Particle and Game Theoretic Methods for Multi-scale and High Dimensional Problems

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Outline

- Fisher-Kolmogorov-Petrovsky-Piskunov Front Speeds in Flows.
- Feynman-Kac Representation and Particle Approximation.
- Learning Invariant Measure w. Physical Parameter Dependence.
- Entropy production in time reversal of diffusion processes.
- Computing principal eigenvalue by interacting particle method.
- Challenges: concentrations, large gradients and high dimensions.
- Curvature G-equation and Two-Player Game Representation.
- One-Way Reachability, Minimum Principle, Cell Problems.
- Bounded Oscillation Estimate, Front Speeds in Cell Flows.
- Conclusions and Future Work.

FKPP Variational Formula in Stationary Ergodic Media

$$u_t = \kappa\, \Delta_x u + \boldsymbol{v}(t,x) \cdot \nabla_x u + u(1-u),\ x \in \mathbb{R}^d,$$

$\boldsymbol{v}$ is space-time stationary ergodic, mean zero, volume preserving. To calculate front speed c^* along direction $\boldsymbol{e}$, let w solve linear equation parameterized by $\lambda > 0$ ($u = \exp\{\lambda\, \boldsymbol{e} \cdot x\}\, w$):

$$w_t = \mathcal{L}w := \kappa\, \Delta_x w + (2\kappa\, \lambda\, \boldsymbol{e} + \boldsymbol{v}) \cdot \nabla_x w + (1 + \kappa\, \lambda^2 + \lambda\, \boldsymbol{e} \cdot \boldsymbol{v})w,$$

with $w(0,x) = 1$. Almost surely,

$$\mu(\lambda) = \lim_{t \to \infty}\ t^{-1}\, \ln w$$

exists as principal Lyapunov exponent, convex and superlinear in large λ.

$$c^*(\boldsymbol{e}) = inf_{\lambda > 0}\, \frac{\mu(\lambda)}{\lambda}.$$

Freidlin, Gärtner, 1979: spatially periodic (1D random) media; Nolen, X, 2009: space-time stationary ergodic flow.

Lagrangian Approximation in Space-Time Periodic Flow

- Write $\mathcal{L} = L + M =$ Markovian + Potential,

$$M \cdot := c(t,x) \cdot = (1 + \kappa \lambda^2 + \lambda \, \boldsymbol{e} \cdot \boldsymbol{v}) \cdot$$

Feynman-Kac formula gives:

$$\mu = \lim_{t \to \infty} t^{-1} \ln \left(\mathbb{E} \exp\{ \int_0^t c(t-s, \boldsymbol{X}_s^{t,\boldsymbol{x}}) \, ds \} \right),$$

$$d\, \boldsymbol{X}_s^{t,\boldsymbol{x}} = \boldsymbol{v}(t-s, \boldsymbol{X}_s^{t,\boldsymbol{x}}) \, ds + \sigma \, d\boldsymbol{W}_s, \; \boldsymbol{X}_0^{t,\boldsymbol{x}} = \boldsymbol{x}.$$

- Direct approximation of this formula is challenging, as the main contribution to $\mathbb{E}$ comes from sample paths that visit maximal points of time-dependent potential c.

Lagrangian Approximation in Space-Time Periodic Flow

- Consider a "normalized version", the Feynman-Kac semi-group:

$$\Phi_t^c(\nu_0)(\phi) := \frac{\mathbb{E}[\phi(\boldsymbol{X}_t^{t,\boldsymbol{x}})\ \exp\{\int_0^t c(t-s, \boldsymbol{X}_s^{t,\boldsymbol{x}})\, ds\}]}{\mathbb{E}[\exp\{\int_0^t c(t-s, \boldsymbol{X}_s^{t,\boldsymbol{x}})\, ds\}]} := \frac{P_t^c(\nu_0)(\phi)}{P_t^c(\nu_0)(1)}$$

  acting on initial probability measure ν_0 ($\boldsymbol{x} \sim \nu_0$), converges weakly to an invariant measure ν_c as $t \uparrow \infty$, for any test function ϕ. Moreover,

$$P_t^c(\nu_c) = \exp\{\mu\, t\}\, \nu_c \ \text{ or } \ \mu = t^{-1} \ln \mathbb{E}_{\nu_c}[P_t^c(\nu_c)].$$

- Discretize $\boldsymbol{X}_s^{t,\boldsymbol{x}}$ as $\boldsymbol{X}_i^{\Delta t}$ by explicit Euler, $i = 1, \cdots, n \times m$, $m = \frac{T}{\Delta t}$, approximate evolution of probability measure $\Phi_t^c(\nu)$ by a particle system, with a resampling technique to reduce variance.

Lagrangian Approximation in Space-Time Periodic Flow

- Let

$$P_n^{c,\Delta t}(\nu_0)(\phi) := \mathbb{E}\left[\phi(\boldsymbol{X}_{nm}^{\Delta t})\ \exp\left\{\Delta t \sum_{i=1}^{m} c((m-i)\Delta t, \boldsymbol{X}_{i+(n-1)m}^{\Delta t})\right\}\right]$$

- As $n \to \infty$, the sampled FK semi-group actions on ν:

$$\mathbb{E}_{\nu_0} \frac{P_n^{c,\Delta t}(\nu_0)(\phi)}{P_n^{c,\Delta t}(\nu_0)(1)} \to \int_D \phi \, d\, \nu_{c,\Delta t}, \quad \forall \text{ smooth } \phi,$$

D: space periodic cell, $\nu_{c,\Delta t}$: approximate invariant measure.

Theorem (Lyu, Wang, X, Zhang, SINUM 2022)

There exists $q \in (0,1)$ so that:

$$\mu_{\Delta t}^n := (nT)^{-1} \ln[P_n^{c,\Delta t}(\nu_0)(1)] \to T^{-1} \ln[P_1^{c,\Delta t}(\nu_{c,\Delta t})(1)] = \mu + o((\Delta t)^q)$$

Genetic Interacting Particle Algorithm

- Initialize 1st generation of particles $\boldsymbol{\xi}_1^0 = (\xi_1^{0,1}, \cdots, \xi_1^{0,N_0}) \in (\mathbb{T}^d)^{N_0}$, unif. distributed over $\mathbb{T}^d$ ($d \geq 2$). Let g be the generation no. in approximating $\nu_{c,\Delta t}$. Each generation moves and mutates m-times, with a life span T (time period), time step $\Delta t = T/m$.

