Equation-free dynamic renormalization: Self-similarity in multidimensional particle system dynamics

Yu Zou and Ioannis Kevrekidis*
Department of Chemical Engineering and Program in Applied and Computational Mathematics, Princeton University, Princeton, New Jersey 08544, USA

Roger Ghanem
Department of Civil Engineering, The University of Southern California, Los Angeles, California 90089, USA
(Received 17 May 2005; published 3 October 2005)

We present an equation-free dynamic renormalization approach to the computational study of coarse-grained, self-similar dynamic behavior in multidimensional particle systems. The approach is aimed at problems for which evolution equations for coarse-scale observables (e.g., particle density) are not explicitly available. Our illustrative example involves Brownian particles in a 2D Couette flow; marginal and conditional inverse cumulative distribution functions (ICDFs) constitute the macroscopic observables of the evolving particle distributions.

DOI: 10.1103/PhysRevE.72.046702 PACS number(s): 11.10.Gh

I. INTRODUCTION

Multiscale phenomena arise naturally in science and engineering. In many cases of current research interest, physical models are available at a *fine, microscopic* scale (atomistic, stochastic, agent-based), while we want to study the system behavior at a *coarse-grained, macroscopic* level. Macroscopic, coarse-grained evolution equations, even when they *conceptually exist* are often unavailable in closed form, due to the lack of accurate explicit closures. The *equation-free* computational framework [1–4] has been recently proposed for the computer-assisted study of precisely such complex, multiscale problems: those for whose macroscopic behavior no *explicit* coarse-grained evolution equations are available. Equation-free methods utilize so-called coarse time steppers, which are used to numerically analyze coarse-grained behavior through appropriately designed short computational experiments performed by the fine-scale models; coarse time stepping is closely related to optimal prediction in the work of Chorin and coworkers [5,6] (see also the discussion in [7]). Quantities necessary for traditional continuum numerical analysis (residuals, the action of Jacobians) are *estimated on demand* from these short fine-scale computational experiments, rather than evaluated from closed-form macrosopic equations. This computational "enabling technology" has been used to perform integration, fixed-point computation, numerical stability and bifurcation analysis as well as control and optimization for the coarse-grained behavior of a number of fine-scale model types (lattice Boltzmann, Monte Carlo, molecular dynamics, Brownian dynamics, etc., see the references in [2,3]).

For problems whose macroscopic behavior is characterized by *scale invariance*, dynamic renormalization methods [8,9] provide tools for locating self-similar solutions and their scaling exponents [10,11]. Recently, we have combined equation-free computation with dynamic renormalization to obtain coarse-grained self-similar solutions based on direct microscopic simulation [12,13]; our particular implementation used a template-based approach [14–17]. Working in a frame of reference that expands (or shrinks) along with the macroscopic system observables turns the self-similar problem into a steady state one, for which fixed-point techniques can be applied. Equation-free dynamic renormalization techniques are used here to investigate macroscopic self-similarity in multidimensional particle system dynamics. This is made possible through a coarse time stepper which utilizes marginal and one-dimensional conditional inverse cumulative distribution functions (ICDFs) as the coarse observables of multidimensional particle systems. Our illustrative example consists of the (self-similar) dynamics of Brownian particles in a Couette flow; the results are validated using known analytical solutions. The paper is organized as follows: we start with a brief description of the coarse time stepper in our framework. We then discuss equation-free dynamic renormalization, present our illustrative example, demonstrate the computation of its self-similar shapes and exponents, and conclude with a brief discussion of limitations and possible extensions of the approach.

II. A COARSE TIME STEPPER FOR MULTIDIMENSIONAL PARTICLE SYSTEMS

In the equation-free framework, short, appropriately initialized computational experiments with a fine-scale model are used to construct the coarse time stepper—the basic element capturing the dynamical interaction between coarse-scale observables and fine-scale model states. There are essentially three components in a coarse time stepper, namely, *lifting, fine-scale evolution*, and *restriction* [1] (Fig. 1). Lifting is a transformation that converts coarse-scale observables to one or more consistent fine-scale realizations;

*Electronic address: yannis@princeton.edu

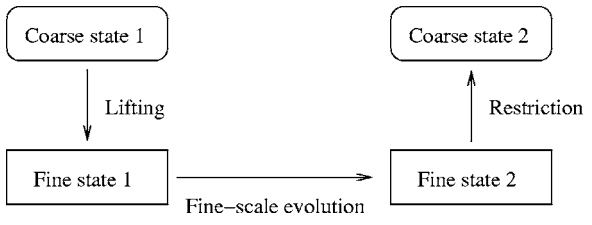

FIG. 1. Schematic of the coarse time stepper.

restriction is the transformation in the reverse direction, from fine-scale states to coarse observables. The specific manner in which these lifting and restriction operators are implemented yields different interscale exchange protocols; one must test that the results at the macroscopic level are relatively insensitive to small details in the protocols (see the discussion in [3]).

