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Adjoint Monte Carlo particle methods with reversible random number generators

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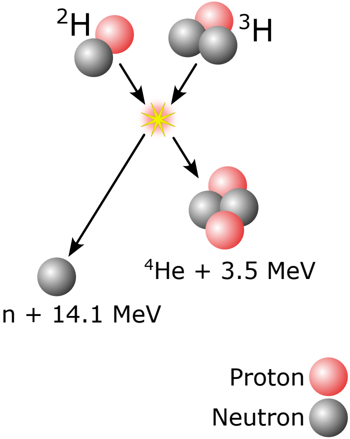
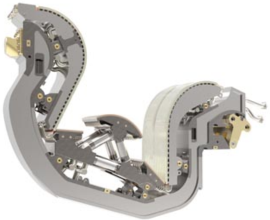
Motivation: nuclear fusion in tokamaks





$$Q \geq 10 : \quad 50\text{MW} \rightarrow 500\text{MW}$$

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Didactical example: Heat equation in 1D

- **Macroscopic view**

$$\frac{\partial}{\partial t}\mathcal{T}(x,t) - \frac{\partial^2}{\partial x^2}\mathcal{T}(x,t) + u(x)\mathcal{T}(x,t) = 0$$

- **Particle view**

$$\{Q_{p,\tau}\}_{p=1}^{P} = \left\{ \begin{bmatrix} X_{p,\tau} \\ W_{p,\tau} \end{bmatrix} \right\}_{p=1}^{P}, \qquad \tau = 0, \ldots, T-1$$

  - Diffusion step

$$X_{p,\tau+1} = X_{p,\tau} + \sqrt{2\Delta t}\,\xi_{p,\tau} \quad \xi_{p,\tau} \sim \mathcal{N}(0,1)$$

  - Reweighting step

$$W_{p,\tau+1} = W_{p,\tau} \exp\left(-\Delta t\, \hat{u}\left(X_{p,\tau+1}\right)\right)$$

Optimization problem

- **Continuous**

$$\min_{u(x)} \mathcal{J}(\mathcal{T}(x,t),u(x,t)) = \int_0^\infty \int_0^L \frac{1}{2}\mathcal{T}(x,t)^2 \mathrm{d}x\,\mathrm{d}t + \kappa \int_0^L \frac{1}{2}u(x)^2 \mathrm{d}x$$

$$\text{subject to } \frac{\partial}{\partial t}\mathcal{T}(x,t) - \frac{\partial^2}{\partial x^2}\mathcal{T}(x,t) + u(x)\mathcal{T}(x,t) = 0,$$

$$\mathcal{T}(x,0) = \mathcal{T}_0(x), \quad \mathcal{T}(0,t) = \mathcal{T}(L,t)$$

- **Discrete**

$$\mathcal{J}(\mathcal{T}(x,t),u(x,t)) \approx \hat{\mathcal{J}}(\hat{\mathcal{T}},\hat{u}) = \Delta t \sum_{\tau=0}^{T}{}'' \Delta x \frac{1}{2}\hat{\mathcal{T}}_\tau^\top \hat{\mathcal{T}}_\tau + \nu \Delta x \frac{1}{2}\hat{u}^\top \hat{u}$$

$$\hat{\mathcal{T}}_{\tau,n} = \sum_{p=1}^{P} \frac{1}{\Delta x}\mathcal{I}_n\left(X_{p,\tau}\right) W_{p,\tau}$$

Adjoint-based optimization

- PDE-constrained optimization

$$\min_{u} \mathcal{J}(q,u), \quad \text{subject to} \quad \mathcal{B}(q;u) = 0$$

- Naive application of chain rule

$$\frac{\mathrm{d}\mathcal{J}}{\mathrm{d}u}(q(u),u) = \frac{\partial \mathcal{J}}{\partial u}(q,u) + \frac{\partial \mathcal{J}}{\partial q}(q,u)\frac{\mathrm{d}q}{\mathrm{d}u}(u)$$

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- Solution: Lagrangian $\mathcal{L}(q,q^*,u) = \mathcal{J}(q,u) + (q^*, \mathcal{B}(q,u))$

$$\mathcal{B}(q,u) = 0 \qquad \text{State equation}$$

$$\frac{\partial \mathcal{J}}{\partial q}^*(q,u) + \frac{\partial \mathcal{B}}{\partial q}^*(q,u)q^* = 0 \qquad \text{Adjoint equation}$$

$$\frac{\partial \mathcal{J}}{\partial u}^*(q,u) + \frac{\partial \mathcal{B}}{\partial u}^*(q,u)q^* = 0 \qquad \text{Design equation}$$

