Random Blob Methods for Diffusion

ASU-UCSB Women in Math Research Minisymposium

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UC Santa Barbara, joint work with Dr. Katy Craig

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The Nonlinear Fokker-Planck Equation

Suppose that

- $v : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$,
- $f : [0, \infty) \to \mathbb{R} \cup \infty$ is l.s.c., coercive, convex, and $f(0) = 0$.

Consider the **nonlinear Fokker-Planck equation**

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This PDE conserves mass, and we assume it has total mass one. Important variants:

0. The Fokker-Planck equation: $f(s) = s \ln(s) - s \Rightarrow \partial_t \rho = \Delta \rho + \nabla \cdot (\rho v)$.

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2. Height-constrained transport [De Philippis et al., 2016; Alexander–Kim–Yao, 2014]:

$$f(s) = \begin{cases} 0 & 0 \leq s \leq 1 \\ \infty & \text{otherwise} \end{cases} \Rightarrow \text{“} \begin{cases} \partial_t \rho + \nabla \cdot (\rho v) = 0 \\ 0 \leq \rho \leq 1. \end{cases} \text{”}$$

Longtime Behavior

Setup: Assume $f : [0, \infty) \to \mathbb{R} \cup \infty$ is differentiable and $v = \nabla V$, where $V : \mathbb{R}^d \to \mathbb{R}$ is continuously differentiable and λ-convex for $\lambda > 0$.

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   1. $\rho(t, x) \to \rho_\infty(x) := Ze^{-V(x)}dx$. Z is a constant chosen s.t. $\int \rho_\infty = 1$.
   2. **PDE perspective:** [Ambrosio–Gigli–Savaré, 2008] If $\rho(t)$ is a solution to the **Fokker-Planck equation** with $v = \nabla V$, then

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2. Nonlinear Fokker-Planck equation
   1. $\rho(t, x) \to \rho_\infty(x) := \max((f')^{-1}(Z - V(x)), 0)$. Z is a constant chosen s.t. $\int \rho_\infty = 1$.
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The nonlinear Fokker-Planck equation is of interest in the sampling literature, as a candidate choice of dynamics to drive particle approximations to ρ_∞, which may be non-log-concave.

Blob Methods for the Nonlinear Fokker-Planck Equation

In recent years, blob methods have shown tremendous promise in simulating a wide range of PDEs [Burger–Esposito, 2023; Carrillo–Craig–Patacchini, 2018; Carrillo–Craig–Yao, 2019; Carrillo et al., 2024; Craig et al., 2023; Craig–Jacobs–Turanova, 2025]. The main challenge in the implementation of these methods is their **computational complexity**.

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Craig, Jacobs, and Turanova (2025) showed convergence of a variant of the **regularized** PDE

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If $\rho_0(x) = \sum_{i=1}^N m_i \delta_{x_i^0}$, then $\rho(t, x) = \sum_{i=1}^N m_i \delta_{x_i(t)}$, where each x_i moves according to the ODE system

$$\begin{cases} \dot{x}_i(t) = -f_\varepsilon'' \left(\sum_{j=1}^N m_j \varphi_\varepsilon(x_i(t) - x_j(t)) \right) \sum_{j=1}^N m_j \nabla \varphi_\varepsilon(x_i(t) - x_j(t)) - v(x_i(t)) \\ x_i(0) = x_i^0. \end{cases} \tag{1}$$

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Our goal is to improve the computational efficiency of blob methods.

Previous Work: The Random Batch Method

The RB method has been successfully used to solve ODE systems that model

1. Opinion dynamics [Pareschi–Zanella, 2024],
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At each time step, particles are split into random "batches" of size p. If I_i equals the index set of all particles in the same batch as particle i,

$$x_i^{m+1} = x_i^m + \Delta t \left(-f_\varepsilon'' \left(\sum_{j \in I_i} \tilde{m}_j \varphi_\varepsilon(x_i^m - x_j^m) \right) \sum_{j \in I_i} \tilde{m}_j \nabla \varphi_\varepsilon(x_i^m - x_j^m) - v(x_i^m) \right),$$

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	Complexity	Error for fixed N
FE	$O(N^2/\Delta t)$	$O(\Delta t)$
RB	$O(Np/\Delta t)$	$O(\sqrt{\Delta t/p})$

