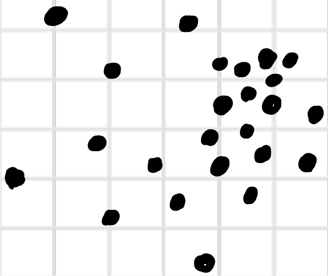
Perspective: Computational methods for coherence and transport based on transfer operators

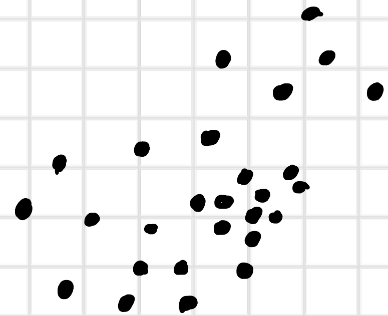
Oliver Junge
Center for Mathematics
Technische Universität München

X state space, $\dot{x} = v(x)$



flow map

φ^t

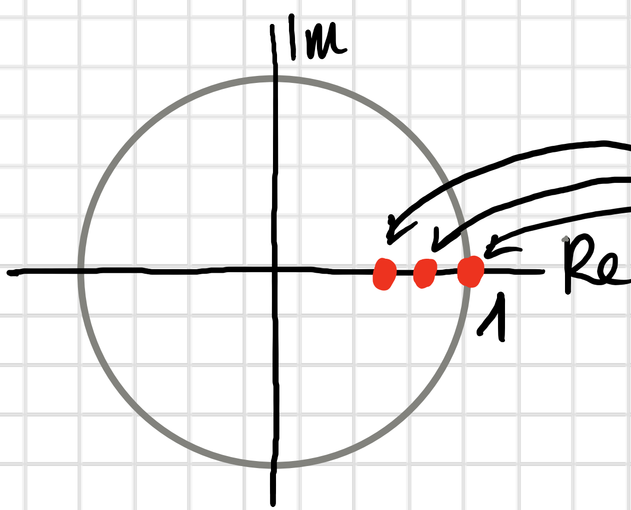


transfer operator

$x_i \sim \mu$

$\varphi^t(x_i) \sim \mu \circ \varphi^{-t} =: \varphi^t_* \mu$

spectrum of φ^t_*



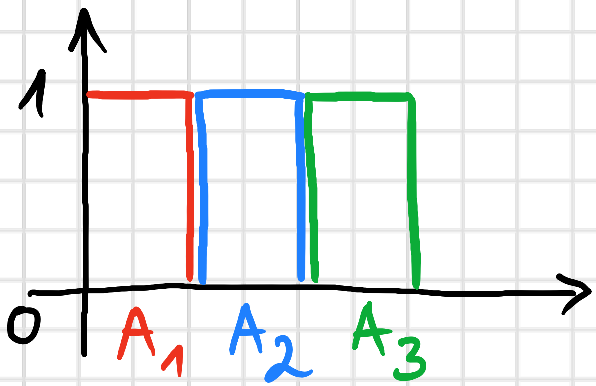
important eigenfunctions

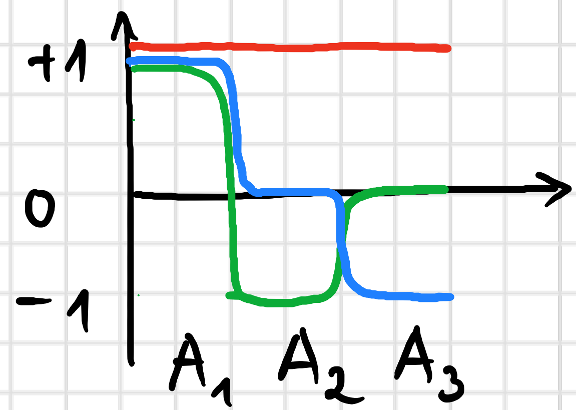
Almost Invariant Sets

P^t has k-fold eigenvalue 1 $\xrightarrow{\text{perturbation}}$ P^t has k eigenvalues close to 1 (including 1)

basis: $1_{A_1}, 1_{A_2}, \dots, 1_{A_{k-1}}$

basis: $u_1, u_2, \dots, u_{k-1}$





$$1_{A_1} \approx \frac{1}{3}(u_1 + u_2 + u_3)$$

[Dellnitz, Junge, 99]

