

VARIATIONAL PRINCIPLE BASED COMPUTATION OF KPP AVERAGE FRONT SPEEDS IN RANDOM SHEAR FLOWS*

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Abstract. Variational principle of Kolmogorov-Petrovsky-Piskunov (KPP) minimal front speeds provides a fast and accurate way for speed calculations. A variational principle based computation is carried out on a large ensemble of KPP random speeds through spatial, mean zero, stationary, Gaussian random shear flows inside two dimensional channel domains. In the regime of small root mean square (rms) shear amplitude, the enhancement of the ensemble averaged KPP front speed obeys the quadratic law. In the large rms amplitude regime, the enhancement follows the linear law. An asymptotic ensemble averaged speed formula is derived and agrees well with the numerics. Related theoretical results are presented with a brief outline of the ideas in the proofs. The ensemble averaged speed is found to increase sublinearly with enlarging channel widths, while the speed variance decreases. Direct simulations in the small rms regime suggest quadratic speed enhancement law for non-KPP nonlinearities.

Key words. KPP front speeds, random shear flows, variational computation

AMS subject classifications. 35K57, 41A60, 65D99

1. Introduction. Front propagation in heterogeneous fluid flows has been an active research area (see [8], [15], [12], [23], [24], [25], [27] and references therein). A fascinating phenomenon is that the large time (large scale) front speed can be enhanced due to multiple scales in fluid flows. Speed characterizations and enhancement laws have been studied mathematically for various flow patterns by analysis of the proto-type models, i.e. the reaction-diffusion-advection equations (see [5, 9, 11, 13, 15, 16, 17, 18, 22, 24, 25, 26] and references therein). The enhancement obeys quadratic laws in the small amplitude flow regime, known as the Clavin-Williams relation [8], which is proved to be true for deterministic shear flows [22], [11], [19], [18]. However, enhancement exponent $4/3$ was proposed based on numerical simulation of random Hamilton-Jacobi models (so called G-equation or KPZ model) on fronts in weak randomly stirred array of vortices [12].

In this work, we consider the reaction-diffusion front speeds through random shear flows in a two dimensional channel domain. We shall address the enhancement laws of the ensemble averaged front speeds. The model equation is:

$$u_t = \Delta_{x,y}u - B \cdot \nabla_{x,y}u + f(u), \quad (1.1)$$

$\Delta_{x,y}$ the two-dimensional Laplacian, $(x, y) \in R \times [0, L]$, $t \in R^+$. The nonlinearity $f = u(1 - u)$, so called Kolmogorov-Petrovsky-Piskunov (KPP) reaction. Other nonlinearities [25] will be discussed later. The vector field $B = (b(y, \omega), 0)$ where $b(y, \omega)$ is a stationary Gaussian process in y , its ensemble mean equal to zero.

Neumann boundary conditions are imposed along the sides of the cylinder: $\frac{\partial u}{\partial y} = 0$ for $y = 0$ or $y = L$. For nonnegative initial data approaching zero and one at x infinities rapidly enough, the KPP solutions propagate as fronts with speed c^* given

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by the variational principle [7, 25, 5]:

$$c^* = c^*(\omega) = \inf_{\lambda > 0} \frac{\mu(\lambda, \omega)}{\lambda}, \quad (1.2)$$

where $\mu(\lambda, \omega)$ is the principal eigenvalue with corresponding eigenfunction $\phi > 0$ of the problem:

$$\bar{L}_\lambda \phi = \phi_{yy} + [\lambda^2 + \lambda b(y, \omega) + f'(0)] \phi = \mu(\lambda, \omega) \phi, \quad y \in (0, L), \quad (1.3)$$

$$\frac{\partial \phi}{\partial y} = 0, \quad y = 0, L. \quad (1.4)$$

The KPP variational speed formula (1.2) offers an efficient and accurate way to compute a large ensemble of random front speeds. Directly solving the original time dependent equation (1.1) to reach steady propagating states can be both slow and less accurate. Numerical difficulties abound for direct simulations due to at least three large parameters. A large ensemble of random fronts requires a large enough truncated domain $(x, y) \in [-x_l, x_r] \times [0, L]$ to contain the front over large times. Due to occasional random excursions in b , the domain size in x has also to be made adaptively large. This can be prohibitively expensive in the regime of large root mean square (rms) shears.

