Brownian-Motion Correspondence Method for Obtaining Approximate Solutions to Nonlinear Reaction-Diffusion Equations

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Consideration is given to equations of the form $\partial n/\partial t = D\nabla^2 n + Q(n)$; the reaction-rate $Q(n)$ is such that $d^2Q/dn^2 \le 0$ for all values of $n \ge 0$. A lower bound $n_- = n_-(\vec{x},t) \equiv \langle\gamma\rangle$ ($\le n$) is obtained as the expectation value of the solution to the associated Brownian-motion equation $\partial\gamma/\partial t = -\vec{u}(t)\cdot\nabla\gamma + Q(\gamma)$, where $\gamma = \gamma(\vec{x},t)$ is an auxiliary stochastic variable and the random velocity $\vec{u}(t)$ is Gaussian. An upper bound n_+ ($\ge n$) emerges as a concomitant of n_-, and an approximate analytical solution is shown to be given by $\tilde{n} \equiv \frac{1}{2}(n_- + n_+)$ with the accuracy bound $|n - \tilde{n}| \le \frac{1}{2}(n_+ - n_-)$ expressed analytically.

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Einstein's relationship[1] between Brownian motion and Fourier diffusion has been utilized recently in time-step algorithms for the efficient numerical integration of reaction-diffusion equations.[2] This stochastic representation for diffusive transport appears to be particularly appropriate in the cases of turbulent fluid flows with and without chemical reactions.[3] The purpose of the present communication is to show that the Brownian-motion correspondence for diffusion also enables one to obtain approximate analytical solutions to reaction-diffusion equations of the basic form

$$\partial n/\partial t = D\nabla^2 n + Q(n), \tag{1}$$

where $n = n(\vec{x},t)$ denotes the concentration of a molecular species or the local value of a thermal variable, D is a diffusivity constant, and the reaction-rate function $Q(n)$ is continuous, at least twice-differentiable, and such that

$$d^2Q/dn^2 \le 0 \quad \text{for all } n \ge 0. \tag{2}$$

Examples of reaction-rate functions satisfying (2) are[4]

$$Q(n) = an - bn^{1+\nu}, \tag{3}$$

in which a, b, ν are positive constants, and

$$Q(n) = -kn^2, \tag{4}$$

with k a positive constant. If supplemented with an initial value through unbounded three-dimensional space

$$n(\vec{x},0) \equiv n_0(\vec{x})\,(\ge 0), \tag{5}$$

the solution to (1) can be approximated analytically by considering the associated Brownian-motion (stochastic-convection) equation[5]

$$\partial\gamma/\partial t = -\vec{u}(t)\cdot\nabla\gamma + Q(\gamma). \tag{6}$$

Here $\gamma = \gamma(\vec{x},t)$ is an auxiliary stochastic variable, and the random velocity $\vec{u}(t)$ is Gaussian with zero mean value and a δ-function covariance,

$$\langle u_i(t)\rangle = 0,$$
$$\langle u_i(t')u_j(t'')\rangle = 2D\delta_{ij}\delta(t'-t''). \tag{7}$$

Subject to the initial value (5), the exact solution to (6) is given implicitly by[6]

$$\int_{n_0(\vec{x}-\vec{\xi})}^{\gamma} Q(\lambda)^{-1}d\lambda = t, \tag{8}$$

where $\vec{\xi} = \vec{\xi}(t) \equiv \int_0^t \vec{u}(t')\,dt'$ is Gaussian with zero mean value and the covariance implied by integrating (7),

$$\langle \xi_i(t)\rangle = 0,$$
$$\langle \xi_i(t')\xi_j(t'')\rangle = 2D\delta_{ij}\min\{t',t''\}. \tag{9}$$

