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Computing reactive front speeds in random flows by variational principle

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ABSTRACT

We study reactive front speeds in randomly perturbed cellular flows using a variational representation for the front speed. We develop this representation into a computational tool for computing the front speeds without resorting to closure approximations. We demonstrate that the front speeds depend on flow statistics and topologies in a complex and dramatic manner.

1. Introduction

Front or interface propagation in complex fluids is an ubiquitous nonlinear phenomenon in various areas of science and technology such as chemical reaction fronts in liquids, population growth of ecological communities (plankton) in the ocean, and premixed flame propagation in fluid turbulence [1–5]. If the fluid velocity is modeled by random processes with known statistics, a fundamental challenge is to characterize the front speed in terms of the given velocity statistics. In such a model, a system of coupled equations that governs the propagating front may be reduced, in the case of equal species diffusion (unit Lewis number), to a reactive passive scalar equation [3,4]:

$$u_t = \kappa \Delta_z u + \vec{B}(z,t)\cdot\nabla_z u + \frac{1}{\tau_r} f(u), \quad z \in \mathbb{R}^n, t > 0. \tag{1}$$

In this paper we use a numerical method to study the speed of fronts governed by Eq. (1) and propagating along the first spatial coordinate axis. We focus on the case $f(u) = u(1-u)$, which is the so-called Kolmogorov–Petrovsky–Piskunov (KPP) nonlinearity. If the initial data for u is nonnegative and wave-like, the large time behavior of u is a propagating front. We will use c^* to denote the asymptotic speed of this front, and we want to understand how this speed depends on the prescribed velocity field $\vec{B}$.

For simplicity, we suppose that the spatial dimension is $n = 2$ and that the spatial coordinate z is decomposed as $z = (x, y)$, where $x \in \mathbb{R}$ parameterizes the unbounded propagation direction, and y belongs to an interval $[0, L]$. So, we are modeling fronts propagating in an infinite channel with cross-section $[0, L]$. In the examples studied here, the vector field $\vec{B}(z,t)$ is a random perturbation of a cellular flow. It is incompressible, random in t and/or x, and periodic with period one in y. Moreover, the field $B(z,t)$ has zero spatial mean. Periodic boundary conditions are imposed in y for u. The two positive constants in the model are: κ, the species diffusion constant; τ_r, the reaction time scale.

For a velocity field that varies randomly or periodically, the front speed c^* is a time-averaged quantity. For an initial condition $u(x, y, 0)$ that is wave-like with sufficiently fast decay away from the interface (for example, $u(x, y, 0) = H(x)$, the Heaviside function in x), the asymptotic speed of the fronts governed by the nonlinear equation (1) may be defined as the unique constant $c^* > 0$ such that

$$\lim_{t\to\infty} \max_{\substack{y\in[0,L]\\ x<-ct}} u(x,y,t) = 0 \quad \text{if } c > c^*,$$

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$$\lim_{t\to\infty} \min_{\substack{y\in[0,L]\\ x>-ct}} u(x,y,t) = 1 \quad \text{if } c < c^*. \tag{2}$$

Although the solution $u(x,t)$ to (1) is random (it depends on the realization of $B(z,t)$), we show in [6,7] that this front speed is well-defined and deterministic, under suitable hypotheses on B. It is known that even when $\vec{B} \equiv 0$, Eq. (1) may admit traveling wave solutions with different speeds. However, the speed defined by (2) is unique, meaning that it is independent of the initial data, under the assumption that the initial data decays very fast away from the interface. Specifically, we assume that $u(x,y,0) \le \min(e^{\lambda^* x}, 1)$ for some constant $\lambda^* > 0$ sufficiently large. We also assume that B is continuous in both z and t, statistically stationary and ergodic with respect to shifts in x and t, and that B satisfies suitable regularity and moment bounds in order to guarantee the existence of a classical solution (almost surely) to Eq. (1) with initial data $u(x,y,t)$. Under these conditions, the asymptotic behavior described by (2) holds with probability one and the front speed is deterministic and independent of the initial data. See [7] for the most general hypotheses required of B. We suspect that a similar convergence result holds for other nonlinearities, but we are not aware that this has been demonstrated rigorously for other nonlinearities. It is not known whether this convergence holds for a velocity field that is white noise in time.

