Lagrangian Approximations and Computations of Effective Diffusivities and Front Speeds in Chaotic and Stochastic Volume Preserving Flows

Jack Xin

Department of Mathematics

University of California, Irvine.

Collaborators and Acknowledgements

- Junlong Lyu
- Zhongjian Wang
- Zhiwen Zhang

  at Hong Kong University.

- Partially supported by NSF.

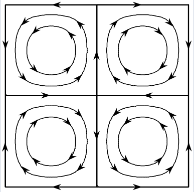
Outline

- Ordered and Chaotic Volume Preserving Flows.
- Enhanced Diffusivity, Mixing and Residual Diffusivity.
- Structure Preserving Methods and Discrete Corrector Problems
- Lagrangian Computation of Effective Diffusivity in 3D Chaotic and Stochastic Flows.
- Kolmogorov-Petrovsky-Piskunov (KPP) Front Speed and HJ.
- Feymann-Kac Representation and Genetic Particle Approximation.
- KPP Front Speed in Time Periodic 3D Kolmogorov Flow.
- Conclusions and Future Work.

Cellular (Beltrami-Childress) Flow

- 2D steady cellular (Hamiltonian) flow:

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



- 2D time periodic cellular flow:

$$\boldsymbol{V}(x,y,t) = (\cos(y) + \theta \sin(y)\cos(t), \cos(x) + \theta \sin(x)\cos(t)),$$

$\theta \in (0,1]$. As θ increases, more and more disorder appears in flow trajectories.

Mixing at $\theta = 1$: snapshots of Lagrangian particles.

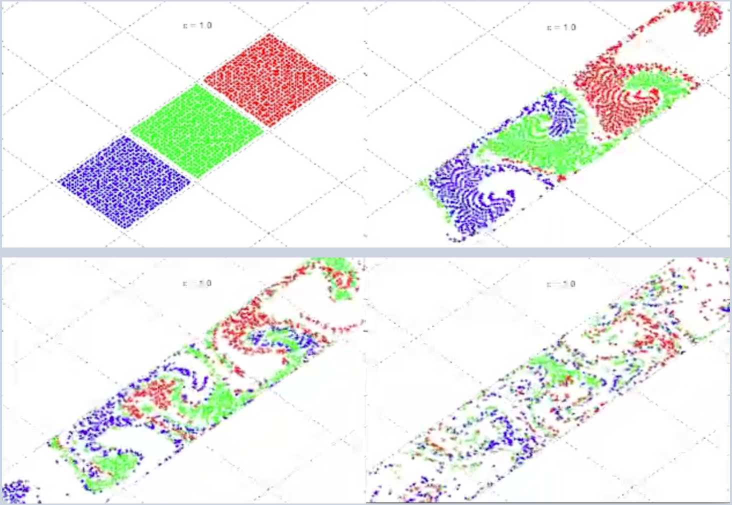


Figure: Courtesy T. McMillen, Cal State Univ. Fullerton.

Arnold-Beltrami-Childress Flows

- Originated in the 1960's:

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

right hand side is a steady state of 3D Euler equation, with dynamic instability (S. Friedlander et al '93: $A = 1, B^2 + C^2 > 1$ or $B, C \ll 1$).

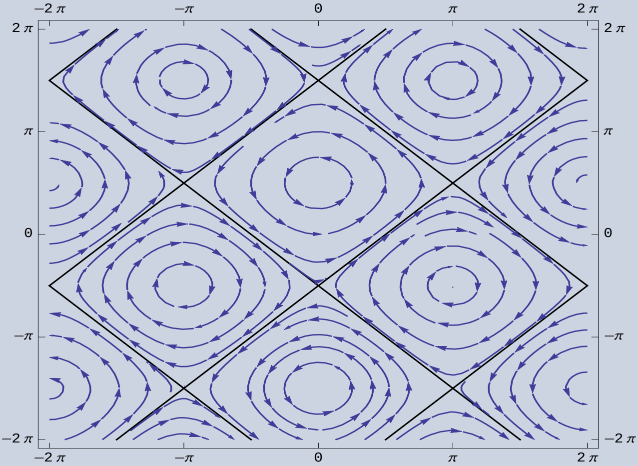
- Another form:

$$\begin{pmatrix} x \\ y \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \nabla H(x,y) + A \begin{pmatrix} \sin z \\ \cos z \end{pmatrix}$$

$$z' = H(x,y) := B\cos x + C\sin y.$$

Integrable (a cellular flow) if A or B or $C = 0$.

Integrable Flow on xy-Plane when $A = 0$



Exact ballistic solution: $(x, y, z) = (0, \pi/2, (B + C)t)$.

Ballistic Spiral Orbit with $(x, y)(t)$ Trapped in a Cell

• When $(x, y)(t)$ stay within a cell, z' does not change sign, implying helical motion with linear growth in z. If $A \ll 1$, the system is a perturbed Hamiltonian in 3 dimensions.