In macroscopically multidimensional particle systems, particle positions are a natural component of the fine-scale state, and marginal and conditional ICDFs of particle positions are good candidate coarse-scale observables. Assuming smoothness, a finite number of marginal and conditional ICDFs can be used to recover the distribution of particle positions (e.g., through interpolation). *Our coarse observables are the leading coefficients of the projection of these ICDFs on an appropriate orthonormal (shifted Legendre) polynomial basis*. Particle positions in one direction are generated using the marginal ICDF, and the corresponding particle positions in the second direction are generated using the conditional ICDFs in our lifting step. For the restriction step, after constructing a smooth multidimensional CDF from particle positions by simple interpolation, marginal and conditional CDFs are first obtained, and then their inverse CDFs are interpolated and their leading expansion coefficients computed.

III. EQUATION-FREE DYNAMIC RENORMALIZATION

For many macroscale systems of practical interest, if the partial differential equations (PDEs) describing their evolution are scale invariant, they may possess self-similar solutions [10,11]. Dynamic renormalization procedures have been used for the study of such self-similar solutions [8,9,18]; recently the template-based method for studying the dynamics of problems with symmetry [16] has been extended to study the dynamics of problems with scale invariance [14,15,17]. When scale invariant evolution PDEs are explicitly available, a template-based approach can be used to derive dynamical equations (termed "MN-dynamics") for the renormalized self-similar solutions and similarity exponents [14]. The idea underlying this approach, especially that of employing template conditions, can be used to obtain renormalized self-similar solutions and similarity exponents in systems whose macroscale governing equations are not explicitly available [12] (see also the approach in [19]).

Consider a PDE of the form

$$\frac{\partial F}{\partial t} = D_{xy}(F), \tag{1}$$

where $F(x,y,t)$ is a CDF of particle positions. We assume that for the differential operator D_{xy} there exist constants p and a such that

$$D_{xy}\left(f\left(\frac{x}{A},\frac{y}{A^p}\right)\right) = A^a D_{uv}(f(u,v)), \quad u=\frac{x}{A}, \quad v=\frac{y}{A^p} \tag{2}$$

for any real function f, real value $A>0$, and coordinate (x,y) (there is no amplitude rescaling since this is a CDF). If a self-similar solution $F(x,y,t)$ exists, it can be written as

$$F(x,y,t) = U\left(\frac{x}{(cs)^{\alpha}},\frac{y}{(cs)^{\alpha p}};c\right), \tag{3}$$

where c is a constant parametrizing the family of renormalized shapes, and $s=t-t_0$ (t_0 is the blowup time for problems with finite time singularities, whether forward or backward in time).

Therefore,

$$\alpha a = -1, \tag{4}$$

and U satisfies the PDE,

$$-\alpha u U_u - \alpha p v U_v = c^{-1} D_{uv}(U), \tag{5}$$

where $u=x/(cs)^{\alpha}$, $v=y/(cs)^{\alpha p}$. For D_{xy} satisfying Eq. (2), the constant a is determined by D_{xy} itself and the similarity exponent α can be obtained by Eq. (4).

If the equation is not explicitly available, one cannot analytically obtain the exponents a and p; tests have to be devised for finding these constants—and thus testing the scale invariance of the operator—before we embark upon the computation of the self-similar solutions themselves.

