The domain dependence of reaction processes in chaotic flows

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Competitive Advantage of Bacteria Swimming

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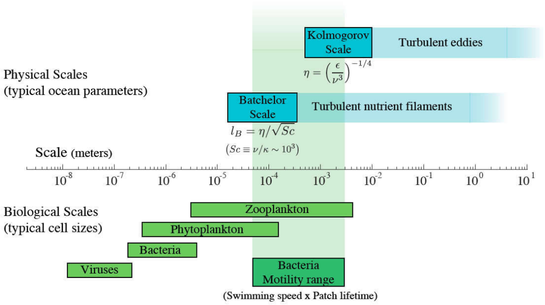

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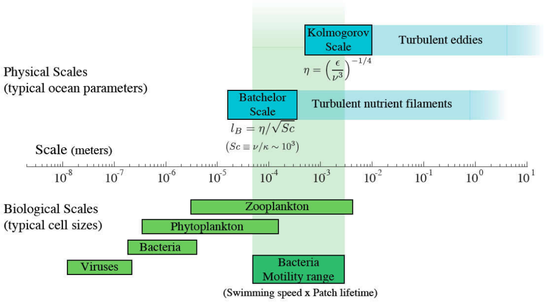

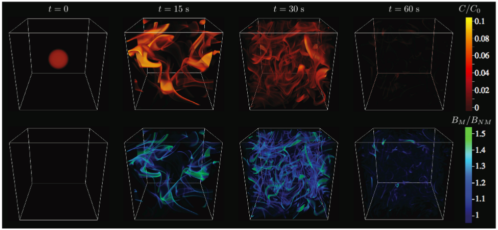

Taylor & Stocker *Science* (2012)

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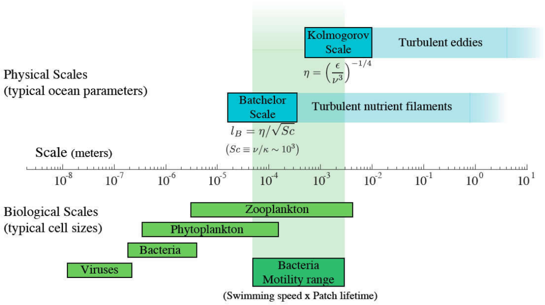

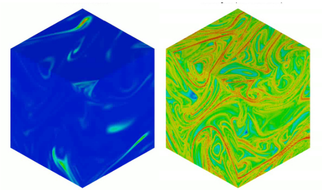

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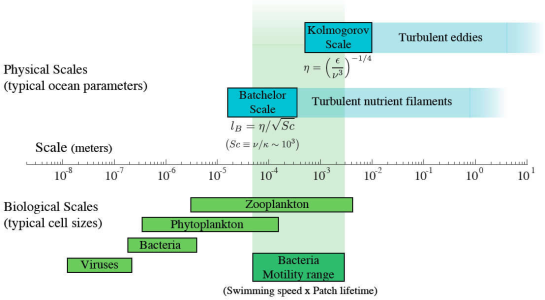

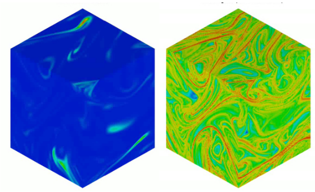

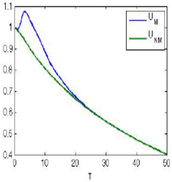

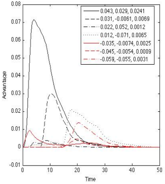

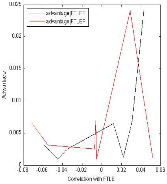

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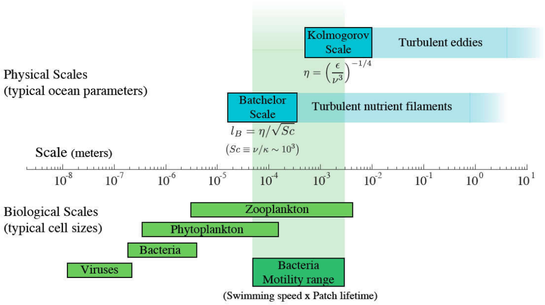
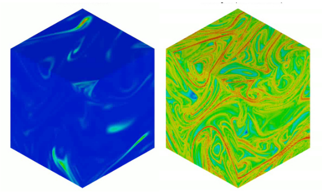
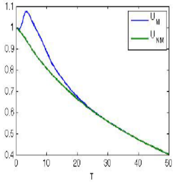
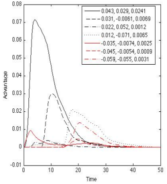
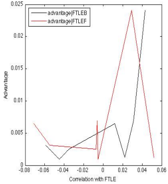




