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# Propagator Based Multi-level Monte-Carlo for Kinetic Neutrals in Edge Plasmas

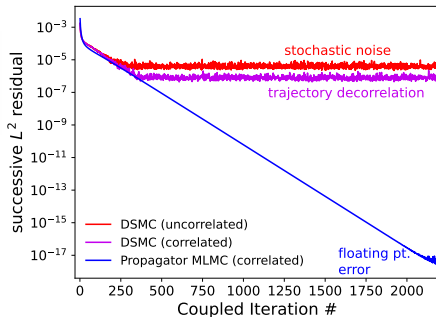
Greg J. Parker (Berkeley, Department of Mathematics)  
UKAEA Exhaust Code Workshop, 7 Oct. 2026

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Berkeley  
UNIVERSITY OF CALIFORNIA

Ref: arXiv:2512.09334 (JCP, 2026)



collaborators: Maxim Umansky and Ben Dudson (LLNL, FES)

# Main Question and Contributions

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Can we unlock deterministic / Jacobian methods with kinetic MC neutrals?

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Introduce new Multi-level MC algorithm that

- ▶ explicitly exploits velocity-localization property
- ▶ displays robust correlation / overcomes decorrelation

# Main Question and Contributions

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This talk:

Introduce new Multi-level MC algorithm that

- ▶ explicitly exploits velocity-localization property
- ▶ displays robust correlation / overcomes decorrelation

Main Question 2:

Can the deterministic methods be used for differentiable code coupling?

# MC noise/decorrelation prevents Jacobian-based methods

Noise demands code-coupling be *explicit*:

- ✗ slow convergence (extreme stiffness).
- ✗ extraneous errors (e.g. poor particle conservation).

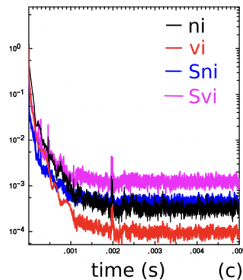
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Jacobian-based methods would enable:

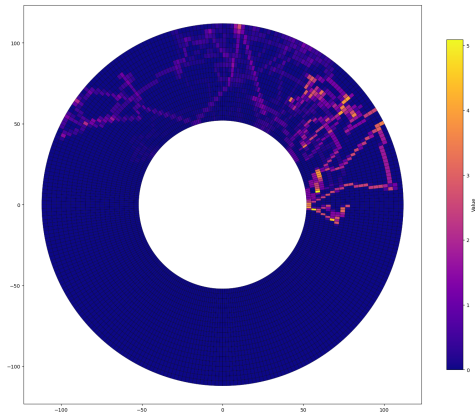
- ▶ Jacobian-free Newton-Krylov (JFNK) solvers for full coupled system.
- ▶ Scan steady state over design parameters.
- ▶ Robust correction methods of approximate solutions (e.g. Neural and tensor network solvers)



[3] I. Joseph *et al* Fig 2(c), convergence.

# Essentials of Neutral Particle Dynamics in Edge Plasmas

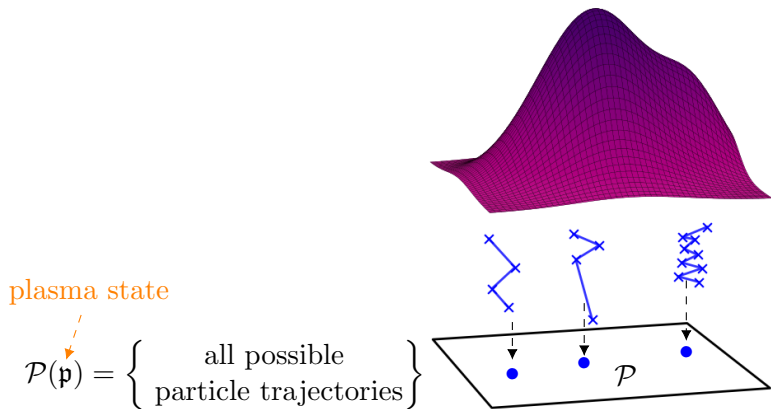
- ▶ H, D, T (main atomic species)
- ▶ He, C, Li, B (impurity species)
- ▶ H<sub>2</sub>, D<sub>2</sub>, T<sub>2</sub> (molecular species)
- ▶ Interactions with plasma
  1. Charge-exchange (resonant, non-resonant)
  2. Wall-scattering
  3. Ionization
  4. Recombination



