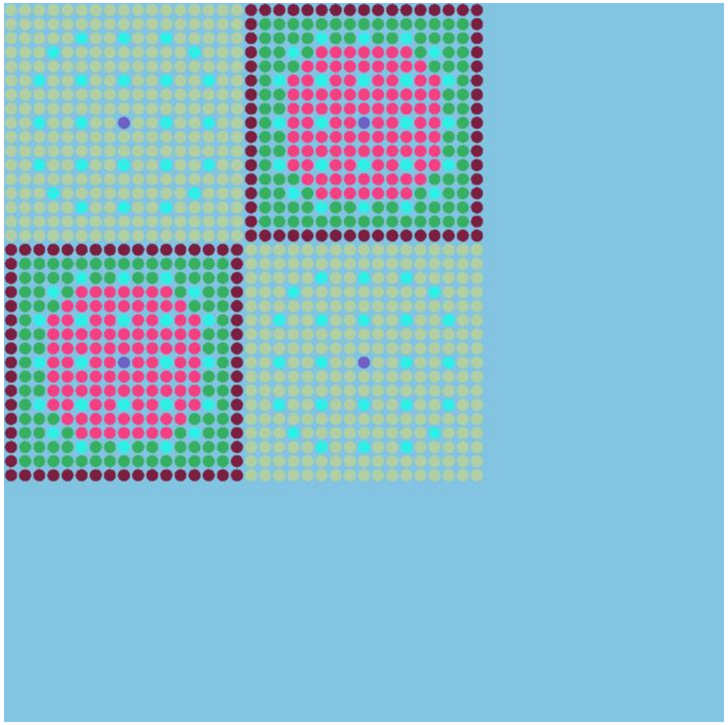
```
Initialize Scalar Fluxes to 1.0
while K-effective and Scalar Flux Unconverged do
    Normalize Scalar Flux to Fission Source
    Compute Source (Equation 9)
    Flatten Scalar Flux to Zero
    Transport Sweep (Algorithm 2)
    Normalize Scalar Flux to Sum of Ray Distances
    Add Source to Scalar Flux (Equation 10)
    Calculate K-effective
end while
```

Kowalski & Cosgrove. (2021). “Acceleration of surface tracking in Monte Carlo transport via distance caching”, Ann. Nucl. Energy

Numerical tests: 2D C5G7

- Used C5G7: standard deterministic transport benchmark with 7 energy groups
- Relatively coarse spatial discretization for TRRM - 142k spatial cells
- C5G7 runs performed on Intel Xeon 8276 with 56 threads