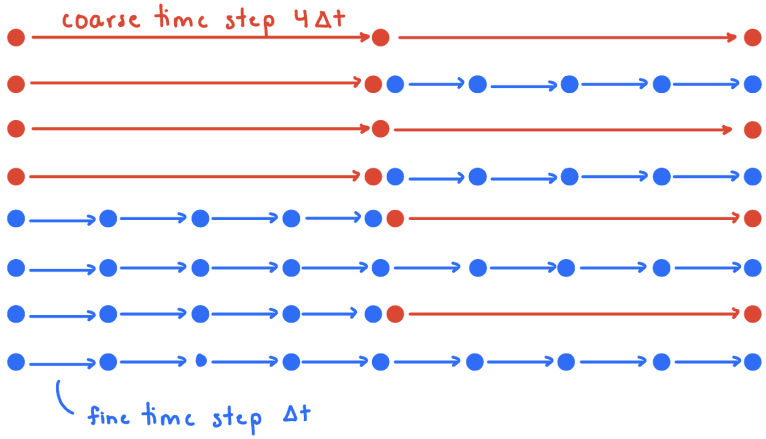
Table: Δt refers to the time step size, N refers to the number of particles, and p refers to the batch size.

As we will see, the random batch method is not well-suited to the ODE system (1).

Our Contribution: The Random Multirate Method

The Random Multirate Method:

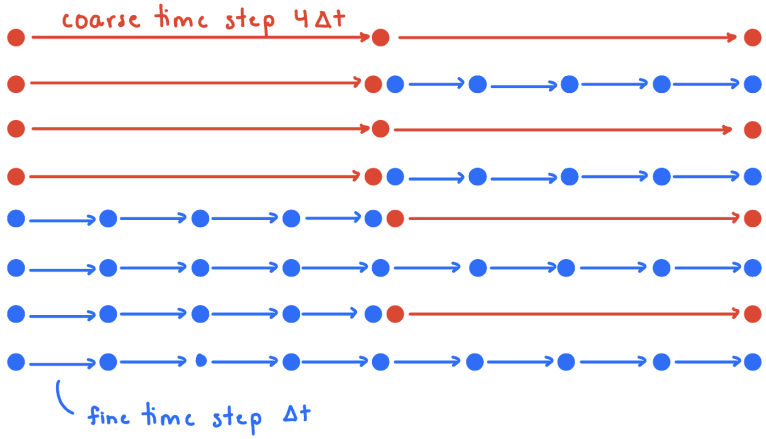
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RB	$O(Np/\Delta t)$	$O\left(\sqrt{\Delta t/p}\right)$
RM	$O\left(\frac{N}{\Delta t}\left(p + \frac{N-p}{k}\right)\right)$	$O(k\Delta t)$

Table: Δt refers to the time step size, N refers to the number of particles, p refers to the batch size, and k refers to the time step ratio.

Height Constraint Results

Height constraint: Our continuum solution cannot rise above height 1.

$$f(s) = \begin{cases} 0 & s \in [0,1] \\ \infty & \text{otherwise} \end{cases} \Rightarrow \text{“} \begin{cases} \partial_t \rho + \nabla \cdot (\rho v) = 0 \\ 0 \leq \rho \leq 1. \end{cases} \text{”}$$

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Continuum behavior with initial condition $\rho_0(x) = \frac{1}{3}\mathbb{1}_{[-1.5,1.5]}$ and external velocity $v(x) = x$.

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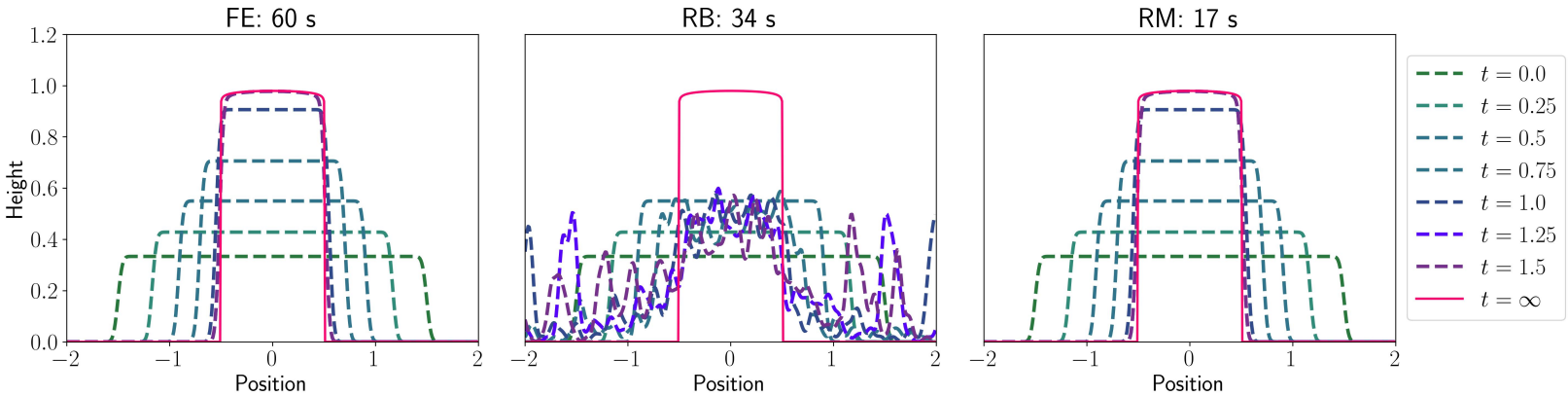


Figure: $N = 600$, $p = 300$, $k = 2$, $\varepsilon = 0.02108$ for φ_ε a Gaussian with standard deviation ε.

