TRANSITORY TRANSPORT

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Madrid

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Aperiodic Time Dependence

- Phase space can no longer be "compactified" in time direction.

Strategies to identify coherent structures

- Look for local instability & distinguished hyperbolicity

  Haller, G. and A. C. Poje (1997). "Finite Time Transport in Aperiodic Flows." Physica D 119: 352-380.
  Shadden, S. C., F. Lekien, et al. (2005). "Definition and properties of Lagrangian coherent structures..." Phys. D 212(3-4): 271-304.
  Mancho, A. M., D. Small, et al. (2006). "A tutorial on ... Lagrangian transport..." Physics Reports 437(3-4): 55-124.

- Look for (Lagrangian) coherent structures (LCS)
  regions bounded by "material lines with locally the longest or shortest stability or instability time"

  Haller, G. and G. Yuan (2000). "Lagrangian coherent structures and mixing in two-dimensional turbulence." Phys. D 147: 352-370.

- Look for approximately invariant regions or "resonance zones"
  regions bounded by nearly invariant sets have small "flux" through boundaries...

  Froyland, G. and K. Padberg (2009). "Almost-invariant sets and invariant manifolds..." Physica D 238: 1507-1523.

- Look for "locally least stretching closed material lines"

  Haller, G. and Beron-Vera, J. (2012). "Geodesic Theory of Transport Barriers..." Physica D in press.

Transitory Dynamics

Past and Future autonomous dynamics:

$$\dot{x} = V(x,t)\ , \quad V(x,t) = \begin{cases} P(x) & t < 0 \\ F(x) & t > \tau \end{cases}$$

for a transition time τ.

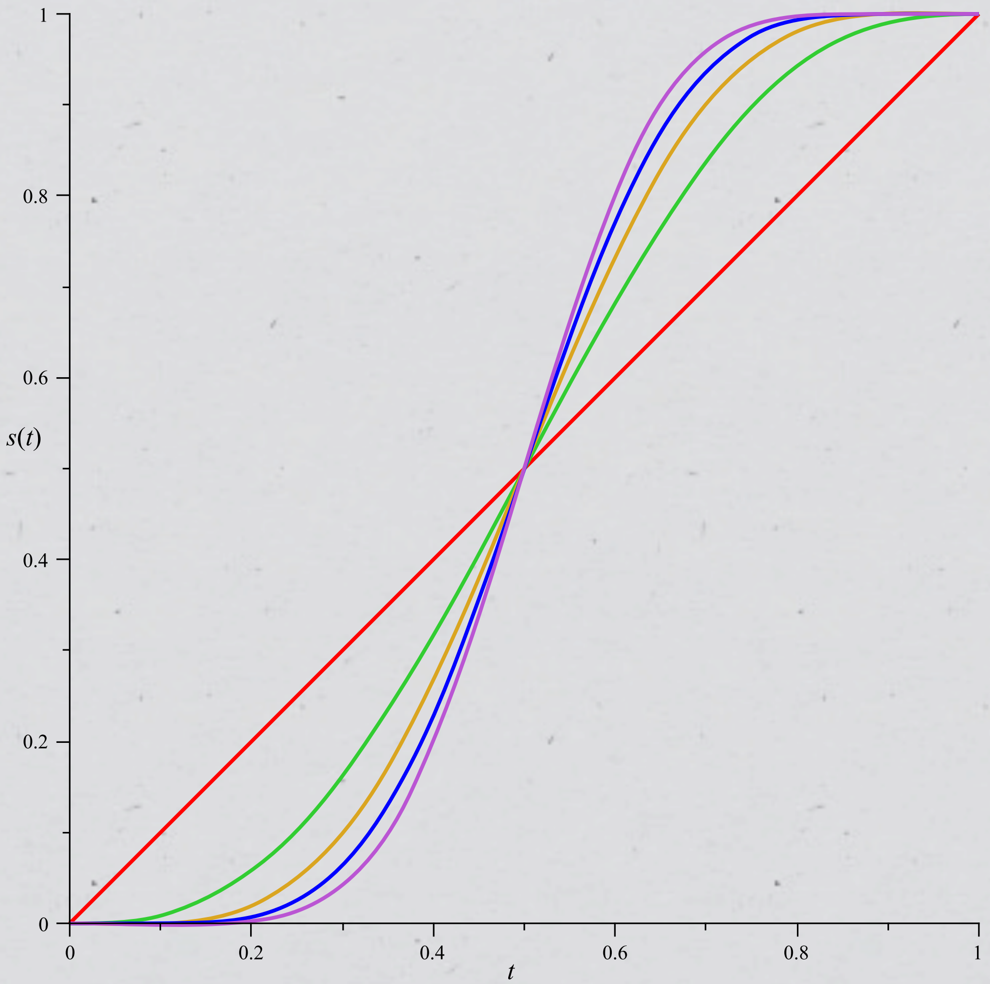
$$V(x,t) = (1 - s(t))P(x) + s(t)F(x)$$

- Transition function

$$s(t) = \begin{cases} 0 & t < 0 \\ 1 & t > \tau \end{cases}$$

- For example:

$$s(t) = \frac{t^2}{\tau^2}\left(3 - 2\frac{t}{\tau}\right)$$

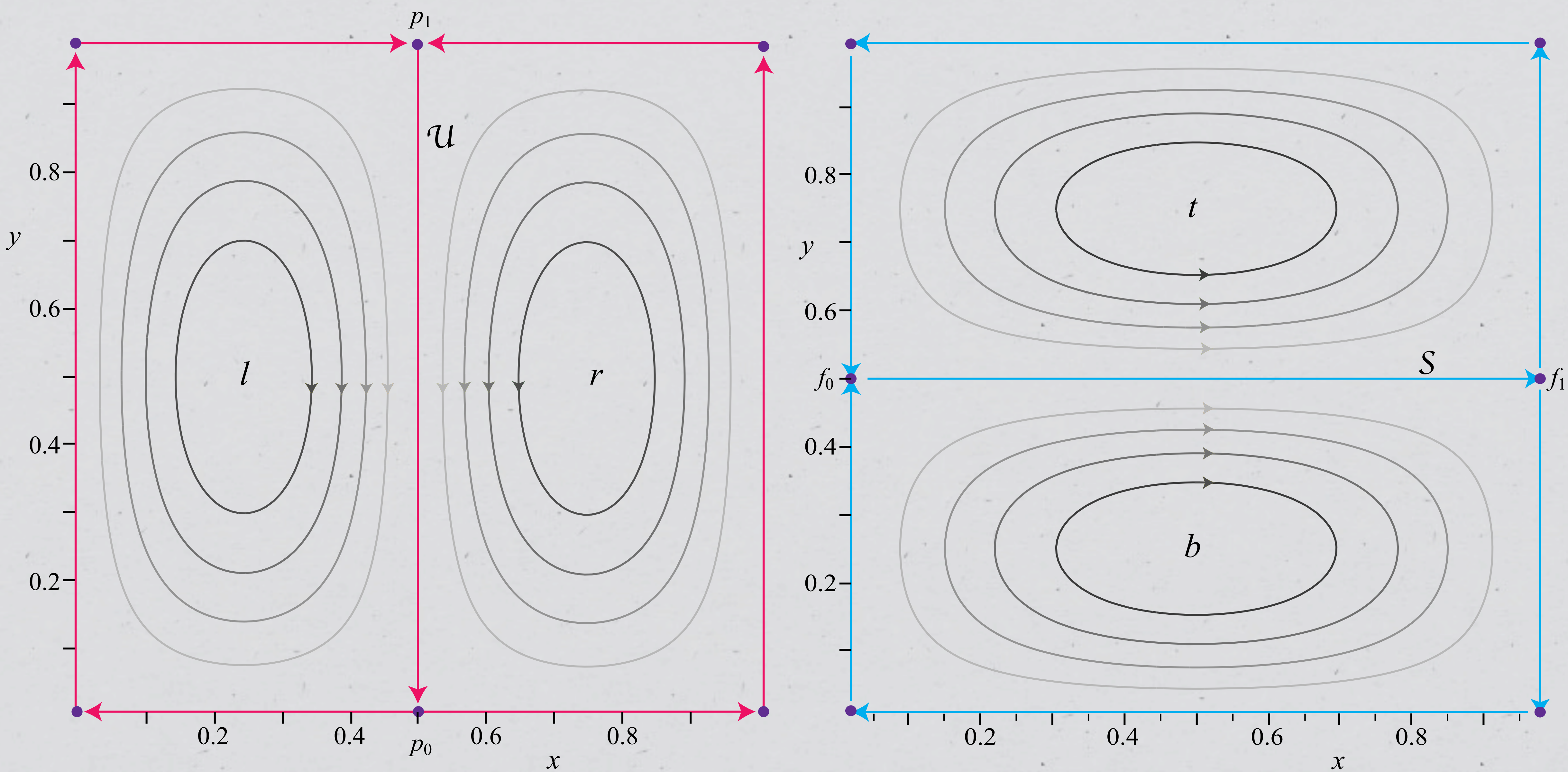


Polynomial $s(t)$

Rotating Double Gyre

Mosovsky, B. A. and J. D. Meiss (2011). "Transport in Transitory Dynamical Systems." SIAM J. Dyn. Sys. **10**(1): 35-65.

$$\psi_P(x,y) = \sin(2\pi x)\sin(\pi y) \qquad \psi_F(x,y) = \sin(\pi x)\sin(2\pi y)$$



$$\dot{x} = -\frac{\partial}{\partial y}\psi\,, \quad \dot{y} = \frac{\partial}{\partial x}\psi \qquad \psi = (1 - s(t))\psi_P + s(t)\psi_F$$

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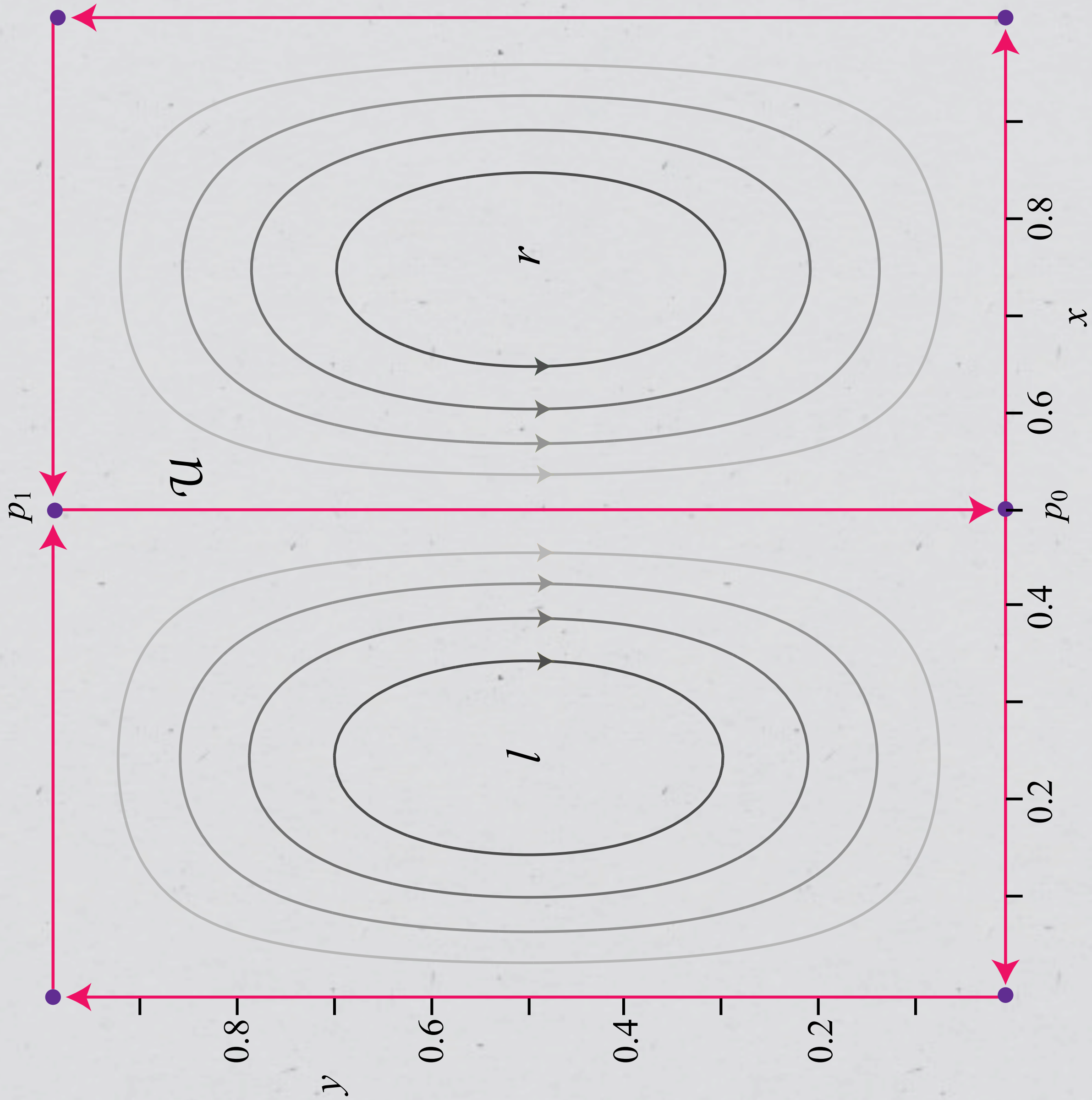
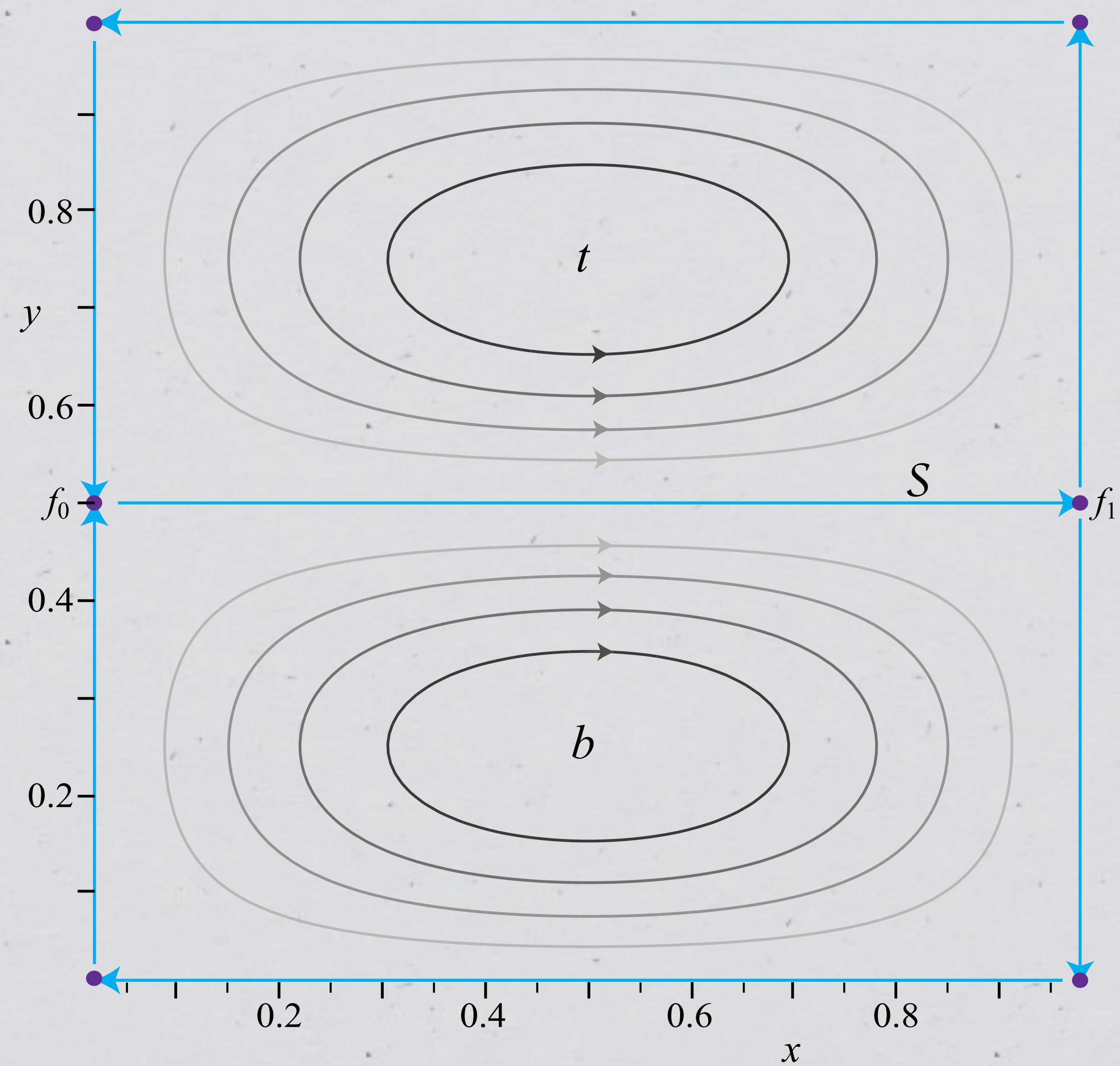




$$\dot{x} = -\frac{\partial}{\partial y}\psi\,, \quad \dot{y} = \frac{\partial}{\partial x}\psi \qquad \psi = (1 - s(t))\psi_P + s(t)\psi_F$$