The variational formula (1.2) allows us to compute fast and accurately the ensemble averaged speeds in both small and large shear rms regimes. An interesting difference from the deterministic case is that the integral average of $b(y, \omega)$ in $y \in [0, L]$, i.e. $\bar{b} = \bar{b}(\omega) = L^{-1} \int_0^L b(y, \omega) dy$, is a random constant not equal to zero. This quantity can be of either sign, and influence greatly the numerical approximation of $E[c^*]$ in the small rms regime, even though it does not contribute to the exact $E[c^*]$. To assess the speed enhancement accurately, we subtract this random constant from each $c^*(\omega)$ before evaluating the expectation numerically. This way, we are able to minimize the errors in approximating $E[c^*]$ in a finite ensemble. In our computation, b is a discrete Ornstein-Uhlenbeck (O-U) process.

The main finding of this article is that the ensemble averaged speed obeys the quadratic law in the small rms regime and linear law in the large rms regime. Without the \bar{b} subtraction technique, the computed average speed enhancement in the small rms regime can give inaccurate scaling exponents significantly below two. The same technique and direct simulations for other nonlinearities (combustion, bistable) suggest quadratic speed enhancement in the small rms regime. We note in passing [26] that if $L \rightarrow \infty$ and b is white in time, then the KPP speed enhancement obeys quadratic (linear) law in the small (large) rms regime; and that the KPP speed logarithmically diverges in time if b is only spatially Gaussian. Our numerical results on channels with enlarging widths are qualitatively consistent, and show that the average speed increases sublinearly while the speed variance decreases.

The rest of this article is organized as follows. In section 2, we discuss properties of the random process $b(y, \omega)$, theorems on ensemble averaged speed enhancement laws, and an asymptotic enhancement formula. In section 3, we describe a numerical method for computing with the variational formula (1.2); show various numerical results, and comparison with the asymptotic formula. The concluding remarks are in section 4. More analytical and numerical findings can be found in the companion paper [20].

2. Speed Formula in Random Setting. Consider scaling the shear amplitude $b(y, \omega) \mapsto \delta b(y, \omega)$, and denote by $c^*(\delta)$ the minimal KPP speed corresponding to the shear δb , so $c_0^* = c^*(0)$ is the minimal speed in the case of zero advection. For a deterministic shear, if the shear integral average $\langle b \rangle = \frac{1}{L} \int_0^L b(y, \omega) dy = 0$, then $c^*(\delta) = c_0^* + O(\delta^2)$ as $\delta \ll 1$. In the large δ regime, $\lim_{\delta \rightarrow \infty} c^*(\delta)/\delta$ exists [4]. In case of a stationary Gaussian shear, we have an ensemble of KPP front speeds $c^*(\delta, \omega)$ in an infinite cylinder $R \times \Omega$, Ω a simply connected bounded domain with smooth boundary in R^{n-1} ($n \geq 2$). Though $\langle b \rangle$ may not be zero, similar enhancement laws holds for the ensemble averaged speeds.

THEOREM 2.1 (Quadratic Law). *Let $b(y, \omega)$ be a stationary random process in R^{n-1} ($n \geq 2$) so that sample paths are almost surely continuous; and that*

$$E[\|b\|_\infty^6] < +\infty. \tag{2.5}$$

Then for δ small, the expectation $E[c^(\delta, \omega)]$ has the expansion*

$$E[c^*(\delta, \omega)] = c_0^* + \delta E[\langle b \rangle] + \frac{c_0 \delta^2}{2|\Omega|} \int_\Omega E[|\nabla \chi|^2] dy + O(\delta^3), \tag{2.6}$$

where $b(y, \omega) = \langle b \rangle(\omega) + b_1(y, \omega)$; and $\chi = \chi(y, \omega)$ solves $\Delta_y \chi = -b_1$, $y \in \Omega$, subject to zero Neumann boundary condition.