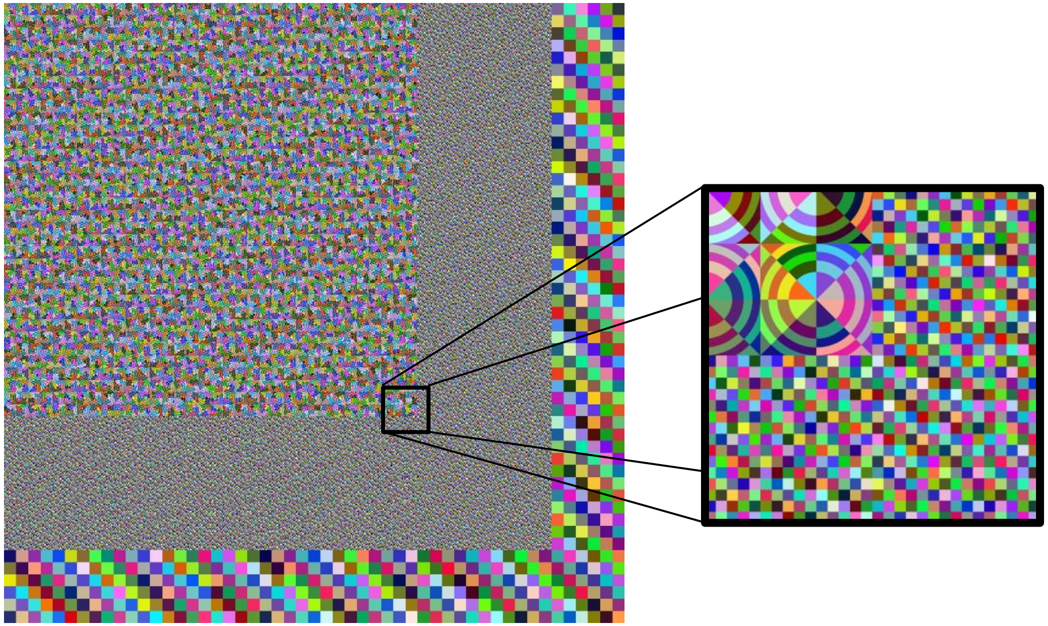
C5G7 geometry



Lewis et al. (2003). “Benchmark Specifications for Deterministic MOX Fuel Assembly Transport Calculations without Spatial Homogenisation”, OECD-NEA

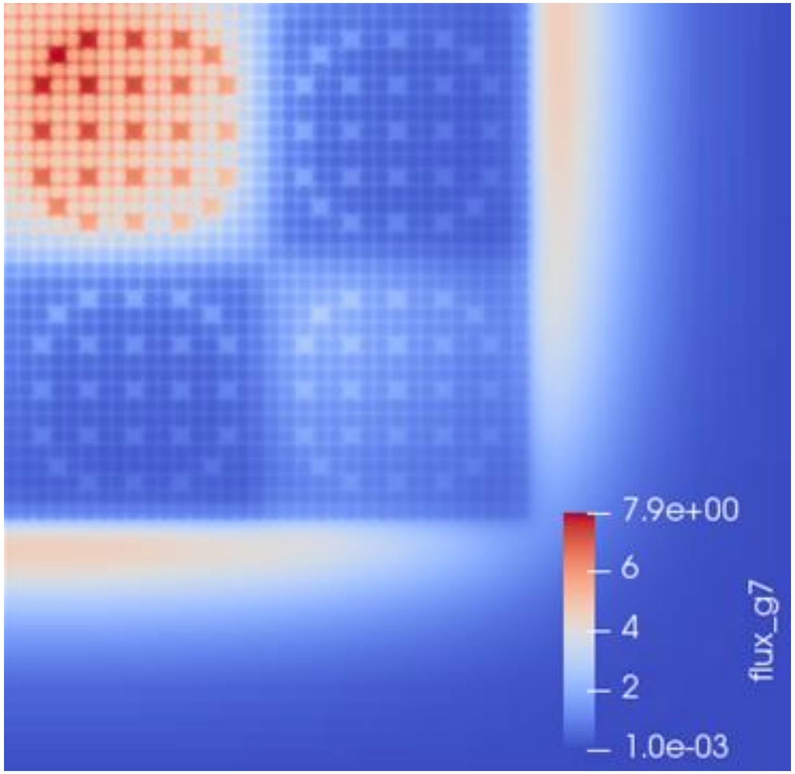
Numerical tests: 2D C5G7

- 1750 rays/iter.
- 1000 inactive iter.
- 2600 active iter.
- 220cm total length
- 20cm dead length