Flow and Transition Map

Time Dependent Flow

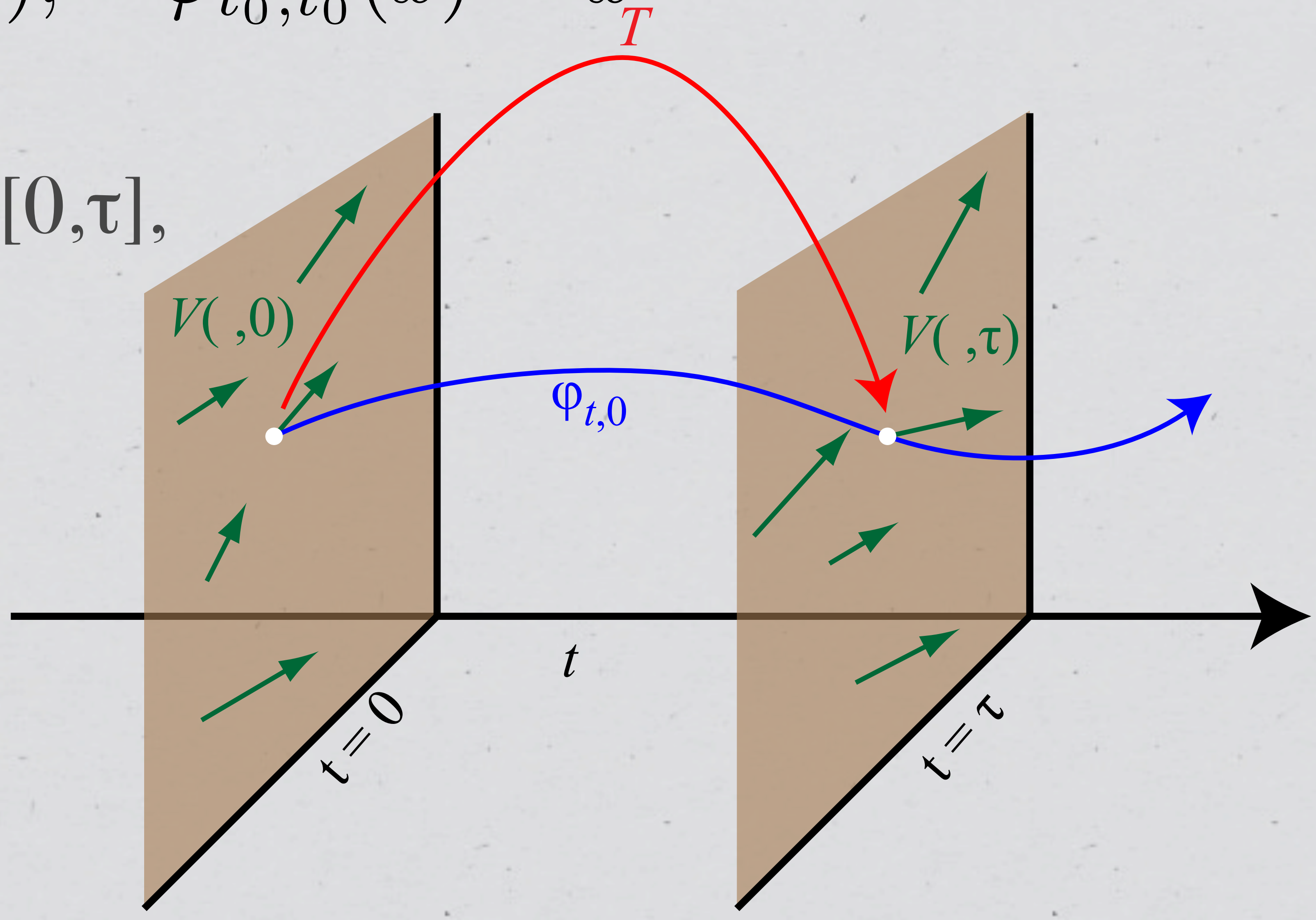
$$\frac{d}{dt}\varphi_{t,t_0}(x) = V(\varphi_{t,t_0}(x), t), \quad \varphi_{t_0,t_0}(x) = x$$

Since V is autonomous for $t \notin [0,\tau]$,

the *Transition map*

$$T = \varphi_{\tau,0}$$

encapsulates the switch



Similar case–Asymptotically Autonomous

see: Markus, L. (1956). Asymptotically Autonomous Differential Systems. Contributions to the Theory of Nonlinear Oscillations. S. Lefschetz. Princeton, Princeton Univ. Press. **3:** 17-29.

Samelson, R. M. and S. Wiggins (2007). Lagrangian transport in geophysical jets and waves : the dynamical systems approach. New York, Springer.

Adiabatic Case

Adiabatic theory for

- τ>> dynamical timescales
- uniform hyperbolicity*

E.g.: Kaper, T. J. and S. Wiggins (1991). "Lobe Area in Adiabatic Hamiltonian Systems." Physica D **51**: 205-212.

Tracking contours
with varying τ

* not satisfied here!

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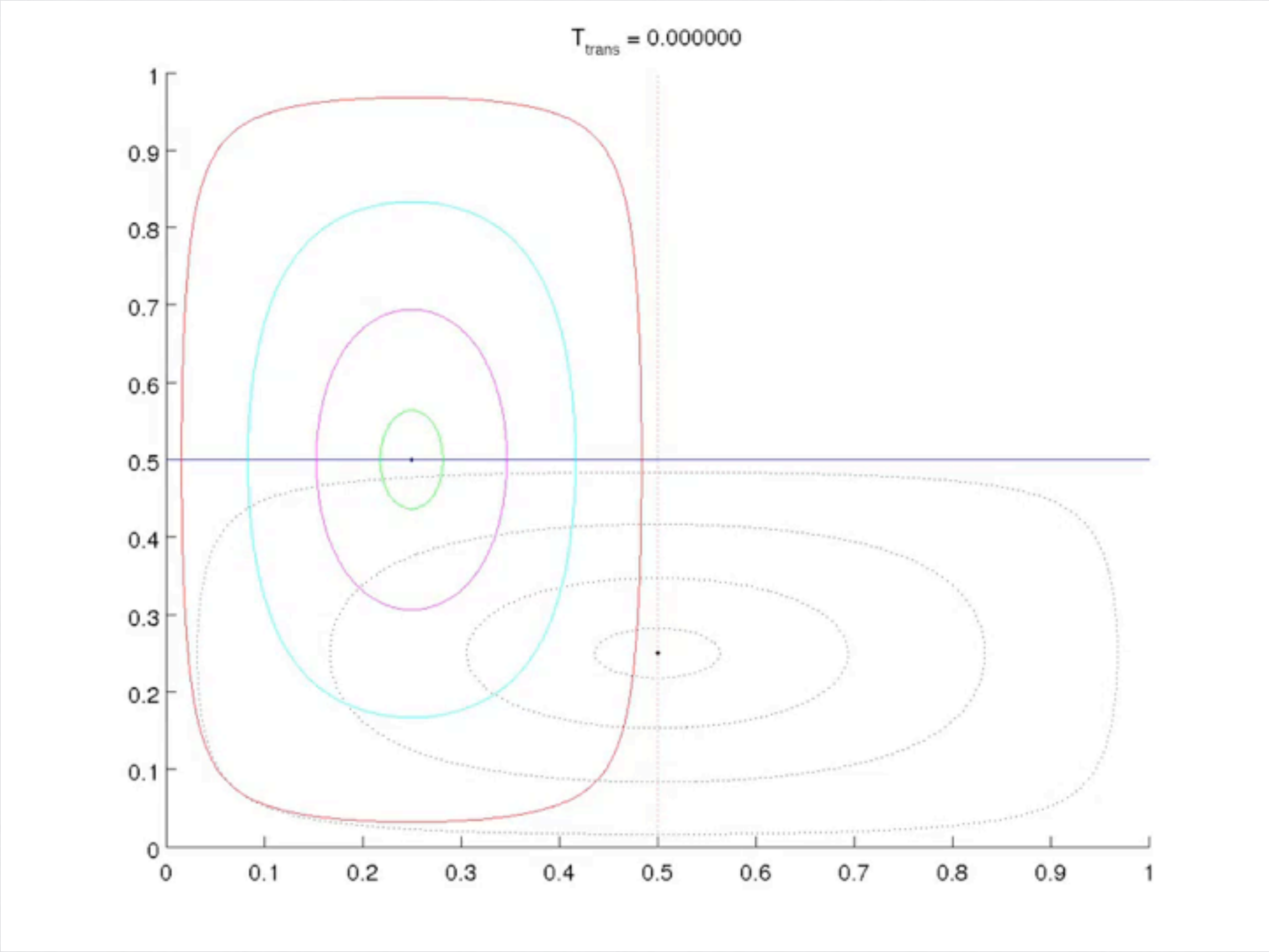

* not satisfied here!

Past & Future Hyperbolicity

Slice: $\Lambda_s = \Lambda \cap \{t = s\}$

- past invariant if $\Lambda_s = \Lambda_0$ for all $s < 0$
- future invariant if $\Lambda_s = \Lambda_\tau$ for all $s > \tau$

Invariant Manifolds

$$W_\tau^u(\Lambda) = \{x \in M : \lim_{t \to -\infty} |\varphi_{t,\tau}(x) - \Lambda_t| = 0\},$$

$$W_\tau^s(\Lambda) = \{x \in M : \lim_{t \to \infty} |\varphi_{t,\tau}(x) - \Lambda_t| = 0\}$$

An invariant set Λ is

- past hyperbolic if, for $t < 0$, it is a hyperbolic set of P
- future hyperbolic, if for $t > \tau$, it is a hyperbolic set of F

Past & Future Hyperbolicity

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- past invariant if $\Lambda_s = \Lambda_0$ for all $s < 0$
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Invariant Manifolds

$$W^u_\tau(\Lambda) = \{x \in M : \lim_{t\to-\infty} |\varphi_{t,\tau}(x) - \Lambda_t| = 0\},$$

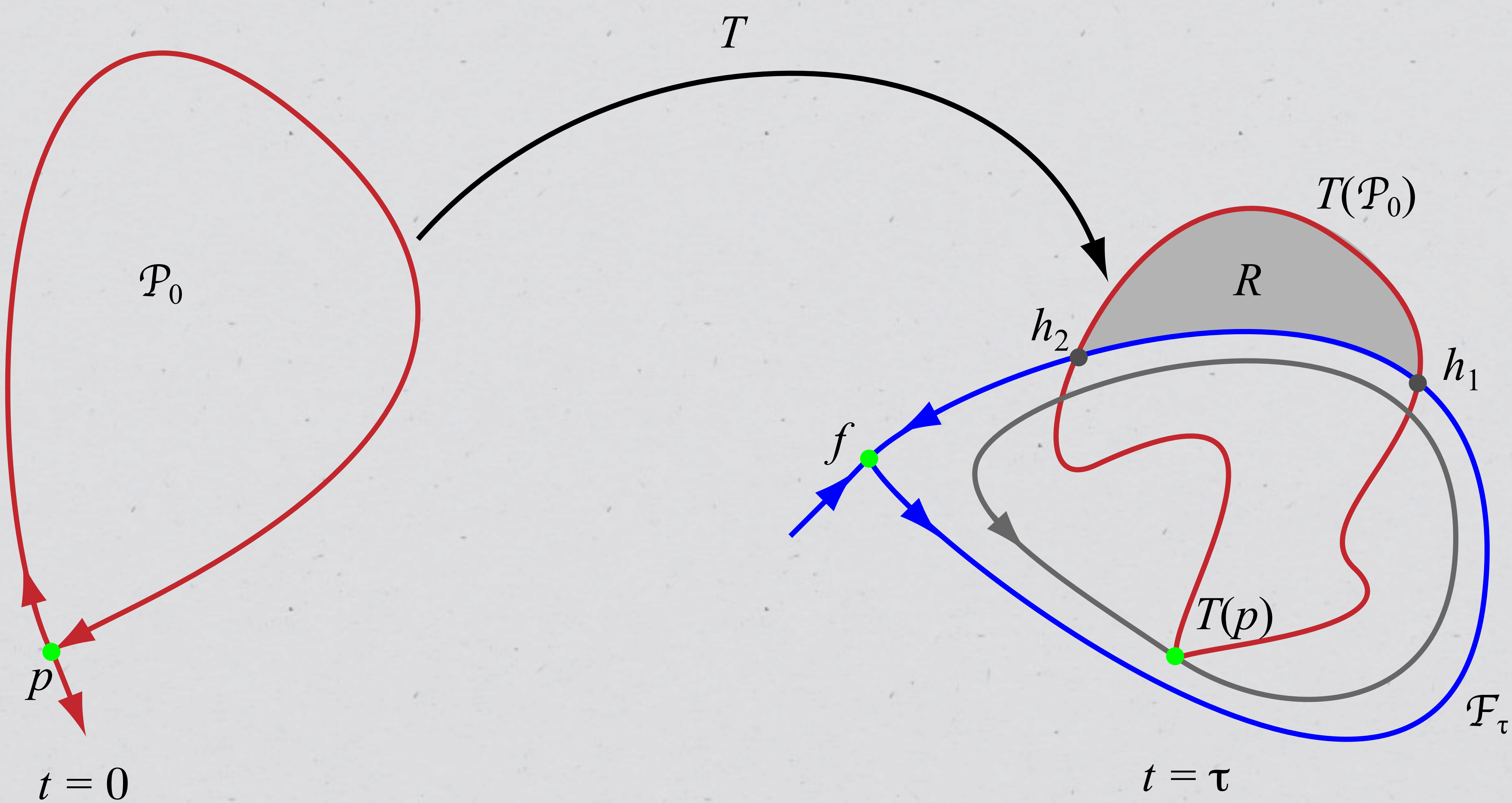
$$W^s_\tau(\Lambda) = \{x \in M : \lim_{t\to\infty} |\varphi_{t,\tau}(x) - \Lambda_t| = 0\}$$

Unstable: look into the past

An invariant set Λ is

- past hyperbolic if, for $t < 0$, it is a hyperbolic set of P
- future hyperbolic, if for $t > \tau$, it is a hyperbolic set of F

Past & Future Hyperbolicity



→ Past-hyperbolic fixed point p with homoclinic loop $\partial\mathcal{P} \subset W^u(p, P)$

→ Future-hyperbolic fixed point f with homoclinic loop $\partial\mathcal{F} \subset W^s(f, F)$

