Aug 06, 2026 | PSD ECA Presentations

From light to discovery:

Advancing DUNE's scientific program with high-fidelity GPU-accelerated optical detector simulation

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From light to discovery:

Advancing DUNE's scientific program with high-fidelity GPU-accelerated optical detector simulation

- **What is DUNE?**
- **Why detector simulation is important and what are the challenges**
- **What can this proposal bring to the DUNE scientific program**
  (If successful)

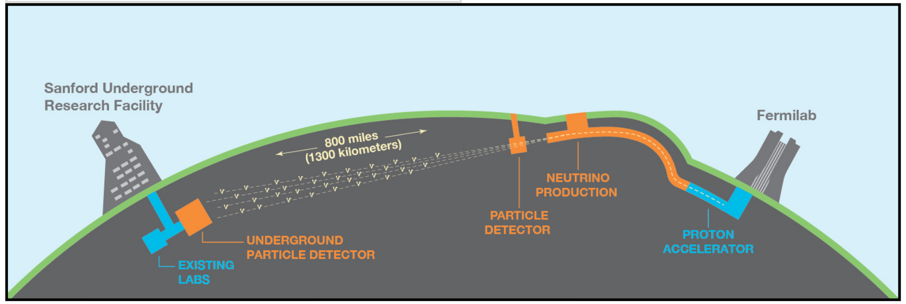
Background

The DUNE experiment and current challenges (on detector simulation)

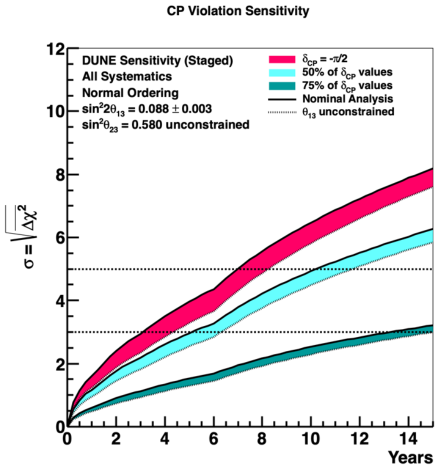
DUNE overview

- Neutrinos may be the strongest case of physics beyond the SM
- DUNE provides a wide scientific program
- **Largest domestic project in the DOE SC**

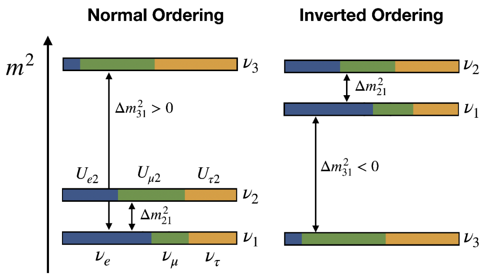
https://www.dunescience.org/



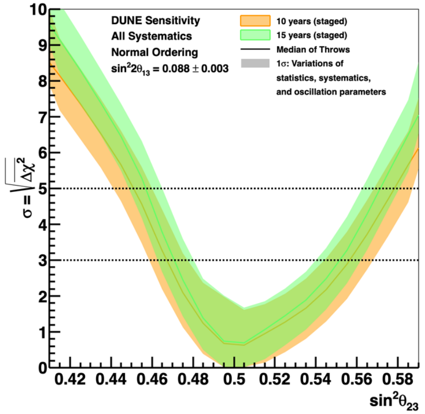
Measure δ_{CP} in the leptonic sector	Solve the neutrino mass ordering	θ_{23} octant determination	Supernova detection	BSM physics



DUNE TDR Vol II arXiv:2002.03005



Phys. Sci. Forum 2023, 8(1), 7



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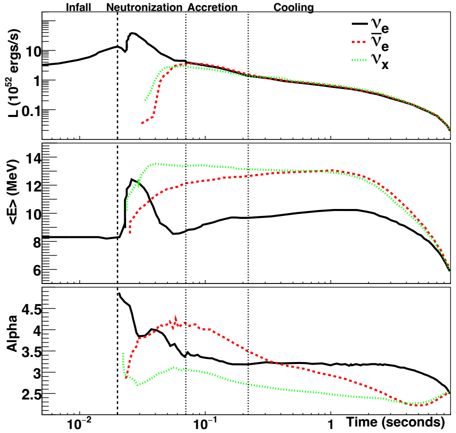
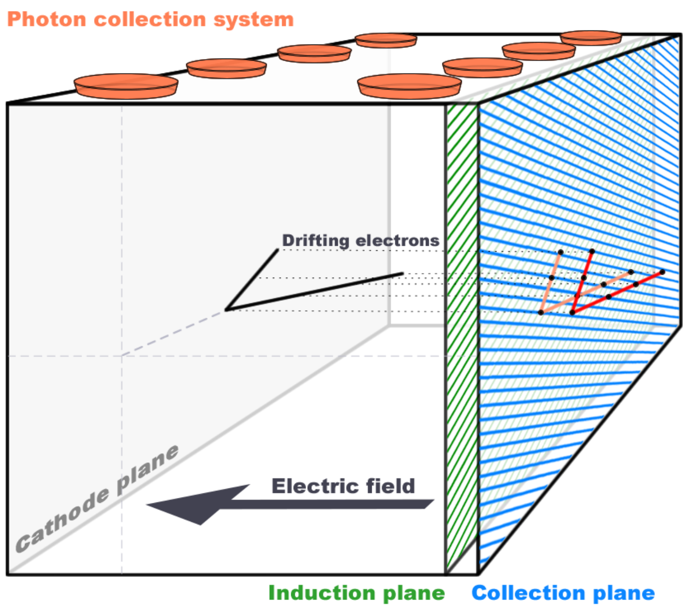


DUNE TDR Vol II arXiv:2002.03005

- Proton decay
- Non-standard Interactions
- CPT violation
- Matter effects
- Heavy neutral leptons

