Hardware Code Generation Techniques for Accelerating Python

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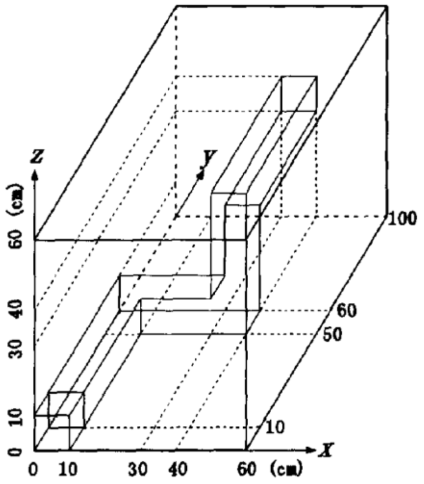
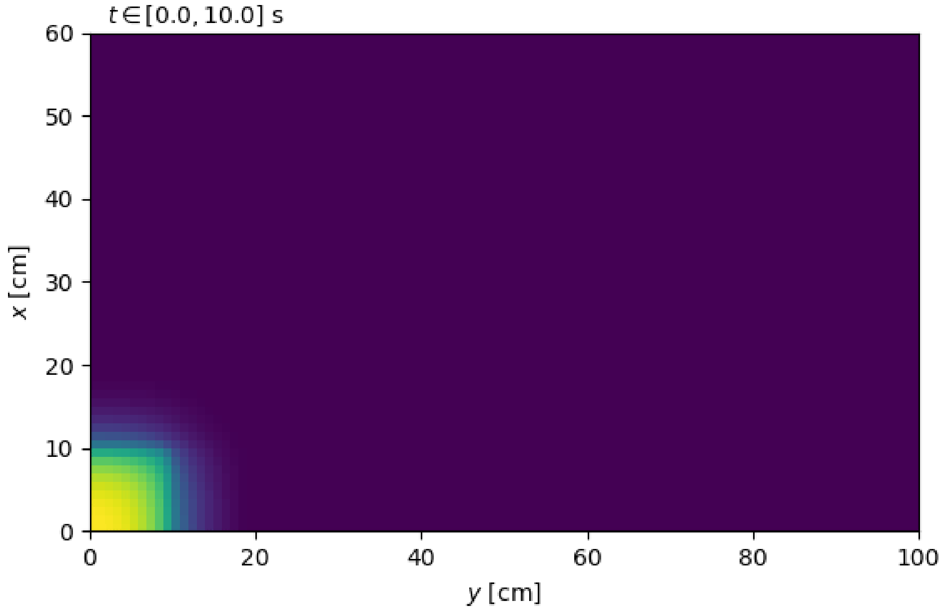
Introduction

MC/DC: Monte Carlo / Dynamic Code

- Dynamic neutron transport solver made for rapid methods exploration at high performance computing and exa-scale
- Target various hardware architectures
- Written in Python





Kobyashi Problem: Image courtesy Ilham Variansyah

MC/DC–TNT: Toy Neutronics Testbed

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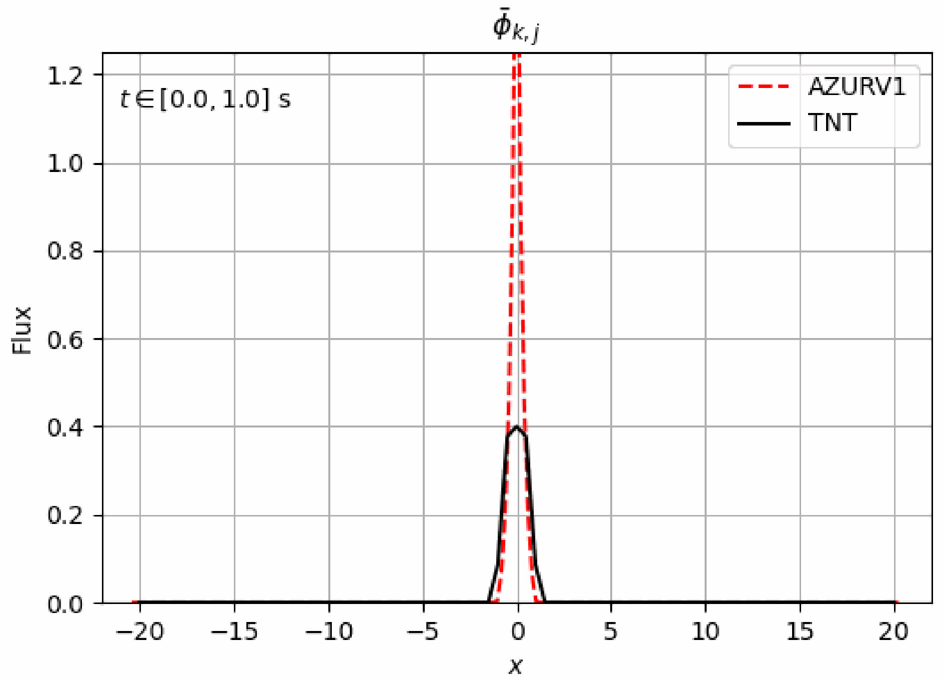
- Mono-energetic, slab-geometry, transient tallies, fission, event-based, with surface tracking
- Architecture targets: Nvidia GPUs and x86 CPUs
- Validated with AZURV1 [1]



