GPU Parallelization of Spin-Tracking Simulations for the nEDM@SNS Experiment

M. Kline[1], D. Mathews[2], L. J. Broussard[3]

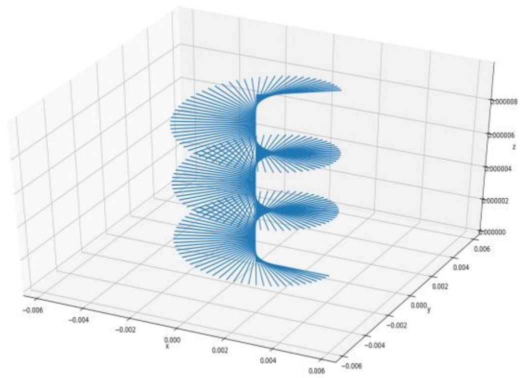
[1]Transylvania University

[2]University of Kentucky

[3]Oak Ridge National Laboratory

Overview

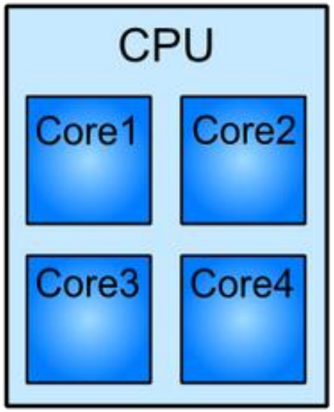
- The nEDM@SNS experiment extracts the EDM from the precession of ^{3}He atoms and spin-dependent signal of neutrons capturing on ^{3}He
- Spin-tracking simulations are very computationally expensive
  - We need these simulations to better understand systematic effects that can lead to a false EDM measurement
  - Need fast spin-tracking simulations for 10^{11} events to have comparable sensitivity to expected experiment precision
  - Use Julia and CUDA to run simulations on GPU to utilize parallelization

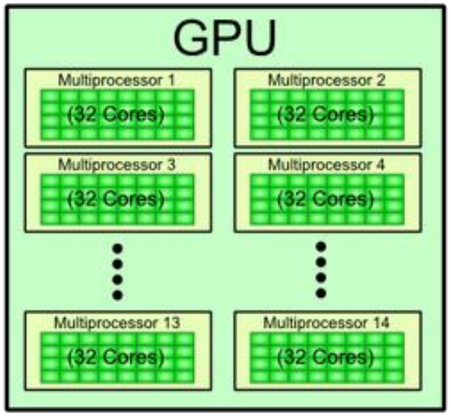


Spin precession of neutron with gravity

Simulations on GPUs

CPU	GPU
Central Processing Unit	Graphics Processing Unit
1-64 cores	100 - 7000 cores
Linear Processing	Parallel Processing
A handful of operations very rapidly	Thousands of operations at once





Images from https://steemit.com/gridcoin/@dutch/hardware-and-project-selection-part-1-cpu-vs-gpu

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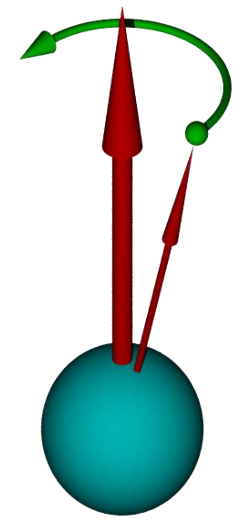
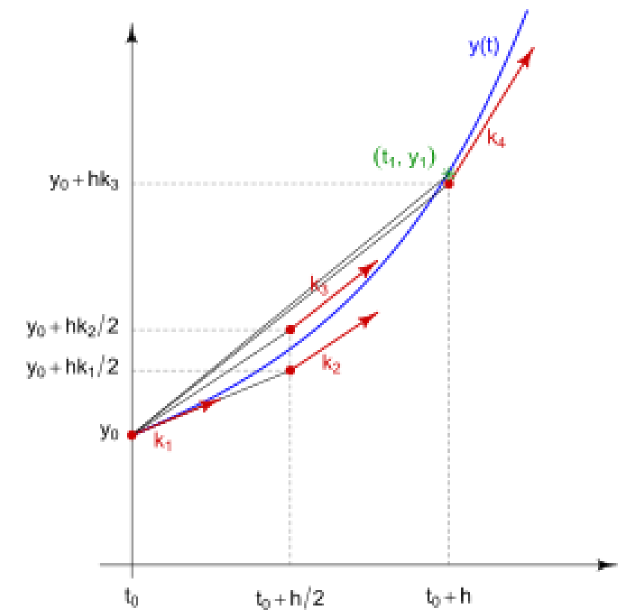
Spin Precession