In the large rms amplitude regime, linear growth of the ensemble averaged speed holds with weaker moment conditions on b :

THEOREM 2.2 (Linear Law). *If the stationary shear process $b(y, \omega)$ has almost surely continuous sample paths and satisfies $E[\|b\|_\infty] < \infty$, then the amplified shear field $\delta b(y, \omega)$ generates the average front speed $E[|c^*(\delta, \omega)|]$ such that $\lim_{\delta \rightarrow \infty} E[|c^*(\delta, \omega)|]/\delta$ exists.*

The above are stochastic analogues of known enhancement laws in deterministic shear flows with the bistable and combustion type nonlinearities. The authors of [11] proved a min-max variational formula for the wave speed in the case of bistable and combustion type nonlinearity, and they used the formula to derive an enhancement law for small shear amplitudes similar to (2.6) (see Theorem 4.2 in [11]). In [10], Hamel proved that the same min-max variational formula holds for c^* in the case of the KPP nonlinearity, but it is not clear that this formula will yield the result of Theorem 4.2 in [11] for the KPP case. The difference lies in the fact that the linearized operator for the traveling wave equation in the KPP case (unlike the bistable and combustion cases) has continuous spectrum with positive real part. As a result, the estimates used to prove Theorem 4.2 of [11] do not extend to the KPP case. Indeed, the estimates needed to prove Theorem 4.2 of [11] are a delicate matter and the technique of [11] must be modified in order to prove the stochastic analogue of (2.6) for the bistable and combustion cases. See [21] for more discussion of this point and an extension of (2.6) to the bistable and combustion cases.

To handle the KPP case and prove (2.6), our strategy is to estimate $c^*(\delta, \omega)$ by analyzing the associated eigenvalues $\mu(\lambda, \omega)$ and applying (1.2). To estimate the eigenvalues $\mu(\lambda, \omega)$, we construct a class of test functions suggested by formal asymptotic expansion of the eigenvalues, and we insert the test functions into well-known variational formulas for the principal eigenvalue of an elliptic operator. For each realization this method yields a speed asymptotic expansion similar to Theorem 4.2 in

[11]. Then combining this with probabilistic estimates on the remainder of the expansion yield the result for the ensemble mean. The linear growth of $E[c^*(\delta, \omega)]$ follows from the dominated convergence theorem and the deterministic result [4]. Details are referred to [20].

The moment conditions for both theorems are satisfied by the Ornstein-Uhlenbeck process restricted to the interval $[0, L]$ as a consequence of Doob's inequality [20]. The expectation integral of the $O(\delta^2)$ term in (2.6) can be calculated in terms of the covariance function $E[b(s)b(y)] = f(|s - y|)$ [20]. In case of O-U process, $E[b] = 0$, $f(|s - y|) = \rho \exp(-a|s - y|)$, $\rho = r^2/(2a)$, for positive constants r and a . Then by (2.6) with $\Omega = [0, L]$, we have the averaged speed formula [20] for δ small:

$$E[c^*(\delta, \omega)] = c_0^* + \frac{c_0^* \delta^2}{2|\Omega|} E[|\chi_x|^2] + O(\delta^3), \tag{2.7}$$

where:

$$E[|\chi_x|^2] = \frac{r^2}{2a} \left(e^{-aL} \left(\frac{4}{L^2 a^4} - \frac{1}{3a^2} \right) + \frac{L}{3a} - \frac{4}{L^2 a^4} - \frac{5}{3a^2} + \frac{4}{La^3} \right). \tag{2.8}$$

We shall see that the average speed formula (2.7)-(2.8) agrees rather well with numerics.

3. Numerical Method and Results.

3.1. Numerical Method. For a given $\lambda > 0$, we compute the principal eigenvalue $\mu(\lambda)$ by solving (1.3)-(1.4) with a standard second order finite-difference method and a second order discretization of the Neumann boundary conditions. The computation is done realization by realization, and we shall omit writing the ω dependence. The problem reduces to finding the principal eigenvalues of symmetric tridiagonal random matrices, easily accomplished with double precision LAPACK routines [2]. Then we compute points on the curve $\frac{\mu(\lambda)}{\lambda}$, and minimize over λ using a Newton's method with line search. This way, our approximation converges quadratically in the region near the infimum and decreases with each iteration. The curves $\frac{\mu(\lambda)}{\lambda}$ may not be convex, but there is always a unique minimum [20].

