Python Development Schemes for Monte Carlo Neutronics on High Performance Computing

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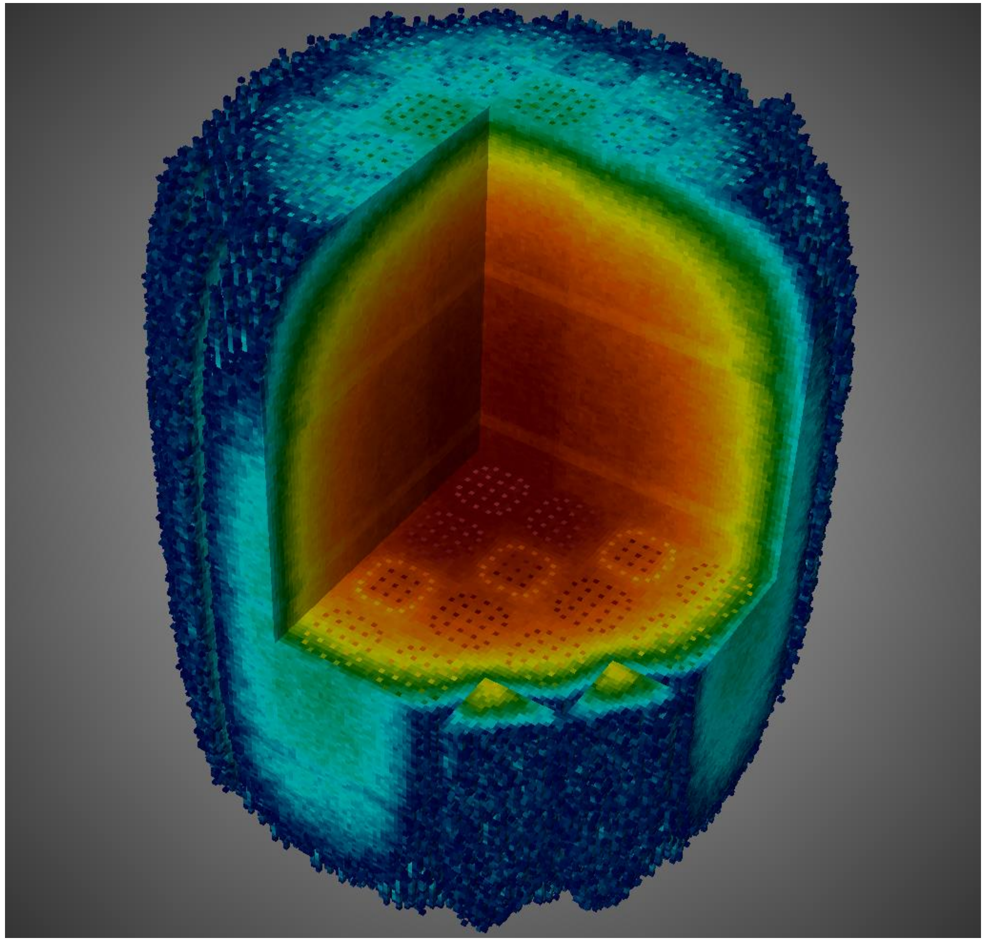
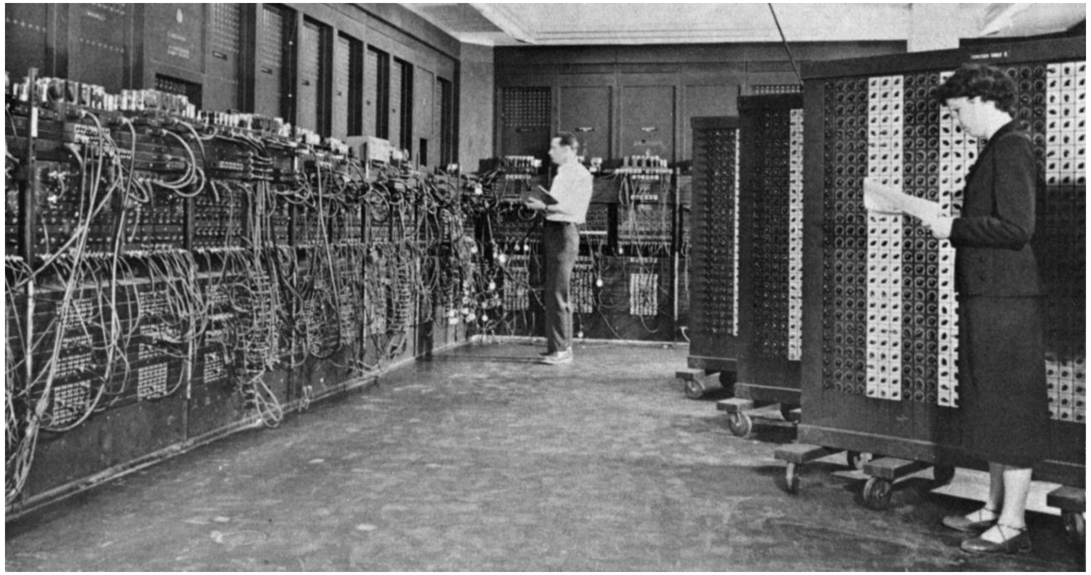
Neutron Transport