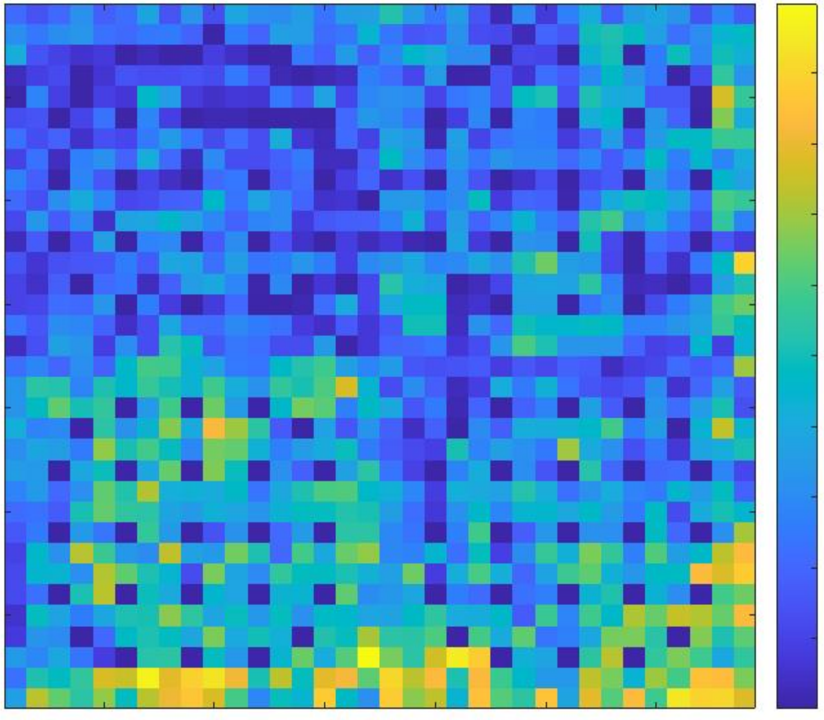


Numerical tests: 2D C5G7

- Runtime of 1.3min, at 1.1ns/integration, and 100MB memory usage
- Keff = 1.18678 +/- 14pcm, Benchmark Keff = 1.18655 +/- 3pcm