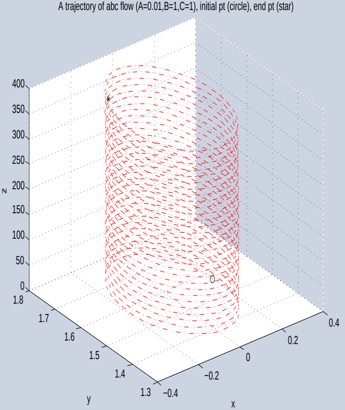
• Contraction mapping principle yields:

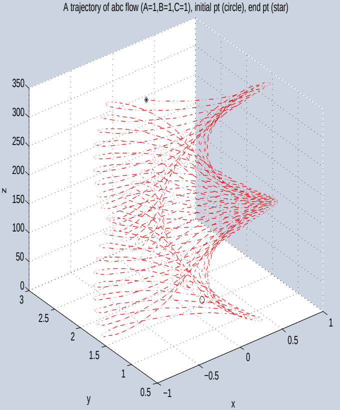
Theorem (McMillen,X,Yu,Zlatos; SIAD 2016)

$\exists$ positive number $A_0 = A_0(B, C)$ s.t. $\forall A \in [0, A_0]$ and $z(0) \in \mathbb{R}$, there is a smooth ABC trajectory $(x, y, z)(t)$ where z is increasing in t, the limit $\lim_{t\to\infty} z(t)/t$ exists and converges to $B + C$ as $A \to 0$, and (x, y) is 2π-periodic in z.

• Quasi-periodic orbits $(x, y)(z)$ exist from a modifed KAM theory based on an action-angle-angle formulation. Higher harmonics, where (x, y) is $2m\pi$-periodic in z, $m \geq 2$, exist by Melnikov method.

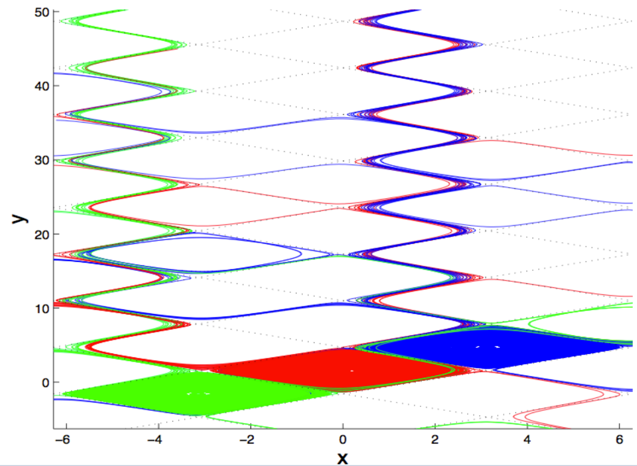
Spiral Orbits: initial pt $(0.2, \pi/2, 0)$ (circle), $A = 0.01(L), 1(R); B = C = 1$; linear growth in z.





Edge Orbits: moving along cell edges on the projected xy-plane, $(A, B, C) = (0.1, 1, 1)$.

Initial position $(x, y)(0)$ close to cell edge. Ballistic motion in x and/or y.



Existence of Mod (2π) Periodic Edge Orbits

Theorem (McMillen,X,Yu,Zlatos, SIAD 2016)

If $A \in (0, A_0]$, $A_0 = A_0(B, C)$ is small enough, there exists $T > 0$ and 4 edge orbits $X(t) = (x, y, z)(t)$ such that

$$\begin{aligned} X(t+T) &= X(t) \pm (2\pi, 2\pi, 0) \\ X(t+T) &= X(t) \pm (2\pi, -2\pi, 0). \end{aligned} \quad (1)$$

Likewise, there exists $T > 0$ and 4 edge orbits $X(t) = (x, y, z)(t)$, s.t.

$$\begin{aligned} X(t+T) &= X(t) \pm (2\pi, 0, 0) \\ X(t+T) &= X(t) \pm (0, 2\pi, 0). \end{aligned} \quad (2)$$

- Edge orbits (2) exist when $A = B = C = 1$ by a **non-perturbative symmetry argument** (X,Yu,Zlatos, SIMA 2016).
- Edge orbits do not exist in the integrable case (e.g. $A = 0$).

ABC and Kolmogorov Flows

- ABC flow has both ordered (ballistic orbits and nearby trajectories, so called vortex tubes) and disordered trajectories (Arnold '65; Hénon '66; Dombre, Frisch, Greene, Hénon, Mehr & Soward '86; ...).
- Vortex tubes in ABC believed to cause maximally enhanced transport.

- Kolmogorov flow (Galloway & Proctor '92, Childress & Gilbert '95):

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

  much more chaotic (visible on Poincaré section) than ABC.
  Disorder dominates order in K flow.

- Ballistic orbits in K flow: Tabrizian, X, Yu (in preparation).
- Quantitative measure of chaos: effective diffusivity.

Effective Diffusivity

- **Lagrangian**. Let $\sigma > 0$, and $\boldsymbol{X}_t$ solve SDE:

$$d\boldsymbol{X}_t = \boldsymbol{V}(t, \boldsymbol{X}_t)\, dt + \sigma\, d\, \boldsymbol{W}_t \qquad (3)$$

  $\boldsymbol{W}_t$: Wiener process. Along $\boldsymbol{e} = (1, 0, \cdots, 0)$, *effective diffusivity is:*

$$D^E = \lim_{t\uparrow+\infty} E[|(\boldsymbol{X}_t - \boldsymbol{X}_0)\cdot \boldsymbol{e}|^2]/(2t)$$

  (known in physics as: Einstein formula. In turbulent diffusion: G.I. Taylor, 1923; simplified models, Majda and Kramer, 1999.)
- **Eulerian.** Let $\boldsymbol{\chi}$ be the unique mean zero time periodic solution of:

$$L\boldsymbol{\chi} := \partial_\tau \boldsymbol{\chi} + (\boldsymbol{V}\cdot\boldsymbol{\nabla}_y)\,\boldsymbol{\chi} + D_0\,\Delta_y \boldsymbol{\chi} = -\boldsymbol{V}(\tau, y), \;\; (\tau, y) \in \mathbb{T}\times\mathbb{T}^d, \; d \geq 2,$$

  corrector (cell) problem (Bensoussan, J-L. Lions, Papanicolaou, 1978),

$$D^E = D_0 + \langle \chi^1\, v^1 \rangle = D_0\,(1 + \langle |\nabla\chi^1|^2 \rangle),$$

