Optimizing exit times

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I. PROBLEM SETUP

Consider the advection-diffusion equation for a passive scalar $\theta(\boldsymbol{x}, t)$, advected by a steady velocity field $\boldsymbol{u}(\boldsymbol{x})$, with Dirichlet boundary conditions on some domain Ω:

$$\partial_t\theta + \boldsymbol{u}\cdot\nabla\theta = D\Delta\theta, \qquad \boldsymbol{u}\cdot\hat{\boldsymbol{n}}|_{\partial\Omega} = 0, \qquad \theta|_{\partial\Omega} = 0, \tag{1}$$

with $\nabla\cdot\boldsymbol{u} = 0$. We take $\theta(\boldsymbol{x}, t_0) = \theta_0(\boldsymbol{x}) \geq 0$, so $\theta(\boldsymbol{x}, t) \geq 0$. Integrating (1) over Ω, we have

$$\partial_t\langle\theta\rangle + \langle\boldsymbol{u}\cdot\nabla\theta\rangle = D\langle\Delta\theta\rangle. \tag{2}$$

The advection term vanishes since the walls are impenetrable, and we have

$$\partial_t\langle\theta\rangle = D\int_{\partial\Omega}\nabla\theta\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S =: -F[\theta] \tag{3}$$

where $\hat{\boldsymbol{n}}$ is the outward normal to $\partial\Omega$. This states that the average θ changes according to the flux through the surface. Since $\theta(\boldsymbol{x}) \geq 0$, $\nabla\theta$ points towards the interior of Ω, and the integrand on the right-hand side of Eq. (3) is negative (or zero). Thus heat is leaking out of the domain, and the ultimate state has $\theta \equiv 0$ everywhere. The heat flux is solely determined by $-D\hat{\boldsymbol{n}}\cdot\nabla\theta$ at the boundary. Our problem is that there is no velocity field in (3), so there is nothing to optimize directly. This is a similar situation to the freely-decaying problem with Neumann boundary conditions.

From (1), we define the linear operator

$$\mathcal{L} := \boldsymbol{u}\cdot\nabla - D\Delta \tag{4}$$

and its formal adjoint

$$\mathcal{L}^\dagger := -\boldsymbol{u}\cdot\nabla - D\Delta\,. \tag{5}$$

The adjoint is computed via integration by parts, which gives rise to three boundary terms:

$$\begin{aligned}\langle f\,\mathcal{L}g\rangle &= \int_\Omega f\,(\boldsymbol{u}\cdot\nabla - D\Delta)g\,\mathrm{d}V \\ &= \int_{\partial\Omega} fg\,\boldsymbol{u}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S - D\int_{\partial\Omega} f\nabla g\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + D\int_{\partial\Omega} g\nabla f\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S \\ &\qquad + \int g\,(-\boldsymbol{u}\cdot\nabla - D\Delta)f\,\mathrm{d}V \\ &= \langle\mathcal{L}^\dagger f\,g\rangle.\end{aligned}$$

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The first boundary term vanishes since $\boldsymbol{u}\cdot\hat{\boldsymbol{n}} = 0$ on the boundary. The next two will typically vanish because of some combination of zero boundary conditions on f and g and their gradients. Here we will typically have $f = g = 0$ on the boundary $\partial\Omega$.

II. DERIVATION OF THE EXIT TIME EQUATION

The Green's function $P(\boldsymbol{x}, t\,|\,\boldsymbol{x}_0, t_0)$ satisfies the Fokker–Planck equation (also called the Kolmogorov forward equation)

$$\partial_t P + \mathcal{L}P = 0, \qquad P|_{\partial\Omega} = 0, \qquad t > t_0, \tag{6}$$

with initial condition $P(\boldsymbol{x}, t_0\,|\,\boldsymbol{x}_0, t_0) = \delta(\boldsymbol{x} - \boldsymbol{x}_0)$. This gives the probability density of finding a particle at $(\boldsymbol{x}, t)$ if it was initially at $(\boldsymbol{x}_0, t_0)$. The *survival probability* of finding the particle anywhere in Ω at time t is

$$S(t\,|\,\boldsymbol{x}_0, t_0) = \int_\Omega P(\boldsymbol{x}, t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}V. \tag{7}$$

From this we find the *first passage time density* $f(t\,|\,\boldsymbol{x}_0, t_0)$, which is the probability that a particle has first reached the boundary at time t:

$$f(t\,|\,\boldsymbol{x}_0, t_0) = -\frac{\partial S}{\partial t} \geq 0. \tag{8}$$