Discrete adjoint

- Linearized discretization around $\hat{q}' = \hat{q}(\hat{u})$

$$\hat{\mathcal{B}}(\hat{q},\hat{u}) \approx \hat{\mathcal{B}}(\hat{q}',\hat{u}) + \frac{\partial \hat{\mathcal{B}}}{\partial \hat{q}}(\hat{q}',\hat{u})(\hat{q}-\hat{q}') = 0$$

is a matrix-vector system

Discrete adjoint

- Linearized discretization around $\hat{q}' = \hat{q}(\hat{u})$

$$\hat{\mathcal{B}}(\hat{q}, \hat{u}) \approx \qquad \frac{\partial \hat{\mathcal{B}}}{\partial \hat{q}}(\hat{q}', \hat{u})(\hat{q} - \hat{q}') = 0$$

  is a matrix-vector system
- Adjoint equation

$$\frac{\partial \hat{\mathcal{J}}}{\partial \hat{q}}^{\top}(\hat{q}', \hat{u}) + \frac{\partial \hat{\mathcal{B}}}{\partial \hat{q}}^{\top}(\hat{q}', \hat{u})\hat{q}^* = 0$$

Monte Carlo as a matrix

- For each particle p and time step τ

$$B_{p,\tau+1}(Q_{p,\tau+1}, Q_{p,\tau}; \hat{u}) = \begin{bmatrix} X_{p,\tau+1} - X_{p,\tau} - \sqrt{2\Delta t}\xi_{p,\tau} \\ W_{p,\tau+1} - W_{p,\tau} \exp\left(-\Delta t\, \hat{u}\left(X_{p,\tau+1}\right)\right) \end{bmatrix} = 0$$

- Particle Jacobian

$$\frac{\partial \hat{\mathcal{B}}_p}{\partial \hat{q}_p}(Q_p, \hat{u}) = \begin{bmatrix} \frac{\partial B_{p,1}}{\partial Q_{p,1}} & & & \\ \frac{\partial B_{p,2}}{\partial Q_{p,1}} & \frac{\partial B_{p,2}}{\partial Q_{p,2}} & & \\ & \ddots & \ddots & \\ & & \frac{\partial B_{p,T}}{\partial Q_{p,T-1}} & \frac{\partial B_{p,T}}{\partial Q_{p,T}} \end{bmatrix}$$

$$\frac{\partial B_{p,\tau+1}}{\partial Q_{p,\tau+1}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \frac{\partial B_{p,\tau+1}}{\partial Q_{p,\tau}} = \begin{bmatrix} -1 & 0 \\ 0 & -\exp\left(-\Delta t\, \hat{u}\left(X_{p,\tau+1}\right)\right) \end{bmatrix}$$

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Adjoint Monte Carlo

- Simulate particles from final state

$$Q^*_{p,T} = \begin{bmatrix} X^*_{p,T} \\ W^*_{p,T} \end{bmatrix} = -\frac{\partial \hat{\mathcal{J}}}{\partial Q_{p,T}}^\top = -\begin{bmatrix} 0 \\ \Delta t \hat{\mathcal{T}}\left(X_{p,T}\right) \end{bmatrix}$$

- Reverse time stepping

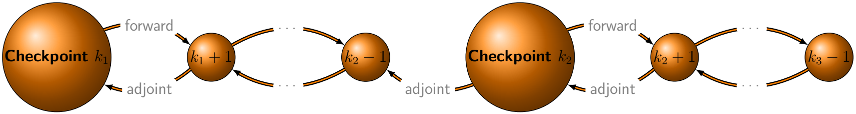
$$\begin{aligned} Q^*_{p,\tau} &= -\frac{\partial B_{p,\tau+1}}{\partial Q_{p,\tau}}^\top Q^*_{p,\tau+1} - \frac{\partial \hat{\mathcal{J}}}{\partial Q_{p,\tau}}^\top \\ &= \begin{bmatrix} X^*_{p,\tau+1} \\ \exp\left(-\Delta t\, \hat{u}\left(X_{p,\tau+1}\right)\right) W^*_{p,\tau+1} \end{bmatrix} - \begin{bmatrix} 0 \\ \Delta t \hat{\mathcal{T}}(X_{p,\tau}) \end{bmatrix} \end{aligned}$$

- Note that $X^*_{p,\tau} = 0$ for all τ

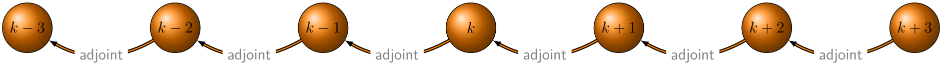
$$W^*_{p,\tau} = \exp\left(-\Delta t\, \hat{u}\left(X_{p,\tau+1}\right)\right) W^*_{p,\tau+1} - \Delta t \hat{\mathcal{T}}(X_{p,\tau})$$

Matching forward and adjoint simulations

- Same paths in forward/backward simulation
- Challenge: $P \times T$ large
- Solutions:
  - Checkpointing: 2 forward simulations + backward simulation