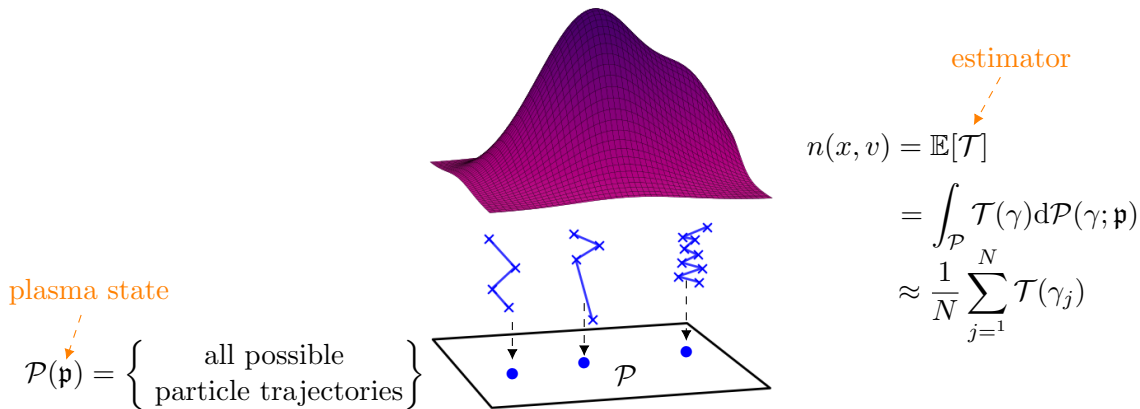
Neutral trajectory in a limiter mesh.

- ▶ A few collisions/trajectory (attached regime) to 1000s of collision/trajectory (fluid, deep detachment regime)

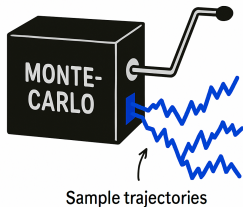
# Monte-Carlo is integration over pathspace



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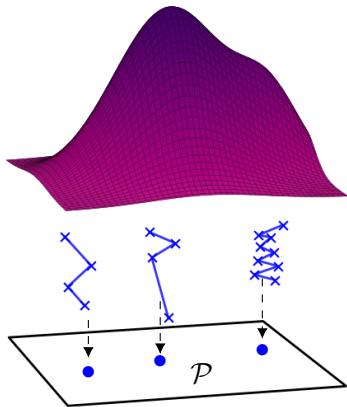


# Monte-Carlo is integration over pathspace



plasma state

$$\mathcal{P}(\mathbf{p}) = \left\{ \begin{array}{l} \text{all possible} \\ \text{particle trajectories} \end{array} \right\}$$

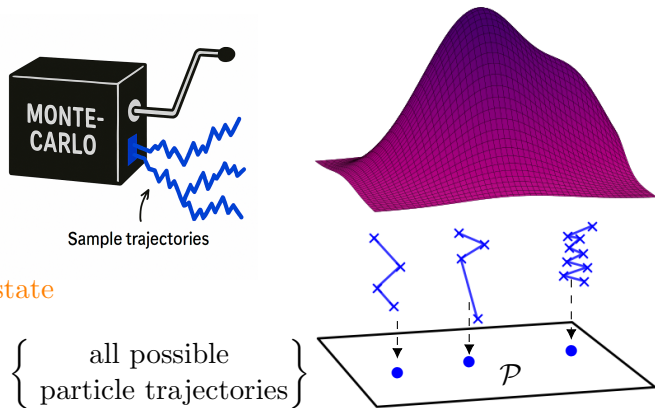


estimator

$$n(x, v) = \mathbb{E}[\mathcal{T}]$$

$$\begin{aligned} &= \int_{\mathcal{P}} \mathcal{T}(\gamma) d\mathcal{P}(\gamma; \mathbf{p}) \\ &\approx \frac{1}{N} \sum_{j=1}^N \mathcal{T}(\gamma_j) \end{aligned}$$

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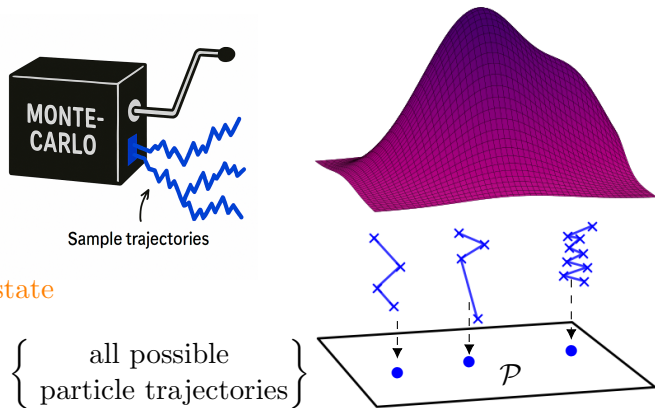


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- ▶ Neutral distribution is  $\mathbb{E}$  over paths of estimator
- ▶ MC code generates unbiased samples of trajectories in plasma

## Charge-exchange localizes velocity

- ▶ Neutrals have the **velocity localization property** (VLP).

