

Accurate discretization of advection-diffusion equations

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We present an exact mathematical transformation which converts a wide class of advection-diffusion equations into a form allowing simple and direct spatial discretization in all dimensions, and thus the construction of accurate and more efficient numerical algorithms. These discretized forms can also be viewed as master equations which provide an alternative mesoscopic interpretation of advection-diffusion processes in terms of diffusion with spatially varying hopping rates.

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I. INTRODUCTION

Advection-diffusion equations (ADEs) describe a broad class of processes in the natural sciences. As their name implies, they provide a continuum (macroscopic) representation of systems whose underlying dynamics combines Brownian motion (diffusion) with some form of deterministic drift (advection). In this paper we shall consider ADEs of the general form

$$\partial_t \rho = \nabla \cdot D \nabla \rho - \nabla \cdot \rho \mathbf{v}. \quad (1)$$

The field ρ typically describes the number density of “particles” which, depending on the application, can range from electrons in a plasma, to chemical molecules advected in solution, to colloidal particles, to biological cells moving along chemical gradients. In principle the diffusion coefficient $D(\mathbf{x}, t)$ and the velocity field $\mathbf{v}(\mathbf{x}, t)$ can depend on the density field ρ . An idea of the ubiquity of ADEs can be gauged from their diverse applications to traditional physics, soft matter systems, and biology. A small subset of examples are magnetic fusion plasmas [1], cosmic ray streaming [2,3], electrons in weakly ionized gases [4], microemulsions under shear flow [5], chemical kinetics in driven systems [6,7], hydrodynamics and chemotaxis of bacterial colonies [8,9], phase field dynamics in directional solidification [10], and a wide array of tracer diffusion problems (for example [11]).

It is generally not possible to analytically solve ADEs, especially since they often appear within sets of non-linear coupled equations. For this reason, great emphasis has been placed on numerical integration methods, typically based on finite differences. It has been found that the advection term, despite its apparent simplicity, is extremely troublesome to handle [12]. There are two major challenges: *stability*, which can be improved using a range of implicit methods, and *accuracy*, which is a delicate issue, requiring the “best possible” form of spatial discretization. Regarding the issue of stability, many schemes are in use, such as the Crank-Nicholson/ADI and fractional step methods [12,13], and the Lax-Wendroff method [14]. The issue of accuracy has re-

ceived somewhat less attention with two spatial discretization schemes (and their immediate variants) commonly in use: these are the simple Taylor expansion [1,15] and the “upwind” scheme [16,17]. One of the main results of this paper is the derivation of a new discretization scheme which is physically appealing, simple to apply in all dimensions, and more accurate than those currently in use.

II. A SIMPLE EXAMPLE

To begin, let us present the key idea in the context of a simple ADE, namely, a one-dimensional system with a velocity function proportional to the spatial derivative of a scalar potential $\phi(x, t)$. Thus, we consider

$$\partial_t \rho = D_0 \partial_x^2 \rho - \alpha \partial_x (\rho \partial_x \phi), \quad (2)$$

where D_0 and α are constants.

Most numerical algorithms designed to integrate an equation such as (2) treat the diffusion and advection terms separately [1,12,17]. The difficulties arise in finding a discretization for the latter term. In doing so, two fundamental properties of the equation must be exactly maintained. These are the non-negativity of ρ and its spatial conservation:

$$\int dx \rho(x, t) = \text{const}. \quad (3)$$

As an illustration, let us write down a common spatial discretization using simple Taylor expansion, which is used both for explicit Euler schemes [18], and as the basis for more advanced implicit algorithms [12,15,16]. We replace the continuous function $\rho(x, t)$ by a set of functions $\{\rho_i(t)\}$ defined on a regular grid with lattice spacing h . The equation of motion for ρ_i is written using centered spatial derivatives:

$$\begin{aligned} \frac{d\rho_i}{dt} = & \frac{D_0}{h^2} (\rho_{i+1} + \rho_{i-1} - 2\rho_i) - \frac{\alpha}{4h^2} [\rho_{i+1} (\phi_{i+2} - \phi_i) \\ & - \rho_{i-1} (\phi_i - \phi_{i-2})]. \end{aligned} \quad (4)$$

It is noteworthy that this simple scheme requires knowledge of the scalar field ϕ at next-nearest neighbor grid points rather than neighboring grid points. For future reference we rewrite this discrete equation in the following manner:

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$$\frac{d\rho_i}{dt} = \frac{1}{h^2} \left\{ \rho_{i+1} \left[D_0 - \frac{\alpha}{4} (\phi_{i+2} - \phi_i) \right] + \rho_{i-1} \left[D_0 + \frac{\alpha}{4} (\phi_i - \phi_{i-2}) \right] - \rho_i [2D_0] \right\}, \quad (5)$$

which we shall hereafter refer to as the ‘‘linear centered discretization’’ (LCD) (and which resembles the backward Euler scheme used for simple advection problems [12]).