Vacuum

$L = 40$cm, $v = 2.3$, $\Delta x = 0.49$cm
$\Sigma_{cap} = \Sigma_{scat} = \Sigma_{fis} = 1/3 cm^{-1}$

Vacuum

MC/DC–TNT

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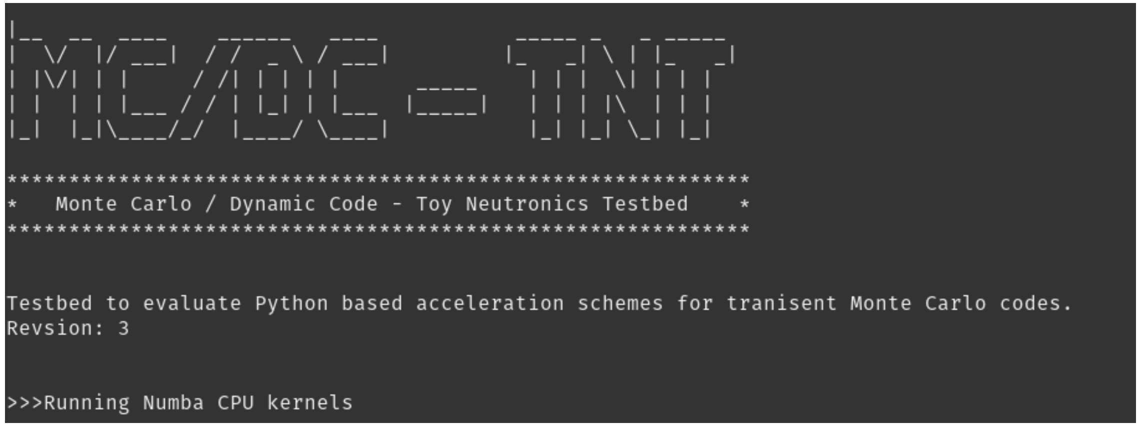
- Modularity in mind
- 10 accelerated functions
- Advance implemented on hardware target