GALERKIN DISCRETIZATION

eigenproblem

$$\varphi_*^t u = \lambda u \quad , \quad u \in U$$

choose subspace $V \subset U$, V finite dimensional

discrete eigenproblem : find $u \in V$, $\lambda \in \mathbb{C}$ s.t.

$$\langle \varphi_*^t u, v \rangle = \lambda \langle u, v \rangle \quad \text{for all } v \in V$$

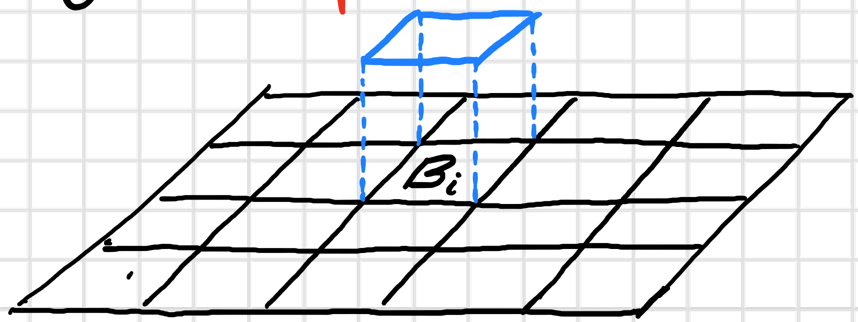
matrix

$$\langle \varphi_*^t v_i, v_j \rangle =: P_{ij}^t$$

$$\approx \varphi_*^t$$

ULAM'S METHOD [Ulam, 60]

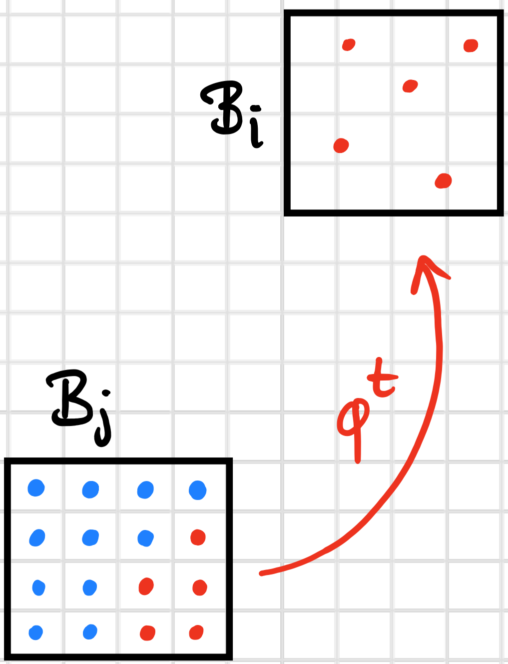
… is choosing V = piecewise constant functions



$$P^t_{ij} = \langle \varphi^t_* \chi_i, \chi_j \rangle$$

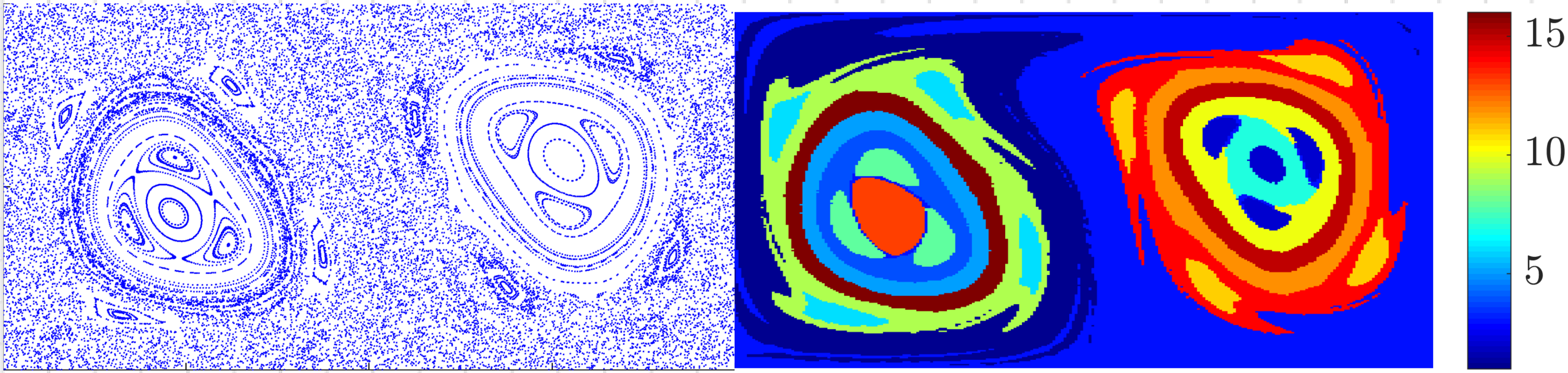
$$= \text{probability to go from } B_j \text{ to } B_i$$