- Trying to answer where, how, and when neutrons interact with a domain
- Applications:
  - Cancer radio therapy development
  - Power reactor analysis
  - Other governmental implementations



Neutron Transport and HPC

There at the beginning…



ENIAC – 1946

First general programable computer circa 1946

https://ieeexplore.ieee.org/document/6880250

There now

El Capitan – 2023

Heterogeneous exa-scale machine

Direct Monte Carlo Simulations

Monte Carlo Methods

Can we use statistics and event rates to model a system?

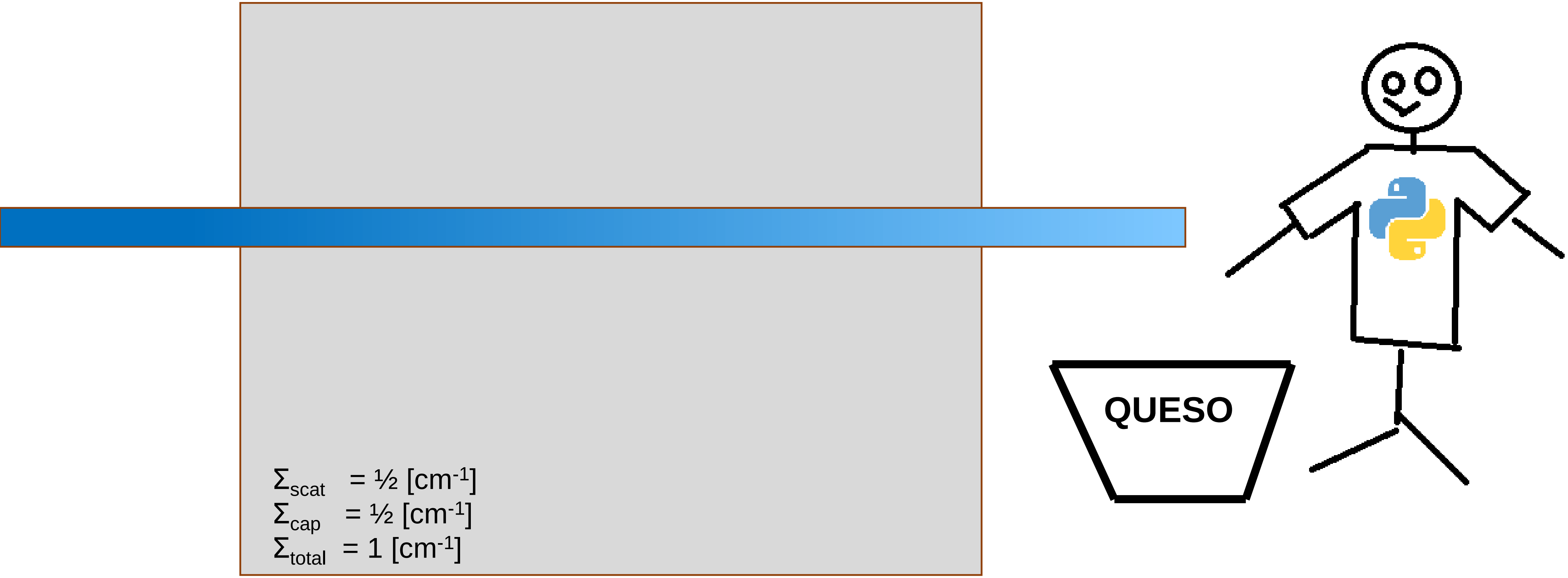
Traditional numerical methods (deterministic methods) get an exact solution to an estimated problem

Monte Carlo gives an estimated solution to an exact problem

Monte Carlo Neutronics

A wild BEAM OF NEUTRONS appeared!

Are we safe?



