SHIFT: A New Monte Carlo Package

Seth R. Johnson
Tara M. Pandya, Gregory G. Davidson, Thomas M. Evans, and Steven P. Hamilton, Cihangir Celik, Aarno Isotalo, Chris Peretti

Oak Ridge National Laboratory

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Shift: a new HPC Monte Carlo package

Seth R Johnson
R&D Staff, Monte Carlo Methods
Radiation Transport Group

Exnihilo team:
Greg Davidson
Tom Evans
Stephen Hamilton
Seth Johnson
Tara Pandya

Associate developers:
Cihangir Celik
Aarno Isotalo
Chris Perfetti
What makes Shift an HPC transport code?

- **Modern framework**
  - Rapid development with C++11, Python, CMake, CTest, …
  - Integration with SCALE, Denovo, VERA, … and Python

- **Extensibility**
  - Multiple geometry, physics packages
  - Easy addition of new tallies, sources, etc.

- **Scalability**
  - State-of-the-art transport methods
  - Hybrid deterministic/MC methods
  - Near-perfect efficiency on leadership-class supercomputers (Titan)
Shift application areas

- Research reactors
  - HFIR target activation
  - HFIR core depletion for HEU→LEU conversion

- Light water reactors
  - SMRs
  - WEC AP1000®

- Neutron sources
  - ITER bioshield dose analysis

- Criticality safety
  - Fuel cask analysis
Exnihilo: radiation transport framework

- **Denovo**: Deterministic ($S_N$ and $SP_N$) transport
  - Uses SCALE cross section processing
  - Powers SCALE hybrid codes

- **Shift**: Monte Carlo transport
  - Uses SCALE CE and MG data
  - Uses ORIGEN depletion
  - General application range

- **Insilico**: PWR physics
  - Uses both Denovo and Shift
  - High-fidelity engine for VERA-CS
Extensibility

- Shift has generic templated geometry, physics, particle interfaces
- One-line input change to switch between physics or geometry models
- Templated/polymorphic interface means all tallying, transport, source algorithms are reused
Extensibility

• Geometry
  – RTK (fast, LWR)
  – SCALE (Atlas library)
  – MCNP (Lava library)
  – CAD (DagMC library)
Extensibility

- **Physics**
  - **Multigroup**
    - Manual XS input
    - SCALE collapsed
    - SCALE processed
  - **Continuous energy**
    - SCALE CE data
    - Coupled (n,\(\gamma\)) physics
Extensibility

• Geometry
  – RTK (fast, LWR)
  – SCALE (Atlas library)
  – MCNP (Lava library)
  – CAD (DagMC library)

• Physics
  – Multigroup
    • Manual XS input
    • SCALE collapsed
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  – Continuous energy
    • SCALE CE data
    • Coupled (n,\gamma) physics

• Sources
  – Multiple sources, particle types, strengths
  – Fission mesh source: fixed source from eigenvalue flux tally
  – MCNP source
Tallies

• Object-oriented design
  – Integrating new application-specific tallies is easy
  – Additional tally types does not affect performance

• High-performance scalability
  – Hash tables for constant-in-cells performance
  – Domain-decomposed mesh tallies for large problems
Scalability: parallel decomposition

- Multi-Set Overlapping Domain (MSOD): adjust from fully decomposed to fully replicated
- Overlap fraction: specifies fraction of each block shared with the adjacent neighboring domain
Decomposed mesh tallies

- Domain-local tally mesh subsumes local “boundary mesh,” including overlap
- Output mesh has unique cells
- Gather/scatter on overlap
- Parallel reduction across equivalent blocks
Fission site rebalance

- Fully parallel fission rebalance
  - Communication with neighbor processors only
  - Iterates until sites are rebalanced
  - Avoids linear-in-time gather/comb

Block-to-block communication during rebalance

Rebalance boundaries across sets
MSOD scaling study

4×4 reactor assembly (17×17 UO₂ pins) with each set decomposed into 2×2 assemblies per block

Strong scaling on Titan

Weak scaling on Titan
Benchmark result: WEC AP1000®

1 trillion particles
240,000 cores
~3 hours
Avg. reported R.E.: 0.1%

Power distribution comparison of AO control rod bank configuration

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<th>RMS Pin %</th>
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Scaling with a real application

- Strong scaling of domain replicated WEC AP1000® on Titan
- $5 \times 10^8$ particle histories per cycle
Current and future work

- Fully integrated hybrid methods
- Sensitivity & uncertainty methods
- High-order transport/depletion solver coupling methods
- Transport on GPU
- Source convergence acceleration
- Covariance and batch statistics for tallies
Conclusions

• Shift is in a good place for a young transport code
• We have shown almost perfect (DR) scaling to $10^5$ cores for real-world engineering applications
• Extensibility allows rapid expansion of application space
• Interfaces (VERA, SCALE, Omnibus) are enabling rapid deployment
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Thursday P.M.: SCALE/Python integration!
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Questions?