Mixing and reaction efficiency in closed domains

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Outline

Advection - Reaction - Diffusion (ARD1)

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta)$$

2 dim. $\mathbf{x} = (x, y)$
$\theta = \theta(\mathbf{x}, t)$, $\theta \in [0, 1]$

Assumptions

- **Reaction term**: $f(\theta) = \theta(1 - \theta)$ (FKPP-like $\Rightarrow$ pulled fronts);
- **Incompressibility condition**: $\nabla \cdot \mathbf{u} = 0 \Rightarrow \mathbf{u} = (\partial_y \psi, -\partial_x \psi)$, being $\psi = \psi(\mathbf{x}, t)$ the stream function;
- **Steep initial condition**: $\theta(\mathbf{x}, 0) \to 1$ for $x \to -\infty$, $\theta(\mathbf{x}, 0) \to 0$ for $x \to +\infty$ (exp. fast);

Asymptotic situation (ARD2)

L linear domain size

ℓ_0 typical length of the flow

$L \gg \ell_0$

front speed: $V(t) = \frac{1}{L_y \Delta t} \int dxdy\, [\theta(x,y,t+\Delta t) - \theta(x,y,t)]$

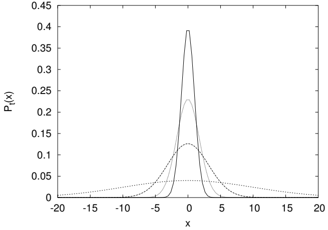
effective diffusion coeff.: $D^E_{ij} = \lim_{t\to\infty} \frac{1}{2t} \langle (x_i - < x_i >)(x_j - < x_j >) \rangle$

$$\mathbf{u} = 0 \quad \Rightarrow V_0 = 2\sqrt{\frac{D}{\tau_r} f'(0)} = 2\sqrt{\frac{D}{\tau_r}}$$

$$\mathbf{u} \neq 0 \quad \Rightarrow V_f \leq 2\sqrt{\frac{D^E}{\tau_r}} \quad (D^E \equiv D^E_{11})$$

- D^E **depends on the velocity field**
- **Typically:** $D^E \gg D \;\Rightarrow\; V_f > V_0$

(ARD3)



Inert tracers

$\mathbf{u} = \mathbf{0}$

$\partial_t \theta = D \nabla^2 \theta$

$\mathbf{u} \neq \mathbf{0}$

$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta$

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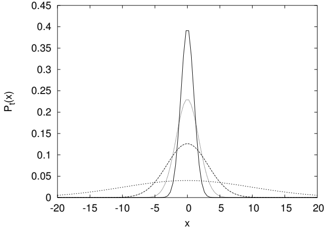

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Reactive particles

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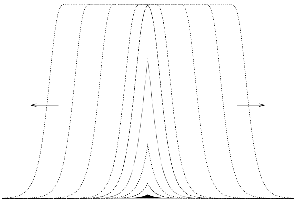

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where ψ_1 is time-periodic (T) $\Longrightarrow$ Lagrangian Chaos

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$r \ll \ell_0$	$r \gg \ell_0$
$\tau_{m_1} \sim \frac{1}{\lambda} \log \frac{L}{\delta_0} \sim \frac{1}{\lambda}$	$\tau_{m_2} \sim \frac{L^2}{D^E}$
...where...	...where...
$\lvert\delta \mathbf{x}(t)\rvert \simeq \lvert\delta \mathbf{x}(0)\rvert e^{\lambda t}$	$\partial_t \theta = D^E \nabla^2 \theta$

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let us observe that...

- $\lambda = \lambda(x) \to$ better to use $h_{KS} = \int_\Omega \lambda(x) \mathrm{d}\mu(x)$;
- τ_{m_1} ignores the existence of barriers and the effect of noise (D);
- τ_{m_2} is appropriate only if $L \gg \ell_0$ and ignores transient effects.

