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Stochastic PDEs: convergence to the continuum?

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Abstract

We examine the convergence properties of stochastic PDEs discretized using finite differences. In one space dimension, where the continuum solution is a stochastic process whose values are continuous functions in space, the transfer integral allows exact calculation of steady state properties, including the corrections due to finite grid spacing. The method applies to arbitrarily nonlinear PDEs, provided they have a stationary density. In two or more space dimensions, however, solution configurations are not continuous functions but only distributions. The stochastic PDE can still be solved on a finite grid of points in space, but the mean squared value at a grid point does not approach a finite limit as the grid spacing is decreased. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

A stochastic partial differential equation (stochastic PDE) describes dynamics with noise in continuous space and time [1–9]. On discretizing space to generate a numerical solution, one obtains a set of coupled stochastic ordinary differential equations. In this article we consider the convergence to the continuum of the finite differences method applied to stochastic PDEs.

We analyse a linear stochastic PDE known as the infinite-dimensional Ornstein–Uhlenbeck process [1–5] in Section 2. A common use of this process is as spacetime colored noise: in the same way as the standard Ornstein–Uhlenbeck stochastic differential equation is used as an auxiliary equation to add colored noise to an ordinary differential equation, the linear stochastic PDE can be used to generate noise with non-delta function correlations in both space and time. For the purposes of this paper, the stochastic PDE is convenient because the initial value problem can be solved analytically in finite differences and in the continuum limit. A Fourier transform in space separates the stochastic PDE into a series of uncoupled SDEs for the Fourier coefficients.

In Section 3, we consider nonlinear stochastic PDEs in one space dimension. Exact calculation, including the lowest-order corrections due to finite grid spacing, is possible for a class of equations that has a steady state density. This class includes stochastic PDEs with nonlinear coherent structures known as kinks.

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2. Linear stochastic PDEs

We consider the following stochastic PDE

$$\mathrm{d}\mathbf{Y}_t(x) = -g\mathbf{Y}_t(x)\,\mathrm{d}t + \sum_{i=1}^{m} \frac{\partial^2}{\partial x_i^2}\mathbf{Y}_t(x)\,\mathrm{d}t + \epsilon\,\mathrm{d}\mathbf{W}_t(x). \tag{1}$$

We take g to be a positive constant, and solve (1) as an initial value problem on $x \in \mathcal{D} = [0, L]^m$, with $L \gg 1$. With initial data $\mathbf{Y}_0(x)$, the solution of (1) can be written [1–5]:

$$\mathbf{Y}_t(x) = \int_{\mathcal{D}} \mathrm{d}^m v\, G(t,0,x,v)\mathbf{Y}_0(v) + \epsilon \int_0^t \mathrm{d}\mathbf{W}_s(v) \int_{\mathcal{D}} \mathrm{d}^m v\, G(t,s,x,v), \tag{2}$$

where $\langle \mathrm{d}\mathbf{W}_t(x)\mathrm{d}\mathbf{W}_t(x')\rangle = \delta(x-x')\,\mathrm{d}t$ and

$$G(t,s,x,v) = \frac{1}{(4\pi(t-s))^{\frac{m}{2}}}\, \mathrm{e}^{-|x-v|^2/4(t-s)}\mathrm{e}^{-g(t-s)}. \tag{3}$$

The analytical solution (2) gives an explicit separation into transient and steady-state solution: the first term on the right-hand-side of (2), the transient, is an ordinary integral over the initial data and is proportional to e^{-gt}. The second term is a space-time stochastic integral; for each t and x, it is a Gaussian random variable with mean 0 and variance that approaches a constant value for $t \to \infty$.