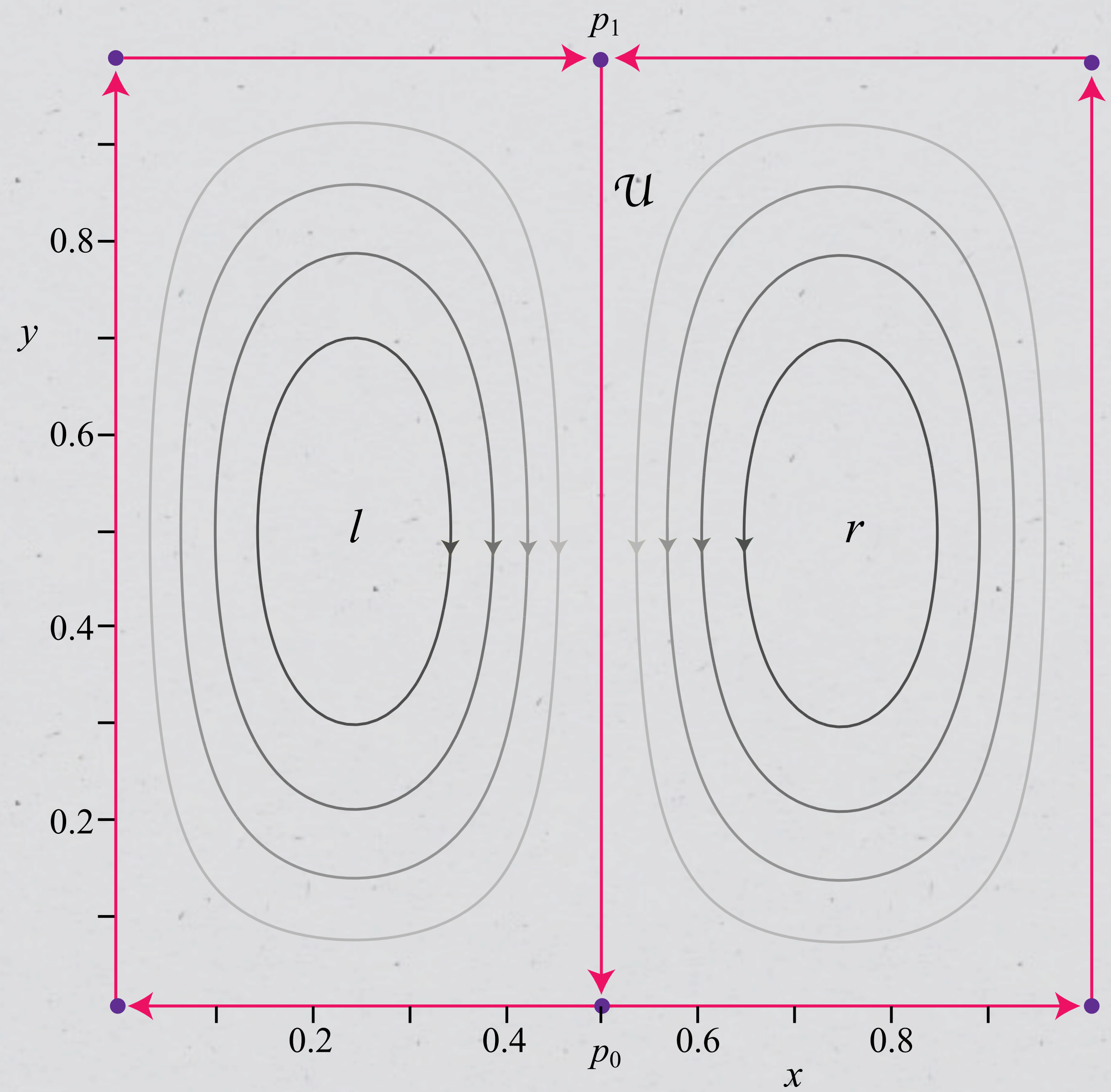
→ Heteroclinic points h_1 and $h_2 \subset \partial P_\tau \cap \partial\mathcal{F}_\tau$ under a transitory flow V.

Rotating Double Gyre

Past Vector field:
Unstable Manifolds

6 past hyperbolic saddles

What is $T(U)$?

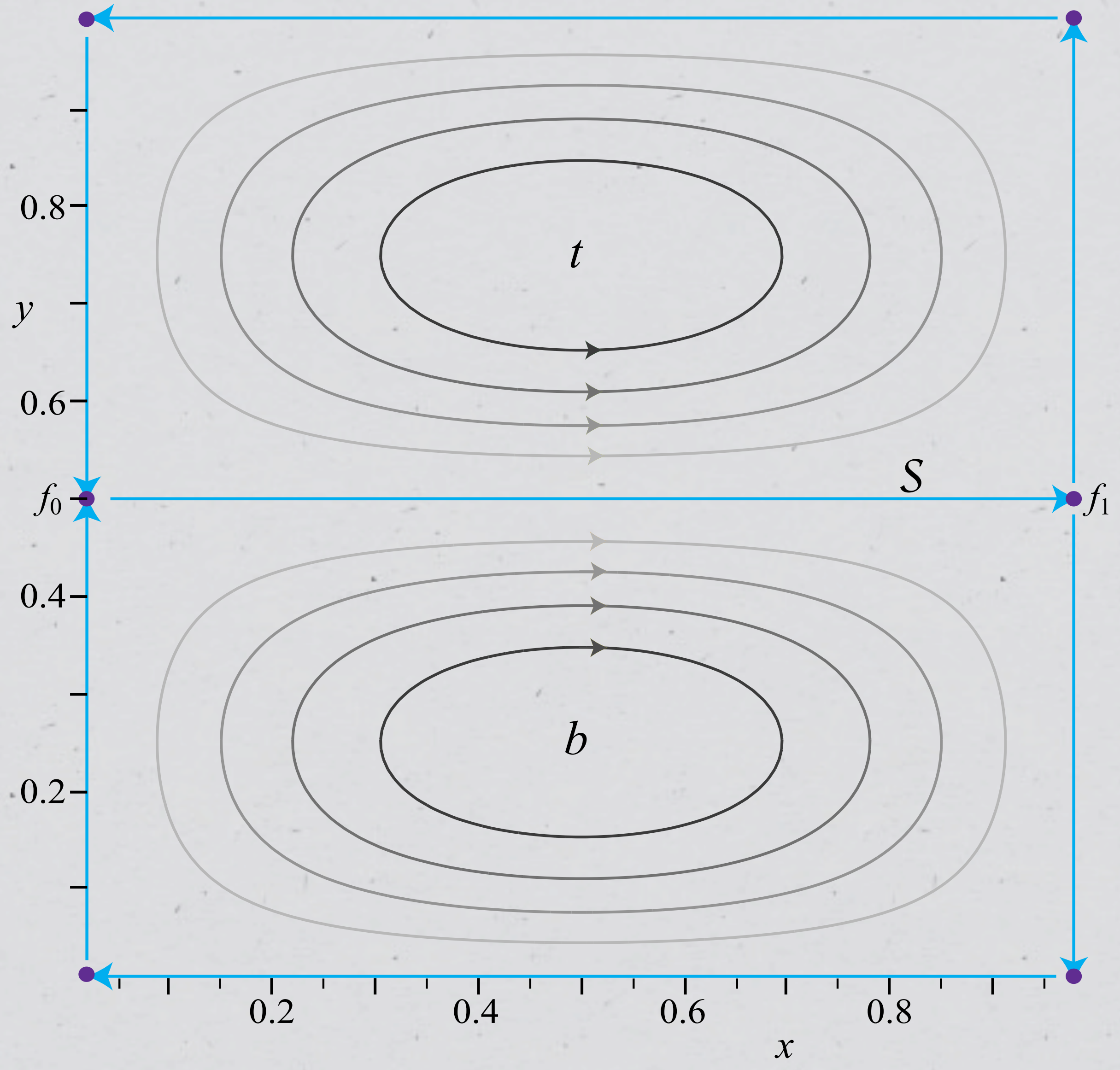


Dynamics for $t < 0$

Rotating Double Gyre

Future Vector field:
Stable Manifolds

6 future hyperbolic saddles



Dynamics for $t > \tau$

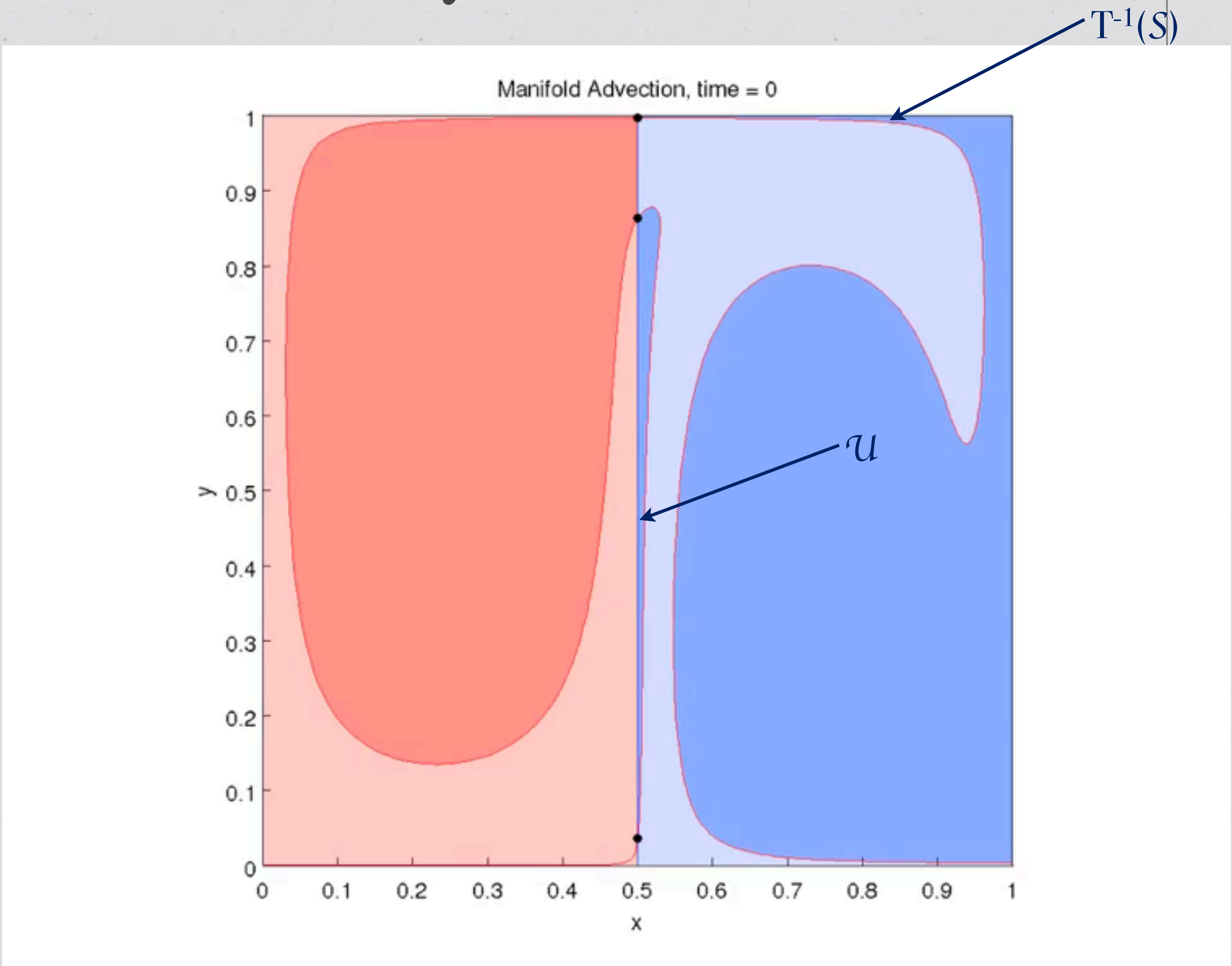
Double Gyre Flow

$\tau = 0.7$

Blue = Right Gyre
Red = Left Gyre

$t = 0$

$t = \tau$



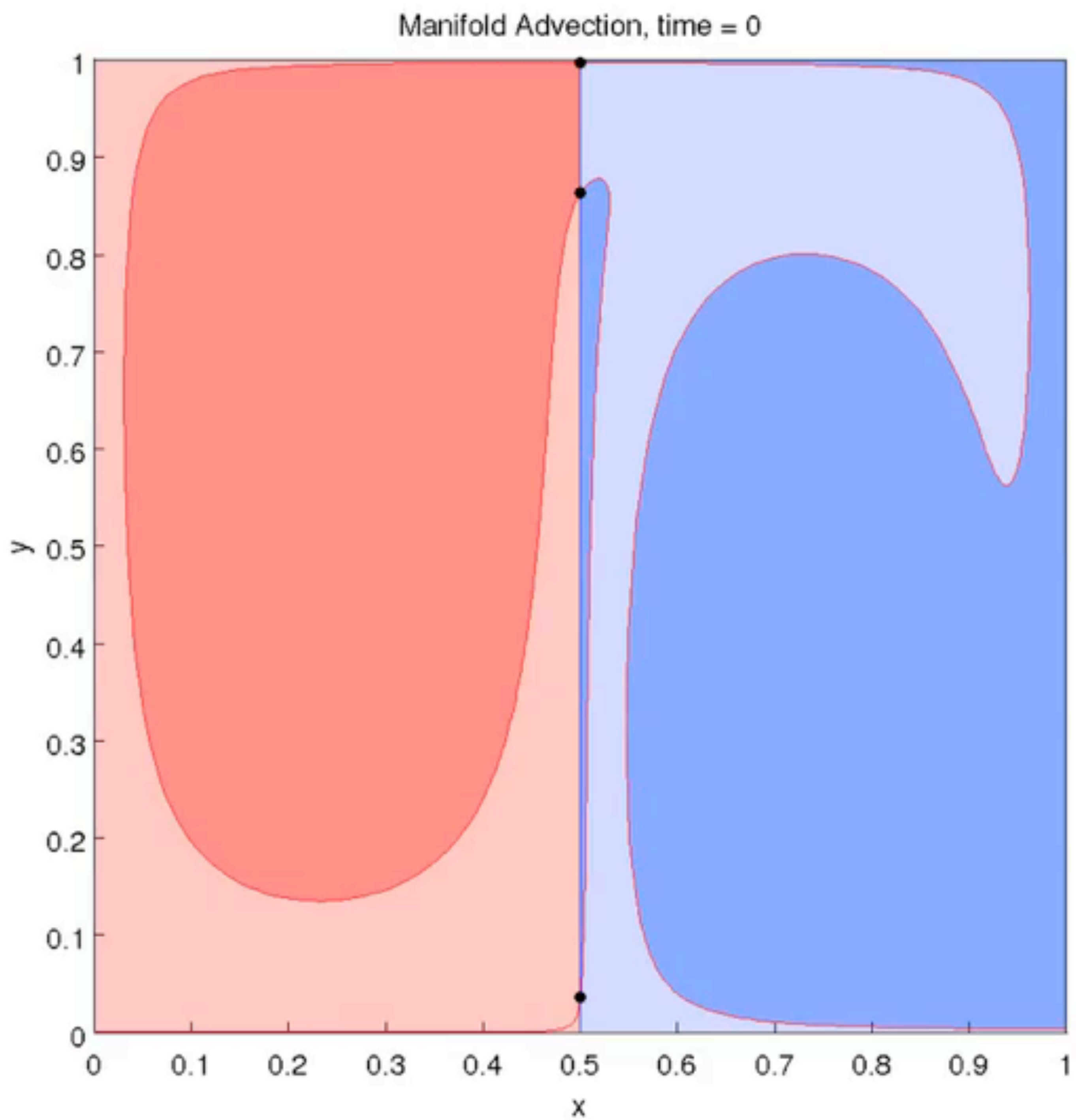
Dark & Light $\Rightarrow$ Top
Light & Dark $\Rightarrow$ Bottom