That γ given by (8) satisfies (6) is verified by differentiating (8) with respect to t and $\vec{x}$,

$$Q(\gamma)^{-1}\frac{\partial\gamma}{\partial t} - Q(n_0(\vec{x}-\vec{\xi}))^{-1}\frac{\partial}{\partial t}n_0(\vec{x}-\vec{\xi}) = 1, \tag{10}$$

$$Q(\gamma)^{-1}\nabla\gamma - Q(n_0(\vec{x}-\vec{\xi}))^{-1}\nabla n_0(\vec{x}-\vec{\xi}) = 0, \tag{11}$$

and using the formula

$$\frac{\partial}{\partial t}n_0(\vec{x}-\vec{\xi}) = -\vec{u}(t)\cdot\nabla n_0(\vec{x}-\vec{\xi}). \tag{12}$$

My main result is that a rigorous lower bound on n, the exact solution to (1) subject to (5), is given generally by the expectation value of γ:

$$n_- = n_-(\vec{x},t) \equiv \langle\gamma\rangle \leq n. \qquad (13)$$

Proof of (13).—Depending algebraically on $\vec{\xi} = \vec{\xi}(t)$ at the instant of time t, γ can be expressed as

$$\gamma = f(n_0(\vec{x}-\vec{\xi}),t), \qquad (14)$$

where $f(\cdot,t)$ is defined by (8). Since (9) produces $\langle \xi_i(t)\xi_j(t)\rangle = 2Dt\delta_{ij}$ and $\vec{\xi}$ is Gaussian, the expectation value in (13) is given by

$$n_- \equiv \langle\gamma\rangle = (4\pi Dt)^{-3/2}\int \gamma \exp(-|\vec{\xi}|^2/4Dt)\,d^3\xi$$
$$= (4\pi Dt)^{-3/2}\int f(n_0(\vec{y}),t)\exp(-|\vec{x}-\vec{y}|^2/4Dt)\,d^3y \qquad (15)$$

with the introduction of (14). In view of (15), (14), and the time-derivative of (8) for fixed n_0, one obtains

$$\frac{\partial n_-}{\partial t} - D\nabla^2 n_- = (4\pi Dt)^{-3/2}\int \frac{\partial f(n_0(\vec{y}),t)}{\partial t}\exp\left(-\frac{|\vec{x}-\vec{y}|^2}{4Dt}\right)d^3y = \langle Q(\gamma)\rangle. \qquad (16)$$

But with $Q'(n) \equiv dQ/dn$, one has

$$Q(\gamma) \leq Q(\langle\gamma\rangle) + (\gamma - \langle\gamma\rangle)Q'(\langle\gamma\rangle) \qquad (17)$$

as a consequence of condition (2), and hence

$$\langle Q(\gamma)\rangle \leq Q(\langle\gamma\rangle). \qquad (18)$$

Thus (16) and (18) yield the differential inequality

$$\partial n_-/\partial t \leq D\nabla^2 n_- + Q(n_-) \qquad (19)$$

from which (13) follows as a consequence of $n_-(\vec{x},0) = n_0(\vec{x})$ and a well-known maximum principle.[7]

An analytically simple upper bound $n_+ = n_+(\vec{x},t)(\geq n)$, defined implicitly by

$$\int_{\bar{n}_0}^{n_+} Q(\lambda)^{-1}d\lambda = t \qquad (20)$$

with

$$\bar{n}_0 \equiv \langle n_0(\vec{x}-\vec{\xi})\rangle, \qquad (21)$$

emerges as a concomitant of the lower bound n_- defined by (8) and (13). To see that $n_+ \geq n$, one notes that the quantity (21) satisfies the linear diffusion equation

$$\partial\bar{n}_0/\partial t = D\nabla^2\bar{n}_0. \qquad (22)$$

Hence, the derivatives of (20) with respect to t and $\vec{x}$ combine to produce

$$\frac{\partial n_+}{\partial t} - D\nabla^2 n_+ - Q(n_+) = DQ(n_+)^{-1}[Q'(\bar{n}_0) - Q'(n_+)]|\nabla n_+|^2. \qquad (23)$$