For a fixed time, the spatial properties of the Gaussian random field $\mathbf{Y}$ are characterized by the correlation function $c(r)$, the mean value of the product of the field measured at two positions:

$$c(r) = \lim_{t\to\infty} \langle \mathbf{Y}_t(x)\mathbf{Y}_t(y)\rangle. \tag{4}$$

Because the processes of interest in this work have the property of invariance under spatial translation, the correlation function depends on $r = |x - y|$ only. It can be evaluated directly from the analytical solution (2) [7,9]:

$$c(r) = \frac{\epsilon^2}{4\sqrt{g}}\mathrm{e}^{-|r|\sqrt{g}} \qquad m = 1; \tag{5}$$

$$= \frac{\epsilon^2}{4\pi} K_0(\sqrt{g}r) \qquad m = 2; \tag{6}$$

$$= \frac{\epsilon^2}{2\pi|r|}\mathrm{e}^{-|r|\sqrt{g}} \qquad m = 3; \tag{7}$$

$$= \frac{2\epsilon^2}{(2\pi)^{m/2}} \frac{\sqrt{g}}{|r|}^{m/2-1} K_{m/2-1}\big(\sqrt{g}|r|\big) \qquad m > 3. \tag{8}$$

(K_m is the modified Bessel function of order m.) For $m > 1$, $c(0)$ is infinite. It is also possible to calculate $\langle \mathbf{Y}_t(x)\mathbf{Y}_s(v)\rangle$ [11].

2.1. Solution by Fourier transform

Let the Fourier coefficients be defined by

$$\widehat{\mathbf{Y}}_t(k) = L^{-m/2} \int_{-\infty}^{\infty} \mathrm{d}^m x\, \mathrm{e}^{\mathrm{i}kx\frac{2\pi}{L}}\, \mathbf{Y}_t(x), \tag{9}$$

where the integral is taken over the domain $[0, L]^m$. Here $k = (k_1, k_2, \dots, k_m)$, each $k_i = \dots -2, -1, 0, 1, 2, \dots$ and $kx = k_1x_1 + k_2x_2 + \cdots + k_mx_m$. For $k \neq 0$, $\widehat{\mathbf{Y}}_t(k)$ is a stochastic process with values in $\mathbb{C}$ satisfying the following SDE

$$\mathrm{d}\widehat{\mathbf{Y}}_t(k) = \bigl(-g - \kappa^2\bigr)\widehat{\mathbf{Y}}_t(k)\,\mathrm{d}t + \frac{\epsilon}{\sqrt{2}}\,\mathrm{d}\widehat{\mathbf{W}}_t(k), \tag{10}$$

where $\kappa = \frac{2\pi}{L}k$ and

$$\bigl\langle \mathrm{d}\widehat{\mathbf{W}}^*(k)\mathrm{d}\widehat{\mathbf{W}}_t(k')\bigr\rangle = 2\delta(k-k')\,\mathrm{d}t. \tag{11}$$

Since $\mathbf{Y}_t(x)$ is real-valued, $\widehat{\mathbf{Y}}_t(-k) = \widehat{\mathbf{Y}}_t^*(k)$. The process $\widehat{\mathbf{Y}}_t(0)$ is real valued and satisfies

$$\mathrm{d}\widehat{\mathbf{Y}}_t(0) = -g\widehat{\mathbf{Y}}_t(0)\,\mathrm{d}t + \epsilon\,\mathrm{d}\widehat{\mathbf{W}}_t(0). \tag{12}$$

Thus

$$\bigl\langle |\widehat{\mathbf{Y}}_t(k)|^2\bigr\rangle_{t\to\infty} \to \frac{\epsilon^2}{2}\bigl(g + \kappa^2\bigr)^{-1}. \tag{13}$$

The correlation function (4) can be obtained using (13)

$$c(r) = \frac{1}{2}\frac{\epsilon^2}{(2\pi)^m}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}\kappa r}}{g+\kappa^2}\,\mathrm{d}^m\kappa. \tag{14}$$

2.2. *Finite differences method*

The finite differences method consists of approximating the infinite dimensional system (1) by N^m ordinary SDEs on a grid of equally-spaced points in $[0, L]^m$. The SDE at position x is

$$\mathrm{d}\boldsymbol{\Upsilon}_t(x) = -g\boldsymbol{\Upsilon}_t(x)\,\mathrm{d}t + \rho\,\tilde{\Delta}\boldsymbol{\Upsilon}_t(x)\,\mathrm{d}t + \rho^{m/4}\epsilon\,\mathrm{d}\mathbf{W}_t(x), \tag{15}$$

where $\langle \mathrm{d}\mathbf{W}_t(x)\mathrm{d}\mathbf{W}_t(x')\rangle = \delta_{x-x'}\,\mathrm{d}t$,

$$\rho = \left(\frac{N}{L}\right)^2 \quad \text{and} \quad \tilde{\Delta}\boldsymbol{\Upsilon}_t(x) = \sum_{x'}\boldsymbol{\Upsilon}_t(x') - 2m\boldsymbol{\Upsilon}_t(x), \tag{16}$$

with the sum over the $2m$ nearest neighbors of x. The distance between neighboring points on the lattice is $\Delta x = \rho^{-1/2}$.