In turbulent combustion, the front speed c^* is called the turbulent front velocity [3,5]. This is an upscaled quantity that depends on the many continuous scales of the flow field $\vec{B}$ as well as the diffusion and reaction scales. Let L be the size of the domain cross section, δ be the root mean square amplitude of $\vec{B}$, and τ_b be the time scale (time correlation length) of $\vec{B}$. Two nondimensional parameters are: the Péclet number $Pe = \frac{L\delta}{\kappa}$ which measures the relative strength of advection and diffusion, and the Damköhler number $Da = \frac{\tau_b}{\tau_r}$, a ratio of advection and reaction time scales. We use the channel width L in the definition of Pe, since the velocity length scale and the channel width are the same in the cases we consider.

Eq. (1) is nonlinear and stochastic. As well as direct numerical simulation, several approximation methods exist. A conventional approach, often employed in studying fluid turbulence, is a closure approximation to construct equations for the moments or probability distribution function of solutions [3,8,9]. Another approach, the renormalization group method (RG), is a procedure to remove length scales in $\vec{B}$ iteratively for approximating c^*. The RG method has been applied to c^* in the regime of thin fronts ($\kappa \ll 1$, $\tau_r \ll 1$) and large Péclet numbers ($Pe \gg 1$), [10,11]. However, the closure method is ad hoc in nature. The RG method, though systematic, lacks control of convergence, and is not a method for robust numerical computation.

In this paper we use an exact variational representation of c^* for the stochastic KPP reactive fronts to study the front speed numerically in a fast advection regime. This representation has been proved rigorously for periodic flows [12–14], for random shear flows [6], and for one-dimensional random potential flows [15]. In a forthcoming paper [7], we prove the representation for general flows that vary randomly in both space and time, without restrictions on the flow geometry. In particular, all of the cases considered in the present article are within the scope of these results. The authors of [16] have developed a strategy for integrating this variational approach into large scale simulation of turbulent premixed flames.

Here we consider two examples of randomly perturbed cellular flows in two space dimensions. The variational representation holds for arbitrarily many dimensions, however. In Section 2, we introduce the variational representation for the front speed c^*, and we describe the numerical simulations. In Section 3, we demonstrate the results of these numerical simulations. The particular flows we study were chosen because the scaling properties of the front speeds in unperturbed cellular flows are known [17,18]. See also [19] for related analytical estimates of c^* in deterministic flows. Numerical computation of front speeds in steady deterministic flows has been carried out in [20,21]. Fronts propagating in deterministic perturbations of cellular flows have been studied experimentally in [2] and numerically in [22] using a simplified geometric front model. We show here that random perturbations can yield strikingly different results.

2. A variational representation for c^*

First, we briefly describe and formally motivate the variational representation for the front speed c^*; for details of the proof see [6,7]. Fronts governed by the KPP nonlinearity are called "pulled fronts" [23] because their speed is determined by the behavior of the solution far beyond the front interface, in the region where u is close to zero, the unstable equilibrium. Linearizing the equation near this unstable equilibrium, we obtain

$$v_t = \kappa \Delta_z v + \vec{B}(z,t)\cdot\nabla_z v + \frac{1}{\tau_r} f'(0) v. \tag{3}$$

Approximate plane wave solutions of (3), which approximate the tails of left-moving KPP fronts, are generated from initial data $v(z,0) = \exp\{\lambda x\}$, for a positive wave number λ. For a large time t, one anticipates that v behaves like $\exp\{\lambda x + \mu(\lambda)t\}$ to leading order, for some positive number μ which is convex and superlinear for large λ. The asymptotic speed of the approximate plane wave is then $\mu(\lambda)/\lambda$.