Particles undergo frequent collisions with outgoing  $\vec{v}$  determined by local plasma parameters.

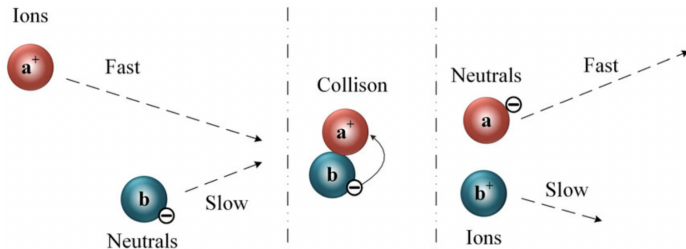
- ▶ Implemented as “velocity swap” collision with thermal ion  $v$  in many codes
- ▶ Holds for *resonant* charge-exchange when neutral energy  $>\sim 0.01\text{eV}$
- ▶ (VLP) could be weakened using higher-order methods.

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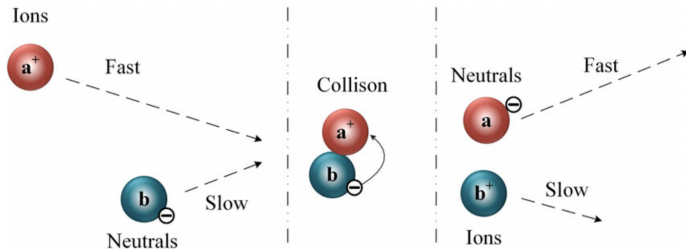


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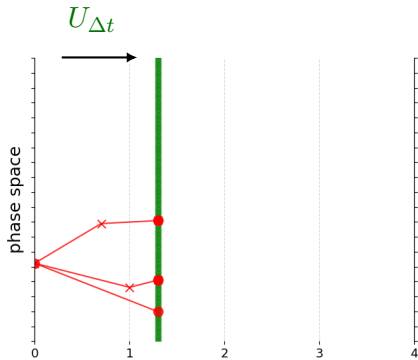


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# Event-manifold slices compress the propagator

- Steady-state or time-stepped MC
  - (1) neutral dynamics non-local
  - (2) distribution is phase space dimension

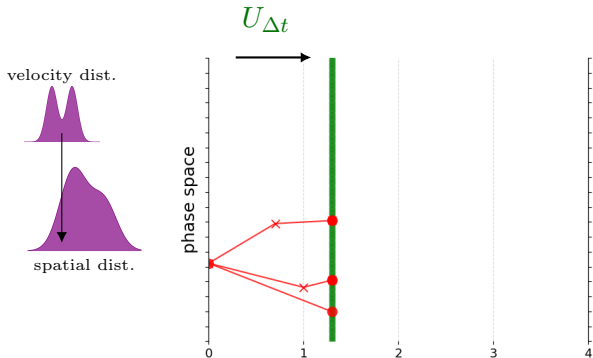
$$n(x, v) = n(x, y, z, v_x, v_y, v_z).$$



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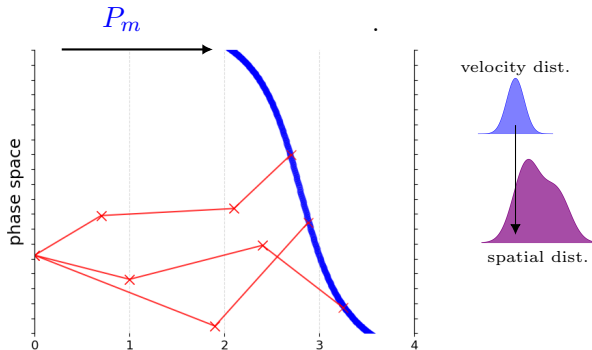
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## ► Propagating to constant CX slices

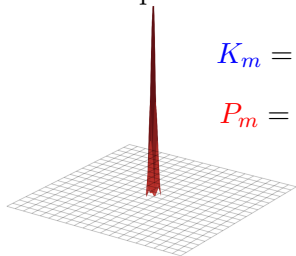
- (1)  $v$  determined by local plasma  $\mathbf{p}(x)$
- (2) distribution collapses to product

$$n(x, v) \longrightarrow f(x) \mathcal{N}_{\mathbf{p}(x)}(v)$$



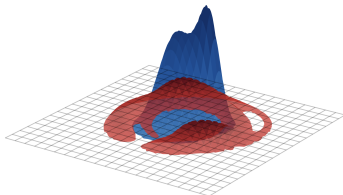
# Propagation by fixed CX collisions defines converging “levels”

- ▶ Propagator by fixed collisions  $P_m$  saved as *real space mesh* sized matrix.
- ▶ Iterative process or linear algebra with  $P_m$  produce equilibrium.