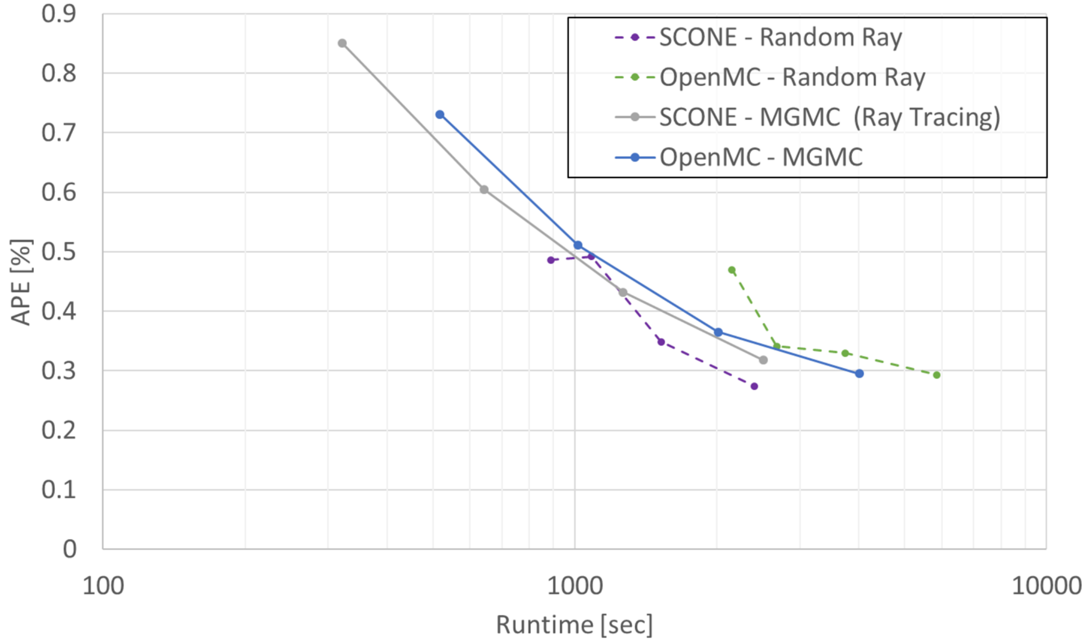
Absolute % Pin Power Errors



Numerical results: 2D C5G7

Serial runs

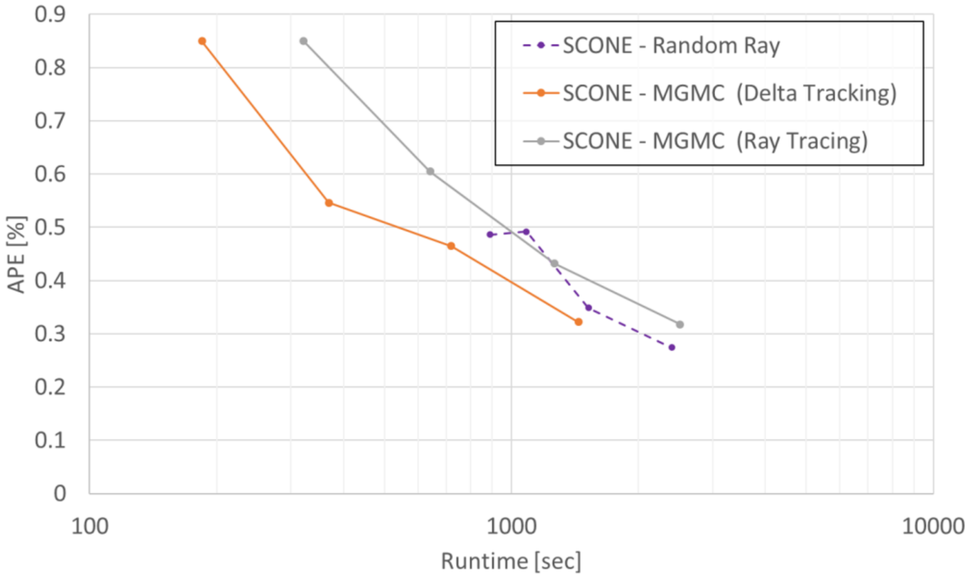
- Both codes show similar performances between MGMC and TRRM
- OpenMC MGMC uses track length estimator
- TRRM should show more benefits when increasing the number of energy groups
- TRRM performance metric ns/integration: 88 (OpenMC), 34 (SCONE)



Numerical results: 2D C5G7

Serial runs

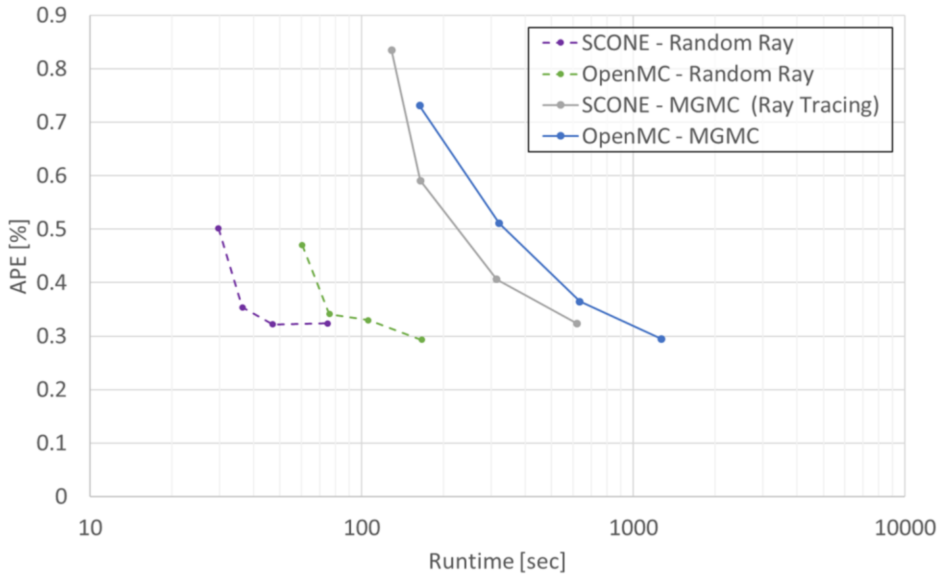
- SCONE also has the possibility to do MGMC particle tracking with Delta Tracking
- In MGMC, the tracking method impacts performance more than in standard CEMC
- Delta Tracking offers a speed-up of a factor ~2