We generate realizations of the shear process $b(y, \omega)$ by applying the Milstein scheme [14] on the stochastic differential equation satisfied by the O-U process. Although the scheme is first order, we select a discrete spacing $\bar{h} \leq h^2$, where h is the discrete grid spacing for the eigenvalue problem. So the method is still second order accurate in the parameter h . Fig. 1 and Fig. 2 show an O-U sample path, numerical and exact covariance functions. The O-U parameters $\rho = 2$, $a = 4$, and 5000 realizations of O-U process are used for calculating the covariance function in Fig. 2.

To approximate the expectation $E[c^*(\delta)]$, we generate N realizations (indexed by $i = 1, \dots, N$) of the shear and compute the corresponding minimal speeds $\{c_i^*\}$ for each δ . Then we compute the average

$$E[c^*(\delta)] \approx \bar{E}(\delta) = c_0^* + \frac{1}{N} \sum_{i=1}^N M_i(\delta), \quad j = 1, \dots, N \tag{3.1}$$

where $M_i(\delta) = c_i^*(\delta) - c_0^* - \delta \bar{b}_i$. That is, we subtract the linear part due to the integral average of the shear being nonzero, as in (2.7).

Once we have the averages $\bar{E}(\delta)$ for each δ , we compute the scaling exponents p using the least square method to fit a line to a log-log plot of averaged speed versus amplitude.

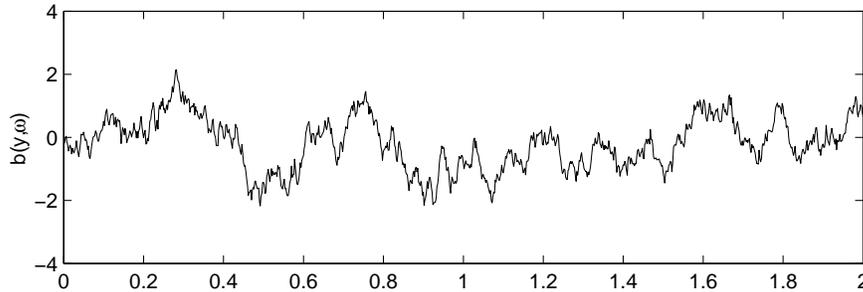


FIG. 1. One sample path of the Ornstein-Uhlenbeck process $b(y, \omega)$.

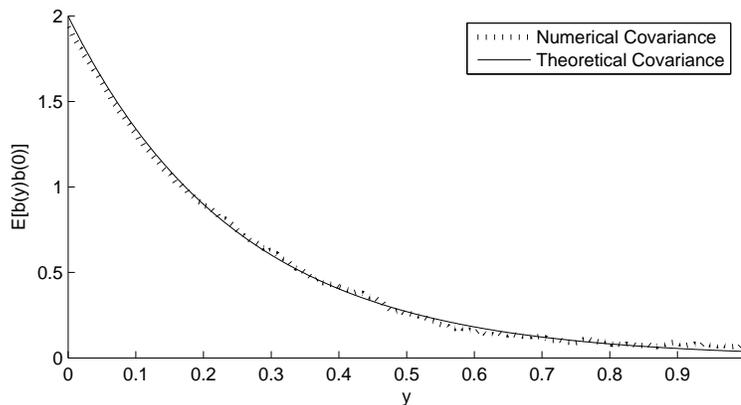


FIG. 2. Numerical and exact covariance functions of the Ornstein-Uhlenbeck process $b(y, \omega)$.

3.2. Numerical Results. Figure 3 and Figure 4 show the results using $N = 10^5$ shear realizations for small rms amplitudes and large rms amplitudes, respectively. The covariance function of the process is $E[b(y)b(s)] = e^{-4|y-s|}$. In each plot, we show multiple curves, corresponding to various domain widths. In Figure 3 in the small δ regime, the solid curves are the numerically computed values; the dashed curves are calculated by formula (2.7). The agreement between the formula and numerics is excellent, especially at small $\delta \in (0, 0.2)$, or smaller domain width $L = 1, 2$. The enhancement of the minimal speed is found to scale quadratically for small rms amplitudes and linearly for large rms amplitudes. The computed scaling exponents are shown in Table 1.