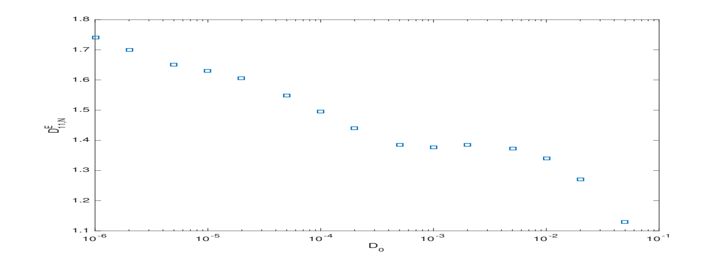
  $D_0 := \sigma^2/2$, the molecular diffusivity; $\langle\cdot\rangle :=$ space time periodic average, $\boldsymbol{V} = (v^1, \cdots, v^d)$, $\boldsymbol{\chi} = (\chi^1, \cdots, \chi^d)$.

Enhanced Diffusivity, Mixing and Residual Diffusivity

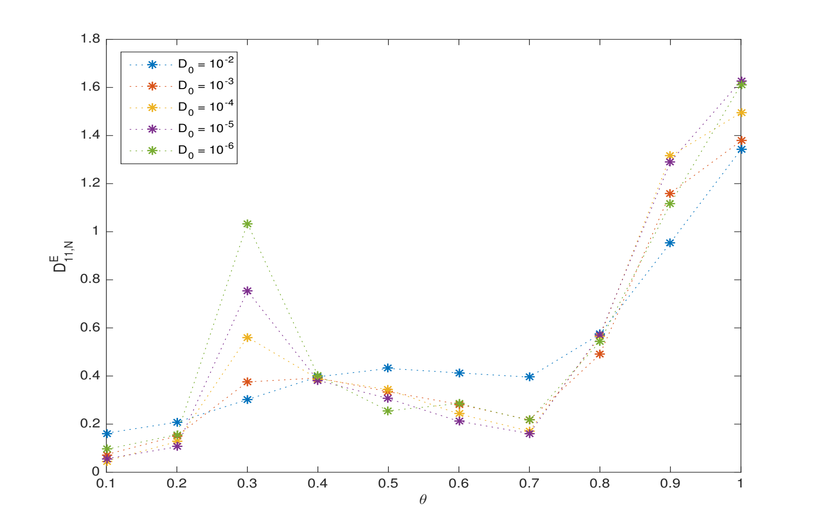
- 2D steady BC flow (Eulerian analysis): $D^E = O(\sqrt{D_0}), \quad \text{as } D_0 \downarrow 0.$
  Childress ('79, boundary layer), Fannjiang and Papanicolaou ('94, variational analysis), Heinze ('03, corrector analysis).
  Lagrangian computation: Pavliotis, Stuart, and Zygalakis,'09.
- 2D time per. mixing flow (num. evidence of **Residual Diffusivity**):

$$D^E = O(1), \quad \text{as } D_0 \downarrow 0, \quad \theta = 1.$$

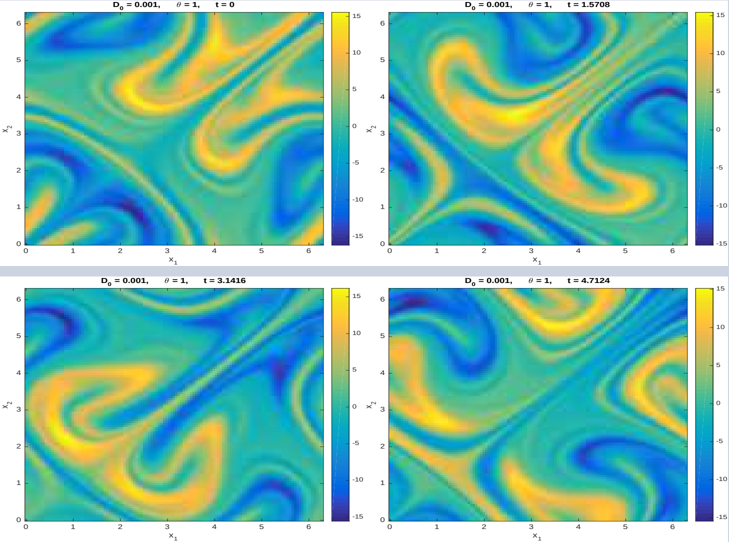
  Biferale, Crisanti, Vergassola, Vulpiani ('95)
  Lyu-X-Yu ('17, spectral method, Figs. below and subsequent).