For D_{xy} satisfying the (unknown) Eq. (2), the constants p and a can be obtained *using a black box simulator* of the equation as follows: Since the unknown Eq. (2) is valid for *any* real function f, let f be a test function, and let us choose the two points (u_1,v_1) and (u_2,v_2) and let $(x_1,y_1)=(u_1A,v_1A^p)$ and $(x_2,y_2)=(u_2A,v_2A^p)$, where A is arbitrarily chosen as a positive real value. Then the following two relations should hold for essentially arbitrary test functions $f(x,y)$ and points $(u_i,v_i), i=1,2$:

$$D_{xy}\left(f\left(\frac{x}{A},\frac{y}{A^p}\right)\right)(x_1,y_1) = A^a D_{uv}(f(u,v))(u_1,v_1),$$

$$D_{xy}\left(f\left(\frac{x}{A},\frac{y}{A^p}\right)\right)(x_2,y_2) = A^a D_{uv}(f(u,v))(u_2,v_2). \tag{6}$$

Comparing the above two equations, we have

$$\frac{D_{xy}\left(f\left(\frac{x}{A},\frac{y}{A^p}\right)\right)(x_1,y_1)}{D_{xy}\left(f\left(\frac{x}{A},\frac{y}{A^p}\right)\right)(x_2,y_2)} = \frac{D_{uv}(f(u,v))(u_1,v_1)}{D_{uv}(f(u,v))(u_2,v_2)}. \tag{7}$$

Equation (7) is solved (using Newton's method) for the constant p. When D_{xy} is not explicitly available, $D_{xy}(f(x,y))$ can

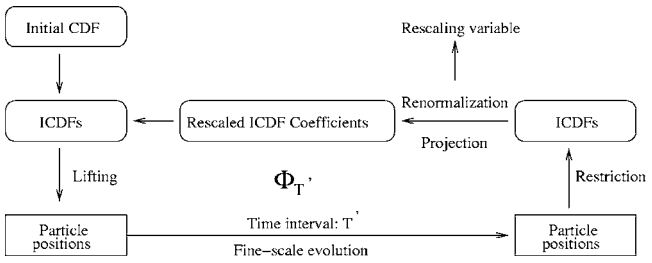

FIG. 2. Illustration for the coarse renormalization.

be obtained by running the microsimulator for a short time and numerically estimating the derivative $\partial f/\partial t$. Given p, the constant a is calculated by

$$a = \log_A \frac{D_{xy}\left(f\left(\frac{x}{A}, \frac{y}{A^p}\right)\right)(x_1, y_1)}{D_{uv}(f(u,v))(u_1, v_1)}. \tag{8}$$

Clearly, other test functions, as well as conditions evaluated at other points (or nonlocal versions of the conditions) can be used; care must be taken also to ensure the finiteness of the estimated quantities.

Given a and p, to determine the self-similar shape of the solution, we consider the general scaling

$$F(x,y,t) = \omega\left(\frac{x}{A(t)}, \frac{y}{A(t)^p}, t\right), \tag{9}$$

where $A(t)$ is an unknown function. The PDE becomes

$$\omega_t - \frac{A_t}{A} u \omega_u - \frac{pA_t}{A} v \omega_v = A^a D_{uv}(\omega). \tag{10}$$

Evidently, U and ω are both rescaled CDFs.

The main idea of dynamic renormalization is to solve Eq. (10) in a "co-exploding" or "co-collapsing" frame by tracking the changes in the *shape* of the solution ω as well as the *scale factor* $A(t)$. This effective decoupling of the shape evolution from the scale evolution is implemented with the help of so-called *template conditions* [16]. Keeping these conditions satisfied [along with Eq. (10)] dictates the evolution of the scale factor (along with the solution shape). In this paper, we choose our template condition to be

$$\omega(e, \infty, t) = m, \quad e < 0, \ 0 < m < 0.5, \tag{11}$$

where e and m are both (essentially arbitrary) constants. Imposing this template condition has the following physical meaning: as the solution evolves both in shape and scale, it is constantly rescaled *so that the template condition remains satisfied*: the u coordinates corresponding to the constantly rescaled marginal CDF $\omega_U = m$ have the same value e for all t. There are no great restrictions in the choice of template functions (see the discussion in [15] as well as different template choices in [12]); later in this paper, we allow our template to vary by changing the value of e.

Applying this template to Eq. (10) and assuming $\partial\omega/\partial v(e, v, t)$ decays exponentially as $v \to \infty$, we have

TABLE I. Iterations in the computation of the constants p and a.