  - Generating the paths in reverse (this work)



Reversing a random number generator

- PCG: permuted congruential generator[1]
  - internal state ζ_k and constant vectors a, c, m

$$\zeta_{k+1} = a\zeta_k + c \mod m,$$

  - 1-way (permutation) function generates output from ζ_k
  - Passes `TestU01` with flying colors
- Reversing modular operations $\rightarrow$ reversed uniform sequence

$$\zeta_k = a^{-1}(\zeta_{k+1} - c) \mod m,$$

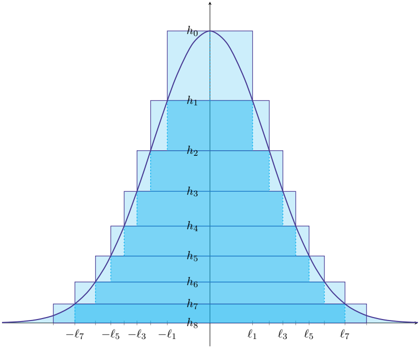
$$a^{-1} \equiv a^{m-2} \mod m$$

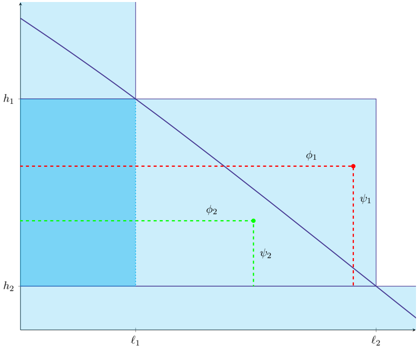
- Exponential distribution through inverse transform:

$$u \sim \mathcal{U}([0,1]) \Rightarrow -\lambda \ln(1-u) \sim \mathcal{E}(\lambda)$$

1: M.E. O'Neill, *PCG: A Family of Simple Fast Space-Efficient Statistically Good Algorithms for Random Number Generation.* Technical report HMC-CS-2014-0905, Harvey Mudd College (2014)

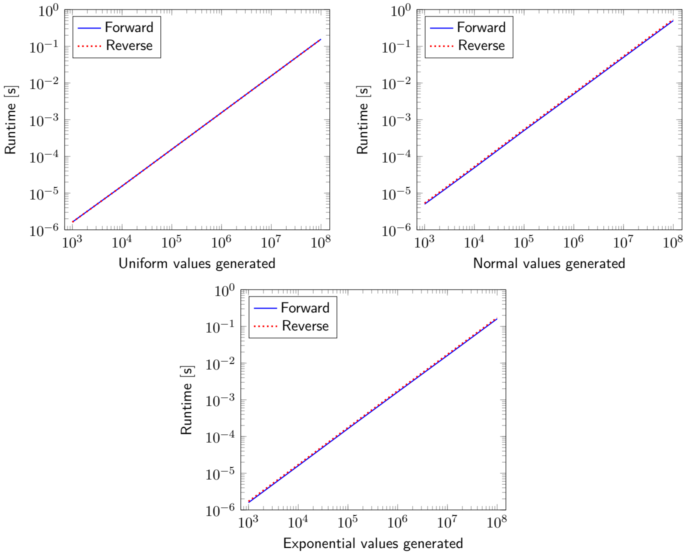
Normal distribution through Ziggurat



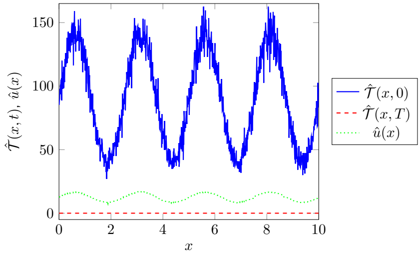


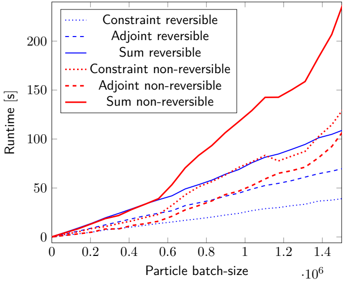
- Uses either 1, 2 or $1 + 2n,\ n = 1, 2, \ldots$ uniform values
- How many depends on the first value
- Solution: Seed second generator