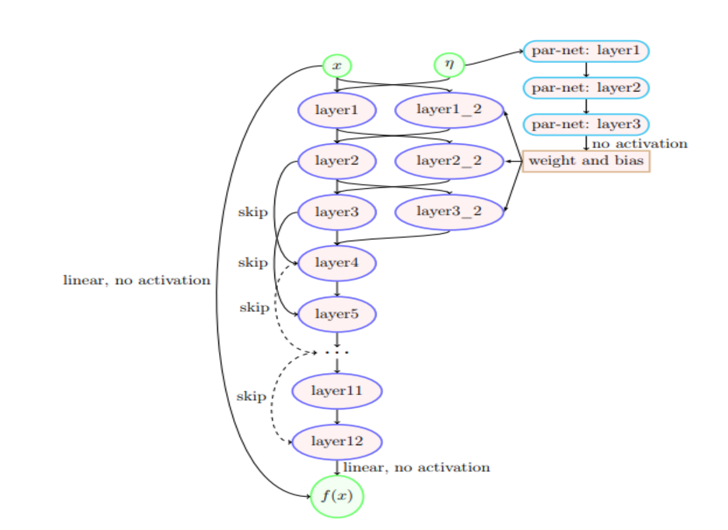
  for $g = 1 : G-1$
  for $i = 0 : m-1$
  $\zeta_g^i \leftarrow$ one-step-advection-diffusion update on $\boldsymbol{\xi}_g^i$
  with fitness $\boldsymbol{F} \leftarrow \exp\{c(T - i\Delta t, \zeta_g^i)\,\Delta t\}$.
  $E_{g,i} := \frac{1}{\Delta t}$ ln (mean population fitness), growth rate.
  Normalize fitness to weight $\boldsymbol{p} := \boldsymbol{F}/SUM(\boldsymbol{F})$.
  $\boldsymbol{\xi}_g^{i+1} \leftarrow$ resample ζ_g^i via multinomial distribution with weight $\boldsymbol{p}$.
  end for
  $\boldsymbol{\xi}_{g+1}^0 \leftarrow \boldsymbol{\xi}_g^m$, $E_g \leftarrow \mathrm{mean}\,(E_{g,i})$ over i.
  end for
- Output: approximate $\mu_{\Delta t} \leftarrow$ mean(E_g), and $\boldsymbol{\xi}_G^0$.

Genetic Algorithm, Bottleneck and Learning

- Feynman-Kac (F-K) semigroup, particle methods of invariant measure and principal eigenvalue, are well-known in physics, large deviation, Monte Carlo.
- Ferré & Stoltz, 2019: error estimates of discrete F-K and particle approximation in *spatially periodic media*.
- Advantages of interacting particle method for generating training data: (1) meshfree, (2) self-adaptive, (3) not sensitive to high dimensions (costs about the same from 2D to 3D).
- Computational bottelneck: long time evolution of large number of particles in the small κ (large Péclet number $\sim \kappa^{-1}$) regime.
- Invariant measure learning: map uniform distribution to invariant measure at κ based on a few less expensive simulations at $\kappa_i > \kappa$.

Nonlocal Resnet for optimal transport (OT) map

η: physical parameter input. $X = Y = \mathbb{R}^d$.



Deep Particle Network Training

- Training data: interacting particle algorithm generates samples of invariant measure at $\kappa_i = 2^{-2-0.25(i-1)}$, $i = 1, \cdots, 8 (= n_\eta)$, and $N_0 = 40000$ particle evolution for $G = 2048$, $\Delta t = 2^{-8}$, $T = 1$.
- At each κ_i, randomly sample $N = 2000$ points $\mathcal{Y}_i$ without replacement.
- $\{\mathcal{Y}_1, \cdots, \mathcal{Y}_8\}$: one mini-batch of training data.
- Total 5 mini-batches for 50000 gradient descent steps of training.
- On a quad-core CPU desktop with an RTX2080 8GB GPU.

Arnold-Beltrami-Childress Flow

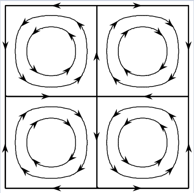
- (Arnold '65; Hénon '66; Dombre, Frisch, Greene, Hénon, Mehr & Soward '86):

$$\begin{aligned} x' &= A \sin z + C \cos y \\ y' &= B \sin x + A \cos z \\ z' &= B \cos x + C \sin y \end{aligned}$$

  weakly chaotic at $A = B = C = 1$.

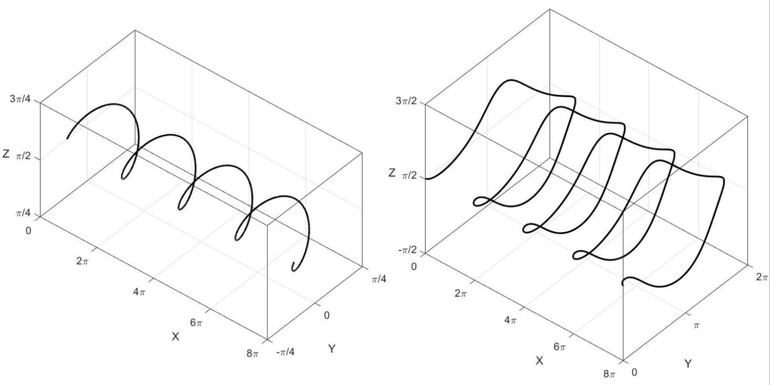
- Cellular (Hamiltonian) flow or BC flow ($A = 0$) with $\pi/4$ rotation:

$$\boldsymbol{v}(x, y) = (\partial_y \mathcal{H}, -\partial_x \mathcal{H}), \;\; \mathcal{H} = \sin(x)\sin(y)$$



Ballistic Orbits in ABC (L), Komogorov(R) Flow

- Kolmogorov (K) flow: ABC (A=B=C=1) with only sine terms.
- Construction of orbits by symmetry: X, Yu, Zlatoš (ABC, SIAM Math Anal. 2016), Kao, Liu, X (K flow, MMS 2022).



