Acceleration of one dimensional mixing by discontinuous mappings

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Abstract

We use a simple model to investigate mechanisms of mixing of a passive tracer into a bulk material that is essentially one dimensional. We examine the relative rates of mixing due to diffusion, stretch and fold operations and permutation of sections of the sample. In particular we show how a combination of diffusion with permutation of sections of the sample ('chopping and shuffling') can achieve a faster rate of mixing than pure diffusion. This is done by numerical approximation of eigenvalues of certain linear operators.

1 Introduction: Mixing in one dimension

Mixing processes in nature and technology are ubiquitous and vitally important, and can occur through a variety of physical mechanisms. For example, mixing can occur purely by diffusion at a molecular scale or it can occur by stretching and folding actions at a lengthscale comparable to the system; this

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can ultimately homogenize the system down to the molecular scale. Mixing via pure diffusion is rarely adequate and so (often turbulent) convection is made use of to increase the rate of mixing over pure diffusion especially for relatively inviscid fluids. However, turbulence is not necessary; there has been a considerable amount of work showing that even steady or time periodic flows may have very good mixing properties, essentially due to deterministic chaos in the Lagrangian particle paths; see [1, 4, 5].

In cases where the substance to be mixed is a polymer or a paste, convection cannot be used so easily; the energetic cost of deformation may be too great or have other undesirable side-effects. Industrial processes usually use static mixers in the form of vanes fixed within pipes to achieve mixing in such cases; see for example [6, 9] for a range of numerical and experimental approaches to this.

A mechanism that has been to a large extent ignored in mathematical modelling of mixing but which is very important especially in the mixing of viscous materials are the effects of discontinuous 'chop and rearrange' transformations on the mixing (though see [2, 3]).

In this paper we investigate and compare some possible mixing methods for materials that are essentially homogeneous in two of their dimensions, i.e. where the mixing only needs to occur in one-dimension. These models are idealized but nonetheless they suggest some interesting effects. Most significantly we show how the use of two processes, diffusion and permutation alternately, can give rise to a much faster rate of mixing than either on its own, provided that the permutation is carefully chosen. The work in this paper is intended as a simple model problem that can be analyzed but which nonetheless has features present in a variety of geometries and mixing methods.

1.1 One-dimensional mixing models

We consider mixing of a passive tracer in a block of material that is essentially one dimensional by application of a sequence of deterministic (i.e. non-random) operations to the block. For the sake of argument we always parameterize the domain describing this block by a nondimensional distance ranging from 0 to 1 and assume that we commence with a distribution of some passive tracer in the block such that the concentration of the tracer does not

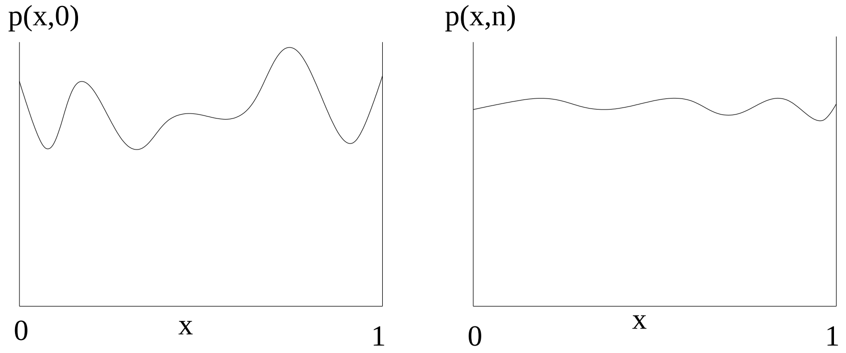


Figure 1: Schematic diagram showing the mixing of a smooth initial concentration profile to produce a progressively more uniform distribution as time progresses. Note that $\int p(x,n)dx = \int p(x,0)dx$ for all $n \geq 0$.

affect the mixing operations. We consider a concentration distribution

$$p(x,t)$$

as a function of location $x \in [0,1]$ and time t, $p(x,t)$ where $x \in [0,1]$ and $p \geq 0$ such that[1]

$$\int_{x=0}^{1} p(x,0)\,dx = 1.$$

Figure 1 shows the development of a concentration profile as time progresses. We normalize the total quantity of tracer to be unit and will only be interested in operations that preserve the total mass of tracer so that

$$\int_{x=0}^{1} p(x,t)\,dx = 1$$

for all $t \geq 0$. For simplicity we consider only discrete time mixing, and so only consider values of $t = 0, 1, 2, \cdots$. We assume that the initial distribution $p(x,0)$ can be differentiated arbitrarily many times in x (we say it is *smooth* in x). This assumption may be justified by the fact that diffusion acting over an arbitrarily small time will regularize any initial discontinuities in the concentration. However, after one mixing operation we may have a concentration that is only smooth on a finite number of pieces (it is *piecewise smooth*) so we widen our interests to this class which we denote $\mathcal{X} = C_p^\infty(0,1)$.

[1]NB integrals without limits are assumed to be definite integrals from $x = 0$ to 1.

