Introduction	MLMC	BIP	SMC	MLSMC	<b>Other</b> 00000000	Summary

### **Multilevel sequential Monte Carlo methods**

### Kody Law



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- 2 Multilevel Monte Carlo sampling
- 3 Bayesian inference problem
- 4 Sequential Monte Carlo samplers
- 5 Multilevel Sequential Monte Carlo (MLSMC) samplers
- Other MLMC algorithms for inference
  - Importance sampling (IS) strategy
  - Coupled algorithm (CA) strategy
  - Approximate coupling (AC) strategy





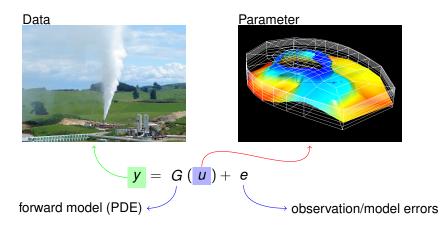
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 $y \in \mathbb{R}^M$ Data y may be limited in number, noisy, and indirect. $u \in E$ Parameter u often a function, discretized. $G: E \to \mathbb{R}^M$ Needs to be **approximated**.



Goal of Bayesian inference: given observed data y, find the posterior distribution

$$\mathbb{P}(du|y) = rac{\mathbb{P}(y|u)\mathbb{P}_0(du)}{\int_{E}\mathbb{P}(y|u)\mathbb{P}_0(du)},$$

and estimate *quantities of interest*, such as, for  $g: E \rightarrow \mathbb{R}$ ,

- expected value,  $\int_E g(u)\mathbb{P}(du|y)$ ;
- variance,  $\int_E g(u)^2 \mathbb{P}(du|y) (\int_E g(u)\mathbb{P}(du|y))^2$ ;
- probability of exceeding some value  $\int_{\{u \in E; g(u) > R\}} \mathbb{P}(du|y)$ .

There exists a connection with a classical inverse problems: identify most probable value,  $\sup_{u \in E} \lim_{\delta \to 0} \frac{\mathbb{P}(B_{\delta}(u)|y)}{\mathbb{P}(B_{\delta}(v)|y)}$ .

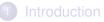


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Orientati	on					

Aim: Approximate expectations with respect to a probability distribution  $\eta_{\infty}$ , which needs to be approximated by some  $\eta_L$ , and can only be evaluated up to a normalizing constant. Solution: The multilevel Monte Carlo (MLMC) framework is extended to Sequential Monte Carlo (SMC) samplers, yielding the MLSMC sampler for Bayesian inference problems (and several other MC methods).

- MLMC methods *reduce cost to* error= O(ε), can be used in the case that η<sub>L</sub> can be sampled from directly [G08].
- Here it is assumed that η<sub>L</sub> cannot be sampled from directly, but can be evaluated up to a normalizing constant (e.g. Bayesian inference problems).
- SMC samplers are a general class of algorithms which are effective for sampling from such distributions [DDJ06,C02].

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Estimation of expectation of solution of intractable stochastic differential equation (SDE).

$$dX = f(X)dt + \sigma(X)dW, \quad X_0 = x_0.$$

- Aim: estimate  $\mathbb{E}(g(X_T))$ . We need to
- (1) Approximate, e.g. by Euler-Maruyama method with resolution *h*:

$$X_{n+1} = X_n + hf(X_n) + \sqrt{h}\sigma(X_n)\xi_n, \quad \xi_n \sim N(0,1).$$

(2) Sample  $\{X_{N_T}^{(i)}\}_{i=1}^N, N_T = T/h.$ 



Aim: Approximate  $\eta_\infty(g):=\mathbb{E}_{\eta_\infty}(g)$  for  $g:E o\mathbb{R}.$ 