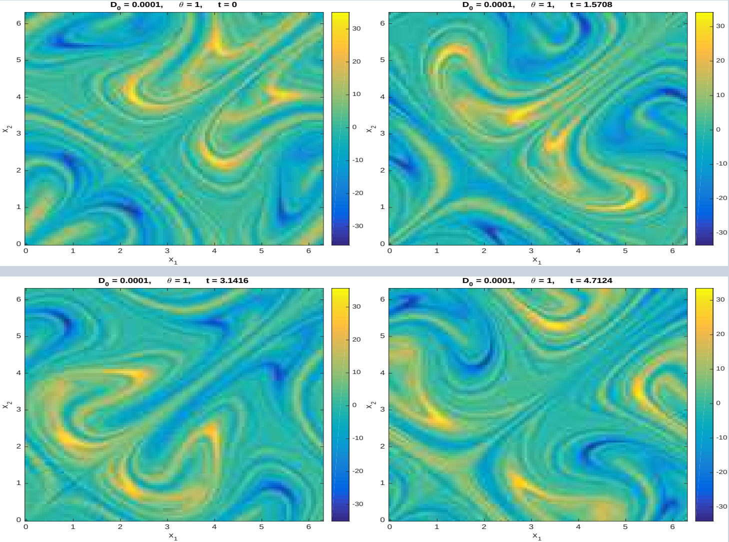
Resonance Phenomenon of Residual Diffusivity in θ



Thin Layers in Snapshots of Corrector at $D_0 = 10^{-3}$



Thinner Layers in Snapshots of Corrector at $D_0 = 10^{-4}$



Structure Preserving Discretization

- The SDE with divergence free advection $\boldsymbol{V}$:

$$d\,\boldsymbol{X}_t = \boldsymbol{V}(t, \boldsymbol{X}_t)\,d\,t + \sigma\,d\,\boldsymbol{W}_t$$

  has uniform invariant measure π_u on the torus $\mathbb{R}^d/\mathbb{Z}^d$ $(d \geq 2)$.
- Let $\boldsymbol{X}_i = (x_i^1, \cdots, x_i^d)$; $i = 0, 1$. Explicit update from $\boldsymbol{X}_0$ to $\boldsymbol{X}_1$ is:

$$\begin{cases} x^{1*} = x_0^1 + \Delta t\, v^1(\frac{\Delta t}{2}, x_0^2, x_0^3, \cdots, x_0^{d-1}, x_0^d) \\ x^{2*} = x_0^2 + \Delta t\, v^2(\frac{\Delta t}{2}, x^{1*}, x_0^3, \cdots, x_0^{d-1}, x_0^d) \\ \cdots\ \cdots\ \cdots \\ x^{d*} = x_0^d + \Delta t\, v^d(\frac{\Delta t}{2}, x_0^{1*}, x_0^{2*}, x_0^{3*}, \cdots, x^{(d-1)*}) \\ \boldsymbol{X}_1 = \boldsymbol{X}^* + \sigma\,\boldsymbol{W}_1 \end{cases}$$

  $\boldsymbol{W}_1$: random vector w. independent entry $\sqrt{\Delta t}\,\xi_j$, ξ_j unit Gaussian.
- The scheme has discrete invariant measure $\pi_{\Delta t} \approx \pi_u$. Deterministic part is volume-preserving or symplectic (K. Feng & Z. Shang, 1995).

Lagrangian Approximation of Effective Diffusivity

Theorem (Wang,X,Zhang '19)

Let $p_n := x_n^1$ be the first component of structure preserving scheme with time step Δt. Let $\boldsymbol{V} = (v^1, \cdots, v^d)(t, \boldsymbol{X})$ be periodic and separable in the sense that v^i does not depend on x^i, $\forall i = 1, \cdots, d$. Then the limit $\lim_{n\to\infty} E[p_n^2]/(2\, n\, \Delta t)$ exists and approximates the effective diffusivity D^E along $\boldsymbol{e} = (1, 0, \cdots, 0)$ with the estimate:

$$\left| \lim_{n\to\infty} E[p_n^2]/(2\, n\, \Delta t) - D^E \right| \leq C\, \Delta t, \quad C \text{ independent of } \Delta t.$$

- In computation, fix Δt and find end time $T = N\Delta t$ so that $E[p_N^2]/(2\, T)$ tends to a constant P which may depend on Δt. The above theorem ensures that P converges to D^E as $\Delta t \downarrow 0$ at a first order rate independent of T.

- Proof casts structure preserving updates as a discrete Markov process, and relates $E[p_n^2]/(2\, n\, \Delta t)$ to the corrector formula of D^E.

Lagrangian Approximation of Effective Diffusivity

- Let $I_{\Delta t,\tau}$ be the density evolution operator of the discrete Markov process generated by the scheme from τ to $\tau + \Delta t$. Let time period be 1, and $\Delta t = 1/N$. Then $(I_{\Delta t,\tau})^n$ converges weakly to an invariant measure $\pi_{\Delta t,\tau}$ on bounded measurable functions on $\mathbb{T}^d$.
- Taking expectation of the 1st eqn of the scheme gives:

$$\begin{aligned} E[x_n^1] &= E[x_{n-1}^1] + \Delta t\, E[v^1(t_{n-1/2}, x_{n-1}^2, \cdots)] \\ &= E[x_0^1] + \Delta t \sum_{k=0}^{n-1} E[v^1(t_{k+1/2}, x_k^2, \cdots)] \end{aligned}$$

motivating the function below in calculating $E[p_n^2]$:

$$\hat{v}_N^1(\tau, x) := \Delta t \sum_{i=0}^{\infty} E[v^1(t_{i+1/2} + \tau, \boldsymbol{X}_i) | \boldsymbol{X}_0 = x].$$

Convergence of infinite sum follows from that of $\pi_{\Delta t,\tau}$.