(AD3)

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Outline

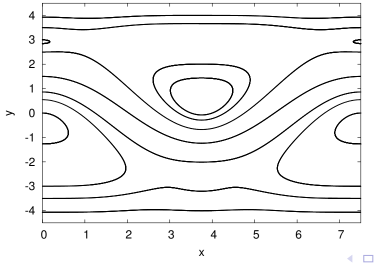
Meandering-jet (AD4)

The **stream function** is:

$$\psi(x,y,t) = -\tanh\left[\frac{y - B(t)\cos kx}{\sqrt{1+k^2 B(t)^2 \sin^2 kx}}\right] + cy$$

$$B(t) = B_0 + \epsilon \cos(\omega t + \phi)$$

The spatial structure of the stationary flow is:



$$B_0 = 1.2$$
$$k = 4\pi/15$$
$$c = 0.12$$

Overlap of the resonances (AD5)

Cross-stream transport can be characterized through the **overlap of the resonances criterion**

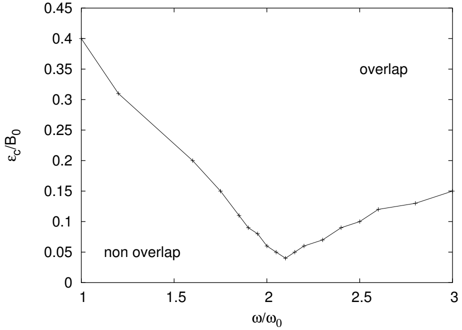
$\epsilon_c = \epsilon_c(\omega)$

$\epsilon < \epsilon_c \Rightarrow$ **local chaos**

$\epsilon > \epsilon_c \Rightarrow$ **global chaos**

$\omega_0 = 0.25$

$\phi = \pi/2$



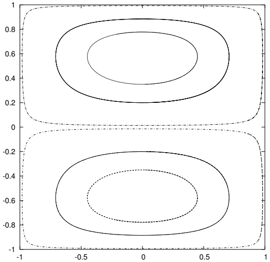
Global chaos allows cross-stream transport

Stokes flow (AD6)

The **stream function** is:

$$\psi(x,y,t) = \frac{1}{2}[(y+1)\cos\phi(t) + (y-1)\sin\phi(t)](1-x^2)(1-y^2)$$
$$\phi(t) = 2\pi t/T$$

The spatial structure of the stationary flow is:



$$V_{top} = \cos(\Phi(t))$$
$$V_{bot} = \sin(\Phi(t))$$
$$V_{top}^2 + V_{bot}^2 = 1$$

Outline

Dispersion of tracers ($D = 0$) (AD7)

local chaos **global chaos**

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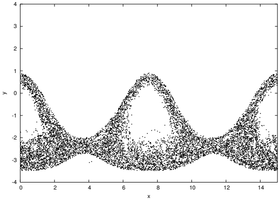
local chaos

$\omega = 0.625$

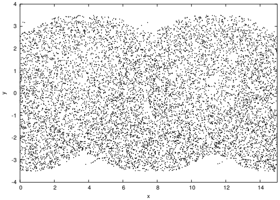
$\epsilon = 0.03$



global chaos

$\omega = 0.625$

$\epsilon = 0.24$



(MJ)

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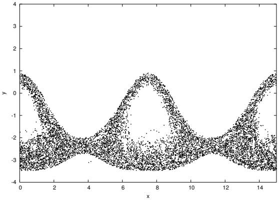

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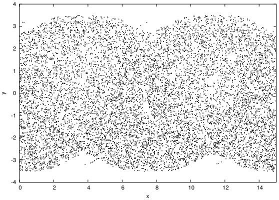
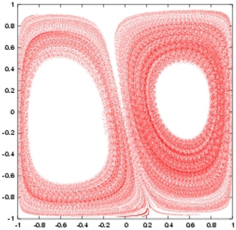
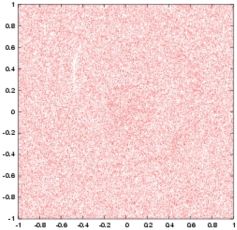


(MJ)