Monte Carlo approach

- Discretize the space  $\Rightarrow$  *approximate* distribution  $\eta_L$ .
- Sample  $U_L^{(i)} \sim \eta_L$  i.i.d., and approximate

$$\eta_L(g) := \mathbb{E}_{\eta_L}(g) pprox \widehat{Y}_L^{N_L} := rac{1}{N_L} \sum_{i=1}^{N_L} g(U_L^{(i)}).$$

• Mean square error (MSE)  $\mathbb{E}\{\widehat{Y}_{L}^{N_{L}} - \mathbb{E}_{\eta_{\infty}}[g(U)]\}^{2}$  splits into

$$\underbrace{\mathbb{E}\{\widehat{Y}_{L}^{N_{L}} - \mathbb{E}_{\eta_{L}}[g(U)]\}^{2}}_{\text{variance} = \mathcal{O}(N_{L}^{-1})} + \{\underbrace{\mathbb{E}_{\eta_{L}}[g(U)] - \mathbb{E}_{\eta_{\infty}}[g(U)]}_{\text{bias}}\}^{2}$$

• Cost to achieve MSE =  $\mathcal{O}(\varepsilon^2)$  is Cost $(U_{L_0}^{(i)}) \times \varepsilon^{-2}$ .





Introduce a hierarchy of discretization levels  $\{\eta_l\}_{l=1}^L$  and define  $Y_l = \{\mathbb{E}_{\eta_l}[g(U)] - \mathbb{E}_{\eta_{l-1}}[g(U)]\}$ , with  $\eta_{-1} := 0$ . Observe the telescopic sum

$$\mathbb{E}_{\eta_L}[g(U)] = \sum_{l=0}^L Y_l.$$

Each term can be unbiasedly approximated by

$$Y_{l}^{N_{l}} = \frac{1}{N_{l}} \sum_{i=1}^{N_{l}} \{g(U_{l}^{(i)}) - g(U_{l-1}^{(i)})\}$$

where  $g(U_{-1}^{(i)}) := 0$ .



Multilevel Monte Carlo approach:

• Sample i.i.d. 
$$(U_l, U_{l-1})^{(i)} \sim \overline{\eta}^l$$
, such that  $\int \overline{\eta}^l du_{l-1,l} = \eta_{l,l-1}$ , and approximate  $\eta_L(g) \approx \widehat{Y}_{L,\text{Multi}} := \sum_{l=0}^L Y_l^{N_l}$ .

Mean square error (MSE) given by

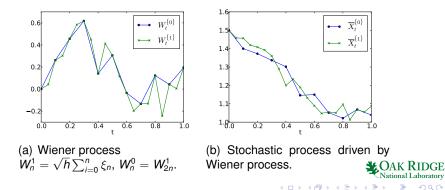
$$\begin{split} \mathbb{E}\{\widehat{Y}_{L,\mathrm{Multi}} - \mathbb{E}_{\eta_{\infty}}[g(U)]\}^2 &= \\ \underbrace{\mathbb{E}\{\widehat{Y}_{L,\mathrm{Multi}} - \mathbb{E}_{\eta_L}[g(U)]\}^2}_{\mathrm{variance} = \sum_{l=0}^{L} V_l/N_l} + \{\underbrace{\mathbb{E}_{\eta_L}[g(U)] - \mathbb{E}_{\eta_{\infty}}[g(U)]}_{\mathrm{bias}}\}^2 \ . \end{split}$$

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• Fix bias by choosing *L*. Minimize cost  $C = \sum_{l=0}^{L} C_l N_l$  as a function of  $\{N_l\}_{l=0}^{L}$  for fixed variance  $\Rightarrow N_l \propto \sqrt{V_l/C_l}$ .