Constraints on time-stepping in the finite differences method arise from the Lax criterion for stability [12,13]. These can be alleviated by using semi-implicit timestepping methods [14] or, for the linear stochastic PDE (1), by generating a solution in Fourier space [15,16]. (However, the finite differences method is more easily adapted to nonlinear stochastic PDEs.) The timestepping algorithm used to generate the figures in this work is the stochastic analogue of the second-order Runge–Kutta method [17–19].

In one space dimension, we examine the behaviour of $\langle \boldsymbol{\Upsilon}_t(x)^2\rangle$ as a function of Δx by taking the discrete Fourier transform:

$$\widehat{\boldsymbol{\Upsilon}}_t(k) = N^{-1/2}\sum_x \boldsymbol{\Upsilon}_t(i)\mathrm{e}^{\mathrm{i}kx2\pi/L}, \quad k = -\frac{N}{2}\dots\frac{N}{2}-1. \tag{17}$$

The imaginary parts of $\widehat{\boldsymbol{\Upsilon}}_t(0)$ and $\widehat{\boldsymbol{\Upsilon}}_t(N/2)$ are zero. The remainder of the $\widehat{\boldsymbol{\Upsilon}}_t(k)$ satisfy

$$\mathrm{d}\widehat{\boldsymbol{\Upsilon}}_t(k) = -\lambda(k)\widehat{\boldsymbol{\Upsilon}}_t(k)\,\mathrm{d}t + \rho^{1/4}\frac{1}{\sqrt{2}}\epsilon\,\mathrm{d}\widehat{\mathbf{W}}_t(k), \tag{18}$$

where $\lambda(k) = g + 2\rho(1 - \cos\frac{2\pi}{N}k)$. Thus

$$\big\langle|\widehat{\boldsymbol{\Upsilon}}_t(k)|^2\big\rangle_{t\to\infty} = \frac{\rho^{1/2}}{2}\frac{\epsilon^2}{\lambda(k)}. \tag{19}$$

Let $C(0) = \langle \boldsymbol{\Upsilon}_t(x)^2\rangle$. Then

$$\begin{aligned} C(0) &= \frac{1}{N}\sum_{k=-N/2}^{N/2-1}|\widehat{\boldsymbol{\Upsilon}}_t(k)|^2 = \frac{\epsilon^2}{2}\rho^{1/2}\frac{1}{N}\sum_{k=-N/2}^{N/2-1}\lambda(k)^{-1} \\ &= \frac{\epsilon^2\rho^{1/2}}{2}\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{1}{g+\rho(2-2\cos x)}\,\mathrm{d}x = \frac{\epsilon^2}{4\sqrt{g}}\frac{1}{\sqrt{1+g/4\rho}} \qquad (20) \\ &= c(0)\left(1+\frac{g}{4}\Delta x^2\right)^{-1/2} \qquad (21) \end{aligned}$$

In the finite differences method in two space dimensions, (1) is solved on N^2 sites $(x_1, x_2) \in [0, L]^2$. Calculation of $c(0)$ using the discrete Fourier transform [7] yields the estimate

$$C(0) \sim \frac{\epsilon^2}{2\pi}\log\frac{2\pi g^{1/2}}{\Delta x}. \tag{22}$$

Thus $c(0)$ is an increasing function of $(\Delta x)^{-1}$ that does not approach a finite limit.