The *expected exit time* $\tau(\boldsymbol{x}_0, t_0)$ (measured from t_0) is then

$$\begin{aligned}
\tau(\boldsymbol{x}_0, t_0) &= \int_{t_0}^{\infty} (t - t_0) f(t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}t \\
&= -\int_{t_0}^{\infty} (t - t_0)\,\frac{\partial S}{\partial t}\,\mathrm{d}t \\
&= -[(t - t_0)S]_{t_0}^{\infty} + \int_{t_0}^{\infty} S(t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}t \\
&= \int_{t_0}^{\infty} S(t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}t.
\end{aligned}$$

Recall that $P(\boldsymbol{x}, t\,|\,\boldsymbol{x}_0, t_0)$ satisfies the Kolmogorov backward equation with respect to $(\boldsymbol{x}_0, t_0)$:

$$-\partial_{t_0} P + \mathcal{L}_0^\dagger P = 0, \qquad P|_{\partial\Omega} = 0, \qquad t_0 < t, \tag{9}$$

with terminal condition $P(\boldsymbol{x}, t\,|\,\boldsymbol{x}_0, t) = \delta(\boldsymbol{x} - \boldsymbol{x}_0)$. We act on τ with $\mathcal{L}_0^\dagger$:

$$\begin{aligned}
\mathcal{L}_0^\dagger \tau(\boldsymbol{x}_0, t_0) &= \int_{t_0}^{\infty} \mathcal{L}_0^\dagger S(t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}t \\
&= \int_{t_0}^{\infty} \int_\Omega \mathcal{L}_0^\dagger P(\boldsymbol{x}, t\,|\,\boldsymbol{x}_0, t_0)\,\mathrm{d}V\,\mathrm{d}t \\
&= \int_\Omega \int_{t_0}^{\infty} \partial_{t_0} P\,\mathrm{d}t\,\mathrm{d}V = \int_{t_0}^{\infty} \partial_{t_0} S\,\mathrm{d}t.
\end{aligned}$$

This last term needs to be computed carefully:

$$\begin{aligned}\int_{t_0}^{\infty} \partial_{t_0} S \,\mathrm{d}t &= \lim_{\epsilon\to 0} \epsilon^{-1} \left\{ \int_{t_0}^{\infty} S(t_0+\epsilon)\,\mathrm{d}t - \int_{t_0}^{\infty} S(t_0)\,\mathrm{d}t \right\} \\ &= \lim_{\epsilon\to 0} \epsilon^{-1} \left\{ \int_{t_0+\epsilon}^{\infty} S(t_0+\epsilon)\,\mathrm{d}t + \int_{0}^{\epsilon} S(t_0+\epsilon)\,\mathrm{d}t - \int_{t_0}^{\infty} S(t_0)\,\mathrm{d}t \right\} \\ &= \partial_{t_0}\tau + \lim_{\epsilon\to 0} \epsilon^{-1} \int_0^{\epsilon} S(t_0+\epsilon)\,\mathrm{d}t \\ &= \partial_{t_0}\tau + S(t_0) \\ &= \partial_{t_0}\tau + 1.\end{aligned}$$

We thus obtain

$$-\,\partial_{t_0}\tau + \mathcal{L}_0^{\dagger}\tau = 1, \qquad \tau|_{\partial\Omega} = 0. \tag{10}$$

The exit time $\tau(\boldsymbol{x}_0, t_0)$ is measured from t_0, so if the velocity field is time-independent then τ does not depend on t_0 (autonomous flow), and we can drop the $-\partial_{t_0}\tau$ term in (10). (For a nonautonomous flow, the situation is a bit more complicated.)

Iyer *et al.* [1] proved an interesting fact: there exist flows that *increase* $\|\tau\|_\infty$ over pure diffusion. These are 'antimixing' flows. These flows are a little peculiar and do not concern us here. They can only exist in noncircular domains.