Discrete Cell Problem (DCP)

- Let v^1 have zero mean over space, then $\hat{v}_N^1(\tau, x)$ is the unique bounded space-time mean zero solution of the DCP equation on $\hat{\chi} = \hat{\chi}(\tau, x)$:

$$(I_{\Delta t,\tau}\, \hat{\chi})(\tau, x) - \hat{\chi}(\tau, x) = -\Delta t\, v^1(\tau + \frac{\Delta t}{2}, x).$$

- Eulerian cell problem gives:

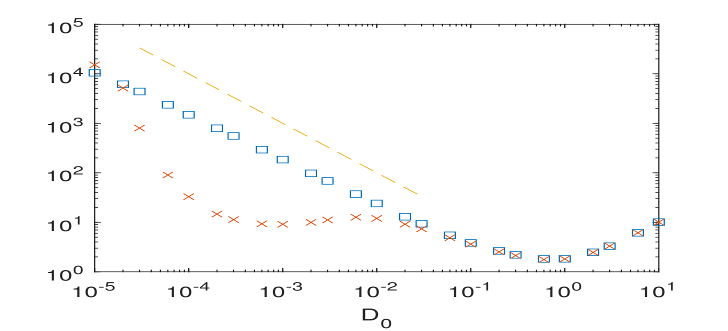
$$\exp\{\Delta t\, L\}\chi^1 - \chi^1 = -\Delta t\, v^1 + O((\Delta t)^2).$$

- $I_{\Delta t,\tau}$ is a 2nd order operator splitting of $\exp\{\Delta t L\}$.
- Example ($d = 2$):

$$I_{\Delta t,\tau} = \exp\{\Delta t\, L_4\} \exp\{\frac{\Delta t}{2} L_1\} \exp\{\Delta t\, L_3\} \exp\{\Delta t\, L_2\} \exp\{\frac{\Delta t}{2} L_1\}.$$

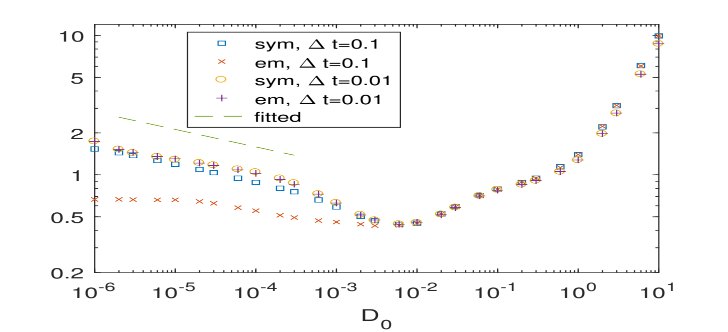
$$L_1 = \partial_\tau,\; L_2 = v^1 \partial_{y_1},\; L_3 = v^2 \partial_{y_2},\; L_4 = D_0\, \Delta_y.$$

Enhanced Diffusivity in ABC Flow: $D^E = O(D_0^{-1})$.



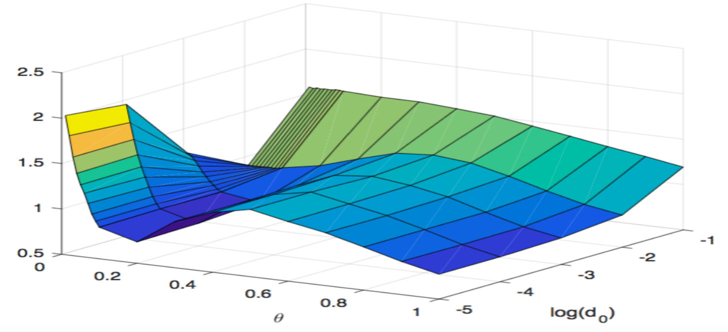
- Maximal enhancement ($A = B = C = 1$): □ structure preserving method, $\times$ Euler's method, $--$ reference line $y = \frac{1}{D_0}$. No. of particles = 120,000; $\Delta t = 0.001$; end time $T = 12000$.
- Robustness of ballistic orbits in the presence of weak Gaussian noise.

Enhanced Diffusivity in K Flow: $D^E = O(D_0^{-0.13})$.



- Sub-maximal enhancement in K flow: "sym" = structure preserving method, "em"= Euler's method, $--$ reference line to fit $y = D_0^{-0.13}$.
- No. of particles = 120,000; end time $T = 12000$.
- Strong Lagrangian chaos: some "remnant structures" in absence of "channels" or "vortex tubes" ?

D^E in time periodic K Flow.



- Time periodic Kolmogorov flow:

$$(\sin(z + \theta \sin 2\pi t), \sin(x + \theta \sin 2\pi t), \sin(y + \theta \sin 2\pi t)).$$

- Resonance in θ is prominent at small D_0.
- Sub-maximal enhancement: $D^E = O(D_0^{-0.2})$, at $\theta = 0.1$.

Time-Mixing Markovian Volume Preserving Flows

- Stationary ergodic in space: prob. space (Ω, F, P_0), with measure preserving group action $\tau_{\boldsymbol{x}}$, $P_0(\tau_{\boldsymbol{x}}(A)) = P_0(A)$, $\forall A \in F$; $P_0(\tau\text{-invariant event})=0$ or 1.
- Let P^t $(t \geq 0)$ be a strongly continuous Markov semigroup on $L^2(\Omega)$: $P^t \mathbf{1} = \mathbf{1}$, positivity and P_0-preserving.
- Random flow $\boldsymbol{b} = \boldsymbol{b}(t, \boldsymbol{x}, \omega) = b(\tau_{\boldsymbol{x}} \omega(t)) \in (L^2(\Omega))^d$ is continuous in $(t, \boldsymbol{x})$, loc. Lipschitz in $\boldsymbol{x}$, divergence-free, finite 2nd moment.
- Let L be the generator of P^t, the corrector problem is $(\kappa = \sigma^2/2)$:

$$\mathcal{L}\psi := (L + \boldsymbol{b} \cdot \nabla + \kappa \, \Delta)\boldsymbol{\psi} = -\boldsymbol{b},$$

  admitting a unique solution in $\mathrm{Dom}(L) \cap C_b^2(\Omega)$ (stationary corrector) under fast time-mixing.
- For each realization ω of the flow, consider SDE:

$$d\, \boldsymbol{X}_t^{\omega} = \boldsymbol{b}(t, \boldsymbol{X}_t^{\omega}, \omega)\, dt + \sigma \, d\boldsymbol{W}_t, \quad \boldsymbol{X}_0^{\omega} = \mathbf{0}.$$