Numerical results: 2D C5G7

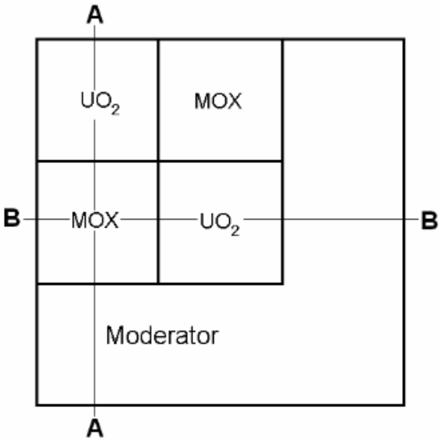
Parallel runs - 56 cores

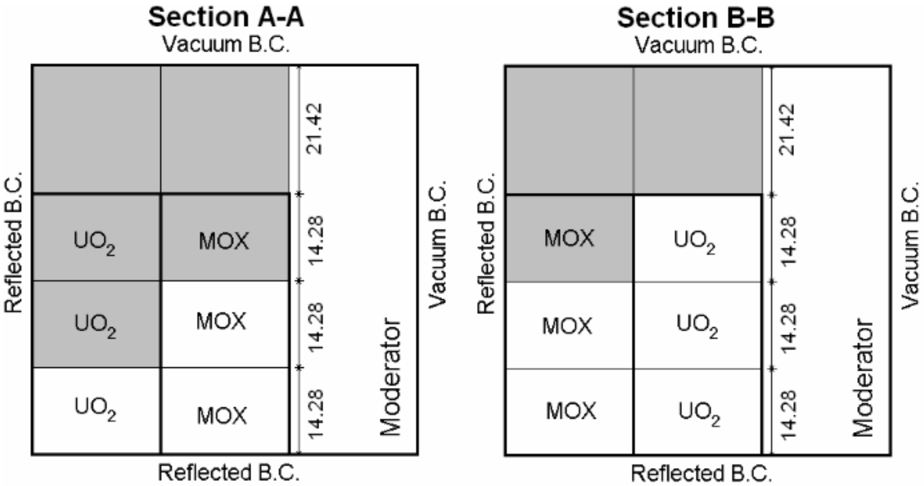
- Both codes presented parallelisation issues in MGMC! Poor SCONE scaling due to false sharing in tallies
- Random Ray is quite easy to write in parallel
- TRRM performance metric ns/integration: 2.5 (OpenMC), 1.26 (SCONE) - both similar to dedicated TRRM code (ARRC) performance



Numerical tests: 3D C5G7, Rodded B

C5G7 geometry





- Axially extruded C5G7 with rods at various insertion depths (grey regions)
- Requires significant axial discretization, dz = 0.357cm, giving 29M spatial cells
- Used quite fine settings:
  117,000 rays/iter.
  950 active iter.
  1525 inactive iter.
  Dead length of 12.56cm
  Total length of 628.12cm

Smith et al. (2005). “Benchmark on Deterministic Transport Calculations without Spatial Homogenisation: MOX Fuel Assembly 3-D Extension Case”, OECD-NEA

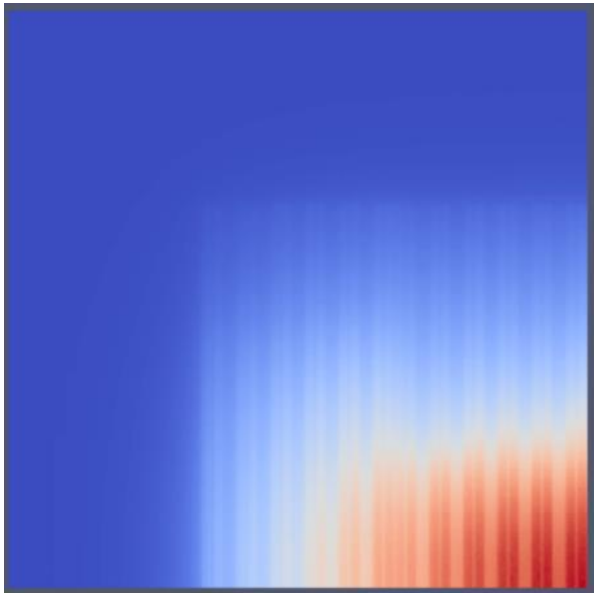
Numerical tests: 3D C5G7, Rodded B

- Runtime of 5.5hrs, at 1.9ns/integration, 7.6GB memory usage
- Keff = 1.07782 +/- 2.4pcm, Benchmark Keff = 1.07777 +/- 3pcm