The quantity $\mu(\lambda)$ may be determined, as follows. Let us write $w(z,t) = \exp\{-\lambda x\} v(z,t)$, and let $\vec{e}$ be the unit vector along the positive x-axis. Then w solves the initial value problem:

$$\begin{aligned} w_t &= \kappa \Delta_z w + (2\kappa\lambda\vec{e} + \vec{B})\cdot\nabla_z w \\ &\quad + (\kappa\lambda^2 + \lambda\vec{e}\cdot\vec{B} + \tau_r^{-1} f'(0)) w, \end{aligned} \tag{4}$$

with initial data $w(z,0) = 1$. By the maximum principle, the function w is positive for all time. The number μ can be expressed as the almost-sure limit:

$$\mu = \lim_{t\to\infty} \frac{1}{t} \ln \int_\Omega w(x,y,t)\,dy, \tag{5}$$

for any x. The number μ is the so-called principal Lyapunov exponent of the parabolic equation (4), and it is deterministic and independent of x. That is, (5) holds with probability one, although w itself is random. Thus, the asymptotic speed of the approximate plane wave, $\mu(\lambda)/\lambda$, is a deterministic quantity.

In [6,7], we demonstrate that for the fronts governed by the original nonlinear equation, the asymptotic front speed satisfies $c^* = \inf_{\lambda>0} \frac{\mu(\lambda)}{\lambda}$. In other words, the minimal plane wave speed of the linearized equation (3) agrees with that of the nonlinear KPP equation (1)! Through this formula, which is exact, one may estimate the speed c^* by estimating the function $\mu(\lambda)$, which is deterministic.

As a function of the parameter λ, μ is convex, and grows super-linearly with large λ, so $\mu(\lambda)/\lambda$ has a unique minimum. The minimum value of $\mu(\lambda)/\lambda$ is the front speed c^*. It is easy to see that the function $\log w$ will solve a nonlinear, Hamilton-Jacobi type equation with an additional viscous term. From this perspective, the same quantity $\mu(\lambda)$ may be recovered as the effective Hamiltonian via homogenization theory [14,24].

Our strategy for computing c^* is to numerically integrate (4), compute the growth rate $\mu(\lambda)$, then minimize $\frac{\mu(\lambda)}{\lambda}$ to yield c^*. In the regime considered here, the minimization step requires only a few (<10) evaluations of $\mu(\lambda)$. The x dimension is truncated into