Double Gyre Flow

$\tau = 0.7$

Blue = Right Gyre
Red = Left Gyre

$t = 0$



$t = \tau$

Dark & Light $\Rightarrow$ Top
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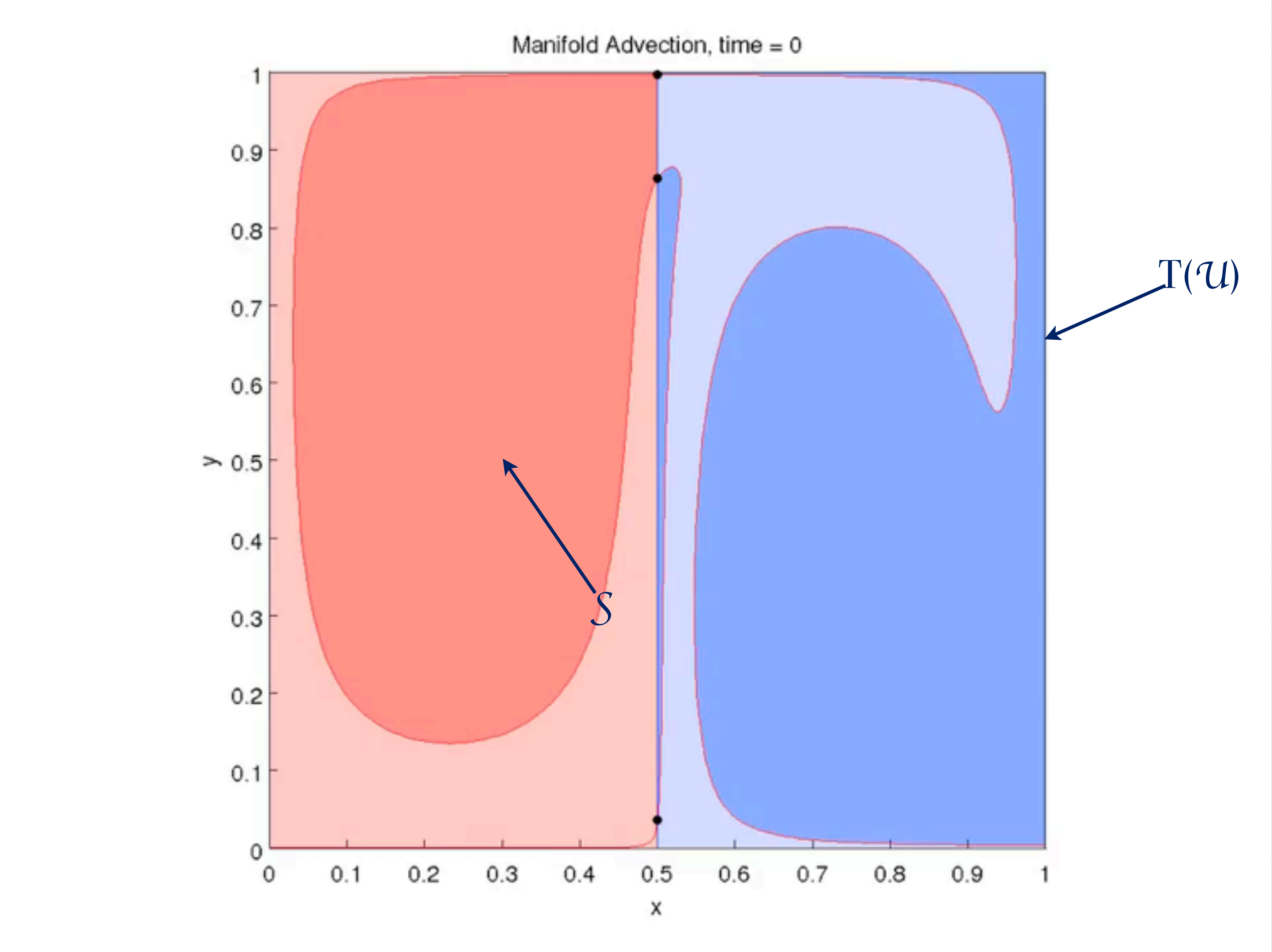
Double Gyre Flow

$\tau = 0.7$

Blue = Right Gyre
Red = Left Gyre

$t = 0$

$t = \tau$

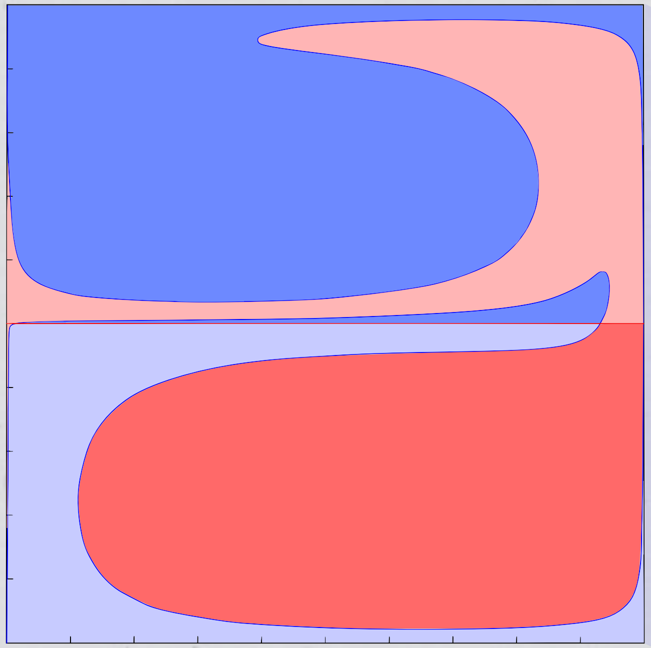


Dark & Light $\Rightarrow$ Top
Light & Dark $\Rightarrow$ Bottom

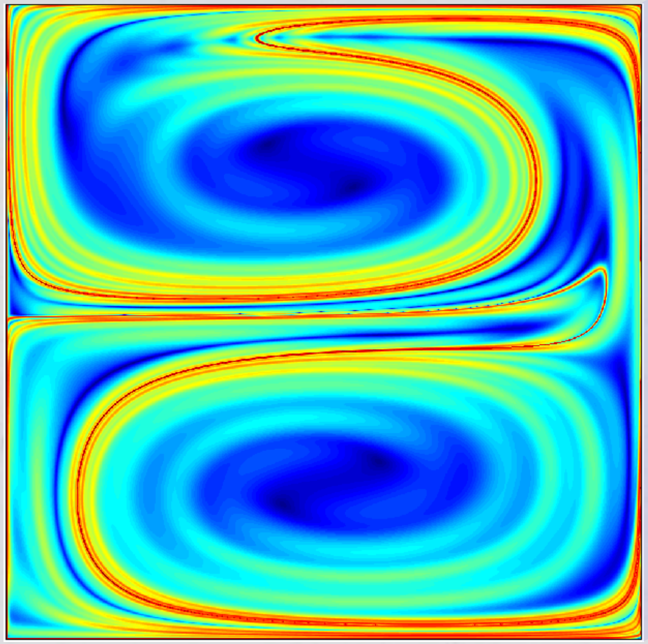
FTLE Comparison

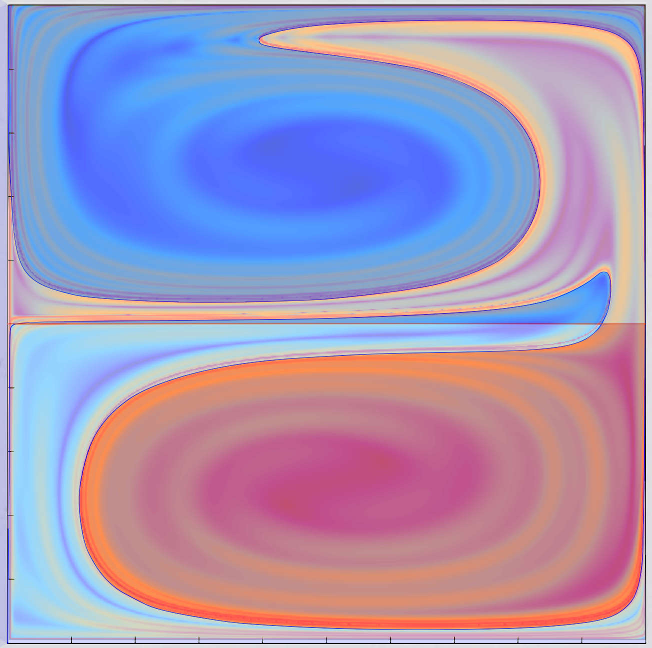
τ = 1.0

Precise Manifolds



"Backwards" FTLE at $t = \tau$ integrating for $\Delta t = 2\tau$





LIOUVILLE VECTOR FIELDS

Liouville Vector Fields

Globally Hamiltonian

- Symplectic form ω = $dq \wedge dp$ + Hamiltonian $H: M \to \mathbb{R}$

$$\mathcal{L}_V\omega \equiv \left. \frac{d}{dt}\varphi_{t,0}^{*}\omega \right|_{t=0}$$

$$\mathcal{L}_V\omega = \imath_V \underbrace{d\omega}_{0} + d(i_V\omega) = 0$$

Locally Hamiltonian

$$\begin{aligned} \mathcal{L}_V\omega &= d\dot{q}\wedge dp + dq \wedge d\dot{p} \\ &= d(\dot{q}dp - \dot{p}dq) \\ &= 0 \end{aligned}$$

Globally Liouville

- Volume form Ω + "F

$$\begin{aligned} \imath_V\Omega =& \dot{x}dy\wedge dz + \\ & \dot{y}dz\wedge dx + \\ & \dot{z}dx\wedge dy \end{aligned}$$

- Example: for standard … $\times \vec{\beta}$

Beltrami Case:

$$\vec{V} = \nabla \times \vec{V} \quad \Rightarrow \quad \beta = V_i dx_i$$

ABC Vector Field

$$\begin{aligned} \dot{x} &= a\sin(z) + c\cos(y) \\ \dot{y} &= b\sin(x) + a\cos(z) \\ \dot{z} &= c\sin(y) + b\cos(x) \end{aligned}$$

Dombre, T., U. Frish, et al. (1986). J. Fluid Mech. 167: 353.

Liouville Vector Fields

Globally Hamiltonian

- Symplectic form $\omega = dq \wedge dp$ + Hamiltonian $H : M \to \mathbb{R}$

$$\imath_V \omega = \dot{q} dp - \dot{p} dq = dH$$

$$\begin{aligned} \mathcal{L}_V \omega &= d\dot{q} \wedge dp + dq \wedge d\dot{p} \\ &= d(\dot{q} dp - \dot{p} dq) \\ &= 0 \end{aligned}$$

Globally Liouville

- Volume form Ω + "Hamiltonian form" $\beta \in \Lambda^{n-2}(M)$

$$\imath_V \Omega = d\beta$$

$$\begin{aligned} \imath_V \Omega = &\dot{x} dy \wedge dz + \\ &\dot{y} dz \wedge dx + \\ &\dot{z} dx \wedge dy \end{aligned}$$

- Example: for standard volume $\Omega = dx \wedge dy \wedge dz$ in $\mathbb{R}^3$: $\vec{V} = \nabla \times \vec{\beta}$

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Globally Liouville

- Volume form Ω + "Hamiltonian form" $\beta \in \Lambda^{n-2}(M)$

$$\begin{aligned}\mathcal{L}_V \Omega &= (\nabla \cdot V)\Omega = 0 \\ &= d(\imath_V \Omega)\end{aligned}$$

Divergence free

$$\begin{aligned}\imath_V \Omega = &\dot{x} dy \wedge dz + \\ &\dot{y} dz \wedge dx + \\ &\dot{z} dx \wedge dy\end{aligned}$$

- Example: for standard ... $\times \vec{\beta}$

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Lagrangian Forms

Symplectic Case: if ω is exact (ω =−*dν* = −*pdq*), then

$$\left.\frac{d}{dt}\right|_V \nu = \mathcal{L}_V \nu = \imath_V d\nu + d(\imath_V \nu) = dL$$

$$-dH \qquad\qquad L = \imath_V \nu - H = p\cdot\dot{q} - H$$

Volume Preserving Case: if Ω = *d*α is exact, then

$$\imath_V \Omega = d\beta$$

$$\left.\frac{d}{dt}\alpha\right|_V = \mathcal{L}_V \alpha = \imath_V d\alpha + d(\imath_V \alpha) = d\lambda$$

$$d\beta \qquad\qquad \lambda = \imath_V \alpha + \beta$$

Lagrangian Forms

$$\frac{d}{dt}\alpha\Big|_V = \mathcal{L}_V\alpha = \imath_V d\alpha + d(\imath_V\alpha) = d\lambda$$

$$\lambda = \imath_V\alpha + \beta$$

In $\mathbb{R}^3$, λ is a one-form

- Beltrami Vector field

$$\Omega = dx \wedge dy \wedge dz$$

$$\alpha = z dx \wedge dy$$

$$\Omega = d\alpha$$

$$\beta = V_x dx + V_y dy + V_z dz$$

$$\lambda = (V_x - zV_y)dx + (V_y + zV_x)dy + V_z dz$$

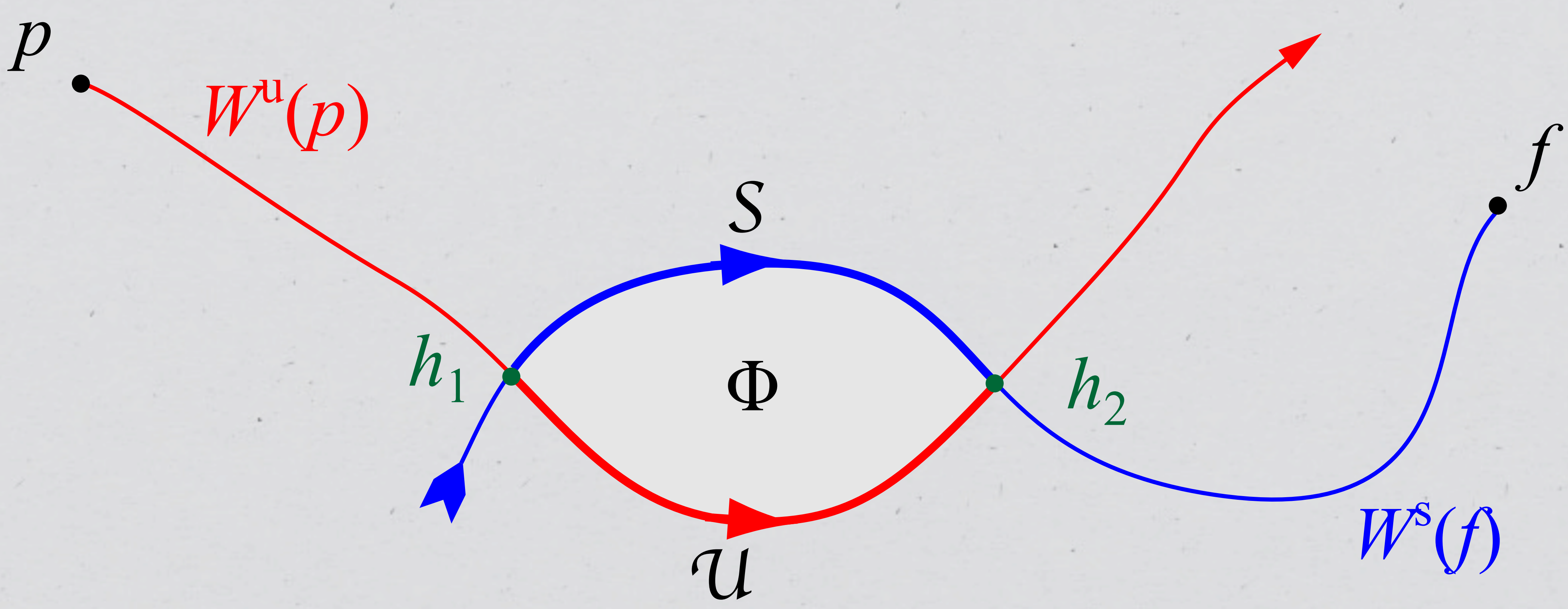
- Analogous forms for exact volume-preserving maps can be used as "generating forms" like those for Hamiltonian dynamics

Lomelí, H. E. and J. D. Meiss (2009). "Generating Forms for Exact Volume-Preserving Maps." Disc. Cont. Dyn. Sys. Series S **2**(2): 361-377.