How LArTPCs observe neutrinos

(Liquid Argon Time Projection Chambers)

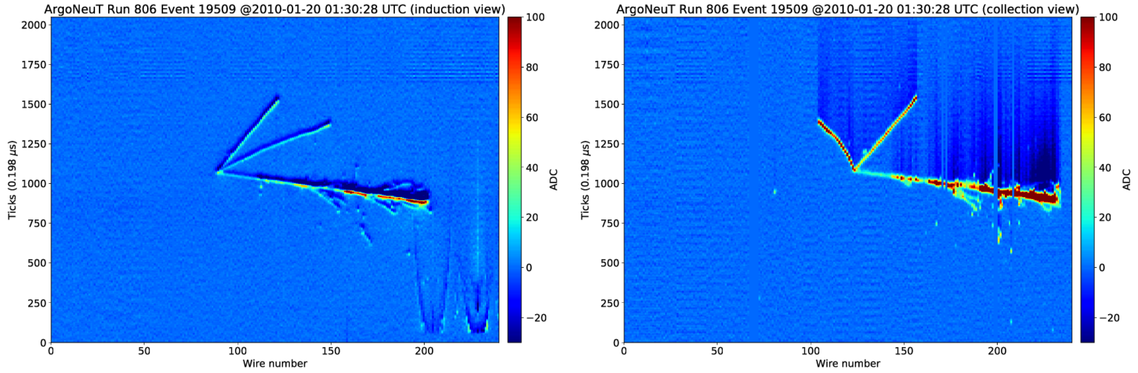


- Particle energy deposition ⇨ scintillation light (t_0) + electron ionization
- Electric field ⇨ electron drift (v_d) ⇨ Induction/collection signals (t_i)

- Signal reconstruction
  - 3D trajectories: $\ell_i = v_d \Delta t = v_d\,(t_i - t_0)$
  - Vertex/energy: $E_T = E_e + E_{light}$

Optical photons

- *Light becomes more important as event energy decreases*



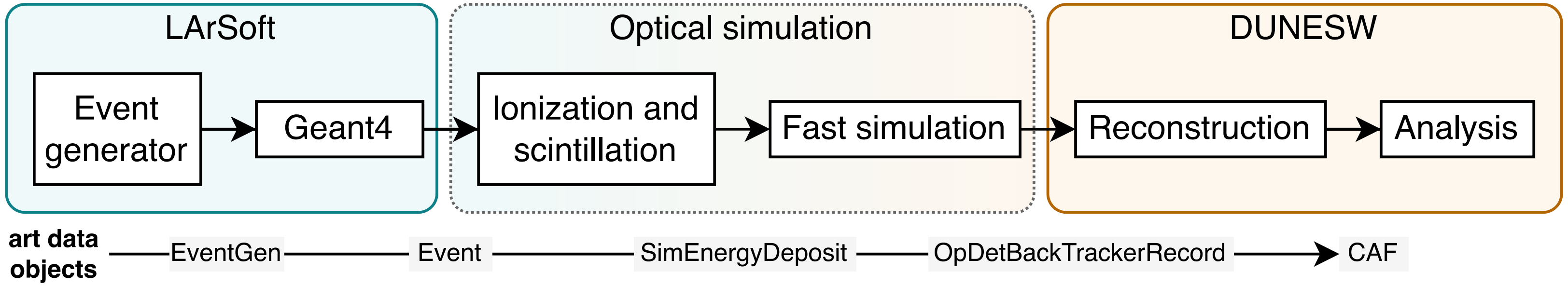
Optical photon MC is a **massive** bottleneck on light-based detectors (>95% of simulation time*)

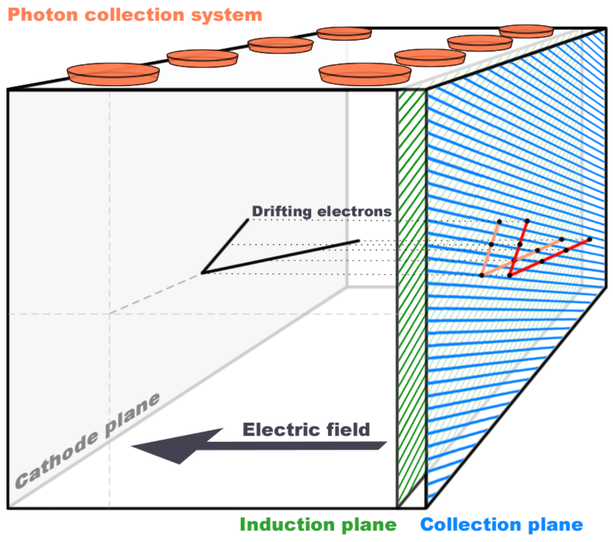
(ArgoNeuT Collab) 2022 *JINST* **17** P01018

*According to LZ, DUNE, COHERENT, and LEGEND

DUNE detector simulation challenges

- **Prohibitive simulation times are currently mitigated with a semi-analytical method** (a.k.a. Fast Simulation)
  - Full Geant4 simulation $\Longrightarrow$ generate visibility maps
  - Production/R&D workflow
    - Geant4 (no optical physics) $\Longrightarrow$ energy deposition per step
    - Visibility maps $\Longrightarrow$ FastSim $\Longrightarrow$ detector response





- **Lack of MC hinders multiple R&D avenues**

ECRP Proposal

Opportunities and benefits to the DUNE physics program

Oak Ridge National Laboratory

DUNE detector simulation ~~challenges~~ Opportunities

- **Fast, high-fidelity optical simulations open multiple opportunities for**
  - Better reconstruction methods
    - Improved t_0 determination
    - Charge + light reconstruction
      - Important for low energy events—supernovas, BSM, NSI physics

$$\boxed{H'(E) \propto H(E) + \delta E}$$

  - Better calibration
    - Detector triggering
    - Existing reconstruction methods
  - Better systematics
  - Enable data generation for AI/ML methods (triggering, reconstruction, event classification, ...)