The right-hand side of (23) is nonnegative as a consequence of (2) and the positive character of (20) for $t>0$, for (20) implies $n_+ > \bar{n}_0$ for $Q(\lambda)>0$ and $n_+ < \bar{n}_0$ for $Q(\lambda)<0$.[6] Therefore (22) yields the differential inequality

$$\partial n_+/\partial t \geq D\nabla^2 n_+ + Q(n_+) \qquad (24)$$

from which $n_+ \geq n$ follows as a consequence of $n_+(\vec{x},0) = n_0(\vec{x})$ and a maximum principle.[7]

Owing to the correspondence between (8) and (20), the upper bound n_+ can also be expressed in terms of the function introduced in (14):

$$n_+ = f(\bar{n}_0,t). \qquad (25)$$

An approximate solution to (1) subject to (5) is given by the arithmetic average of the lower and upper bounds,

$$\tilde{n} \equiv \tfrac{1}{2}(n_- + n_+), \qquad (26)$$

for it follows from $n_- \leq n \leq n_+$ that

$$|n-\tilde{n}| \leq \frac{1}{2}(n_+ - n_-)$$
$$= \tfrac{1}{2}[f(\bar{n}_0,t) - \langle f(n_0(\vec{x}-\vec{\xi}),t)\rangle] \qquad (27)$$

where (15) is recalled. Hence, the global accuracy of the approximation $n \cong \tilde{n}$ can be determined for all $\vec{x}$ and $t \geq 0$ by evaluating the final member of (27) for prescribed $Q(n)$ and $n_0(\vec{x})$.

Consider as an example the reaction-rate expression (4), for which (8) yields

$$\gamma = [n_0(\vec{x}-\vec{\xi})^{-1} + kt]^{-1}$$
$$\equiv f(n_0(\vec{x}-\vec{\xi}),t) \qquad (28)$$

and the quantities (15) and (20) are

$$n_- = (4\pi Dt)^{-3/2}\int [n_0(\vec{y})^{-1} + kt]^{-1}\exp(-|\vec{x}-\vec{y}|^2/4Dt)\,d^3y$$
$$= \bar{n}_0 - (4\pi Dt)^{-3/2}\int [n_0(\vec{y}) + (kt)^{-1}]^{-}n_0(\vec{y})^2\exp(-|\vec{x}-\vec{y}|^2/4Dt)\,d^3y \tag{29}$$

$$n_+ = (\bar{n}_0^{-1} + kt)^{-1}, \tag{30}$$

with

$$\bar{n}_0 = (4\pi Dt)^{-3/2}\int n_0(\vec{y})\exp(-|\vec{x}-\vec{y}|^2/4Dt)\,d^3y \tag{31}$$

according to (21). By subtracting (29) from (30), the final member of (27) is obtained as

$$\tfrac{1}{2}(n_+ - n_-)$$
$$= \tfrac{1}{2}kt\{(4\pi Dt)^{-3/2}\int [1 + ktn_0(\vec{y})]^{-1}n_0(\vec{y})^2\exp(-|\vec{x}-\vec{y}|^2/4Dt)\,d^3y - (1+kt\bar{n}_0)^{-1}\bar{n}_0^2\}. \tag{32}$$

Since the curly-bracketed expression is asymptotic to $2Dt|\nabla n_0(\vec{x})|^2$ for small t, the right-hand side of (32) is generally of $O(t^2)$ for small t. One must fix the initial value (5) in order to evaluate the accuracy bound (32) for larger values of t. In particular, in cases for which $n_0(\vec{x}) \geq n_{\min}(\equiv$ positive const), it follows from (31) that $\bar{n}_0 \geq n_{\min}$ for all $\vec{x}$ and t; thus (29), (30) and (26) are asymptotic to $(kt)^{-1}$ for large t, while the right-hand side of (32) is asymptotic to a quantity of $O(t^{-2})$, i.e., $\frac{1}{2}(kt)^{-2}[\langle n_0(\vec{x}-\vec{\xi})^{-1}\rangle - \bar{n}_0^{-1}]$.