CALCULATING FLUX

Flux—2D

- Transport from a past invariant region $\mathcal{P}_\text{o}$ to a future invariant region $\mathcal{F}_\tau$ is localized to one or more lobes

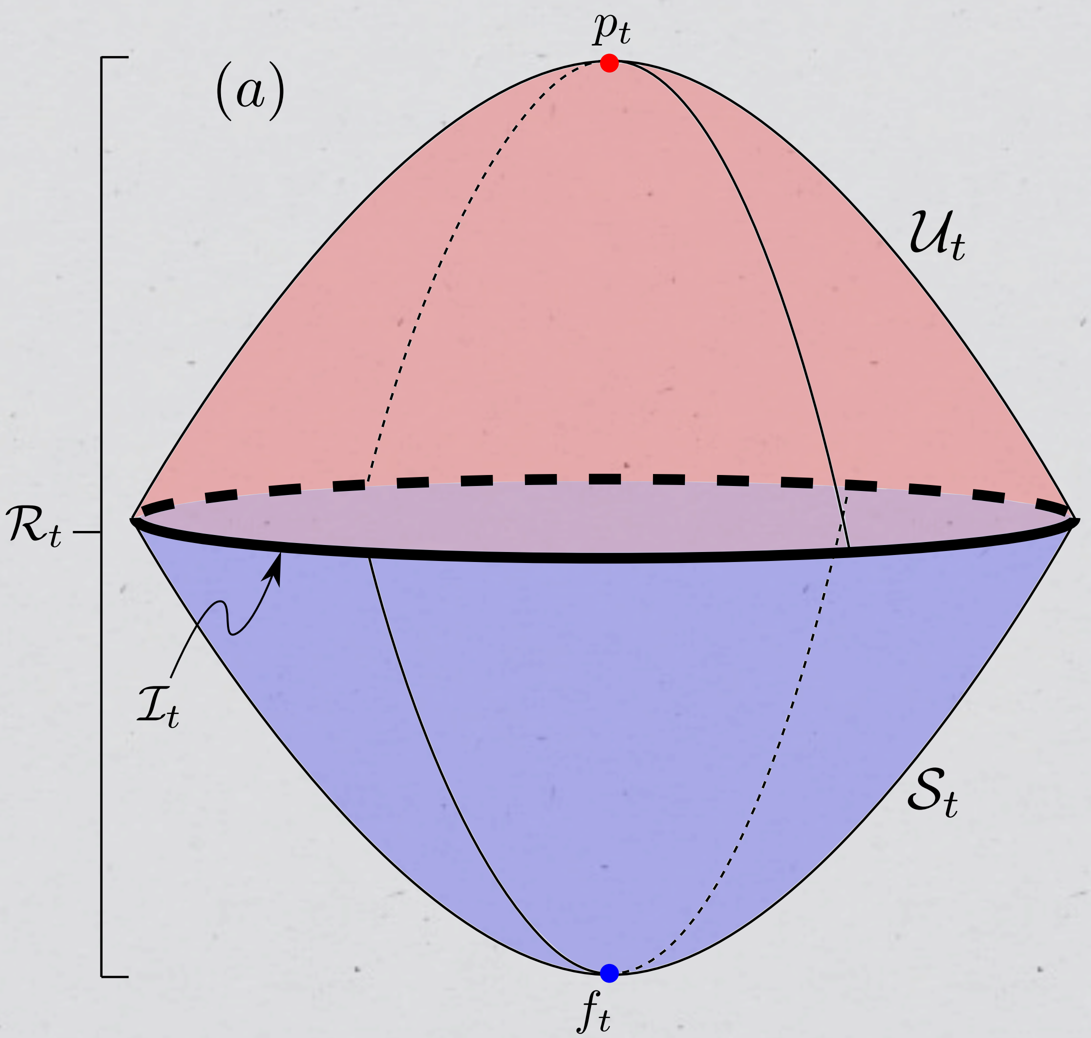


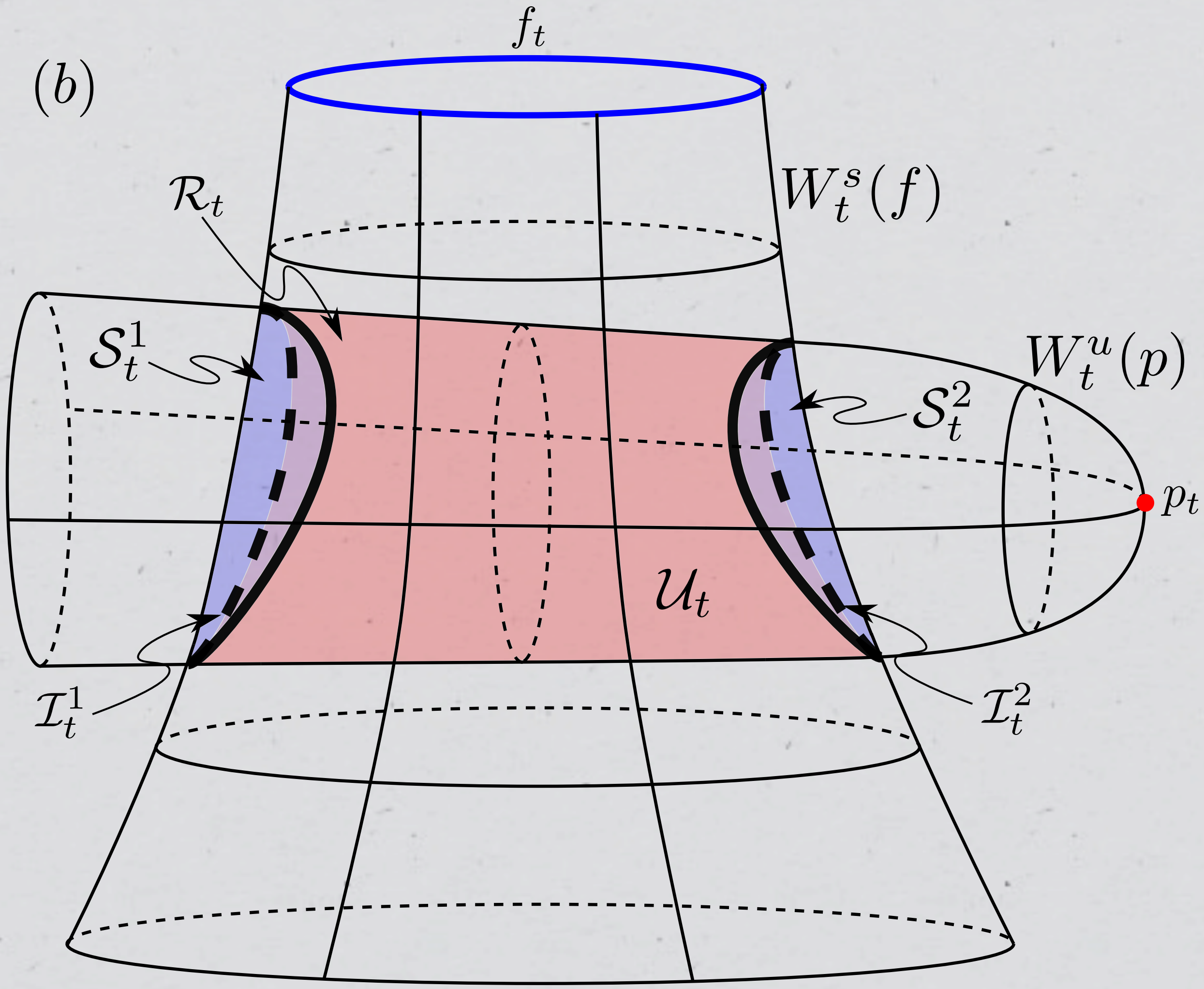
$$\Phi = \mathrm{Vol}(\mathcal{P}_t \cap \mathcal{F}_t)$$

Flux–3D

Transport from a past invariant region $\mathcal{P}_\circ$ to a future invariant region $\mathcal{F}_\tau$ is localized to one or more lobes

$$\Phi = \mathrm{Vol}(\mathcal{P}_t \cap \mathcal{F}_t)$$





$$\partial \mathcal{R}_t = \mathcal{U}_t + \mathcal{S}_t$$

Flux

$$\Omega = d\alpha$$

Stokes's Theorem: codimension-one reduction to boundary

$$\Phi = \mathrm{Vol}(\mathcal{R}_t) = \int_{\mathcal{R}_t} \Omega = \int_{\partial \mathcal{R}_t} \alpha.$$

$$\Omega = dx \wedge dy \wedge dz$$

$$\partial \mathcal{R}_t = \mathcal{U}_t + \mathcal{S}_t \qquad \alpha = z dx \wedge dy$$

Action-Flux Formula: codimension-two reduction (+ time)

- Theorem: Suppose that $\Omega = d\alpha$ is exact and Γ_t is a codimension-one slice of an invariant set of a **globally** Liouville flow φ. Then for any $r \in \mathbb{R}$,

$$\int_{\Gamma_t} \alpha = \int_r^t \left(\int_{\partial \Gamma_s} \lambda \right) ds + \int_{\Gamma_r} \alpha$$

Action Flux: Stable & Unstable Manifolds

$$\int_{\Gamma_t} \alpha = \int_r^t \left(\int_{\partial \Gamma_s} \lambda \right) ds + \int_{\Gamma_r} \alpha$$

If $\Gamma = \mathcal{U}$ an unstable manifold: take $r \to -\infty$:

$$\int_{\mathcal{U}_\tau} \alpha = \int_{-\infty}^{\tau} \left(\int_{\partial \mathcal{U}_s} \lambda \right) ds$$

If $\Gamma = S$ a stable manifold: take $r \to \infty$:

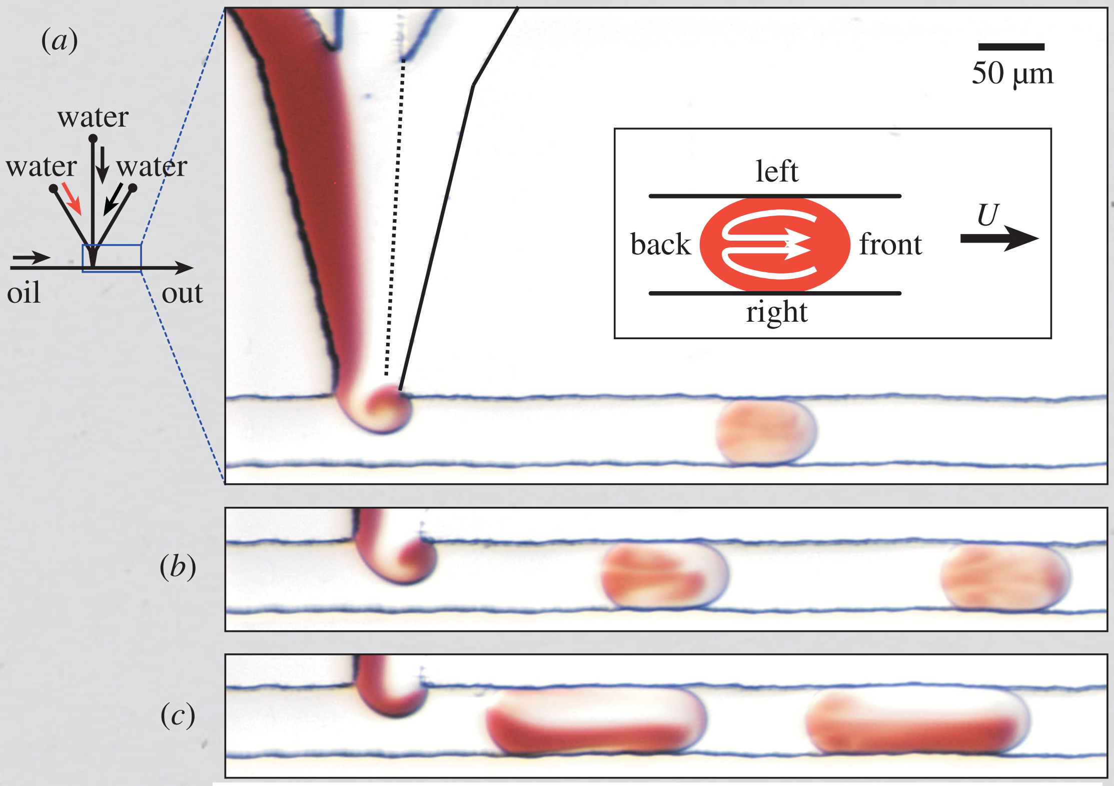
$$\int_{\mathcal{S}_\tau} \alpha = -\int_{\tau}^{\infty} \left(\int_{\partial \mathcal{S}_s} \lambda \right) ds$$

Often: $\mathcal{I}_t = \partial \mathcal{U}_t \cap \partial \mathcal{S}_t$

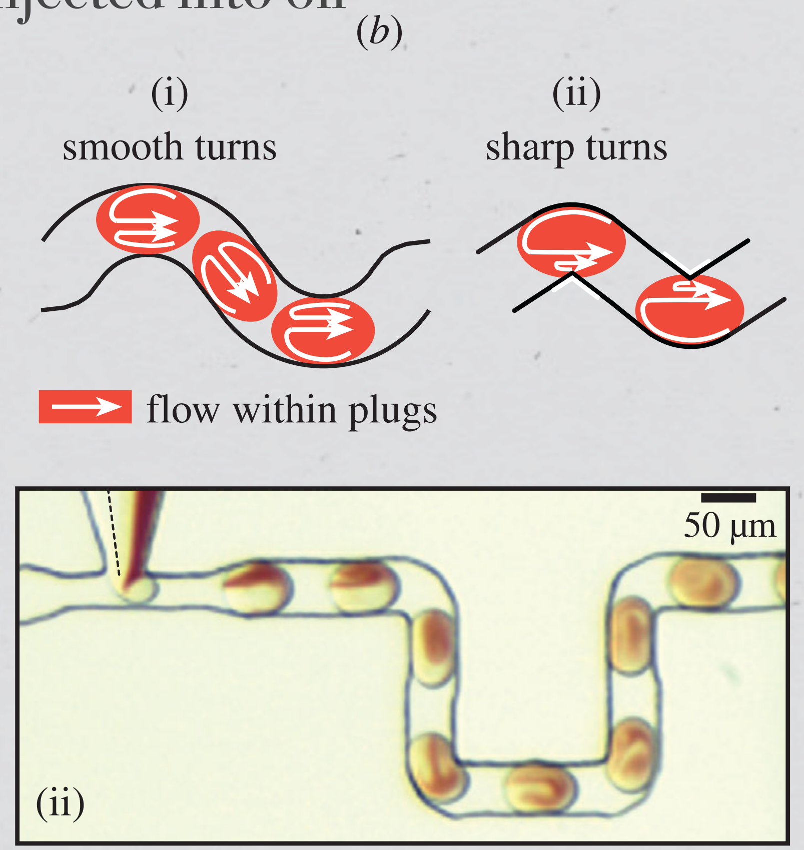
APPLICATION: DROPLET MIXING

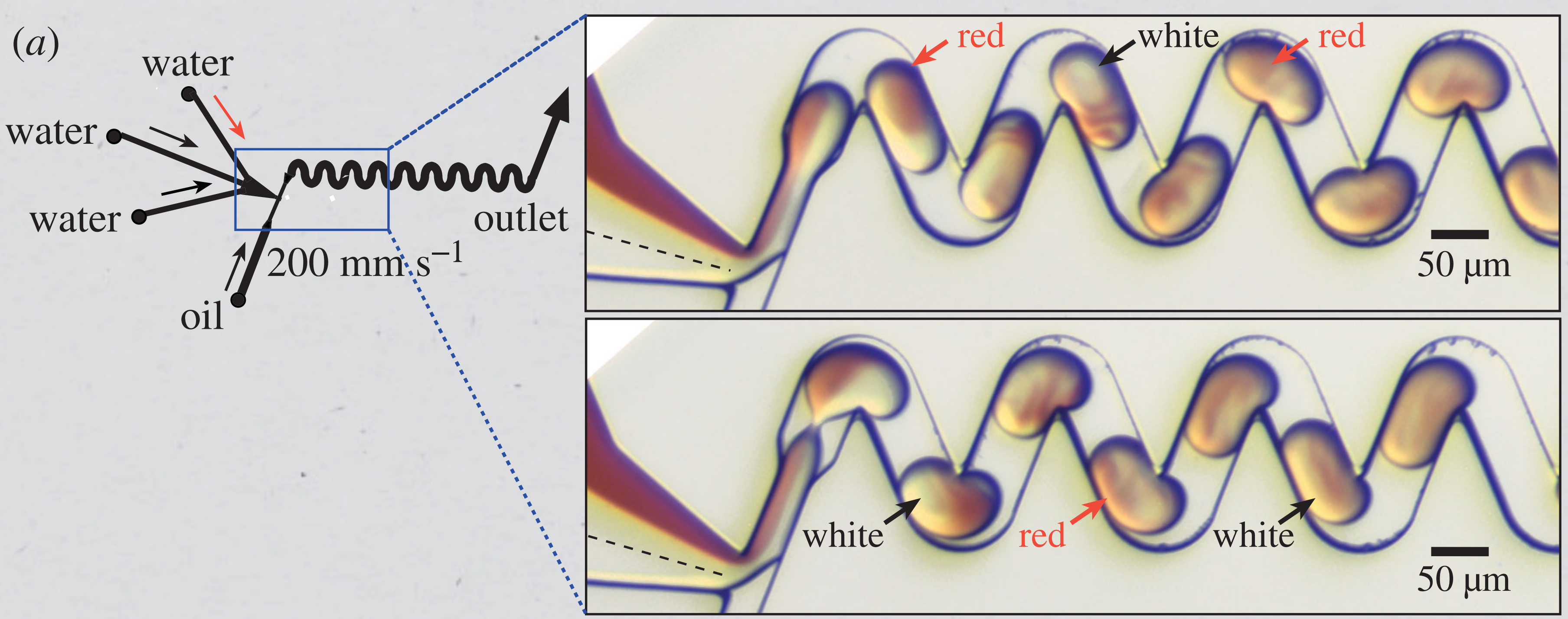
MicroDroplet Mixers

M. R. Bringer and others



Water injected into oil





Bringer, M., C. J. Gerdts, et al. (2004). "Microfluidic systems for chemical kinetics that rely on chaotic mixing in droplets." Phil. Trans. R. Soc. Lond. A **362**(1818): 1087-1104.