Using the direct second order upwind finite difference method described in [18], we observe similar results for small rms amplitudes in case of generalized KPP ($f(u) = u^2(1 - u)$), combustion [18], or bistable [18] front speeds, as shown in Table 2. The numerical domain in the direct simulation is $(x, y) \in (0, 30) \times (0, 4\pi)$. For front containment in this domain during its evolution, the diffusion coefficient in front of $\Delta_{x,y} u$ is 0.025 (instead of one), so to have sharper fronts moving at slower velocities. The initial front is located near $x = 0$. The number of realizations for the average speeds to stabilize is on the order of 10^3 . The range of computed δ is $[0.01, 0.05]$. Due to the long time required for direct simulation, we have not pursued direct computation of the scaling exponents for large rms shear amplitudes.

TABLE 1

Scaling exponents p in $E[c^*(\delta)] = c_0^* + O(\delta^p)$, with KPP nonlinearity, computed by variational formula for various L .

	$L = 1.0$	$L = 2.0$	$L = 3.0$	$L = 4.0$
$\delta \ll 1$	2.00	1.98	1.96	1.93
$\delta \gg 1$	1.09	1.05	1.04	1.03

TABLE 2

Scaling exponents p in $E[c^*(\delta)] = c_0^* + O(\delta^p)$, computed by direct simulation for various nonlinearities.

	KPP	Combustion	Bistable	Generalized KPP
$\delta \ll 1$	1.98	2.00	1.99	1.99

We also observed that as we increase the width L of the channel, with δ fixed, the expectation $E[c^*(\delta)]$ grows sublinearly and the variance $Var[c^*(\delta)]$ decreases. Figure 5 illustrates the variation of the distribution of $c^*(\delta)$ as $L = 4, 16, 30$. For this figure (and later Fig. 6 and Fig. 7), $\delta = 50$, and the diffusion constant equals 0.01 (set to 1 in equation (1.1)). Also, the covariance of the shear process has been modified from Fig. 3 and Fig. 4 to give optimal enhancement for the larger amplitude and larger domain widths (see [20] for more details about enhancement versus covariance of b). The distribution curves get narrower and shifted to the right with increasing L . A theoretical explanation is as follows. The average speed obeys the upper bound

$$E[c^*(\delta)] \leq c_0^* + \delta E\left[\sup_{y \in [0, L]} b(y)\right]. \quad (3.2)$$

From the theory of extremal distributions for stationary Gaussian fields with covariance function being Hölder continuous near the origin ([1], Chapter 6), we have as $L \rightarrow \infty$:

$$\begin{aligned} E\left[\sup_{y \in [0, L]} b(y)\right] &\equiv A(L) \sim O(\sqrt{\log(L)}), \\ \text{Var}\left[\sup_{y \in [0, L]} b(y)\right] &\equiv B(L) \sim O\left(\frac{1}{\sqrt{\log(L)}}\right), \\ \text{Prob}(B^{-1}(L)\left(\sup_{y \in [0, L]} b(y) - A(L)\right) < u) &\rightarrow \exp\{-\exp\{-u\}\}. \end{aligned} \quad (3.3)$$

The O-U process satisfies (3.3), its covariance is Lipschitz near the origin. In view of (3.2), we see that the growth of $E[c^*(\delta)]$ with respect to L could be no more than $O(\sqrt{\log L})$. It is known [3, 6] that for deterministic shear flows, if the diffusion coefficient (instead of being one in (1.1)) is small enough, the ratio $c^*(\delta)/\delta$ is close to $\sup_{y \in [0, L]} b(y)$ as $\delta \gg 1$. We observed that at $\delta = 50$, diffusion constant = 0.01, the mean and variance of $c^*(\delta)/\delta$ mimic the mean and variance of $\sup_{y \in [0, L]} b(y)$ as $L \gg 1$. In Fig. 6 and Fig. 7, we compare $E[c^*(\delta)]$ with $E[g_1(L)]$ and $Var[c^*(\delta)]$ with $Var[g_1(L)]$, where

$$g_1(L) = c_0^* + \delta \sup_{y \in [0, L]} b(y).$$

The figures show a close correlation between the speed and the global maximum of the shear on $[0, L]$, but the curves are clearly not identical. While they suggest that asymptotic convergence may hold for the speed distribution function up to a