No. of iterations	p	a
0	6.0	−3.862 87
1	2.794 41	−1.830 47
2	2.978 49	−1.979 27
3	3.001 32	−2.001 14
4	2.998 04	−1.997 32
5	2.996 70	−1.996 12
6	2.994 41	−1.996 75
7	2.993 43	−1.991 13
8	2.994 00	−1.994 59

$$A_t e \frac{\partial \omega}{\partial u}(e, \infty, t) + A^{a+1} D_{uv}(\omega)(e, \infty, t) = 0. \tag{12}$$

Equations (10) and (12) are solved for the rescaled CDF $\omega(u, v, t)$ and rescaling variable $A(t)$ if the operator D_{xy} is explicitly known. As the time $t \to \infty$, ω may approach a steady state, which is a stable self-similar shape for the solutions to Eq. (1).

The value for α can be calculated in the long-time limit (i.e., after ω reaches steady state). Indeed, let t_1 and t_2 be distinct times after ω reaches the steady state, then

$$\alpha = \frac{t_2 - t_1}{\frac{A(t_2)}{A_t(t_2)} - \frac{A(t_1)}{A_t(t_1)}}. \tag{13}$$

In many cases, the macroscale equation for the CDF of particle positions may not be explicitly known. However, the template conditions can still be used to renormalize the CDF itself, evolved via microscale models, and rescaling variables are obtained during the course of renormalization. In these cases, a coarse time stepper is employed to evolve the coarse system using the marginal and conditional ICDFs (actually, the leading coefficients of their projection on an appropriate basis) as coarse observables.

The procedure for equation-free renormalization, depicted in Fig. 2, consists of the following six steps: (i) Generate the marginal and conditional ICDFs according to the initial CDF or according to the coefficients of dominant modes of the ICDFs. (ii) Generate particle positions based on these ICDFs using the *lifting* procedure in the coarse time stepper. (iii) Evolve particle positions over a time interval T' using the fine-scale model. (iv) Obtain ICDFs from particle positions using the *restriction* procedure in the coarse time stepper. (v) Rescale the marginal ICDF according to the template condition and obtain the rescaling variable A. We then rescale the conditional ICDFs by A^p [recall that p has been independently computed through Eq. (7)]. This step can be justified by Eq. (9). Indeed, obtaining the rescaled solution ω_{k+1} from ω_k via the dynamics (10) and (12) is equivalent to starting from the initial condition ω_k, running the original dynamics for a while to get F_{k+1}, obtaining the rescaling variable A, and rescaling F_{k+1} by A and A^p respectively in the x and y

directions. (vi) Project the rescaled ICDFs onto the appropriate orthonormal basis and obtain the coefficients of its dominant modes. Go back to step (i).

The above procedure can be viewed as an iterative algorithm to solve for the fixed point of a nonlinear operator $\Phi_{T'}$, written as

$$\alpha - \Phi_{T'}(\alpha) = 0. \tag{14}$$

This fixed point can be written in component form as $\alpha^r_{i,j}, i=1,\ldots,M+1, j=0,\ldots,P$ [12], or

$$\alpha = (\alpha^r_{1,0}, \alpha^r_{1,1}, \ldots, \alpha^r_{1,P}, \alpha^r_{2,0}, \alpha^r_{2,1}, \ldots, \alpha^r_{2,P}, \ldots, \alpha^r_{M+1,0}, \alpha^r_{M+1,1}, \ldots, \alpha^r_{M+1,P})^T,$$

where $\alpha^r_{1,j}, j=0,1,\ldots,P$ stands for the projection of the marginal ICDF onto a jth-order mode; $\alpha^r_{i,j}, i=2,\ldots,M+1; j=0,1,\ldots,P$ is the projection of the $(i-1)$th conditional ICDF onto a jth-order mode; and the superscript r refers to the fact that this is, in fact, the renormalized self-similar shape. These coefficients correspond to the renormalized ICDFs and CDF of the multidimensional particle system. Equation (14) can also be solved using any numerical algorithm such as direct iteration or matrix-free implementations of Newton's method (e.g., Newton-GMRES [20]).

IV. BROWNIAN PARTICLES IN COUETTE FLOW

We now illustrate our computational approach to self-similarity in a two-dimensional Brownian model of particle dispersion in Couette flow [21]. Let $X(t)$ and $Y(t)$ represent particle positions in the x and y directions, respectively, at time t on the plane. The particle positions evolve according to

$$dX(t) = D d\omega_X(t), \quad dY(t) = X dt, \tag{15}$$

where $\omega_X(t)$ is a Wiener process [22] and D is the diffusion coefficient. The discretized dynamics of (15) is given by [23]

$$X_{k+1} = X_k + D\,\eta_{X,k}\sqrt{\Delta t}, \quad Y_{k+1} = Y_k + X_k \Delta t, \tag{16}$$

where $\eta_{X,k}$ are independently and identically distributed standard Gaussian random variables and Δt is the discrete time step.

