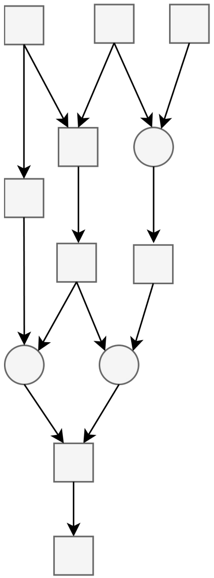


ML4Lattice ETH Zurich

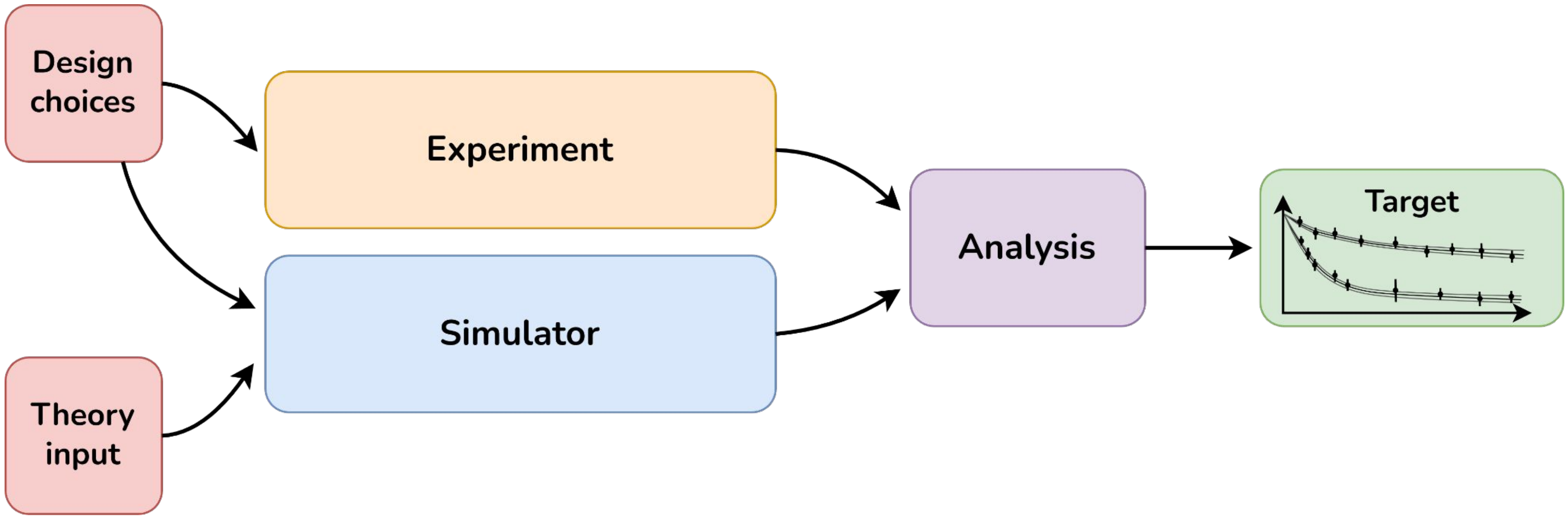
10.06.2025

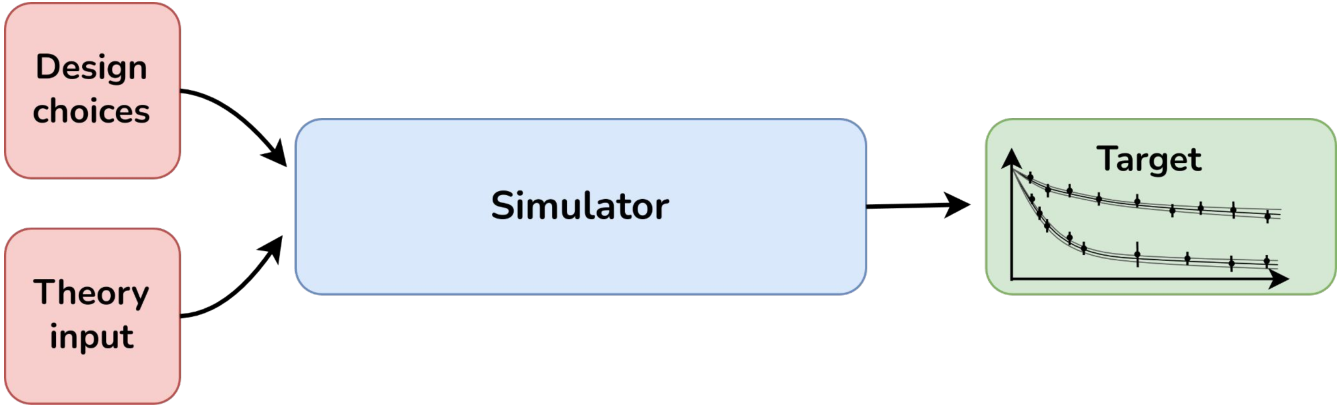
Stochastic differentiation of Monte Carlo simulations for parameter inference in quarkonium suppression

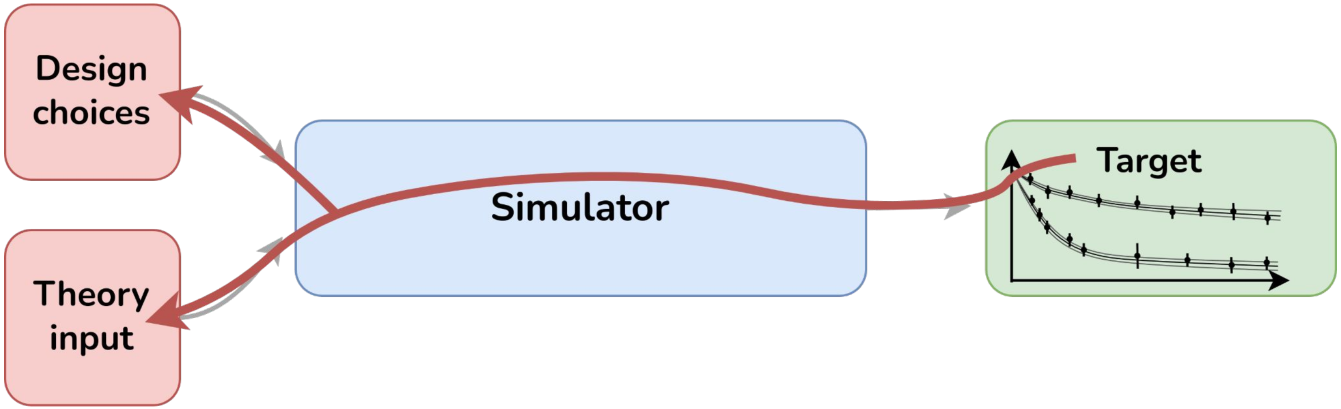
Tom Magorsch
Technical University of Munich

in collaboration with

Lukas Heinrich
Technical University of Munich


Design choices
Experiment
Simulator
Theory input
Analysis
Target


Design choices
Theory input
Simulator
Target

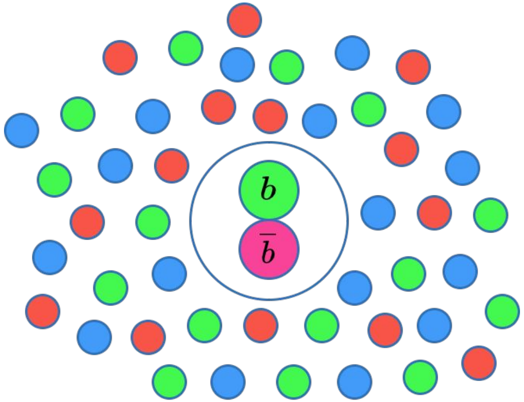

Design choices
Theory input
Simulator
Target

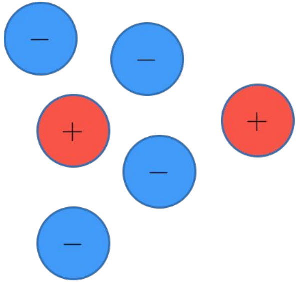
Quarkonium Suppression

Veres, Gábor I. "Heavy ion physics at CMS and ATLAS: hard probes." *arXiv preprint arXiv:1905.10461* (2019).

