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Scalable algorithms for domain decomposition of Monte Carlo neutral particle transport simulations on unstructured mesh

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Scalable algorithms for domain decomposition of Monte Carlo neutral particle transport simulations on unstructured mesh

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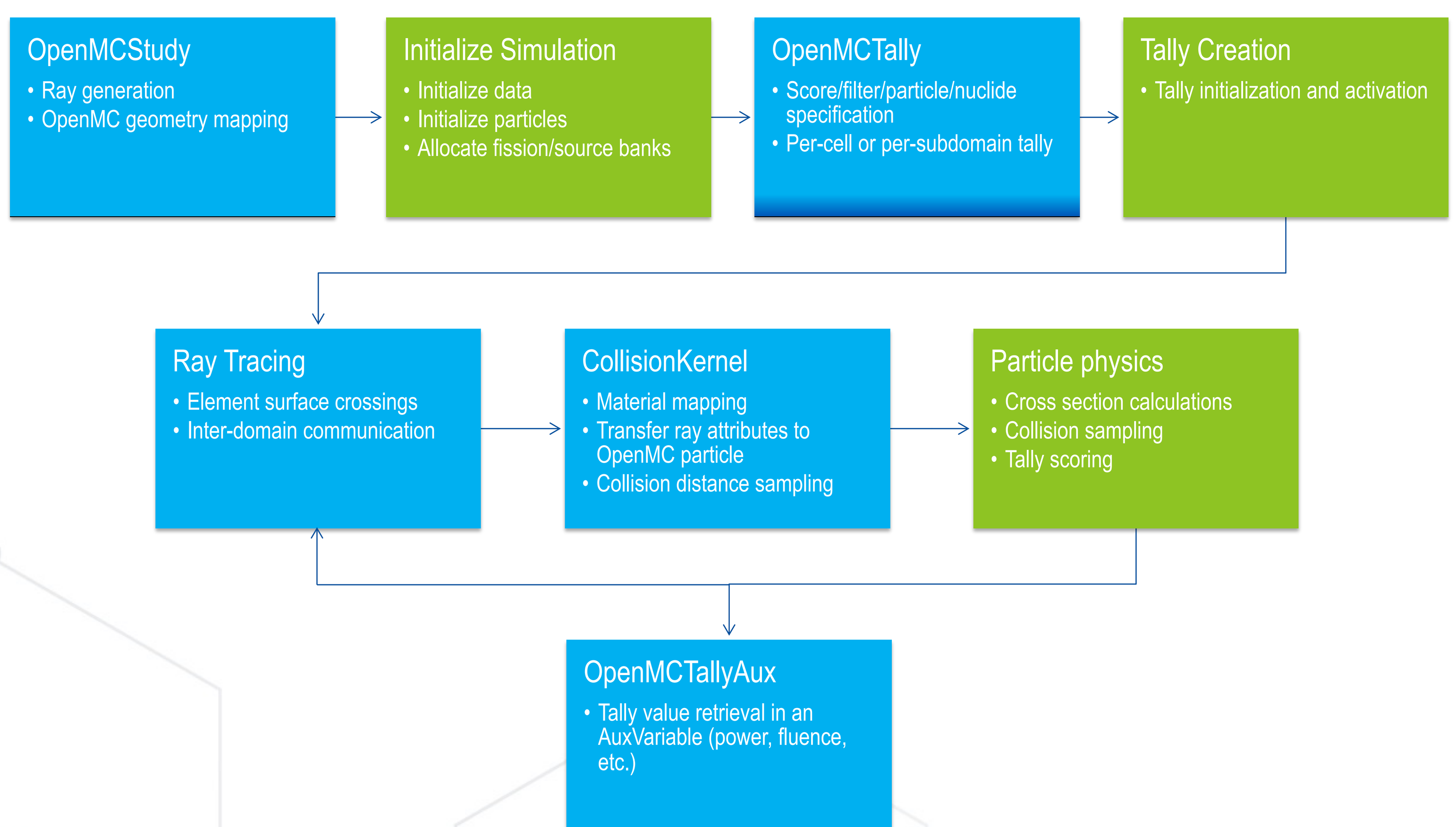
Introduction