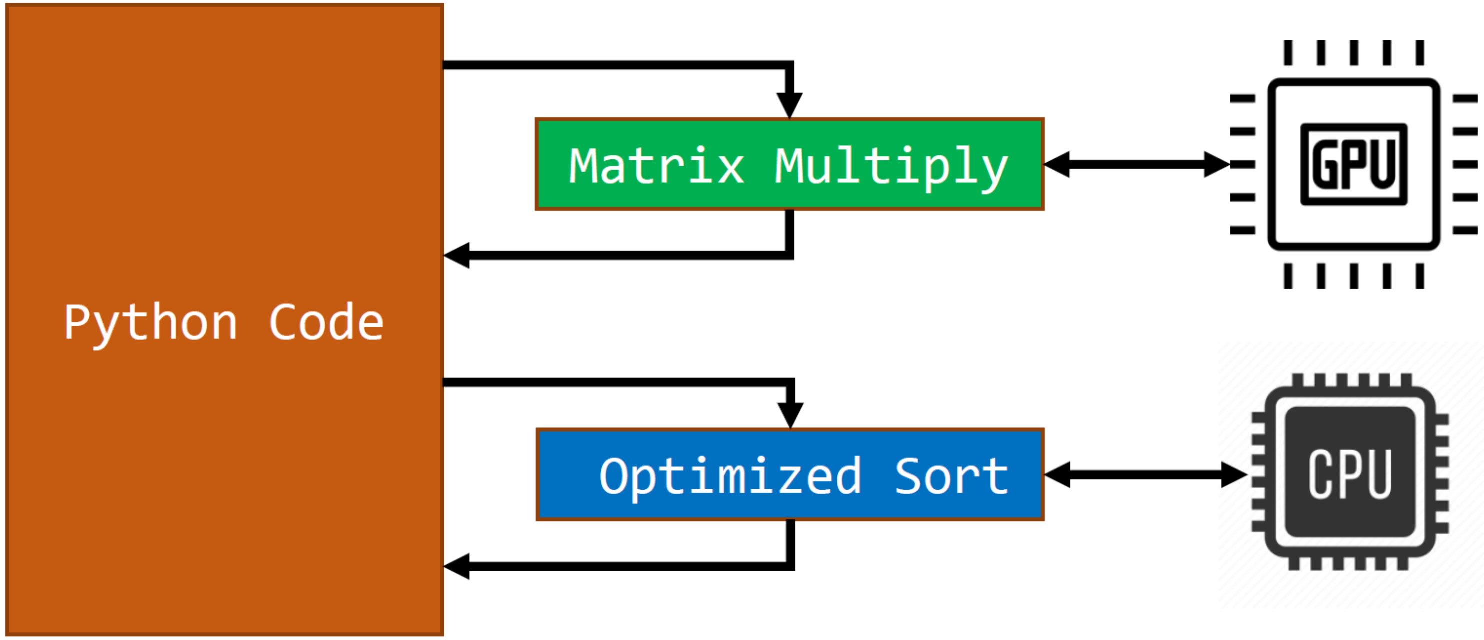



```
.
└── mcdc_tnt
    ├── numba_kernels
    │   ├── cpu
    │   ├── pyopenmp
    │   └── cuda
    ├── pk_kernels
    ├── hcgl_kernels
    └── pure_py_kernels
```