For general review: Wiggins, S. and J. M. Ottino (2004). "Foundations of chaotic mixing." Phil. Trans. R. Soc. Lond. **362**(1818): 937-970.

MicroDroplet Mixers

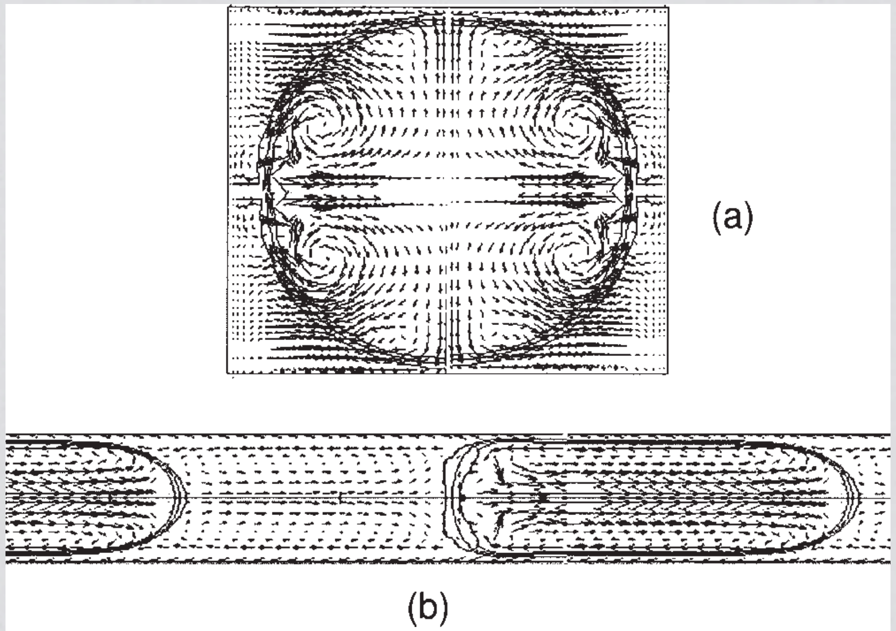


Figure 7. Velocity field in the reference frame of the droplet obtained inside the droplet and the continuous phase by 3D computations.

(a) View of the (*xy*) section at half of the droplet length. (b) View in the (*yz*) plane at $x/D = 0.4$. The interfacial region is represented by isovalues (*C*) of 0.05, 0.5, and 0.95.

50 x 40 µm rectangular channel
Water Droplet in silicone oil

Sarrazin, F., K. Loubière, et al. (2006). "Experimental and numerical study of droplets hydrodynamics in microchannels." AIChE journal **52**(12): 4061-4070.

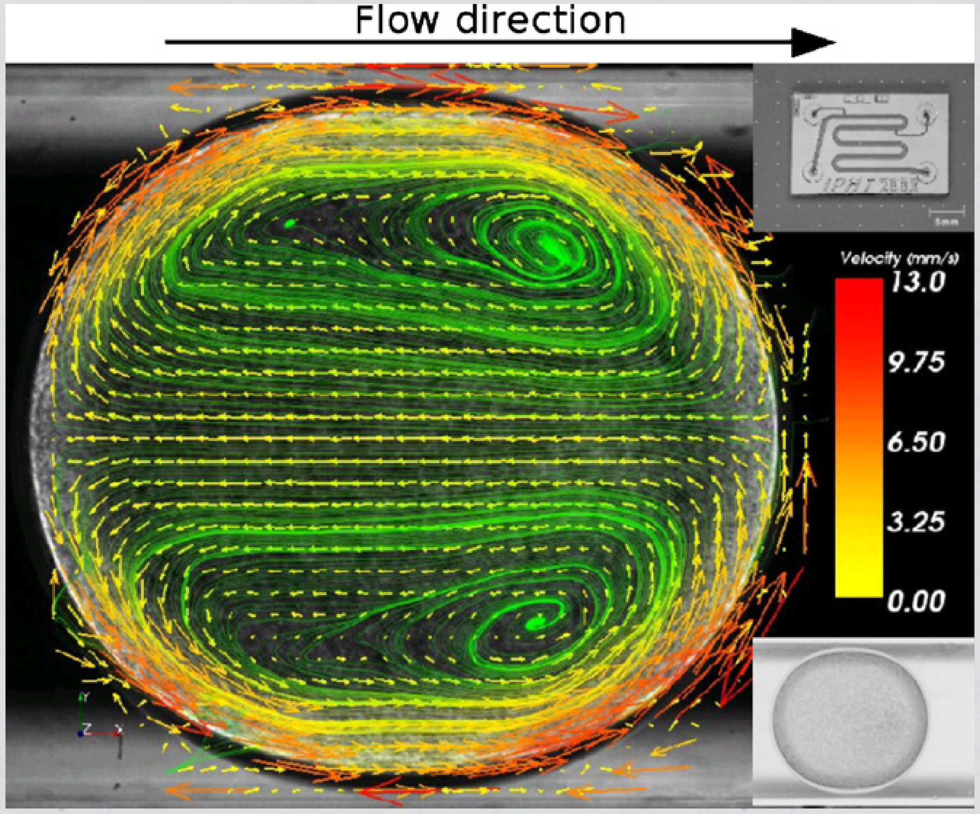


Fig. 9. Reversed symmetrical flow fields are induced by the translation of micro droplets through linear micro channels (transport velocity 7.6 mm/s). Mixing is suppressed. The measured internal flow inside a micro droplet is shown for a micro channel with dimensions of 780 µm × 260 µm. Internal flow is induced at the liquid/liquid interface with four regions of maximum flow.

Malsch, D., M. Kielpinski, et al. (2008). "µPIV-Analysis of Taylor flow in micro channels." Chem. Eng. J. **135**(Suppl. 1): S166-S172.

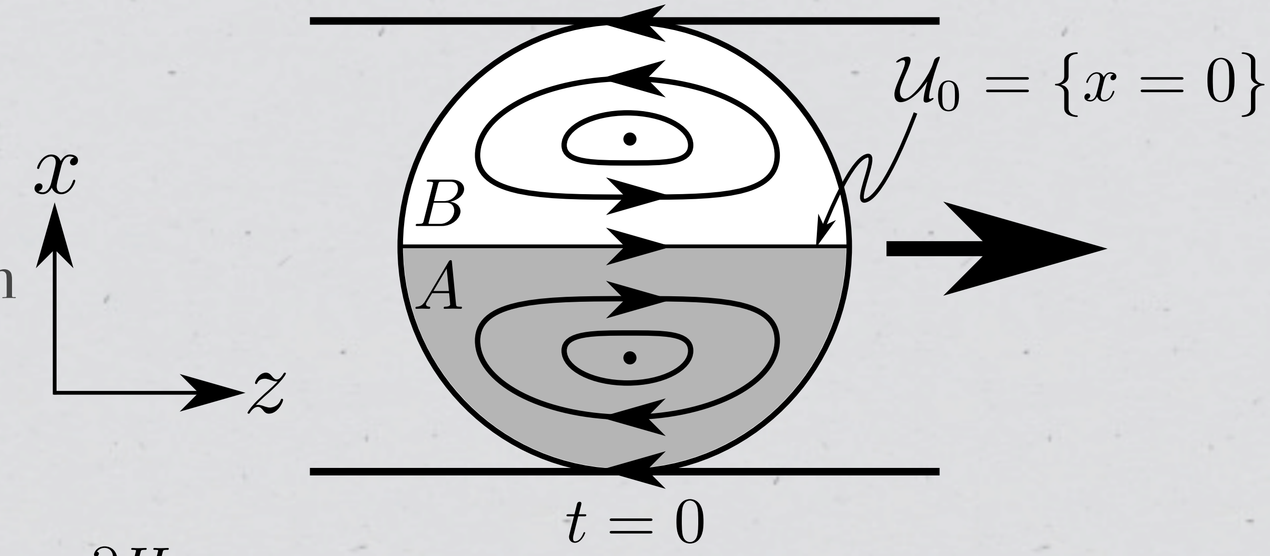
780x260 µm rectangular channel
Water Droplet in oil

Modeling Droplet Flow

Stone, Z. B. and H. A. Stone (2005). “Imaging and quantifying mixing in a model droplet micromixer.” Phys. Fluids **17**: 063103.

Hadamard-Rybczynski Flow

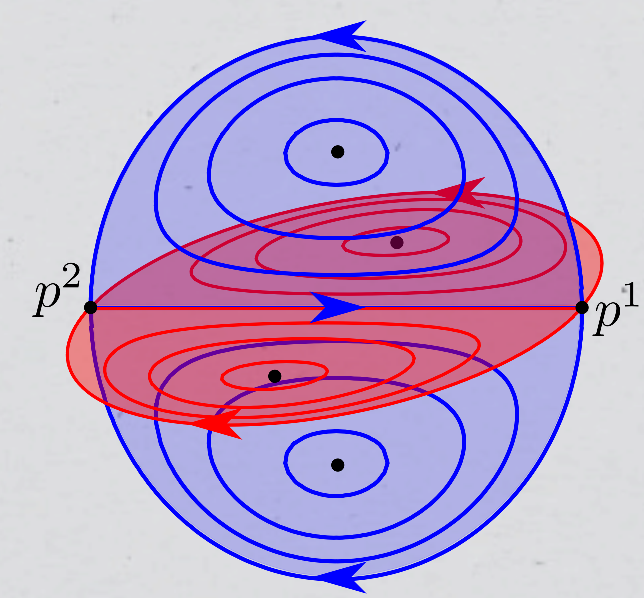
- Assume droplet in infinite fluid with steady flow
- Surface tension and viscosity difference maintain droplet shape and integrity
- Velocity field in droplet frame:



$$V_0 = \begin{pmatrix} 2xz \\ 2yz \\ 2(1 - 2x^2 - 2y^2 - z^2) \end{pmatrix} = \begin{pmatrix} -\frac{\partial H}{\partial z} \\ -\frac{\partial K}{\partial z} \\ \frac{\partial H}{\partial x} + \frac{\partial K}{\partial y} \end{pmatrix}$$

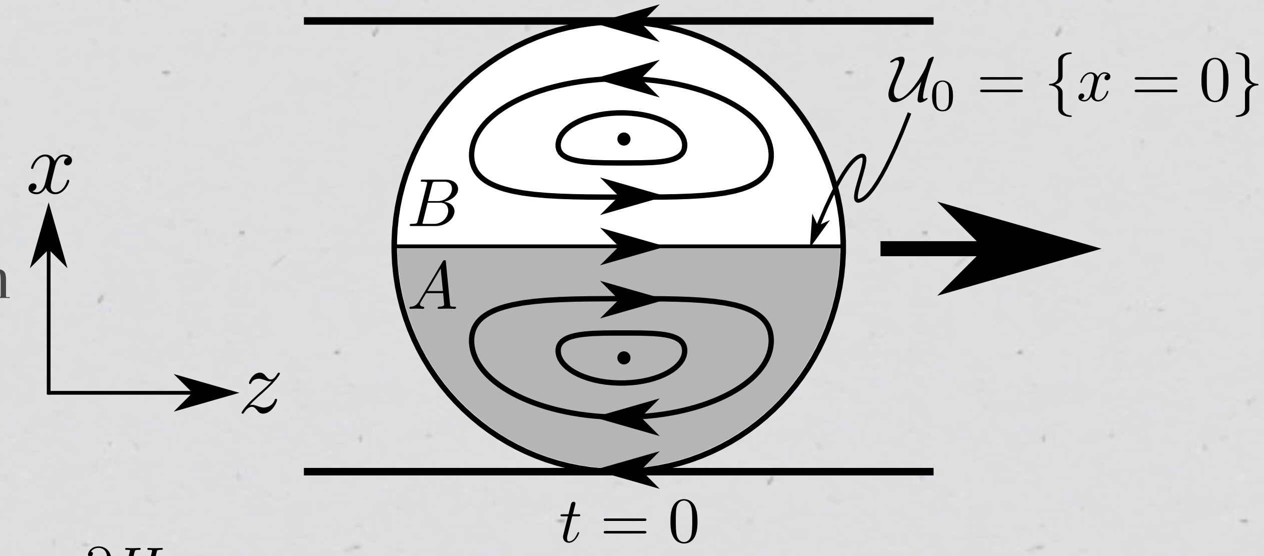
$$H(\vec{x}) = (1 - x^2 - y^2 - z^2)x$$

$$K(\vec{x}) = (1 - x^2 - y^2 - z^2)y$$



Modeling Droplet Flow

Stone, Z. B. and H. A. Stone (2005). “Imaging and quantifying mixing in a model droplet micromixer.” Phys. Fluids **17**: 063103.



Hadamard-Rybczynski Flow

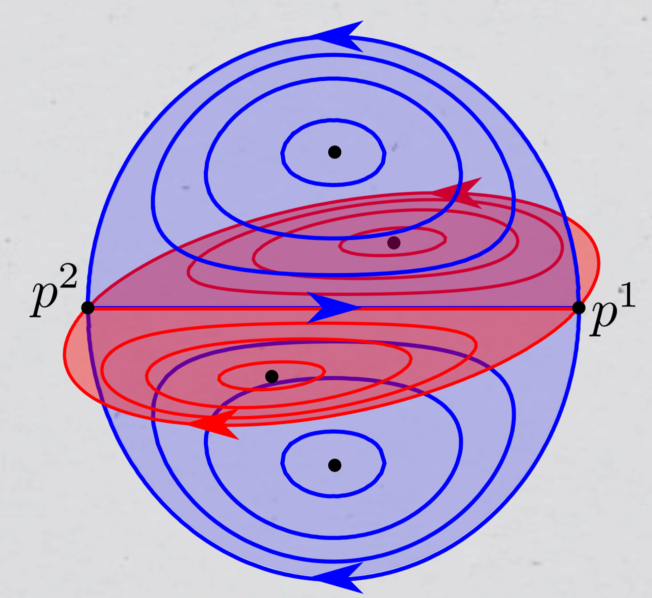
- Assume droplet in infinite fluid with steady flow
- Surface tension and viscosity difference maintain droplet shape and integrity
- Velocity field in droplet frame:

$$V_0 = \begin{pmatrix} 2xz \\ 2yz \\ 2(1 - 2x^2 - 2y^2 - z^2) \end{pmatrix} = \begin{pmatrix} -\frac{\partial H}{\partial z} \\ -\frac{\partial K}{\partial z} \\ \frac{\partial H}{\partial x} + \frac{\partial K}{\partial y} \end{pmatrix}$$

$$H(\vec{x}) = (1 - x^2 - y^2 - z^2)x$$
$$K(\vec{x}) = (1 - x^2 - y^2 - z^2)y$$

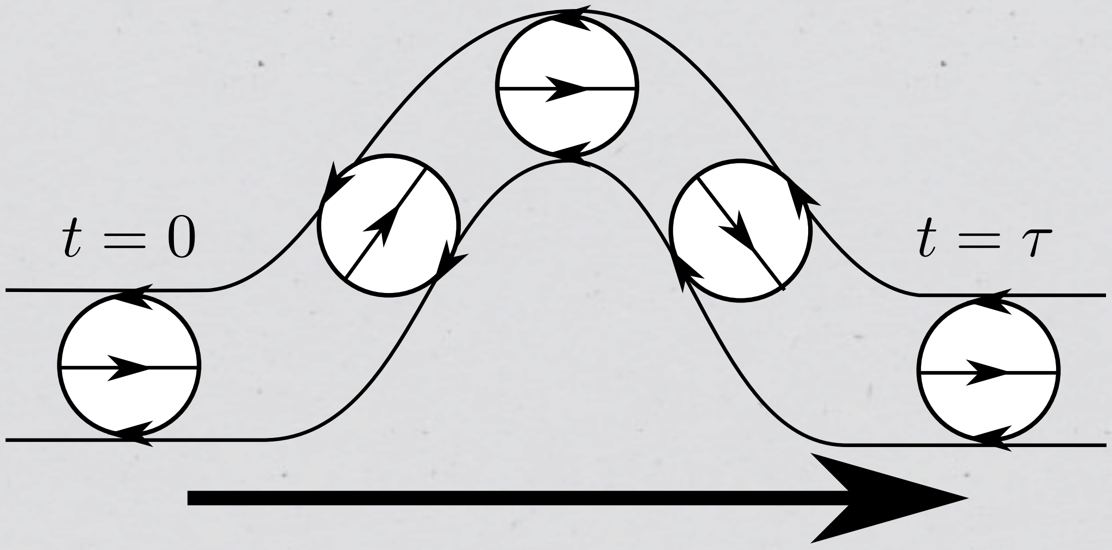
Globally Liouville: $\lambda = \imath_V \alpha + \beta$

$$\beta_0 = H\,dy - K\,dx,$$
$$\lambda_0 = (z\dot{x} + H)\,dy - (z\dot{y} + K)\,dx.$$



