Lecture 6: Mixing in the presence of sources and sinks

Jean-Luc Thiffeault

Notes by Sam Pegler and Woosok Moon

28 June 2010

1 Norms

In this section we define a measure of mixing that does not necessarily require diffusion to measure the amount of homogenization that occurs during the mixing process. Recall the advection-diffusion equation

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta = \kappa \nabla^2 \theta, \tag{1}$$

where θ is a concentration field in a finite domain Ω, with no-net-flux boundary conditions. We assume without loss of generality that

$$\int_\Omega \theta \, \mathrm{d}\Omega = 0, \tag{2}$$

and define the L^2-norm, or variance, as

$$\|\theta\|_2^2 = \int_\Omega \theta^2 \, \mathrm{d}\Omega. \tag{3}$$

Recall from Lecture 1 that the variance evolves according to

$$\frac{d}{dt}\|\theta\|_2^2 = -2\kappa \|\boldsymbol{\nabla}\theta\|_2^2, \tag{4}$$

and decays in time as the system mixes. The variance indicates the extent to which the concentration has homogenized and is thus a good measure of the amount of mixing that has occurred. However, the variance requires knowledge of small scales in θ, which we are not necessarily interested in. A measure of how well-mixed the concentration is does not necessarily require knowledge of how much homogenization has occurred due to diffusion at small scales. This is more in keeping with the definition of mixing in the sense of ergodic theory [2]. In this regard, we proceed to consider the pure advection equation

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta = 0. \tag{5}$$

Note that in this case equation (4) predicts that the variance satisfies

$$\frac{d}{dt}\|\theta\|_2^2 = 0, \tag{6}$$

and cannot therefore be used as a measure of mixing.

The advection equation (5) takes us closer to the ergodic sense of mixing in which we think of the advection due to the velocity field as a time-dependent operator $S^t : \Omega \to \Omega$ that moves an initial patch of dye according to

$$\theta_0(\boldsymbol{x}) \mapsto \theta(\boldsymbol{x}, t) = S^t \theta_0(\boldsymbol{x}). \tag{7}$$

If we consider a region A of uniform concentration defined by

$$\theta_0(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in A, \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

then the volume of the patch

$$\mathrm{Vol}[\theta(\boldsymbol{x}, t)] = \mathrm{Vol}(A), \tag{9}$$

remains constant in time by incompressibility. We can associate the volume of the patch with the Lebesgue measure and, because of the result (9) above, S^t is measure-preserving.

We define mixing in the sense of ergodic theory by

$$\lim_{t\to\infty} \mathrm{Vol}[A \cap S^t(B)] = \mathrm{Vol}(A)\mathrm{Vol}(B), \tag{10}$$

for all patches $A, B \in \Omega$. This definition follows our intuition for what good mixing is. Referring to figure 1, when the system is well-mixed the intersection of A and $S^t B$ is proportional to both $\mathrm{Vol}(A)$ and $\mathrm{Vol}(B)$. Thus, if the condition (10) holds then S^t must spread any initial patch throughout the domain. This condition is referred to as *strong mixing* and can be shown to imply ergodicity.

The intersection of the advected patch B with the reference patch A is analogous to projection onto L^2 functions. This motivates the following *weak convergence* condition

$$\lim_{t\to\infty} \langle \theta(\boldsymbol{x}, t), g \rangle = 0, \tag{11}$$

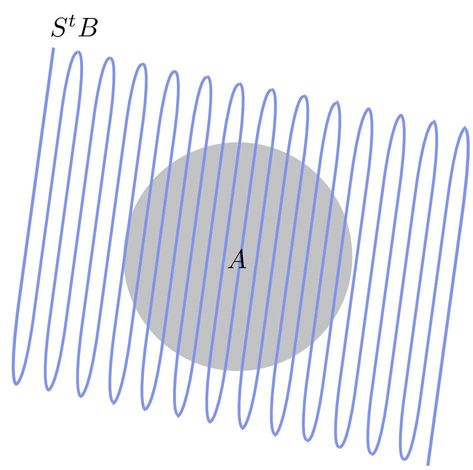

Figure 1: An advected patch $S^t B$ that has undergone strong mixing. At late times the patch covers an arbitrary reference patch A.