III. RELATING τ AND THE HEAT FLUX

The equation for the *expected exit time* $\tau(\boldsymbol{x})$ of a Brownian particle starting at $\boldsymbol{x}$ [1] is (see Section II)

$$\mathcal{L}^{\dagger}\tau = 1, \qquad \tau|_{\partial\Omega} = 0. \tag{11}$$

We multiply the advection-diffusion equation (1) by τ and integrate. From (11), we have

$$-\,\langle \tau\, \partial_t\theta\rangle = \langle \tau\, \mathcal{L}\theta\rangle = \langle \mathcal{L}^{\dagger}\tau\, \theta\rangle = \langle\theta\rangle. \tag{12}$$

Using Hölder's inequality, we can then bound the $\langle \tau\, \partial_t\theta\rangle$ term as

$$|\langle \tau\, \partial_t\theta\rangle| \le \|\partial_t\theta\|_q \|\tau\|_p, \qquad p^{-1} + q^{-1} = 1. \tag{13}$$

so that

$$\|\partial_t\theta\|_q \ge |\langle\theta\rangle| / \|\tau\|_p\,. \tag{14}$$

If θ is an eigenmode with eigenvalue λ, this becomes a bound on $\operatorname{Re}\lambda \ge 0$:

$$\operatorname{Re}\lambda^{-1} \le |\lambda|^{-1} \le \left(\|\theta\|_q / |\langle\theta\rangle|\right)\, \|\tau\|_p\,. \tag{15}$$

If we prefer, we can use the inequality

$$\operatorname{Re}\lambda^{-1} = \frac{\operatorname{Re}\lambda^*}{|\lambda|^2} = \frac{\operatorname{Re}\lambda}{|\lambda|^2} \ge (\operatorname{Re}\lambda)^{-1}, \qquad \operatorname{Re}\lambda > 0, \tag{16}$$

to obtain a lower bound on $\operatorname{Re}\lambda$ instead.

Another interesting limit of (14) is when $\partial_t\theta \le 0$ everywhere. Then

$$\|\partial_t\theta\|_1 = \langle\partial_t\theta\rangle = -\partial_t\langle\theta\rangle = F[\theta], \tag{17}$$

and so

$$F[\theta] \geq \langle\theta\rangle / \|\tau\|_\infty \,. \tag{18}$$

Of course, $\langle\theta\rangle$ is time-dependent, so this doesn't tell us much yet; we thus use (3) to obtain

$$\partial_t \langle\theta\rangle = -F[\theta] \leq -\langle\theta\rangle / \|\tau\|_\infty \,, \tag{19}$$

so that

$$\langle\theta\rangle \leq \langle\theta_0\rangle \exp(-t/\|\tau\|_\infty), \tag{20}$$

but this bound is only valid for $\partial_t \theta \leq 0$ everywhere, which is not very realistic.

IV. OPTIMIZATION

The functional to optimize:

$$\mathcal{F}[\tau, \boldsymbol{u}, \vartheta, \mu, p] = \tfrac{1}{m}\|\tau\|_m^m - \langle\vartheta(\mathcal{L}^\dagger\tau - 1)\rangle + \tfrac{1}{2}\mu(\|\boldsymbol{u}\|_2^2 - 2E) - \langle p\nabla\cdot\boldsymbol{u}\rangle, \tag{21}$$

with $m \geq 1$. Here ϑ, μ, and p are Lagrange multipliers. This functional is analogous to (10.11) in [2], but the boundary condition on τ is different. The variations with respect to the Lagrange multipliers just return the constraints; the other variations give

$$\frac{\delta\mathcal{F}}{\delta\tau} = -\mathcal{L}\vartheta + \tau^{m-1} = 0; \tag{22}$$

$$\frac{\delta\mathcal{F}}{\delta\boldsymbol{u}} = \mu\boldsymbol{u} - \tau\nabla\vartheta + \nabla p = 0. \tag{23}$$

Using $\mathcal{L}^\dagger\tau = 1$ and (22), we have $\langle\tau^m\rangle = \langle\vartheta\rangle$. From (23) we get

$$\mu\|\boldsymbol{u}\|_2^2 = -\int_\Omega \vartheta\,\boldsymbol{u}\cdot\nabla\tau\,\mathrm{d}V = \int_\Omega \vartheta\,(1 + \Delta\tau)\,\mathrm{d}V = \langle\vartheta\rangle - \int_\Omega \nabla\tau\cdot\nabla\vartheta\,\mathrm{d}V. \tag{24}$$

In 2D, we use a streamfunction $\boldsymbol{u} = \hat{\boldsymbol{z}} \times \nabla\psi$, and take the curl of (23):

$$\mu\Delta\psi = (\nabla\tau \times \nabla\vartheta)\cdot\hat{\boldsymbol{z}} =: J(\tau, \vartheta). \tag{25}$$