T. Matsui, H. Satz, Phys. Lett. B 178 (1986) 416

Propagation through QGP



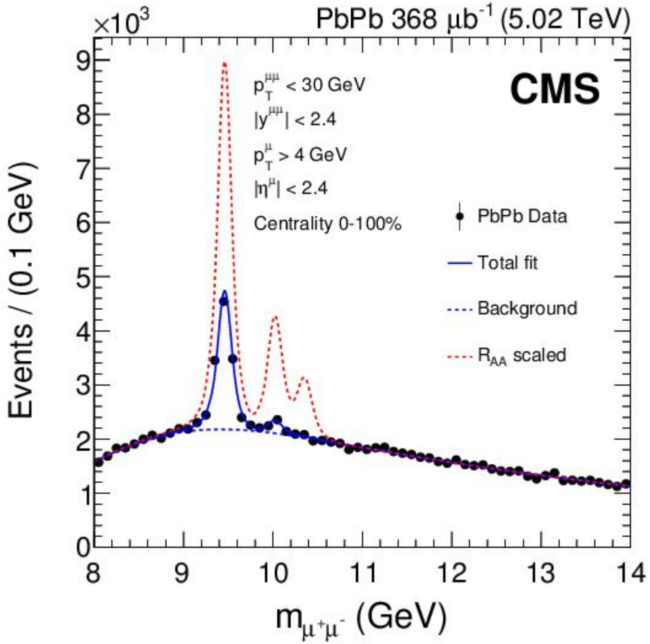


$$V(r) = -\frac{\alpha}{r}$$

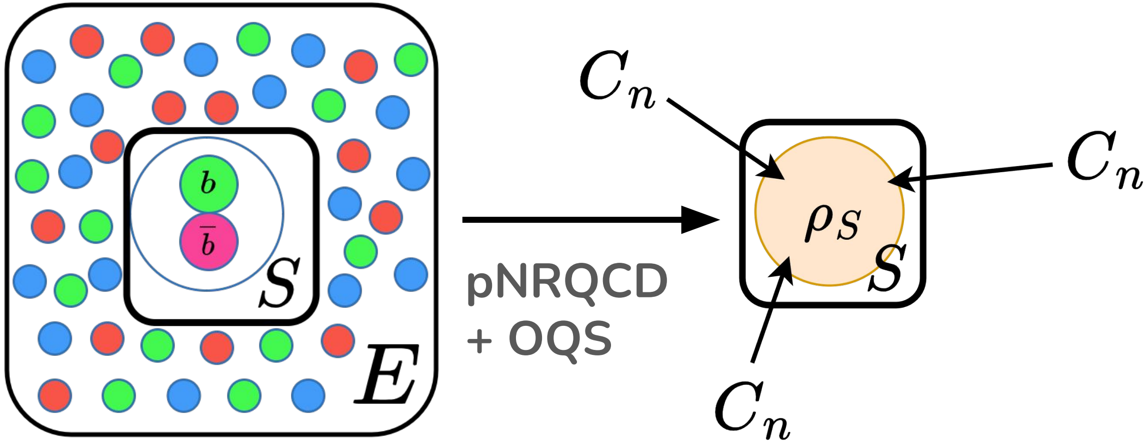
$$\downarrow$$

$$V(r) = -\frac{\alpha}{r}\mathrm{e}^{-m_D r}$$

Debye-screening in medium



Quarkonium Suppression Simulator



$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_l \otimes \mathcal{H}_r$$

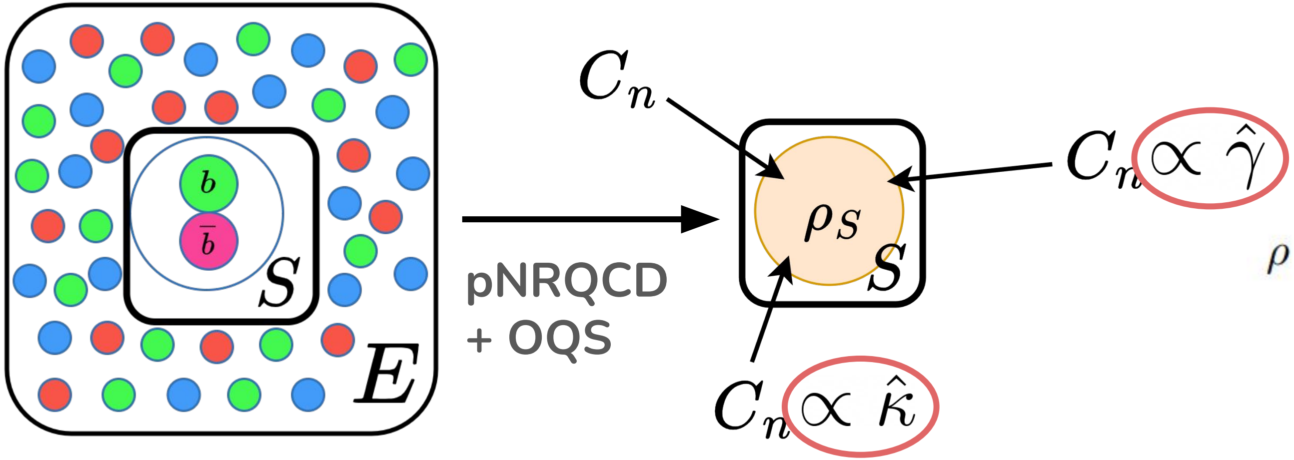
$$\rho = \begin{pmatrix} \rho_s^0 & 0 & \dots & 0 & 0 & \cdots \\ 0 & \rho_s^1 & \dots & 0 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \\ 0 & 0 & \dots & \rho_o^0 & 0 & \dots \\ 0 & 0 & \dots & 0 & \rho_o^1 & \dots \\ \vdots & \vdots & & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2}\left\{ C_n^\dagger C_n, \rho_S \right\} \right)$$

E.g. 40000×40000 matrix

Stochastic unraveling

Quarkonium Suppression Simulator



$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_l \otimes \mathcal{H}_r$$

$$\rho = \begin{pmatrix} \rho_s^0 & 0 & \dots & 0 & 0 & \cdots \\ 0 & \rho_s^1 & \dots & 0 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \\ 0 & 0 & \dots & \rho_o^0 & 0 & \dots \\ 0 & 0 & \dots & 0 & \rho_o^1 & \dots \\ \vdots & \vdots & & \vdots & \vdots & \ddots \end{pmatrix}$$