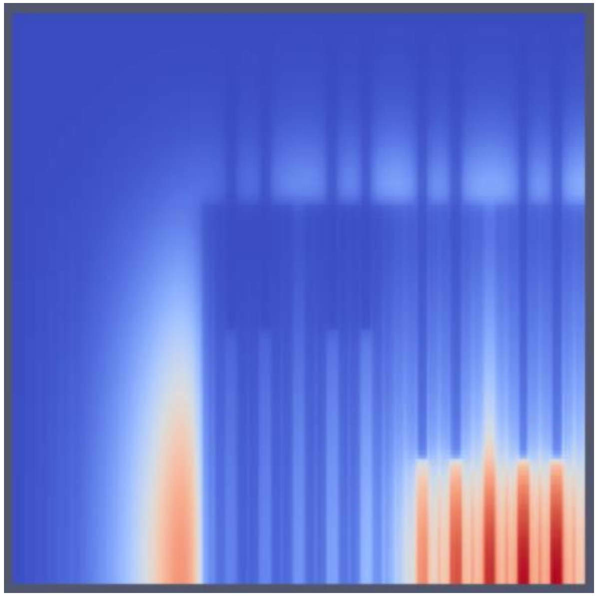
Benchmark comparison

	Reference	TRRM
Peak Power	1.835	1.825
Inner UO2	395.4	393.9
MOX	236.6	237.3
Outer UO2	187.3	187.5

Fast flux (g = 1)



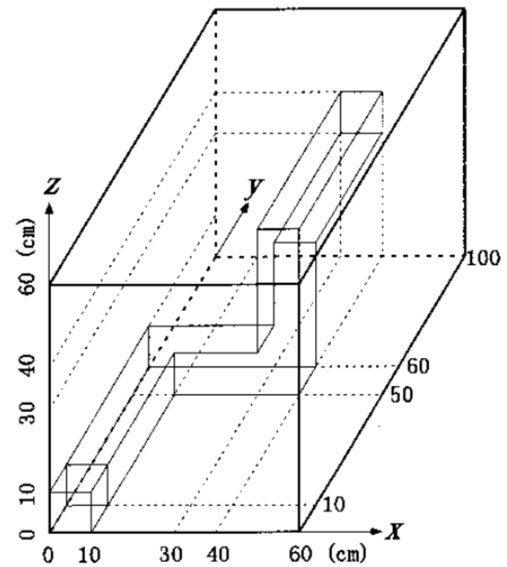
Thermal flux (g = 7)

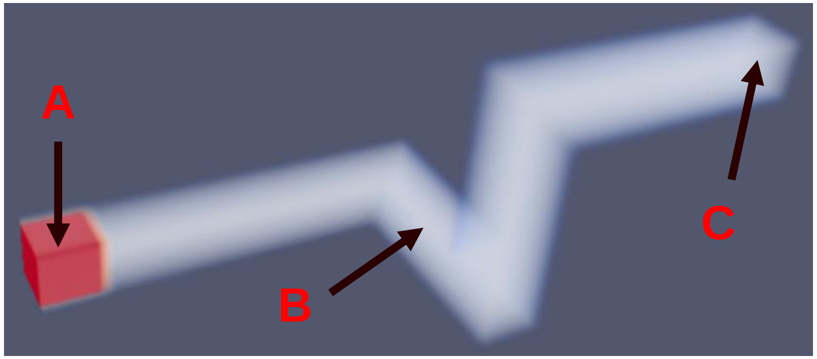


Smith et al. (2005). "Benchmark on Deterministic Transport Calculations without Spatial Homogenisation: MOX Fuel Assembly 3-D Extension Case", OECD-NEA