ECRP proposal: Enable GPU detector simulations on DUNE & explore all of the physics above

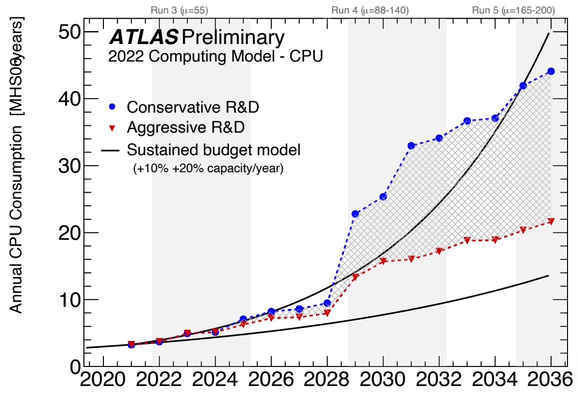
CELERITAS

Celeritas overview

GPU-optimized MC particle transport code

celeritas.ornl.gov

- Motivated by computational challenges on all HEP Frontiers



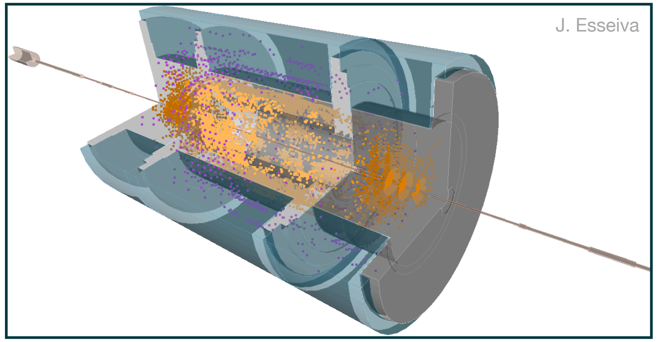
ATLAS Collaboration: CERN-LHCC-2022-005; LHCC-G-182

Energy
- ATLAS
- CMS
- LHCb
- …

Intensity
- DUNE
- LEGEND
- …

Cosmic
- LZ
- …

Credit: 2014 P5 Report, Building for Discovery



- **GOAL** Faster & more energy efficient MC simulations
- GPU platform-portable | CPU-compatible
- G4 *Geant4 API for integrated workflows*

Informal core collaborators

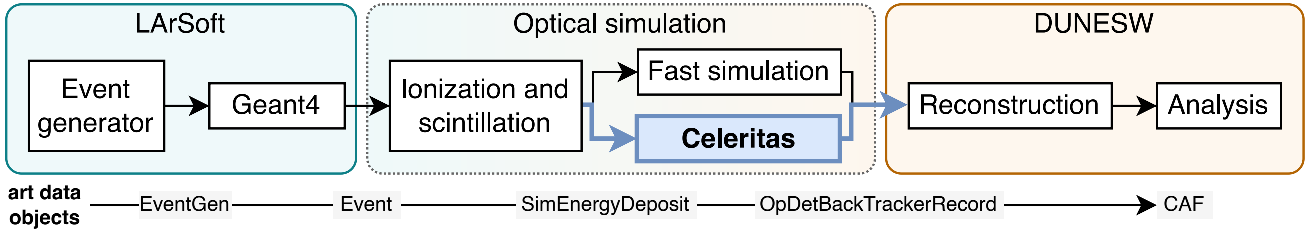
OAK RIDGE National Laboratory

ECRP proposal overview

Advance DUNE’s scientific program with Celeritas

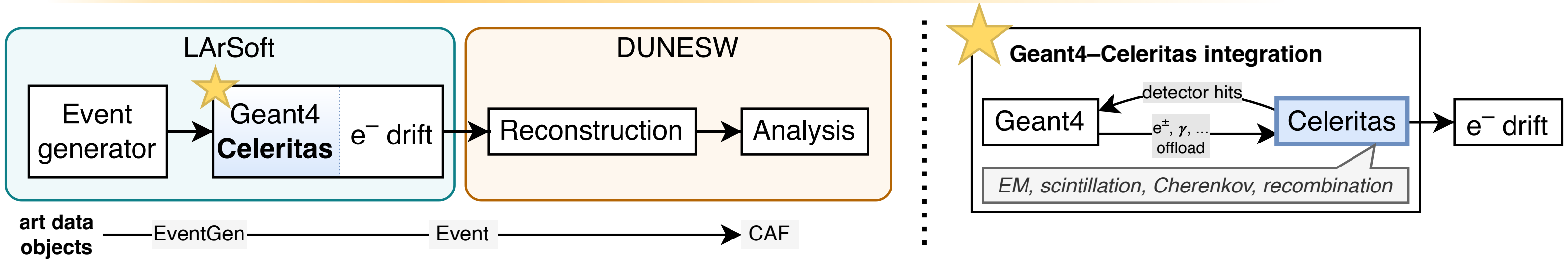
- **Maximize use of GPUs on DUNE using Celeritas**
  - Optical simulation only:

Proof-of-principle integration is complete (-ish)



  - EM + optical simulation:

Proposed



- **Benefits**
  - Full MC for R&D and production
  - Fast generation optical maps
  - Inclusion of better LAr scintillation and recombination models
  - Addition of Cherenkov effects (currently not quantified)
  - Generation of better AI/ML data

Integration with COHERENT

COHERENT simulation and data will help validate Celeritas physics implementation and add confidence to DUNE simulations