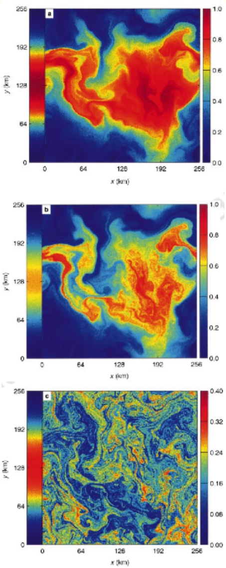






Flow topology seems to be relevant, but unable to explain

Effects of Chaotic Advection on Reaction Processes



Abraham *Nature* (1998)

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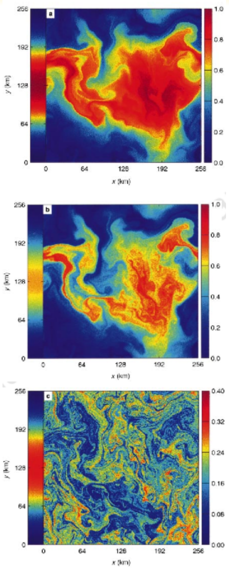

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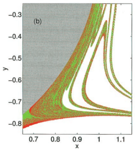
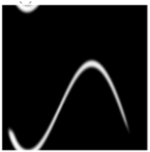
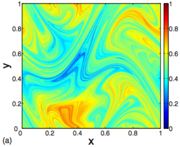
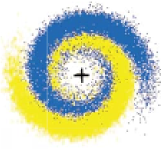




Neufeld *PRL* (2001)

Tzella & Haynes *PRE* (2010)





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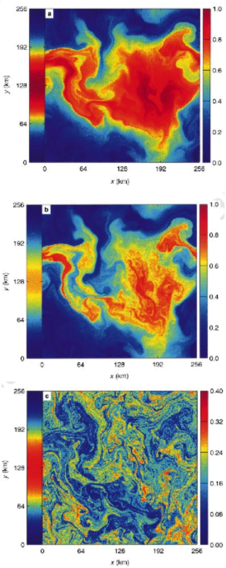

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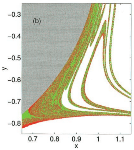

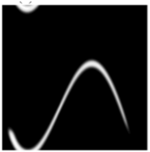

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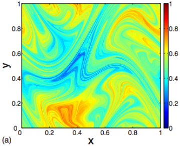

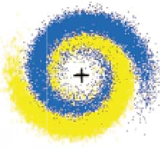

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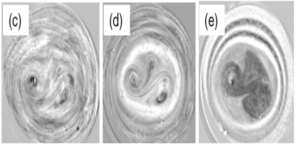

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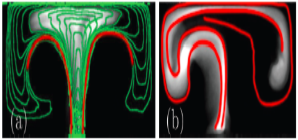

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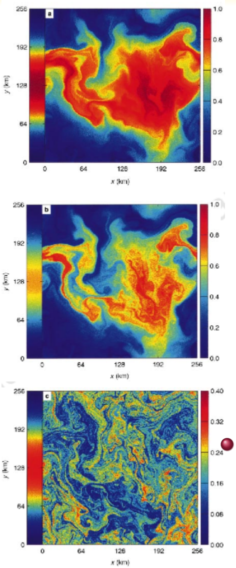

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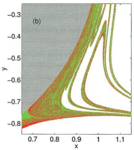

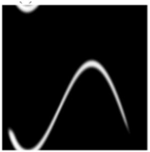

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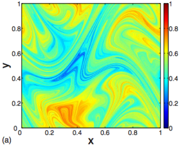