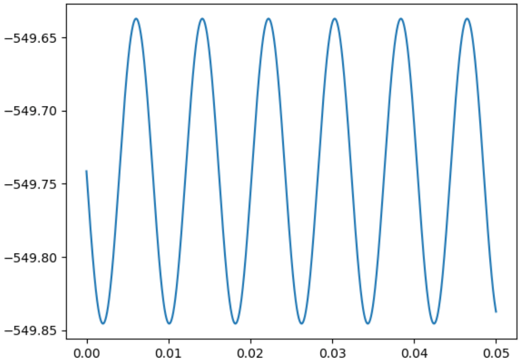


- Spin precession described by the Bloch equation
  - $\dot{\sigma} = \gamma_n \sigma \times B - \frac{2d_n}{\hbar} \sigma \times E$
- Numerically integrated using 5th order Runge-Kutta method
  - Used Cash-Karp parameters
  - $\frac{dy}{dt} = f(t, y)$
  - $k_i = h\, f(x_n + a_i h, y_n + \sum_{j=1}^{i-1} b_{ij} k_j)$
  - $y_{n+1} = y_n + \sum_{i=1}^{6} c_i k_i$



Other Integration Methods

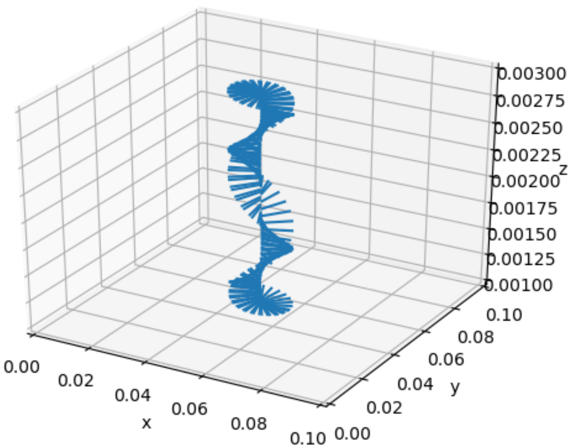
- Symplectic integration
  - More stable than Runge-Kutta over long durations
  - Used for Hamiltonian where $\mathcal{H} = T(p) + V(q)$
    - Great for UCN in gravitational/magnetic fields
    - Reflections/variable step size become problematic
  - $\frac{dx}{dt} = f(t, v)$ and $\frac{dv}{dt} = g(t, x)$ satisfy the Hamiltonian
    - $\mathcal{H} = -\mu_n \sigma \cdot B - d_n \sigma \cdot E$
    - We investigated the transformation $\sigma = x$ and $\dot{\sigma} = v$
- Turn RK/SI step into a matrix equation
  - The differential equation must be linear (like the Bloch equation)
  - Matrix operations are fast on GPUs
  - Adding physics (reflections, etc.) slows it down
  - Time dependence is difficult
  - Magnetic field nonuniformities cause problems



