1 Sources and Sinks

Consider the situation with a sources-sink term $s(\boldsymbol{x}, t)$,

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = \kappa \nabla^2 \theta + s \left(\boldsymbol{x}, t \right), \tag{1}$$
$$\nabla \cdot \boldsymbol{u} = 0.$$

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 $\theta(\mathbf{x})$ that satisfies

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

We define the operator

$$\mathcal{L} \equiv \boldsymbol{u} \cdot \nabla - \kappa \nabla^2 \tag{3}$$

so that (2) can be written

$$\mathcal{L}\theta = s. \tag{4}$$

The steady solution is then

$$\theta = \mathcal{L}^{-1}s \tag{5}$$

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*:

$$\varepsilon_q = \frac{\|\theta\|_{\dot{H}^q}}{\|\theta\|_{\dot{H}^q}},\tag{6}$$

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

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

^{*}Notes by Sam Pegler and Woosok Moon of lectures delivered at the 2010 Woods Hole Summer Program in Geophysical Fluid Dynamics.



Figure 1: Sources and sinks: CO in the atmosphere. Red corresponds to high levels of CO (450 parts per billion) and blue to low levels (50 ppb). Note the immense clouds due to grassland and forest fires in Africa and South America. (Photo NASA/NCAR/CSA.)

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 [3], and Thiffeault and Pavliotis [5]; see also the review by Thiffeault [4]. 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

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

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

$$egin{aligned} &\langle heta \mathcal{L} heta
angle &= \langle heta u \cdot
abla heta
angle - \kappa \left\langle heta
abla^2 heta
ight
angle \ &= \langle
abla \cdot (u heta^2/2)
ight
angle - \kappa \left\langle heta
abla^2 heta
ight
angle \ &= \kappa \left\langle |
abla heta|^2
ight
angle . \end{aligned}$$

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

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

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

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

We conclude that

$$\|\theta\|_{\dot{H}^1} \le \|\tilde{\theta}\|_{\dot{H}^1} \iff \varepsilon_1 \le 1.$$
⁽⁷⁾

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



Figure 2: The pattern of velocity field and source for the 'unmixing' flow and source distribution (8).

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:

$$u = (2\sin x \cos 2y, -\cos x \sin 2y), \qquad (8a)$$

$$s = \left(\cos x - \frac{1}{2}\right)\sin y \,. \tag{8b}$$

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 2. 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.

2 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 $u = U\hat{x}$, which is constant flow from the hot region to the cold region [2,3,5] (figure 3). This example demonstrates that, with body sources, the best 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 4 shows contours of the streamfunction for the optimal stirring velocity (lines) for a source $s(x) = \sin x \sin y$, 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 5, for the source distribution $s(x) = \cos x \cos y + \cos 3y + (1/4) \sin 3y$. 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 6 shows this for the source (8b) 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 (8a), 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.



Figure 3: The optimal velocity field (solid arrows) for the source distribution $s(x) = \sin x$.



Figure 4: Optimal stirring velocity field (solid lines) for the source $s(x) = \sin x \sin y$ (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.)



Figure 5: 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 6: 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.)

Appendix: Matlab code

1 Program file example.m

```
function example(ex)
if nargin < 1, ex = 1; end
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, 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*((Dv*theta) *(Dv*chi) = (Dv*theta) *(Dv*chi));
```

```
gradHq2 = 2*((Dx*theta).*(Dy*chi) - (Dy*theta).*(Dx*chi));
varargout{2} = gradHq2(2:end) / N^2 * scalefac;
end
```

```
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
```

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