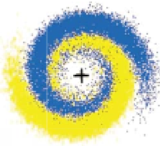

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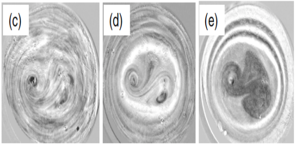

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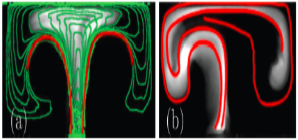

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- Tél *et al.* *Phys. Rep.* (2005), Neufeld & Hernández-García (2009)

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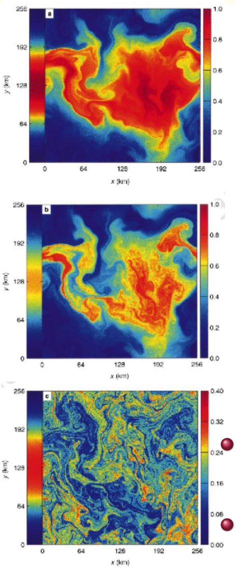

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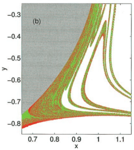

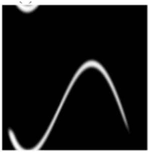

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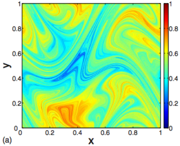

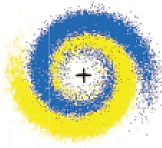

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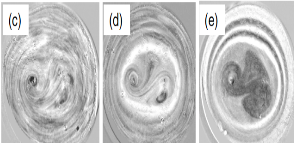

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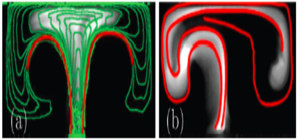

Mitchell & Mahoney *Chaos* (2012)

- Tél *et al.* *Phys. Rep.* (2005), Neufeld & Hernández-García (2009)
- Finite-time? Bulk behavior (Neufeld *et al.* 2002)? Transport barriers?

Distinct limits of scalar diffusion

- Batchelor regime
  L_B : balance - stirring & molecular diffusion

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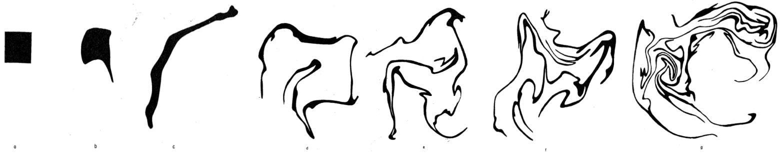

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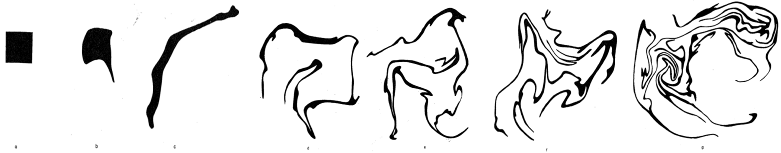

- Small-scale sink/source/biology, long-term correlation make transient-time dynamics important

Reaction Model 1 — Single Stable State (with C. Luna *PoF* 2013)

- Autocatalytic reaction in chain vortex flow

$$c_t + \mathbf{u} \cdot \nabla c - \mathrm{Pe}^{-1} \nabla^2 c = \mathrm{Da}\, c(1-c),$$

$$\mathrm{Pe} \equiv UL/\kappa_{eddy} \sim 10 - 10^4, \qquad \mathrm{Da} \equiv kC_0 L/U \sim 1$$

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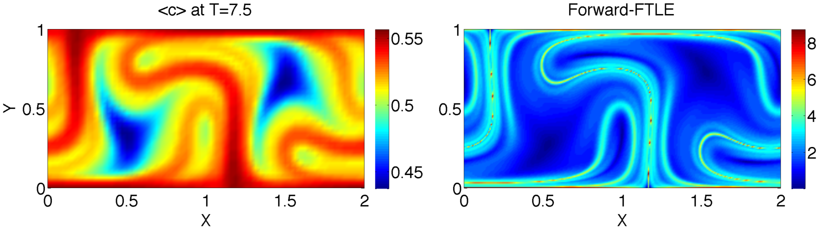
- Spatially periodic flow → homogenization, what about transient?