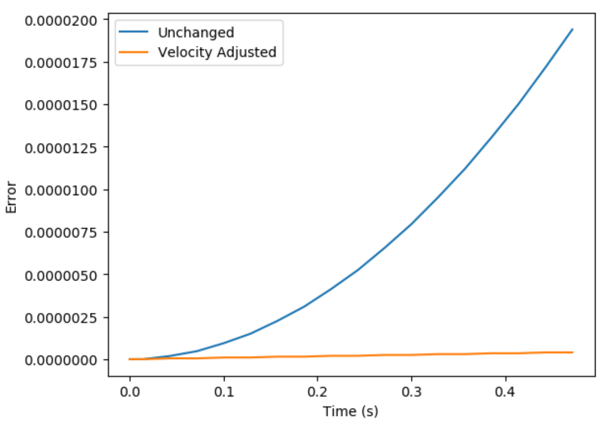
Spin precession frequency vs time with symplectic integration

Wall Interactions

- Wall reflections are difficult
  - Magically change neutron's direction in the middle of a solver step
  - To avoid errors, you have to change the step size to reach the wall exactly
- Side walls are periodic to avoid variable step size
  - Achieved with a GPU kernel
- Problem: top/bottom walls break symmetry because of gravity
- Solution: duplicate measurement cell
  - Top cell has normal gravity
  - Bottom cell has "antigravity"
- Still run into problem of wrong gravity during part of step
  - Solved by scaling velocity



Neutron oscillating between top and bottom cells



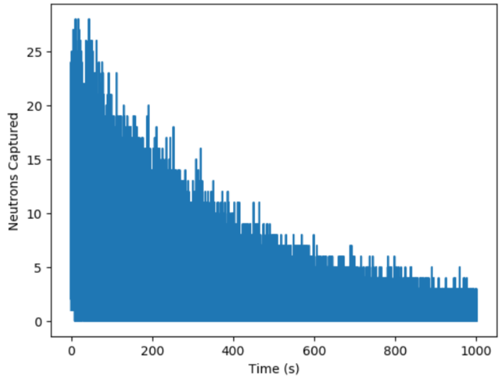
Error accumulation with and without adjusting velocity after crossing top/bottom wall

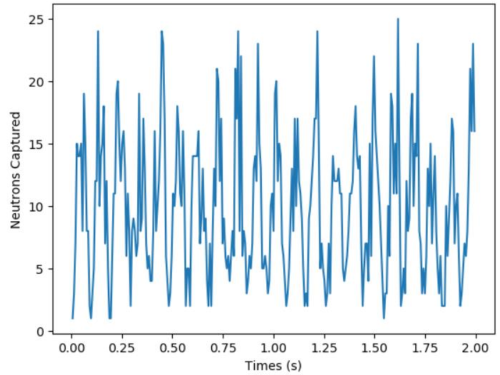
Wall Interactions

- Probability of diffuse reflections $\propto \cos\theta_i$
  - $\approx$20% for normal incident angle
- Diffuse reflections must preserve detailed balance
  - For random number $y \in [0,1]$, $\theta = \cos^{-1}\left[(1-y)^{1/3}\right]$
  - Azimuthal angle ϕ can be chosen from uniform distribution in 2π
- Wall losses added with constant probability to match expected lifetime of 2000s
  - Lifetime will be experimentally determined for each measurement cell

n+^{3}He capture and β decay

- At each step, probability of n+^{3}He capture event is dependent on relative spin between UCN and ^{3}He
  - $h\Gamma_3(1-\cos\theta)$
- Probability of β decay is constant
  - $h\Gamma_\beta$
- Γ_3 and Γ_β come from lifetimes
  - $\Gamma_3 = \frac{1}{\tau_3} = \frac{1}{500\ s} \qquad \Gamma_\beta = \frac{1}{\tau_\beta} = \frac{1}{881.5\ s}$
- Plot binned events vs time
- Large-scale decay caused by decrease in number of neutrons in the cell
- Zooming in shows oscillation
  - Frequency of oscillation with 3He precession signal used to determine nEDM