- Monte Carlo simulations are the gold standard in particle transport simulations for shielding and nuclear reactor simulations
- Full core simulations can require terabytes of memory for tracking pin-resolved (up to 50,000 pins), nuclide (200 tracked), and axial (20-200 zones) reaction rates
- Domain decomposition (splitting the calculation and the memory storage among several nodes) is challenging [3,4,5] as it involves communication of particles across domain boundaries
- New MOOSE application: MaCaw
- Algorithms developed for ray tracing in MOOSE were adapted for simulating neutral particle transport
- Physics and tally routines in OpenMC, dynamically linked, are called from the application.

OpenMC – MOOSE coupling



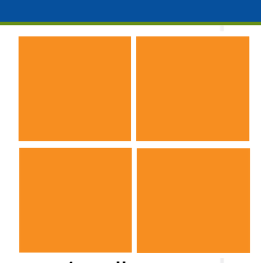
- Temperature field on unstructured mesh is used for cross-section sampling
- AuxVariable output can be transferred to other applications for coupling or cross-section generation (potential future work).

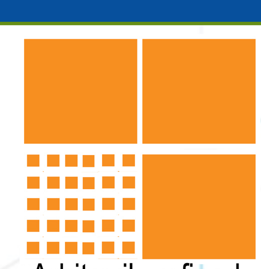
Test cases

Infinite medium:
- Provide simple interpretable insight into algorithm performance

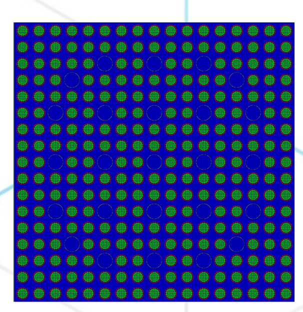
Assembly
- Typical single-node workload
- Realistic pin-discretization (4–10 rings) provides realistic number of surface crossings

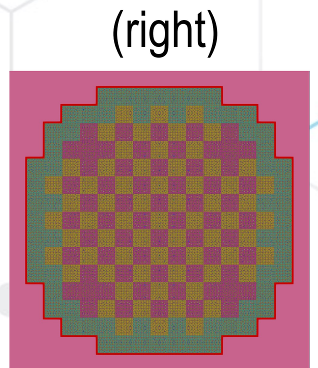
Full core
- Requires domain decomposition
- Challenging benchmark [6] wherein few codes have solved, especially with unstructured mesh
- Load imbalance for naïve decompositions.


4-cell case


Arbitrarily refined

17x17 lattice (right)




BEAVRS core (left)

References

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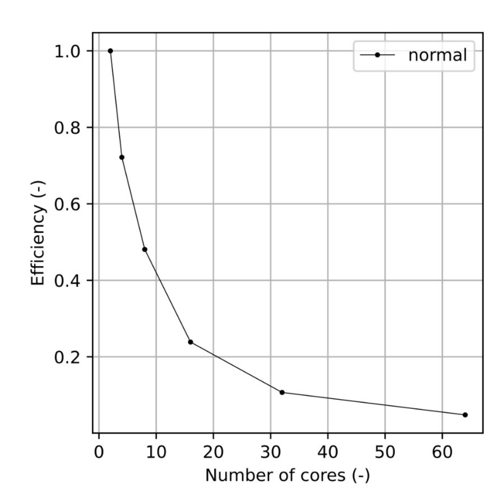
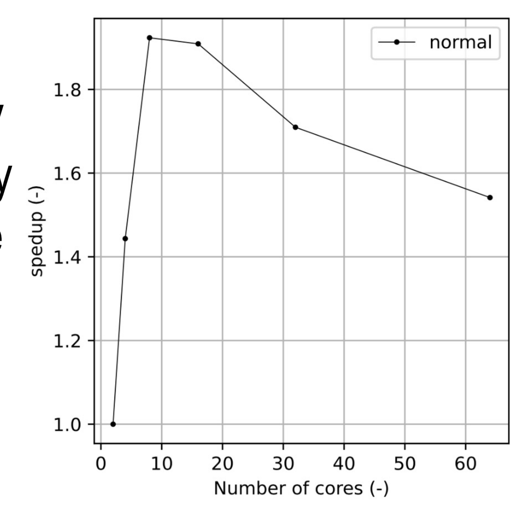
[6] N. Horelik, B. Herman, B. Forget, and K. Smith. 2013. "Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)." American Nuclear Society M&C 2013: International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Sun Valley, ID. May 5–9, 2013.