3. Exact analysis for nonlinear stochastic PDEs

We now consider the stochastic PDE

$$\mathrm{d}\boldsymbol{\phi}_t(x) = f\big(\boldsymbol{\phi}_t(x)\big)\,\mathrm{d}t + \sum_{i=1}^{m}\frac{\partial^2}{\partial x_i^2}\boldsymbol{\phi}_t(x)\,\mathrm{d}t + \left(\frac{2}{\beta}\right)^{1/2}\mathrm{d}\mathbf{W}_t(x), \tag{23}$$

where $\boldsymbol{\phi}_t(x)$ is scalar valued and $f(x)$ is a nonlinear function. A general time-dependent solution cannot be written down, but a steady state solution can be shown to exist under fairly general conditions [10] and can be analyzed using the transfer integral [21–24].

The steady state density of the field at a point (no longer Gaussian) is given as follows. Let ϵ_n and $\psi_n(u)$ be the eigenvalues and corresponding normalized eigenfunctions of the equation

$$\left(-\frac{1}{2\beta^2}\frac{\partial^2}{\partial u^2} + V(u)\right)\psi_n(u) = \epsilon_n\psi_n(u), \tag{24}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}u}V(u) = -f(u) \tag{25}$$

and $n = 0$ corresponds to the eigenfunction with the smallest eigenvalue. Let $R(u) = \frac{\mathrm{d}}{\mathrm{d}u}\mathcal{P}[\boldsymbol{\phi}_t(x) < u]$. Then $R(u) = \psi_0(u)^2$ for $t \to \infty$.

In Fig. 1 we plot the steady state density for the stochastic PDE (23) with the potential $V(u) = -\frac{1}{2}u^2 + \frac{1}{4}u^4$. This double-well potential t configurations with long areas wht the field is close to $+1$ or to -1, sparated by narrow interpolating regions known asnks and antikinks [20].

Thte correlation function of the field $\boldsymbol{\phi}_t(x)$

$$_t(x+r)\boldsymbol{\phi}_t(x)\big\rangle = \sum s_n^2\exp\big(-\beta|r|(\epsilon\ \ -\epsilon\ \ )\big),$$

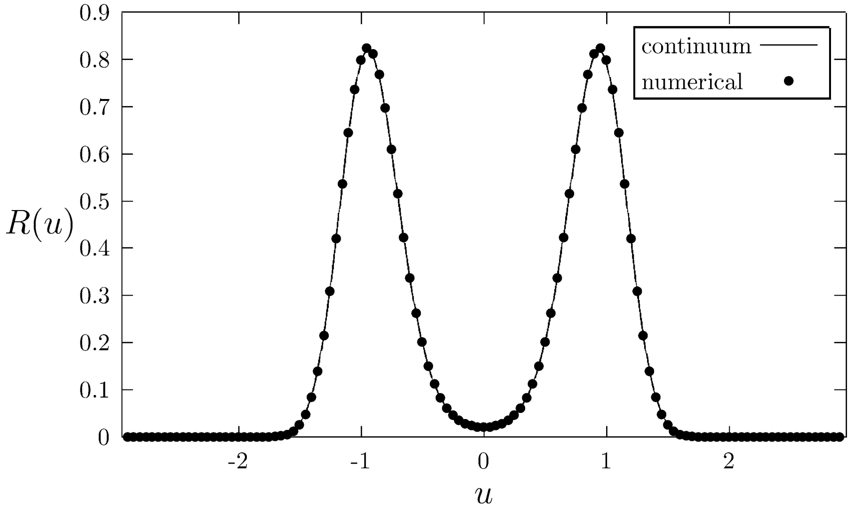

Fig. 1. *Steady state density* $R(u) = \frac{d}{du}\mathcal{P}[\boldsymbol{\phi}_t(x) < u]$, for $\beta = 7$. The solid line is $\psi_0(u)^2$, predicted from the first eigenfunction of (24). The dots are obtained from a numerical histogram, run with grid spacing $\Delta x = 0.2$.