Height Constraint Continued

For different choice of Δt, how is the computational complexity and accuracy of the FE, RB, and RM methods affected?

We measure accuracy using an approximation of the 2-Wasserstein distance between the particle solution and the exact continuum solution at final time $T = 1.5$.

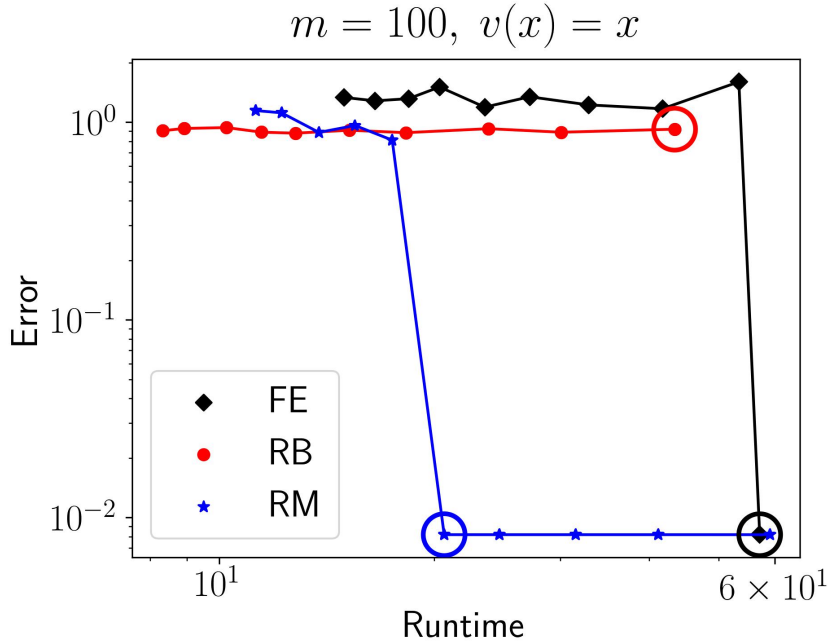


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Diffusion Regime Results

Diffusion: We simulate nonlinear diffusion with

$$f(s) = \begin{cases} s\ln(s) - s & m = 1 \\ \frac{s^m}{m-1} & m \neq 1 \end{cases} \Rightarrow \partial_t \rho = \Delta \rho^m + \nabla \cdot (\rho v)$$

and $v(x) = \frac{x}{m+1}$ up to final time $T = 1$.

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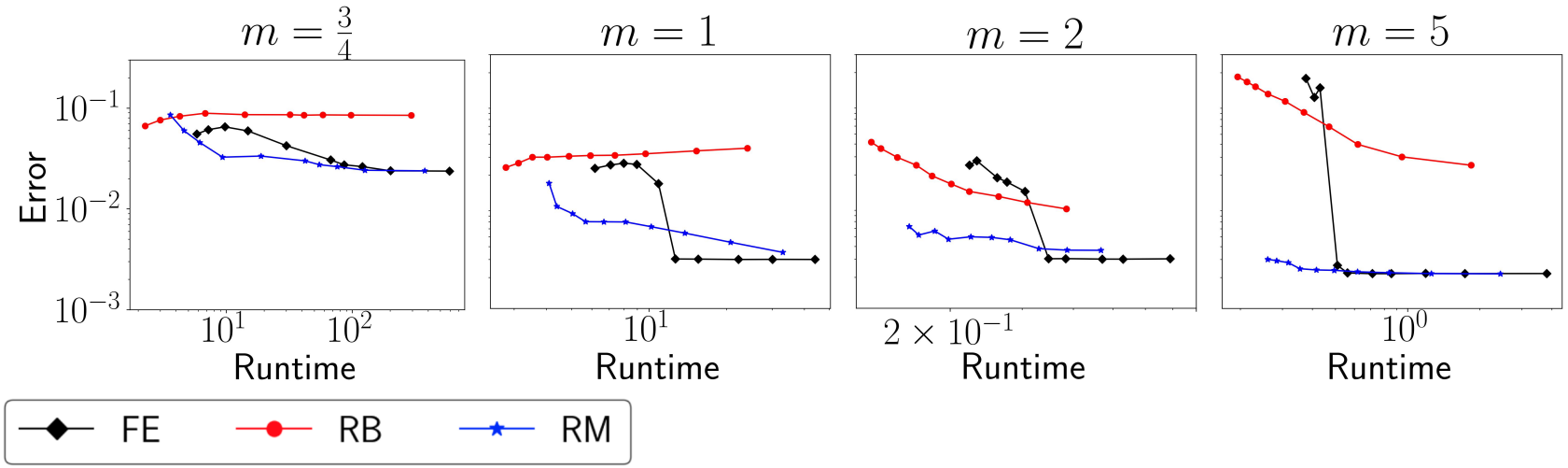