Comparisons

- Initial stretching dictates reaction variability



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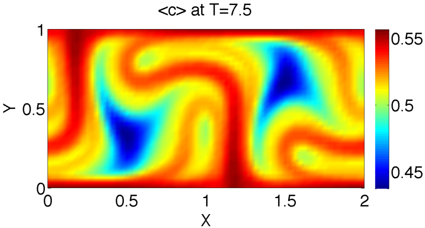
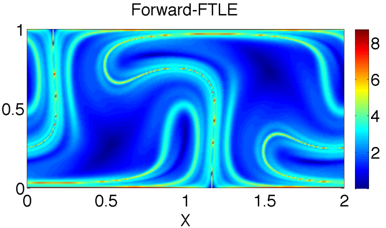
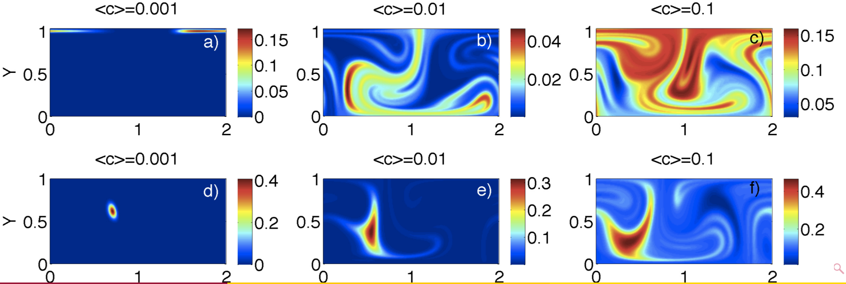




- Four stages of the ADR process based on scalar budget $\langle c \rangle$



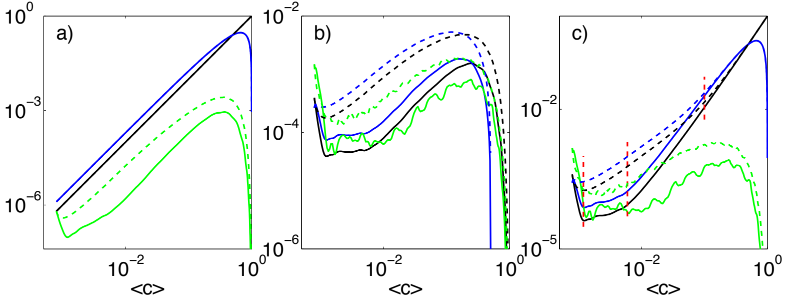
Scalar budget

- Evolution of scalar density and related quantities

$$\frac{\mathrm{d}\langle c\rangle}{\mathrm{d}t} = \mathrm{Da}\langle c\rangle - \mathrm{Da}\langle c^2\rangle \equiv \mathrm{Da}\langle c\rangle - \mathrm{Da}\langle c\rangle^2 - \mathrm{Da}\langle c'^2\rangle,$$

$$\frac{\mathrm{d}\langle c\rangle^2}{\mathrm{d}t} = 2\mathrm{Da}\langle c\rangle^2 - 2\mathrm{Da}\langle c\rangle^3 - 2\mathrm{Da}\langle c\rangle\langle c'^2\rangle,$$

$$\frac{\mathrm{d}\langle c'^2\rangle}{\mathrm{d}t} = -\frac{2}{Pe}\langle|\nabla c'|^2\rangle + 2\mathrm{Da}\langle c'^2\rangle - 4\mathrm{Da}\langle c\rangle\langle c'^2\rangle - 2\mathrm{Da}\langle c'^3\rangle.$$



Behavior at different stages

- Stage 1: decay due to scalar dissipation

$$c_t - \lambda \hat{x} c_{\hat{x}} + \lambda \hat{y} c_{\hat{y}} = \frac{1}{Pe}(c_{\hat{x}\hat{x}} + c_{\hat{y}\hat{y}})$$

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$$G(\hat{x}, \hat{y}, t; x', y') = \frac{Pe}{4\pi t} \exp\left\{ -\frac{Pe[(\hat{x} - x')^2 e^{2\lambda t} + (\hat{y} - y')^2 e^{-2\lambda t}]}{4t} \right\},$$