$T = 1$



$T = 16$

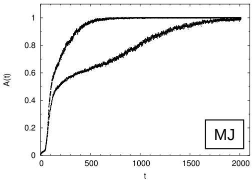


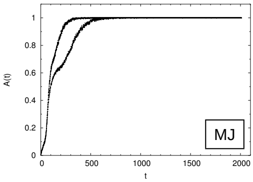
(Stokes)

Mixing (AD8)

Occupied area

$D = 0.001$





$D = 0.004$

Mixing (AD8)

Occupied area

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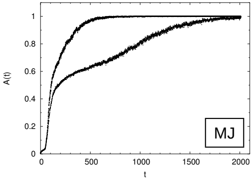
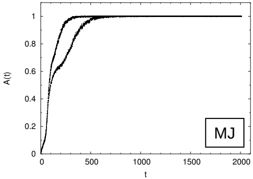




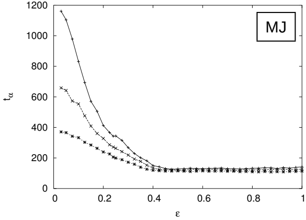
$D = 0.004$

Mixing times t_α: $A(t_\alpha) = \alpha$; $\alpha = 0.9$

$D = 0.001$

$D = 0.002$

$D = 0.004$



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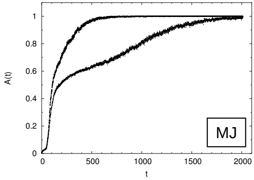

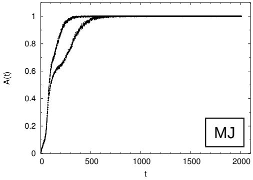

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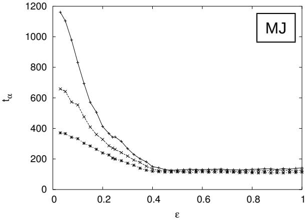

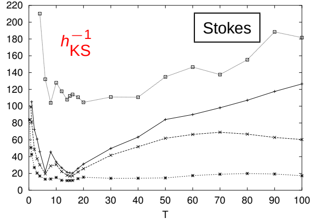

$D = 0.0005$

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$D = 0.004$

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Discrete-time approach $\longrightarrow$ numerical integration 3-step process:

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2. **backward advection**: $\mathbf{x} - \sqrt{2D\Delta t}\mathbf{w} \to \mathbf{F}_{\Delta t}^{-1}(\mathbf{x} - \sqrt{2D\Delta t}\mathbf{w})$
3. **forward reaction**: $\theta(t + \Delta t) = G_{\Delta t}(\theta(t))$

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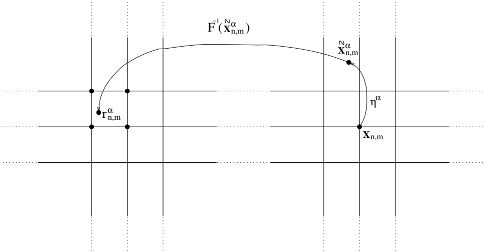

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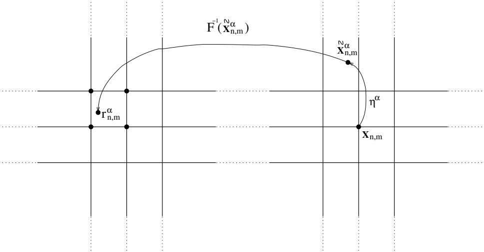

$$\mathbf{x}(t + \Delta t) = F_{\Delta t}(\mathbf{x}(t)) + \sqrt{2D\Delta t}\mathbf{w}(t) \quad \text{(lagrangian map)}$$

$$\theta(t + \Delta t) = G_{\Delta t}(\theta(t)) \quad \text{(reaction map)}$$

$$F_{\Delta t}(\mathbf{x}) \simeq \mathbf{x} + \mathbf{u}(\mathbf{x})\Delta t, \quad G_{\Delta t} \simeq \theta + \frac{\Delta t}{\tau_r} f(\theta)$$

$$\theta(\mathbf{x}, t + \Delta t) = \left\langle G_{\Delta t}\left(\theta(\mathbf{F}_{\Delta t}^{-1}(\mathbf{x} - \sqrt{2D\Delta t}\mathbf{w}(t)), t)\right)\right\rangle$$