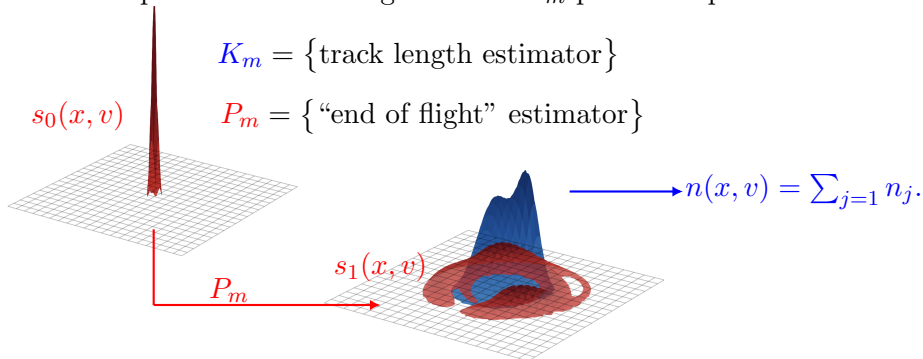
$$K_m = \{\text{track length estimator}\}$$

$$P_m = \{\text{“end of flight” estimator}\}$$



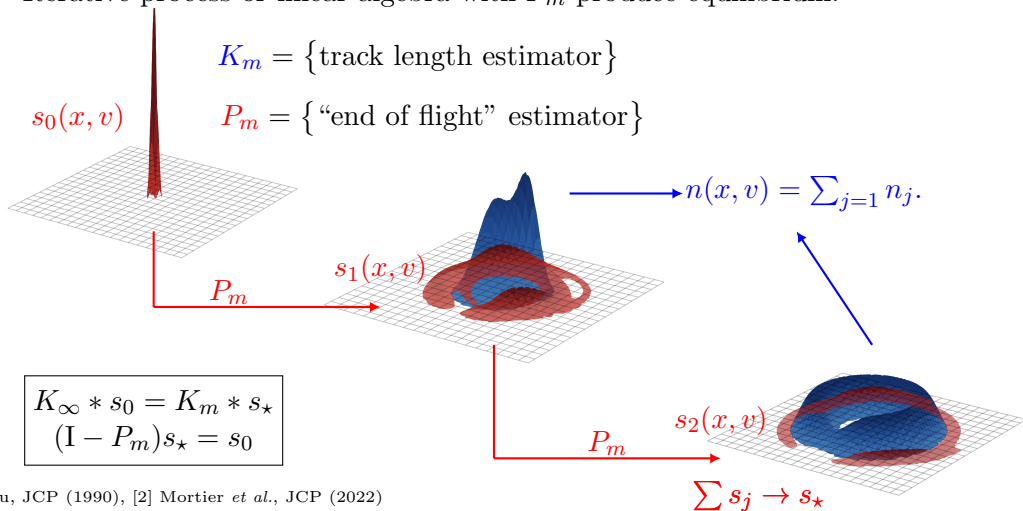
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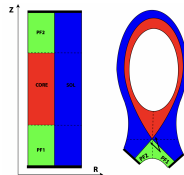
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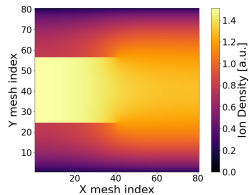


# Home-made 2D MC code is used for numerical experiments

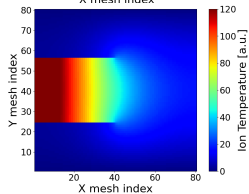
- ▶ Standard MC algorithm for neutral transport [4]
- ▶ Modern CPU-parallel implementation in Julia
- ▶ Simplifying assumptions for atomic physics
- ▶ Rectilinear tokamak geometry
- ▶ Verified on several test problems w/ exact solutions



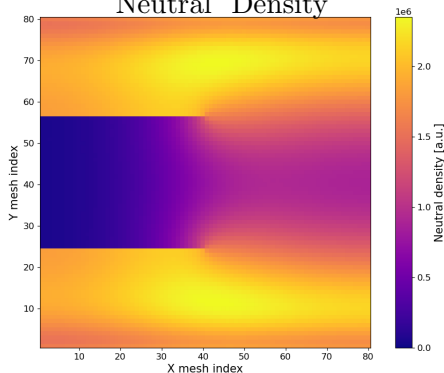
Plasma  
density



Ion Temp.