The dynamics (15) represent the motion of particles *which only diffuse in the x direction* in a Couette flow (see the discussion for both x and y diffusion). It can be shown that the coarse-scale dynamics for the pair distribution function (PDF), $P_{XY}(x,y,t)$, of a particle position, corresponding to the fine-scale dynamics (15), is governed by the following equation [24]:

$$\frac{\partial P_{XY}}{\partial t} + x\frac{\partial P_{XY}}{\partial y} = \frac{D^2}{2}\frac{\partial^2 P_{XY}}{\partial x^2}, \tag{17}$$

where P_{XY} is assumed to be second-order differentiable. Hence the dynamics for the CDF, $F_{XY}(x,y,t)$, associated with (17) is given by

$$\frac{\partial F_{XY}}{\partial t} + x\frac{\partial F_{XY}}{\partial y} - \int_{-\infty}^{x} \frac{\partial F_{XY}}{\partial y} dx = \frac{D^2}{2}\frac{\partial^2 F_{XY}}{\partial x^2}. \tag{18}$$

In the above equation, the operator D_{xy} is written as

$$D_{xy} = -x\frac{\partial}{\partial y} + \int_{-\infty}^{x} \frac{\partial}{\partial y} dx + \frac{D^2}{2}\frac{\partial^2}{\partial x^2}. \tag{19}$$

This operator satisfies the invariance property (2), with constants $p=3$ and $a=-2$.

The analytical self-similar solution to the PDF equation (17) is

$$P_{XY}(x,y,t) = \frac{\sqrt{3}}{\pi D^2 (t-t_0)^2} \times \exp\left[-\left(\frac{6(y-0.5x(t-t_0))^2}{D^2(t-t_0)^3} + \frac{x^2}{2D^2(t-t_0)}\right)\right], \tag{20}$$

where t_0 is the blowup time (forward or backward in time); the corresponding CDF self-similar solution to (18) is

$$F_{XY}(x,y,t) = \frac{\sqrt{3}}{\pi D^2 (t-t_0)^2} \times \int_{-\infty}^{x}\int_{-\infty}^{y} \exp\left[-\left(\frac{6(y-0.5x(t-t_0))^2}{D^2(t-t_0)^3} + \frac{x^2}{2D^2(t-t_0)}\right)\right] dy dx. \tag{21}$$

Let $u' = x/(c(t-t_0))^{1/2}$ and $v' = y/(c(t-t_0))^{3/2}$; then

$$F_{XY}(x,y,t) = F_{UV}(u',v') = \frac{\sqrt{3}}{\pi D^2/c^2} \times \int_{-\infty}^{u'}\int_{-\infty}^{v'} \exp\left[-\left(\frac{6(v-0.5u/c)^2}{D^2/c^3} + \frac{u^2}{2D^2/c}\right)\right] \times dv du. \tag{22}$$

Hence for the integro-differential equation (18), the similarity exponent α in (3) is $\alpha = 1/2$. For the CDF in (22), its standard deviations in two directions and correlation are $\sigma_X = D/c^{1/2}$, $\sigma_Y = D/(\sqrt{3}c^{3/2})$, and $\rho_{XY} = \sqrt{3}/2$, respectively.

V. NUMERICAL RESULTS

We now compute the self-similar solutions *without* the macroscopic equations, based only on the particle simulator.