For $m = 1$, $\|\tau\|_1$ is the integral of τ over Ω, since $\tau \geq 0$. We have $\mathcal{L}^\dagger\tau = 1$ and $\mathcal{L}\vartheta = 1$. Since (4) and (5) only differ in the sign of $\boldsymbol{u}$, we have $\vartheta(\boldsymbol{x}) = \tau(-\boldsymbol{x}) =: \tau_-(\boldsymbol{x})$, as long as the domain and boundary conditions are symmetric under inversion $\boldsymbol{x} \to -\boldsymbol{x}$. (In 2D this is a rotation by π about the origin.) Hence, for $m = 1$ and a centrally-symmetric domain (circle, square, rectangle. . .) we do not need to solve the ϑ equation. From (25) we then see that $\psi(\boldsymbol{x}) = -\psi(-\boldsymbol{x})$.

To summarize, in 2D for $m = 1$ we must solve

$$-\Delta\tau = J(\psi, \tau) + 1, \qquad \tau|_{\partial\Omega} = 0; \tag{26a}$$

$$\mu\Delta\psi = J(\tau, \tau_-), \qquad \psi|_{\partial\Omega} = 0, \tag{26b}$$

with $\tau_-(\boldsymbol{x}) = \tau(-\boldsymbol{x})$.

Consider now a channel of with 1, $-\frac{1}{2} \leq y \leq \frac{1}{2}$, with period $k = 2\pi/L$ in x. This is symmetric under rotation by π, so $\vartheta(\boldsymbol{x}) = \tau_-(\boldsymbol{x}) = \tau(-\boldsymbol{x})$. The conduction solution is

$$\tau_0(y) = \vartheta_0(y) = \tfrac{1}{2}\left(\tfrac{1}{4} - y^2\right). \tag{27}$$

The L^1 norm of the conduction solution is

$$\|\tau_0\|_1 = L\int_{-1/2}^{1/2} \tfrac{1}{2}\left(\tfrac{1}{4} - y^2\right)\,\mathrm{d}y = \frac{\pi}{6k}. \tag{28}$$

This depends on k, since it is an integral 'per period.'

The Péclet number is proportional to U. For small U, we can solve the optimization problem from the previous section perturbatively. Let's do the case $m = 1$. We let $\varepsilon = U$ and expand as

$$\begin{aligned}
\tau &= \tau_0 + \varepsilon\tau_1 + \varepsilon^2\tau_2 + \ldots, \\
\vartheta &= \vartheta_0 + \varepsilon\vartheta_1 + \varepsilon^2\vartheta_2 + \ldots, \\
\psi &= \qquad \varepsilon\psi_1 + \varepsilon^2\psi_2 + \ldots, \\
\mu &= \mu_0 + \varepsilon\mu_1 + \varepsilon^2\mu_2 + \ldots.
\end{aligned}$$

We won't give the details here, but the perturbation is relatively straightforward. In the x direction we expand in $\sin kx$, $\cos kx$, and the wavenumbers are not coupled at leading order. We then minimize $\|\tau\|_1/\|\tau_0\|_1$ over k, to find the wavenumber that minimizes the exit time. Numerically, we find the maximum enhancement occurs at $k \simeq 14.3$, where $\mu_0 \simeq .00061$. Even this maximal enhancement is very small:

$$\frac{\|\tau\|_1}{\|\tau_0\|_1} = 1 - \varepsilon^2\frac{\tfrac{1}{2}\mu_0}{\pi/6k} + \ldots \simeq 1 - (0.0083)\,\varepsilon^2 + \mathrm{O}(\varepsilon^4), \qquad k \simeq 14.3. \tag{29}$$

The two types of solutions are shown in Fig. 1. We can see that the solutions do what seems to be exactly the same thing in each quadrant. These are really the same type of solution, but their linear combination could look a bit funny. For instance, the sum has rolls only in the bottom, with each roll turning twice as fast! We can also sum the two patterns in Fig. 1(a) and 1(b) with different phases, and get tilted rolls as in Fig. 1(c).

Simulations at larger Pe in a closed box still resemble the stacked roll structure (Fig. 2), but this is very much ongoing work.