$\Sigma_{scat} = ½ \text{ [cm}^{-1}]$
$\Sigma_{cap} = ½ \text{ [cm}^{-1}]$
$\Sigma_{total} = 1 \text{ [cm}^{-1}]$

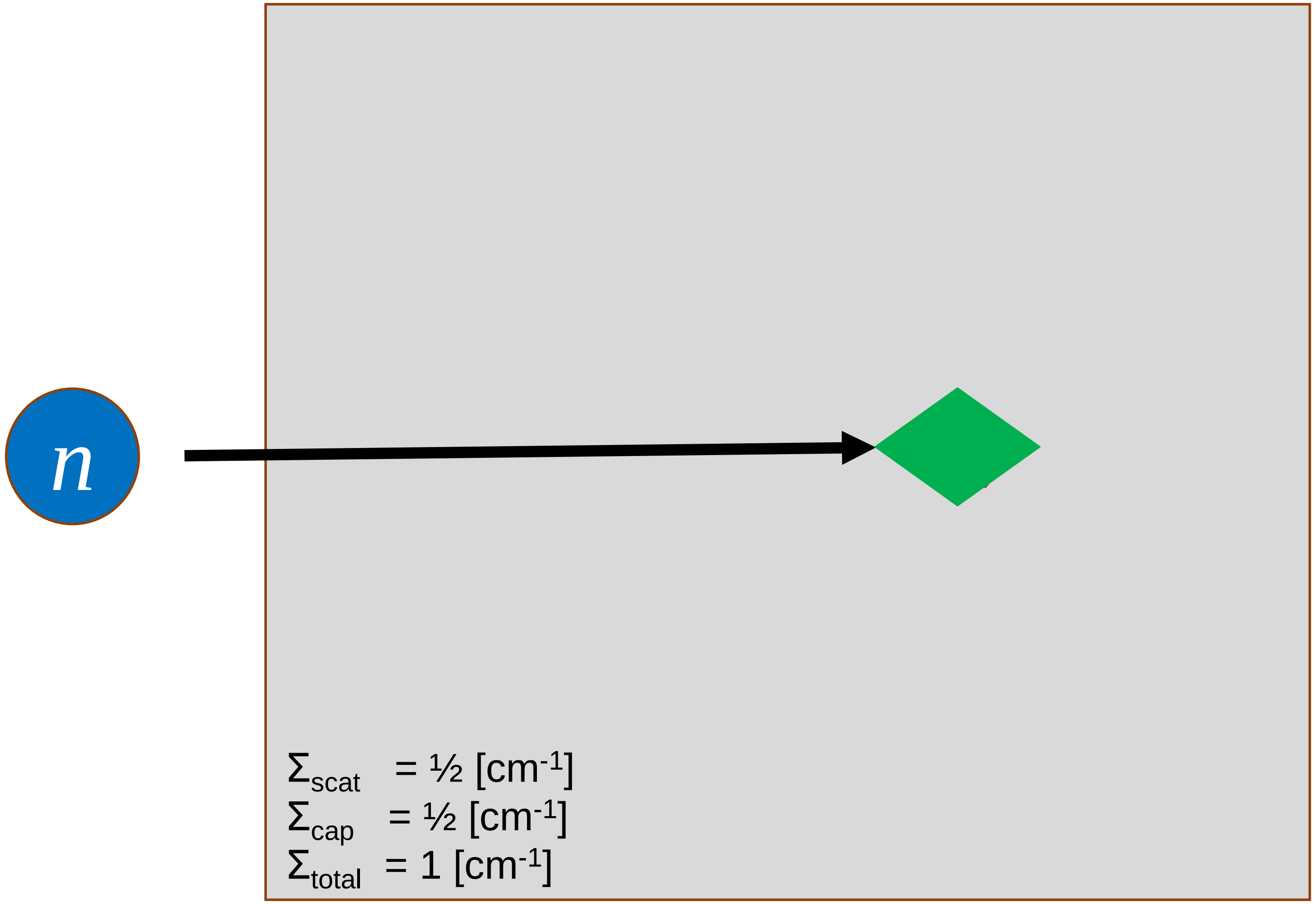
Monte Carlo Neutronics

- Material Data (statistical likelihoods)
- Equations where can relate a distance to a probability
- List of events that could possible happen (scatter, absorption, transmission)

$$S = -\frac{\ln(\xi)}{\Sigma_t}$$

ξ: random number [0,1]
Σ_t: total cross section

Monte Carlo Neutronics



Events:

1. Roll a random number
   `ξ = 0.345`
2. Compute distance to event
   `S = 1.06 cm`
3. Move the particle
4. Roll a new random number
   `ξ = 0.544`
5. Determine new event type
   `ξ > 0.5`
6. Tally
   `Absorption`