A=B=C=1, plus random shear perturbation

- $\delta\,(\sin(z)+\cos(y),\ \sin(x)+\cos(z)+\epsilon\cdot\xi(x,\omega),\ \sin(y)+\cos(x))$, $\kappa=1,\ T=512,\ \Delta t=2^{-11},\ T=512,\ N=100,000$ particles.

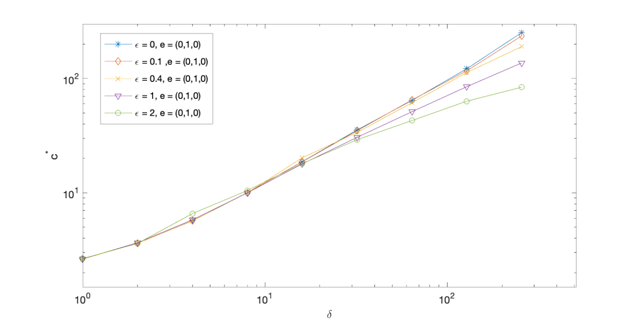
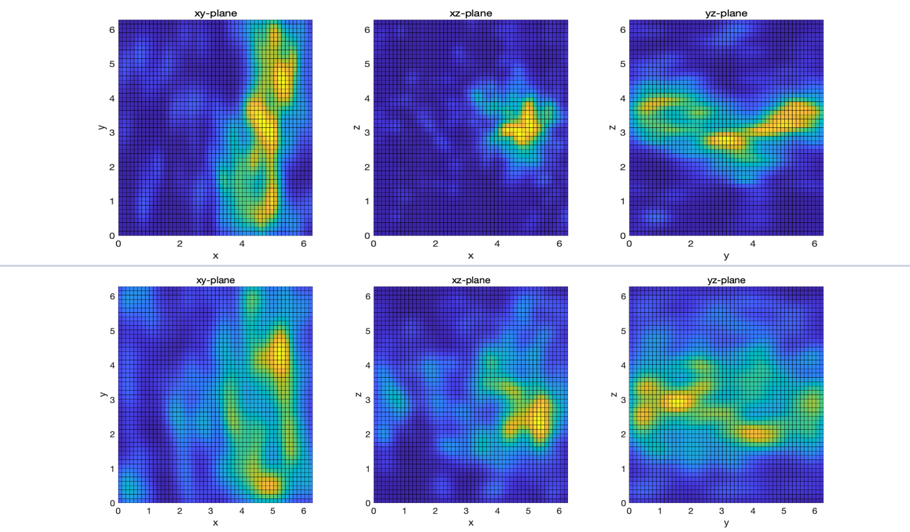


Figure: $\xi \approx$ OU process, generated by random Fourier series.

- $c^\star = O(\delta^{0.9842})$ at $\delta \approx 100$, $\epsilon = 0$. As $\epsilon \uparrow$, vortex tube structure in ABC flow facilitating transport is destroyed by $(0,\xi(x,\omega),0)$, $c^\star \downarrow$.

Defocusing of invariant measure: $\epsilon = 0$ (top), 2 (bottom).



Kolmogorov Flows

- Galloway & Proctor 1992, Childress & Gilbert 1995:

$$\begin{aligned} x' &= \sin z \\ y' &= \sin x \\ z' &= \sin y \end{aligned}$$

  Disorder (mixing) dominates phase space, integrable regions shrink to small islands.

- Time-Periodic Kolmogorov flow field (strongly mixing):

$$\boldsymbol{v} = (\sin(z + \sin(2\pi t)), \sin(x + \sin(2\pi t)), \sin(y + \sin(2\pi t))).$$

DP Generated Invariant Measure Projected on yz plane

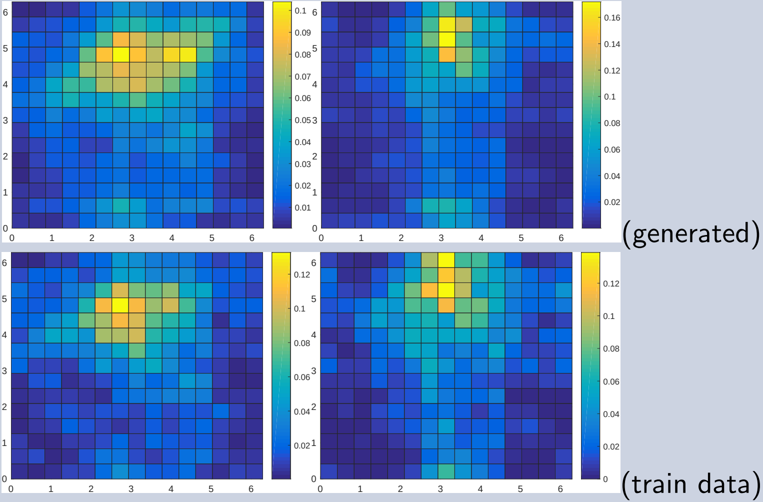


Figure: 1st/2nd col: $\kappa = 2^{-2.5}/2^{-3}$ in time-periodic K flow.

DP Predicted Inv. Meas. vs. Ground Truth on *yz* plane

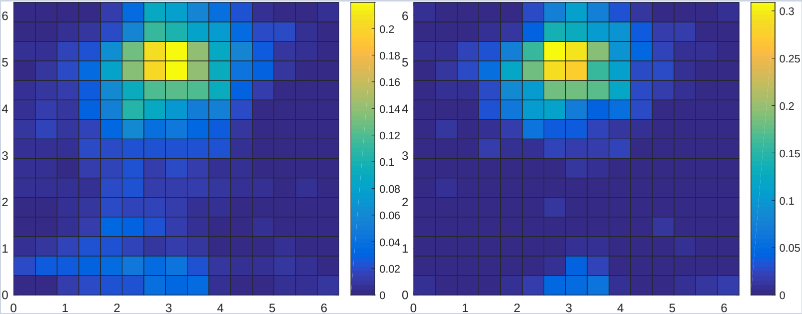


Figure: Invariant measures projected to *yz* plane in time-periodic K flow at $\kappa = 2^{-4}$: prediction (left), ground truth (right), at test value $\kappa = 2^{-4}$.