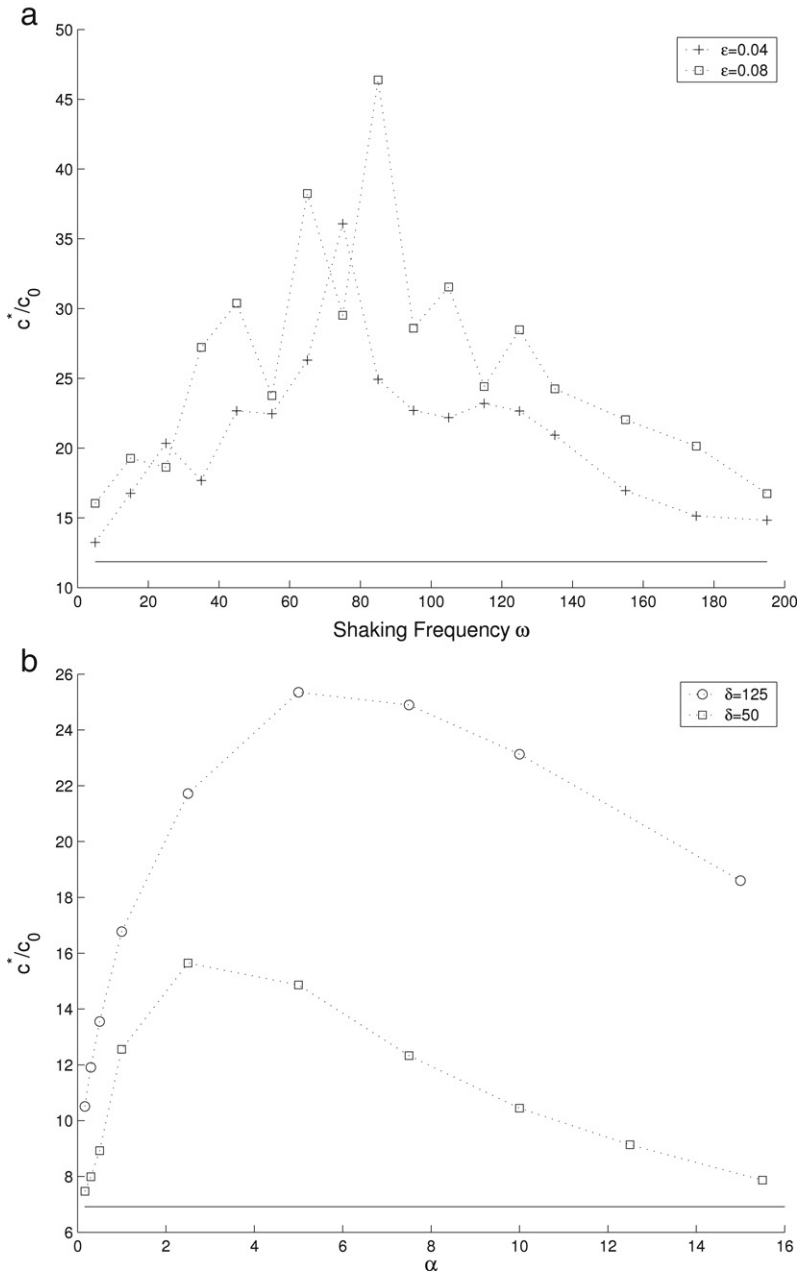

Fig. 1. Top: c^* as a function of ω for $\delta = 80$ ($Pe = 8.0 \times 10^3$), $\epsilon = 0.04, 0.08$. The solid line is the front speed in the unperturbed flow ($\epsilon = 0, \delta = 80$). Bottom: c^* as a function of α (the inverse of the correlation time), $\delta = 125, 50$ ($Pe = 1.25 \times 10^4,\ 5.0 \times 10^3$), $\epsilon = 2.0$. The solid line is the front speed in the unperturbed flow ($\epsilon = 0, \delta = 50$).

a finite and large enough interval $[0, L_x]$ with periodic boundary conditions at $x = 0, L_x$.

Our first set of numerical examples is where $\vec{B}$ is a temporally perturbed cellular flow in two space dimensions (δ, ϵ are constant parameters):

$$\vec{B}(x, y, t) = \delta 2\pi(-\sin(2\pi(x + \epsilon\gamma(t))) \times \cos(2\pi y), \cos(2\pi(x + \epsilon\gamma(t)))\sin(2\pi y)).$$

As $\vec{B}$ has period one in x and y, the spatial domain for (4) is the unit square. We examine how temporally random perturbations influence c^* in the case where $\gamma(t)$ is an Ornstein-Uhlenbeck process (Gaussian and Markov), and we compare the results with the case where $\gamma(t)$ is periodic in time. As $\gamma(t)$ has an intrinsic parameter, the time correlation length (denoted by $\frac{1}{\alpha}$), the front speed depends on three parameters $c^* = c^*(\delta, \epsilon, \alpha)$. The parameter α has the unit of frequency. If $\gamma(t) = \cos(\omega t)$, then $c^* = c^*(\delta, \epsilon, \omega)$.

Our second example is when the perturbation is a spatially random shear flow so that $\vec{B}$ is random in x:

$$\vec{B}(x, y) = \delta[2\pi(-\sin(2\pi x)\cos(2\pi y), \cos(2\pi x) \times \sin(2\pi y)) + \epsilon(0, \xi(x))], \quad (6)$$

where $\xi(x)$ is a mean zero stationary ergodic process, and we examine how the spatial randomness influences the front speed c^*.