Dead Slow

To get a decent solution we will need to do this over

and over…
and over…
and over…
and over…
and over…
and over…

⋮ ⋮

$$\mathcal{O} = \frac{1}{\sqrt{n}}$$

The Problem Fully Defined

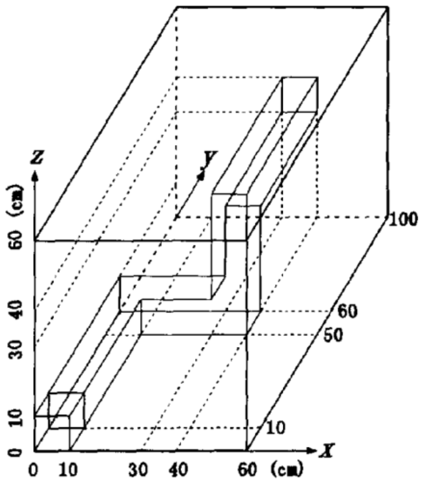
How do we

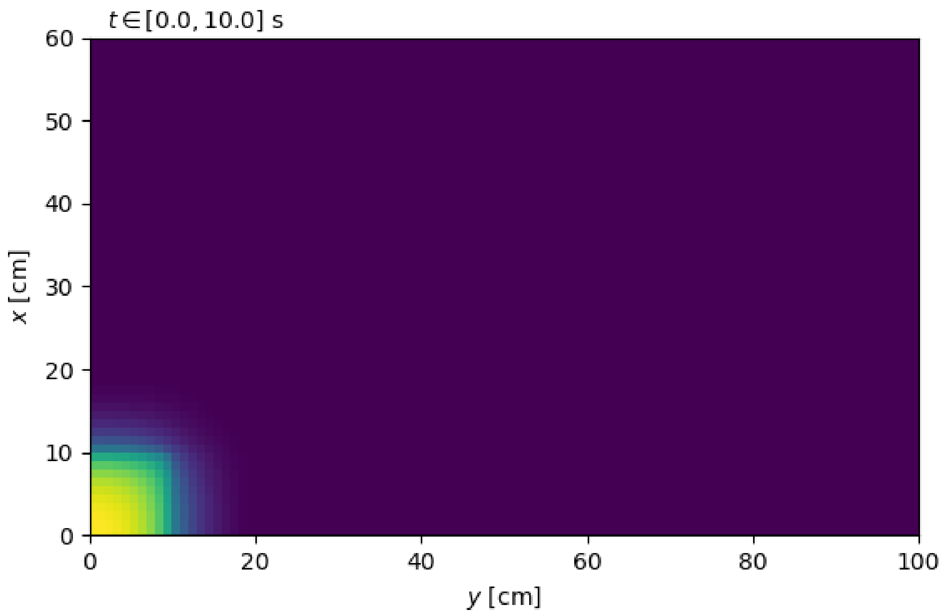
1. *Write high performance compute kernels*
2. *That can't use off the shelf libraries*
3. *For heterogeneous machines*
4. *That isn't too syntactically dense so all can participate*
5. *And maybe even total abstraction of hardware target or at least abstract vector machines from CPUs*

MC/DC

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 architecture
- Currently parallelized with mpi4py





Kobyashi Problem: Image courtesy Ilham Variansyah

GitHub: https://github.com/CEMeNT-PSAAP/MCDC

MC/DC–TNT: Toy Neutronics Testbed

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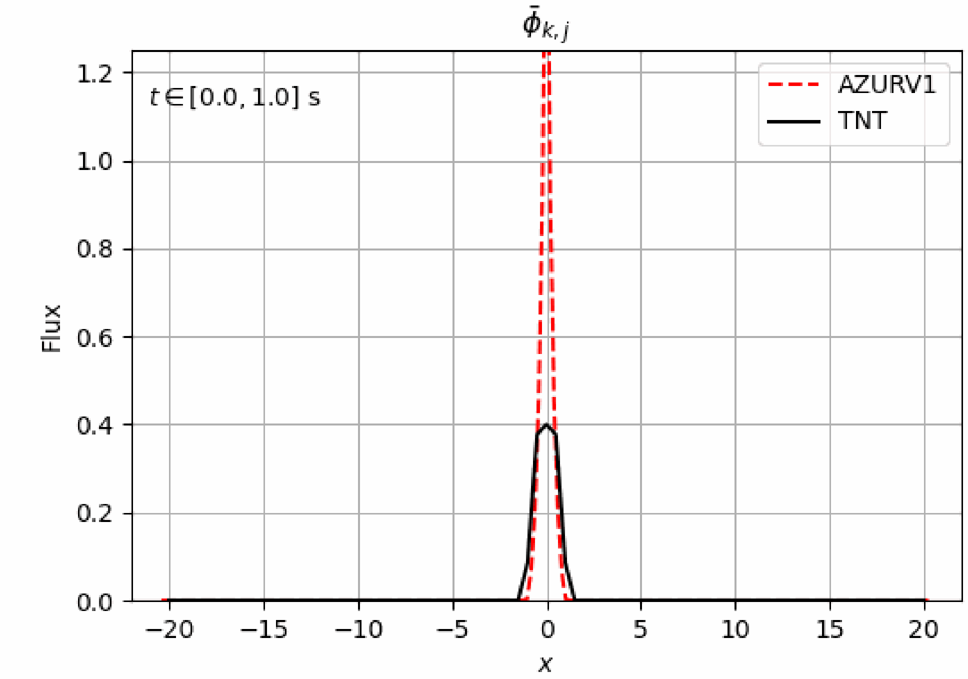
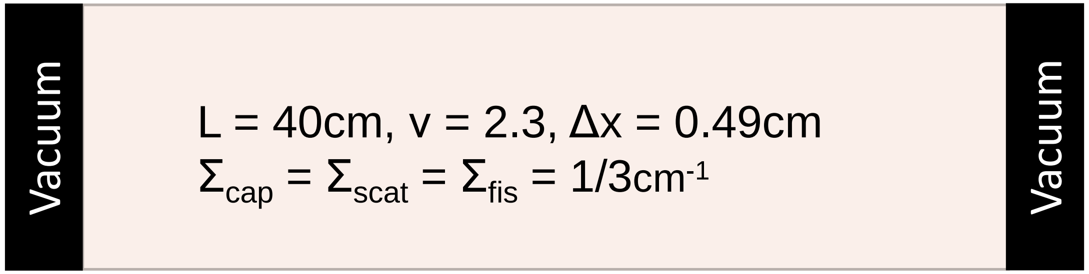
- Mono-energetic, slab-geometry, transient tallies, fission, event-based, with surface tracking