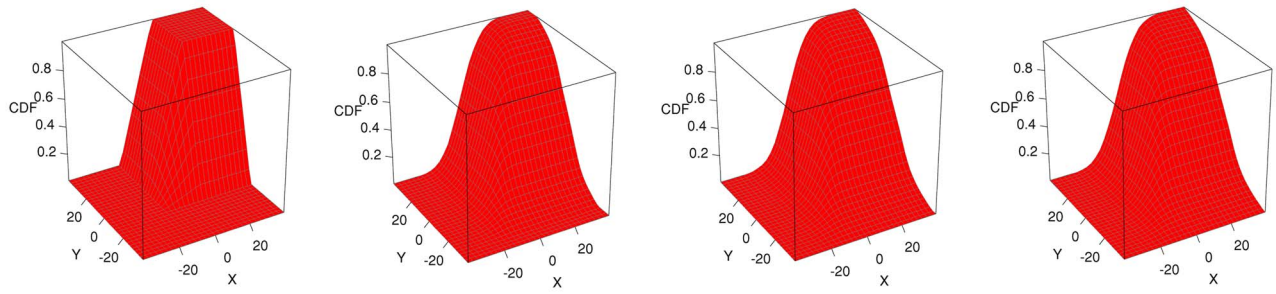

FIG. 3. (Color online) Renormalized CDFs. Top left: initial CDF; top right: renormalized CDF after second iteration; bottom left: renormalized CDF after fourth iteration; bottom right: renormalized CDF after sixth iteration (see text).

The invariance property of the (presumed unavailable) macroscale differential operator D_{xy} has to be established first. Then the fixed-point algorithm is used to solve for the renormalized CDF steady-state shape, and the similarity exponent is computed. The diffusion coefficient D and simulation time step Δt in the fine-scale model are set to 5.0 cm/s$^{1/2}$ and 0.01 s, respectively. An ensemble of 9000 ($N=9000$) particles is typically used in the fine-scale simulations.

Without the macroscale equation (18), we use Newton's method to solve Eq. (7) for p. Our test function f is a two-dimensional joint Gaussian, $f(x,y)=1/4.5^2 N(x/4.5) \times N(y/4.5)$, where $N(x)$ and $N(y)$ are standard Gaussian distributions. The positive real number $A=2.0$. The two coordinates (u_1,v_1) and (u_2,v_2) in (7) are chosen as $(-2.5,-2.5)$ and (3.5,3.5), respectively. To reduce fluctuations of values for the operator D_{xy}, 200 copies of values for D_{xy} and D_{uv} are averaged in the computation.

Starting from the initial value $p_0=6.0$, iterative values for p are stabilized at 3.0 after three iterations. Accordingly, the converged value for a is approximately -2.0 (Table I) (other test functions and test point selections gave similar results).

This suggests that the unavailable differential operator D_{xy} corresponding to the microsimulator (15) does indeed possess the invariance property (2) for constants $p=3.0$ and $a=-2.0$.

To determine the self-similar shape, the template condition for the x direction was chosen as $\omega(-2.266,\infty,t)=0.4$, i.e., the x coordinate corresponding to the renormalized marginal CDF $\omega_U=0.4$ always has the same value, -2.266 cm. For the analytical solution (22) and our template, $c=0.3125$ s^{-1} and the corresponding standard deviations are $\sigma_X=4\sqrt{5}$ cm and $\sigma_Y=12.8\sqrt{15}/3$ cm, respectively.

A uniform particle CDF over the space domain $(-10\text{ cm},10\text{ cm})\times(-10\text{ cm},10\text{ cm})$ is used as the initial condition for our equation-free fixed-point algorithm. Direct iteration is used to solve the fixed point of Eq. (14). The time interval T' is $150\Delta t$. The number of conditional ICDFs is 20 ($M=20$) and the bases for the both types of ICDF are the shifted Legendre polynomials of order up to and including 5 ($P=5$). In this simulation, 200 copies of 5000 particle positions are generated according to the ICDF mode coefficients at the beginning of each iteration and let to evolve for time T'. The mode coefficients at the end of each iteration are obtained by averaging over these 200 copies. After the second, fourth, and sixth iterations, mode coefficients of renormalized ICDFs are used to generate particle positions, out of which the CDFs are computed and plotted respectively in Fig. 3. It can be seen that the renormalized solutions reach a steady state quickly.

To verify the self-similar shape of the solution, the standard deviations and correlation of the simulated self-similar shape are compared with those of the analytical self-similar shape. The standard deviations and correlations of the rescaled CDFs are calculated via the ensemble particle positions corresponding to these CDFs. The comparison is shown in Fig. 4. The standard deviations and correlations of rescaled CDFs approach those of the analytical self-similar shape, which means that the rescaled CDF quickly approaches a member of the family of theoretical self-similar shapes expressed by Eq. (22).