Pairwise coupling of trajectories of an SDE:

$$\begin{aligned} X_{n+1}^{1} &= X_{n}^{1} + hf(X_{n}^{1}) + \sqrt{h}\sigma(X_{n}^{1})\xi_{n}, \quad \xi_{n} \sim N(0,1), \quad n = 0, \dots, N_{1} \\ X_{n+1}^{0} &= X_{n}^{0} + (2h)f(X_{n}^{0}) + \sqrt{2h}\sigma(X_{n}^{0})(\xi_{2n} + \xi_{2n+1}), \quad n = 0, \dots, (N_{1} - 1)/2 \end{aligned}$$



#### Introduction MLMC MLSMC Other Summary Multilevel vs. Single level

Assume  $h_l = 2^{-l}$  and there are  $\alpha$ , and  $\beta > \zeta$  such that

- (i) weak error  $|\mathbb{E}[q(U_l) q(U)]| = \mathcal{O}(h_l^{\alpha})$ .
- (ii) strong error  $\mathbb{E}|g(U_l) g(U)|^2 = \mathcal{O}(h_l^\beta) \Rightarrow V_l = \mathcal{O}(h_l^\beta)$ ,
- (iii) computational cost for a realization of  $g(U_l) g(U_{l-1})$ ,  $C_l \propto h_l^{-\zeta}$ .

Both cases require  $h_{L}^{\alpha} = \mathcal{O}(\varepsilon) \Rightarrow L \propto |\log \varepsilon|$ .

- Single level cost  $C = O(e^{-\zeta/\alpha-2})$ : cost per sample is  $C_{I} \propto \varepsilon^{-\zeta/\alpha}$ , and fixed  $V \propto \varepsilon^{2} \Rightarrow N_{I} \propto \varepsilon^{-2}$ .
- Multilevel cost  $C_{\rm ML} = \mathcal{O}(\varepsilon^{-2})$ :  $N_l \propto \varepsilon^{-2} K_l h_l^{(\beta+\zeta)/2}$ , so  $V \propto \varepsilon^2$  and  $C \propto \varepsilon^{-2} K_l^2$  for  $K_L = \sum_{l=0}^L h_l^{(\beta-\zeta)/2} = \mathcal{O}(1)$ [G08] – cost of simulating a scalar random variable.
- Example: Milstein solution of SDE

$$C = \mathcal{O}(\varepsilon^{-3})$$
 vs.  $C_{\mathrm{ML}} = \mathcal{O}(\varepsilon^{-2})$ .

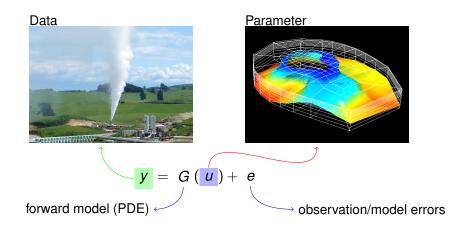
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Let  $V := H^1(\Omega) \subset L^2(\Omega) \subset H^{-1}(\Omega) =: V^*, \Omega \subset \mathbb{R}^d$  with  $\partial \Omega$  convex, and  $f \in V^*$ . Consider

$$-\nabla \cdot (\widehat{\boldsymbol{u}} \nabla \boldsymbol{p}) = \boldsymbol{f}, \quad \text{on } \Omega$$
$$\boldsymbol{p} = \boldsymbol{0}, \quad \text{on } \partial \Omega,$$

where

$$\widehat{u}(x) = \overline{u}(x) + \sum_{k=1}^{K} u_k \sigma_k \Phi_k(x)$$
.

Define  $u = \{u_k\}_{k=1}^{K} \in E := \prod_{k=1}^{K} [-1, 1]$ , with  $u_k \sim U[-1, 1]$ i.i.d. This determines the prior distribution for u. Assume  $\bar{u}, \Phi_k \in C^{\infty}$ , and  $\|\Phi_k\|_{\infty} = 1$  for all k, and require

$$\inf_{x} \widehat{u}(x) \geq \inf_{x} \overline{u}(x) - \sum_{k=1}^{K} \sigma_{k} \geq u_{*} > 0.$$

Let  $p(\cdot; u)$  denote the weak solution for parameter value u, and define

$$\mathcal{G}(\boldsymbol{p}) = [g_1(\boldsymbol{p}), \cdots, g_M(\boldsymbol{p})]^\top$$

where  $g_m \in V^*$  for  $m = 1, \ldots, M$ .