We now turn to a new discretization scheme which emerges from a simple mathematical transformation of the ADE (2). Defining $\gamma = \alpha/2D_0$ it can be verified by direct differentiation that Eq. (2) may be written as

$$\partial_t \rho = D_0 [e^{\gamma\phi} \partial_x^2 (\rho e^{-\gamma\phi}) - e^{-\gamma\phi} \rho \partial_x^2 (e^{\gamma\phi})]. \quad (6)$$

A similar transformation involving exponential functions is known for Fokker-Planck equations [19]. The simple ADE given in (2) can indeed be formally interpreted as such an equation, although the physical origin is quite different. We will shortly be considering more general ADEs in which the diffusion coefficient and velocity function can be functions of the density ρ . Clearly then the simple correspondence with Fokker-Planck equations breaks down, although we are still able to achieve a transformation of the kind given above. The crucial feature of Eq. (6) is that spatial derivatives only enter in the form of a second derivative ∂_x^2 which is straightforward to discretize. Using the simplest such discretization we immediately have

$$\frac{d\rho_i}{dt} = \frac{D_0}{h^2} [\rho_{i+1} e^{-\gamma(\phi_{i+1}-\phi_i)} + \rho_{i-1} e^{-\gamma(\phi_{i-1}-\phi_i)} - \rho_i (e^{-\gamma(\phi_i-\phi_{i+1})} + e^{-\gamma(\phi_i-\phi_{i-1})})]. \quad (7)$$

There are a number of points to make concerning this equation. First, in contrast to the LCD (4), the scalar field appears in a non-linear fashion, and is sampled at nearest-neighbor positions. Second, the new equation is of the same form as a master equation [15,19,20]. Within this analogy one can think of ρ_i as the probability that a fictitious particle is located at grid position i . The transition rate for the particle to hop from grid point i to a neighboring point j is of the Arrhenius form

$$W_{i \rightarrow j} = (D_0/h^2) \exp[-\gamma(\phi_i - \phi_j)]. \quad (8)$$

Given this formal analogy with a master equation for a probability function, one immediately sees that Eq. (7) exactly maintains conservation of the function ρ (normalization of probability) and its non-negativity. Due to this analogy we hereafter refer to Eq. (7) as the ‘‘master equation discretization’’ (MED).

Our numerical work (see Sec. V) shows that the MED is more accurate than the LCD and other popular discretizations. To appreciate the underlying reason for this, it is helpful to consider the case of $\gamma\delta\phi \ll 1$ in which case we can expand the exponential functions in Eq. (7) to first order. One then finds

$$\frac{d\rho_i}{dt} = \frac{1}{h^2} \left\{ \rho_{i+1} \left[D_0 - \frac{\alpha}{2} (\phi_{i+1} - \phi_i) \right] + \rho_{i-1} \left[D_0 + \frac{\alpha}{2} (\phi_i - \phi_{i-1}) \right] - \rho_i \left[2D_0 - \frac{\alpha}{2} (2\phi_i - \phi_{i+1} - \phi_{i-1}) \right] \right\}. \quad (9)$$

Comparison of this form with Eq. (5) gives useful insight into the potential weakness of the LCD. Namely, it neglects an important curvature term in the scalar field. In fact, this omission is directly related to artificial (or ‘‘numerical’’) diffusion, which is a common failing of other discretization schemes, most notably, the ‘‘upwind’’ scheme [12,16,17]. The linear scheme given above in Eq. (9) can of course be regarded as one of many possible linear discretizations, but without the derivation given here one would have no *a priori* reason to prefer it over forms such as the LCD, since they both have non-vanishing second-order errors in space. Continuing the expansion of the exponential terms in powers of α yields crucial non-linear corrections to Eq. (9) which have no analogy within linear discretization schemes. As shall be seen below, the MED is easily formulated for the d -dimensional extension of Eq. (2) as well as for a range of more general ADEs.

III. THE GENERAL CASE

Consider the general ADE in d -dimensions given in Eq. (1). We shall now proceed to transform this equation into a form amenable to the MED. In one dimension we shall find that this is possible for general functions D and v . In higher dimensions the vectorial nature of the velocity field will place a constraint on the transformation.