As the renormalized CDF $\omega(u,v,t)$ reaches the steady state, we can set this CDF as the initial condition and run the

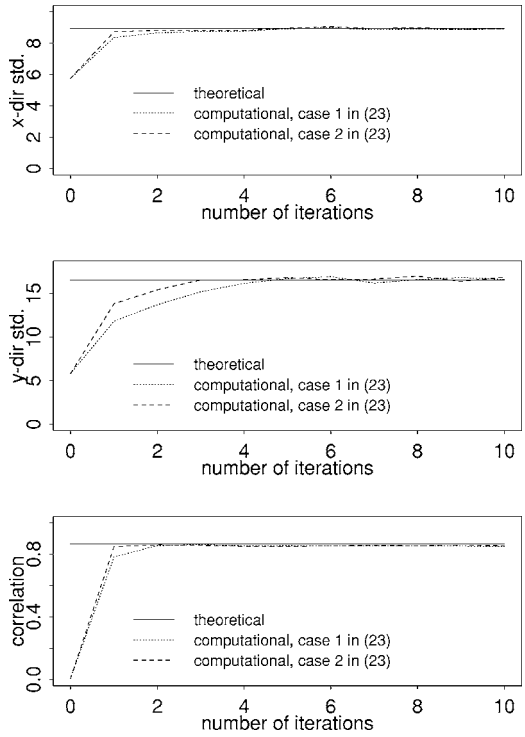

FIG. 4. Computational vs theoretical values for the standard deviations and the correlation of the self-similar shapes. Cases (1), (2) in Eqs. (23a) and (23b) (see text).

TABLE II. Values of the rescaling variable $A(t)$ in Eq. (13).

t (sec)	$A(t)$	$A_t(t)$
0	1.000 00	—
1.5	1.208 72	0.139 15
3.0	1.382 43	0.115 81

microscale dynamics (16) for two more loops with $t_1=150\Delta t$ and $t_2=300\Delta t$. The rescaling variable $A(t)$ is listed in Table II. Note that $A(t)=1$ at $t=0$. By Eq. (13), the similarity exponent α is approximately estimated as 0.461, which is within 8% of the theoretical value 1/2.

We now study the effect of varying templates and reporting horizons in the fixed-point operator $\Phi_{T'}$ on our results; different templates should give different members in the family of Eq. (5), while T' should not affect the computed fixed points.

Four combinations of template condition and evolution times including the one above are investigated as follows: for Case (1)

$$\omega(-2.266,\infty,t)=0.4, \quad T'=150\Delta t, \tag{23a}$$

for Case (2)

$$\omega(-2.266,\infty,t)=0.4, \quad T'=250\Delta t, \tag{23b}$$

for Case (3)

$$\omega(-0.227,\infty,t)=0.4, \quad T'=150\Delta t, \tag{23c}$$

for Case (4)

$$\omega(-0.227,\infty,t)=0.4, \quad T'=250\Delta t. \tag{23d}$$

The iterative values of standard deviations and correlation for the four cases are shown in Figs. 4 and 5. Comparison with theoretical calculations shows that variation of templates and evolution times indeed does not cause deviation of the converged rescaled CDF from the family of self-similar solutions.

VI. CONCLUSIONS

We presented a coarse dynamic renormalization technique, based on a coarse time stepper using marginal and conditional ICDFs as coarse-scale observables, for the computer-assisted analysis of multidimensional self-similar particle systems. For coarse-grained differential operators that possess a scale-invariance property of the type arising in our numerical example, a single template condition is necessary for rescaling the ICDFs. In our example, we confirmed

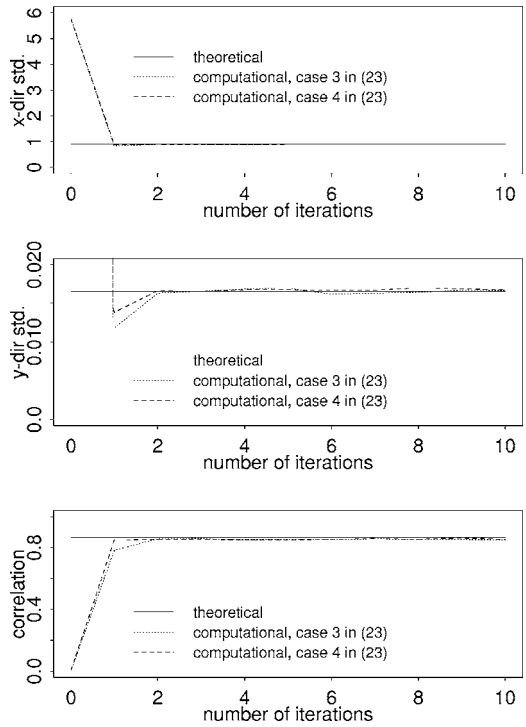

FIG. 5. Computational vs theoretical values for the standard deviations and the correlation of the self-similar shapes. Cases (3), (4) in Eqs. (23c) and (23d) (see text).

that the steady-state shape of the renormalized CDFs of particle positions is not affected by the template condition and evolution time interval in our coarse time stepper.