When the concentration is fully mixed we have $\overline{p}(x) = 1$ for all $x \in [0, 1]$; we refer to this as the *uniform state*; the aim of mixing is simply to cause $p(x, t)$ to converge to $\overline{p}$ as fast as possible.

1.2 Mixing in different norms

There are many ways of measuring how far $p(x, t)$ is from uniform; which one is important depends on the application considered. For example, if one is trying to Dis infect some food substance it is important that effectively all locations are smoothly covered during the mixing process; we need the L^∞ norm

$$\|p(x,t) - 1\|_\infty = \text{ess sup}_{x\in[0,1]}|p(x,t) - 1|$$

to converge to zero as time progresses (this norm on $\mathcal{X}$ is equivalent to finding the supremum over all points where the function is continuous). If instead we are trying to use the mixing process to achieve as high a yield as possible, then a more appropriate criterion would be the L^p norm

$$\|p(x,t)\|_p = \left(\int_0^1 |p(x,t) - 1|^p \, dx\right)^{\frac{1}{p}}.$$

Which $p \geq 1$ we choose governs how much weight is given to unmixed 'outliers'. Note that if $\|p(x, t) - 1\|_\infty \to 0$ then $\|p(x, t) - 1\|_2 \to 0$ but the converse is not true.

Unfortunately, any given type of mixing will typically mix at different rates depending on which norm we choose; this is an unavoidable problem. In this paper, mostly for convenience of the mathematics, we will consider mixing either using $\|\cdot\|_\infty$ or $\|\cdot\|_2$. Mixing with respect to the former norm denotes a very strong sort of mixing; the latter can be much weaker. For practical purposes one would like to know when the concentration has been mixed to within 5% of uniform; we refer this to the *time to* 95% *mixing*, t_{95} and defined to be the smallest $t > 0$ such that

$$\|p(x, t_{95}) - 1\| \leq 0.05$$

and we aim to give some predictions on this (dependent on the mixing norm chosen); naturally such predictions will depend on the initial distribution.

2 Methods of mixing

We now characterize some mixing processes either generated by diffusion or by point operations (in other words maps of $[0,1]$ to itself) as detailed in Section 2.2.

2.1 Mixing by diffusion

We consider diffusion occurring over a time step of 1 unit at a normalized rate $D > 0$. For simplicity we suppose that the domain is periodic during a diffusion step but one could similarly consider different boundary conditions (for example Neumann/no-flux) as long as they do not allow concentration to leak out of or into the domain. Although the following calculation is routine we emphasis that one can explicitly solve the diffusion equation

$$p_t = Dp_{xx} \tag{1}$$

over one unit time in the following way. Assume that $p(x,0) \in \mathcal{X}$ has Fourier expansion

$$p(x,0) = \sum_{n=-\infty}^{\infty} a_n e^{2\pi inx}$$

(assumed to be real, so $a_{-n} = a_n^*$, where $*$ denotes complex conjugation) where as usual we can compute $a_n = \int p(x,0)e^{-2\pi inx}\,dx$ (note that $a_0 = \int p(x,0)\,dx = 1$) so that

$$p(x,t) = \sum_{n=-\infty}^{\infty} a_n e^{2\pi inx} e^{-4\pi^2 n^2 Dt}.$$

We can thus write one time step of diffusion as the operator

$$P_{\mathrm{diff}} : \mathcal{X} \to \mathcal{X}$$

which is explicitly

$$(P_{\mathrm{diff}}(p))(x) = \sum_n e^{2\pi inx} \left(e^{-4\pi^2 n^2 D} \int p(y) e^{-2\pi iny}\,dy \right).$$

Note that all Fourier modes decay at an exponential rate. The slowest decaying mode has the longest wavelength and decays at the rate $4\pi^2 D$. This means that the decay in the L^2 norm is as follows:

$$\|p(x,t) - 1\|_2^2 = \sum_{n\neq 0} |a_n|^2 e^{-8\pi^2 n^2 Dt}$$

$$\leq e^{-8\pi^2 Dt} \sum_{n \neq 0} |a_n|^2 = \|p(x,0) - 1\|_2^2 e^{-8\pi^2 Dt}.$$

Thus $\|p(x,t) - 1\|_2 \leq \|p(x,0) - 1\|_2 e^{-4\pi^2 Dt}$ which means that a lower bound on the time to 95% mixing for $\|.\|_2$ can be found as

$$t_{95} = \frac{\log(20\|p(x,0) - 1\|_2)}{4\pi^2 D}.$$

2.2 Mixing by point operations

Several mixing operations T that we consider will deform the material; we call these *point operations*. They can be considered as mappings of $[0,1]$ to itself i.e.

$$T : [0,1] \to [0,1]$$

such that the map is surjective, i.e. such that $T([0,1]) = [0,1]$, however we do not require the map to be invertible. We assume that the map is piecewise smooth. For any such map T we can derive an associated action on $p \in \mathcal{X}$ called the *Perron-Frobenius operator* [8] in the dynamics literature

$$(P(T)p)(x) = \sum_{y = T^{-1}(x)} \frac{p(y)}{|T^{'}(y)|}.$$

In fact $P(T)$ is a linear operator that takes a density function $p \in \mathcal{X}$ and maps it to another density function $P(T)p \in \mathcal{X}$ ($T'(x)$ denotes the derivative of T with respect to its argument). This operator expresses how the mapping of the domain changes a concentration on that domain. The term $|T^{'}(y)|$ denotes the local stretching or compression of the domain and ensures that the total concentration is preserved by the map.