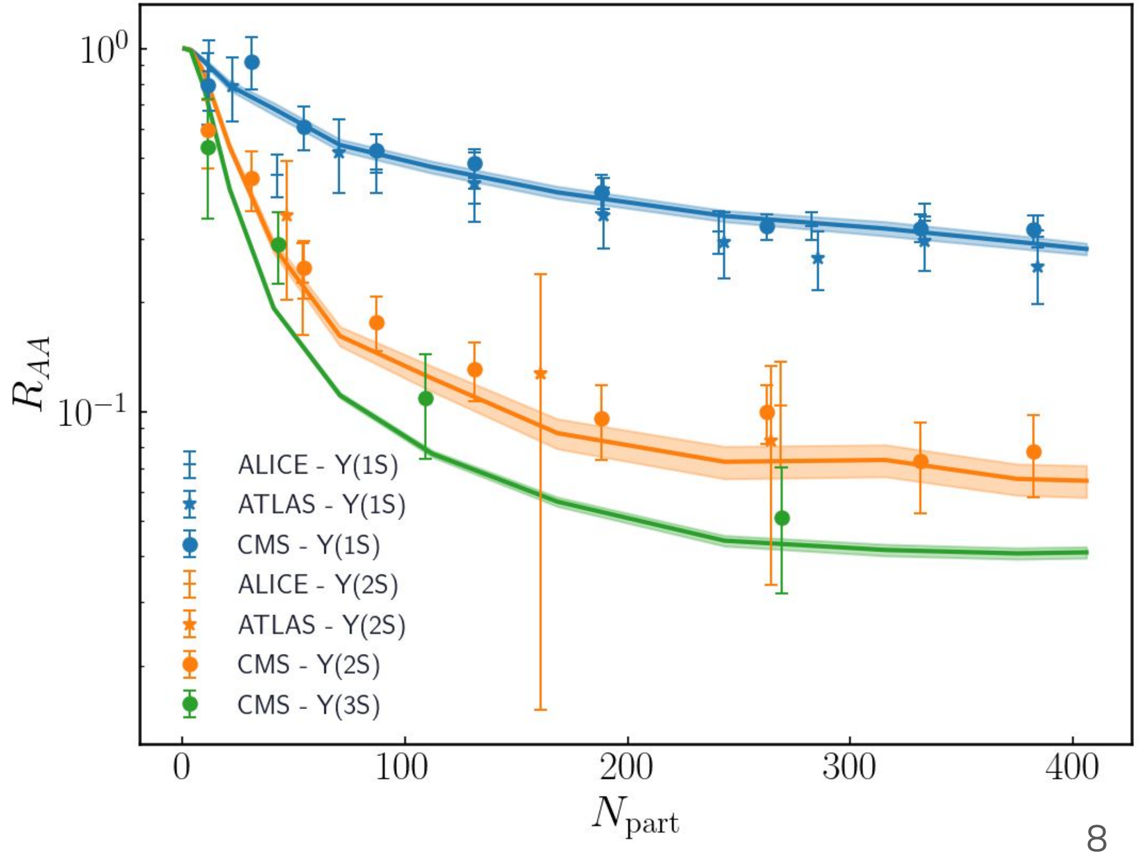
$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2}\left\{C_n^\dagger C_n, \rho_S\right\}\right)$$

E.g. 40000×40000 matrix

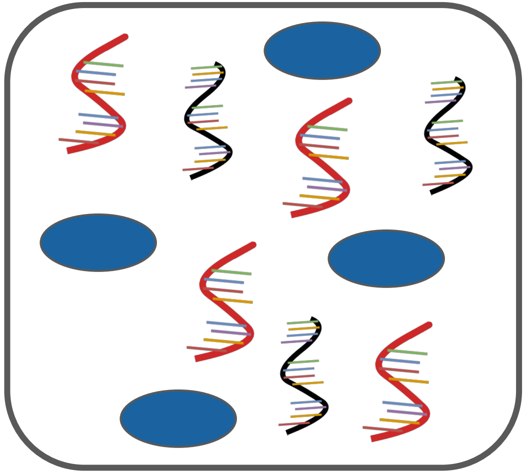
Stochastic unraveling

Nuclear modification factor

$$\langle 1S|\rho(t_{\max})|1S\rangle$$



Stochastic simulation in Biophysics:



 RNA A

 RNA B

 Enzyme E

Reactions:

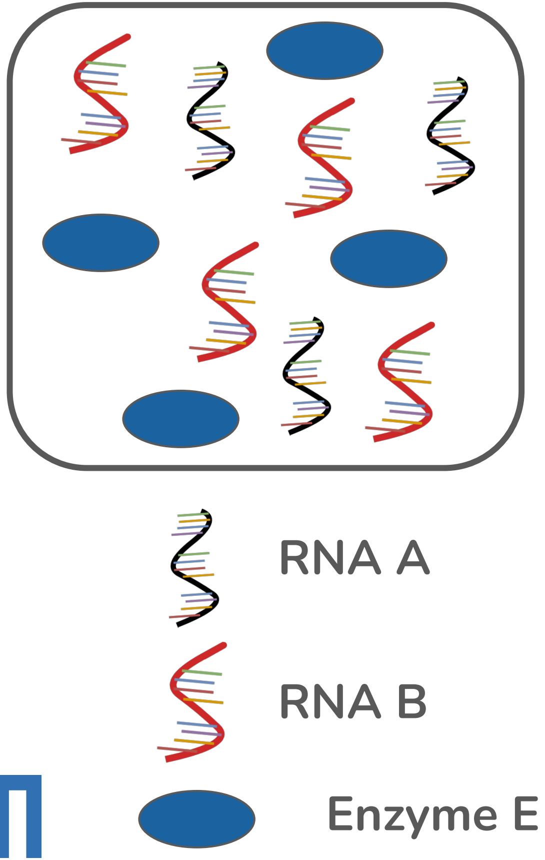
$$A + E \xrightarrow{k_{\mathrm{on},A}} AE$$

$$AE \xrightarrow{k_{\mathrm{rep},AE}} A + B + E$$

$$B + E \xrightarrow{k_{\mathrm{on},B}} BE$$

$$BE \xrightarrow{k_{\mathrm{rep},BE}} A + B + E$$

Stochastic simulation in Biophysics:



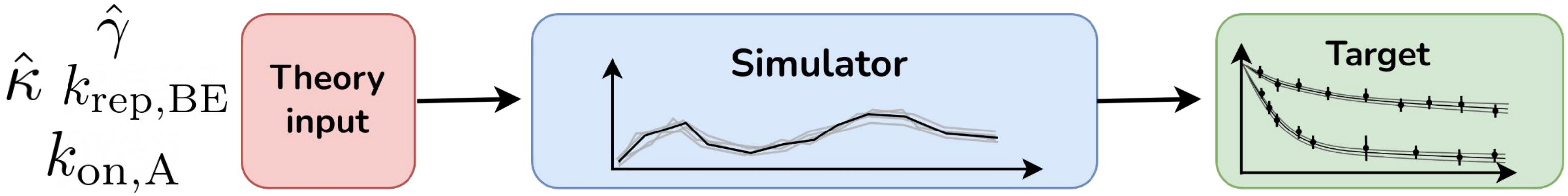
Reactions:

$$A + E \xrightarrow{k_{\mathrm{on},A}} AE$$

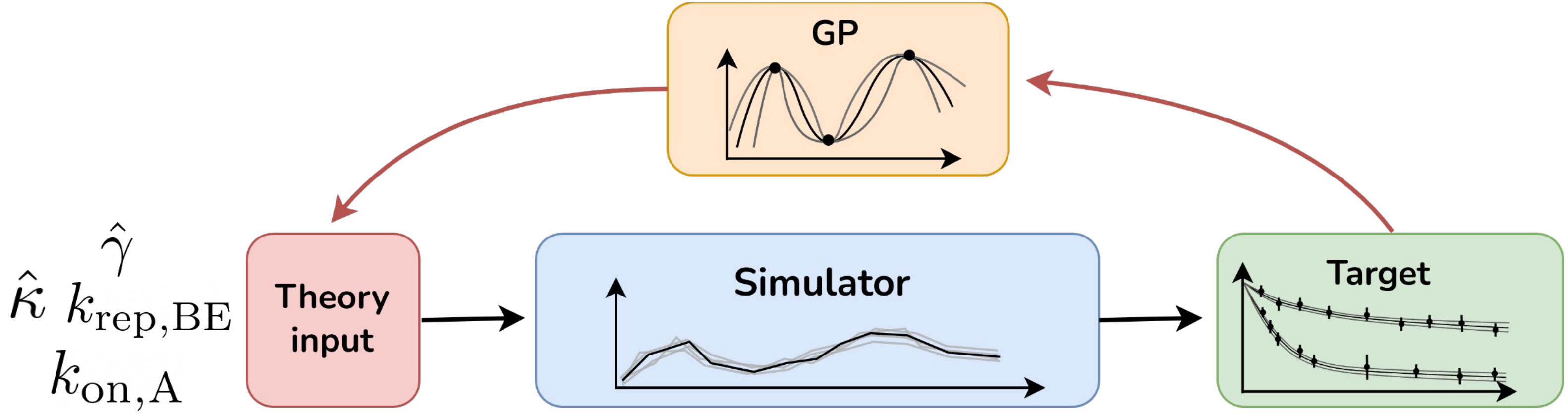
$$AE \xrightarrow{k_{\mathrm{rep},AE}} A + B + E$$

