# Neutron Transport Days 2021

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Branching Structures Meeting Bath, September 17, 2021

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Large deviations

Monte Carlo methods

Stochastic control + PDEs and variational problems

Large deviations

Monte Carlo methods

2

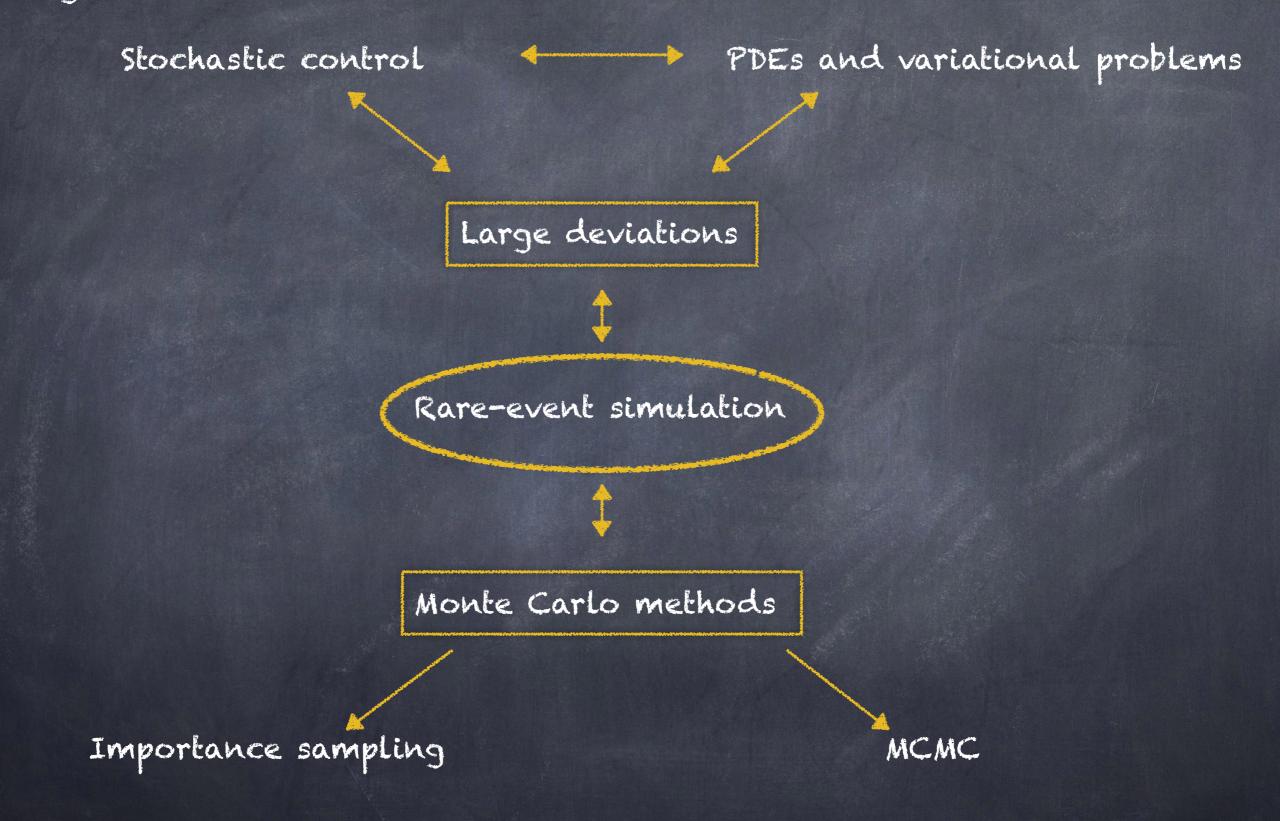
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Importance sampling

MCMC



#### 9. Discussion and numerical comparison of methods.

9.1. Towards Improved Monte-Carlo Methods for the NTE. The results of the previous section (in particular Remark 8.1) suggests that extremely efficient methods for estimating  $\lambda_*$  can be developed if the eigenfunction  $\varphi$  is known. Unfortunately, finding the optimal  $\varphi$  is generally at least as hard as finding the optimal  $\lambda_*$ , so this is not immediately helpful. However, importance sampling can still be highly effective in reducing the variance of the numerical scheme even when the function  $\varphi$  is not known. The key question is how to construct informative functions h which might approximate  $\varphi$  well.

The benefits of combining SMC methods with importance sampling has been investigated by (e.g. [29]). It is in this combination that we expect the results in Sections 7 and 8 to be of most benefit. Specifically, we would anticipate using SMC methods to sample/resample from a population of particles, which themselves undergo motion according to an h-transformed version of the NRW. We aim to write more about this in forthcoming work.

A further difficulty that arises in the use of *h*-transformed motion for the estimation of  $\lambda_*$  is that the estimates can be dominated by large-deviation effects. Specifically, although the estimates remain unbiased, for large *t* a substantial contribution to the expectation in (7.11) comes from rare particles with large weights (the exponential, product and indicator terms

Relies on choosing new sampling dynamics (previous quote: h function). Rare-event simulation: Large deviation asymptotics guides the choice.

Ex: Estimate the probability of exiting A for a process  $\{X^n(t); t \in [0,T]\}$ :

 $p_n = P(X^n(\tau) \in \partial A, \text{ some } \tau \leq T).$ 

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(Standard) Monte Carlo: Sample trajectories  $\{X_i^n\}_{i=1}^N$  from original dynamics  $P^n$ . Estimator

$$\hat{p}_{N,n} = \frac{1}{N} \sum_{i=1}^{N} I\{X_i^n(\tau) \in A, \text{ some } \tau \leq T\}$$

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Importance sampling: Sample trajectories  $\{X_i^n\}_{i=1}^N$  from alternative dynamics  $Q^n$ . Estimator

$$\tilde{p}_{N,n} = \frac{1}{N} \sum_{i=1}^{N} I\{X_i^n(\tau) \in A, \text{ some } \tau \leq T\} \frac{dP^n}{dQ^n}(X_i^n)$$

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Choice of  $Q^n$  main challenge for IS. Two common approaches:

- Lyapunov inequalities
- Control approach/HJ equations

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A large deviation-style analysis of associated control problem suggests  $Q^n$  according to  $\nabla_x W$ , W a subsolution of a HJ equation:

 $\begin{cases} W_t(t,x) - H(x, -\nabla_x W(t,x)) \ge 0, (t,x) \in (0,T] \times A, \\ W(t,x) \le 0, \qquad (t,x) \in (0,T] \times \partial A. \end{cases}$ 

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In general: <u>Very</u> difficult to construct "optimal" subsolution. So far, mostly toy-ish problems studied in full detail.

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- Control-perspective on the choice of h,
- Provably efficient methods for interacting particle systems,
- Combination with on-line estimates and updates,
- Measure-valued processes, different from standard setting.

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(similar ideas can be applied for MCMC, splitting, genealogical methods...)

### Possible alternative: Efficient numerical methods for QSDs



Recent work studies connections between QSDs and stochastic control: Budhiraja, Dupuis, N., Wu – Quasi-stationary distributions and ergodic control problems (arXiv:2103.00280)

- Introduce ergodic stochastic controls problems associated with the QSD of a diffusion process.
- Prove well-posedness of HJB eq:s and describe how they characterise important properties of the QSD.
- Opens up for numerical methods, from the control community, for approximating the rate (eigenvalue) and the QSD.

(very early in the development, much to do for this to be viable...)

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