Time Reversal of Diffusion Processes

- Stochastic differential equation (SDE) in $\mathbb{R}^d$:

$$d\,X_s = h(X_s, s)\,ds + g(s)\,d\,W_s := -\nabla V(X_s)\,ds + b(X_s)\,ds + \sqrt{2\,\epsilon}\,d\,W_s \tag{1}$$

  where V is a smooth potential function with at least quadratic growth at infinity, b is a bounded divergence free and smooth vector field, $\epsilon \in (0,1)$, and W is standard Wiener process.

- Kolmogorov (1937): The initial distribution $\sim \exp\{-V/\epsilon\}$ is realized by solving (1) backward in time from terminal distribution iff $b = 0$.

- Let terminal (prior) distribution p_T at time T be normal. MCMC sampler: $p_{data} = Z^{-1}\exp\{-V\}$, V is a closed form log-likelihood function.

- Mapping p_{prior} to p_{data} (since 2010's): variational autoencoder, generative adversarial network, flow-based models (e.g. neural ODEs, finding h from data), deep particle (2022).

Entropy Production

- Denoising diffusion probabilistic (score-based generative) modeling.
- Map p_{data} to p_{prior} by (1) or adding noise in time to increase entropy.
- Invert the map (denoising) by solving SDE (in reverse time):

$$d\,\tilde{X}_s = [h(\tilde{X}_s, s) - g^2(s)\nabla_{\tilde{X}_s} \log p_s(\tilde{X}_s)]\, ds + g(s)\, d\,\tilde{W}_s, \qquad (2)$$

Anderson (1982), where p_s is distribution of forward time SDE (1).

- Entropy integral to quantify reversability:

$$S_t = \epsilon^{-1} \int_0^t \langle\, b(X_s), \circ\, d\, X_s \rangle$$

work done by non-gradient part of the drift h.

Entropy Production

- Let $P_t^{\lambda,\,\epsilon}$ be the probability measure of (1) from initial measure λ. Its moment generating function is ($\alpha \in \mathbb{R}$):

$$\chi_t^{\epsilon}(\alpha) = \int_{C([0,t];\mathbb{R}^d)} \exp\{-\alpha\, S_t^{\epsilon}\}\, d\, P_t^{\lambda,\,\epsilon}$$

with representation:

$$\chi_t^{\epsilon}(\alpha) = \int_{\mathbb{R}^d} d\xi\, (\exp\{t\, A^{\varepsilon,\alpha}\}1)(\xi)$$

where $A^{\varepsilon,\alpha}$ acts on smooth and compactly supported functions f as:

$$\begin{aligned} A^{\varepsilon,\alpha} f &= \varepsilon \Delta f + < -\nabla V + (1-2\alpha) b, \nabla f > - \frac{\alpha(1-\alpha)}{\varepsilon} |b|^2 f \\ &\quad + \frac{\alpha}{\varepsilon} < b, \nabla V > f + \alpha (\nabla \cdot b) f \end{aligned}$$

over $\alpha \in [-\delta, 1+\delta]$ for some small $\delta > 0$.

Entropy Production and Leading Eigenvalue

- Let $\lambda^{\varepsilon,\alpha}$ be the leading eigenvalue (the one with the largest real part) of $A^{\varepsilon,\alpha}$. Then:
$$\lim_{t\to\infty}\frac{1}{t}\log\chi_t^{\epsilon}(\alpha)=\lambda^{\varepsilon,\alpha} \tag{3}$$
convex in α and symmetric about $\alpha=1/2$.

- Legendre transform of $\lambda^{\varepsilon,\alpha}$ in α is the large deviation rate function of $t^{-1}S_t^{\epsilon}$, so characterizes the stochastic growth rate of entropy.

- $A^{\varepsilon,\alpha}$ shares $\lambda^{\varepsilon,\alpha}$ with operator:

$$\begin{aligned}B^{\varepsilon,\alpha}f:=&\exp((-2\varepsilon)^{-1}V)A^{\varepsilon,\alpha}(\exp((2\varepsilon)^{-1}V))\\ =&\varepsilon\Delta f+\langle(1-2\alpha)b,\nabla f\rangle-\frac{1}{4\varepsilon}|\nabla V|^2f+\frac{1}{2\varepsilon}\langle b,\nabla V\rangle f\\ &-\frac{\alpha(1-\alpha)}{\varepsilon}|b|^2f+\frac{1}{2}(\Delta V)f-\alpha(\nabla\cdot b)f:=(L+U)\,f.\end{aligned}$$

Probabilistic Representation

- Markov generator:

$$L f := \varepsilon \Delta f + \langle (1-2\alpha) b, \nabla f \rangle$$

with corresponding SDE:

$$dX_t = (1-2\alpha) b(X_t)\, dt + \sqrt{2\varepsilon}\, dB_t.$$

- Assume: at least quadratic growth of potential $|\nabla V|^2 \geq a|x|^2$ for $|x| \geq R$, consts. $(a, R) > 0$, $\lim_{|x|\to\infty} \Delta V / |\nabla V| = 0$; and bounded drift $\|b\|_{C^1(\mathbb{R}^d)} \leq C$.
- Evolution operator P_t^U:

$$P_t^U \varphi(x) = \mathbb{E}\left[\varphi(X_t) \exp\left(\int_0^t U(X_s)\, ds\right) \Big| X_0 = x\right], \qquad (4)$$

$\mathbb{E}[\cdot]$ on Brownian motion and φ measurable.
- Let $\hat{P}_t^U$ be the time discretized P_t^U, $t = n\Delta t$.

Discrete FK semigroup

- $\exists$ invariant measure $\hat{\nu}_*$ under discrete FK semigroup so that:

$$\hat{P}_t^U(\hat{\nu}_*) = \exp\{\hat{\lambda}_{\Delta t}^{\varepsilon,\alpha}\, t\}\, \hat{\nu}_* \ \text{ or } \ \hat{\lambda}_{\Delta t}^{\varepsilon,\alpha} = t^{-1} \ln \mathbb{E}_{\hat{\nu}_*}[\hat{P}_t^U(\hat{\nu}_*)]$$

  and

$$\hat{\lambda}_{\Delta t}^{\varepsilon,\alpha} = \lim_{k\to+\infty} \frac{1}{k\Delta t} \log \mathbb{E}\left[\exp\left(\Delta t \sum_{j=1}^{k-1} U(X_{j\Delta t})\right) \middle| X_0 \sim \nu\right].$$

- Interacting Particle method + HKU cluster: 2 Intel Xeon Gold 6226R (16 Core) CPU's and 96GB RAM.
- Experiments: #(particles)=$500,000$, $\Delta t = 2^{-8}$; $\varepsilon = 0.1, 0.01, 0.001$. At each ε, $\alpha \in \left[-\frac{1}{10}, \frac{11}{10}\right]$, compute $\lambda^{\varepsilon,\alpha}$ for $\alpha = -\frac{1}{10} + \frac{j}{31}\frac{12}{10}$ with $j = 0, 1, \ldots, 31$. The computation of $\lambda^{\varepsilon,\alpha}$ for each ε with 32 different values of α is performed in parallel on 32 cores of the CPU's.