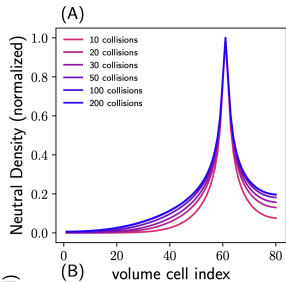


Neutral Density

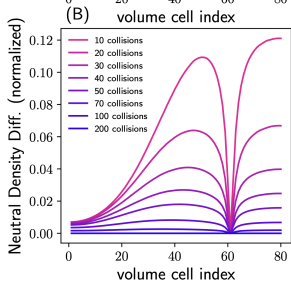


# Propagator MLMC reproduces standard MC

- Comparison on 2D rectilinear tokamak grid  $80 \times 80$



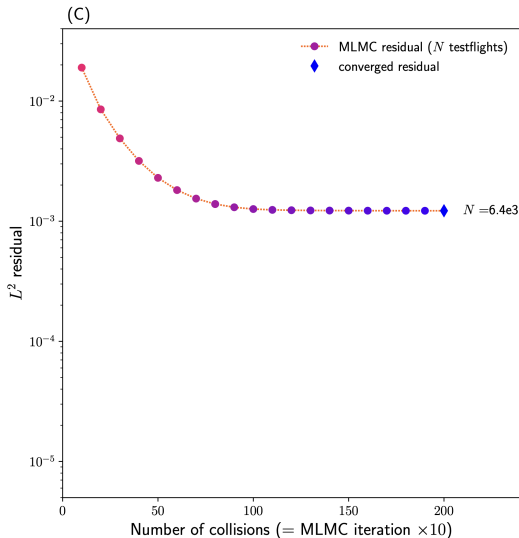
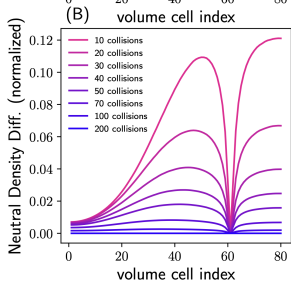
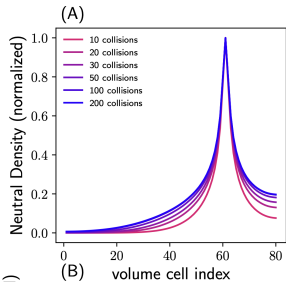
$$K_{10} *^m \rightarrow K_{\infty}$$



$$K_{10} *^m - K_{\infty}$$

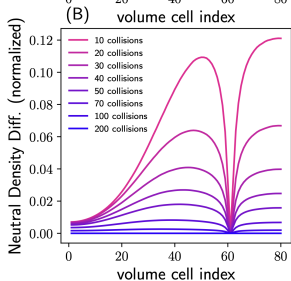
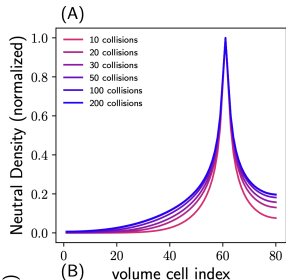
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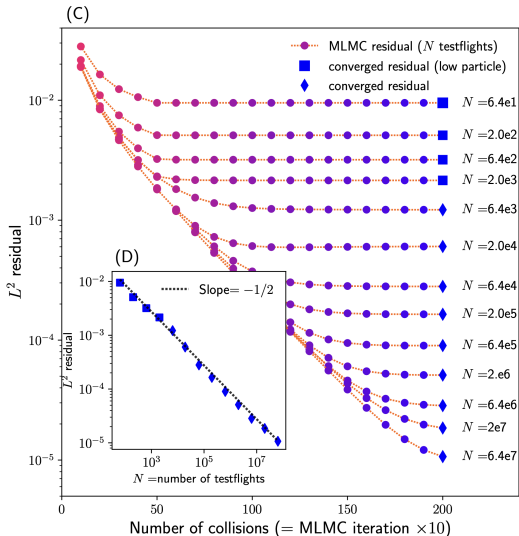
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- ▶ coupled to simple non-linear diffusion plasma model