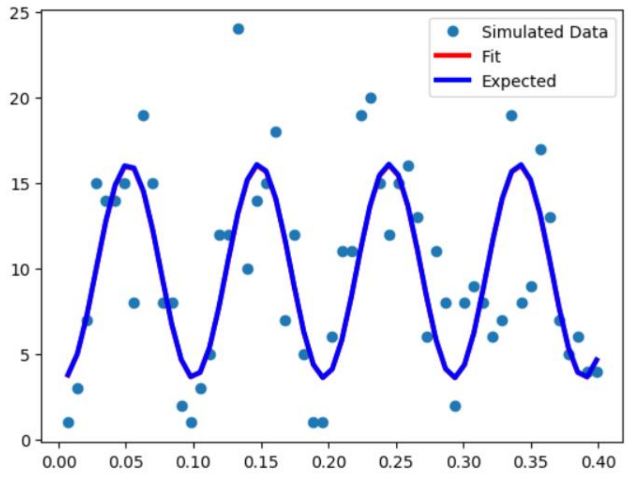




Simulated scintillation signal vs time

Simulated Signal Fit & Analysis

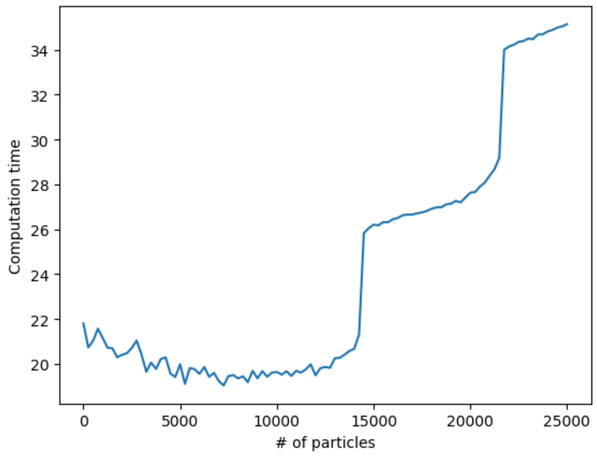
- Rate of events is
  - $\Gamma(t) = N(t) \times \left[\Gamma_\beta + \Gamma_3(1 - \cos[\omega t + \phi_0])\right] + \Gamma_B(t)$
  - $N(t) = N_0 e^{-t/\tau_{eff}}$
- Maximize log likelihood to obtain fit parameters
- $\chi^2 \approx -2 \log \Lambda$
  - $\Lambda = \mathcal{L}/\hat{\mathcal{L}}$ is the maximum likelihood ratio
- $\log \Lambda = \sum_{i=1}^{N_{bins}} [k_i \log\left(\frac{\lambda_i}{k_i}\right) - (\lambda_i - k_i)]$
- $\omega = (\gamma_3 - \gamma_n)\frac{\omega_3}{\gamma_3} + \frac{2d_n}{\hbar} E$
- $1\sigma \approx 2.5 \times 10^{-23}\ e \cdot cm$



Maximum likelihood fit of simulated scintillation signal

GPU Computation Time

- Simulate $\approx 15{,}000$ particles simultaneously per GPU
- At $\approx 15{,}000$, another set of streaming multiprocessors is required for the task, causing a jump in computation time
  - Will remain approximately constant until another set is required
- Preliminary computation time per particle per iteration
  - CPU: 2 μs/CPU
  - GPU: 8 ns/GPU (with 225,000 particles)



Computation time vs number of particles simulated

GPU: Nvidia GeForce GTX 1080 Ti

Summary and Future Work

- GPUs look promising for studying computationally expensive systematic effects
- Investigating additional physics
  - Realistic B-field maps
  - Time-dependent systematics
  - Tracking of ^{3}He particles
- Optimize GPU code to get better performance
- Compare with CUDA C
- Goal: run hybrid CPU/GPU version on Summit supercomputer

Thank You!

Questions?

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