$$\approx \sum_k \chi_i(\varphi^t(x_k)) \quad , \quad x_k \in B_j$$



- simple, robust – but slow
- software : GAIO

example: double gyre



convergence [Li 76], [Ding, Du, Li, 82], [Froyland, 95], ...

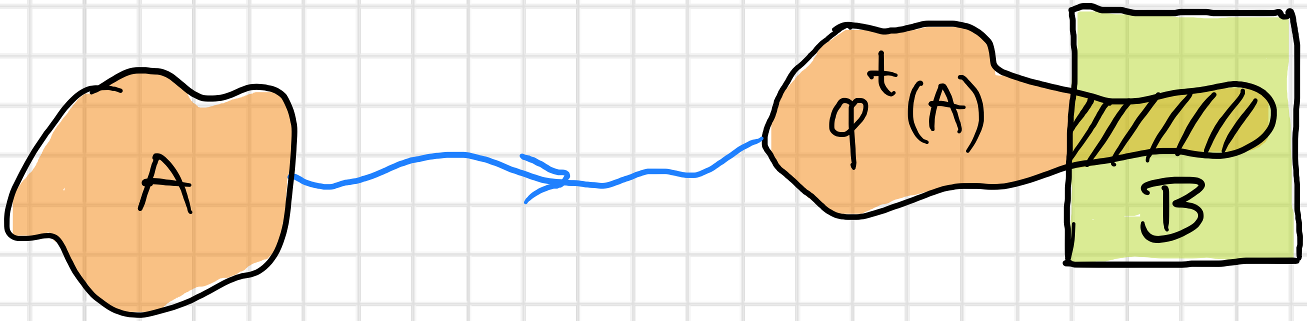
higher order [Ding, Du, Li, 86 – ...]

clustering of eigenfunctions [Deuflhard, Huisinga, Schmidt]

exhaustion technique [Dellnitz, Kreuzer, 99]

Petrov–Galerkin [Aston, J, 09]

TRANSPORT RATES



$$m\left(\varphi^t(A) \cap B\right) \approx \mathbb{1}_B^T P^t \mathbb{1}_A$$

[Dellnitz, J., Padberg, et al 05]

[Marsden, Ross, 09]

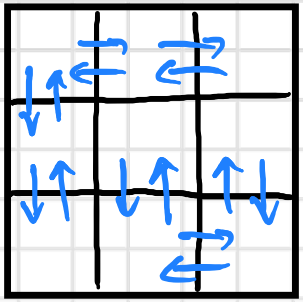
[Balasuriya, Froyland, Santitisadeekorn, 14]

THE GENERATOR OF φ_*^t

$$\frac{d}{dt}\varphi_*^t u = -\operatorname{div}(v u) =: G u$$

$\rightarrow$ compute eigenvectors of $-\operatorname{div}(v\,\cdot)$

via Ulam's method:



(finite volume scheme)

- simple and robust
- integrals have one dimension less
- sparse eigenproblem
- first order only
- large numerical diffusion, linked to cell size

[Froyland, J, Koltai, 13]

THE GENERATOR OF φ_*^t

via spectral collocation

$$\mathcal{G}u_j(x_i) = \lambda u_j(x_i), \qquad i = 1:N$$

with $u_j(x) = e^{-ijx}$, $j = 1:N$.