for all functions $g \in L^2(\Omega)$, where the inner product is defined by

$$\langle f, g \rangle = \int_\Omega f(\boldsymbol{x}) g(\boldsymbol{x}) \, \mathrm{d}\Omega, \tag{12}$$

and $f \in L^2(\Omega)$ if $\int_\Omega |f|^2 \, \mathrm{d}\Omega < \infty$. Weak convergence is equivalent to mixing as a consequence of the Riemann–Lebesgue lemma. The equivalent conditions (10) and (11) require computing over all patches A or functions g, respectively. Thus, neither of these conditions is useful in practice. However, we proceed to describe a theorem that shows there is a simpler way to determine whether or not weak convergence is satisfied.

Mathew, Mezic and Petzold [5] introduced the mix-norm, which for mean-zero functions is equivalent to

$$\|\theta\|_{\dot{H}^{-1/2}} := \|\nabla^{-1/2}\theta\|_2 \,. \tag{13}$$

Doering and Thiffeault [1] and Lin, Thiffeault and Doering [3] generalized the mix-norm to

$$\|\theta\|_{\dot{H}^q} := \|\nabla^q \theta\|_2, \qquad q < 0, \tag{14}$$

which is a negative homogeneous Sobolev norm. This norm can be interpreted for negative q via eigenfunctions of the Laplacian operator. For example, in a periodic domain, we have

$$\|\theta\|^2_{\dot{H}^q} = \sum_{\boldsymbol{k}} |\boldsymbol{k}|^{2q} |\hat{\theta}_{\boldsymbol{k}}|^2, \tag{15}$$

from which we see that, for $q < 0$, $\|\theta\|^q_{\dot{H}}$ smooths θ before taking the L^2 norm. The theorem

$$\lim_{t\to\infty} \|\theta\|_{\dot{H}^q} = 0, \quad q < 0 \quad \iff \quad \theta \text{ converges weakly to } 0, \tag{16}$$

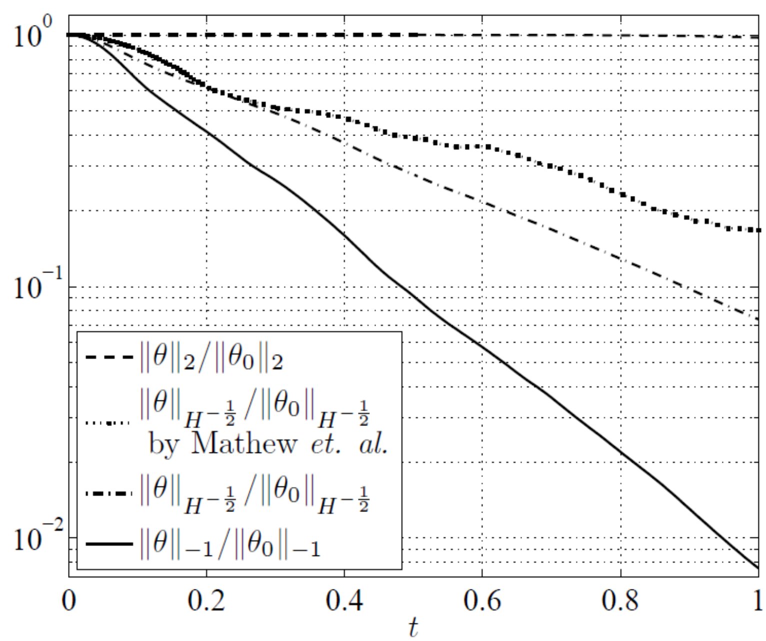

Figure 2: Comparison of the mix-norms for a flow optimized using the separate methods of optimal control and optimal instantaneous decay. Figure from Lin *et al.* [3].