Figure: The performance of the FE, RB, and RM methods in the case $p = N/2$ and $k = 2$.

2D Results: The Navier-Stokes Equation

We use the RM method to simulate the viscosity formulation of the 2D Navier-Stokes equation

$$\partial_t \rho + v \cdot \nabla \rho = \nu \Delta \rho,$$

where $v = K * \rho$ for K the Biot-Savart kernel. Nordmark (1996) utilized regridding to simulate this equation with a "double bump" initial condition. We avoid regridding, instead using the RM method to simulate the solution.

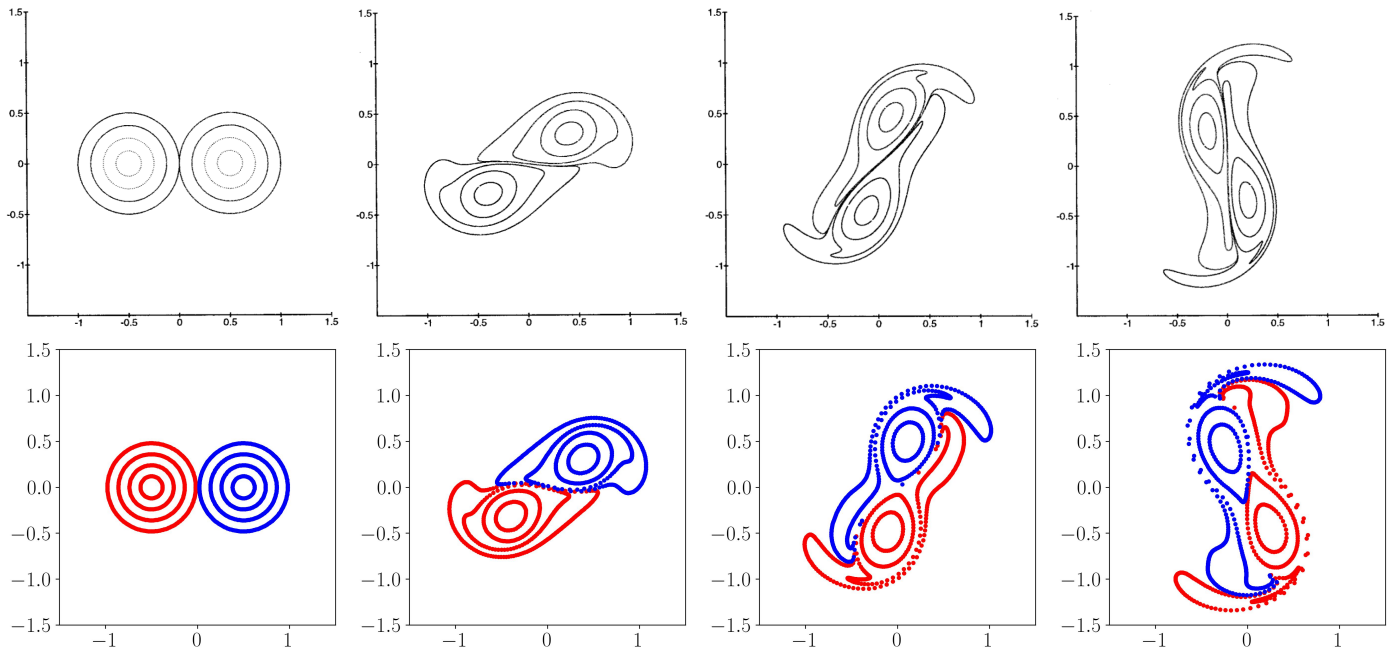


Figure: $N = 4688$, $\Delta t = 0.05$, $p = 2344$, $k = 2$, $\nu = 0.0005$, $\varepsilon = 0.08319$ for φ_ε a Gaussian with standard deviation ε.

Conclusions

Major takeaways

1. The RM method improves computational efficiency and preserves accuracy of blob methods for diffusion equations.
2. We see best performance of the RM method in the slow diffusion regime.
3. The RM method is compatible with a wide choice of linear and nonlinear diffusion equations.

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THANK YOU!!!

References

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