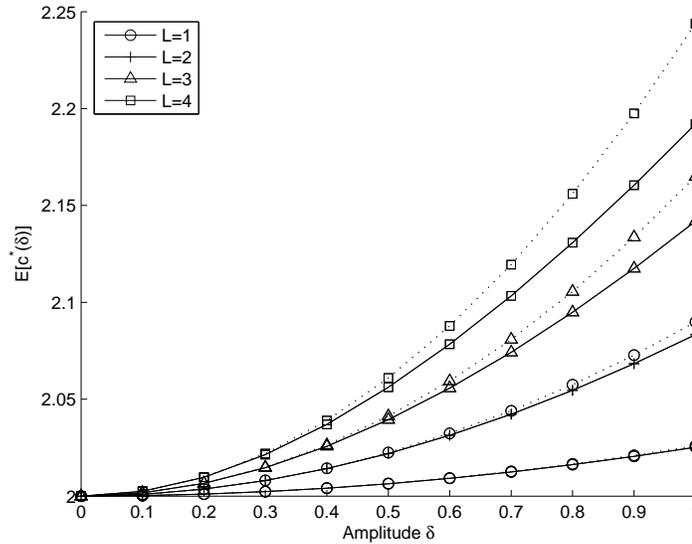


FIG. 3. Enhancement of ensemble averaged KPP minimal speeds in the small rms shear amplitude regime and varying domain widths. Solid curves are the numerically computed values; the dashed curves are calculated by asymptotic formula (2.7).

normalization similar to (3.3), they do not suggest that the $E[c^*(\delta)/\delta]/E[\sup b] \rightarrow 1$. Because of the very slow convergence of these quantities as $L \rightarrow \infty$, additional computation of these curves as $L \rightarrow \infty$ does not yield more insight into the subtle behavior of $c^*(\delta)$ in the limit.

4. Concluding Remarks. Variational principle of KPP front speeds allows us to perform an accurate computation of a large ensemble of speeds through random shears inside two dimensional channel domains. In the regime of small rms shear amplitude, the enhancement of the ensemble averaged speed obeys the quadratic law. In the large rms regime, the enhancement follows the linear law. An asymptotic averaged speed formula is found to agree well with the numerics. Enlarging the channel width increased the averaged front speed, and decreased the speed variance. The correlation between the KPP speed and the shear maximum was observed in the large rms regime of the shear. A mean shear subtraction technique helps to numerically approximate the average front speeds accurately in the small rms regime. The technique and direct simulations suggest quadratic enhancement law for non-KPP nonlinearities.

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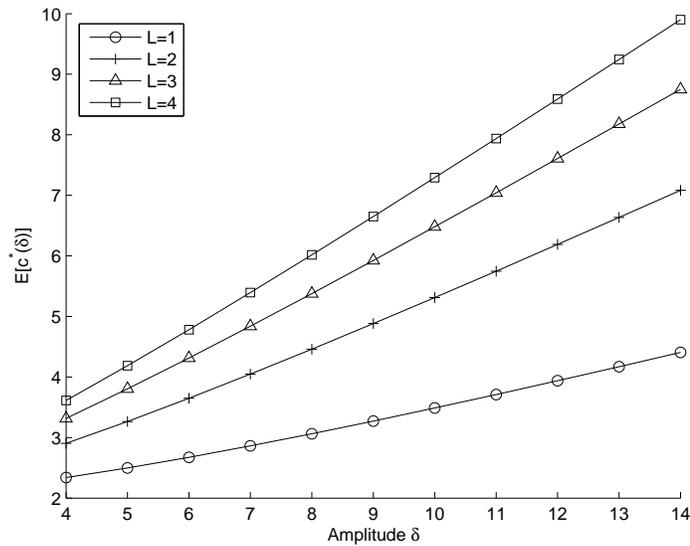


FIG. 4. Enhancement of ensemble averaged KPP minimal speeds in the large rms shear amplitude regime with varying domain widths.