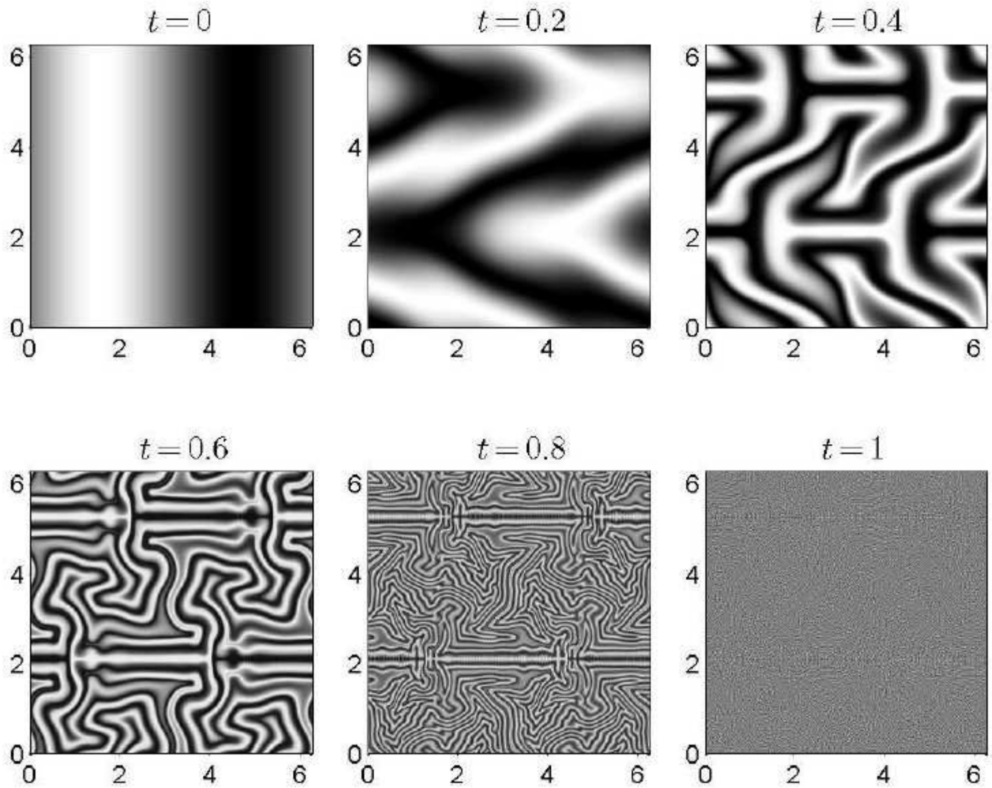

Figure 3: Evolution of the concentration field for the flow optimized in the case $q = -1$ as computed by Lin *et al.* [3].

due to Mathew, Mezic and Petzold [5] and Doering, Lin and Thiffeault [3] shows that we can track any mix-norm to determine whether a system is mixing (in the weak sense). The existence of this quadratic norm makes optimization of the velocity field for good mixing considerably easier. Mathew, Mezic, Grivopoulos, Vaidya and Petzold [4] have used optimal control to optimize the decay of the $q = -1/2$ mix-norm. Lin, Doering and Thiffeault [3] have optimized the instantaneous decay rate of the $q = -1$ norm using the method of steepest descent, which is easier to compute numerically but yields suboptimal, but nevertheless very effective, stirring velocity fields. A comparison of the methods for optimized mixing is shown in figure 2. The solid line decays faster, but this is merely because the $\dot{H}^{-1}$ cannot be compared directly with $\dot{H}^{-1/2}$. The corresponding evolution of the concentration field for the case $q = -1$ from Lin *et al.* [3] is shown in figure 3.

2 Sources and Sinks

Now let us consider the situation with a sources-sink term $s(\boldsymbol{x}, t)$,

$$\begin{aligned} \partial_t \theta + \boldsymbol{u} \cdot \nabla \theta &= \kappa \nabla^2 \theta + s\left(\boldsymbol{x}, t\right), \\ \nabla \cdot \boldsymbol{u} &= 0. \end{aligned} \tag{17}$$

For simplicity, assume that $\int_\Omega s(\boldsymbol{x}, t) d\Omega = 0$. Otherwise, we can subtract the mean of θ. It is convenient to think of sources and sinks as hot and cold regions.