DATA : 
$$y = \mathcal{G}(p(\cdot; u)) + e, \quad e \sim N(0, \Gamma), \quad e \perp u.$$

The *unnormalized* density of u|y over  $u \in E$  is given by

$$\kappa(u) = e^{-\Phi[\mathcal{G}(p(\cdot;u))]}; \quad \Phi(\mathcal{G}) = \frac{1}{2} |\mathcal{G} - y|_{\Gamma}^2.$$

TARGET: 
$$\eta(u) = \frac{\kappa(u)}{Z}, \quad Z = \int_E \kappa(u) du.$$



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Distributions  $\eta_l$  dictated by an accuracy parameter  $h_l$  (here FEM mesh diameter)  $\infty > h_0 > h_1 \dots > h_\infty = 0$ . Approximate  $\mathbb{E}_{\eta_L}[g(U)] = \eta_L(g) = \int_E g(u)\eta_L(u)du$ .

Idea: interlace sequential importance resampling (selection) along the hierarchy, and mutation by MCMC kernels.

- Initialize i.i.d.  $U_0^i \sim \eta_0, i = 1, ..., N$ . For  $I \in \{0, ..., L-1\}$ :
- Resample  $\{\widehat{U}_{l}^{i}\}_{i=1}^{N}$  according to the weights  $\{w_{l}^{i}\}_{i=1}^{N}$ ,  $w_{l}^{i} = G_{l}^{i} / \sum_{j=1}^{N} G_{l}^{j}$ ,  $G_{l}^{j} = (\kappa_{l+1} / \kappa_{l})(U_{l}^{i})$ .
- Draw  $U_{l+1}^i \sim M_{l+1}(\widehat{U}_l^i, \cdot)$ , where  $M_{l+1}$  is an MCMC kernel such that  $\eta_{l+1}M_{l+1} = \eta_{l+1}$ .

For  $g: E \to \mathbb{R}$ ,  $l \in \{0, \dots, L\}$ , we have the following estimators

$$\mathbb{E}_{\eta_l}[g(U)] pprox \eta_l^N(g) := rac{1}{N} \sum_{i=1}^N g(U_l^i) \;.$$

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Notice

$$egin{aligned} \mathbb{E}_{\eta_L}[g(U)] &= \mathbb{E}_{\eta_0}[g(U)] + \sum_{l=1}^L \left\{ \mathbb{E}_{\eta_l}[g(U)] - \mathbb{E}_{\eta_{l-1}}[g(U)] 
ight\} \ &= \mathbb{E}_{\eta_0}[g(U)] + \sum_{l=1}^L \mathbb{E}_{\eta_{l-1}}\Big[ \Big( rac{\kappa_l(U) Z_{l-1}}{\kappa_{l-1}(U) Z_l} - 1 \Big) g(U) \Big]. & \dagger \end{aligned}$$

Idea: Approximate † using SMC sample hierarchy.

Key: Subsample  $(U_0^{1:N_0}, \ldots, U_{L-1}^{1:N_{L-1}})$  as in single level SMC, but with  $+\infty > N_0 \ge N_1 \cdots \ge N_{L-1} \ge 1$  appropriately chosen.