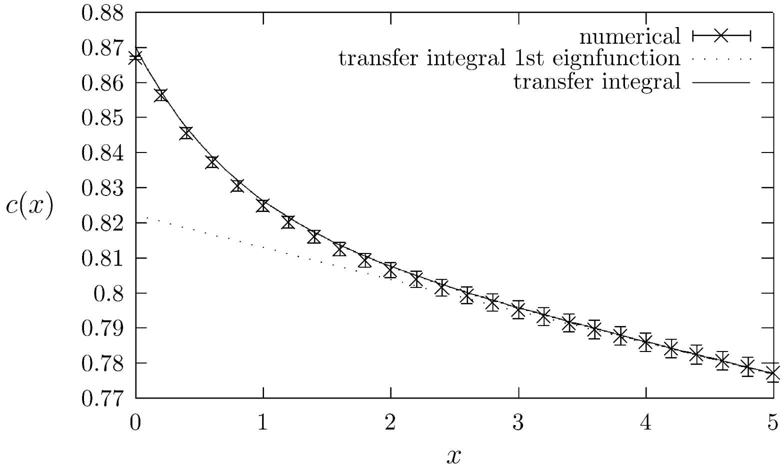

Fig. 2. *Correlation function for* $\beta = 7$. The solid line is $\sum_n s_n^2 \exp(-\beta|r|(\epsilon_n - \epsilon_0))$ and the dotted line is $s_1^2 \exp(-\beta|r|(\epsilon_1 - \epsilon_0))$. The crosses with error bars are numerical results, obtained with $\Delta x = 0.2$.

where $s_n = \int_{-\infty}^{\infty} u\psi_n(u)\psi_0(u)\mathrm{d}u$. For $r \to \infty$, the correlation function is dominated by the exponential term with exponent $\beta(\epsilon_1 - \epsilon_0)$, where ϵ_1 is the next-to-smallest eigenvalue (Fig. 2).

3.1. Correction for finite grid spacing

Eq. (24) can be modified to include powers of Δx^2. The lowest-order correction to the continuum is obtained by replacing the on-site potential $V(u)$ by [23,24]

$$U(u, \Delta x) = V(u) - \frac{\Delta x^2}{24} V'(u)^2. \tag{27}$$

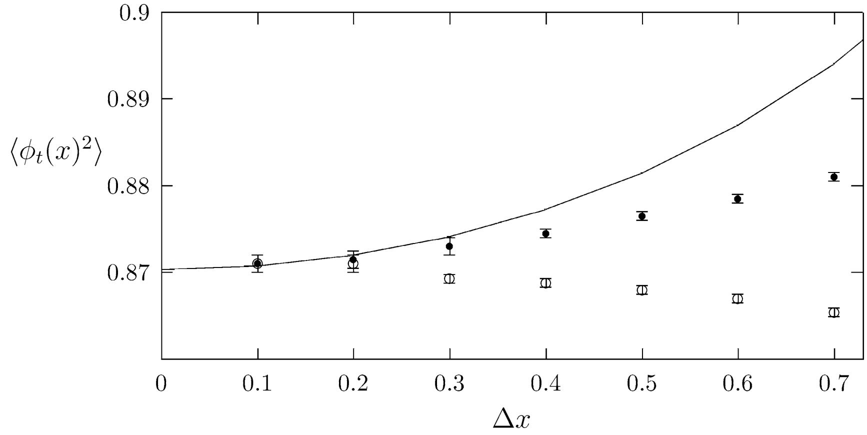

Fig. 3. *Mean squared field versus grid spacing for* $\beta = 7$. The solid line is $\int_{-\infty}^{\infty} u^2 \psi_0(u)^2 \, du$, where the eigenfunction $\psi_0(u)$ is found using the potential (27). The dots with error bars are obtained from numerical runs at finite values of Δx. The circles with error bars are obtained from numerical results where the $f(x)$ in (23) is replaced by $f(x) + \frac{1}{12}\Delta x^2 V'(x)V''(x)$.

The solid line in Fig. 3 shows the effect of this modification on the steady state value of $\langle \boldsymbol{\phi}_t(x)^2 \rangle$. Also shown in Fig. 3 are two series of numerical results. The first is from simulations done using the standard method and coincide with the modified analytical results for sufficiently small Δx. Also shown are the results of a numerical experiment in which the nonlinear function $f(x)$ in (23) is replaced by $f(x) + \frac{1}{12}\Delta x^2 V'(x)V''(x)$ in the numerical timestepping [24]. This correction appears to improve the accuracy of the finite difference discretization.