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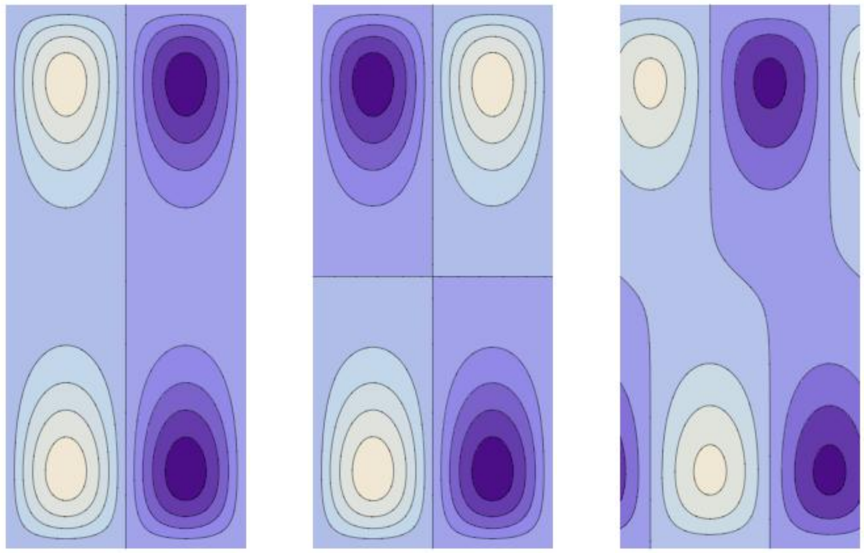
[1] G. Iyer, A. Novikov, L. Ryzhik, and A. Zlatoš, SIAM J. Math. Anal. **42**, 2484 (2010).
[2] J.-L. Thiffeault, Nonlinearity **25**, R1 (2012), arXiv:1105.1101.



(a) (b) (c)

FIG. 1. The optimal streamfunction $\psi_1(\boldsymbol{x})$ at leading order, for the optimal enhancement wavenumber $k \simeq 14.3$. (a) ψ_1 even in y; (b) ψ_1 odd in y; (c) The sum of (a) and (b), with (b) out of phase by $\pi/2$.

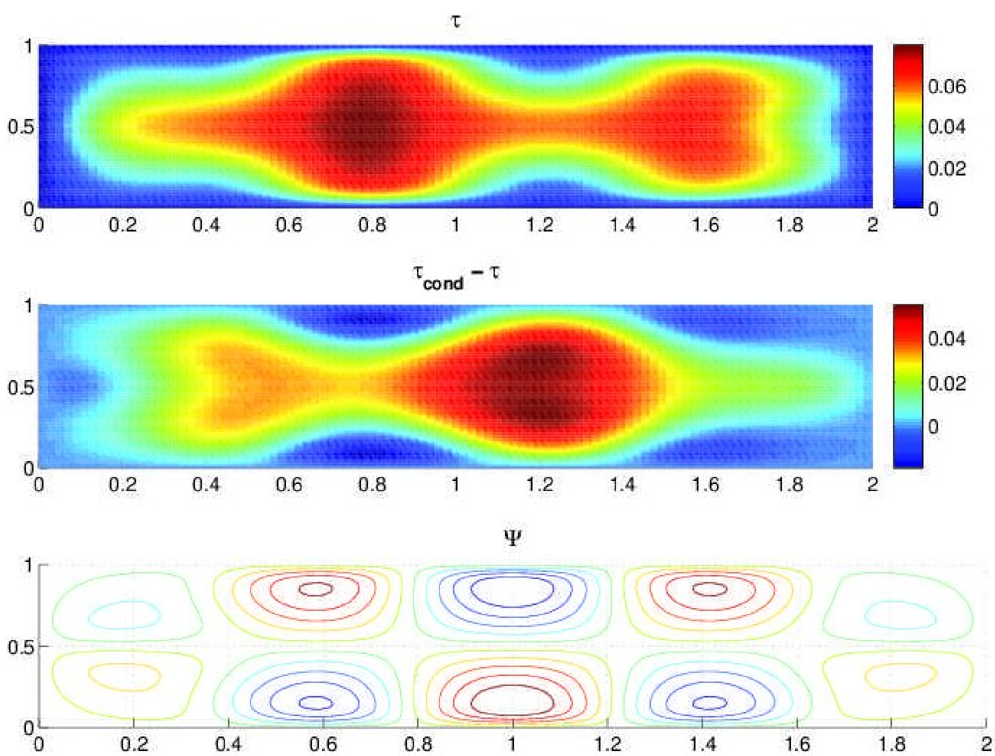


FIG. 2. Numerical optimization for Pe = 200, in a closed rectangular container. The 'stacked rolls' structure persists even at this larger Pe = 200 and for a finite box. The improvement over pure conduction is significant ($\|\tau_0\|_1/\|\tau\|_1 \sim 1.4$). [Numerical simulations by Florence Marcotte.]