The MLSMC consistent estimator of  $\eta_L(g)$  is given by

$$\widehat{Y} := \eta_0^{N_0}(g) + \sum_{l=1}^L \Big\{ rac{\eta_{l-1}^{N_{l-1}}(gG_{l-1})}{\eta_{l-1}^{N_{l-1}}(G_{l-1})} - \eta_{l-1}^{N_{l-1}}(g) \Big\}.$$

i) the *L* + 1 terms above are *not* unbiased estimates of  $\mathbb{E}_{\eta_l}[g(U)] - \mathbb{E}_{\eta_{l-1}}[g(U)]$ , so decompose MSE as:

$$egin{aligned} & \mathbb{E}ig[\{\widehat{Y}-\mathbb{E}_{\eta_{\infty}}[g(U)]\}^2ig] \leq \ & 2\,\mathbb{E}ig[\{\widehat{Y}-\mathbb{E}_{\eta_L}[g(U)]\}^2ig]+2\,\{\mathbb{E}_{\eta_L}[g(U)]-\mathbb{E}_{\eta_{\infty}}[g(U)]\}^2\,. \end{aligned}$$

ii) the same L + 1 estimates are *not* independent, so a more complex error analysis will be required to characterize  $\mathbb{E}[\{\widehat{Y} - \mathbb{E}_{\eta_L}[g(U)]\}^2].$ 

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(A1) There exist  $0 < \underline{C} < \overline{C} < +\infty$  such that

$$\sup_{1 \le l \le L} \sup_{u \in E} G_l(u) \le \overline{C},$$
  
$$\inf_{1 \le l \le L} \inf_{u \in E} G_l(u) \ge \underline{C}.$$

(A2) There exist a  $\rho \in (0, 1)$  such that for any  $1 \le p \le L - 1$ ,  $(u, v) \in E^2$ ,  $A \in \sigma(E)$ ,

$$\int_{\mathcal{A}} M_{\rho}(u, du') \geq \rho \int_{\mathcal{A}} M_{\rho}(v, du').$$

(A3) There is a  $\beta > 0$  such that

$$V_l := \|rac{Z_{l-1}}{Z_l} G_{l-1} - 1\|_\infty^2 = \mathcal{O}(h_l^eta) \; .$$



Introduction	MLMC	BIP	SMC	MLSMC	Other 000000000	Summary
Main res	sult					

#### Theorem (BJLTZ16 – Stoch. Proc. App.)

Assume (A1-3). For any  $g: E \to \mathbb{R}$  bounded

$$\mathbb{E}\left[\{\widehat{Y} - \mathbb{E}_{\eta_L}[g(U)]\}^2\right] = \frac{V}{2}$$

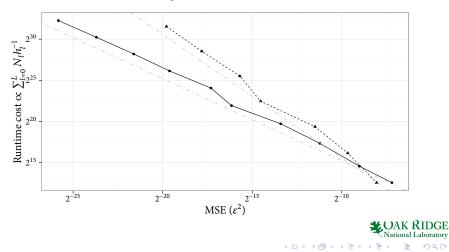
$$\lesssim \frac{1}{N_0} + \sum_{l=1}^{L} \left(\frac{V_l}{N_l} + \left(\frac{V_l}{N_l}\right)^{1/2} \sum_{q=l+1}^{L} \frac{V_q^{1/2}}{N_q}\right)$$

In particular, for  $\beta > \zeta$ , L and  $\{N_l\}_{l=0}^{L}$  can be chosen such that  $MSE = \mathcal{O}(\varepsilon^2)$  for computational cost=  $\mathcal{O}(\varepsilon^{-2})$ , the optimal case.





Algorithm - MLSMC - - SMC



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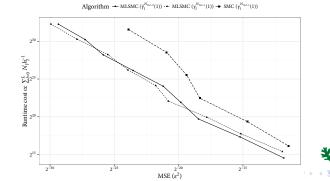
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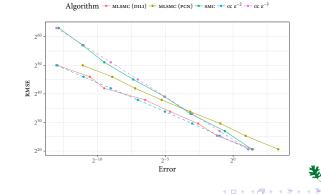


- In case g = 1, the original estimator does not make sense.
- Two *unbiased* estimators proposed which provide the optimal rate with a logarithmic penalty on the cost: MSE  $\mathcal{O}(\varepsilon^2)$  for cost  $\mathcal{O}(|\log \varepsilon|\varepsilon^{-2})$  [DJLZ16 Trans. Mod. Comp. Sim.] Here one can also construct estimators of Rhee&Glynn type.