Modeling Droplet Flow

Sinuous Channel



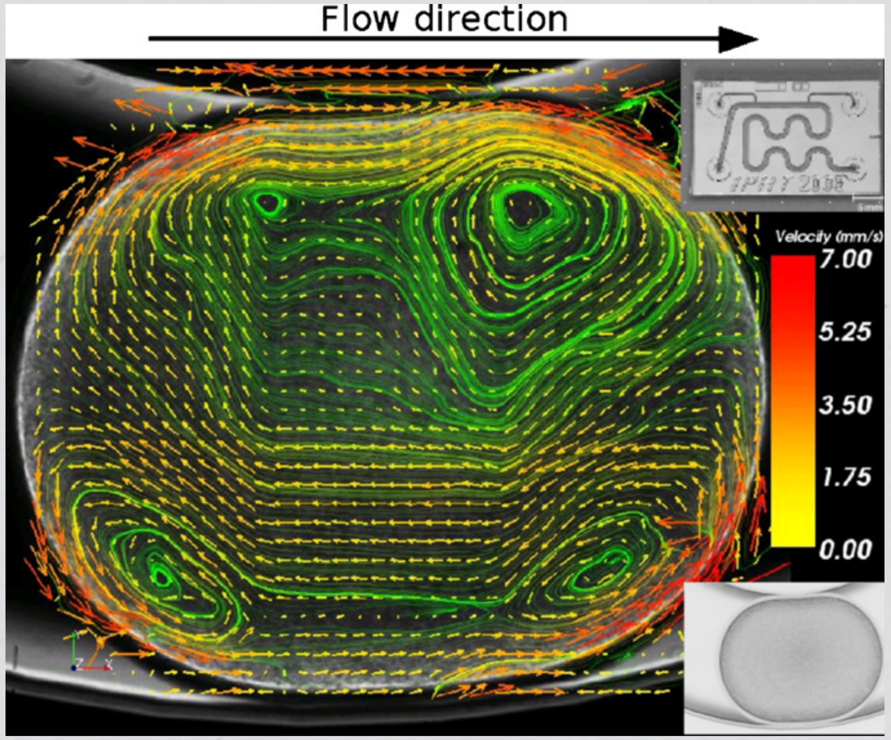
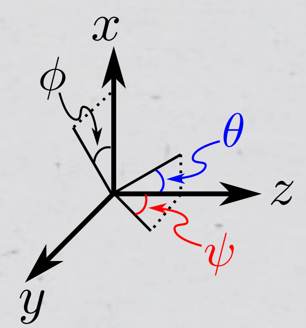
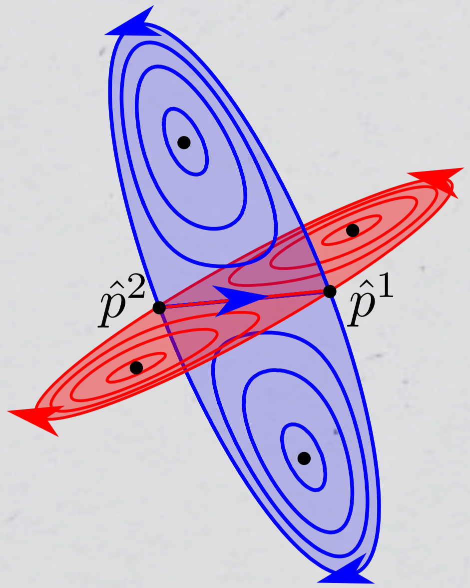


Fig. 10. Translation of droplets through winding channels (transport velocity 7.6 mm/s) induces complex internal flow for efficient mixing. Maximum flow is observed at the liquid/liquid interface which dominates the phase internal flow.

Make it 3D!





$$R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$

$$R_x(\psi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & \sin\psi \\ 0 & -\sin\psi & \cos\psi \end{bmatrix}$$

Modeling Droplet Flow

Sinuous Pipe: Push Forward velocity

$$V(\vec{x},t) = R_*(t)V_0(\vec{x})$$

$$R(t) = R_y(\theta(t))R_x(\psi(t))$$

Transitory Case:

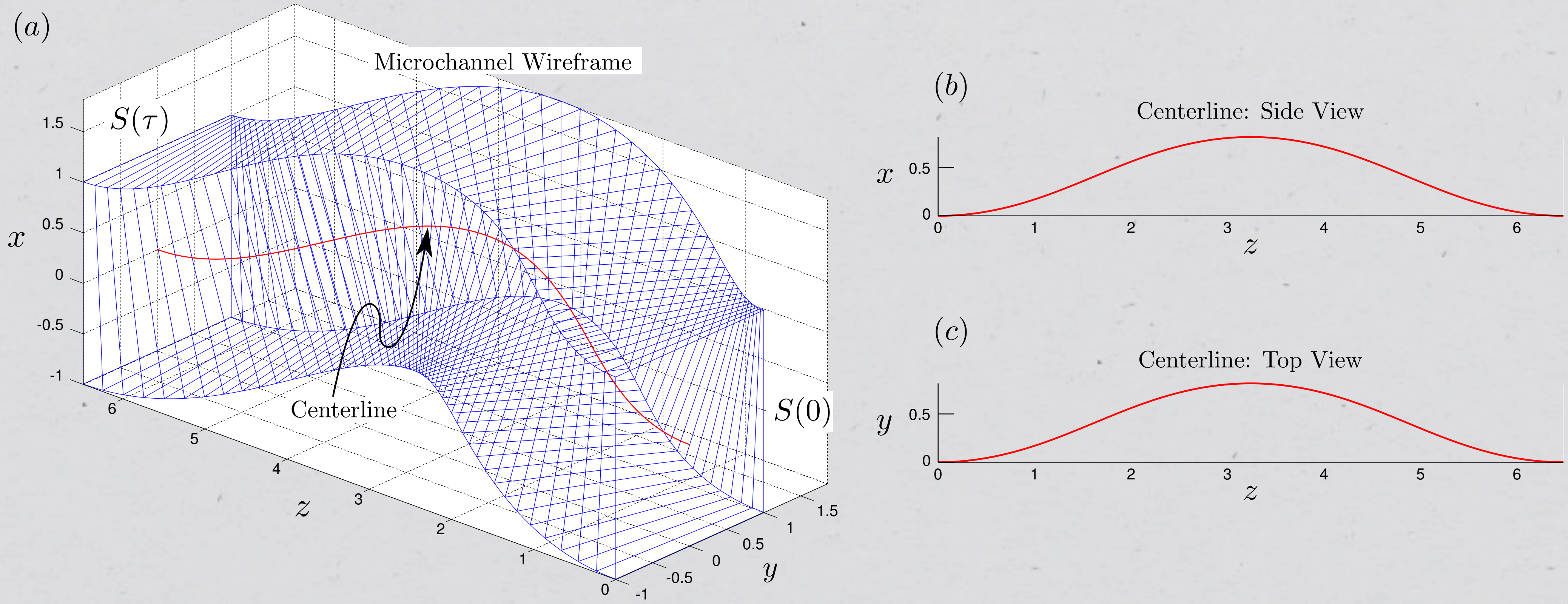
$$R(0) = R(\tau) = I$$

Simple Example:

$$\theta(t) = \psi(t) = \xi \sin(2\pi t/\tau)$$

τ = 3.5

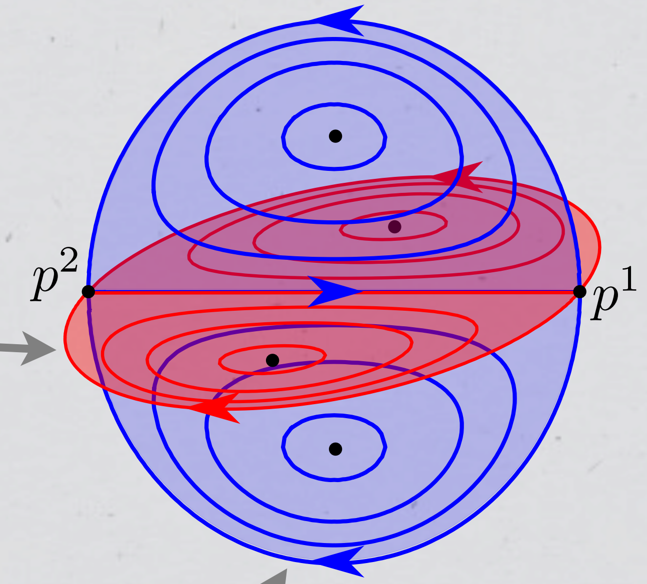
ξ = π/8



Transport

Inject fluid in $x < 0$ hemisphere

- Injection plane: $\mathcal{U}_0 = \{(0, y, z)\}$

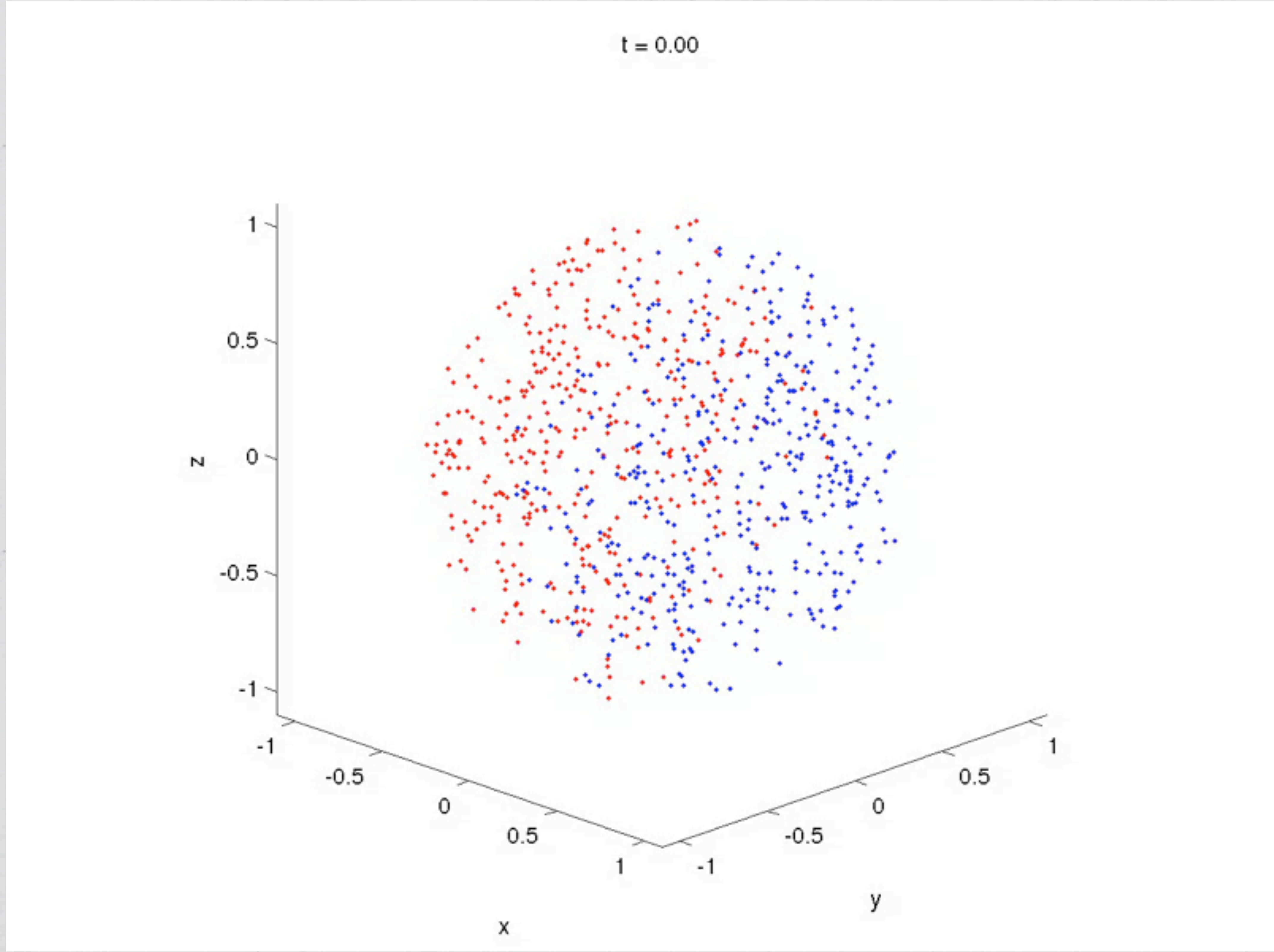


Extract fluid in $x > 0$ or $y > 0$ hemisphere

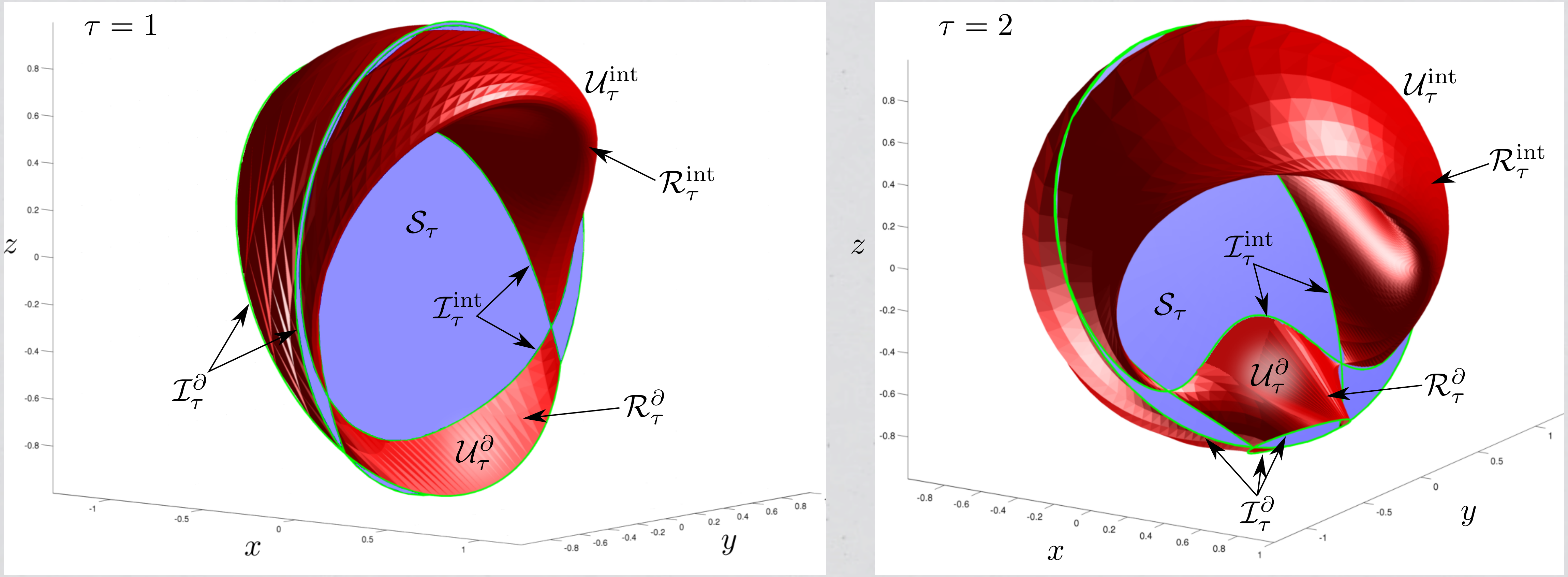
- Extraction planes $\mathcal{S}_\tau = \{(0, y, z)\}$ or $\mathcal{S}_\tau = \{(x, 0, z)\}$