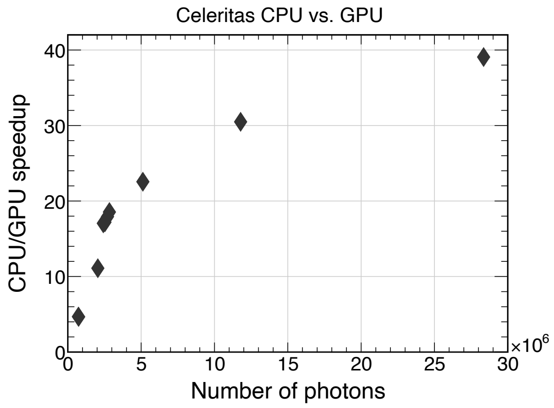
PRELIMINARY

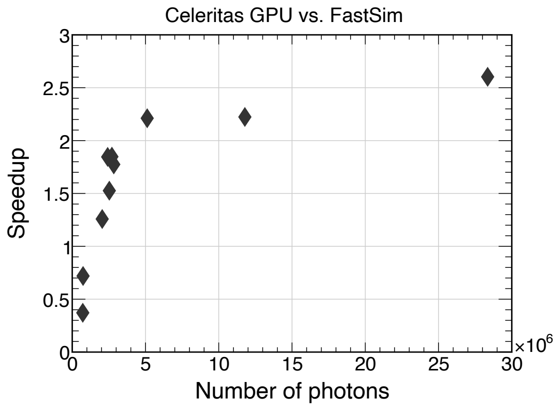
ECRP proposal overview

Advance DUNE's scientific program with Celeritas

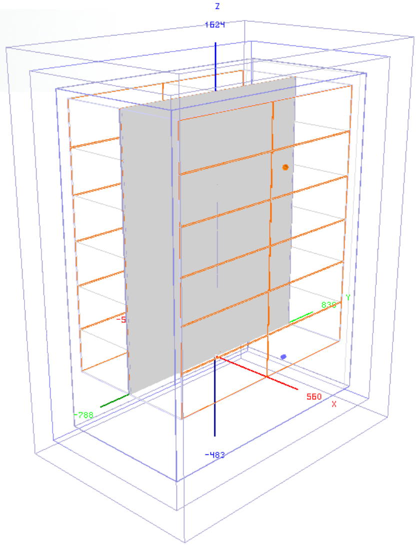
- **Performance of GENIE events on ORNL ExCL**
  AMD EPYC 7513; Nvidia Tesla V100

art Module	Arch.	Avg. event time (s)		Memory CPU + GPU (MB)	
		Full geometry	Z wires only	Full geometry	Z wires only
FastSim	CPU	2.5	2.5	823	808
Celeritas	CPU	119.4	25.6	912	894
Celeritas	GPU	7.6	2.3	1061 + 1198	1040 + 1196





- **Celeritas GPU is ~10% *faster* than Fast Simulation (on a 10 year old GPU)**
  - Celeritas GPU speedup against FastSim plateaus at ~2.5x (on the Nvidia V100)
  - Memory footprint is roughly equivalent



Optimizations & newer GPU hardware will yield better results still

OAK RIDGE National Laboratory

ECRP proposal overview

Advance DUNE's scientific program with Celeritas

What physics will this proposal focus on?

- **Event reconstruction**
  - Better t_0 determination via detailed optical detector simulations, important for
    - ND pile-up—expected $O(100)$ neutrino interactions per beam spill
    - Background rejection (beam spill edges)
  - Better energy reconstruction methods
    - Combined charge + light signals
    - Better recombination/fluctuation modeling (↑recombination $\Longrightarrow$ ↑light & ↓electrons)
- **Online triggering**—better calibration means better sensitivity
- **Re-calculate ND/FD systematics** once better triggering/reconstruction are implemented
- **Support AI/ML** workflows

Community engagement through workshops is integral to the proposal

Summary

- If funded, the proposal will bring new computing capabilities to DUNE and COHERENT
  - Multiple physics topics will be explored, opening novel scientific avenues on DUNE
- Community engagement will solidify the use of GPUs for detector simulation in HEP

Task / Milestone	**FY27**				**FY28**				**FY29**				**FY30**				**FY31**			
Business quarter	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
1. Computing R&D																				
1.a Framework integration																				
1.b Software development																				
1.c Benchmarking & validation																				
2. Physics research																				
2.a Event t_0 reconstruction																				
2.b Background rejection																				
2.c Event reconstruction																				
2.d ND optical simulation																				
2.e Online triggering																				
2.f ND/FD systematics																				
2.g AI and ML R&D																				
Community engagement																				
a Long-term documentation																				
b DUNE HPC workshops																				

Celeritas v0.7 code contributors:

- Seth R. Johnson (@sethrj)
- Amanda Lund (@amandalund)
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- Julien Esseiva (@esseivaju)
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- Greg Davidson (@davidsgr)
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Celeritas core team:

- Elliott Biondo *(ORNL)*
- Greg Davidson *(ORNL)*
- Julien Esseiva *(LBNL)*
- Rashika Gupta *(ORNL)*
- Hayden Hollenbeck *(UVA)*
- Seth R Johnson *(ORNL)*
- Soon Yung Jun *(FNAL)*
- Guilherme Lima *(FNAL)*
- Amanda Lund *(ANL)*
- Ben Morgan *(U Warwick)*
- Sakib Rahman *(BNL)*
- Stefano Tognini *(ORNL)*

Celeritas core advisors:

- Tom Evans (ORNL)
- Philippe Canal (FNAL)

Past code contributors:

- Paul Romano (@paulromano)
- Vincent R. Pascuzzi (@vrpascuzzi)
- Tom Evans (@tmdelellis)
- Vidor Heli Lujan Montiel (@VHLM2001)
- Damien L-G (@dalg24)
- Doaa Deeb (@DoaaDeeb)
- Andrey Prokopenko (@aprokop)
- Shane Hart (@hartsw)
- Peter Heywood (@ptheywood)