Let us also assume that our sources and sinks are time-independent. Then, the system eventually achieves a steady state $\theta(\boldsymbol{x})$ that satisfies

$$\boldsymbol{u} \cdot \nabla \theta = \kappa \nabla^2 \theta + s. \tag{18}$$

We define the operator

$$\mathcal{L} \equiv y \cdot \nabla - \kappa \nabla^2 \tag{19}$$

so that (18) can be written

$$\mathcal{L}\theta = s. \tag{20}$$

The steady solution is then

$$\theta = \mathcal{L}^{-1} s \tag{21}$$

where the mean-zero condition on θ makes this unique. Note that $\kappa \neq 0$ is needed to achieve a steady state. So, assuming the system has reached a steady-state, we have to determine how we measure the quality of mixing. One of the possible ways is to look at the norms $\|\theta\|_{\dot{H}^q}$, where $q = 0$ represents standard derivation. But we have to decide what we will compare to. One possibility is $\|\theta\|_{\dot{H}^q} / \|s\|_{\dot{H}^q}$. This ratio is a reasonable choice, but has units of inverse time. It is preferable to use a dimensionless quantity for measuring the quality of mixing. In this spirit, we define *mixing enhancement factors*:

$$\varepsilon_q = \frac{\|\tilde{\theta}\|_{\dot{H}^q}}{\|\theta\|_{\dot{H}^q}}, \tag{22}$$

where $\tilde{\theta}$ is the purely-diffusive solution which satisfies

$$\tilde{\mathcal{L}}\tilde{\theta} = s.$$

Here, $\tilde{\mathcal{L}} = -\kappa \nabla^2$ is the pure diffusive operator, so $\tilde{\theta}$ can be interpreted as the solution in the absence of stirring. Since $\|\theta\|_{\dot{H}^q}$ is usually decreased by stirring, ε_q measures the enhancement over the pure-diffusion state. Several properties are given in Doering and Thiffeault [1], Shaw, Thiffeault and Doering [7], and Thiffeault and Pavliotis [8]. We interpret a large ε_q as ‘good stirring,’ since it in that case the norm is decreased by stirring.

A natural question is whether ε_q can ever be less than unity, that is, if stirring can ever be worse than not stirring. Let’s consider

$$\varepsilon_1 = \frac{\|\nabla \tilde{\theta}\|_2}{\|\nabla \theta\|_2}$$

Here,

$$\tilde{\theta} = \tilde{\mathcal{L}}^{-1} s = \left(-\kappa \nabla^2\right)^{-1} s = -\kappa^{-1} \nabla^{-2} s \Rightarrow \nabla \tilde{\theta} = -\kappa^{-1} \nabla^{-1} s$$

Also, from $\mathcal{L}\theta = s$, we can multiply θ on both sides and take spatial average and then get

$$\langle \theta \mathcal{L} \theta \rangle = \langle s\theta \rangle \,,$$

where $\langle \cdot \rangle = \int_\Omega \cdot \, d\Omega$. We expand the left-hand side:

$$\begin{aligned} \langle \theta \mathcal{L} \theta \rangle &= \langle \theta u \cdot \nabla \theta \rangle - \kappa \left\langle \theta \nabla^2 \theta \right\rangle \\ &= \left\langle \nabla \cdot \left(u\theta^2/2 \right) \right\rangle - \kappa \left\langle \theta \nabla^2 \theta \right\rangle \\ &= -\kappa \left\langle \theta \nabla^2 \theta \right\rangle = \kappa \left\langle |\nabla \theta|^2 \right\rangle . \end{aligned}$$

As for the right-hand side,it can be written as

$$\langle \theta s \rangle = \left\langle \theta \nabla \cdot \nabla^{-1} s \right\rangle = - \left\langle \nabla \theta \cdot \nabla^{-1} s \right\rangle = \kappa \left\langle \nabla \theta \cdot \nabla \tilde{\theta} \right\rangle ,$$

where we used

$$\begin{aligned} &\tilde{\theta} = \tilde{\mathcal{L}}^{-1} s = \left(-\kappa \nabla^2\right)^{-1} s = -\kappa^{-1} \nabla^{-2} s \\ &\iff \nabla \tilde{\theta} = -\kappa^{-1} \nabla^{-1} s \,. \end{aligned}$$