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- Based on this approximation dissipation rate is (σ^2 : initial variance)

$$\left\langle |\nabla c|^2 \right\rangle = \frac{\pi \sigma^4 e^{\lambda t} (\sigma^2 e^{2\lambda t} + t e^{4\lambda t} Pe^{-1} + t Pe^{-1})}{(\sigma^2 e^{2\lambda t} + 2t Pe^{-1})^{3/2} (\sigma^2 + 2t e^{2\lambda t} Pe^{-1})^{3/2}},$$

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- Small t behavior is $\pi[1 + 3t\lambda(1 - \sigma^2) + 2t(1/\sigma^2 - 3)/Pe]$

Behavior at different stages

- Stage 2: maintenance of filament width at Batchelor scale

$$c_t - \lambda \hat{x} c_{\hat{x}} = \frac{1}{Pe} c_{\hat{x}\hat{x}} + \mathrm{Da} c.$$

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$$\begin{aligned} X &= c_1 exp(-\lambda Pe \hat{x}^2/2) \\ T &= e^{\mathrm{Da} t} \end{aligned}$$

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$$\begin{aligned} X &= c_1 exp(-\lambda Pe \hat{x}^2/2) \\ T &= e^{\mathrm{Da} t} \end{aligned}$$

- Amplitude c_1 decays as $e^{-\lambda t}$
- Scalar dissipation scales as $\mathcal{O}(e^{-2\lambda t} e^{\lambda t} e^{\mathrm{Da} t}) = \mathcal{O}(e^{(\mathrm{Da}-\lambda)t})$
- The larger the stretching, the smaller the dissipation

Behavior at different stages

- Stage 2: maintenance of filament width at Batchelor scale

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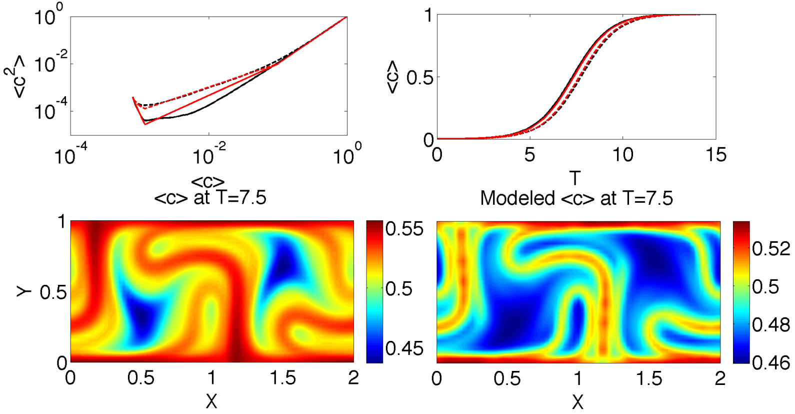
- Stage 3: homogenization in different zones
- Stage 4: almost uniform reaction

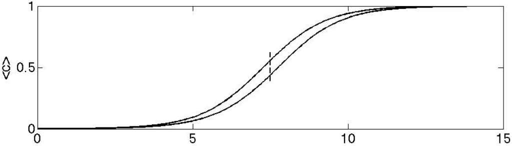
Modeling based on Lagrangian stretching rate

- Model effective reaction rate $\langle c^2 \rangle = f(FTLE_w, \langle c \rangle)$



Parametric dependence

- Quantify variability based on gap at intermediate time to saturation



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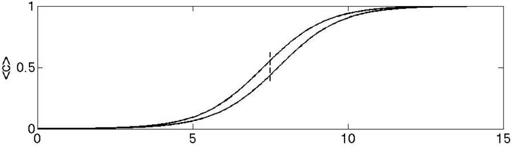
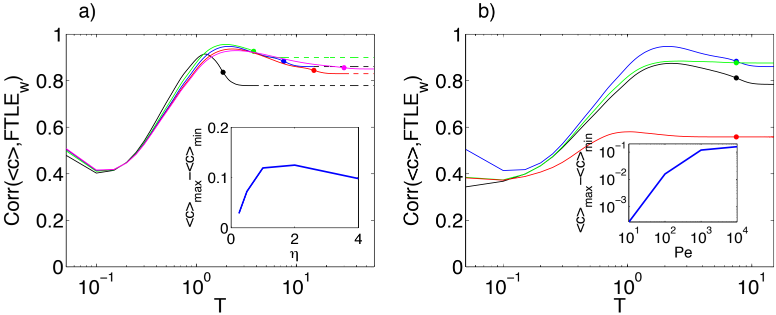