2.3 Stretching and folding

The first point operation we consider is an m-fold stretch and fold. We stretch out the interval $[0,1]$ to be m-times its length, cut them into m equal sized sections and superimpose them on each other. This can be represented as a transformation

$$T(x) = mx \pmod{1}$$

where $m \geq 2$ is an integer. Note that since m is an integer T is a smooth mapping. $T : [0,1] \to [0,1]$ is an expanding map of the interval and much is known about its mixing properties. In particular $T^{'}(x) = m > 1$ and one can show [8] that the Perron-Frobenius operator $P(T)$ has a unique fixed point that is the uniform density, $\overline{p}(x) = 1$. Moreover, for any smooth normalized initial density $p(x,0)$ the resulting density will approach this uniform density at an exponential rate determined by the maximum derivative of $p(x)$ and m. We write

$$p(x,n) = (P(T)^n)p(x,0),$$

and note that under the assumption $p(x,0)$ is C^1 one can show

$$\|p(x,n) - 1\|_\infty \leq \frac{\|p_x(x,0)\|_\infty}{m^n}$$

where $p_x(x,0)$ is the partial derivative in the x direction. Note that the Perron-Frobenius operator does not increase the maximal spatial derivative i.e.

$$|p_x(x,n)|_\infty \leq |p_x(x,0)|_\infty.$$

To see this, define $g(x) = p(x,0) - 1$ so that $\int g(x)dx = 0$. Furthermore $P(T)g(x) = \frac{1}{m}\sum_{j=0}^{m-1} g(\frac{x+j}{m})$. Since $\sum_{j=0}^{m-1}\int_{\frac{j}{m}}^{\frac{j+1}{m}} g(t)dt = 0$ and

$$\begin{aligned}\left|g\left(\frac{x+j}{m}\right) - m\int_{\frac{j}{m}}^{\frac{j+1}{m}} g(t)dt\right| &\leq m\int_{\frac{j}{m}}^{\frac{j+1}{m}} \left|g(t) - g\left(\frac{x+j}{m}\right))\right| dt \\ &= m\int_{\frac{j}{m}}^{\frac{j+1}{m}} |\epsilon(x,j)|dt\end{aligned}$$

(where $|\epsilon(x,j)| \leq \frac{\|p_x(x,0)\|_\infty}{m}$ by the mean value theorem), we can estimate

$$\frac{1}{m}\sum_{j=0}^{m-1} g\left(\frac{x+j}{m}\right) = \sum_{j=0}^{m-1}\int_{\frac{j}{m}}^{\frac{j+1}{m}} g(t)dt + \frac{1}{m}\sum_{j=0}^{m-1}\epsilon(x,j).$$

Thus $|\frac{1}{m}\sum_{j=0}^{m-1} g(\frac{x+j}{m})| \leq \frac{\|p_x(x,0)\|_\infty}{m}$ and by induction we have[2]

$$\|p(x,n) - 1\|_\infty \leq \frac{\|p_x(x,0)\|_\infty}{m^n}.$$

Using this we obtain a prediction of the time to 95% mixing (i.e. $\|p(x,n) - 1\|_\infty < \frac{1}{20}$) for m-fold stretch and fold, namely

$$t_{95} = \frac{\log(20\|p_x(x,0)\|_\infty)}{\log m}.$$

[2]In general if $p(x,0)$ is r-times continuously differentiable then the rate of mixing is m^r, but the estimate of the constant of proportionality is not as straightforward.

2.4 Permutation of cells.

A second class of point operations that we consider consist of ones that chop the domain into a finite number of equal sized pieces and shuffling them; we refer to this as *permutation of cells*. Suppose that the interval is divided into N subintervals (called "cells")

$$[0, 1/N), [2/N, 3/N), ..., [(N-1)/N, 1)$$

We consider a permutation $\sigma \in S_N$ where S_N is the group of all permutations of the symbols $\{1, \cdots, N\}$. This defines a mapping on $[0, 1]$ defined by

$$T_\sigma(x) = x + \frac{\sigma(i) - i}{N}$$

whenever $x \in [(i-1)/N, i/N)$. The permutation acts on $p(x)$ as $P(T_\sigma) \circ p(x) = p(T_\sigma^{-1} x)$.

Note that after applying T_σ a finite number of times we must return to the original density:

$$P(T_\sigma)^K p(x) = p(x).$$

This is because each σ is of finite order. Therefore permutation of cells cannot lead to mixing on its own. Moreover each point in the domain must return to its original location in a periodic manner. In other words if $p(x, t) = P(T_\sigma)^t p(x, 0)$ then $\|p(x, t) - 1\| \not\to 0$ for any norm we choose where the initial state is not uniform: $\|p(x, 0) - 1\| \neq 0$.