- Architecture targets: Nvidia GPUs and x86 CPUs

- Validated with analytic solutions (AZURV1 [1])



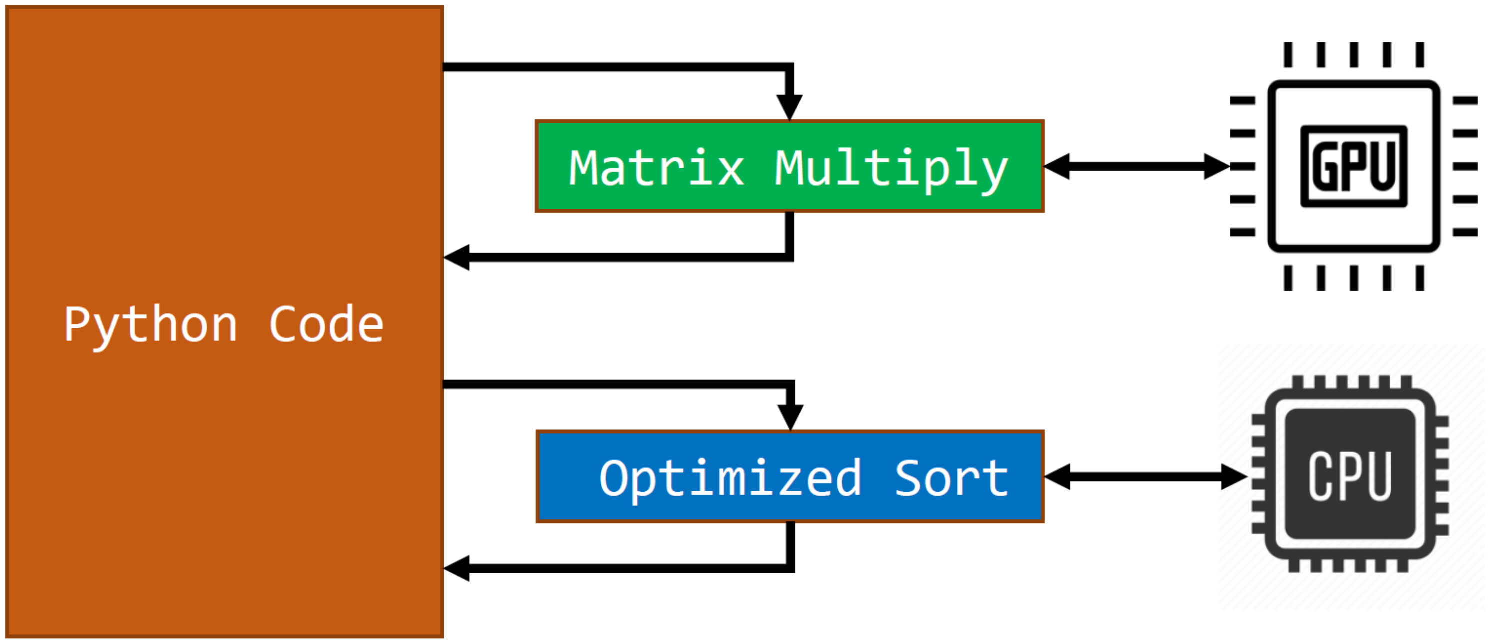


GitHub: https://github.com/CEMeNT-PSAAP/MCDC-TNT

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



A potential accelerated Python program

PyKokkos

```python
import math
import numpy as np
import pykokkos as pk

@pk.workload
class vecLog:
    def __init__(self, vec, total, N):
        self.vec: pk.View1D[pk.float] = vec
        self.total: pk.View1D[pk.float] = total
        self.N: int = N

    @pk.main
    def run(self):
        pk.parallel_for(self.N, self.vecLog_wu)

    @pk.workunit
    def vecLog_wu(self, i: int):
        self.vec[i] = math.log(self.vec[i])
        pk.atomic_fetch_add(self.total, [0], self.vec[i])


if __name__ == '__main__':
    space = pk.ExecutionSpace.Cuda #pk.ExecutionSpace.OpenMP
    pk.set_default_space(space)

    data_type = np.float32
    N: int = 32

    vec = np.random.random(N).astype(data_type)
    vec_pyk = pk.from_numpy(vec)
    total = np.zeros(1, data_type)
    total_pyk = pk.from_numpy(total)