Recall that $\left\langle |\nabla \theta|^2 \right\rangle = \|\theta\|^2_{\dot{H}^1}$. Therefore,

$$\|\theta\|^2_{\dot{H}^1} = \left\langle \nabla \theta \cdot \nabla \tilde{\theta} \right\rangle \;\leq\; \|\nabla \theta\|_2 \|\nabla \tilde{\theta}\|_2 = \|\theta\|_{\dot{H}^1} \|\tilde{\theta}\|_{\dot{H}^1} \,.$$

We conclude that

$$\|\theta\|_{\dot{H}^1} \;\leq\; \|\tilde{\theta}\|_{\dot{H}^1} \;\iff\; \varepsilon_1 \;\leq\; 1 \,. \tag{23}$$

This is somewhat counter-intuitive because gradients are usually increased by stirring. However, the gradients in a steady-state have been affected by diffusion.

What about ε_q for values of q other than 1? We tried and failed to prove $\varepsilon_q \leq 1$, simply because it is not true. Following a challenge by Charlie Doering at a workshop at the IMA in 2010, Jeff Weiss came up with something like:

$$u = (2 \sin x \cos 2y \,, -\cos x \sin 2y) \,, \tag{24a}$$

$$s = \left(\cos x - \tfrac{1}{2}\right) \sin y \,. \tag{24b}$$

This velocity field manages to concentrate the source and sink distribution more than diffusion alone. Streamlines of u and level sets of s are shown in figure 4. In this example, we could get $\varepsilon_0 \simeq 0.978$ and $\varepsilon_{-1} \simeq 0.945$, which are slightly less than 1. It is an open problem to characterize such ‘unmixing’ flows.

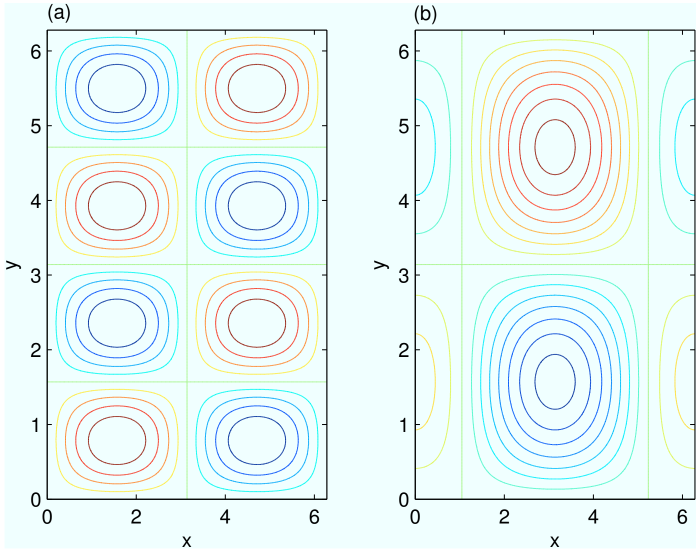

Figure 4: The pattern of velocity field and source for the 'unmixing' flow and source distribution (24).

3 Optimization

We defined the mixing enhancement factors based on Sobolev norms. Large mixing enhancement factor indicates good mixing for a given source and sink pattern. One of the relevant questions in this step is what kinds of flow give the largest ε_q given source and sink distribution $s(\boldsymbol{x})$.

Here is a simple but surprising example. The source and sink distribution is given by $s(x) = \sin x$ with periodic boundary conditions on θ. The optimal solution for this source and sink distribution is $\boldsymbol{u} = U\hat{x}$, which is constant flow from the hot region to the cold region [6–8] (figure 5). This example demonstrates that, with body sources, the best

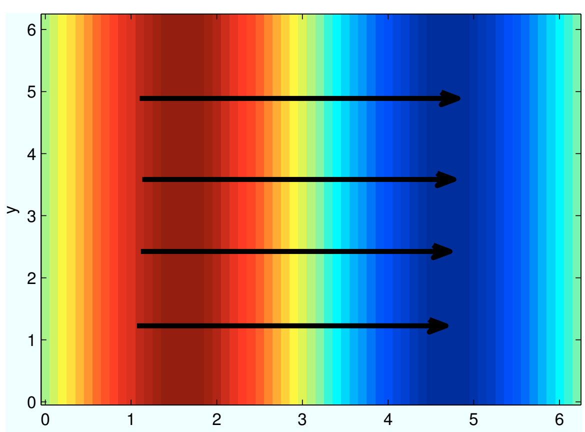

Figure 5: The optimal velocity field (solid arrows) for the source distribution $s(x) = \sin x$.