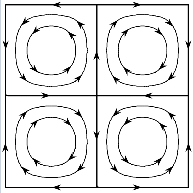
2D example

- Double-well potential

$$V(x_1, x_2) = x_1^4 - 2x_1^2 + (1 + a\,(x_1 - 1)^2)x_2^2 + x_2^4$$

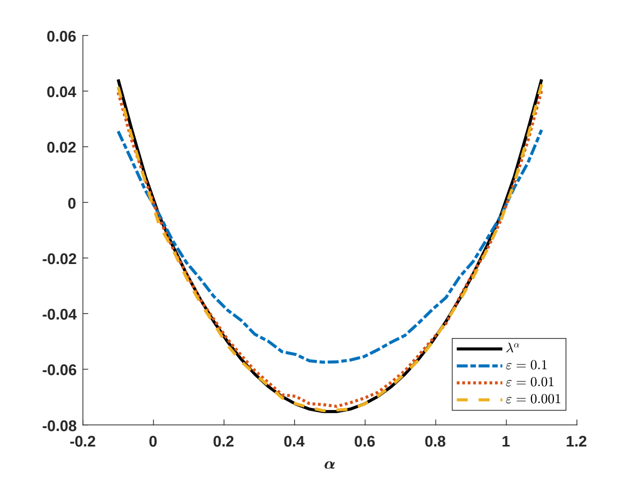
with $a = 0.4$, and cell (Hamiltonian) flow

$$b(x_1, x_2) = \pi^{-1}(\cos(\pi x_1)\sin(\pi x_2), -\sin(\pi x_1)\cos(\pi x_2))$$



- $\lambda^{\alpha} = \lim_{\varepsilon \to 0} \lambda^{\varepsilon,\alpha}$ known in closed-form.

2D example: computed $\lambda^{\varepsilon,\alpha}$ and exact λ^{α} as $\varepsilon \downarrow 0$



2D example: approximate invariant measures

- $\varepsilon = 0.1$ 0.01 0.001

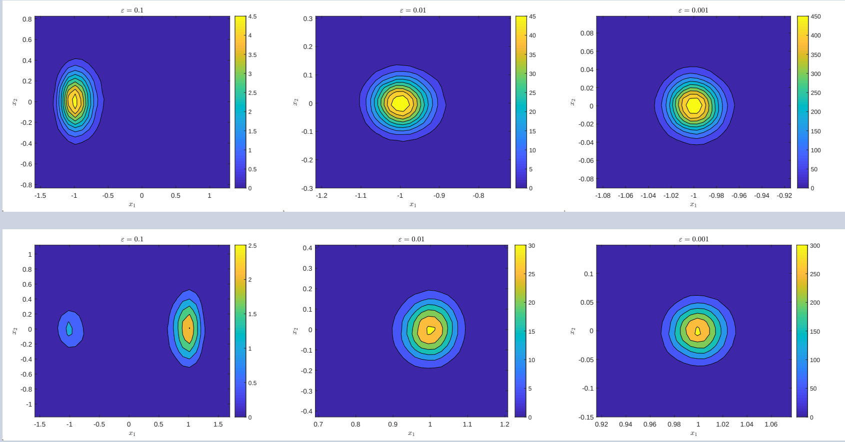
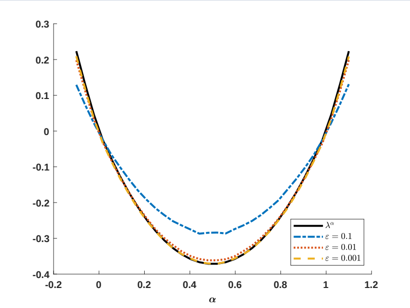


Figure: Distribution of particles at $T = 2048$, and $\alpha \approx 0.5968\,(top)/1.0613$.

4D example: $\lambda^{\varepsilon,\alpha}$ in doublewell potential ($a = 0.4$)

$$\begin{aligned} V(x_1,x_2,x_3,x_4) &= x_1^4 - 2x_1^2 + (1 + a(x_1-1)^2)\, x_2^2 + \\ &\quad x_2^4 + x_3^4 - 2x_3^2 + (1 + a(x_3-1)^2)\, x_4^2 + x_4^4 \end{aligned}$$

$$\begin{aligned} b(x_1,x_2,x_3,x_4) &= \pi^{-1}(\cos(\pi x_1)\sin(\pi x_2), -\sin(\pi x_1)\cos(\pi x_2), \\ &\quad 2\cos(\pi x_3)\sin(\pi x_4), -2\sin(\pi x_3)\cos(\pi x_4)), \end{aligned}$$



8D example: $\lambda^{\varepsilon,\alpha}$ in potential and Hamiltonian flow.

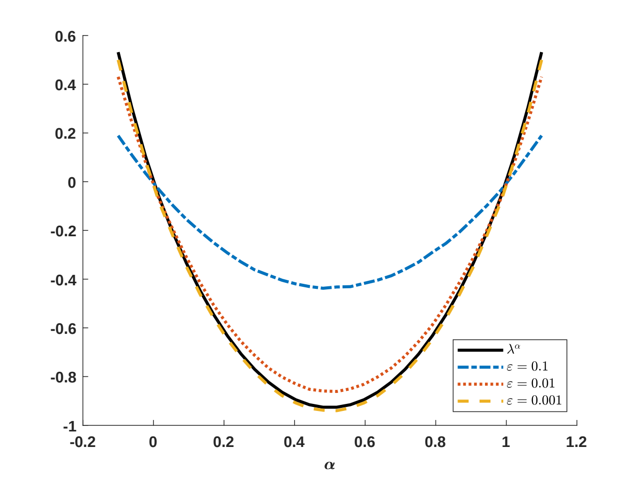
$$\begin{aligned} V(x_1,x_2,x_3,x_4,x_5,x_6,x_7,x_8) = {} & \frac{x_1^2+x_2^2}{2} + \frac{x_1^4+x_2^4}{8} + \frac{x_3^2+x_4^2}{2} + \frac{x_3^4+x_4^4}{8} \\ & + x_5^4 - 2x_5^2 + (1+a(x_5-1)^2)x_6^2 + x_6^4 \\ & + x_7^4 - 2x_7^2 + (1+a(x_7-1)^2)x_8^2 + x_8^4 \end{aligned}$$

with $a = 0.3$.