$$B + E \xrightarrow{k_{\mathrm{on},B}} BE$$

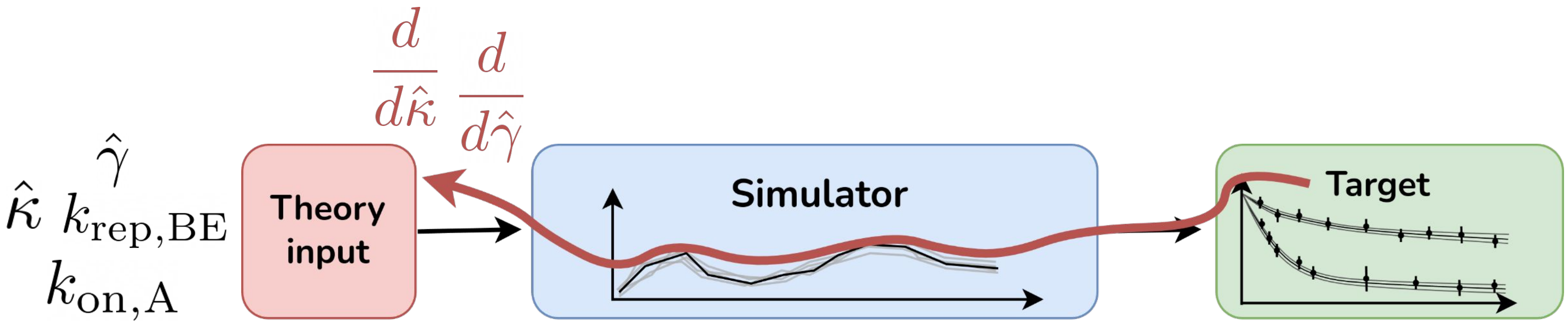
$$BE \xrightarrow{k_{\mathrm{rep},BE}} A + B + E$$


$\hat{\gamma}$
$\hat{\kappa}$ $k_{\mathrm{rep,BE}}$
$k_{\mathrm{on,A}}$
Theory input
Simulator
Target