3 Permutation of cells

In this section we examine permutation of cells in more detail. Although it cannot mix on its own, it turns out that it can considerably accelerate mixing by diffusion. We consider an initial $p(x) \in \mathcal{X}$ in terms of its Fourier expansion

$$p(x) = \sum_{-\infty}^{\infty} a_n e^{2\pi i n x}$$

with $a_n = \int p(x) e^{-2\pi i n x}\, dx$ (sums without limits in this section are assumed to run from $-\infty$ to ∞). This initial distribution is transformed to a distribution $q(x)$ where

$$q(x) = \sum_n b_n e^{2\pi i n x}.$$

We may calculate

$$\begin{aligned} b_n &= \int_0^1 p(T_\sigma^{-1}(x)) e^{-2\pi i n x} dx \\ &= \int_0^1 p(x) e^{-2\pi i n T_\sigma(x)} dx \\ &= \sum_k a_k \int e^{2\pi i k x - 2\pi i n T_\sigma(x)} dx. \end{aligned}$$

Thus if we write

$$q(x) = \sum_n b_n e^{2\pi i n x}$$

then the transformation is a linear transformation of the complex Fourier coefficients:

$$b_n = \sum_{k=-\infty}^{\infty} \tau_{nk} a_k$$

where for any n we have $\sum_k |\tau_{nk}|^2 = 1$ (and thus $|\tau_{nk}| \leq 1$). We can compute

$$\tau_{nk} = \int e^{2\pi i k x - 2\pi i n T_\sigma(x)} dx = \sum_{l=1}^{N} \int_{(l-1)/N}^{l/N} e^{2\pi i k x - 2\pi i n x - \frac{2\pi i n}{N}(\sigma(l) - l)} dx$$

$$= \sum_{l=1}^{N} e^{\frac{-2\pi i n}{N}(\sigma(l)-l)} \int_{\frac{l-1}{N}}^{\frac{l}{N}} e^{2\pi i (k-n) x} dx$$

Define the primitive Nth root of unity as follows

$$w = e^{\frac{-2\pi i}{N}}$$

and then the diagonal terms can be written:

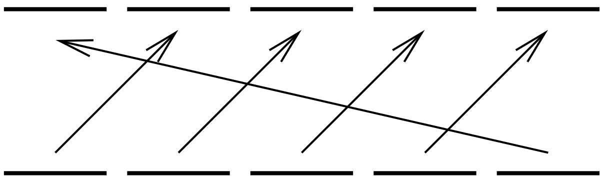
$$\tau_{nn} = \frac{1}{N} \sum_{l=1}^{N} w^{n(\sigma(l)-l)}. \tag{2}$$

When $k \neq n$ we obtain the off-diagonal terms:

$$\tau_{nk} = \frac{(1 - w^{(k-n)})}{2\pi i (k-n)} \sum_{l=1}^{N} w^{n\sigma(l) - kl}. \tag{3}$$

3.1 Some example permutations

We now consider some example permutations and the structure of the associated transformation (τ_{nk}).



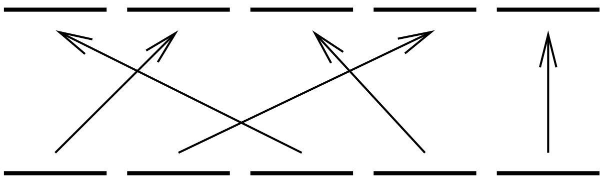


Figure 2: Schematic diagram showing the action of primary rotation and discrete doubling with $N = 5$ equal sized cells on the one-dimensional domain.

Simple rotation A simple rotation of the cells can be expressed as the permutation

$$\sigma(j) = j + m(\mathrm{mod} N)$$

where m gives the shift in cells; this corresponds to the map $T(x) = x + m/N(\mathrm{mod} 1)$ on the domain; see Figure 2(a). In this case we can compute

$$\tau_{nn} = w^{nm}, \quad \tau_{nk} = 0 \ \text{ for } n \neq k.$$

Thus the transformation is diagonal and moreover $|\tau_{nn}| = 1$ for all n. This means that the only effect of the simple rotation is to shift the phase of the modes but no energy is exchanged between the modes.

Secondary rotation Now suppose that $N = ab$ is a product of two integers $a > 1$ and $b > 1$. Let $1 \leq r < a$. We consider a permutation σ which within each block of a cells performs a rotation by r, i.e. given any $0 \leq k < b$ and $1 \leq l < a$ we define

$$\sigma(ka + l) = ka + (l + r(\mathrm{mod} a)).$$

This transformation can transport energy between modes and will typically introduce discontinuities to $p(x)$; however the entries in τ_{nk} are more difficult to compute and we do not have explicit formulae for all (a, b).

Discrete doubling Now we consider a permutation we refer to as 'discrete doubling' because of its resemblance to the doubling map $x \to 2x \pmod 1$. In shuffling terms we split the cells into two groups of almost equal size and then reassemble by interleaving them; see Figure 2(b).