Code ***Documentation*** ***Publication***

CELERITAS

Thank you

Backup

Neutrino oscillations

$$|\nu_\ell\rangle = U|\nu_i\rangle \implies |\nu_\ell(t)\rangle = Ue^{iEt}|\nu_i\rangle$$

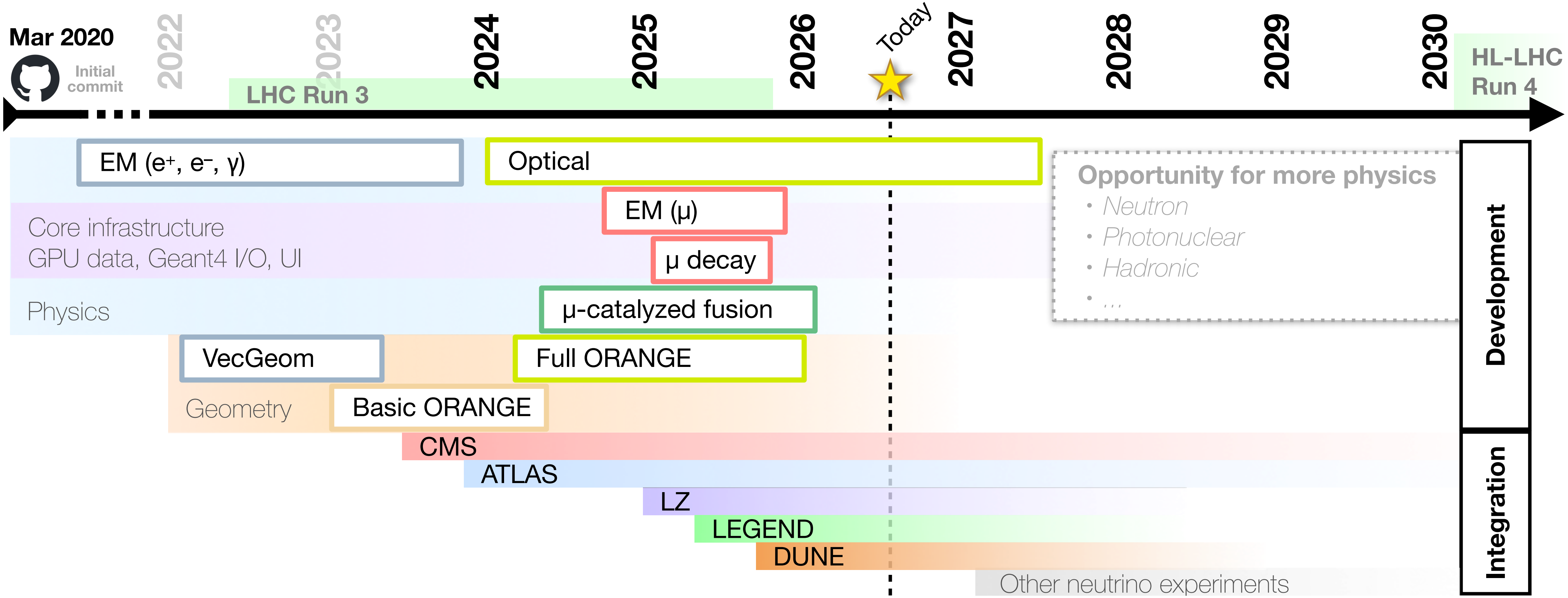
$$\begin{pmatrix}\nu_e\\ \nu_\mu\\ \nu_\tau\end{pmatrix} = \begin{pmatrix}U_{e1} & U_{e2} & U_{e3}\\ U_{\mu 1} & U_{e\mu 2} & U_{\mu 3}\\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3}\end{pmatrix} = \begin{pmatrix}\nu_1\\ \nu_2\\ \nu_3\end{pmatrix} \implies \begin{pmatrix}\nu_e\\ \nu_\mu\\ \nu_\tau\end{pmatrix} = \begin{pmatrix}1 & 0 & 0\\ 0 & c_{23} & s_{23}\\ 0 & -s_{23} & c_{23}\end{pmatrix}\begin{pmatrix}c_{13} & 0 & s_{13}e^{-i\delta}\\ 0 & 1 & 0\\ -s_{13}e^{+i\delta} & 0 & c_{13}\end{pmatrix}\begin{pmatrix}c_{12} & s_{12} & 0\\ -s_{12} & c_{12} & 0\\ 0 & 0 & 1\end{pmatrix} = \begin{pmatrix}\nu_1\\ \nu_2\\ \nu_3\end{pmatrix}$$

$$P_{\nu_\alpha \to \nu_\beta}(L/E) = \delta_{\alpha\beta} - 4\sum_{k>j}^{n} \mathfrak{Re}[U^*_{\alpha k}U_{\beta k}U_{\alpha j}U^*_{\beta j}]\sin^2\left(\frac{\Delta m^2_{kj}L}{4E}\right) + 2\sum_{k>j}^{n} \mathfrak{Im}[U^*_{\alpha k}U_{\beta k}U_{\alpha j}U^*_{\beta j}]\sin\left(\frac{\Delta m^2_{kj}L}{2E}\right)$$

Slide from APS DPF 26: https://indico.fnal.gov/event/72820/contributions/341182/

Updated timeline based on https://meetings.aps.org/Meeting/APR24/Session/D14

Celeritas overview



Optical physics efforts

MOTIVATION Optical photon MC is a **massive** bottleneck on light-based detectors (>95% of simulation time*)