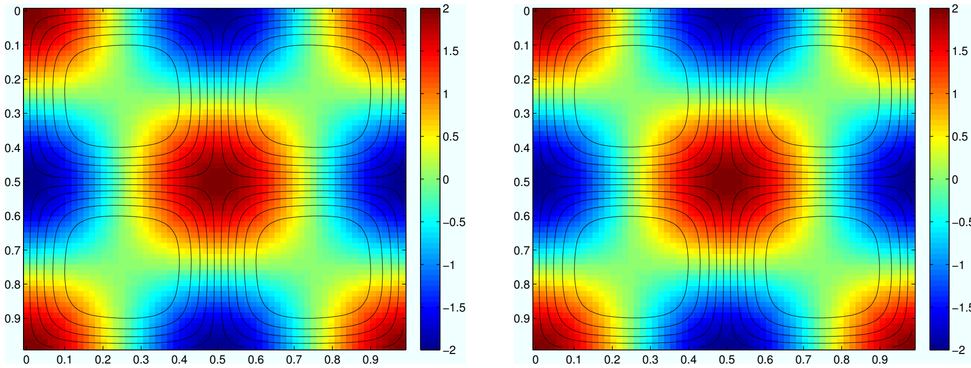

Figure 6: Optimal stirring velocity field (solid lines) for the source $s(\boldsymbol{x}) = \sin x \sin y$ (colored background), for $q = 0$ (left) and $q = -1$ (right). The optimal velocity is the same in both cases because the source is an eigenfunction of the Laplacian. (Matlab programs `example(1)` and `example(2)` in the Appendix.)

stirring often has more to do with transport than with creation of small scales.

More generally, we have to solve the optimization problem numerically. Figure 6 shows contours of the streamfunction for the optimal stirring velocity (lines) for a source $s(\boldsymbol{x}) = \sin x \sin y$, for $q = 0$ and $q = -1$. The optimal velocity fields are identical for the two values of q, because the source is an eigenfunction of the Laplacian.

Contrast this to the optimal solutions in figure 7, for the source distribution $s(\boldsymbol{x}) = \cos x \cos y + \cos 3y + (1/4) \sin 3y$. This source is not an eigenfunction of the Laplacian, and we expect optimal solutions to depend on q. Comparing the left ($q = 0$) and right ($q = -1$) figures, we see this is indeed the case, though the difference in this case is fairly small.

Finally, given an optimization code, it is simple to turn it around to anti-optimize, that is, find the *worst* stirring velocity for a given source distribution. Figure 8 shows this for the source (24b) and $q = 0$. Note how the velocity field seems to work to concentrate the source sink, thereby increasing the variance. The efficiency for this anti-optimal solution is $\varepsilon_0 = 0.9736$, which is not much lower than Jeff Weiss's unoptimized flow (24a), which had $\varepsilon_0 \simeq 0.978$.

To reproduce the 5 figures in this section run the program `example`(n) in the Appendix, where n is a number from 1 to 5.

Appendix: Matlab code

1 Program file `example.m`

```
function example(ex)

% util folder contains Diffmat2.m, fourdif.m, refine.m, refine2.m, refinek.m
% Contact author to obtain these functions.
addpath util

if nargin < 1, ex = 1; end
```