Assume N is odd and define $\sigma(l) = 2l \pmod N$ where mod takes the representative in $\{1, \cdots, N\}$. We calculate

$$\tau_{nn} = \frac{1}{N}\sum_{l=1}^{N} w^{nl} \tag{4}$$

Thus $\tau_{nn} = 0$ if N is not a factor of n and 1 if N is a factor of n. It is possible to calculate

$$\tau_{nk} = \frac{(1 - w^{(k-n)})}{2\pi i(k-n)}\sum_{l=1}^{N} w^{2nl-kl} \tag{5}$$

which is equal to zero if N is not a factor of $(2n - k)$ and $\frac{N(1-w)}{2\pi i(k-n)}$ otherwise. Thus

$$|\tau_{nk}| = \begin{cases} 0 & N \text{ is not a factor of } (2n-k) \\ \leq 1 & \text{if it is a factor} \end{cases}$$

3.2 Discrete doubling with $N = 3$.

For the special case of discrete doubling ie $N = 3$ we calculate the entries τ_{nk} explicitly using (4) and (5). This gives

$$\tau_{nk} = \frac{(1 - w^{(n-k)})}{2\pi i(k-n)}\sum_{l=1}^{3} w^{(2n-k)l}$$

$$= \frac{(1 - w^{(n-k)})}{2\pi i(k-n)}\left(w^{(2n-k)} + w^{2(2n-k)} + w^{3(2n-k)}\right)$$

where $w = e^{\frac{2\pi i}{3}}$. A straightforward calculation produces the matrix below (only the positive indices of $\{\tau_{ij}\}$ are shown here):

$$\{\tau_{ij}\} = \left(\begin{array}{c|c|cccccc}
. & . & . & . & . & . & . & . & . \\
\hline
. & \tau_{00}=1 & 0 & 0 & 0 & 0 & 0 & 0 & . \\
\hline
. & 0 & 0 & \frac{3(1-w^{-1})}{2\pi i} & 0 & 0 & \frac{3(1-w^{-1})}{8\pi i} & 0 & . \\
. & 0 & \frac{3(1-w)}{-2\pi i} & 0 & 0 & \frac{3(1-w)}{4\pi i} & 0 & 0 & . \\
. & 0 & 0 & 0 & 1 & 0 & 0 & 0 & . \\
. & 0 & 0 & \frac{3(1-w^{-1})}{-4\pi i} & 0 & 0 & \frac{3(1-w^{-1})}{2\pi i} & 0 & . \\
. & 0 & \frac{3(1-w)}{-8\pi i} & 0 & 0 & \frac{3(1-w)}{-2\pi i} & 0 & 0 & . \\
. & 0 & 0 & 0 & 0 & 0 & 0 & 1 & . \\
. & . & . & . & . & . & . & . & .
\end{array}\right).$$

As an example, Figure 3 illustrates the effect of applying τ to a simple cosine mode $p(x) = \cos(x)$; this was computed using the algebraic manipulation package *Maple* truncating to a finite number of modes

$$\{a_n \;:\; -N_t \leq n \leq N_t\}$$

with $N_t = 50$ in this case.

One can check that the matrix with entries (τ_{nk}) is orthonormal in the sense that

$$\sum_n \tau_{nk}\tau^*_{nl} = \delta_{kl}$$

and the sum of the moduli of entries in each row and column equals 1 i.e. for all k, n, $\sum_{j=-\infty}^{\infty} |\tau_{nj}|^2 = \sum_{j=-\infty}^{\infty} |\tau_{jk}|^2 = 1$. For example, the sum of the entries of the n^{th} row in the discrete doubling case is given by

$$\sum_{n=-\infty}^{\infty} |\tau_{n1}|^2 = \sum_{m=-\infty}^{\infty} \left| \frac{3(1-w)}{2\pi i(3m-2)} \right|^2$$
$$= \sum_{m=-\infty}^{\infty} \frac{27}{4\pi^2(3m-2)^2} = 1.$$

where the sum is computed using standard complex variable methods.

4 Mixing using permute-diffuse

We now consider mixing via multi-stage mixing protocols, namely when a members of a sequence of maps are applied one after the other. Namely,