- Vary Da, Pe independently



Reaction Model 2 — Bistable Equilibria with A. Dhumuntarao, submitted

- Bistable dynamics with single scalar

$$(c_t + \mathbf{u} \cdot \nabla c) - \mathrm{Pe}^{-1}\nabla^2 c = \mathrm{Da}\, c(\alpha - c)(c-1),$$
$$\mathrm{Pe} = 1000, \qquad \alpha = 0.2, \qquad \mathrm{Da} \text{ varies}$$

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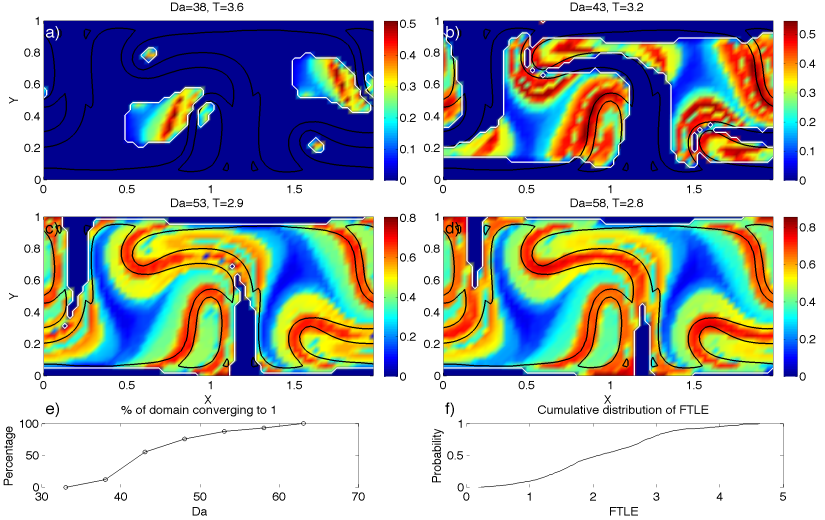
- Without flow, $c = 1$ is more stable. With flow (Da=53):