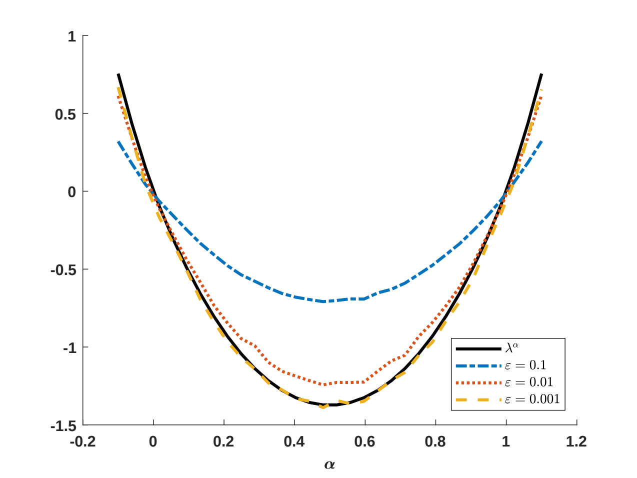
$$\begin{aligned} b(x_1,x_2,x_3,x_4,x_5,x_6,x_7,x_8) = {} & \pi^{-1}(\cos(\pi x_1)\sin(\pi x_2), -\sin(\pi x_1)\cos(\pi x_2), \\ & \widetilde{b}_2\cos(\pi x_3)\sin(\pi x_4), -\widetilde{b}_2\sin(\pi x_3)\cos(\pi x_4), \\ & \cos(\pi x_5)\sin(\pi x_6), -\sin(\pi x_5)\cos(\pi x_6), \\ & 2\cos(\pi x_7)\sin(\pi x_8), -2\sin(\pi x_7)\cos(\pi x_8)), \end{aligned}$$

with $\widetilde{b}_2 = 0.5$.

8D example: computed $\lambda^{\varepsilon,\alpha}$ and exact λ^{α} as $\varepsilon \downarrow 0$



16D example: computed $\lambda^{\varepsilon,\alpha}$ and exact λ^{α} as $\varepsilon \downarrow 0$



16D example: projected invariant measures

- $\varepsilon = 0.1$ 0.01 0.001

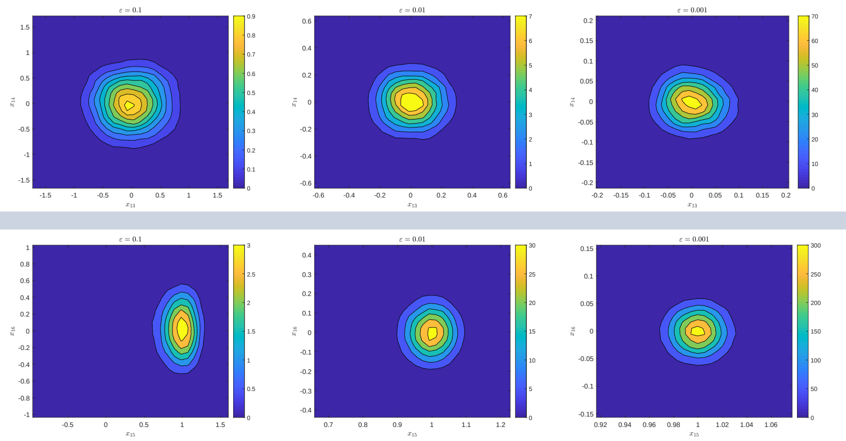
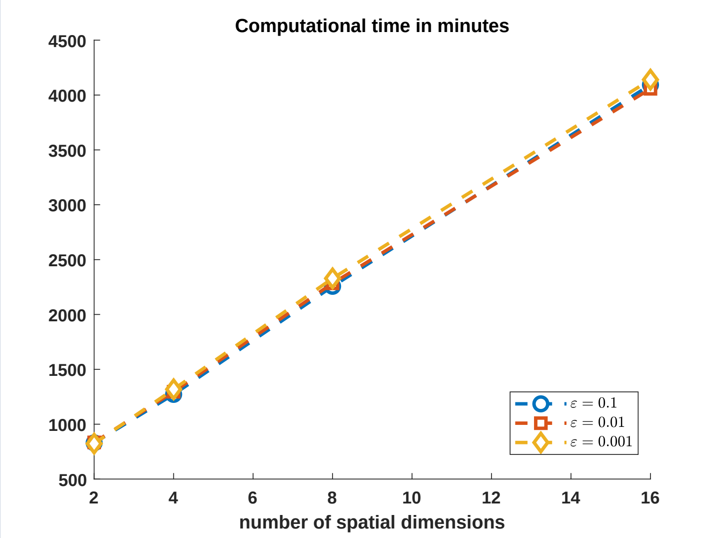


Figure: $T = 2048$, $\alpha \approx 0.2097$, projected on (x_{12}, x_{14}) (top)/(x_{15}, x_{16}).

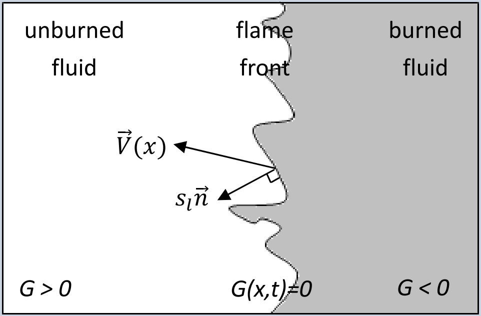
Linear Growth: comput. time (min) vs. dimension.



G-equation: Hamilton-Jacobi Level Set Equation

- Markstein (1950's), Williams (1980's): convex yet non-coercive Hamiltonian.