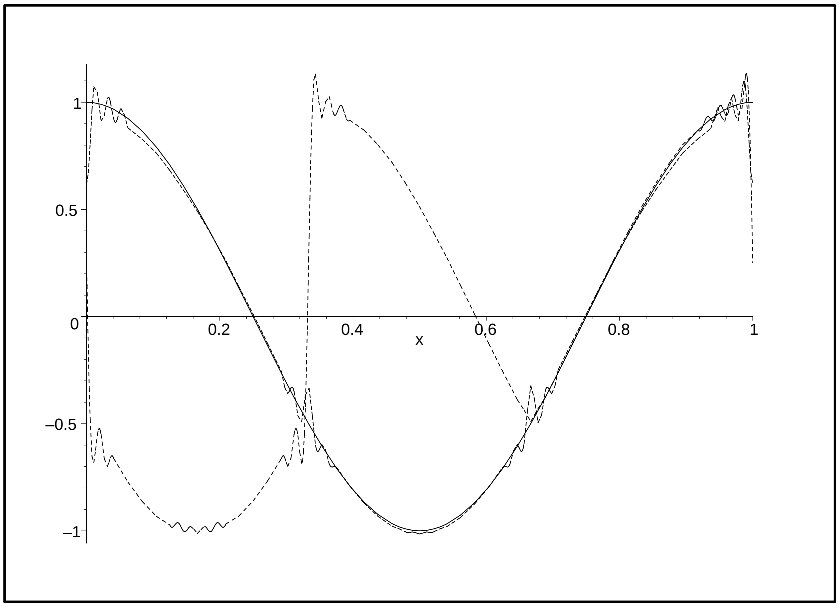


Figure 3: Illustration of the action of the permutation of discrete doubling on the perturbation to uniform concentration in the form of $\cos 2\pi x$. Note that the average deviation from uniform is zero. This was computed using a Fourier truncation $N_t = 50$. The original distribution is shown with the solid line, after one iteration with a dotted and after two with a dashed line. After two applications of the permutation the distribution approaches close to this original distribution. Note the presence of high order harmonics induced by the truncation of discontinuities in the distributions.

we consider $P_{\text{diff}} \circ P(T_\sigma)$ where T_σ is some permutation of cells (given two operators A and B the composition is written $A \circ B$). If the action of $P(T_\sigma)$ introduces discontinuities to a continuous function then in doing so it will send energy into modes $e^{2\pi ikx}$ with k high. In this way it can increase the rate of mixing over that by pure diffusion. How much this is achieved and how effectively depends on a permutation chosen. We first consider some generalities before re-examining the examples discussed in Section 3 in turn.

Note that P_{diff} acts on Fourier coefficients as a diagonal operation where the nth entry is $e^{-4\pi^2n^2D}$. Hence if we commence with a concentration density

$$p(x) = \sum_n a_n e^{2\pi inx}$$

after one timestep we have

$$q(x) = P_{\text{diff}}(P(T_\sigma)(p)(x) = \sum_{n=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} e^{-4\pi^2n^2D} \tau_{nk} a_k.$$

In terms of the Fourier coefficients b_n of $q(x) = \sum b_n e^{2\pi inx}$ we have

$$b_n = \sum_k e^{-4\pi^2n^2D} \tau_{nk} a_k = \sum_k m_{nk} a_k$$

where we define $m_{nk} = \rho^{n^2} \tau_{nk}$ and $\rho = e^{-4\pi^2D}$.

Let us now consider the specific case of the discrete doubling permutation with $N = 3$ for which τ was calculated in Section 3.2. The optimal rate of mixing for pure diffusion is given by

$$\|p(x, n) - 1\| \leq C\rho^n.$$

This mixing rate is governed by ρ, the largest eigenvalue of the diagonal matrix with entries $d_{ii} = \rho^{i^2}$ (excluding the eigenvalue 1).

We approximate the Fourier expansion using the finite number of modes $\{a_n \ : \ -N_t \leq n \leq N_t\}$ and compute the truncated matrices $\{d_{ij}\}$, $\{\tau_{ij}\}$ and $\{m_{ij}\}$ above as a function of the diffusion parameter $\rho = e^{-4\pi^2D}$. The (typically complex) eigenvalues of the truncated matrices were found using Maple, λ_d^i being the ith eigenvalue of $\{d_{ij}\}$ and λ_{pd}^i being the ith eigenvalue of $\{m_{ij}\}$. Table 1(a) shows the first five eigenvalues for $\rho = 0.5$ computed by this method to six decimal places. Observe that the combination of permute-diffuse gives rise to a leading eigenvalue (eigenvalue with maximum modulus)

i	0	1	2	3	4
$\|\lambda_d^i\|$	1.0	0.5	0.5	0.0625	0.0625
$\|\lambda_{pd}^i\|$	1.0	0.279769	0.279769	0.085946	0.085946

(a)

i	0	1	2	3	4
$\|\lambda_d^i\|$	1.0	0.1	0.1	0.001	0.001
$\|\lambda_{pd}^i\|$	1.0	0.041514	0.041514	0.000185	0.000185

(b)

	Fourier	Finite Difference	
	$N_t = 30$	$(N_s, N_t) = (90, 25)$	$(N_s, N_t) = (45, 10)$
$\|\lambda_d^1\|$	0.5	0.5001	0.5005
$\|\lambda_{pd}^1\|$	0.2797	0.2805	0.2813

(c)

Table 1: Absolute values of the eigenvalues of the pure diffusion operator λ_d^i and the permute-diffuse operator λ_{pd}^i ordered by decreasing size for the cases (a) $\rho = 0.5$ and (b) $\rho = 0.1$ from the truncated Fourier expansion (FE) calculations. Observe the unity eigenvalues corresponding to the uniform state and that the eigenvalues (except for 1) come in pairs corresponding to the real and imaginary parts of complex modes. For both cases of ρ, one step of permute-diffuse achieves considerably more mixing than just one step of diffusion. These eigenvalues were computed using a Fourier truncation $N_t = 30$. Table (c) compares the leading eigenvalues for the FE with finite-difference (FD) calculations for grid-size (N_s, N_t) (see text).

that is appreciably smaller than the pure diffusion case. Table 1(b) illustrates the same thing for the case of stronger diffusion, $\rho = 0.1$.