- Posterior over function-space, levels include refinement in parameter and model 
   *η*<sub>l</sub>(u<sub>0:l</sub>).
- Covariance-based LIS (cLIS) introduced and incorporated in DILI proposals [CLM16, BJLMZ17] – substantial reduction in cost.



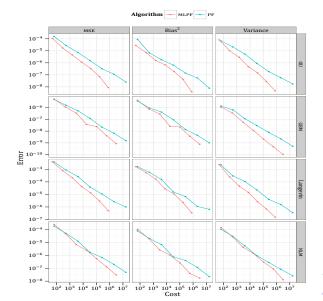
### (CA) ML particle filter (MLPF) for SDE

- Filtering involves a sequence of Bayesian inversions, separated by propagation in time (in this case through an SDE).
- Coupled traditional SMC algorithms (particle filters) can be used for each level.
- Mutation M<sup>ℓ</sup> is now coupled propagation of a pair of initial conditions through an SDE discretized at two successive mesh-refinements, for ℓ = 0,..., L.
- Selection is performed by novel pairwise coupled resampling which preserves marginals.
- MLMC results carry over with somewhat weaker rate  $\beta \rightarrow \beta/2$  [JKLZ15].

(a)



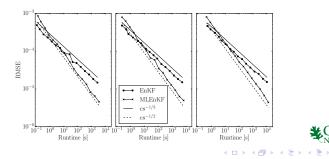
### (CA) MLPF numerical experiments





# Introduction MLMC BIP SMC MLSMC Other<br/>occoo Summary (CA) ML ensemble Kalman filter (MLEnKF) for SDE

- EnKF uses sample covariance from an ensemble of particles to approximate a linear Gaussian Bayesian update, given by an affine transformation of particles.
- Multilevel approximation of the covariance improves cost for MSE O(ε<sup>2</sup>) [HLT16].
  - Best theoretical bound (at step *n*):  $\mathcal{O}(|\log \varepsilon|^{2n} \varepsilon^{-2})$ .
  - Numerically (uniformly in *n*):  $\mathcal{O}(\varepsilon^{-2})$ .







- Aim: estimate E[φ(θ)|y], where y is a finite set of partial observations of the SDE X<sup>θ</sup><sub>t</sub> on [0, T], parameterized by θ.
- particle MCMC: Iterate
  - propose  $\theta' \sim q(\theta, \theta')$ ,
  - simulate  $\{X^{\theta',i}\}_{i=1}^{M} \approx \pi(X|\theta',y)$  with particle filter,
  - compute non-negative and unbiased estimator  $p^{M}(y|\theta') = \prod_{p=1}^{n} (\frac{1}{M} \sum_{i=1}^{M} g_{p}(X_{p}^{\theta',i})),$
  - accept/reject according to

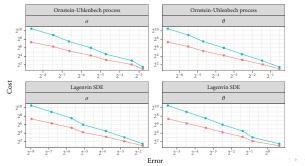
$$1 \wedge rac{ \pmb{p}^{\mathcal{M}}(\pmb{y}| heta') \pi( heta') \pmb{q}( heta', heta)}{ \pmb{p}^{\mathcal{M}}(\pmb{y}| heta) \pi( heta) \pmb{q}( heta, heta')}.$$