The evolution problem (4) is solved with an operator splitting technique to handle diffusion and advection-reaction time stepping separately. After a long enough evolution period, we sample the logarithm of the spatial integral of w at many points in time and let μ be the slope of the best-fit line through these points. For the advection-reaction step, we use a semi-Lagrangian scheme [25], which permits larger time steps and minimal numerical diffusion. For the diffusive step, we use the implicit unconditionally stable Crank–Nicholson scheme in time and spectral method in space.

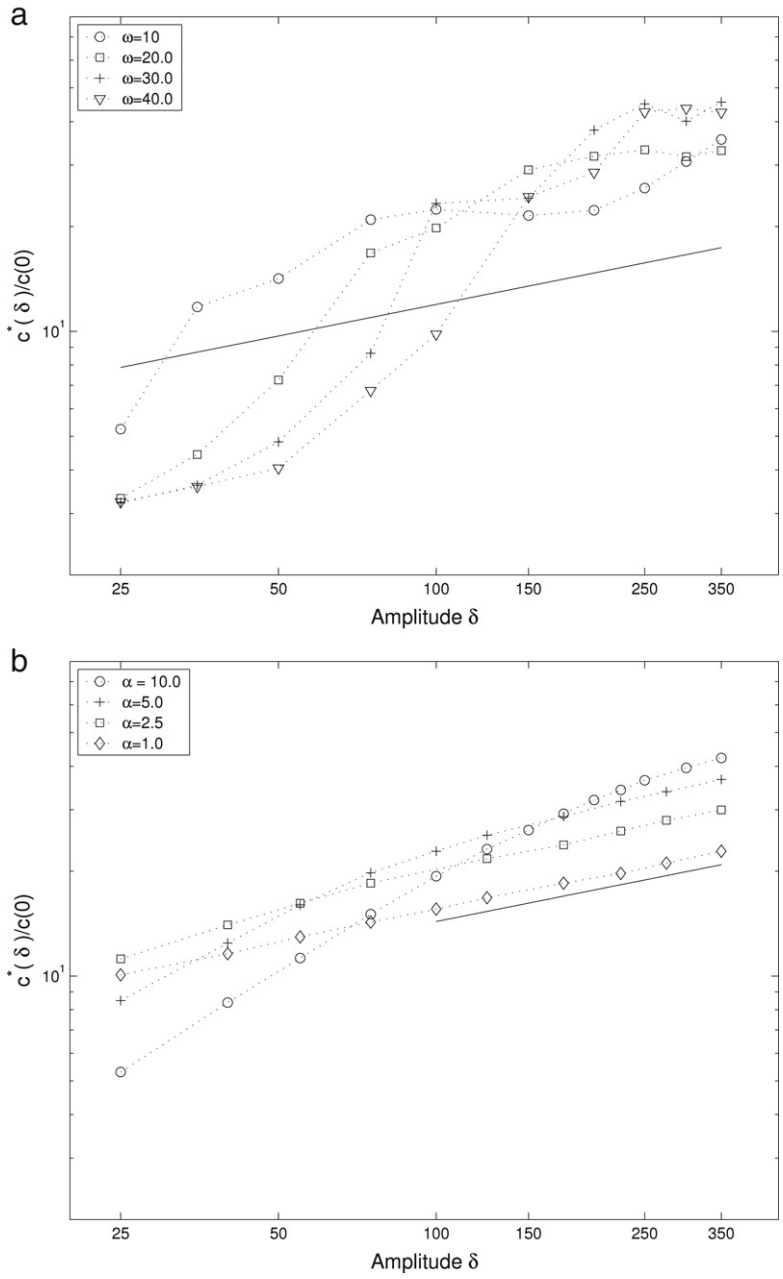

Fig. 2. Top: Log–log plot of c^* versus flow amplitude δ for various periodic shaking frequencies. Bottom: Log–log plot of c^* versus flow RMS amplitude δ for various correlation times $1/\alpha$. For both plots, the perturbation amplitude is fixed at $\epsilon = 2.0$. For comparison, the two solid lines have slope $p = 0.3$.