Time-Mixing Markovian Volume Preserving Flows

- Homogenization (Fannjiang & Komorowski '99): let $\boldsymbol{e}$ be a unit vector, the process $\epsilon\, \boldsymbol{e}^T \boldsymbol{X}^{\omega}_{t/\epsilon^2}$ converges weakly to a Brownian motion as $\epsilon \downarrow 0$ with diffusivity:

$$\boldsymbol{e}^T D^E \boldsymbol{e} := \kappa + (-\mathcal{L}\psi \cdot \boldsymbol{e}, \psi \cdot \boldsymbol{e})_{L^2(\Omega)}.$$

- Split out $\sigma\, d\boldsymbol{W}_t$ and adopt a volume-preserving integrator on the flow $\boldsymbol{b}$:

$$\boldsymbol{X}^{\omega}_{n+1} = \boldsymbol{\Phi}^{\omega(t_n)}_{\Delta t}(\boldsymbol{X}^{\omega}_n),$$

  $\omega(t_n)$ refers to realization of $\boldsymbol{b}$ at times $t_n = n\Delta t$.
- Due to lack of separability of $\boldsymbol{b}$ in general, $\boldsymbol{\Phi}^{\omega(t_n)}_{\Delta t}$ is implicit.
- Example ($d = 2$):

$$\boldsymbol{X}^{\omega}_{n+1} = \boldsymbol{X}^{\omega}_n + \Delta t\, \boldsymbol{b}(t_n, mean(\boldsymbol{X}^{\omega}_n, \boldsymbol{X}^{\omega}_{n+1}), \omega).$$

Time-Mixing Markovian Volume Preserving Flows

- In $d \geq 3$, decompose $\boldsymbol{b}$ into a sum of $d-1$ velocity fields, each of them equivalent to a two-component problem (Feng & Shang '95).
- Environment processes (view from the particle position):

$$\eta_t := \tau_{\boldsymbol{X}_t^\omega} \omega(t), \quad \eta_n := \tau_{\boldsymbol{X}_n^\omega} \omega(t_n)$$

- Strongly continuous Markov semigroup on $L^2(\Omega)$ with generator $\mathcal{L}$:

$$S_t f = \mathbb{E}[f(\eta_t] := M\, E_\Omega[f(\eta_t)], \; S_n f := \mathbb{E}[f(\eta_n)], \quad M\; w.r.t.\; W$$

representing solution to corrector problem as:

$$\boldsymbol{\psi} = \int_0^\infty S_t\, \boldsymbol{b}\, dt.$$

- Define:

$$\boldsymbol{B}_{\Delta t} := \boldsymbol{\Phi}_{\Delta t}^{\omega(t_n)}(\boldsymbol{X}_n^\omega) - \boldsymbol{X}_{\boldsymbol{n}}^{\boldsymbol{\omega}}, \; \bar{\boldsymbol{B}}_{\Delta t} = \mathbb{E}[\boldsymbol{B}_{\Delta t}].$$

Time-Mixing Markovian Volume Preserving Flows

- The function

$$\psi_{\Delta t} = \sum_{n=0}^{\infty} S_n \left(\boldsymbol{B}_{\Delta t} - \bar{\boldsymbol{B}}_{\Delta}\right),$$

is the unique zero mean solution in $(L^2(\Omega))^d$ to the discrete corrector problem:

$$(S_1 - I)\, \psi_{\boldsymbol{\Delta t}} = -(\boldsymbol{B}_{\Delta t} - \bar{\boldsymbol{B}}_{\Delta}).$$

Theorem (Lyu,Wang,X,Zhang, '19)

For time-mixing Markovian volume preserving random flow $\boldsymbol{b}$, $\exists\, p \in (0,1)$,

$$\lim_{n\to+\infty} (2n\,\Delta t)^{-1}\, \mathbb{E}[(\boldsymbol{X}_n^{\omega} - n\bar{\boldsymbol{B}}_{\Delta t}) \otimes (\boldsymbol{X}_n^{\omega} - n\bar{\boldsymbol{B}}_{\Delta t})] = D^E + o((\Delta t)^p).$$

Time-Mixing Markovian Volume Preserving Flows

- Random Fourier representation:

$$\boldsymbol{b}(t,\boldsymbol{x}) = \frac{1}{\sqrt{M}} \sum_{m=1}^{M} [\boldsymbol{u}_m \cos(\boldsymbol{k}_m \cdot \boldsymbol{x}) + \boldsymbol{v}_m \sin(\boldsymbol{k}_m \cdot \boldsymbol{x})], \quad \boldsymbol{x} \in \mathbb{R}^3$$

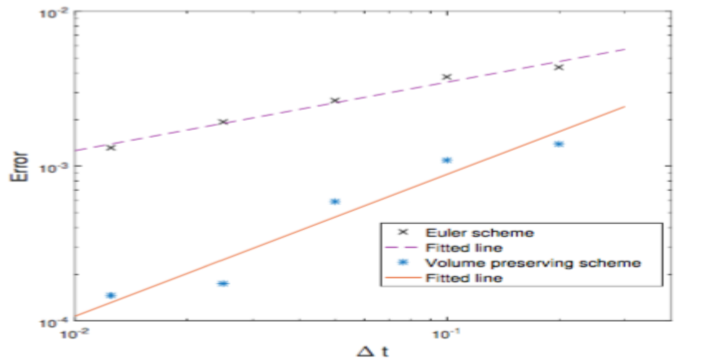
  $\boldsymbol{k}_m$'s are independent with directions unif. distributed on unit sphere, lengths (r) in the interval $[0, K]$ with density $\propto r^{1-2\alpha}$, $\alpha \in (0.5, 1)$, to mimic energy spectrum of physical flows. K ultraviolet cut-off, $M = 100$, $K = 10$, $\alpha = 0.75$ in simulation.