- MLMC version [JKLZ16]:
  - Construct approximate coupling π̃<sub>l,l-1</sub>(θ, X<sup>l</sup>, X<sup>l-1</sup>): usual coupled forward kernel, and coupled selection function G<sub>p,θ</sub>(X<sup>l</sup>, X<sup>l-1</sup>) = max{g<sub>p,θ</sub>(X<sup>l</sup>), g<sub>p,θ</sub>(X<sup>l-1</sup>)}.
     Let H<sub>l</sub>(θ, X<sup>l</sup>, X<sup>l-1</sup>) = Π<sup>n</sup><sub>p=1</sub> g<sub>p,θ</sub>(X<sup>l</sup>)/G<sub>p,θ</sub>(X<sup>l</sup>, X<sup>l-1</sup>). Then
  - $\begin{array}{l} \overset{\bullet}{=} \operatorname{Let} H_{l}(\theta, X, X) = \prod_{p=1} g_{p,\theta}(X) / \operatorname{G}_{p,\theta}(X, X). \text{ Then} \\ & \mathbb{E}_{\pi_{l}}[\varphi(\theta)] \mathbb{E}_{\pi_{l-1}}[\varphi(\theta)] = \\ & \frac{\mathbb{E}_{\pi_{l,l-1}}[\varphi(\theta)H_{l}(\theta, X', X^{l-1})]}{\mathbb{E}_{\pi_{l,l-1}}[H_{l}(\theta, X', X^{l-1})]} \frac{\mathbb{E}_{\pi_{l,l-1}}[\varphi(\theta^{l-1})H_{l-1}(\theta, X', X^{l-1})]}{\mathbb{E}_{\pi_{l,l-1}}[H_{l-1}(\theta, X', X^{l-1})]}. \end{array}$
- Optimal results hold with **same** rate as forward.

Algorithm - ML-PMCMC - PMCMC





 If spatio-temporal approximation dimension *d* > 1, then MIMC is preferable to MLMC [HNT15]. *α* ∈ N<sup>d</sup>

• 
$$\Delta_i \mathbb{E}_{\alpha}(\varphi(u)) = \mathbb{E}_{\alpha}(\varphi(u)) - \mathbb{E}_{\alpha - e_i}(\varphi(u)), \Delta = \Delta_d \cdots \Delta_1,$$

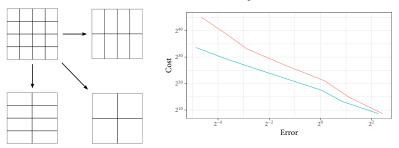
$$\mathbb{E}(arphi(u)) = \sum_{lpha} \Delta \mathbb{E}_{lpha}(arphi(u)) pprox \sum_{lpha \in \mathcal{I}} \Delta \mathbb{E}_{lpha}(arphi(u))$$

Approximate coupling can be applied to the 2<sup>d</sup> probability measures in each summand.



Introduction	MLMC	BIP	SMC	MLSMC	Other ○○○○○○○●	Summary

### • Optimal results hold for appropriate regularity [JKLZ17]



Algorithm — мсмс — мімсмс



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Summar	у					

- MLSMC sampler can perform as well as MLMC.
- For our example β > ζ. If β ≤ ζ, cost is somewhat higher, analogous to standard MLMC.
- If ζ > 2α then the optimal cost is ε<sup>-ζ/α</sup>, the cost of a single simulation at the finest level.
- New importance sampling: MLSMC with DILI mutations.
- Coupled algorithms: MLPF strong error is effectively reduced by coupled resampling  $\beta \rightarrow \beta/2$ .
- Coupled algorithms: MLEnKF has a spurious n-dependent logarithmic penalty | log ε|<sup>2n</sup> on cost.
- New approximate couplings: ML PMCMC for SDE parameter estimation preserves strong error β.
- New approximate couplings: MIMCMC can perform as well as MIMC; also for *d* = 1 new MLMCMC.
- We are keen to do more applications (on HPC) ! Looking for students/postdocs with similar interests.





- **[BJLTZ15]**: Beskos, Jasra, Law, Tempone, Zhou. "Multilevel Sequential Monte Carlo samplers." SPA 127:5, 1417–1440 (2017).
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### Thank you