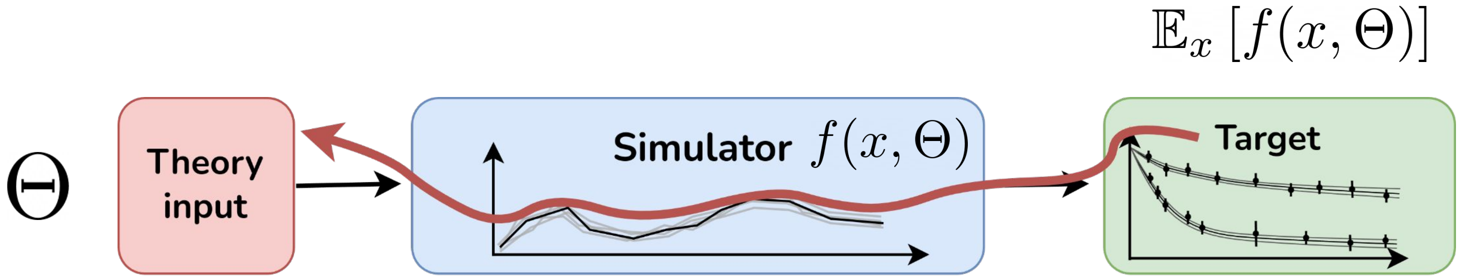
Bayesian optimization



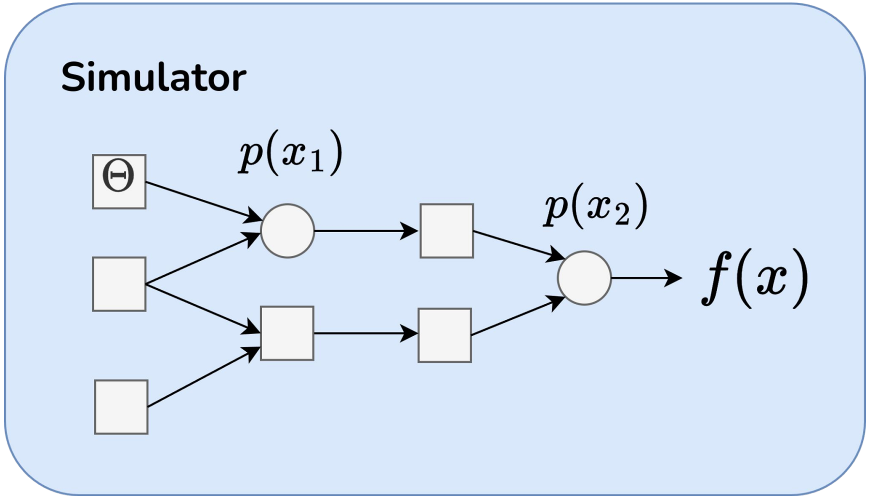
Gradient based optimization

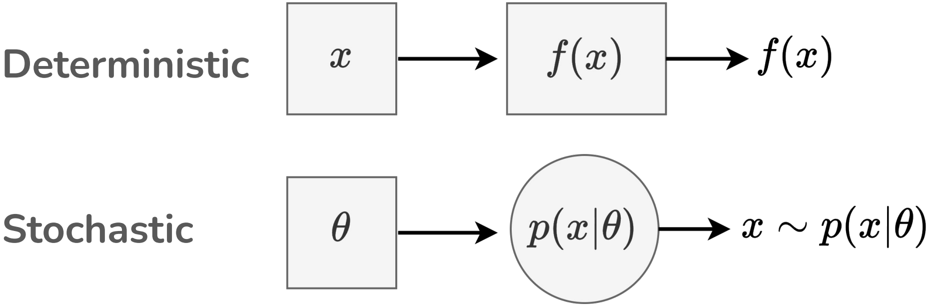


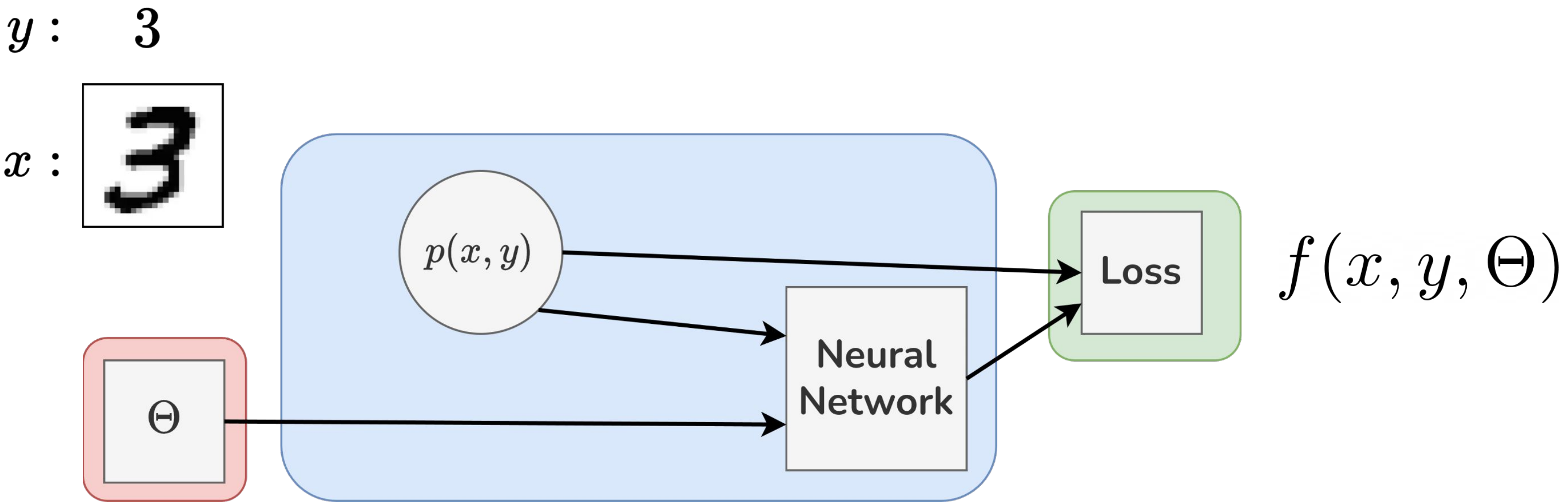
Stochastic simulator



$$\nabla_\Theta \mathbb{E}_x\left[f(x,\Theta)\right]$$

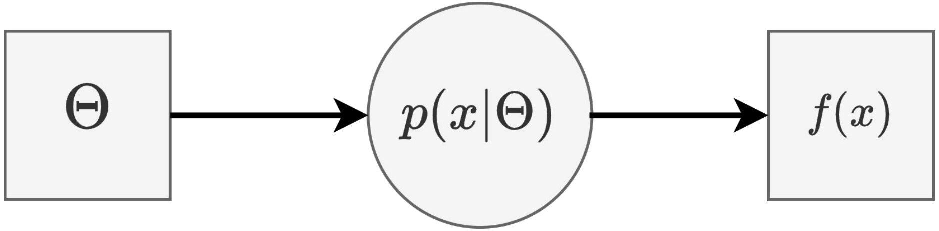

Simulator
Θ
$p(x_1)$
$p(x_2)$
$f(x)$


Deterministic
x
$f(x)$
$f(x)$
Stochastic
θ
$p(x|\theta)$
$x \sim p(x|\theta)$

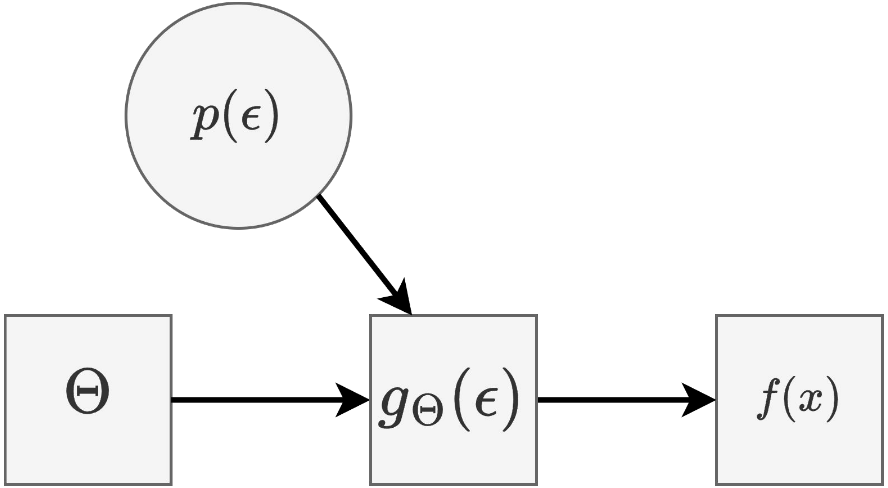


$$\nabla_\Theta \mathbb{E}_{p(x,y)}[f(x,y,\Theta)] = \mathbb{E}_{p(x,y)}[\nabla_\Theta f(x,y,\Theta)]$$

Stochastic gradient



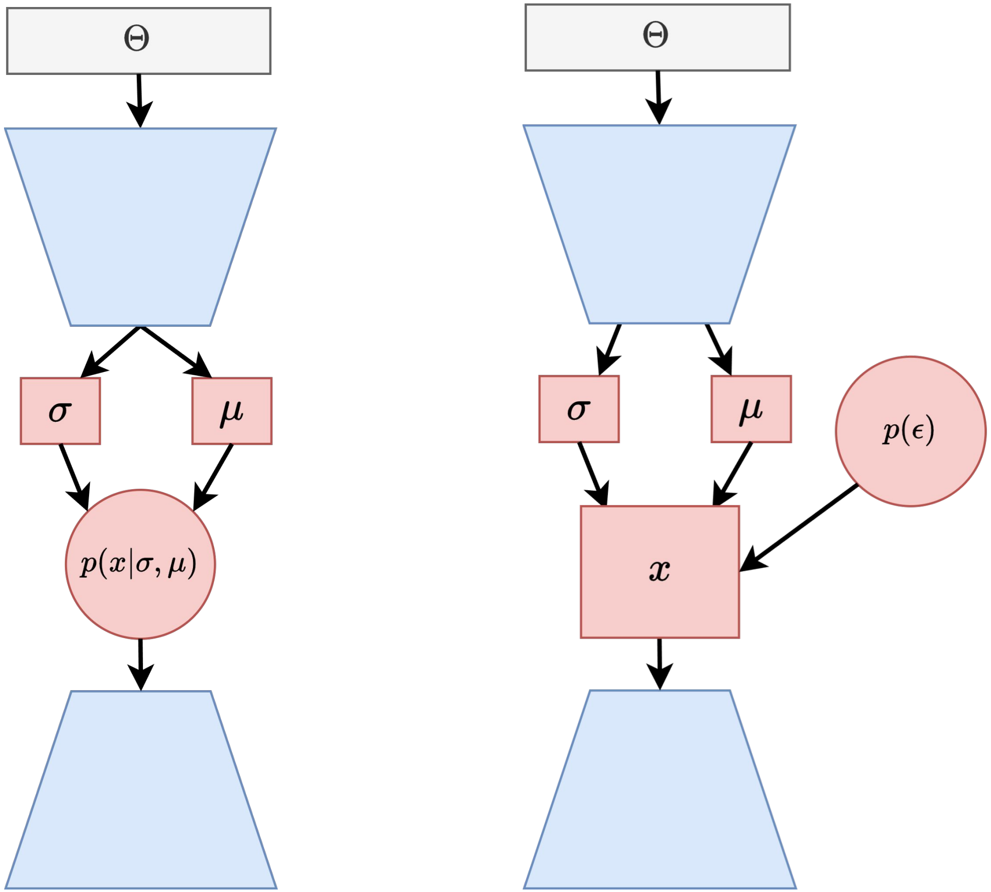
$$\nabla_\Theta \mathbb{E}_{p(x|\Theta)}[f(x)]$$



$$x = g_\Theta(\epsilon)$$
$$\epsilon \sim p(\epsilon)$$

$$\nabla_\Theta \mathbb{E}_{p(x|\Theta)}[f(x)]$$
$$= \nabla_\Theta \mathbb{E}_{p(\epsilon)}[f(g_\Theta(\epsilon))]$$
$$= \mathbb{E}_{p(\epsilon)}[\nabla_\Theta f(g_\Theta(\epsilon))]$$

VAE



Discrete distributions are not reparametrizable

$$\pi(x|s,\Theta)$$

$$x = \{\rightarrow \downarrow \leftarrow \uparrow \text{A} \; \text{B}\}$$

https://en.wikipedia.org/wiki/File:NES_Super_Mario_Bros.png

REINFORCE gradient estimator

$$\frac{d}{d\Theta} E_{x \sim p(x|\Theta)} [f(x, \Theta)]$$

$$= \int dx \frac{d}{d\Theta} [p(x|\Theta) f(x, \Theta)]$$

$$= \int dx \, p(x|\Theta) \left[\frac{d \log(p(x|\Theta))}{d\Theta} f(x, \Theta) + \frac{d}{d\Theta} f(x, \Theta) \right]$$

$$\boxed{= E_{x \sim p(x|\Theta)} \left[\frac{d \log(p(x|\Theta))}{d\Theta} f(x, \Theta) + \frac{d}{d\Theta} f(x, \Theta) \right]}$$