- Time-Mixing Markovian: let $\boldsymbol{\xi}_m(t)$, $\boldsymbol{\eta}_m(t)$ be independent 3D random vectors with components being independent stationary OU process having covariance function $\exp\{-\theta|t_1 - t_2|\}$, $\theta > 0$.
- Volume Preserving:

$$\boldsymbol{u}_m = \boldsymbol{\xi}_m(t) \times \boldsymbol{k}_m/|\boldsymbol{k}_m|, \ \boldsymbol{v}_m = \boldsymbol{\eta}_m(t) \times \boldsymbol{k}_m/|\boldsymbol{k}_m|.$$

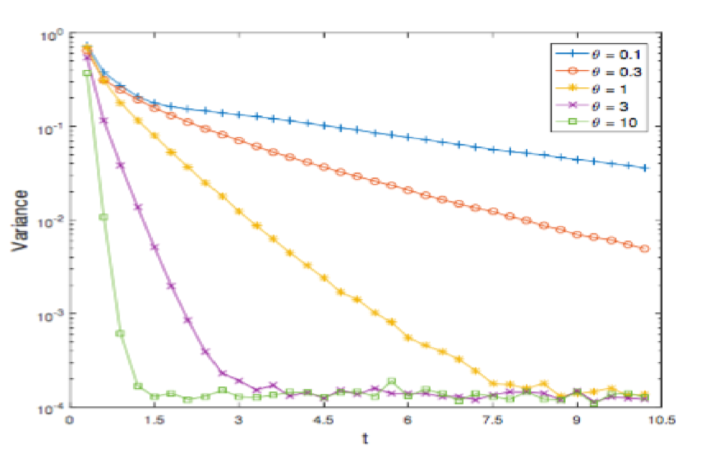
Time-Mixing Markovian Volume Preserving Flows

- Reference solution: $\Delta t_{ref} = 0.003125$, $T = 40$, $\sigma = 0.1$, $\theta = 4$, with $N_{mc} = 100,000$ (no. of Monte-Carlo realizations), resulting in $D_{11}^E = 0.2266$. Comparison runs: $N_{mc} = 50,000$.
- Compare error $(O(\Delta t)^p)$ in computing D_{11}^E: p of Euler scheme $= 0.44$, of volume preserving scheme $= 0.86$.



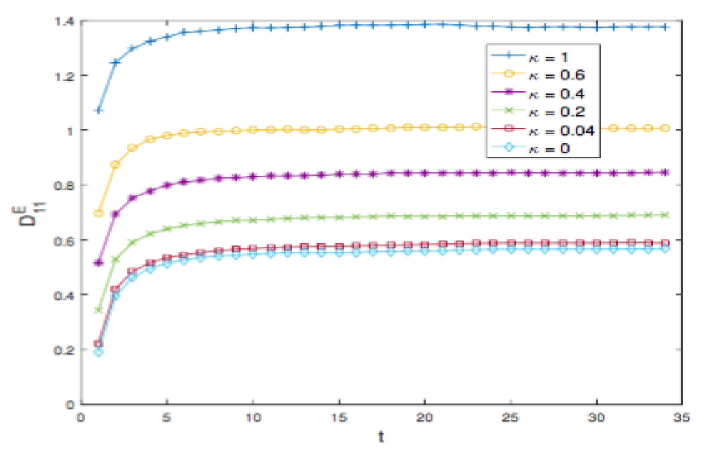
Time-Mixing Markovian Volume Preserving Flows

Larger θ, less temporal correlation, faster decay of variance of D_{11}^E approximation in time.



Time-Mixing Markovian Volume Preserving Flows

Let $\kappa = \sigma^2/2$, $\theta = 1$, $\Delta t = 0.05$, observed convergence of $D^E_{11}(\kappa)$ to $D^E_{11}(0) > 0$ as κ approaches 0 (Fannjiang & Komorowski '99).



KPP Variational Formula in Stationary Ergodic Media

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

where $\boldsymbol{B}$ is space-time stationary ergodic, mean zero, div-free. To calculate front speed c^* along direction $\boldsymbol{e}$, let w solve linear equation parameterized by $\lambda > 0$:

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

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.

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

Space periodic media: Gärtner & Freidlin '79. Space-time periodic flow: Nolen, Rudd, X, '05. Space-time stationary ergodic flow: Nolen, X, '09.

Viscous HJ and Effective Hamiltonian

$v := \lambda\, \boldsymbol{e} \cdot x + \ln w$, a plane wave at large time, solves viscous HJ equation:

$$v_t = \kappa\, \Delta\, v + \kappa\, |\nabla v|^2 + \boldsymbol{B}(t, x) \cdot \nabla v + 1,$$

and $\mu(\lambda)$ is its homogenized (effective) Hamiltonian.