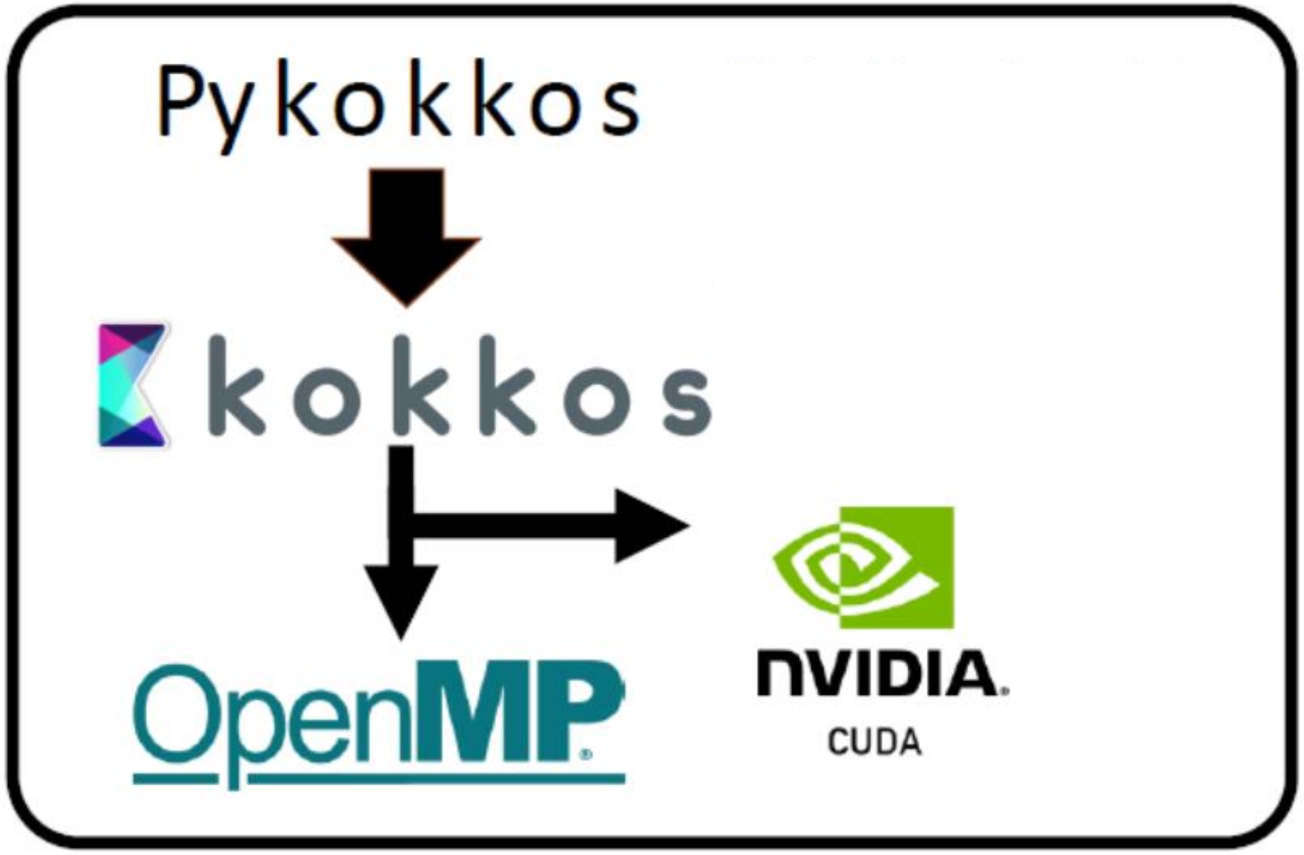
Methods of Acceleration

Heterogeneous Targeting: Python Glue

- Python serves as glue code
- Native Python modules used produce and just-in-time (JIT) schemes
- Can target multiple architecture types



PyKokkos



- Python library that implements parts of Kokkos Portability framework [2]
- Brand new and under active development
- Currently building out HIP functionality

Numba + CUDA

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- Converts Python code then implements the LLVM compiler [3]
- Industry support and active development
- Often operates on pure Python code
- Experimental full implementation of OpenMP [4]