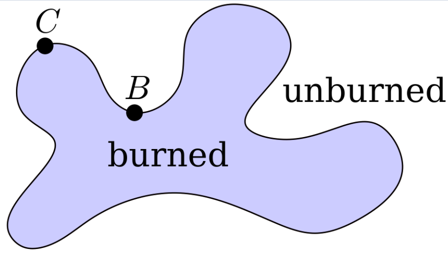
$$G_t + s_l|DG| + V(x)\cdot DG = 0.$$



- **Motion law**: normal velocity $v_{\vec{n}} = \vec{V}\cdot\vec{n} + s_l$,
  s_l laminar speed, $\vec{n} = \frac{DG}{|DG|}$.

Curvature Effect on Laminar Speed

- **Curvature effect**, Markstein (1951): as flame front bends toward cold region (unburned area, point C), propagation slows down. As flame bends toward hot spot (burned area, point B), it burns faster.



- Empirical linear relation proposed by Markstein:

$$s_l = s_l^0 (1 - \tilde{d}\ \kappa)_+$$

κ: mean curvature along the flame front. $\tilde{d}$: Markstein length. $(\cdot)_+$ prevents "unburn". Folklore: curvature slows flame on average.

Curvature G-equation in Cell Flow

- After normalizing consts, a non-convex & non-coercive Hamiltonian:

$$G_t + \left(1 - d\ \mathrm{div}\left(\frac{DG}{|DG|}\right)\right)_+ |DG| + V(x) \cdot DG = 0$$

- Let $V(x) = A\, D^{\perp} \sin(x_1) \sin(x_2)$, intensity $A > 0$.

Theorem (Gao, Long, X, Yu. J. Geometric Analysis, 2024)

For any unit vector $p \in \mathbb{R}^2$ and initial data $G(x, 0) = p \cdot x$, there exists a positive number $\overline{H}_{A,d}(p)$ such that

$$\left| G(x, t) - p \cdot x + \overline{H}_{A,d}(p)\, t \right| \leq C, \quad \forall\, (t, x) \in \mathbb{R}^2 \times [0, \infty),$$

for a constant C depending only on A and d.

Corrector

- Look for a solution of the form $p \cdot x - \overline{H}(p)t + v(x)$, v is the so called corrector satisfying (a.k.a. cell problem):

$$\left(1 - d\ \operatorname{div}\left(\frac{p + Dv}{|p + Dv|}\right)\right)_{+} |p + Dv| + V(y) \cdot (p + Dv) = \overline{H}(p), \quad (5)$$

  subject to 2π-periodic boundary condition in y.
- Theorem follows by comparing G with $v\pm$ const.
- To construct a solution, consider a modified cell (discount) problem as Lions-Varadhan-Papanicolaou (1980's, *coercive* periodic Hamiltonian):

$$\lambda v + \left(1 - d\ \operatorname{div}\left(\frac{p + Dv}{|p + Dv|}\right)\right)_{+} |p + Dv| + V(y) \cdot (p + Dv) = 0, \quad (6)$$

  for a parameter $\lambda > 0$,.
- Existence and uniqueness of $v = v_\lambda$ to (6) known by Perron's method (Crandall-Ishii-Lions 1992). Comparison principle implies: $\max_{x \in \mathbb{R}^2} |\lambda v_\lambda(x)| \leq 1 + \max_{\mathbb{R}^2} |V|$.

- Aim to show

$$\lim_{\lambda\to 0} \lambda\, v_\lambda(x) = -\overline{H}(p) \quad \text{uniformly on } \mathbb{R}^2$$

then (6) $\to$ (5) with standard sub/super-solution technique on v_λ.

- Key is the *bounded oscillation* estimate:

$$\max_{x,\, y\, \in[-\pi,\pi]^2} |v_\lambda(x) - v_\lambda(y)| \le C = C(d, A). \tag{7}$$

- In the absence of curvature ($d = 0$), (7) follows from mutual reachability of x and y by a controled trajectory (X-Yu, 2010). If y is reachable from x by ξ for $|\alpha(t)| \le 1$,

$$\dot{\xi}(t) = \alpha(t) - V(\xi(t))$$

subject to $\xi(0) = x$ within time T, then

$$v_\lambda(x) \le v_\lambda(y) + C\,T,$$

for incompressible V in any dimension.

Deterministic Two-Person Game in 2D

- A deterministic game (Kohn-Serfaty, 2006): consider the discrete dynamical system $\{x_n\}_{n=1}^N \subset \mathbb{R}^2$ associated with the game starting from $x_0 = x$: for $n = 0, 1, 2, .., N-1$,

$$\begin{cases} x_{n+1} = x_n + \tau\sqrt{2d}\, b_n\, \vec{\eta}_n + \tau^2\, \vec{\eta}_n^{\perp} - \tau^2\, V(x_n) \\ x_0 = x, \end{cases}$$

  where $|\vec{\eta}_n| \leq 1$ and $b_n \in \{-1, 1\}$.
- Player I controls direction via $\vec{\eta}_n$ and player II controls sign via b_n.
- Let $g = g(x)$ be a final payoff function. Player I (II) aims to minimize (maximize) $g(x_N)$. If both players proceed optimally, the value function

$$u(x, N\tau^2) := g(x_N),$$

  converges to the solution of curvature G-eq with initial data $g(x)$:

$$\lim_{N\tau^2 \to t, \tau \to 0} u(x, N\tau^2) = G(x, t).$$

Inequalities from One-Way Reachability via Game

- A typical scenario to get an upper bound of the game value is for player I to devise a strategy so that the game trajectory, starting at a point P, ends at a point Q in a desired region U in N moves despite any strategy of player II; then

$$u(P, N\tau^2) \le g(Q) \le \max_{q\in U} g(q).$$

- For stationary equation, suppose: (1) w satisfies

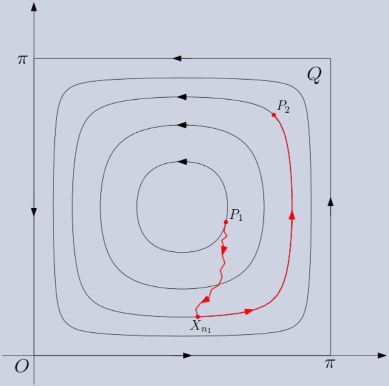
$$\left(1 - d\ \mathrm{div}\left(\frac{Dw}{|Dw|}\right)\right)_+ |Dw| + V(x)\cdot Dw \le C$$

implying $w - Ct$ is a sub-solution to G-eq; (2) player I has a strategy to steer the game trajectory from x to a region D (invariant under $-V$ flow) within time T regardless how player II plays; then

$$w(x) - CT \le G(x, N\tau^2) \le \max_{y\in D} w(y).$$

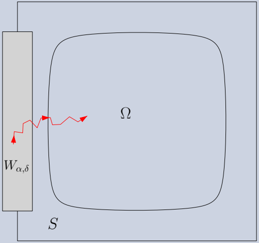
- Unlike the $d = 0$ case, two-way reachability does NOT hold.