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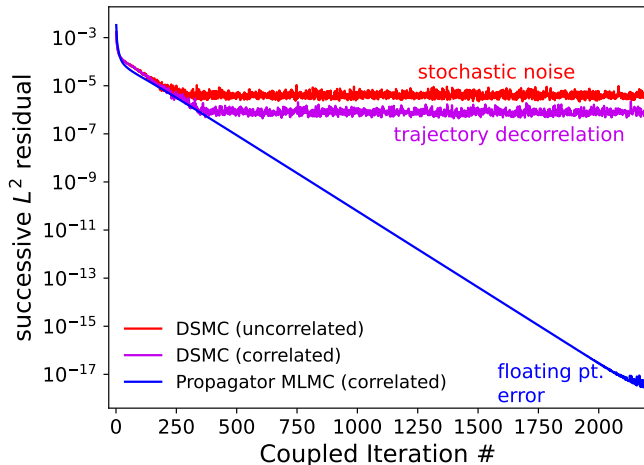
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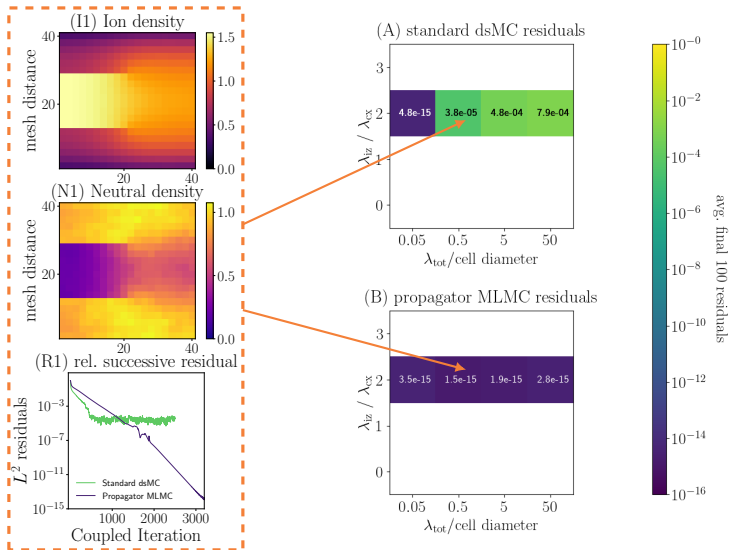
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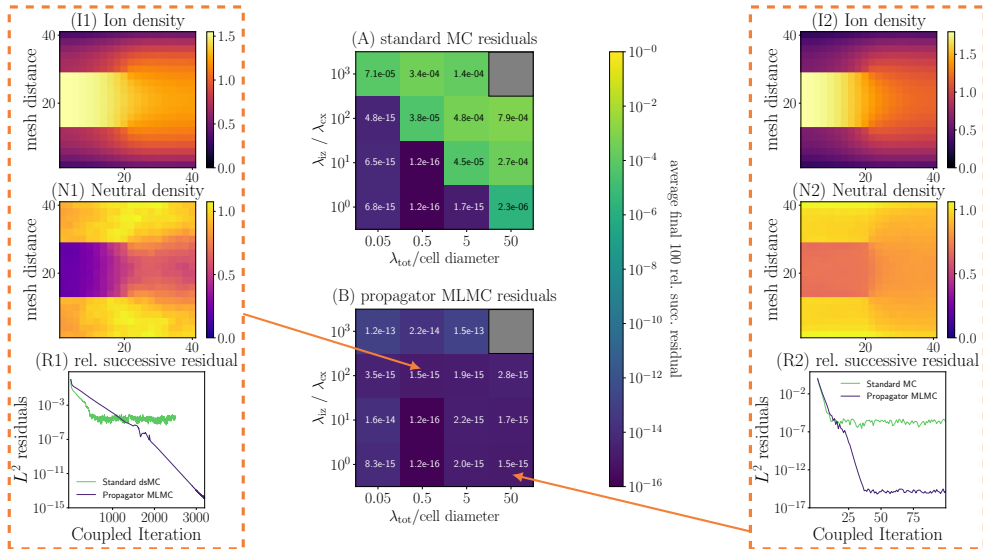
# Effect persists for varying lengthscale and collisionality

- varying  $\sigma_{cx}, R_{iz}$  used as a proxy for different regimes in simplified model