HCGL and Mako Templating Engine

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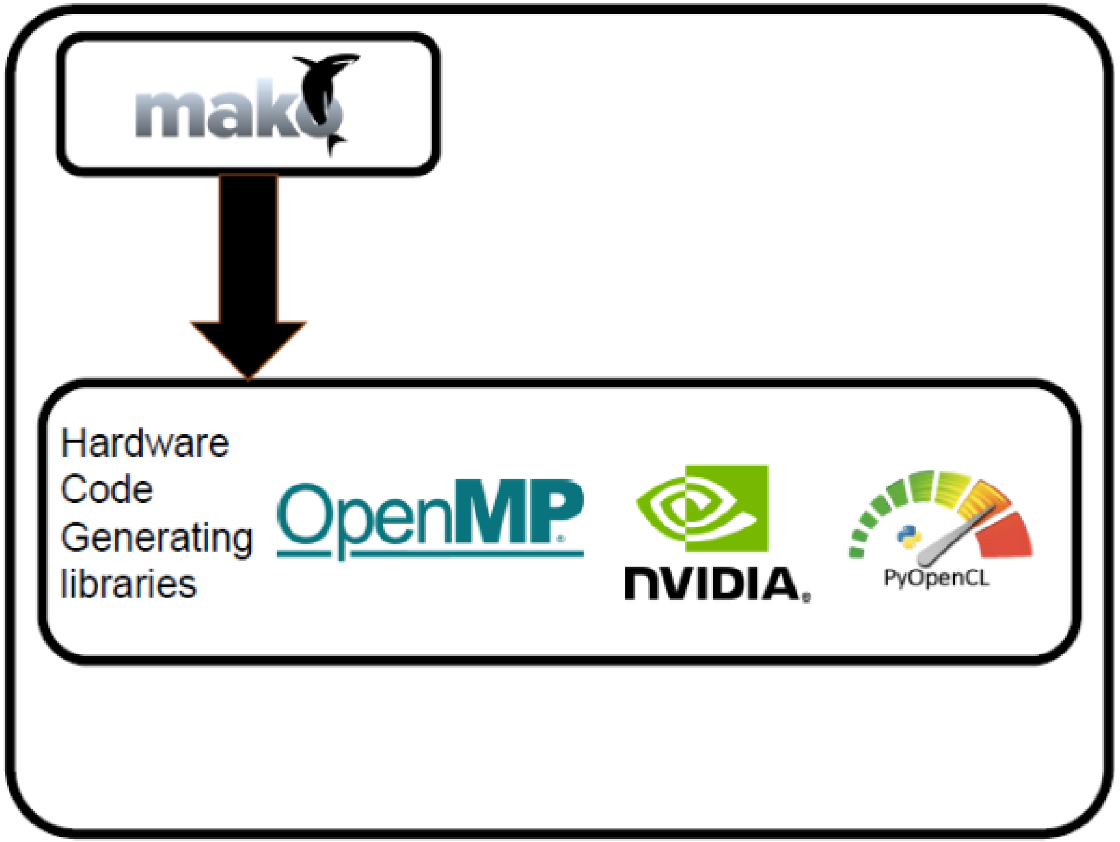
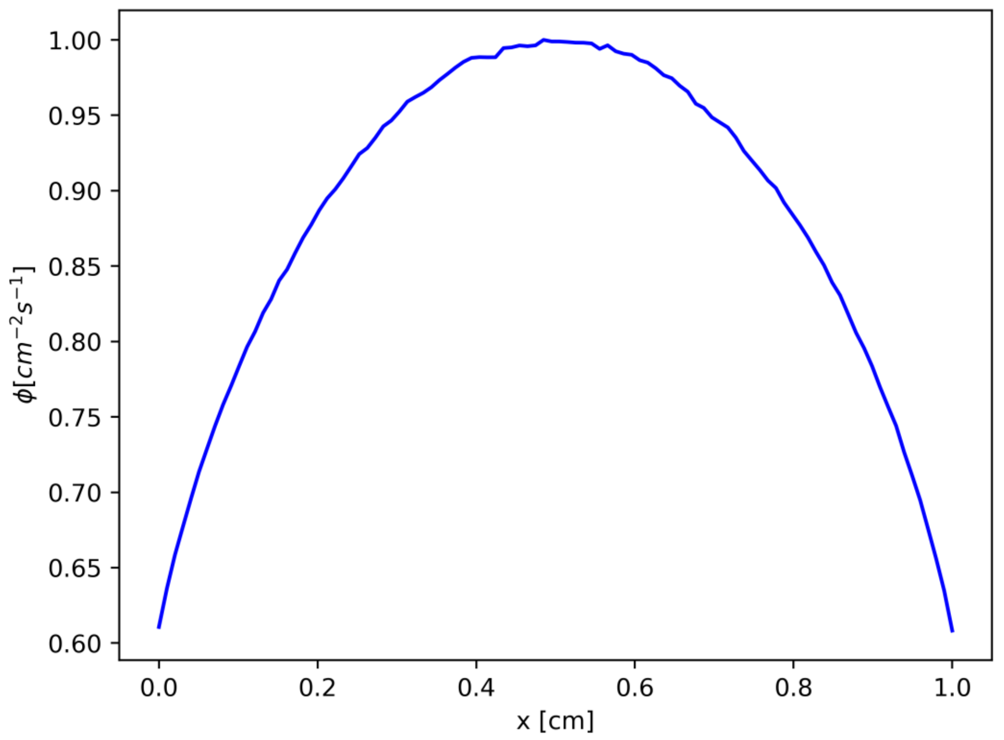
- Implemented on PyFR [5] at petascale [6]
- Code-generating libraries to compile templated code
- Our implementation plugs into PyCUDA and g++