    pk.execute(space, vecLog(vec, total, N))
```

- Python library that implements parts of Kokkos Portability framework [2]
- Brand new and under active development
- Treats functions as objects to run in pyk commands

Numba + CUDA

- 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]

```python
import numpy as np
import numba as nb
import math
from numba import cuda


@cuda.jit
def vecLog(vec, total):
    i: int = cuda.grid(1)

    vec[i] = math.log(vec[i])
    cuda.atomic.add(total, [0], vec[i])

if __name__ == '__main__':
    data_type = np.float32
    N: int = 32

    vec = np.random.random(N).astype(data_type)
    total = np.zeros(1, data_type)

    vec_cuda = cuda.to_device(vec)
    total_cuda = cuda.to_device(total)

    threadsperblock = 32
    blockspergrid = (N + (threadsperblock - 1)) // threadsperblock

    vecLog[blockspergrid, threadsperblock](vec, total, N)
```

HCGLs (PyCUDA)

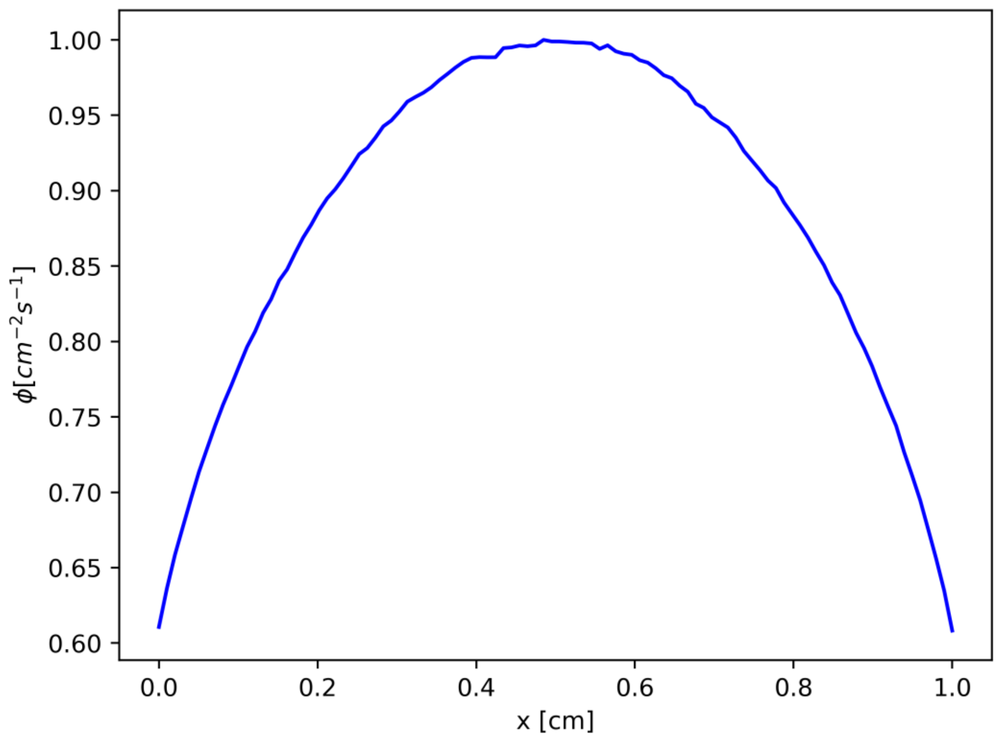
- Implemented on PyFR [5] at petascale [6]
- Code-generating libraries to compile code
- Have to write our own source