With the constants $\mu(\lambda)$ computed in this way, we minimize the function $\mu(\lambda)/\lambda$ using a standard algorithm based on a golden section search [26].

3. Numerical results

We first study c^* in unsteady cellular flows. Due to "shaking" by $\gamma(t)$, the positions of the saddle points in the flows oscillate in time. At a fixed time t_0, the streamlines of the flow $B(z, t_0)$ are bounded. When $\gamma(t)$ is periodic with frequency $\omega \ll 1$, nearly ballistic trajectories may result from the creation of oscillating unbounded channels within the shaken reference frame. In this regime, the temporal perturbation γ allows Lagrangian particles to hop from one bounded cell to another, traveling a distance of order ω^{-3} in a time scale of order $\omega^{-3} \log \omega$ [27]. Consequently, the front speed in such a shaking flow may be significantly larger than that in the unperturbed steady flow.

In the periodic case, with $\gamma(t) = \epsilon \cos(\omega t)$, there appears an intriguing resonance pattern when c^* is plotted as a function of ω for fixed δ and ϵ. The frequency range spans the interval $\omega \in [5.0, 195.0]$. The diffusion constant is $\kappa = 0.01$, and the reaction time scale is $\tau_r = 0.5$. In Fig. 1(top), c^* is plotted as a function of ω at flow amplitude $\delta = 80$, and $\epsilon = 0.04, 0.08$. We observe multiple resonance peaks. The peaks become more pronounced as ϵ or δ gets larger.

Resonance peaks of c^* in periodically shaking cellular flows were computed previously from a simplified geometric front model [22] (the so called G equation). This model is an approximation to the front in the thin front regime when the reaction time scale is much smaller than the diffusive and advective time scales. Here we consider a different regime in which the advective time scale is much smaller than the reactive time scale (fast advection). In this regime, the geometric front approximation may be very inaccurate, even for steady shear flows [28]. The variational