For comparison, Table 1(c) compares the results for the Fourier expansion (FE) with a finite difference (FD) computation, using Crank-Nicolson with N_t timesteps and N_s gridpoints in space, for each diffusive step. The two methods can be seen to produce similar results for the leading eigenvalue in this case $\rho = 0.5$ ($D = 0.017557$ in (1)). For the finite difference calculations, the eigenvalues of the associated linear transformation were computed using Maple. The leading eigenvector (slowest decaying mode) is shown in Figure 4 computing by the FD computation.

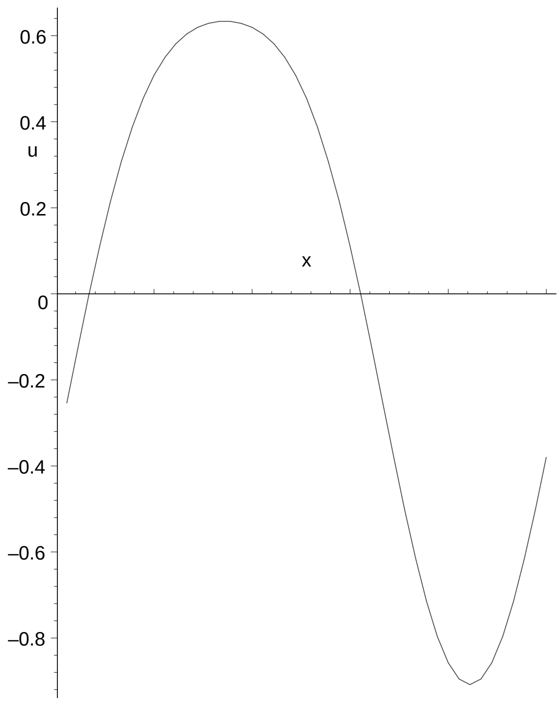


Figure 4: The slowest decaying eigenvector corresponding to the leading eigenvalue, computed using finite difference with $(N_s, N_t) = (45, 10)$ for $N = 3$ discrete doubling followed by diffusion with $\rho = 0.5$. Observe the asymmetry; it is clearly not a pure Fourier mode. This profile shifted by one third of a period will also decay at the same rate, interchanging with the same profile shifted by two thirds of a period.

One can similarly compute the increase in mixing rate as a function of ρ; Figure 5 plots

$$R = \left| \frac{\lambda^1_{pd}}{\lambda^1_d} \right|$$

from the FE calculations, on varying ρ between 0 and 1. Note that (a) $R < 1$ for all $0 < \rho < 1$; this means that permute-diffuse mixes better than pure diffusion for all diffusion rates; (b) near $\rho = 1$ we see that R is proportionate to ρ, implying that for slow diffusion we have a speed-up such that one step of permute-diffuse is almost as good as two steps of pure diffusion; (c) It appears that $R \geq R_0 = 0.4135$ and R approaches this value as $\rho \to 0$. This implies that we cannot speed up the decay of the L^2 norm better that by this ratio at every step. The limiting value R_0 seems to correspond to $\frac{3\sqrt{3}}{4\pi} = 0.4134966717$. Note that there is one term of order ρ in $\{m_{ij}\}$ which has coefficient $\frac{3\sqrt{3}}{2\pi}$ which suggests that the limit can be understood by analytical methods.

Implications for time to 95% mixing Over long time intervals we have

$$\|p(x,n) - 1\| < \|p(x,0) - 1\| e^{n \log |\lambda^1|}$$

where $p(x,n) = P^n p(x,0)$ and $|\lambda^1|$ is the leading eigenvalue of P. Thus the time to 95% mixing is

$$t_{95} = \frac{\log(20\|p(x,0) - 1\|)}{-\log |\lambda^1|}$$

and we see for the above example that for the same initial distribution we expect t_{95} to be decreased by a factor given by the logarithm of the leading eigenvalues. For example, for $N = 3$ and $\rho = 0.5$ we see that 95% mixing using permute-diffuse will happen in 0.54 the time it would take to achieve 95% mixing using pure diffusion. Obviously, by taking a greater number of cells a much greater speedup would be obtained.

4.1 Optimal speedup of permute-diffuse

From the numerical calculations above we see that, at least for the case of discrete doubling with $N = 3$ there will be a speedup of mixing by using a mixture of permutation and diffusion over that obtained just using diffusion.