4. Conclusion

In the finite differences method, independent mean-zero Gaussian random variables are added at each timestep and at each grid point, with variance proportional to the length of the timestep Δt and to $\Delta x^{-m/2}$, where Δx is the distance between grid points and m the number of space dimensions. In one space dimension, the continuum solution takes values in a space of continuous functions. That is, in a fixed realization at a given time, one obtains a configuration that is a continuous function of space. In more than one space dimension, the configurations are not necessarily continuous functions but only distributions [1]. Such stochastic PDEs can be solved on a finite grid of points in space; however the mean squared value at a grid point does not approach a finite limit as the grid spacing is decreased.

References

[1] J.B. Walsh, An introduction to stochastic partial differential equations, in: P.L. Hennequin (Ed.), Ecole d'été de probabilités de St-Flour XIV, Springer, Berlin, 1986, pp. 266–439.
[2] T. Funaki, Nagoya Math. J. 89 (1983) 129–193.
[3] C.R. Doering, Commun. Math. Phys. 109 (1987) 537–561.
[4] G. Da Prato, J. Zabczyk, Stochastic Equations in Infinite Dimensions, Cambridge University Press, Cambridge, 1992.
[5] I. Gyöngy, E. Pardoux, Probab. Theory Relat. Fields 94 (1993) 413–426.
[6] C.R. Doering, in: R. Cerdeira (Ed.), Lectures on Path Integration, World Scientific, Singapore, 1992, pp. 184–214.
[7] G.D. Lythe, Stochastic slow-fast dynamics, PhD thesis, University of Cambridge, 1994.
[8] G. Lythe, Phys. Rev. E 53 (1996) R4271–R4274.
[9] G.D. Lythe, Anales de Fisica 4 (1998) 55–62 (available as http://xxx.lanl.gov/abs/cond-mat/9808242).
[10] W. Gardiner, Handbook of Stochastic Methods, Springer, Berlin, 1990.

[11] P.-M. Lam, D. Bagayoko, Phys. Rev. E 48, 3267–3270.
[12] L. Lapidus, G.F. Pinder, Numerical Solution of Partial Differential Equations in Science and Engineering, Wiley, New York, 1982.
[13] W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling, Numerical Recipes — The Art of Scientific Computing, Cambridge University Press, Cambridge, 1986.
[14] P.D. Drummond, I.K. Mortimer, J. Comput. Phys. 93 (1991) 144–170;
M.J. Werner, P.D. Drummond, J. Comput. Phys. 132 (1997) 312–326.
[15] J. García-Ojalvo, J.M. Sancho, L. Ramírez-Piscina, Phys. Rev. A 46 (1992) 4670–4675.
[16] A. Careta, F. Sagués, J.M. Sancho, Phys. Rev. E 48 (1993) 2279–2287;
J. García-Ojalvo, J.M. Sancho, Phys. Rev. E 49 (1994) 2769–2778.
[17] A. Greiner, W. Strittmatter, J. Honerkamp, J. Stat. Phys. 51 (1988) 95–108.
[18] P.E. Kloeden, E. Platen, Numerical Solution of Stochastic Differential Equations, Springer, Berlin, 1992.
[19] K. Jansons, G. Lythe, J. Stat. Phys. 90 (1998) 227.
[20] S. Habib, G. Lythe, Phys. Rev. Lett. 84 (2000) 1070.
[21] D.J. Scalapino, M. Sears, R.A. Ferrell, Phys. Rev. B 6 (1972) 3409;
J.A. Krumhansl, J.R. Schrieffer, Phys. Rev. B 11 (1975) 3535;
J.F. Currie, J.A. Krumhansl, A.R. Bishop, S.E. Trullinger, Phys. Rev. B 22 (1980) 477.
[22] A. Khare, S. Habib, A. Saxena, Phys. Rev. Lett. 79 (1997) 3797;
S. Habib, A. Khare, A. Saxena, Physica D 123 (1998) 341.
[23] S.E. Trullinger, K. Sasaki, Physica D 28 (1987) 181.
[24] L.M.A. Bettencourt, S. Habib, G. Lythe, Phys. Rev. D 60 (1999) 105 039.