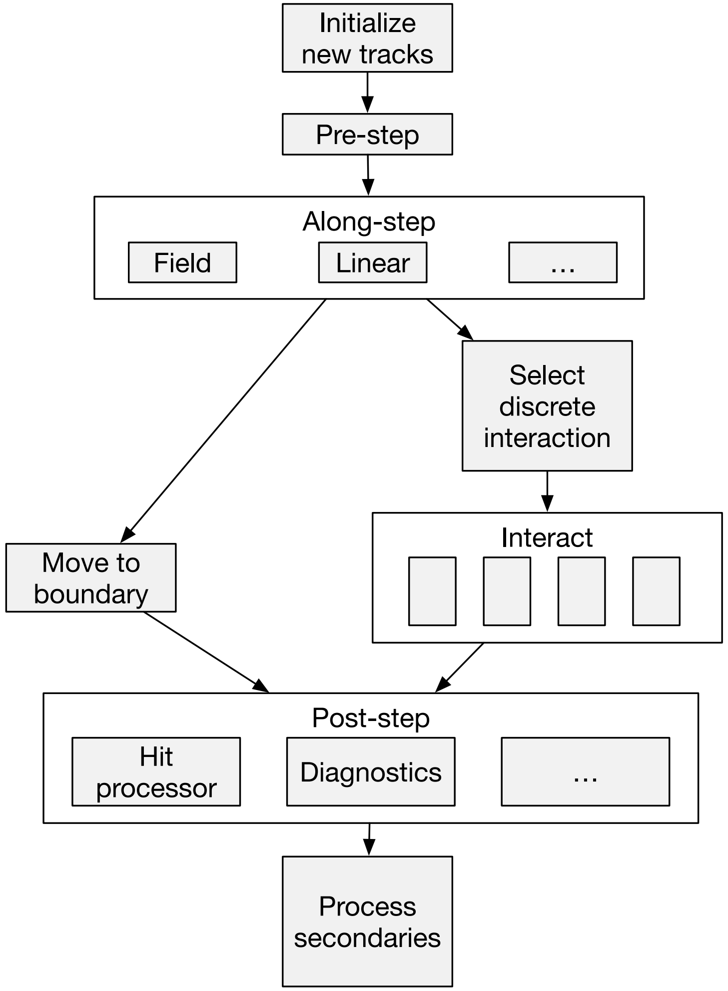
- **Optical physics imported automatically via GDML**
  - Currently supported models: `G4OpticalSurfaceModel { glisur, unified }`
- **Generalized scintillation per particle:** any particle, any number of components
  - Geant4 only allows a few different scintillation yields/components
    `enum G4MaterialPropertyIndex { p, d, t, α, ion, e± }`
    Up to 3 components: `kSCINTILLATIONCOMPONENT[1, 2, 3]`
- **Generalized number of surface physics layers:** n-layers per surface
  - Not limited to `G4OpticalSurfaceFinish { polished, ground, polishedfrontpainted, ... }`
  - Each surface is a `std::vector<VecInterstitialMaterials>`, each with its own properties and interaction model

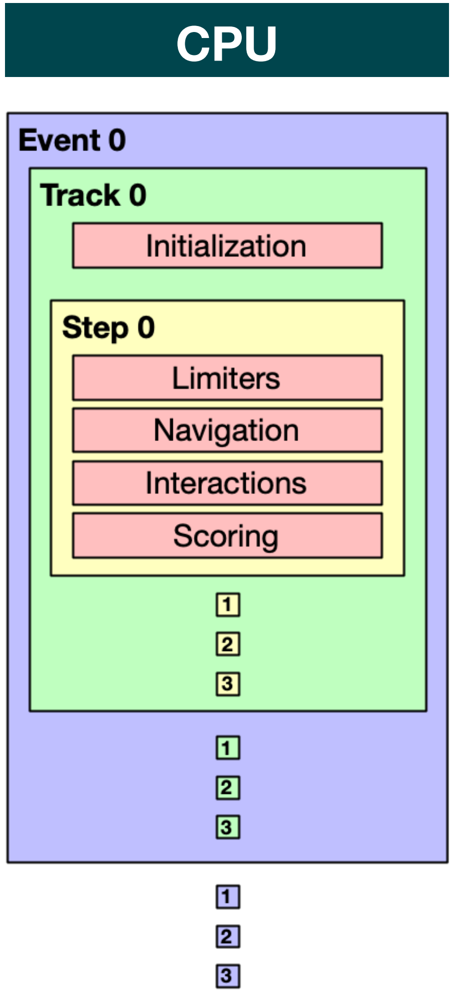
Optical physics
Cerenkov
Scintillation
Wavelength-shifting
Refraction / Reflection
Absorption
Rayleigh scattering
Mie scattering

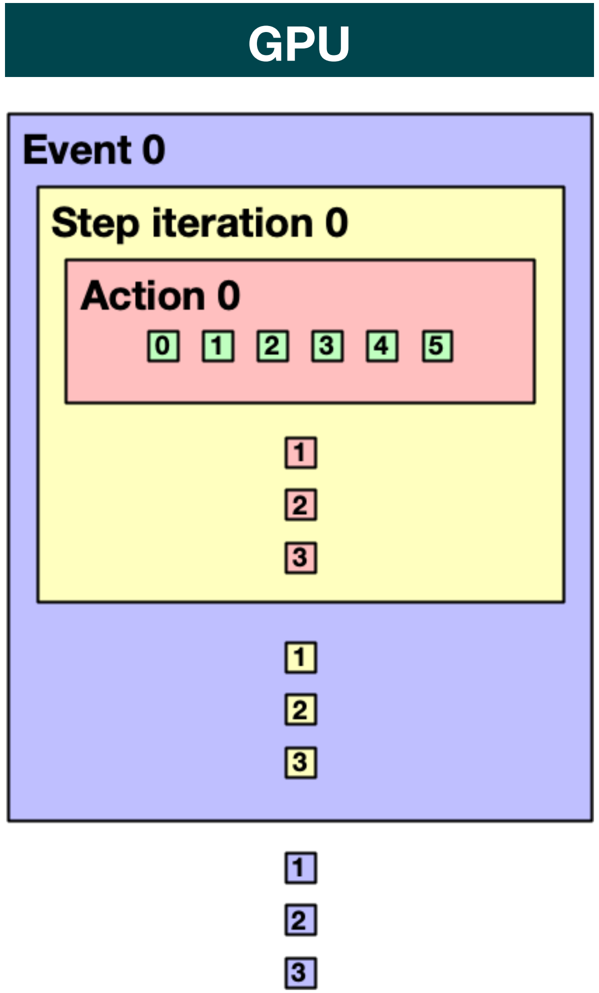
	CPU	Nvidia	AMD
Geant4	✅	❌	❌
Opticks	❌	✅	❌
Celeritas	✅	✅	✅