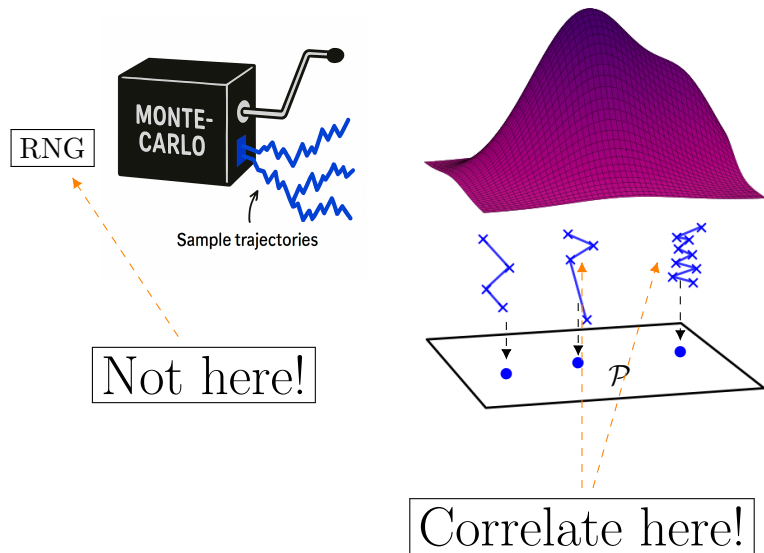


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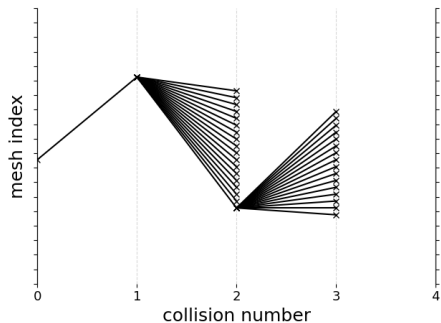
## Why it works: higher correlation



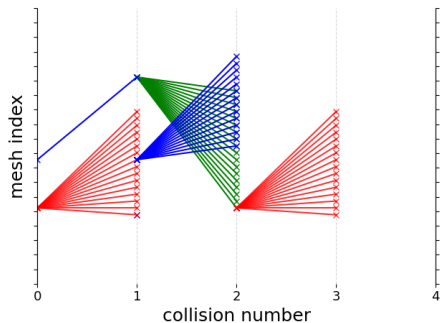
estimator

$$n(x, v) = \mathbb{E}[\mathcal{T}]$$
$$= \int_{\mathcal{P}} \mathcal{T}(\gamma) d\mathcal{P}(\gamma; u)$$
$$\approx \frac{1}{N} \sum_{j=1}^N \mathcal{T}(\gamma_j)$$

# Propagator MLMC samples correlated branching trees



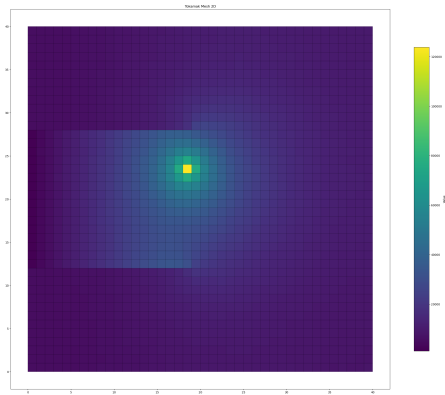
Multiplying propagator extends trajectory samples to exponentially branching trees.



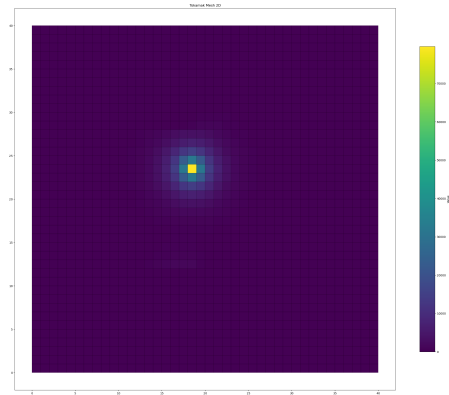
Correlation of seeds results in exponentially many cross-correlations between trees.

- Divergences “caught” and recollected every few collisions

# Propagator localizes geometry and solution operator



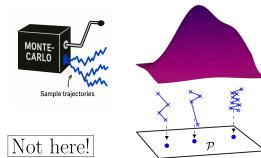
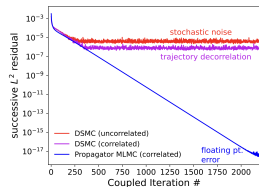
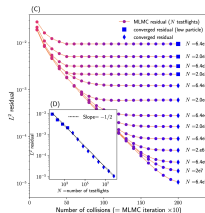
Steady-state solution operator requires resolving full domain geometry