As an example of a practical application of (26), consider the diffusion and recombination of a very large number N of free radicals which are distributed uniformly within a sphere of radius r_0 at $t=0$,

$$n_0(\vec{x}) = \begin{cases} 3N/4\pi r_0^3 & \text{for } |\vec{x}| = r \leq r_0, \\ 0 & \text{for } r > r_0, \end{cases} \tag{33}$$

and have a distribution governed by (1) with (4) for $t > 0$.[8] The integral in (31) is evaluated in the case of (33) to yield $\bar{n}_0 = (3N/4\pi r_0^3)\mathscr{F}$ where the positive function $\mathscr{F} = \mathscr{F}(r,t)\,(\leq 1)$ is given by[9]

$$\mathscr{F} = \tfrac{1}{2}\left[\operatorname{erf}\left(\frac{r_0 - r}{2(Dt)^{1/2}}\right) + \operatorname{erf}\left(\frac{r_0 + r}{2(Dt)^{1/2}}\right)\right] + \left(\frac{Dt}{\pi}\right)^{1/2} r^{-1}\left[\exp\left(-\frac{(r_0+r)^2}{4Dt}\right) - \exp\left(-\frac{(r_0-r)^2}{4DT}\right)\right]. \tag{34}$$

Since the quantities (29) and (30) are obtained as $n_- = [(4\pi r_0^3/3N) + kt]^{-1}\mathscr{F}$ and $n_+ = [(4\pi r_0^3/3N\mathscr{F}) + kt]^{-1}$, an upper bound on the fractional error in (26) follows from (27) as

$$|n - \tilde{n}|/\tilde{n} \leq (n_+ - n_-)/(n_+ + n_-) = kt(1-\mathscr{F})[(8\pi r_0^3/3N) + kt(1+\mathscr{F})]^{-1}. \tag{35}$$

Subject to desired accuracy, the fractional error bound (35) delineates the (r,t) values for guaranteed usefulness of the approximation $n \cong \tilde{n}$; high accuracy is attained for all r with $t \ll (8\pi r_0^3/3Nk)$ and for (r,t) values such that $\mathscr{F}$ given by (34) is close to unity.

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[5] For an introduction to the mathematical theory of Brownian motion, see: *Selected Papers on Noise and Stochastic Processes,* edited by N. Wax (Dover, New York, 1954). The "white noise" $\vec{u}(t)$ in (6) is employed here in the manner

of R. L. Stratonovich, *Conditional Markov Processes and Their Application to the Theory of Optimal Control* (American Elsevier, New York, 1968), pp. 42–49, 234, 290.

[6]The ordinary Riemann integral (8) features the stochastic quantity $\vec{\xi}$ in its lower limit, but it is unrelated to the stochastic integral of Itô [discussed, e.g., by H. P. McKean, *Stochastic Integrals* (Academic, New York, 1969)]. If $Q(\lambda)$ possesses a zero for some positive value of λ [e.g., as in (3)], then condition (2) guarantees that the associated singularity in $Q(\lambda)^{-1}$ is nonintegrable. Hence, $Q(\lambda)$ is either positive or negative for all λ in (8).

[7]M. H. Protter and H. F. Weinberger, *Maximum Principles in Differential Equations* (Prentice-Hall, Englewood Cliffs, N. J., 1967), p. 187.

[8]A version of this recombination-diffusion problem with different boundary conditions has been treated numerically by E. P. Gray and D. E. Kerr, Ann. Phys. (N.Y.) **17**, 276 (1962).

[9]The error function or probability integral is defined as $\mathrm{erf}(x) = 2\pi^{-1/2}\int_0^x \exp(-\alpha^2)\,d\alpha$.