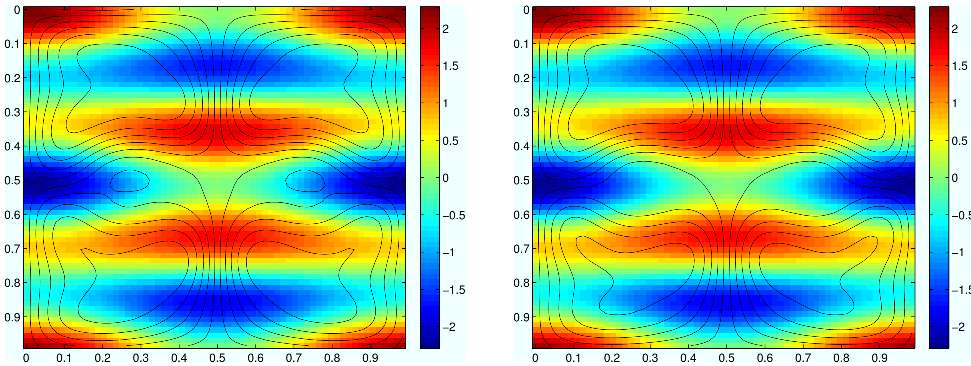

Figure 7: Optimal stirring velocity field (solid lines) for the source $\cos x \cos y + \cos 3y + (1/4) \sin 3y$ (colored background), for $q = 0$ (left) and $q = -1$ (right). The optimal velocities are different since the source is not an eigenfunction of the Laplacian. (Matlab programs `example(3)` and `example(4)` in the Appendix.)

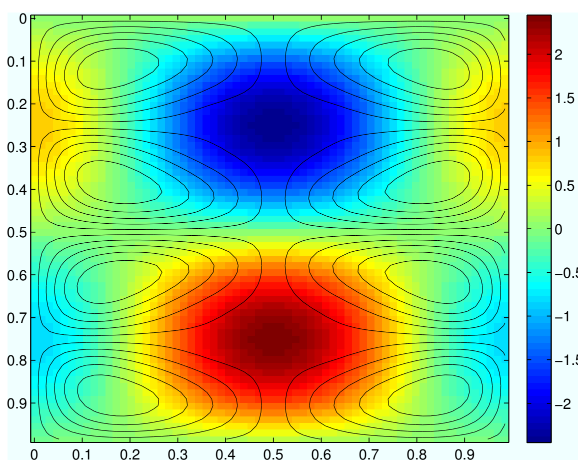

Figure 8: Optimal 'unmixing' solution for the source $\left(\cos x - \frac{1}{2}\right) \sin y$, with mixing efficiency $\varepsilon_0 = 0.9736$. (Matlab program `example(5)` in the Appendix.)

```
N = 11; % Number of gridpoints
L = 1; k1 = 2*pi/L; % Physical size of domain
x = L*(0:N-1)/N; y = x'; [xx,yy] = meshgrid(x,y);

switch ex
 % Examples 1 and 2 use the same cellular source, for q=0 and q=-1.
 % Since the source is an eigenfuntion of the Laplacian, the optimal
 % flow is the same for q=-1.
 case {1,2}
  src = cos(k1*xx).*cos(k1*yy) * 2/L;
  psi0 = sin(k1*xx).*sin(k1*yy) * 1/sqrt(2)/pi;
  kappa = .1; q = 1-ex;
 % Examples 3 and 4 use the same two-mode source, for q=0 and q=-1.
 % Since the source is not an eigenfuntion of the Laplacian, so the optimal
 % flow is different for q=-1.
 case {3,4}
  src = (cos(k1*xx).*cos(k1*yy)+cos(3*k1*yy)+.25*sin(3*k1*yy)) * 4*sqrt(2)/5/L;
  psi0 = sin(k1*xx).*sin(k1*yy) * 1/sqrt(2)/pi;
  kappa = .1; q = 3-ex;
 case 5
  % Unmixing solution
  src = (cos(k1*xx) - .5).*sin(k1*yy) * 2*sqrt(2/3)/L;
  psi0 = sin(k1*xx).*sin(2*k1*yy) * 1/sqrt(5)/pi;
  scalefac = -N^2; % Set scale factor negative to minimize instead
  kappa = 1/4; q = 0;
end

if ~exist('scalefac'), scalefac = N^2; end

[psi,Effq] = velopt(psi0,src,kappa,q,L,scalefac);

fprintf(1,'Eff_%d=%f\n',q,Effq)

figure(1)
Nplot = 64; % Interpolate solution for plotting
psir = refine2(psi,Nplot); srcr = refine2(src,Nplot);
xplot = L*(0:Nplot-1)/Nplot; yplot = xplot';
imagesc(xplot,yplot,srcr), colorbar, hold on
contour(xplot,yplot,psir,10,'EdgeColor','k'), hold off
```