Gradient Estimation Using Stochastic Computation Graphs

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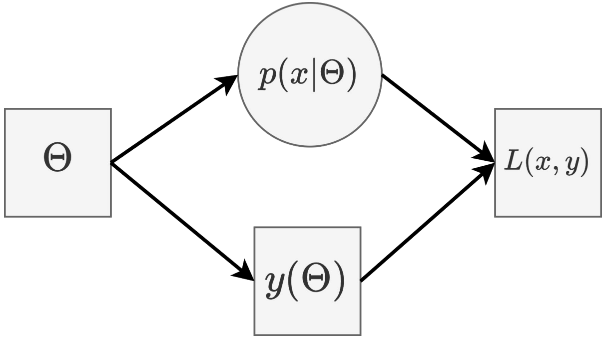
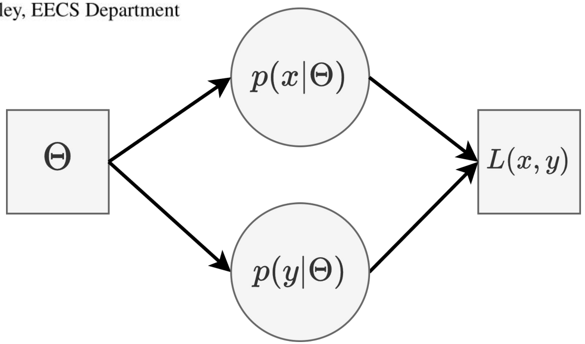
Theophane Weber[1] theophane@google.com

Pieter Abbeel[2] pabbeel@eecs.berkeley.edu

[1] Google DeepMind [2] University of California, Berkeley, EECS Department





$$\frac{\partial}{\partial\Theta}\mathbb{E}_x[L(x,y)]$$

$$= \mathbb{E}_x\left[\frac{\partial}{\partial\Theta}\log p(x|\Theta)L(x,y) + \frac{\partial L}{\partial y}\frac{\partial y}{\partial\Theta}\right]$$

$$\frac{\partial}{\partial\Theta}\mathbb{E}_{x,y}[L(x,y)]$$

$$= \mathbb{E}_{x,y}\left[\left(\frac{\partial}{\partial\Theta}\log p(x|\Theta) + \frac{\partial}{\partial\Theta}\log p(y|\Theta)\right)L(x,y)\right]$$

Stochastic unraveling

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2} \{C_n^\dagger C_n, \rho_S\} \right)$$

- **Stochastic** evolution of states $|\psi(t)\rangle$
- Full solution as **expectation** over sampled trajectories:

$$\rho(t) = \mathbb{E}\left[|\psi(t)\rangle\langle\psi(t)|\right]$$

Stochastic unraveling

e.g.: $U = 1 - iH_{\text{eff}}\delta t$

ψ_0

1. Evolve state $|\psi(t)\rangle$ with $H_{\text{eff}} = H - \frac{i}{2}C^\dagger C$

$$|\psi'(t+\delta t)\rangle = U|\psi(t)\rangle$$

2. Compute norm

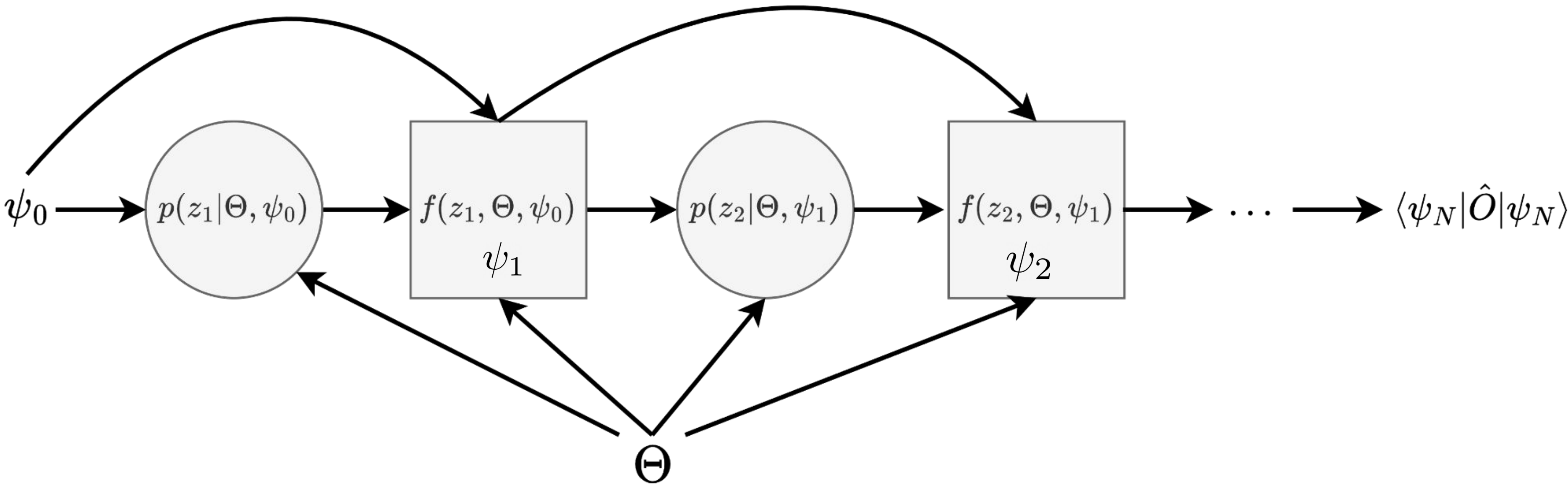
$$\langle\psi'(t+\delta t)|\psi'(t+\delta t)\rangle = 1 - \delta p < 1$$

3. Apply jump operator C with probability δp

$$P\left(|\psi(t+\delta t)\rangle = C|\psi(t)\rangle\right) = \delta p$$

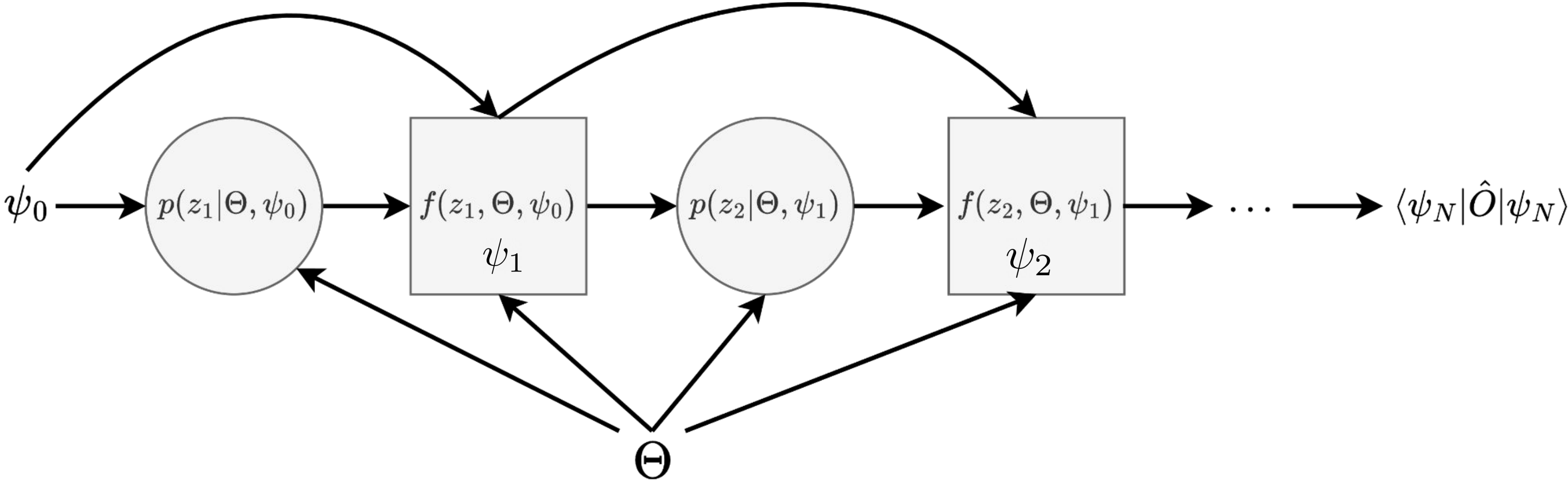
$$P\left(|\psi(t+\delta t)\rangle = |\psi'(t+\delta t)\rangle\right) = 1 - \delta p$$