*According to LZ, DUNE, COHERENT, and LEGEND

Celeritas stepping loop design





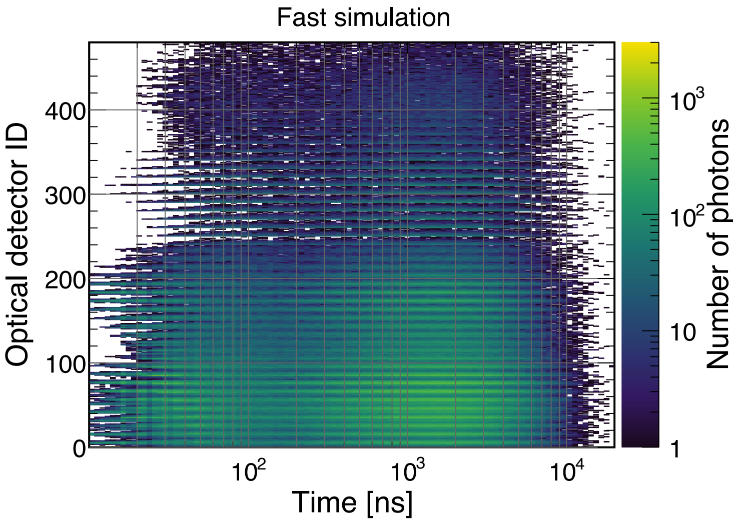


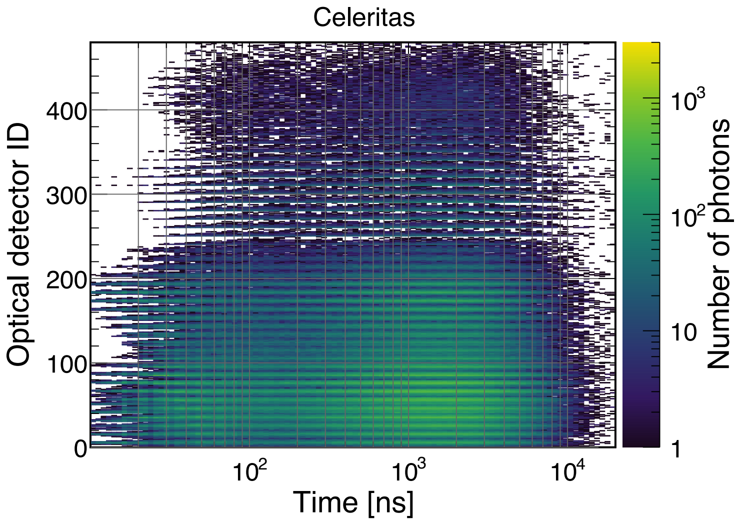
PRELIMINARY

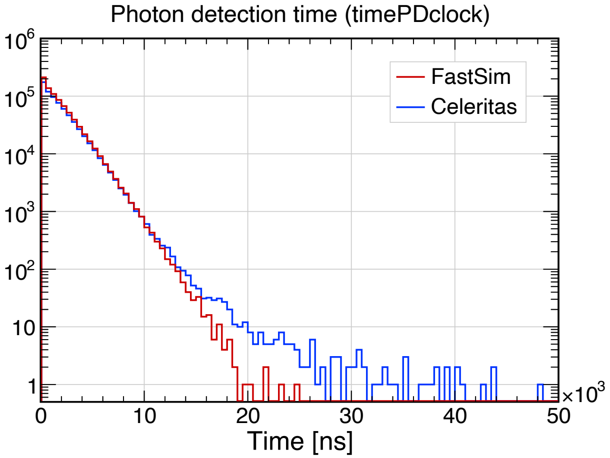
Validation and performance

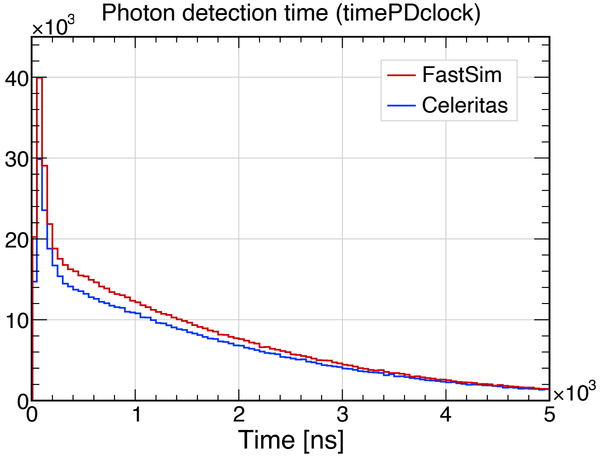
LArSoft: Celeritas vs. Fast Simulation in dunesw v10_20_00d00

- **Physics comparison of GENIE events on ORNL ExCL** *(dune10kt_v6_refactored_1x2x6.gdml with optical data)*
  AMD EPYC 7513; Nvidia Tesla V100