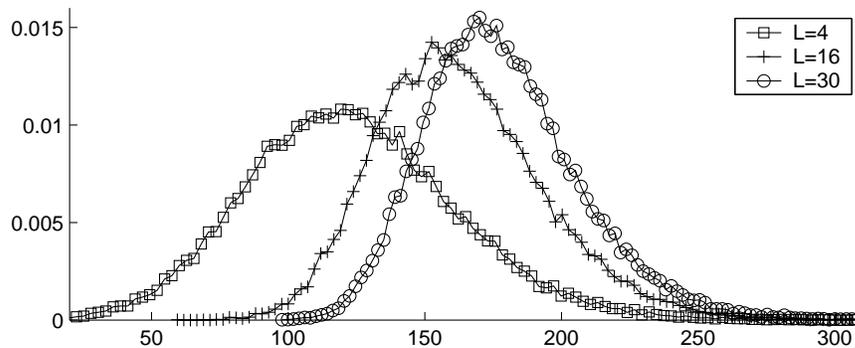


FIG. 5. Distribution of KPP minimal speeds in the large rms shear amplitude regime with varying domain widths, $\delta = 50$.

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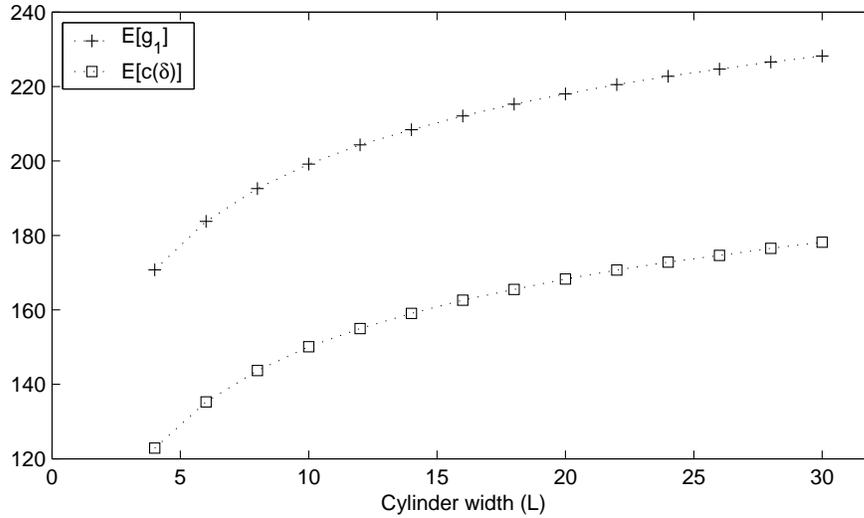


FIG. 6. Sublinear growth of ensemble averaged speed as domain width increases, $\delta = 50$.

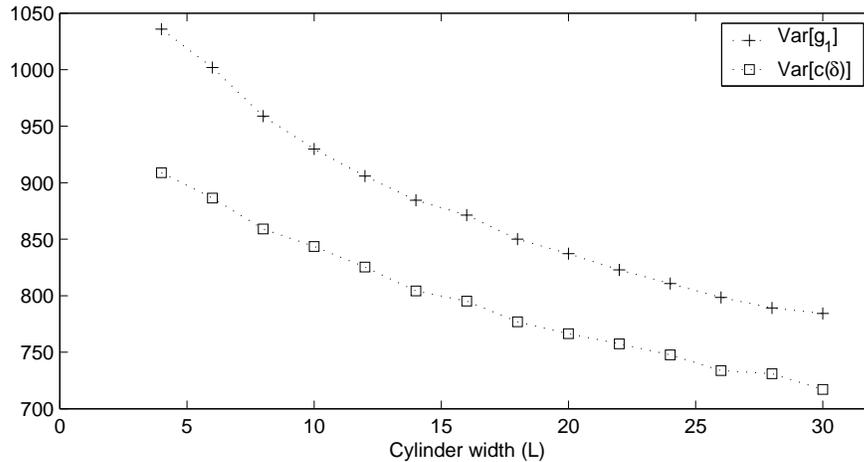


FIG. 7. Decay of the speed variance as domain width increases, $\delta = 50$.

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