Outline

Concentration field (MJ) (R2)

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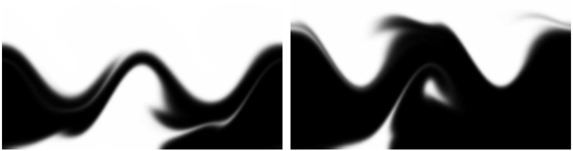
- In a **non asymptotic situation** the evolution is **not** characterized by **front propagation**

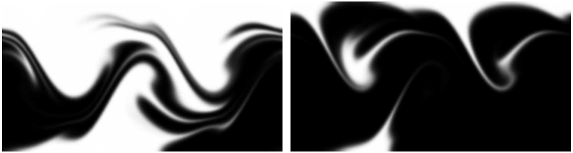


local chaos

$L_x = 15$

$\omega = 0.625$ $\epsilon = 0.03$

$\tau_r = 2$



global chaos

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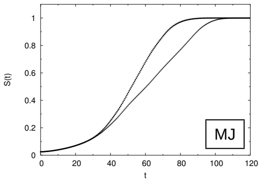
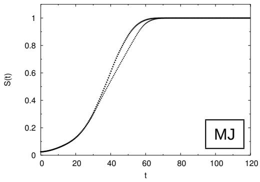
$$\boxed{t_\alpha : \quad S(t_\alpha) = \alpha}$$ $\longleftarrow$ burning time

(R4)

Burnt area

$D = 0.001$



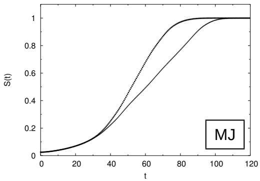


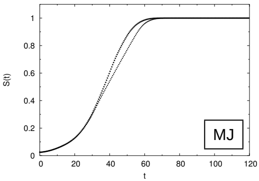
$D = 0.004$

(R4)

Burnt area

$D = 0.001$





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Burning times t_α: $S(t_\alpha) = \alpha$; $\alpha = 0.9$

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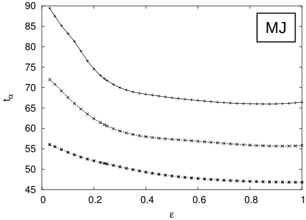
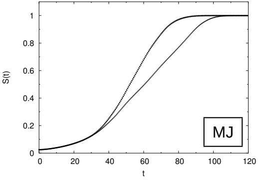
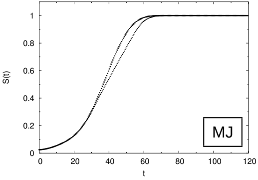


(R4)

Burnt area

$D = 0.001$





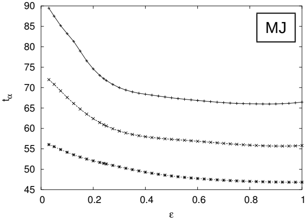
$D = 0.004$

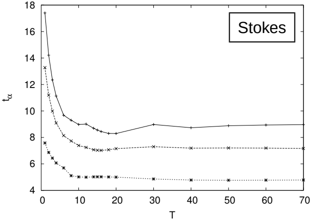
Burning times t_α: $S(t_\alpha) = \alpha;\ \alpha = 0.9$

$D = 0.001$

$D = 0.002$

$D = 0.004$





$D = 0.0005$

$D = 0.001$

$D = 0.004$

Conclusions

Non asymptotic situation $\boxed{L \simeq \ell_0}$

- In the **inert case** different dynamical regimes (local or global chaos) imply very different mixing properties.
- **The reactive case** is substantially unaffected by the presence of global chaos. The details of the velocity field have weak influence on the “burning” process, so that a more efficient mixing seems not to imply a better reaction efficiency.

For Further Reading I

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