Interior One-way Reachability



Player I's strategy: at each step, choose $\eta = \frac{V}{|V|}$ until it reaches the target lower level set of $\mathcal{H}$: $\mathcal{H}(X_{n+1}) - \mathcal{H}(X_n) \leq -|DH(X_n)|\,\tau^2 + O(\tau^3)$.
Then switch to $\eta = 0$ to reach the target point P_2.

Quarter Cell Boundary Crossing: PDE Method



Evolve G-equation with initial data ($\Omega \subset S = (0,1)^2$):
$g_S(x) = -\frac{2}{\pi}\arctan(\mathrm{dist}(x, \partial S))$, for $x \in S$; else, $\frac{2}{\pi}\arctan(\mathrm{dist}(x, \partial S))$.
The edge $\{0\} \times (0,1)$ is part of the zero level set of G where:

$$v_{\vec{n}} = (1 - d\kappa)_+ + V(x) \cdot \vec{n} \approx 1,$$

so $\exists t_\delta > 0$ s.t. $G((0,\theta), t) < 0 \quad$ for $(\theta, t) \in [\delta, 1-\delta] \times (0, t_\delta]$. An optimal game trajectory starting from $W_{\alpha,\delta}$ must pass through the edge $\{0\} \times [\delta, 1-\delta]$ during the time interval $(0, t_\delta]$.

PDE estimates from: 1-Way Reachability

Lemma

Let $G(x,t)$ be the unique solution with $G(x,0) = p \cdot x$. There exist positive constants β and C depending only on d and V s.t. for all $(x,t) \in \mathbb{R}^2 \times [0,\infty)$,

$$G(x,t) - p \cdot x \leq -\beta\, t + C \tag{8}$$

and

$$\max_{x \in \mathbb{R}^2} \lambda\, v_\lambda(x) < -\frac{\beta}{2} + \lambda\, C. \tag{9}$$

Inequality (8) follows from estimating travel times of game trajectories across cells and 1-way reachability inequalities.

Inequality (9) from constructing a super-solution to a time-dependent variant of the discount cell problem via the inequality (8).

Minimum Principle from: 1-Way Reachability

- Applying inequality (9) at $\lambda < \beta/(4C)$, we have from the discount cell problem:

$$\left(1 - d \ \mathrm{div}\left(\frac{p + Dv_\lambda}{|p + Dv_\lambda|}\right)\right)_+ |p + Dv_\lambda| + V(y) \cdot (p + Dv_\lambda) \geq \beta/4$$

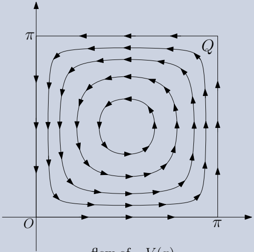
- $\rightarrow$ minimum principle: The minimum value of $u_\lambda := p \cdot x + v_\lambda$ in a domain can only be attained on its boundary.
- $u = u_\lambda$ is a viscosity sub-solution of the stationary G-equation:

$$\left(1 - d \ \mathrm{div}\left(\frac{Du_\lambda}{|Du_\lambda|}\right)\right)_+ |Du_\lambda| + V(y) \cdot (Du_\lambda) = 1 + \max_{[-\pi,\pi]^2} |V|(y) := \alpha$$

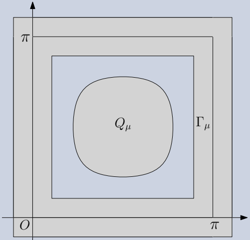
$$\text{satisfying} \quad u_\lambda(x_0) \leq \max_{y \in \bar{S}} u_\lambda(y) + \alpha\, T_0$$

if a bounded set S is reachable from x_0 within T_0, and S is invariant under $-V$ flow.

Quarter Cell Interior Oscillation Estimate



flow of $-V(x)$



Q_μ and Γ_μ

- For each point $x \in \partial Q_\mu$ and each point $y \in \overline{Q}_\mu$, $u_\lambda(x) \geq u_\lambda(y) - C_\mu$ for some constant $C_\mu > 0$. Accordingly:

$$\min_{x \in \partial Q_\mu} u_\lambda(x) \geq \max_{x \in \overline{Q}_\mu} u_\lambda(x) - C_\mu.$$

- By minimum principle: $\min_{x \in \partial Q_\mu} u_\lambda(x) = \min_{x \in \overline{Q}_\mu} u_\lambda(x)$, and so:

$$\max_{x \in \overline{Q}_\mu} u_\lambda(x) - \min_{x \in \overline{Q}_\mu} u_\lambda(x) = \max_{x,y \in \overline{Q}_\mu} |u_\lambda(x) - u_\lambda(y)| \leq C_\mu.$$

Conclusions and Future Work

- Deep Particle (DP) framework to compute and learn multi-scale PDEs with physical parameter dependence based on data from stochastic interacting particle (SIP) systems.
- Learned and generated complex phenomena of FKPP in 3D flows.
- Computed 1st eigenvalue of advection dominated reaction-diffusion operators on $\mathbb{R}^d$ ($d = 16$) by SIP with linear complexity.
- Integrated two-person game and PDE method for existence of average curvature dependent front speeds in cell flows.
- Ongoing/future: (1) DP for reaction-diffusion models with interacting particle description arising in cancer cell spreading. (2) curvature G-equation in 3D: non-existence of $\bar{H}_+$ in shear flow $V = (0, 0, A\, f(x_1, x_2))$ if A exceeds a finite value, i.e. averaging fails in some direction (Mitake, Mooney, Tran, X, Yu, '23).