- very fast, spectral convergence
- dense eigenproblem
- only simple geometries
- needs explicit noise

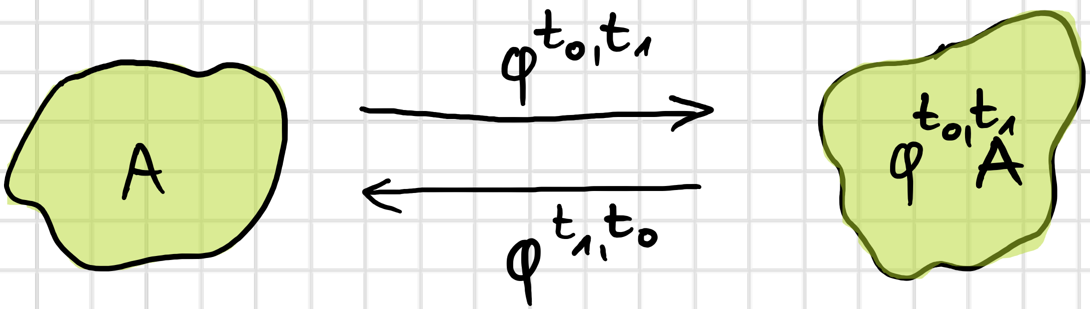
→ Fokker-Planck operator $\varepsilon\Delta u - \operatorname{div}(vu)$

[Froyland, J, Koltai, 13]

Finite Time Coherent Sets

now: $\dot{x} = v(t, x) \rightsquigarrow \varphi^{t_0, t_1}$

idea: consider $\varphi^{t_1, t_0} \circ \varphi^{t_0, t_1}$ (+ noise)



eigenvectors of $\varphi_*^{t_1,t_0} \varphi_*^{t_0,t_1}$ are singular vectors of $\varphi_*^{t_0,t_1}$

- standard methods apply
- needs noise (explicit or numerially induced)

[Froyland, Lloyd, Santitissadeekorn, '10]

DIRECT SOLUTION OF FOKKER-PLANCK

$\varphi_*^{t_0,t_1} u_0$ for noisy ODE is solution of

Fokker-Planck equation

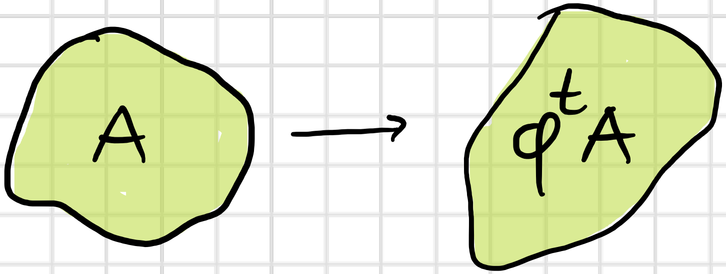
$$u_t = \varepsilon^2 \Delta u - \operatorname{div}(uv)$$

spectral discretization $\rightsquigarrow$ Δ = diagonal matrix

stiffness : linear implicit time-stepping

- no need to compute Lagrangian trajectories
- dense eigenproblem
- only simple geometries

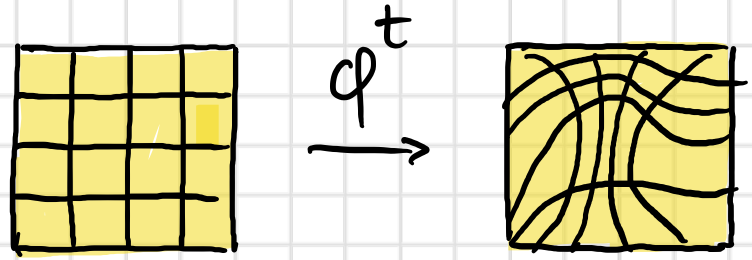
[Denner, J, Matthes, 16]



want $\frac{|\partial A|}{|A|}$ and $\frac{|\partial \varphi^t A|}{|\varphi^t A|}$ small

dynamic isoperimetry

[Froyland 15]