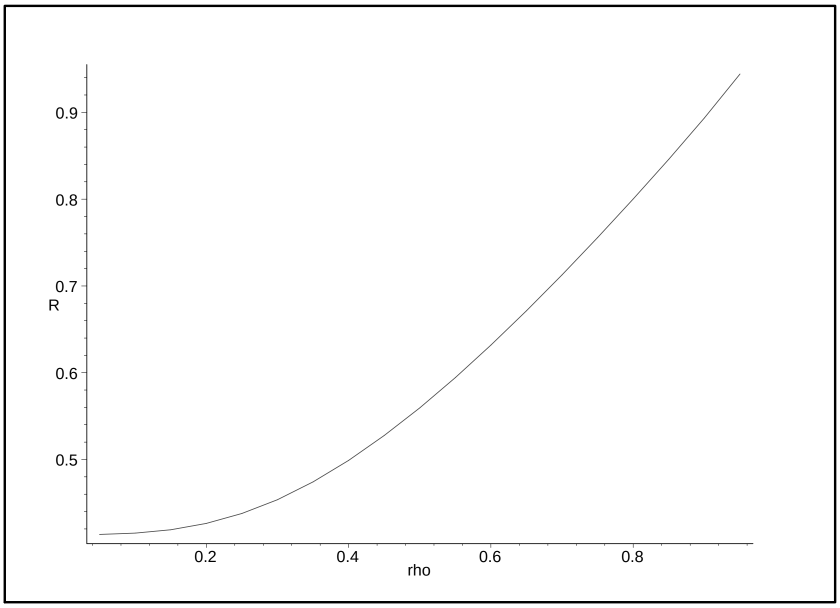


Figure 5: The rate R of increase of mixing as a function of ρ for the discrete doubling with $N = 3$. Note that this lies below $R = 1$ at all values and so the transformation leads to faster mixing than pure diffusion for all diffusion rates. This was computed using the truncation $N_t = 30$. Note the approach to $R = 0.4135$ as $\rho \to 0$.

Unfortunately, up to now we have not been able to quantify this speedup other than numerically although it appears to be considerable. Note that the speedup will depend on N, the diffusion rate ρ and the particular permutation σ chosen. In order to get any speedup over pure diffusion it is obvious that we need to choose a nontrivial perturbation. However many nontrivial perturbations will give no speedup; for example the simple rotation will do nothing. These observations suggest two rather interesting questions:

Q1 For a given number of cells N and diffusion constant ρ, what is the permutation that leads to the optimum speedup, i.e. what is the $\sigma \in S_N$ such that

$$P_{\mathrm{diff}} \circ P(T_\sigma)$$

has leading eigenvalue with minimal modulus? (We suspect that the optimal speedup permutation may be related to the Ulam metric of the permutation).

Q2 Is this optimal permutation independent of ρ?

The σ obtained in answer to **Q1** would be in some sense the best way to shuffle the cells after cutting them up. Note that if σ is an optimal shuffle then any conjugate of σ by the N-cycle $(12..N)$ would also be optimal and so one cannot expect the optimal shuffle to be unique.

In the case $N = 3$, the numerics above suggest that permutations of the form $(12)(3)$ will be the best as in fact there are only six elements in S_3; all the others are either conjugate to this one or are simple rotations (123). Similarly, the evidence of Figure 5 implies that the answer to **Q2** is true for the permutation with $N = 3$.

Another question one might consider is the following: suppose instead of taking the same permutation every time, we choose one from a number of possible shuffles before applying the diffusion constant. Is there any way to improve the mixing rate over what one could obtain using an optimal permutation repeatedly? We leave these intriguing questions open for future research.

5 Discussion

In summary we have shown that using a mixture of discontinuous (permutation) and smooth mixing processes one can improve the mixing rates in one-dimensional domains. This work complements much of that done on deterministic mixing in that it is merely one-dimensional, but uses the discontinuity in an important way.

In this paper we have only considered one-dimensional domains, but suggest that in principle one could make progress on two or three dimensional domains. More direct derivations from practical (non-turbulent) mixing regimes would be very helpful- in fact necessary to make the project worthwhile. One could in principle model mixing by turbulent flow by a mixing protocol including discontinuous maps (approximating detached boundary layers within the turbulence) that vary chaotically with time.

Other point transformations It is clear one can consider a large variety of families of possible permutations such as 'discrete tripling' or indeed 'discrete m-tupling' with permutations of the form $\sigma(l) = ml \pmod N$ whenever m and N have no common factors. In such cases we believe that essentially the same effects as discrete doubling will appear, except that clearly, choosing higher N will allow faster mixing rates.

A generalization of the permutation of cells considered would be the so-called *interval exchange maps* [7, p470]; these allow us to model permutations of cells of differing sizes and can give rise to maps that are not periodic. Note however that $\|p(x,t) - 1\|$ will still not change with t and so they trivially cannot mix in the sense of any such norm decaying. In fact, the mixing properties of interval exchange maps are very subtle and relatively poorly understood and depend on parameters in a very sensitive way. Hence we do not address these maps other than as permutations of equal-sized cells although there may be some advantage in using them.

Further questions We finish by stating some other interesting questions that present themselves as possible extensions of this work:

1. Can one design an experimental setup that precisely corresponds to this model that would allow further exploration of this model?

2. Rather than fixing on a mixing protocol one could consider the following control problem: Given a distribution can we pick the best permutation to mix it? This would mean we need to split up regions with the largest gradients most of all. By comparison with [2, 3] we expect simple periodic protocols to work best.

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