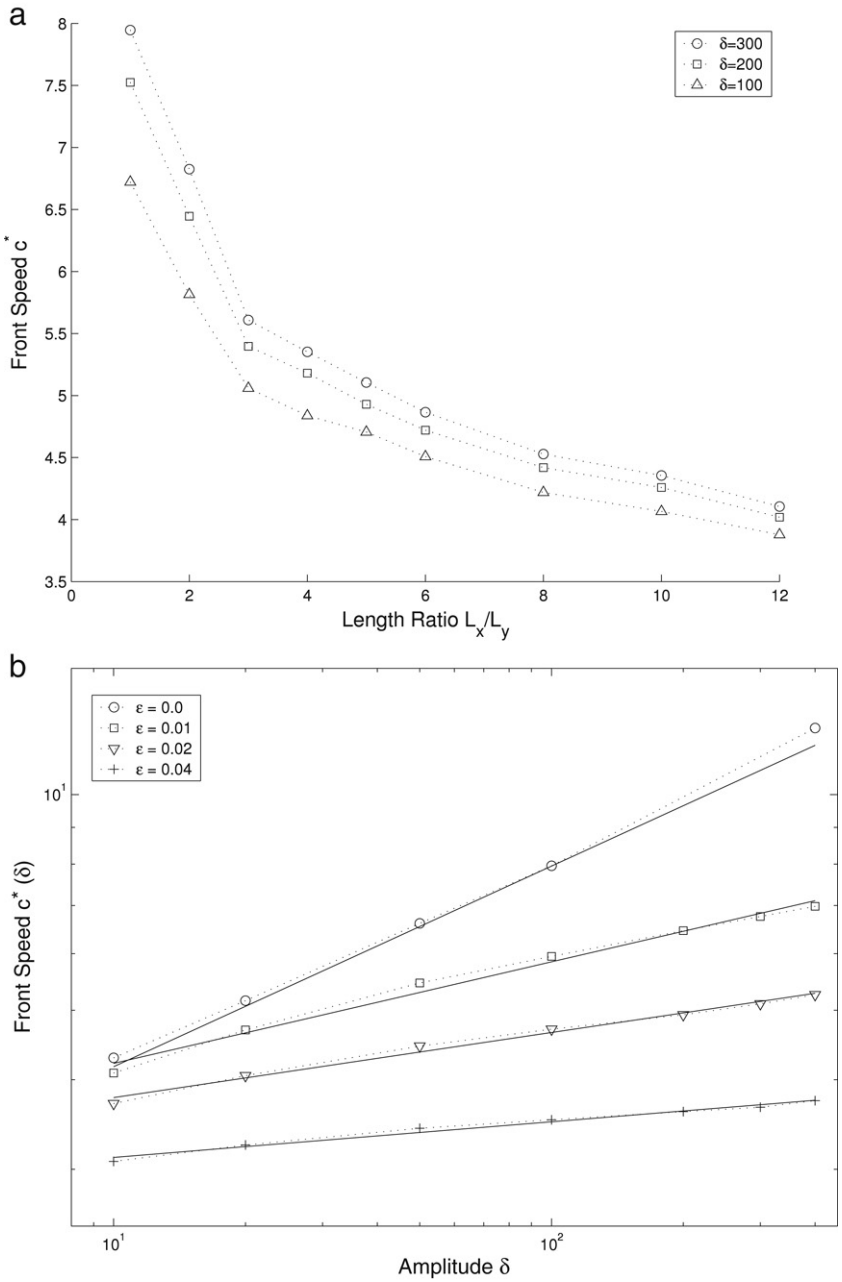

Fig. 3. Top: Front speed c^*/c_0 versus channel length ratio L_x/L_y for fixed flow amplitudes $\delta = 100, 200, 300$. Bottom: Log–log plot of c^*/c_0 as a function of amplitude δ for various values of ϵ, at $L_x/L_y = 5$. Diffusion constant κ is fixed at $\kappa = 0.01$, the Péclet number ranges from 1.0×10^3 to 4.0×10^4.

representation of c^* is exact, however. Thus we should expect our results to differ from those of [22]. For example, for the range of parameters shown in Fig. 1(top), the speed in the perturbed flow is always greater than the speed of the corresponding unperturbed flow ($\epsilon = 0, \delta = 80$). This is different from the results of [22] where the fronts governed by the G-equation may travel faster or slower than the fronts in the unperturbed flow. We observe a slow-down of front speeds as $\omega \to \infty$ and $\omega \to 0$.

Now we plot c^* as a function of δ for fixed values of ω or α. Fig. 2(top) shows that the front speed in the periodically shaking flows may not be a monotonic function of the flow amplitude δ. When δ is large, $c^*(\delta)$ scales sub-linearly, approximately $O(\delta^{0.3})$ at $\epsilon = 2$, larger than $O(\delta^{1/4})$ in the steady flows [17,18]. This may be explained in terms of the competing effects of the underlying cellular flow and the nature of oscillatory channels created by the temporal shaking. When ω is very small, the channels have small width, of order $O(\omega)$. The diffusing Lagrangian particles may easily hop out of these channels, which may result in less enhancement of the front speed. As the frequency increases, the channels widen, leading to greater enhancement of the Lagrangian transport and front speed. However, for very large frequencies, the perturbation destroys more of the cellular structure so that over a large time interval the flow is closer to a purely oscillatory flow. It can be shown analytically that a purely oscillatory flow $B = B(t)$ does not enhance the front speed. So, if too much of the cellular structure is destroyed by very fast perturbation, the front speed cannot be greater than the speed corresponding to unperturbed flow.