Goal: Find Fraction of injected fluid extracted

Transitory Transport: Particle Tracking



Transitory Transport: Boundary Tracking

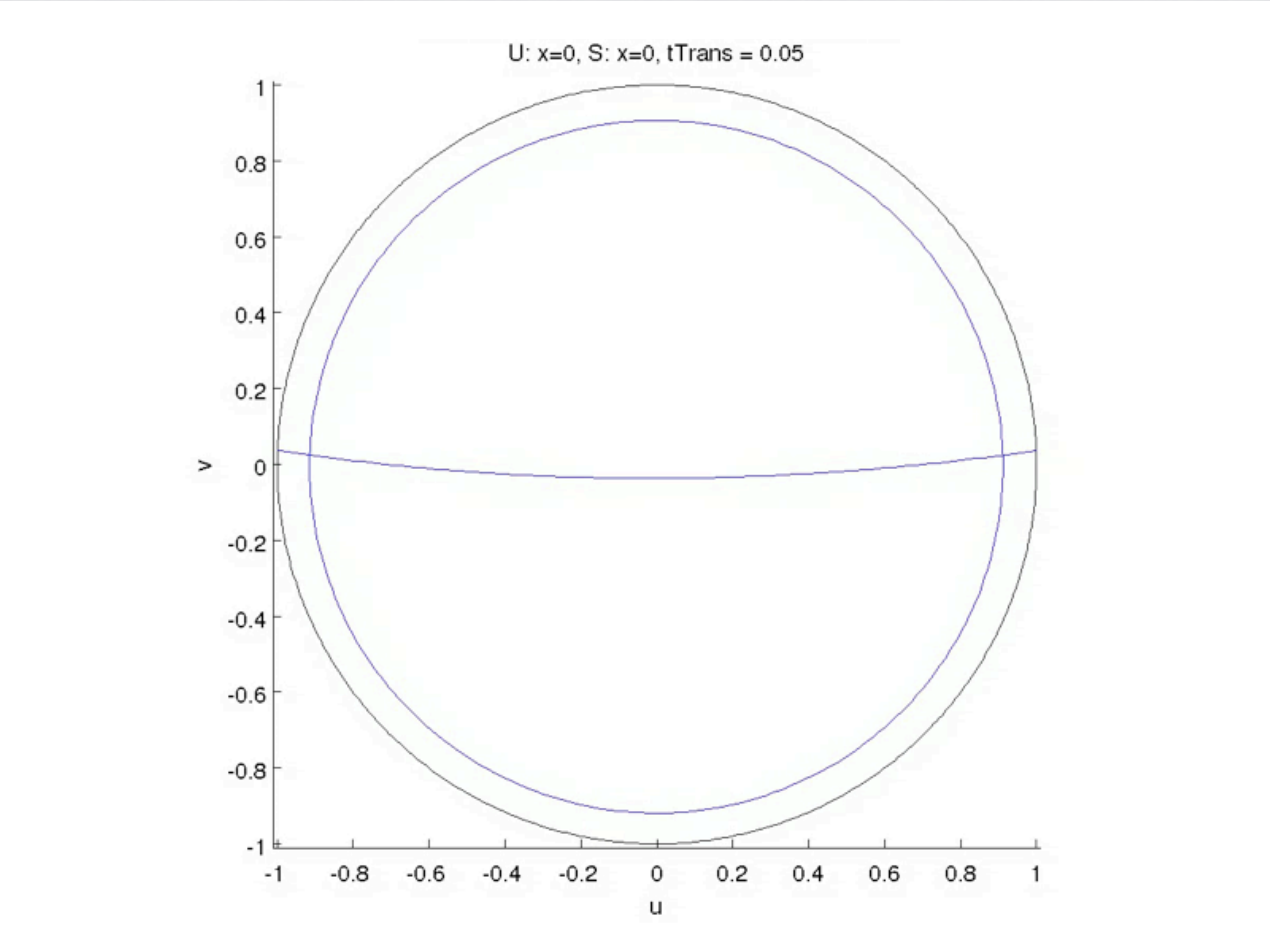


Action-Flux Formula

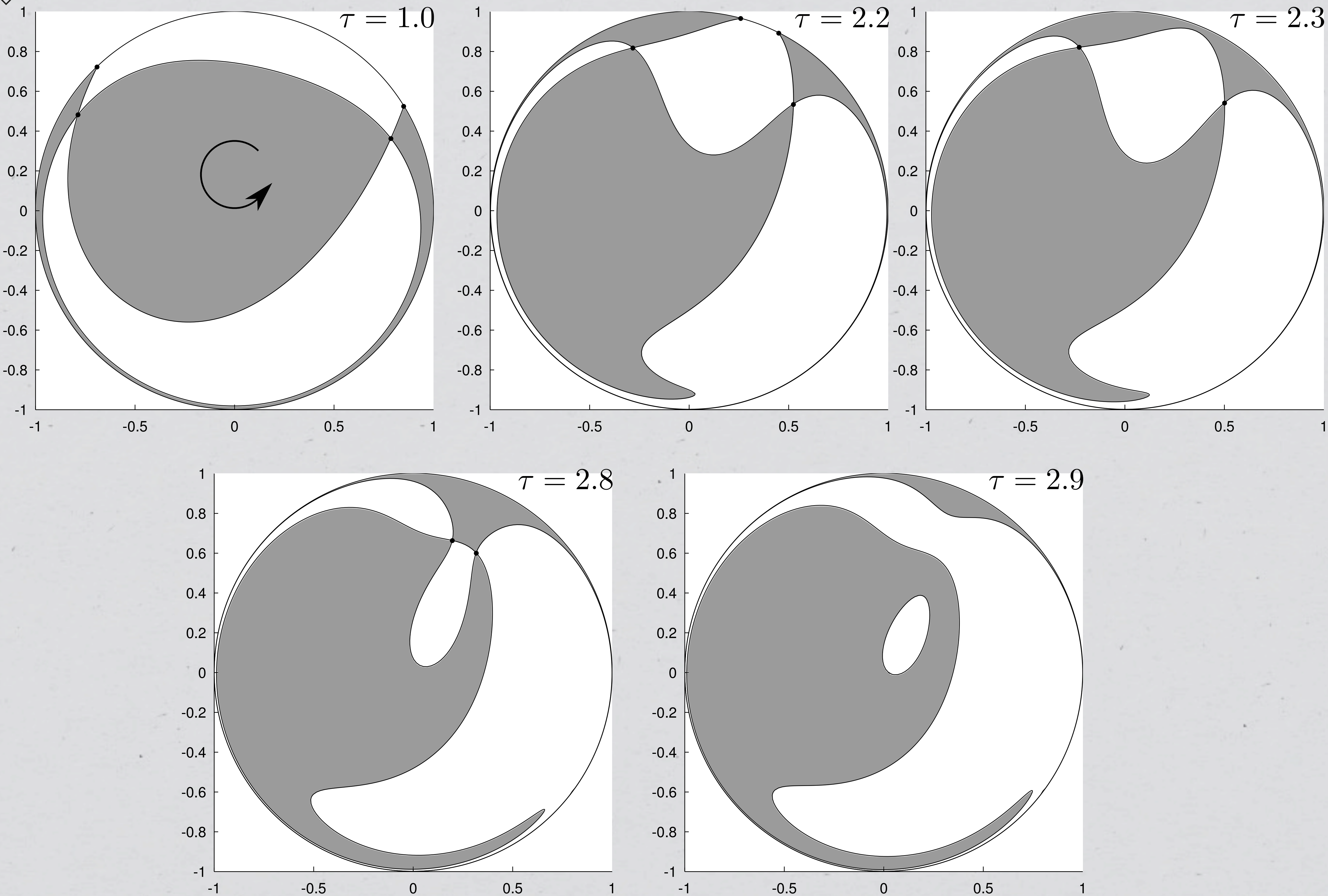
- Computation relies on finding $\mathcal{I}_\tau^{\text{int}} = T(\mathcal{U}_0) \cap \mathcal{S}_\tau$.

$$\int_{\mathcal{U}_\tau} \alpha = \int_0^\tau \left(\int_{\partial \mathcal{U}_s} \lambda \right) ds + \int_{\mathcal{U}_0} \alpha.$$

Intersection Curves

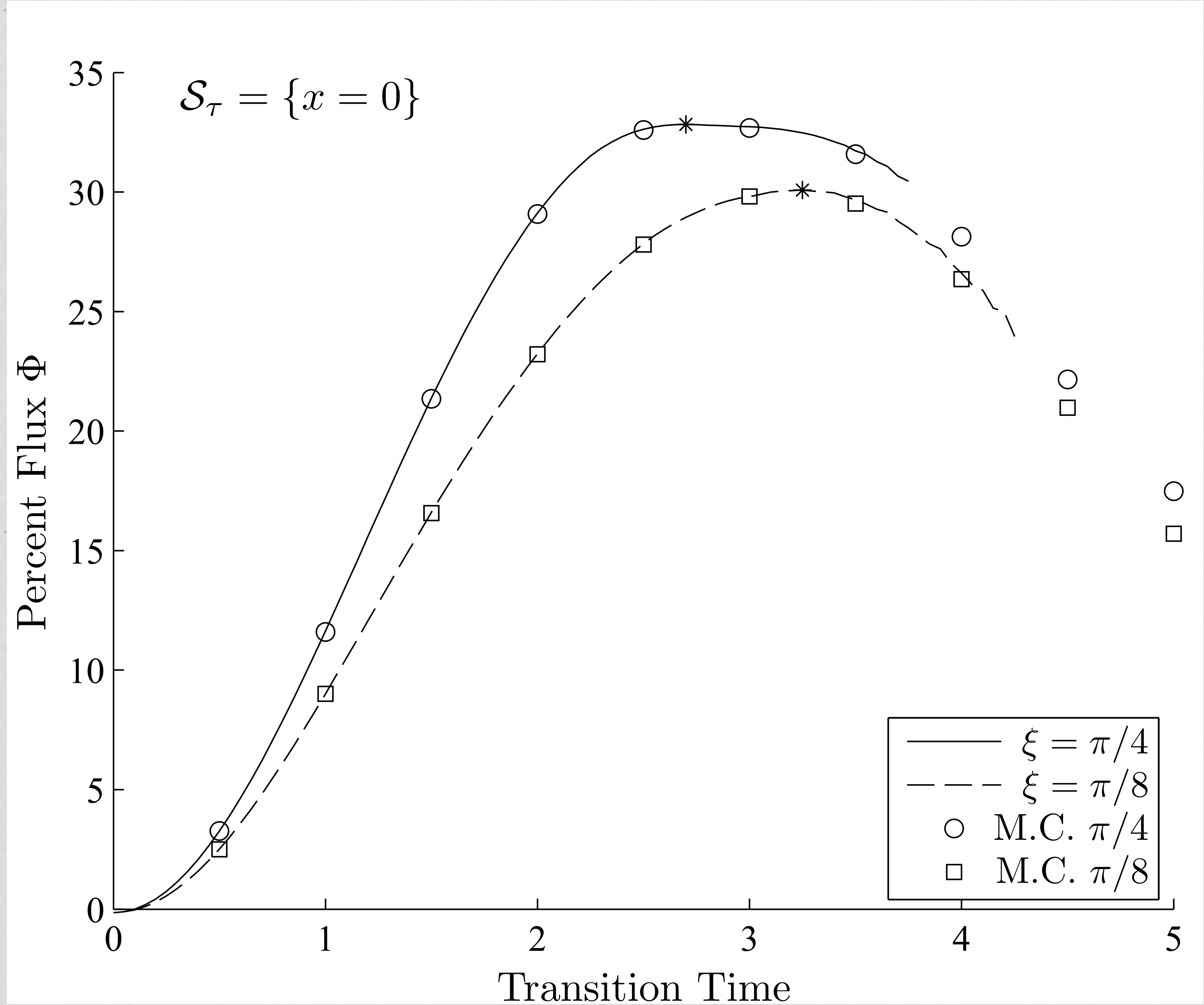


Intersection Curves



Flux

$$\theta(t) = \psi(t) = \xi \sin(2\pi t/\tau)$$



Comparison with Monte Carlo

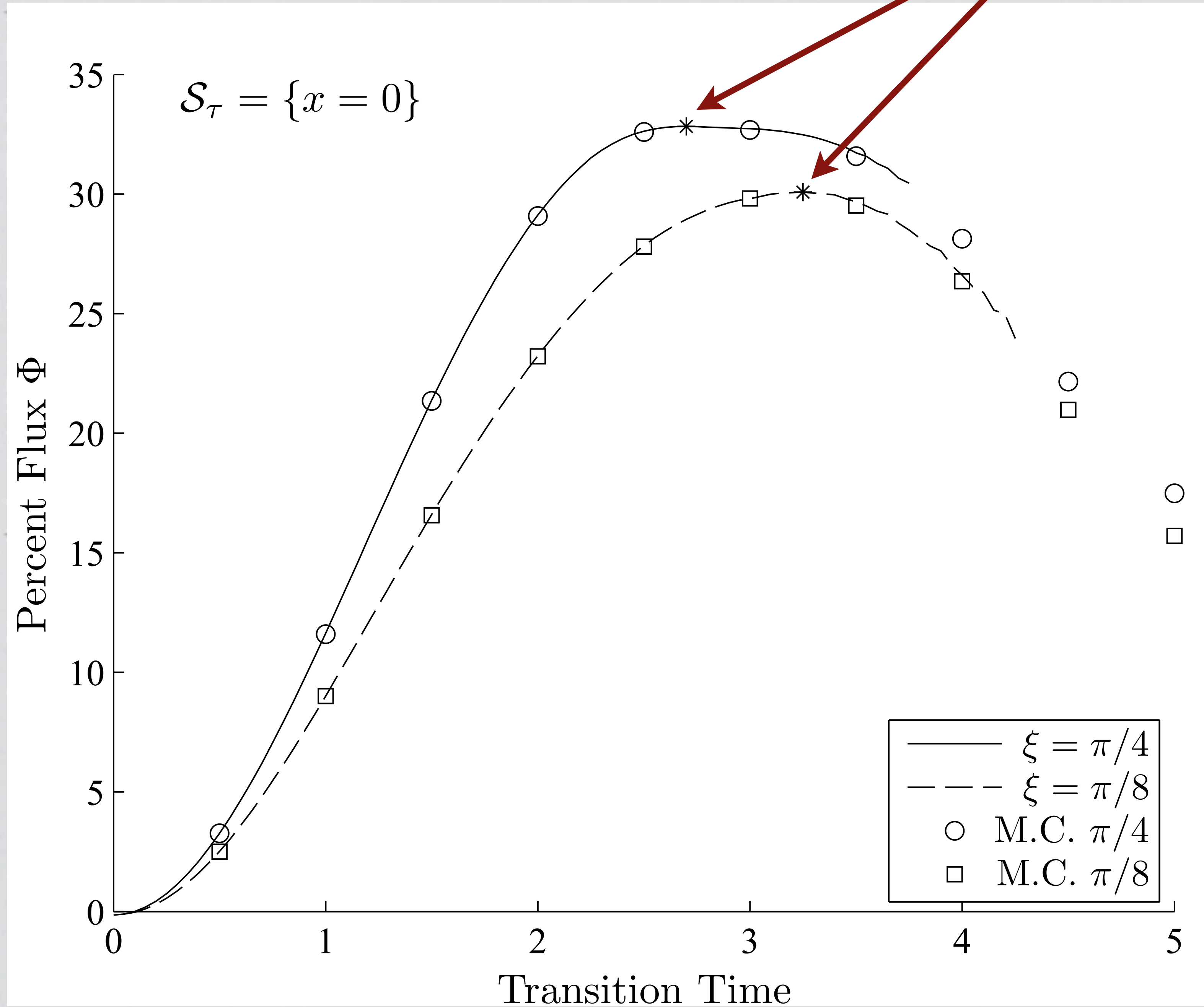
$$\Phi \approx \frac{2}{3}\pi\frac{N_{in}}{N}$$

$N = 10^6$ particles to give M.C. errors $O(10^{-3})$ when $\Phi = O(1)$.

Flux

$$\theta(t) = \psi(t) = \xi \sin(2\pi t/\tau)$$

Optimal Shapes!



Comparison with Monte Carlo

$$\Phi \approx \frac{2}{3}\pi\frac{N_{in}}{N}$$

$N = 10^6$ particles to give M.C. errors $O(10^{-3})$ when $\Phi = O(1)$.

Future Goal: Optimize Channel Shape

Conclusions / Future Work

* Globally Liouville Flows have Lagrangian Forms
* Action-Flux Formulas reduce Lagrangian information needed for transport computations
* Optimal bend may be intermediate.

* Develop techniques for computing Lagrangians from data?
* Optimize channel shape for transport?
* Measure mixing instead of transport?

See http://arXiv.org/abs/1203.3821