• Stochastic homogenization of viscous HJs (convex & uniformly coercive):
space: P-L Lions, Souganidis, '05; Kosygina, Rezakhanlou, Varadhan '06.
space-time: Kosygina, Varadhan, '08; Schwab, '09.
KPP problem in space-time random $\boldsymbol{B}$ (Nolen, X, '09): uniform coercivity relaxed to a finite 2nd moment condition (allowing unbounded $\boldsymbol{B}$).

• Prior KPP Computations based on Linearized Corrector (w) Equation:

1) space-time stationary ergodic ($d = 2$), semi-Lagrangian (Nolen, X, '08).
2) adaptive FEM (Shen, X, Zhou, '13): 3D steady periodic flows, ABC flow & maximal speed enhancement.
3) residual speed in time-periodic mixing cellular flow ($d = 2$): edge-averaged FEM w. algebraic multigrid acceleration (Zu, Chen, X, '15).

Lagrangian Approximation in Space-Time Periodic Media

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

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

  Feymann-Kac formula gives:

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

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

- 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 Media

- An altenative is to study a "normalized version", the Feymann-Kac semi-group:

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

  acting on any initial probability measure ν, converges weakly to an invariant measure ν_c as $t \to \infty$, for any test function ϕ. Moreover,

$$P_t^c(\nu_c) = \exp\{\mu\, t\}\,\nu_c.$$

- Discretize $\boldsymbol{X}_s^{t,\boldsymbol{x}}$ as $\boldsymbol{X}_i^{\Delta t}$, approximate the evolution of probability measure $\Phi_t^c(\nu)$ by a particle system, and use resampling technique to reduce variance.

Lagrangian Approximation in Space-Time Periodic Media

- Let

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

- As $n \to \infty$, the discrete semi-group

$$\Phi_n^{c,\Delta t}(\nu)(\phi) = \frac{P_n^{c,\Delta t}(\nu)(\phi)}{P_n^{c,\Delta t}(\nu)(1)} \to \int_D \phi\, d\,\nu_{c,\Delta t}, \quad \forall \text{ smooth } \phi,$$

D is the space-time periodic cell, $\nu_{c,\Delta t}$ is invariant measure.

Theorem (Lyu, Wang, X, Zhang, '20)

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

$$\mu_{\Delta t} := \frac{1}{\Delta t} \ln[P_1^{c,\Delta t}(\nu_{c,\Delta t})(1)] = \mu + o((\Delta t)^p).$$

Genetic Algorithm

- Initialize first generation of N particles $\boldsymbol{\xi}_1^0 = (\xi_1^{0,1}, \cdots, \xi_1^{0,N}) \in (\mathbb{T}^d)^N$, 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 replicates m-times, with a life span T (time period), time step $\Delta t = T/m$.

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

Genetic Algorithm

- Feymann-Kac (F-K) semigroup, particle method of its invariant measure and principal eigenvalue, are well-known in physics, large deviation, sequential/population/diffusion Monte Carlo.
- Ferré & Stoltz, '19: error estimates of discrete F-K and particle approximation in spatially periodic media.
- 3D time periodic Kolmogorov flow with large amplitude A:

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

- By scaling property of D^E and computed exponent,

$$D^E(A) = A\,D^E(A^{-1}) = O(A^{1.2}).$$

- Scaling analysis of front speed linear growth rate:

$$\mathrm{LGR} := c^*(A)/A \approx \sqrt{D^E(A)}/A = O(A^{-0.4}),$$

suggesting sublinear (sub-maximal) growth law: $c^*(A) = O(A^{0.6})$.

Submaximal Growth of $c^*(A)$ $(A \gg 1)$ in K flow

- $G = 150$, $N = 800,000$, $\kappa = 3$, $\Delta t = 2^{-7} = 0.0078$, Euler on $\boldsymbol{X}^{\Delta t}$.

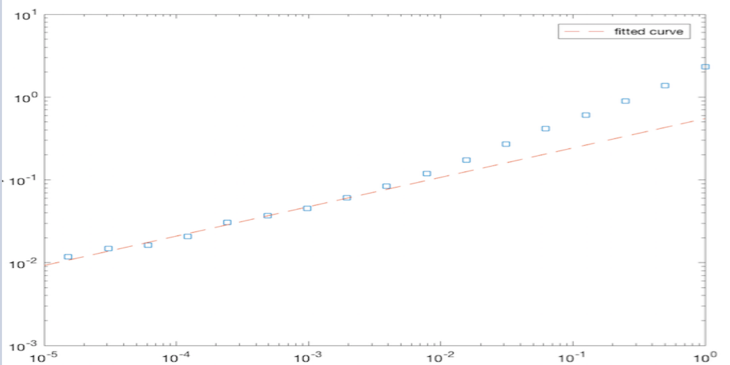


Figure: Linear growth rate (LGR=$c^*(A)/A$) vs. A^{-1}.

- Computed $\mathrm{LGR} = O(A^{-0.35}) \to c^*(A) = O(A^{0.65})$.

Conclusions and Future Work

- Developed Lagrangian methods and their approximation theory for computing effective diffusivity and front speed in high dimensional volume preserving chaotic/stochastic flows.
- Explored discrete corrector approximations of continuous PDE corrector problems via volume-preserving schemes /genetic particle evolution algorithm.
- Enhanced diffusivity in chaotic flows shows a myriad of scalings near small molecular diffusivity, and poses interesting open problems for analysis.
- Ongoing work: genetic algorithm for KPP fronts in random media.
- Future work: 1) generate adaptive initial measure to speed up genetic computation with deep learning tools, 2) transport in rough flows.