Now compare these results to the case of random perturbations. Let $\gamma(t)$ be the Ornstein-Uhlenbeck process defined by the Ito equation: $d\gamma(t) = -a\gamma(t)dt + rdW(t)$, where W is the Wiener process, a and r are positive constants. We choose $r = \sqrt{2}\alpha^{3/4}$ so that the covariance function is $\sqrt{\alpha}e^{-\alpha|t-s|}$. The total energy

in the power spectrum is invariant with α. We integrate the Ito equation by an implicit second-order strong Taylor scheme [29]. Fig. 1(bottom) shows c^* as a function of α, the inverse of the time correlation length, with $\delta = 50$ and $\delta = 125$ fixed. There is an optimal time correlation length leading to maximal speed enhancement. As α goes to $+\infty$, the correlation length goes to zero, and the front speed decreases to the speed in the unperturbed steady flow. When the α is less than the optimal value, the front speed c^* decreases with decreasing α. In the randomly shaking flows, multiple resonance peaks disappear in contrast to the case of periodically shaking flows. Moreover, for the range of parameters we simulated with the randomly shaking flows, the front speed is always greater than the speed in the unperturbed flow.

Fig. 2(bottom) shows c^* as a function of flow amplitude for various fixed correlation times at $\epsilon = 2$. We observe that c^* scales sub-linearly with large δ. In the randomly shaking flows, however, c^* increases monotonically in δ, without local resonance peaks. The continuously many scales in the random shaking removes resonance. The speed scaling in large δ is also $O(\delta^{0.3})$. However, the range of values of δ over which this scaling is manifested changes with α. Specifically, we observe that when α is large (e.g. $\alpha = 10$) this scaling $O(\delta^{0.3})$ is manifested only at larger values of δ, compared to the case of smaller α (e.g. $\alpha = 1$). A rigorous justification of this observed scaling is not known to the authors.

Next, we consider spatial randomness in the direction of front propagation. The shear perturbation ξ is generated by the random Fourier method: $\xi(x,\omega) \approx \sum_{j=0}^{F_m} E^{1/2}(j\Delta k)\sqrt{\Delta k}(\zeta_j \cos(2\pi j \Delta k x) + \eta_j \sin(2\pi j \Delta k x))$, where Δk is the wavenumber spacing and F_m is the highest Fourier mode included in the approximation. The variables ζ_j and η_j are independent unit Gaussians. We take $E^{1/2}(k) = \frac{1}{k}$ and $F_m = 30$, and use a uniform grid of 1000×200 ($L_x \times 1$ with $L_x = 5.0$) to approximate the truncated channel. Fig. 3(top) shows the dependence of c^* on the channel length L_x for values in the range $L_x = 1.0$ to $L_x = 12.0$. The front speed is seen to converge to a deterministic constant as L_x increases.

We observe that the random transverse perturbation destroys the $O(\delta^{1/4})$ growth law of the front speed in steady cellular flows [18]. Fig. 3(bottom) is a log–log plot of the front speed as a function of flow amplitude for various values of the perturbation strength ϵ. The plots demonstrate the power-law scaling of c^* with respect to δ; the solid lines fitting the data have slopes 0.28, 0.14, 0.09, and 0.05, respectively. This demonstrates a significant reduction of the front speed due to the transverse random perturbation breaking the cellular structures at many places along the channel.

In conclusion, we have developed a variational principle based numerical method to compute reactive front speeds in random flows. With this method we discover new phenomena in front speeds in randomly perturbed cellular flows. When a cellular flow is perturbed by temporally random oscillations, the front speed c^* does not exhibit a resonance between spatial and temporal scales, as in the case of time periodic oscillation of cellular flows. On the other hand, random spatial oscillations significantly diminish the speed-enhancing effect of the underlying cellular flow. The variational approach is a promising tool for studying stochastic reactive fronts arising in other scientific areas such as multiscale surface reactions [30], among other problems of front propagation into unstable states [23].

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