The equation-free dynamic renormalization technique was applied only to a simple two-dimensional Brownian particle system in this paper. In our computations, we had already factored out translational invariance; we also knew the particular coordinate system (the x and y axis) in which the macroscopic differential operator is scale invariant. Finding this information, if unknown, can be incorporated in the test procedure for scale invariance. For higher-dimensional diffusive particle systems, this technique may still be used. In these cases, conditional ICDFs in third or higher dimensions have to be utilized, thus rendering the computations slightly more complicated, yet still qualitatively similar to the ones presented here. Using appropriately selected template conditions, this technique can also be used to approximate coarse-grained *asymptotically* self-similar shapes; this is the case for our Couette example when the particles diffuse in *both* the x and y directions (work in progress). Several other examples of coarse self-similarity (e.g., models of glassy dynamics, KPZ-type evolution of interfaces, dynamics of energy spectra in randomly forced PDEs) are also being explored.

[1] C. W. Gear, I. G. Kevrekidis, and C. Theodoropoulos, Comput. Chem. Eng. **26**, 941 (2002).
[2] I. G. Kevrekidis, C. W. Gear, and G. Hummer, AIChE J. **50**, 1346 (2004).
[3] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg, and K. Theodoropoulos, Commun. Math. Sci. **1**, 715 (2003).
[4] K. Theodoropoulos, Y-H. Qian, and I. G. Kevrekidis, Proc. Natl. Acad. Sci. U.S.A. **97**, 9840 (2000).
[5] A. J. Chorin, O. H. Hald, and R. Kupferman, Physica D **166**, 239 (2002).
[6] A. J. Chorin, R. Kupferman, and D. Levy, J. Comput. Phys. **162**, 267 (2000).
[7] D. Givon, R. Kupferman, and A. M. Stuart, Nonlinearity **17**, R55 (2004).
[8] B. J. LeMesurier, G. C. Papanicolaou, C. Sulem, and P. L. Sulem, Physica D **31**, 78 (1988).
[9] D. W. McLaughlin, G. C. Papanicolaou, C. Sulem, and P. L. Sulem, Phys. Rev. A **34**, 1200 (1986).
[10] G. I. Barenblatt, *Scaling, Self-Similarity and Intermediate Asymptotics* (Cambridge University Press, Cambridge, UK, 1996).
[11] N. D. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Addison-Wesley, Reading, MA, 1992).
[12] L. Chen, P. G. Debenedetti, C. W. Gear, and I. G. Kevrekidis, J. Non-Newtonian Fluid Mech. **120**, 215 (2004).
[13] L. Chen, I. G. Kevrekidis, and P. G. Kevrekidis, e-print cond-mat/0412773.
[14] D. G. Aronson, S. I. Betelu, and I. G. Kevrekidis, e-print cond-mat/0111055.
[15] C. W. Rowley, I. G. Kevrekidis, J. E. Marsden, and K. Lust, Nonlinearity **16**, 1257 (2003).
[16] C. W. Rowley and J. E. Marsden, Physica D **142**, 1 (2000).
[17] C. I. Siettos, I. G. Kevrekidis, and P. G. Kevrekidis, Nonlinearity **16**, 497 (2003).
[18] B. J. LeMesurier, G. C. Papanicolaou, C. Sulem, and P. L. Sulem, Physica D **32**, 210 (1988).
[19] A. J. Chorin, Multiscale Model. Simul. **1**, 105 (2003).
[20] C. T. Kelley, *Iterative Methods for Linear and Nonlinear Equations* (SIAM, Philadelphia, 1995).
[21] Ronald L. Panton, *Incompressible Flow*, 2nd ed.(J. Wiley, New York, 1996).
[22] I. I. Gihman and A. V. Skorohod, *Stochastic Differential Equations* (Springer Verlag, Berlin, 1972).
[23] G. N. Milshtein, Theor. Probab. Appl. **19**, 557 (1974).
[24] A. J. Majda and P. R. Kramer, Phys. Rep. **314**, 237 (1999).