Shared memory scalability

- With a non-decomposed single domain, shared memory parallelism allows for a smaller memory footprint on a single node
- Efficient shared memory parallelism is achieved by distributing most calculation phases and avoiding false sharing
- MaCaw shows limited scalability on infinite medium and assembly cases, prompting further investigation



Weak scalability efficiency (**left**) and strong scalability speedup (**right**) on infinite medium/assembly case



Distributed memory scalability

- Domain decomposition entails using distributed memory.
- Fission bank management: renormalization using random sampling.

800 particles/sites generated in batch

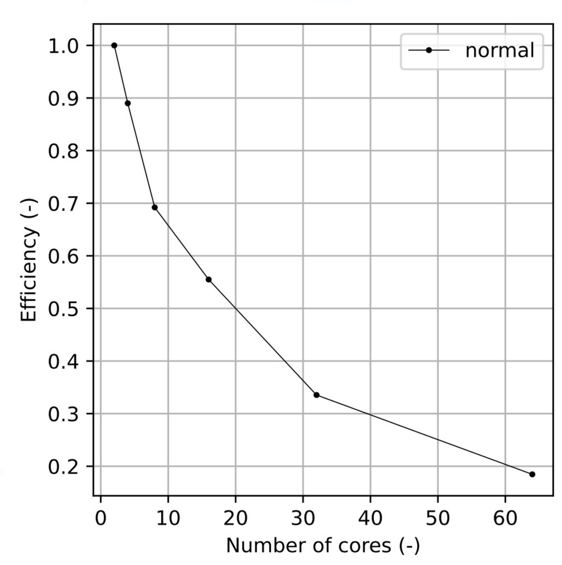
237	160
202	201

1,000 particles sampled in next batch

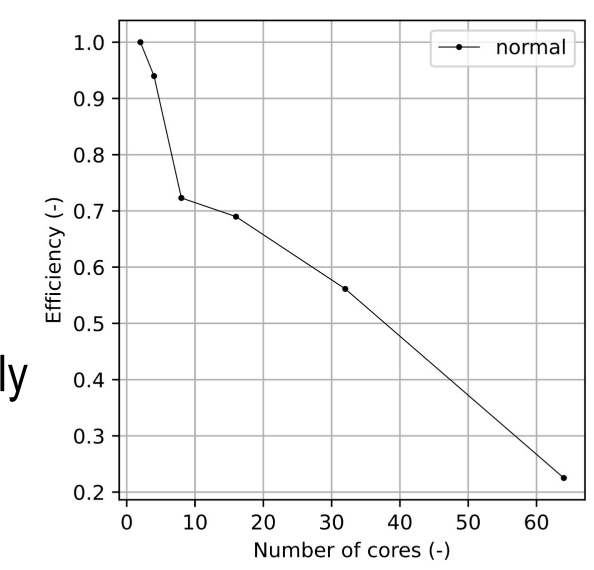
297	202
251	250

Algorithm for node-to-node communication [2]:
- Asynchronous ray transfers executed simultaneously with the simulation.