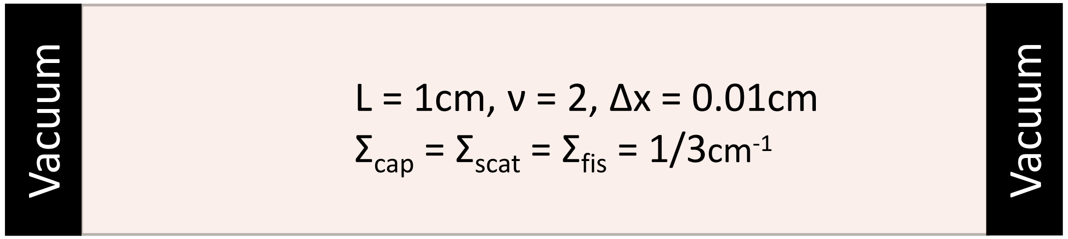


Results

Runtime Test Problem

- Sub-critical slab with initial population of 1×10^8 particles
- Validated with MC/DC
- Follow particles till death





Performance: CPU

Integration test problem: $L = 1cm$, $\Delta x = 0.01cm$, $\Sigma_f = \Sigma_c = \Sigma_s = 1/3\ cm^{-1}$, $\nu = 2$, vacuum boundary conditions on LHS and RHS w/ 1×10^8 Initial particles

Method of Implementation	Compile Time [s]	Run Time [s]
Pure Python*	N/A	52970
Numba (Native threading)	5.28	232.3
Numba PyOmp	5.66	382.3
PyKokkos	37.50	158.4

16 threads on an i7-10875H CPU
*one thread

Performance: GPU Implementation

Integration test problem: L = 1cm, Δx = 0.01cm, $\Sigma_f = \Sigma_c = \Sigma_s = 1/3\ cm^{-1}$, ν = 2, vacuum boundary conditions on LHS and RHS w/ 1×10^8 Initial particles

Method of Implementation	Compile Time [s]	Run Time [s]
Numba	6.25	179.36
PyKokkos	39.72	385.24
HCGL (PyCUDA)	2.45	160.53

1 single GPU (NVIDIA TeslaV100 at 1530MHz w/ 16GB) on 1 Lassen node

Conclusions and Future Work

Difficulty of Implementation

- Numba is simple
- Pykokkos is more difficult
- HCGL is very difficult but more performant

Performance

- Ease of use inversely proportional to max performance
- Every method is very performant! (relative to Python)
- Diminishing returns for more difficult implementations

Future Work

- Complete transient tally implementation for all methods
- Test deployment on new hardware
- Implement testbed in C++
- Implement Numba on MC/DC to accelerate pure Python code and gain *fine grain parallelism*

Acknowledgments

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- CEMeNT Team and Associated Folks!