$$u_t = \Delta_t u$$

geometric heat flow

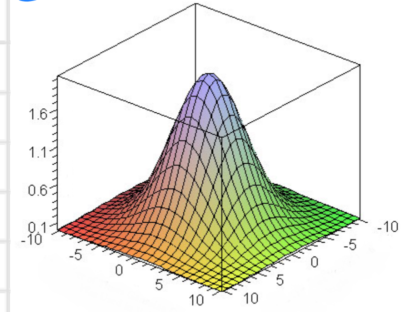
[Karrasch, Keller 16]

compute eigenvectors of $\frac{1}{2}\left(\Delta + \varphi_*^{-t}\Delta\varphi_*^{t}\right) =: \Delta^t$

- real and discrete spectrum
- no explicit artificial noise

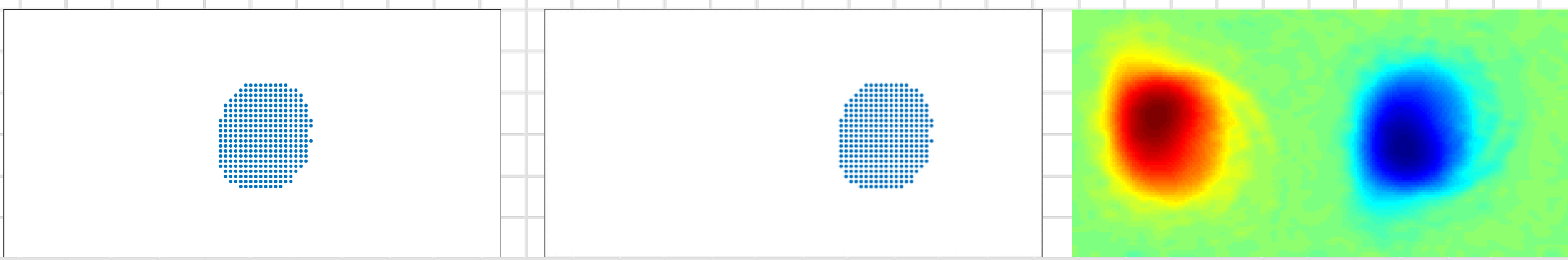
Collocation with Radial Basis Functions

$$u = \sum_k u_k \varphi_k \qquad \varphi_k =$$



$$\Delta^t u(x_i) \overset{!}{=} \lambda u(x_i) \quad , \quad i = 1:n$$

- very high order, sparse data suffices
- issues: free parameter, boundary conditions, ...



[Froyland, J 15], [Rowley et al, 15]

DISCRETIZATION BY FINITE ELEMENTS

$$\Delta^t u = \lambda u \quad + \text{ Neumann b.c.}$$

weak form, Galerkin, ...

$$D^t \tilde{u} = \lambda M \tilde{u}$$

two approaches:

(1) on inital domain only / using $D\varphi^t$
(2) on initial & final domain / without $D\varphi^t$

- sparse data suffices
- matrices sparse and symmetric ($\rightarrow$ real spectrum)
- no boundary conditions

[Froyland, J, Karrasch, in prep.]

Perspective

- 3D ✓
- higher-order elements ✓
- sparse spectral methods

Questions:

(1) How to combine with other diagnostics?

(2) How to make it fully „black-box"?

(3) Applications!

ALMOST INVARIANT SETS

$$p(A,B) = \frac{\langle \varphi_*^t 1_A, 1_B \rangle}{\langle 1_A, 1_A \rangle}$$

transition probability $A \to B$

Under certain assumptions on φ_*^t,

$$p(A_1,A_1) + \cdots + p(A_n,A_n) \leq 1 + \lambda_2 + \cdots + \lambda_n$$

$$1 + c_2\lambda_2 + \cdots + c_n\lambda_n \leq p(A_1,A_1) + \cdots + p(A_n,A_n)$$

where $c_j \approx 1$, if $u_i|_{A_\cdot} \approx$ constant.

Dellnitz, Junge, Huisinga, Schmidt, Deuflhard, Schütte, ...

- clustering

- William's / Rowley's ?

DMD^2