Propagator reduces to local (potentially lower rank) operator

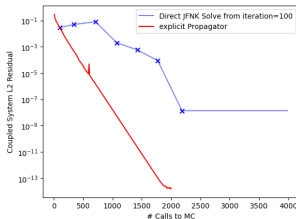
# Summary

- (1) propagator MLMC introduced and verified
- (2) demonstrates advantages for smoothness and stability across regimes in simple 2d coupled plasma-neutral model
- (3) “higher correlations” on pathspace provide robust framework for eliminating diverging trajectories
- (4) excellent candidate for proceeding to test Jacobian-based methods



# We are still far from optimal algorithms

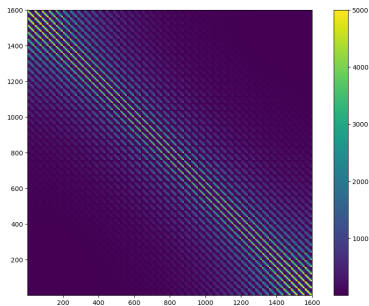
1. New families of “hybrid” models could provide “best of both” options scenarios
  - ▶ e.g. baseline kinetic model + MC rare species
2. Can MC be used as a residual correction for simpler models
  - ▶ Newton-solve with JFNK



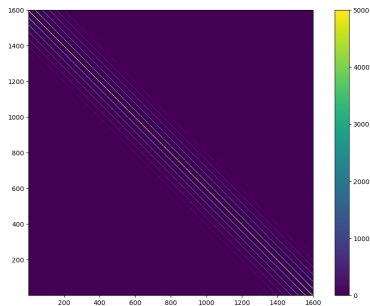
- ▶ [Roberts et. al] , [Pozulp and Haut] Surrogate correction schemes, higher moment MC corrections, ...

## Additional Slides

# Neural Network surrogates for propagators



Sparsity of steady-state operator

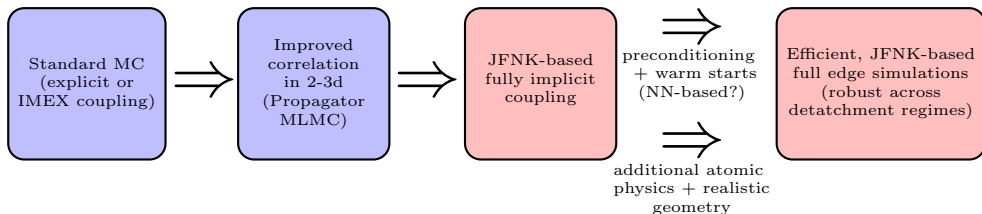


Sparsity of Propagator  $K_{10}$

- ▶ propagator capabilities being explored for PPPL's DEGAS2 MC neutral code (Dr. Georgie Wilkie).
- ▶ demonstrated Propagator learning in 1D (Umansky, P. Smirnov, CPP 2026)
- ▶ joint project developing propagator-based surrogates in general geometries between LLNL, UC Berkeley, PPPL.

# Conclusions and Outlook

1. Propagator MLMC proposed for edge plasma modeling (retains robust correlation)
  - ▶ eliminates key barriers (diverging trajectories) to Jacobian-based methods
  - ▶ numerical experiments with homemade 2D MC code show promising stability for use in JFNK methods
  - ▶ higher correlation provides updated framework to achieve stability & smoothness
2. Towards operational fully-implicit JFNK-based coupling



## Additional Slides

## References

- [1 ] G.P., Umansky, Dudson. “A propagator-based Multi-level Monte-Carlo scheme for kinetic neutral species in edge plasmas” (submitted).  
(main text )
- [2 ] G.P. Umansky, Dudson. Journal of Nuclear Materials **42**, 101889 (2025).  
(1d JFNK methods coupling correlated MC and UEDGE)
- [3 ] Carney *et al* Annals of Nuclear Energy **73**, 423-431 (2014).  
(review of event-based Fission-matrix Monte-Carlo in Neutron transport)
- [4 ] P.M. Valanju. Journal of Computational Physics **88**, 114130 (1990).  
(propagator methods for continuum models of kinetic neutral transport)
- [5 ] Mortier *et al.* Journal of Computational Physics **450** 110736 (2022).  
(Multi-level Monte-Carlo for neutral transport with similar themes)

# MLMC samples rare trajectories

1d reduction in fluid limit: analytic solution

$$N(x) = N_0 \text{Exp} \left( -\frac{|x-x_0|}{L} \right).$$

- ▶ Standard use case for MLMC
  - (1) Similar effect to stratified sampling/ “russian roulette” sampling.
  - (2) Number of propagator flights can be adjusted locally in space.
- ▶ Correct distribution is achieved w/ good sampling of even rare particle trajectories.