Numerical tests: fixed source, dog-leg problems

- Common benchmark: monoenergetic, 3D shielding problem, no scattering
- Easy/immediate convergence but induces ray effect/negativity in deterministic solvers
- Use a coarse $(2\text{cm})^3$ mesh, ~45k cells
- 500,000 rays/iter., 100 active, 10 inactive, 60cm dead, 650cm total
- Compare flux in source, middle of duct, and end of duct

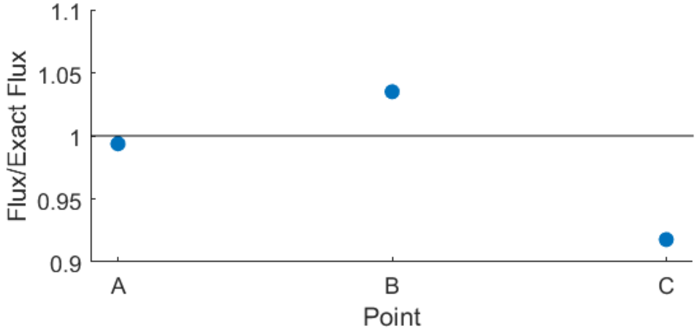


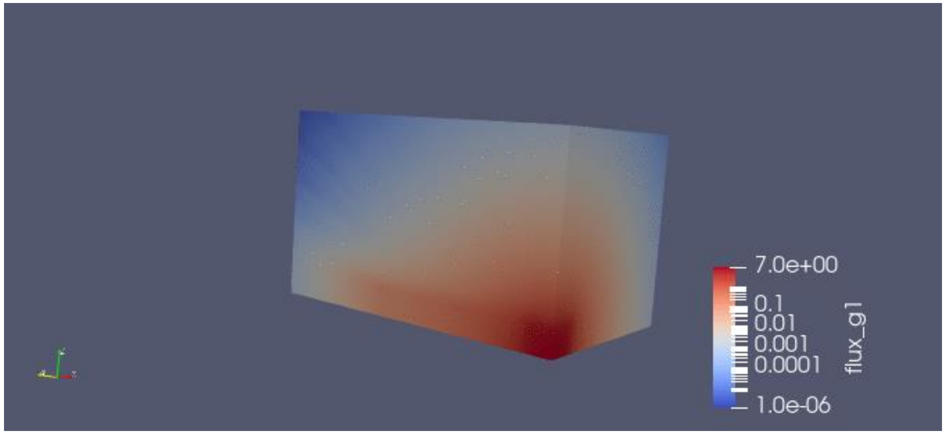


Kobayashi et al. (2000). "3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions", NEA-OECD

Numerical tests: fixed source, dog-leg problems

- 6min15s on 26 cores (Intel Xeon 6130), ~14ns/integration, 10.5MB memory
- Higher variance in the extremes, but agrees well with benchmark values





Conclusions and future work

- Random Ray can be quickly implemented by using the existing infrastructures of Monte Carlo transport codes
- It remains a fast 3D transport solver with good performance on reactor problems
- One of the first MoC fixed source solvers has been implemented and tested in 3D

Future Work

- Need to add acceleration – while the solver is fast, convergence is a bottleneck
- 90% sure some sub-optimal scaling problem is lurking, need to nail down what’s going on with error convergence on C5G7

THANK YOU FOR YOUR ATTENTION

MaThRad

- Translate mathematical advances in probability theory and inverse problems to MC radiation transport
- Reactor analysis, criticality, shielding, medical and space applications
- £7M, 5-year UKRI-sponsored Program Grant
- 26 partners from industry and academia
- 30 postdoc-years, up to 10 PhDs
- Internships and hosting visitors
- Industry workshops and symposia
- UCLH proton treatment team + beam time