2 Program file velopt.m

```
function [psi,Effq] = velopt(psi0,src,kappa,q,L,scalefac)

% Problem parameters for Matlab's optimizer fmincon.
psi0 = psi0(:); problem.x0 = psi0(2:end);
problem.objective = @(x) normHq2(x,src,kappa,q,L,scalefac);
problem.nonlcon = @(x) nonlcon(x,src,kappa,q,L,scalefac);
problem.solver = 'fmincon';
problem.options = optimset('Display','iter','TolFun',1e-10,...
   'GradObj','on','GradConstr','on',...
   'algorithm','interior-point');

[psi,Hq2] = fmincon(problem);

% Mixing efficiency: call normHq2 with no flow to get pure-conduction solution.
Effq = sqrt(normHq2(zeros(size(psi)),src,kappa,q,L,scalefac) / Hq2);

psi = reshape([0;psi],size(src)); % Convert psi back into a square grid

%======================================================================
function [varargout] = normHq2(psi,src,kappa,q,L,scalefac)

N = size(src,1); src = src(:);
```

```
% 2D Differentiation matrices and negative-Laplacian
[Dx,Dy,Dxx,Dyy] = Diffmat2(N,L); mlap = -(Dxx+Dyy);
if q ~= 0 && q ~= -1, error('This code only supports q = 0 or -1.'); end

psi = [0;psi]; ux = Dy*psi; uy = -Dx*psi;
ugradop = diag(sparse(ux))*Dx + diag(sparse(uy))*Dy;

if q == 0
  Aop2 = (-ugradop + kappa*mlap);
elseif q == -1
  Aop2 = mlap*(-ugradop + kappa*mlap);
end
Aop1 = (ugradop + kappa*mlap)*Aop2;
% Solve for chi, dropping corner point to fix normalisation.
chi = [0; Aop1(2:end,2:end) \ src(2:end)];
theta = Aop2*chi;

% The squared H^q norm of theta.
varargout{1} = L^2*sum(theta.^2)/N^2 * scalefac;

if nargout > 1
  % Gradient of squared-norm Hq2.
  gradHq2 = 2*((Dx*theta).*(Dy*chi) - (Dy*theta).*(Dx*chi));
  varargout{2} = gradHq2(2:end) / N^2 * scalefac;
end

%=====================================================================
function [c,ceq,gc,gceq] = nonlcon(psi,src,kappa,q,L,scalefac)

psi = [0;psi]; N = size(src,1);
c = []; gc = [];

[Dx,Dy,Dxx,Dyy] = Diffmat2(N,L); % 2D Differentiation matrices
U2 = L^2*(sum((Dx*psi).^2 + (Dy*psi).^2)/N^2);
ceq(1) = (U2-1) * scalefac;

if nargout > 2
  % Gradient of constraints
  mlappsi = -(Dxx+Dyy)*psi;
  gceq(:,1) = 2*mlappsi(2:end) / N^2 * scalefac;
end
```

References

[1] C. R. Doering and J.-L. Thiffeault, *Multiscale mixing efficiencies for steady sources*, Phys. Rev. E, 74 (2006), p. 025301(R).

[2] A. Lasota and M. C. Mackey, *Chaos, Fractals, and Noise*, Springer-Verlag, New York, 1994.

[3] Z. Lin, C. R. Doering, and J.-L. Thiffeault, *An optimal stirring strategy for passive scalar mixing*, 2010. preprint.

[4] G. Mathew, I. Mezić, S. Grivopoulos, U. Vaidya, and L. Petzold, *Optimal control of mixing in Stokes fluid flows*, J. Fluid Mech., 580 (2007), pp. 261–281.

[5] G. Mathew, I. Mezić, and L. Petzold, *A multiscale measure for mixing*, Physica D, 211 (2005), pp. 23–46.

[6] S. Plasting and W. R. Young, *A bound on scalar variance for the advection–diffusion equation*, J. Fluid Mech., 552 (2006), pp. 289–298.

[7] T. A. Shaw, J.-L. Thiffeault, and C. R. Doering, *Stirring up trouble: Multi-scale mixing measures for steady scalar sources*, Physica D, 231 (2007), pp. 143–164.

[8] J.-L. Thiffeault and G. A. Pavliotis, *Optimizing the source distribution in fluid mixing*, Physica D, 237 (2008), pp. 918–929.