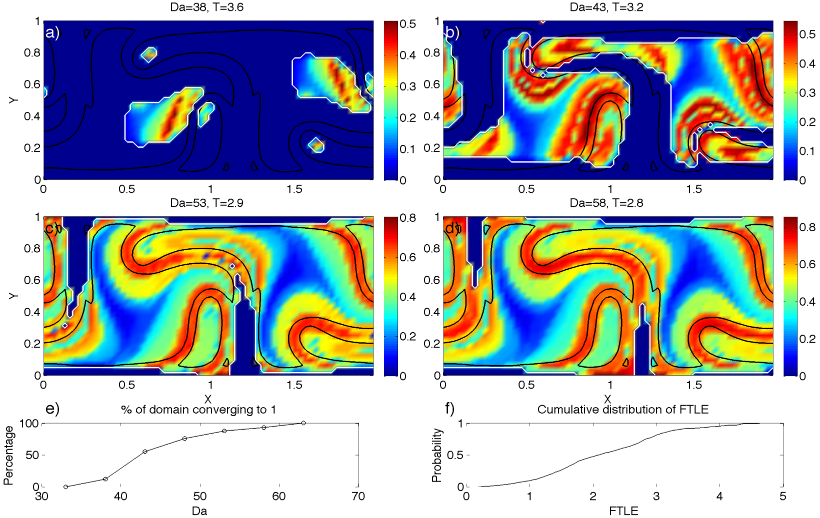
Domain Partition

- Dependence on *Da*



Domain Partition

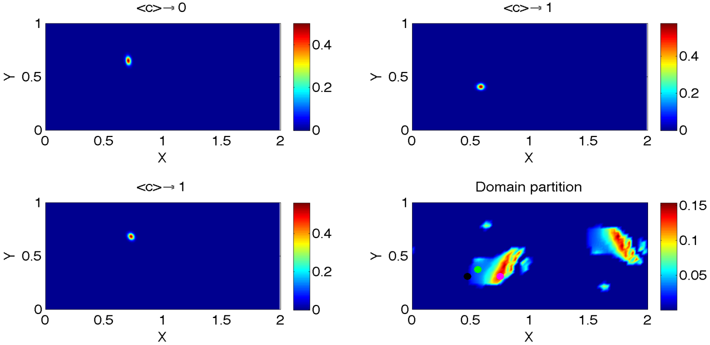
- Dependence on *Da*



- FTLE (with T=1) alone insufficient to explain (at least for $Da = 38$)

Closer look for small *Da*

- $Da = 38$, lower stretching $\to 0$, higher stretching $\to 1$



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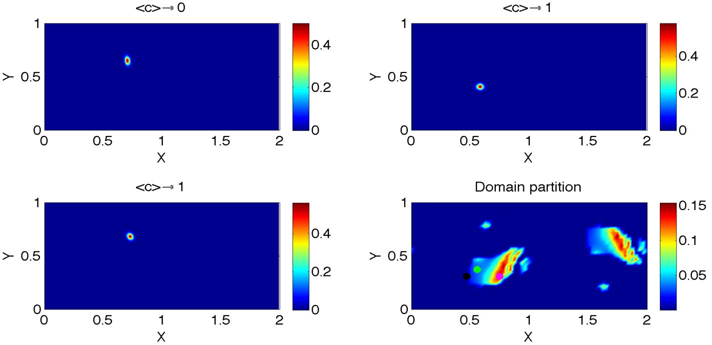
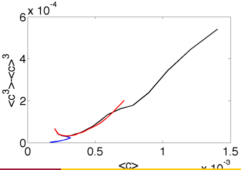
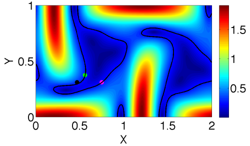


- Bifurcation location (I.C. dependent)





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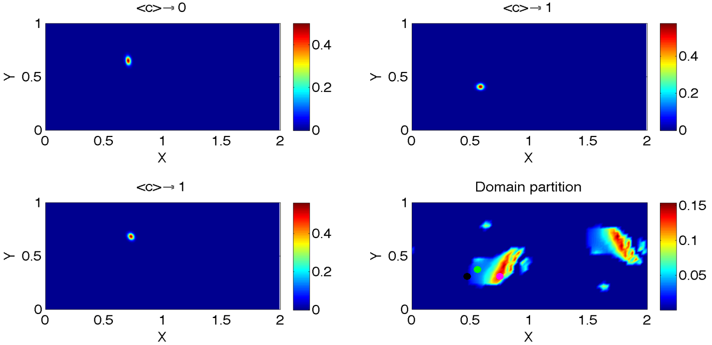
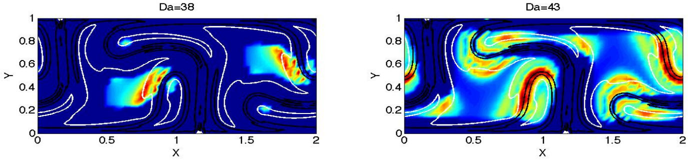


- $Da = 38$ vs $Da = 43$



Turbulence

- 2D turbulence randomly forced to maintain modal energy at medium wavenumber and low-mode damped to avoid inverse cascade

$$\omega_t + J[\psi, \omega] = \frac{1}{Re}\nabla^2\omega + \psi + f, \qquad \omega = \nabla^2\psi$$

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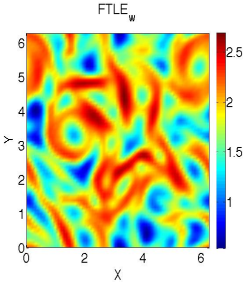
$$\omega_t + J[\psi, \omega] = \frac{1}{Re}\nabla^2\omega + \psi + f, \qquad \omega = \nabla^2\psi$$