4. Normalize $|\psi(t+\delta t)\rangle$



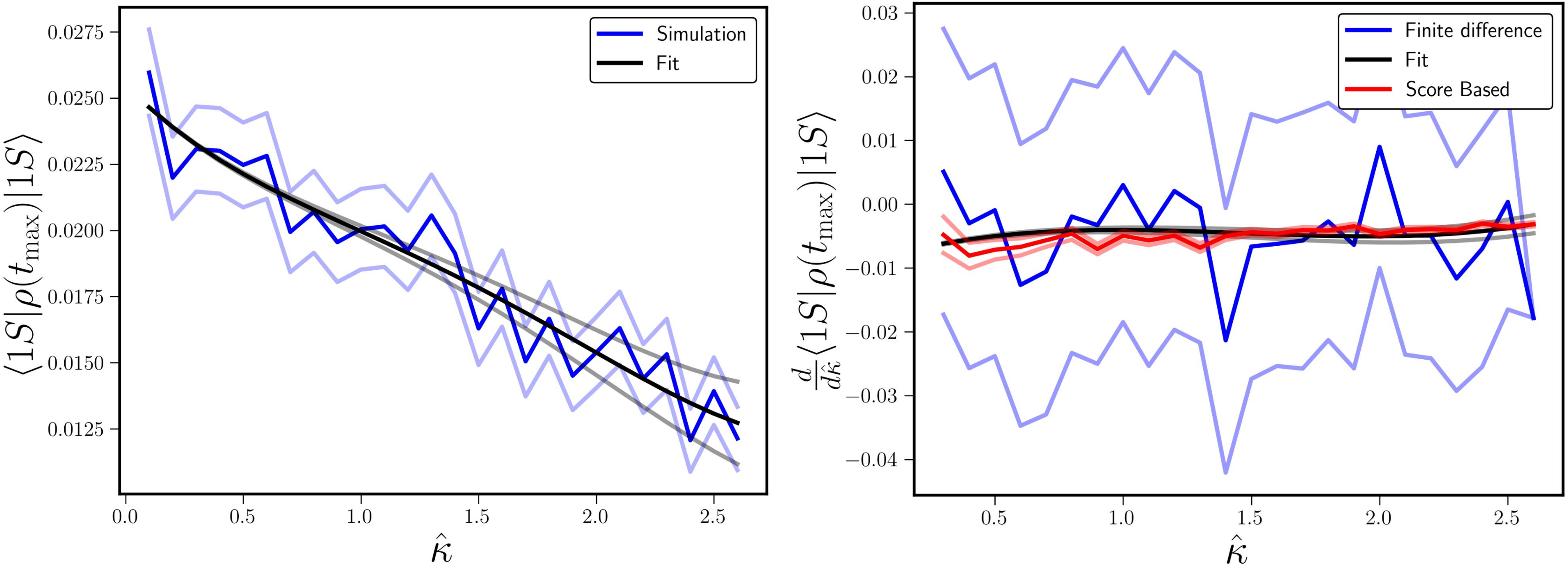
$$p(z|\Theta, \psi_{n-1}) = \begin{cases} 1 - \delta p(\Theta, \psi_{n-1}) & , z = 1 \\ \delta p(\Theta, \psi_{n-1}) & , z = 0 \end{cases}$$

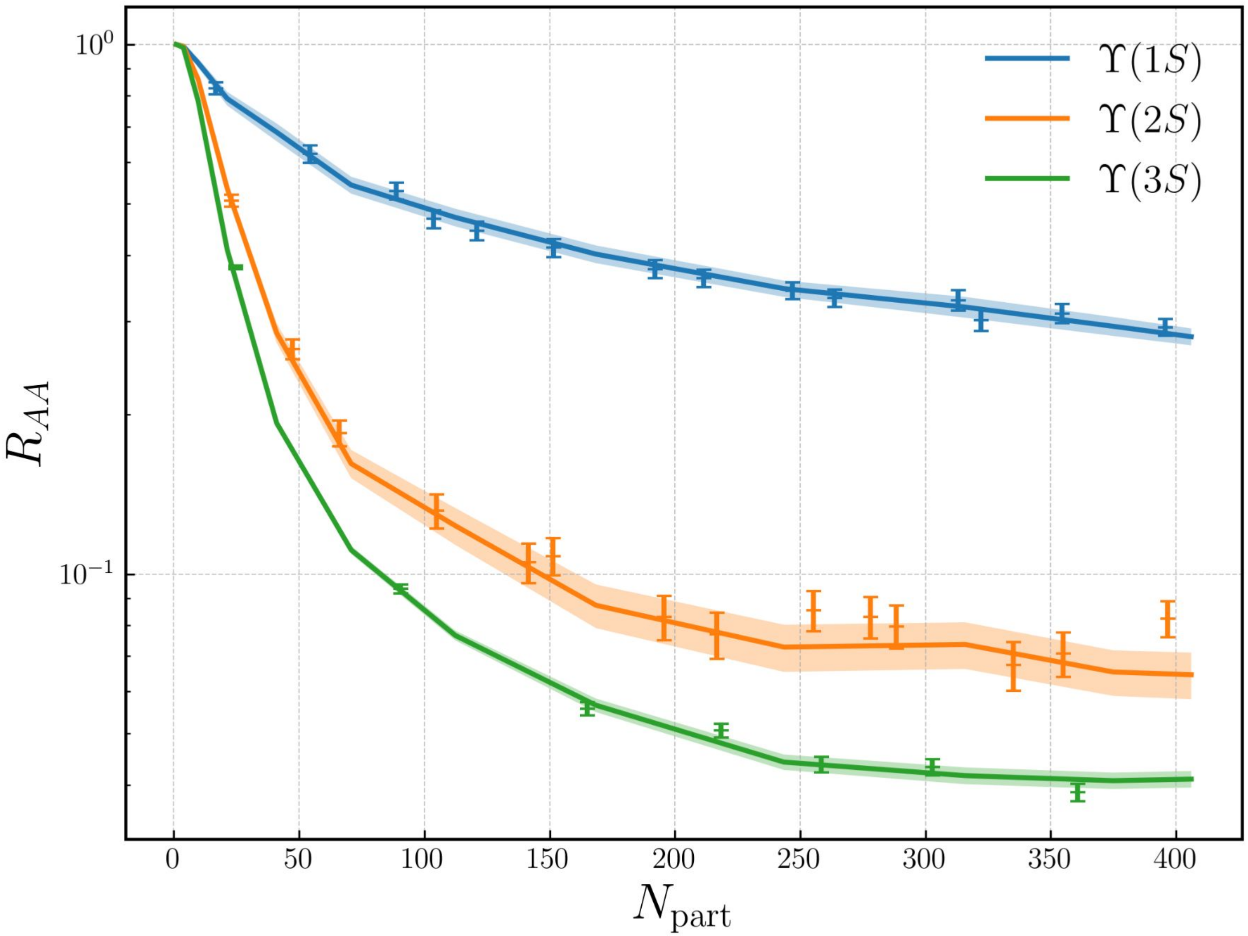
$$f(z, \Theta, \psi_n) = z \frac{U(\Theta)|\psi_n\rangle}{||U(\Theta)|\psi_n\rangle||} + (1 - z) \frac{C(\Theta)|\psi\rangle}{||C(\Theta)|\psi\rangle||}$$