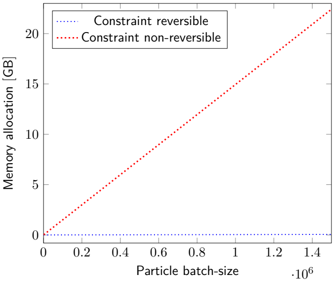
Generator timings



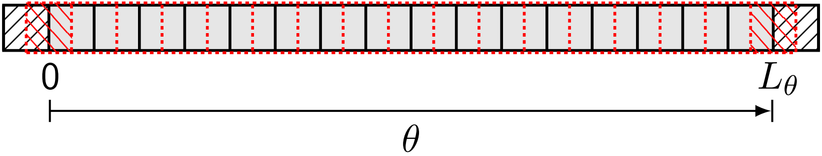
Optimal cooling







Fusion example: domain length optimization[2]



$$\mathcal{J}(q, L_\theta) = \frac{1}{2}\left(n_{\mathbf{i}} b_\theta u_{\|} - \Gamma_d \right)^2 \Big|_{L_\theta} + \frac{\kappa}{2}\left(L_\theta - L_0\right)^2$$

$$q = \left(n_{\mathbf{i}}, u_{\|}, f_{\mathbf{n}} \right)^\top$$

$n_{\mathbf{i}}$	plasma density
$u_{\|}$	plasma velocity
$f_{\mathbf{n}}$	neutral position-velocity

2: W. Dekeyser, *Optimal Plasma Edge Configurations for Next-Step Fusion Reactors.* PhD thesis (2014)

Plasma edge model

- Plasma $\Rightarrow$ Finite volume

$$\frac{\partial}{\partial\theta}\left(n_{\mathbf{i}} b_\theta u_\parallel\right) = S_{n_{\mathbf{i}}} - K_{\mathsf{d}} n_{\mathbf{i}}$$

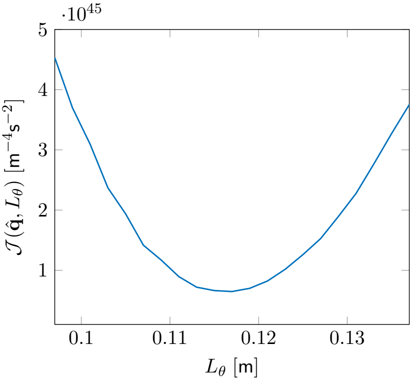
$$\frac{\partial}{\partial\theta}\left(m n_{\mathbf{i}} b_\theta {u_\parallel}^2 - \nu_{\mathsf{d}} \frac{\partial u_\parallel}{\partial\theta}\right) = S_{u_\parallel} - b_\theta \frac{\partial p}{\partial\theta}$$

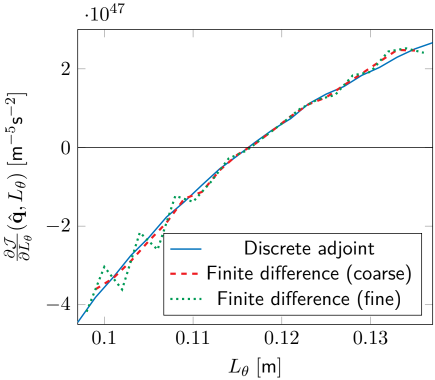
$$S_\psi = \int f_{\mathbf{n}}(\theta, v)\Psi(\theta, v)\mathrm{d}v, \quad \psi \in \{n_{\mathbf{i}}/u_\parallel\} \quad \Rightarrow \quad \text{Low-dimensional}$$

- Neutrals $\Rightarrow$ Monte Carlo

$$v\frac{\partial}{\partial\theta} f_{\mathbf{n}}(\theta, v) + K_{\mathsf{i}} f_{\mathbf{n}}(\theta, v) = S_{f_{\mathbf{n}}}\left(n_{\mathbf{i}}, u_\parallel\right) + K_{\mathsf{cx}} \int f_{\mathbf{n}}(\theta, v') C(v' \rightarrow v)\mathrm{d}v'$$

Preliminary results

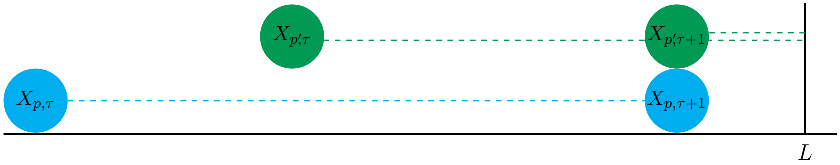




	$n_\mathbf{i}$-solver	$u_\parallel$-solver	Neutral solver
State	3.5×10^{-5} s	4.1×10^{-5} s	6.6 s
Adjoint	3.1×10^{-5} s	3.6×10^{-5} s	9.8 s

Can all simulations be reversed?

- In theory yes!
- ... but at what cost?
  - Reflections
  - Collisions in batched simulations
  - ...



Løvbak, E., Blondeel, F., Lee, A., Vanroye, L., Van Barel, A., Samaey, G., *Reversible random number generation for adjoint Monte Carlo simulation of the heat equation.* Monte Carlo and Quasi-Monte Carlo Methods - MCQMC 2022. **Submitted** (2023) *arXiv:2302.02778*

Løvbak, E., *Multilevel and adjoint Monte Carlo methods for plasma edge neutral particle models.* PhD thesis (2023)