- Scintillation data used to generate visibility maps is not clear
- Ongoing work: regeneration of Fast Simulation maps for full reproducibility

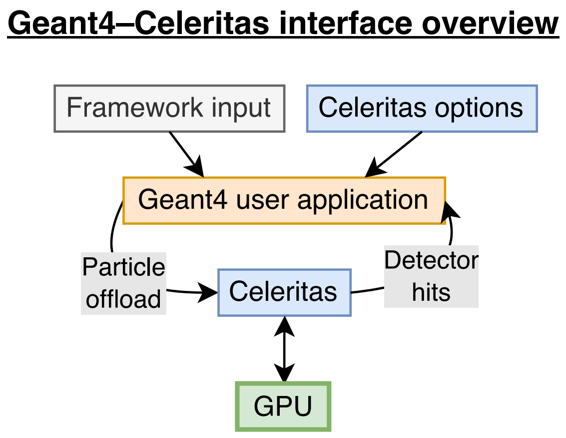
Beyond full MC, Celeritas can generate better optical maps, faster

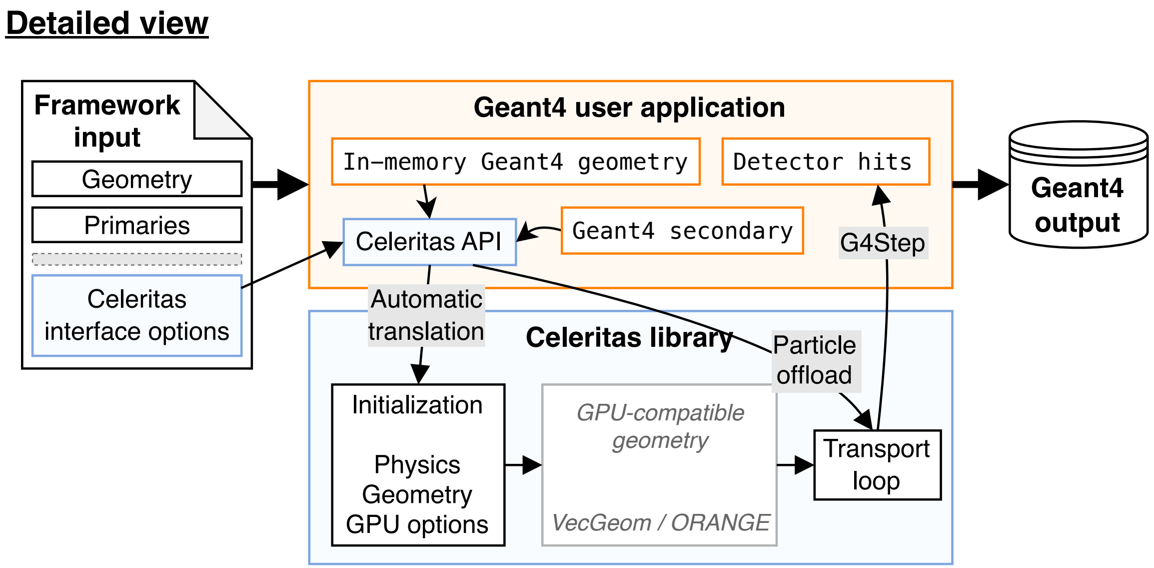
Celeritas overview

Celeritas library usage

Standalone Loads XS/material/particle data from Geant4 at startup and transports all particles

Geant4 API Initialized *within* a Geant4 application; offloads a subset of particles to GPU





Multiple examples of both use-cases can be found in the Celeritas Project GitHub

PRELIMINARY

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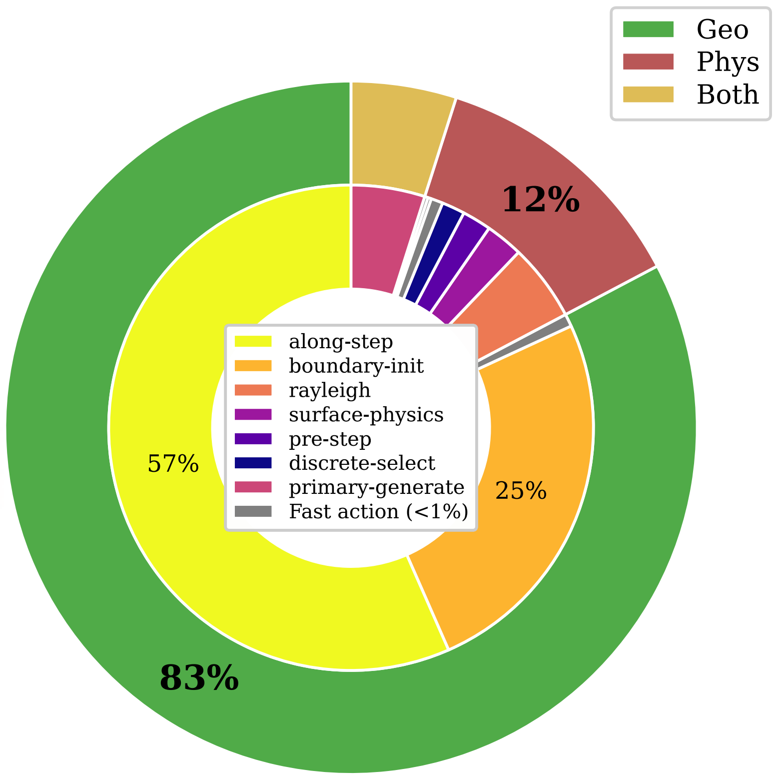

- **Geometry navigation is the largest bottleneck**
  - UV wire design on DUNE compounds the inefficiencies
  - Optimization ideas are being discussed