Distributed memory scaling



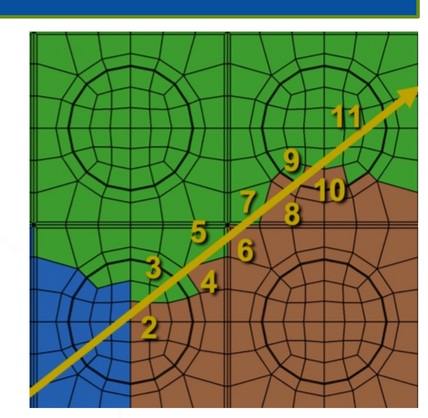
Weak scalability efficiency (**left**) and strong scalability speedup (**right**) on infinite medium/ assembly case currently show only limited scaling.

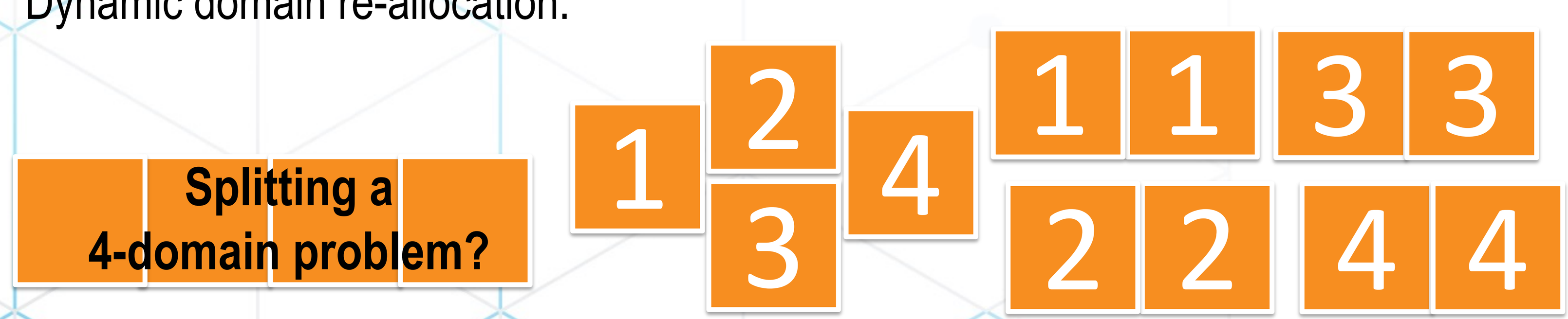


Further investigation into load balancing or communication reduction strategies is warranted to improve scaling.

Ongoing & future work

- Ghosting of a single element layer avoids numerous communications along jagged domain edges. [2]
- Requires reduction of tallies across boundaries. Worth it for Monte Carlo methods?
- Multi-scale calculation strategies replicate part of the geometry to limit communication.
- Dynamic domain re-allocation.

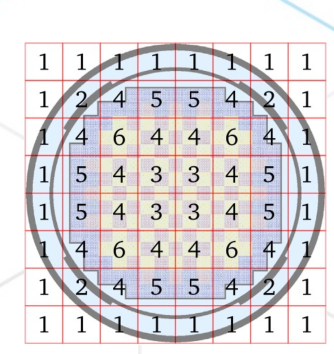


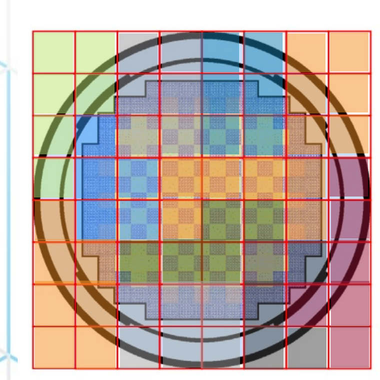


Full distribution

Partial replication

Different neutron flux cause load imbalance in the simulation. This can be handled ahead of time by assigning more nodes to high-flux regions [**left**, 4], or dynamically by moving domain boundaries [**right**, 12 domains].





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