Citations

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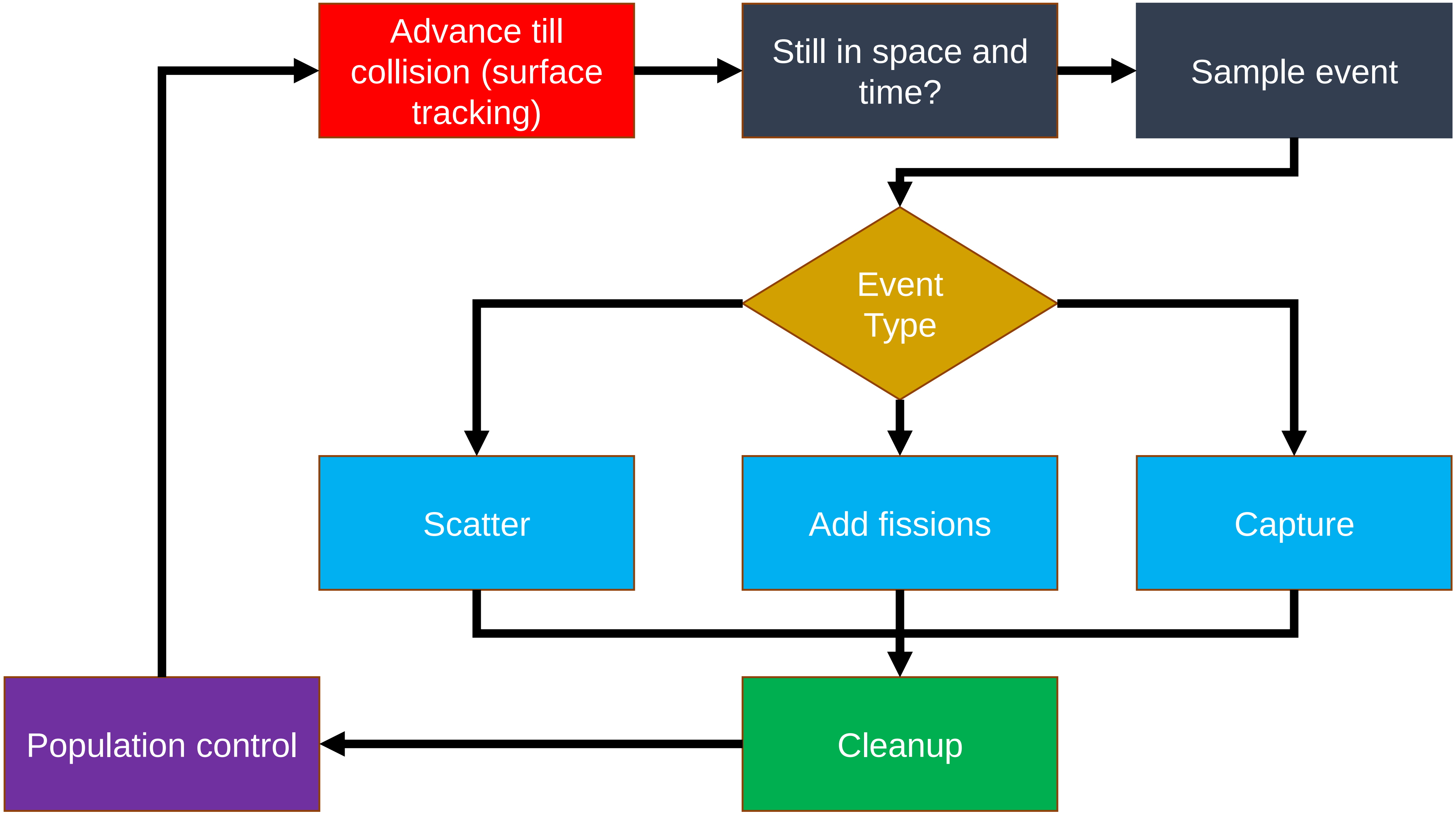
Backmatter Slides

Event-Based MC Transport Flow Chart



Other Acceleration Techniques in Python

- Cython (able to use C++ standard parallelism)
- PyCUDA and PyOpenCL (used but not directly)
- MPI4Py (Does not accelerate code, only runs more of it)
- Python CUDA
- Pure Numba / SciPy implementations (C under the hood)
- Build your own!

Planed Explorations within MC/DC

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- Fully transient Monte Carlo
- Intrusive UQ
- Dynamic Quasi Monte Carlo
- Dynamic Weight Windows
- Population Control Methods
- Python Based Parallelization
- Asynchronous GPU scheduling
- Machine Learning MPI scheduling

Future Development Path of MC/DC

1. Address Numba issues in MC/DC
   - Replace JITClass with Numba structured array
   - Runtime and memory profiling
2. Write event-based MC/DC (pure Python + MPI4Py)
   - Reuse and exploit existing MC/DC (history-based) modules
     - with Python decorator
3. Integrate findings from MC/DC-TNT
   - PyKokkos, Numba, PyOMP, Mako templating

AVURV Benchmark Descirption

We can simulate fission by having c>1

$$\Phi(x,t) = \frac{e^{-t}}{2t}\left[1 + \frac{c\,t}{4\pi}\left(1-\eta^2\right)\int_0^{\pi} \sec^2\left(\frac{u}{2}\right)\Re\left(\xi^2 e^{\frac{c\,t}{2}\left(1-\eta^2\right)\xi}\right)\,du\right] H(1-|\eta|)$$

NTE with initial source

$$\left[\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x} + 1\right]\Psi(x,\mu,t) = \frac{c}{2}\int_{-1}^{1}\Psi(x,\mu',t)\,d\mu + \frac{1}{2}\delta(x)\,\delta(t)$$

Science Python & HPC: Bigger Picture

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- Enables rapid methods development for complex systems [7]
- Off the shelf codes for science applications available [8]
- There ***is*** a trade off in performance in benchmarks [9]
- A rich environment or high productivity in science [10]
- Allows nuclear folks to better interface with other fields!
- Can alleviate the need for C++ testbeds as initial performance analysis of methods can be examined

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