- $Re = 1000, Sch = 1$, distinct behaviors at $Da = 8$



Domain Partition

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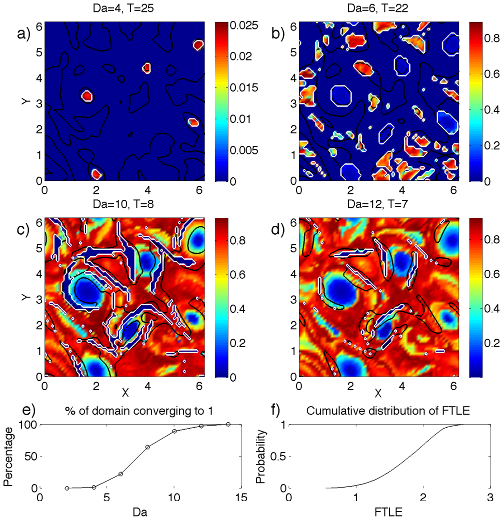

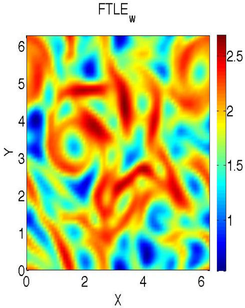

Reaction Model 3 — Chemotaxis in 2D with K. Jones, in preparation

- Motile species move via chemotaxis

$$
\begin{aligned}
(C_t + \mathbf{u}\cdot\boldsymbol{\nabla} C) - \mathrm{Pe}^{-1}\nabla^2 C &= -\mathrm{Da}\, C(B+1), \\
(B_t + \mathbf{u}\cdot\boldsymbol{\nabla} B) - \mathrm{Pe}^{-1}\nabla^2 B &= -\chi\nabla(B\nabla C), \\
\mathrm{Pe} = 1000,\ \mathrm{Da} = 0.001,\ \chi &= 0.01
\end{aligned}
$$

Reaction Model 3 — Chemotaxis in 2D with K. Jones, in preparation

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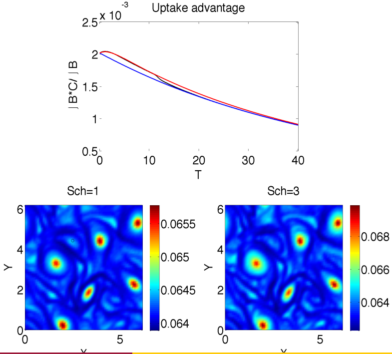
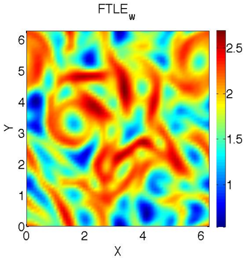
$$(B_t + \mathbf{u}\cdot\boldsymbol{\nabla} B) - \mathrm{Pe}^{-1}\nabla^2 B = -\chi\nabla(B\nabla C),$$
$$\mathrm{Pe} = 1000,\ \mathrm{Da} = 0.001,\ \chi = 0.01$$

- $\mathrm{U}_M = \int_D B_M \cdot C dD / \int_D B_M dD$, $\mathrm{U}_{NM} = \int_D B_{NM} \cdot C dD / \int_D B_{NM} dD$,





Summary

- Conclusions
  - FKPP
    - Spread further to react fast
    - Chaotic advection affects early reaction, dictates bulk reaction speed
    - Lagrangian measures (FTLE) can be used to parameterize this variability, even with transport barriers
  - Bistable Equilibria
    - Flow topology can lead to distinct states
    - Similarity and distinction from FKPP
    - Distinct fates even when eddies are transient
- Current work
  - Determination of bifurcation boundary for bistable reaction
  - Mixing between fixed point and limit cycle
  - Domain dependence for chemotaxis
- References

  - Tang,W. & Luna, C., Dependence of advection-diffusion-reaction on flow coherent structures. Phys. Fluids, 25 (2013): 105602
  - Tang,W. & Dhumuntarao, C., Bistability in inhomogeneity — effects of flow coherent structures on the fate of a bistable reaction. submitted
  - Tang,W. & Jones, K., The domain dependence of chemotactic advantage in two-dimensional flows. in preparation