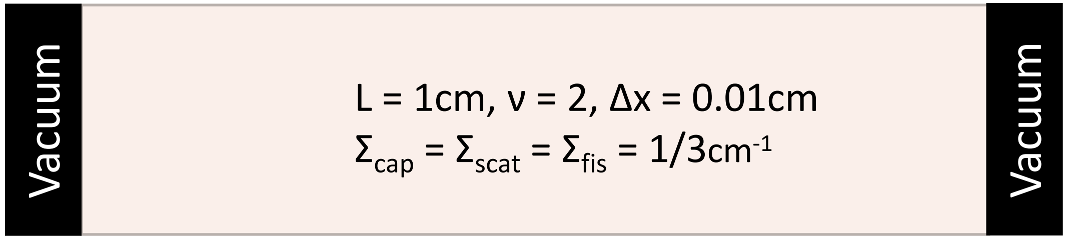
```python
import numpy as np

import pycuda.autoinit
import pycuda.driver as drv
from pycuda.compiler import SourceModule

mod = SourceModule("""
__global__ void vecLog(float *vec, float *total){
    const int i = threadIdx.x + blockIdx.x * blockDim.x;

    float vec[i] = log(vec[i]);
    atomicAdd(&total[0], vec[i]);

}""")



if __name__ == '__main__':
    data_type = np.float32
    N: int = 32

    vec = np.random.random(N).astype(data_type)
    total = np.zeros(1, data_type)

    threadsperblock = 32
    blockspergrid = (N + (threadsperblock - 1)) // threadsperblock

    vecLog = mod.get_function("vecLog")

    vecLog(drv.InOut(vec), drv.InOut(total),
           block=(threadsperblock, 1, 1), grid=(blockspergrid, 1))
```

Results

Runtime Test Problem

- Sub-critical slab with initial population of $1{\times}10^8$ particles
- Validated with MC/DC
- Follow particles till death





Performance: CPU

Integration test problem: $L = 1\text{cm}$, $\Delta x = 0.01\text{cm}$, $\Sigma_f = \Sigma_c = \Sigma_s = 1/3\ \text{cm}^{-1}$, $\nu = 2$, 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

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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

Future Work

- Complete transient tally implementation for all methods
- Test deployment on new hardware
- Accelerated as compered to what
- Implement Numba on MC/DC*
- *And much much much more!*

How to Slay the Dragons

- Data type hygiene
- Keep an errors diary
- Actually implement testing and run your tests after EVERY commit
- Use CONDA for everything possible
- Log build commands

Acknowledgments

Special thanks to:

- Post Docs: Ilham Variansyah; Aaron Reynolds
- CEMeNT Team and Associated Folks!
- *All the packages, their developers and the open science community*

Please Reach Out!

Contact

- Discord: `jpmorgan34#9493`
- Email: morgjack@oregonstate.edu
- Slack!

Repos

- MC/DC: https://github.com/CEMeNT-PSAAP/MCDC
- MC/DC – TNT: https://github.com/CEMeNT-PSAAP/MCDC-TNT

Citations

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[1] Ganapol B.D., Baker, R. S., Dahl, J. A., & Alcouffe, R. E. (2001). Homogeneous Infinite Media Time-Dependent Analytical Benchmarks. *International Meeting on Mathematical Methods for Nuclear Applications*, *836*(December), 1–4.

[2] Awar, N. Al, Zhu, S., Biros, G., & Gligoric, M. (2021). A performance portability framework for python. *Proceedings of the International Conference on Supercomputing*, 467–478. https://doi.org/10.1145/3447818.3460376

[3] Lam, S. K., Pitrou, A., & Seibert, S. (2015). Numba: A LLVM-Based Python JIT Compiler. *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*. https://doi.org/10.1145/2833157.2833162

[4] T. G. Mattson, T. A. Anderson, G. Georgakoudis, K. Hinsen, and A. Dubey, “PyOMP: Multithreaded Parallel Programming in Python,” *Comput. Sci. Eng.*, vol. 23, no. 6, pp. 77–80, Nov. 2021, doi: 10.1109/MCSE.2021.3128806.

[5] Witherden, F. D., Farrington, A. M., & Vincent, P. E. (2014). PyFR: An open source framework for solving advection-diffusion type problems on streaming architectures using the flux reconstruction approach. *Computer Physics Communications*, *185*(11), 3028–3040. https://doi.org/10.1016/j.cpc.2014.07.011

[6] Witherden, F. (2021). Python at petascale with PyFR or: how I learned to stop worrying and love the snake. *Computing in Science & Engineering*, *9615*(c), 1–1. https://doi.org/10.1109/mcse.2021.3080126

Backmatter Slides

Neutron Transport Equation

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Time Rate of Change

Streaming through space

Collision

$$\left(\frac{1}{v(E)}\frac{\partial}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_t(\mathbf{r}, E, t)\right)\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) =$$