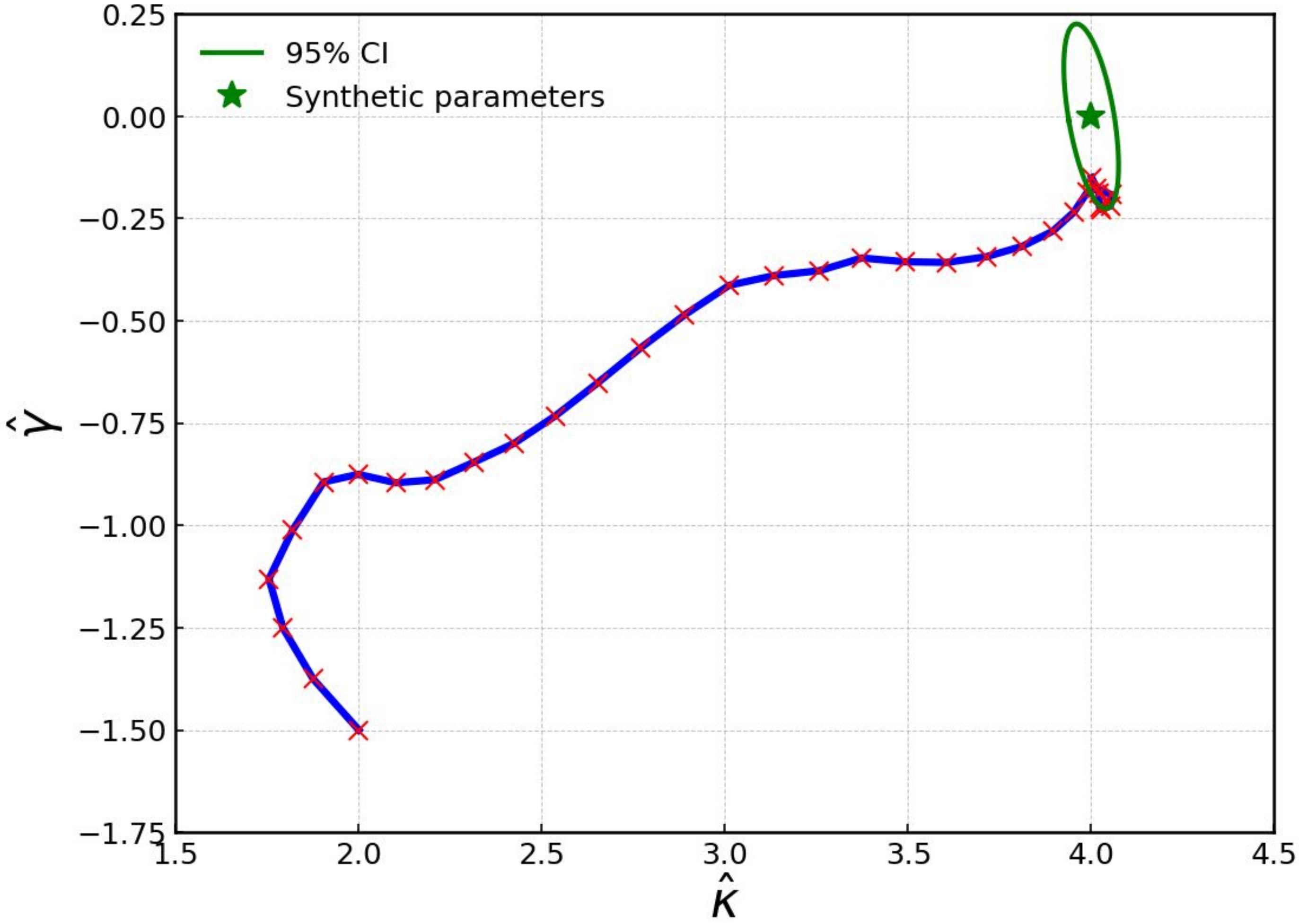
$$\nabla_\Theta \mathbb{E}_{\prod_n p(z_n|\Theta,\psi_{n-1})}\left[\langle\psi_N|\hat{O}|\psi_N\rangle\right]$$

$$= \mathbb{E}_{\prod_n p(z_n|\Theta,\psi_{n-1})}\left[\sum_n \frac{d\log p(z_n|\Theta,\psi_{n-1})}{d\Theta}\langle\psi_N|\hat{O}|\psi_N\rangle + \frac{d}{d\Theta}\langle\psi_N|\hat{O}|\psi_N\rangle\right]$$


Simulation
Fit
$\langle 1S|\rho(t_{\max})|1S\rangle$
$\hat{\kappa}$
Finite difference
Fit
Score Based
$\frac{d}{d\hat{\kappa}}\langle 1S|\rho(t_{\max})|1S\rangle$
$\hat{\kappa}$



$$\hat{\kappa} = 4$$
$$\hat{\gamma} = 0$$

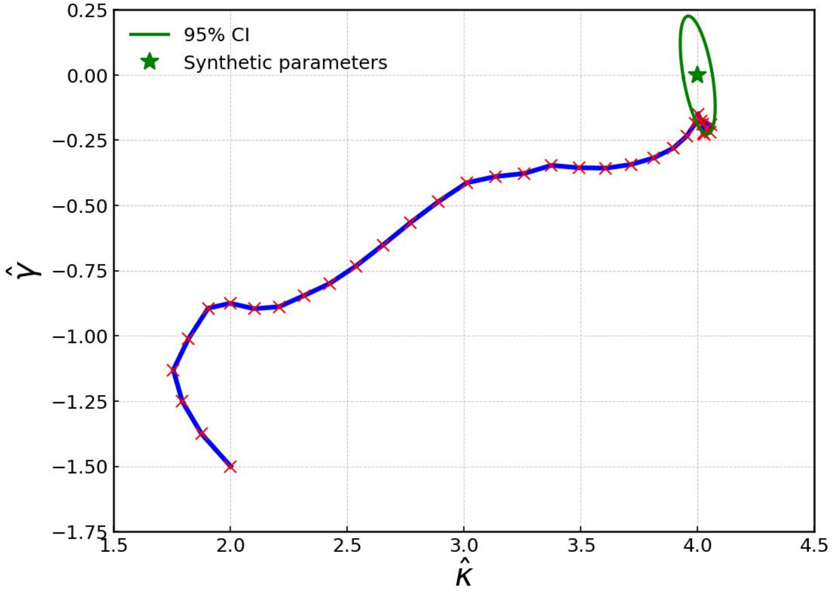


$$\hat{\kappa} = 4.01$$
$$\hat{\gamma} = -0.16$$

Summary & Outlook

- REINFORCE for stochastic gradients of MC simulators
- Gradient descent works with small number of samples

- Potentially design optimizer for reducing required samples
- Apply to more transport coefficients in Quarkonium Suppression



Backup

Gillespie Algorithm

N_i Number of Molecules of type i

1. Randomly draw time t ***when*** the next reaction will happen: depends on $\sum_i k_i N_i$
2. Randomly draw which reaction will happen: depends on $k_i N_i$
3. Adjust N_i

Variance reduction

$$\boxed{E_{x\sim p(x|\Theta)}\left[\frac{d\log(p(x|\Theta)}{d\Theta}f(x,\Theta) - h(x) + \frac{d}{d\Theta}f(x,\Theta)\right]}$$

Unbiased if: $E_{x\sim p(x|\Theta)}\left[h(x)\right] = 0$

Variance changes: $\mathrm{Var}(g(x) - h(x)) = \mathrm{Var}(g) + \mathrm{Var}(h) - 2\mathrm{Cov}(g,h)$

$$E_{x\sim p(x|\Theta)}\left[\frac{d\log(p(x|\Theta))}{d\Theta}\right] = 0$$

$$E\left[\frac{d\log(p(x|\Theta))}{d\Theta}f(x,\Theta)\right] = E\left[\frac{d\log(p(x|\Theta))}{d\Theta}(f(x,\Theta) - b(\Theta))\right]$$