Particles produced from delayed fission

Particles produced from prompt fission

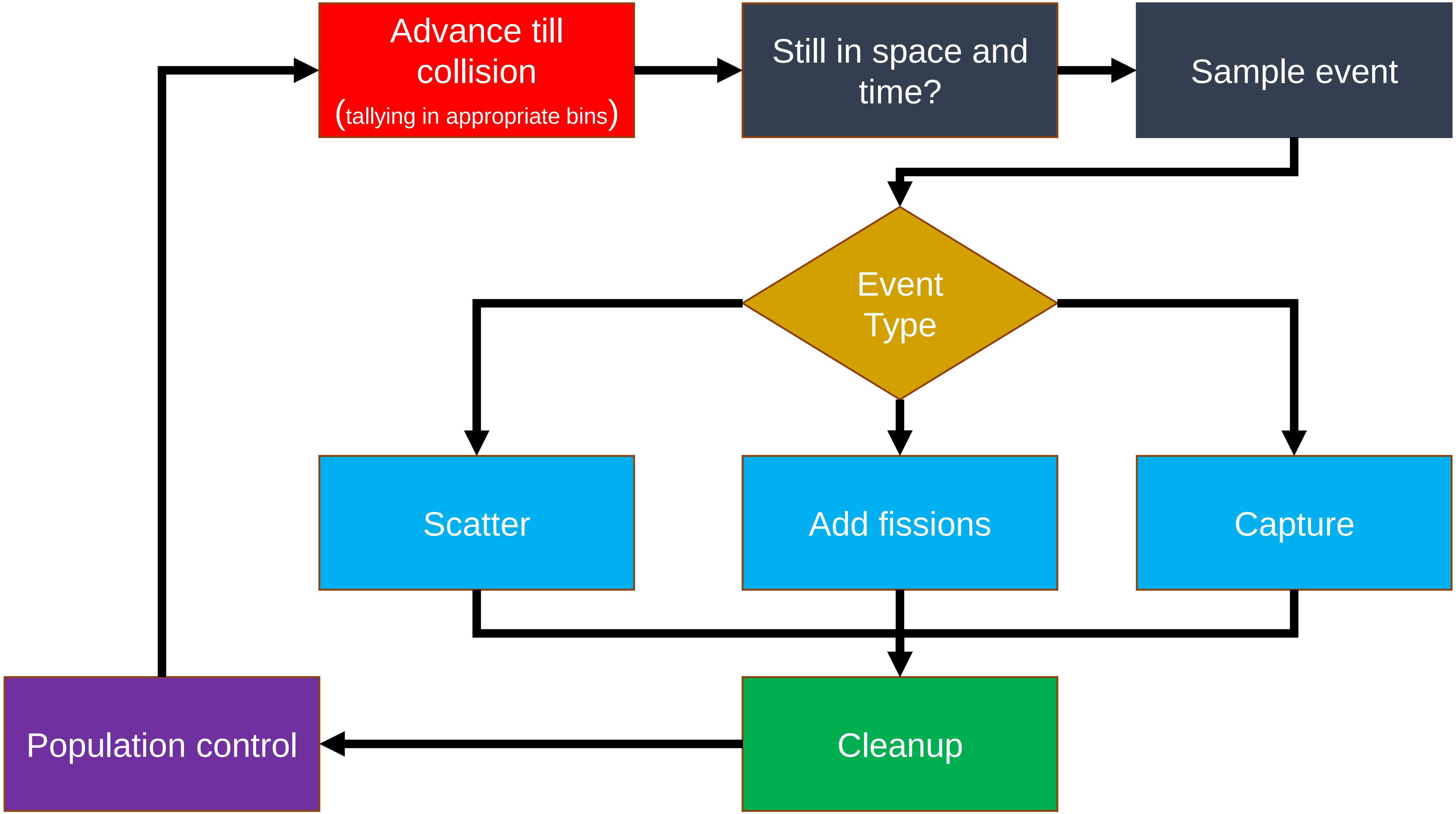
$$\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\,\nu_p(E')\,\Sigma_f(\mathbf{r}, E', t)\,\phi(\mathbf{r}, E', t) + \sum_{i=1}^{N}\frac{\chi_{di}(E)}{4\pi}\lambda_i C_i(\mathbf{r}, t) +$$

$$\int_{4\pi} d\Omega' \int_0^\infty dE'\,\Sigma_s(\mathbf{r}, E' \to E, \hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}}, t)\psi(\mathbf{r}, E', \hat{\mathbf{\Omega}}', t) + s(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

In scattering

Direct source

MC Transport Flow Chart



Other Acceleration Techniques in Python

- Cython (able to use C++ standard parallelism)
- MPI4Py (Does not accelerate code, only runs more of it)
- DASK
- Python CUDA
- Pure Numpy / SciPy implementations (C under the hood)
- Build your own! (PyBind11, SciKit-Build)

Planed Explorations within MC/DC

- 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

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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 Description

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

- 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

[7] Barba, L. A., Klockner, A., Ramachandran, P., & Thomas, R. (2021). Scientific Computing With Python on High-Performance Heterogeneous Systems. *Computing in Science & Engineering*. https://doi.org/10.1109/MCSE.2021.3088549
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