Let us introduce two scalar functions $f(\mathbf{x}, t)$ and $g(\mathbf{x}, t)$ defined via the relations

$$D = fg, \quad (10)$$

$$\mathbf{v} = g \nabla f - f \nabla g. \quad (11)$$

Then the ADE (1) has the explicit form

$$\partial_t \rho = \nabla \cdot [fg \nabla \rho] - \nabla \cdot [\rho(g \nabla f - f \nabla g)]. \quad (12)$$

By direct differentiation one can show that this equation may be rewritten as

$$\partial_t \rho = f \nabla^2 (g\rho) - g \rho \nabla^2 f. \quad (13)$$

Once again, we see that the spatial derivatives appear only as Laplacians, which allows us to immediately write down a simple discrete form. Let us define the discrete Laplacian via

$$\nabla^2 Q(\mathbf{x}) = \frac{1}{h^2} \sum_j (Q_j - Q_i), \quad (14)$$

where the sum is over nearest neighbors j of the grid point i , which corresponds to the continuum position \mathbf{x} . Then the MED corresponding to Eq. (13) is

$$\partial_t \rho_i = \sum_j [W_{j \rightarrow i} \rho_j - W_{i \rightarrow j} \rho_i], \quad (15)$$

where the transition rate for ‘‘hopping’’ from site i to site j is

$$W_{i \rightarrow j} = f_j g_i / h^2. \quad (16)$$

Having formulated the MED in this general manner, let us examine some particular cases. We stress that once the functions f and g are determined the discrete algorithm is completely defined via the transition rate given above.

First, we consider one dimension. In this case it is possible to integrate Eqs. (10) and (11) exactly to find the necessary auxiliary functions f and g in terms of the physically relevant diffusion coefficient and velocity. One finds

$$f(x, t) = C \sqrt{D(x, t)} \exp(S), \quad S(x, t) = \frac{1}{2} \int^x dx' \frac{v(x', t)}{D(x', t')}, \quad (17)$$

with g then given trivially from (10). The transition rate is easily evaluated from (16) to give

$$W_{i \rightarrow j} = \frac{\sqrt{D_i D_j}}{h^2} \exp[-(S_i - S_j)]. \quad (18)$$

A non-trivial application of this general solution would be advection-diffusion in the kinetic theory of gases where the diffusion coefficient is non-constant, and actually depends on the density as $D \propto 1/\rho$ [21]. In higher dimensions a general solution for f and g is not possible. Solvable cases will rely on special conditions for D and \mathbf{v} reminiscent of the potential conditions for the existence of steady-state solutions to the multi-variate Fokker-Planck equation [19,20].

For many problems the diffusion coefficient is constant (D_0) and the velocity function is associated with a scalar potential via $\mathbf{v} = \alpha \nabla \phi$. In these cases, the analysis leading to Eq. (8) is easily generalized to d dimensions and one finds the discrete equation (15) with

$$W_{i \rightarrow j} = (D_0/h^2) \exp[-\gamma(\phi_i - \phi_j)], \quad (19)$$

where we remind the reader that $\gamma = \alpha/2D_0$. As found in one dimension, this scheme includes important curvature terms, even within a linear approximation, which are absent in conventional LCD algorithms. Numerical analysis shows such terms to be essential in regions where ϕ has maxima or minima.

The MED scheme encapsulated in Eqs. (15) and (19) can be used to model more complicated ADEs in which there is non-linear feedback. An interesting example of this is the continuum theory of group dynamics, in which a non-linear and non-local feedback mechanism is imposed via the velocity potential [22,23]. In particular one has

$$\phi(x, t) = \int d^d x' V(\mathbf{x} - \mathbf{x}') \rho(\mathbf{x}', t), \quad (20)$$

where V is analogous to a potential, and is responsible for long-range attraction and short-range repulsion of individuals. If V is a Dirac δ -function then $\phi \propto \rho$. Such models are used to describe density-dependent dispersal in population

dynamics [22] and have recently been shown to arise from excluded volume effects in models of interacting cellular systems [24]. A second well-known example is the Keller-Segel model for chemotactic motion [9]. Here, the potential ϕ represents the chemoattractant concentration field and is coupled to the cell density field ρ via

$$\partial_t \phi = \nu \nabla^2 \phi - \lambda \phi + \beta \rho, \quad (21)$$

where ν , λ , and β are the diffusion constant for the chemical field and its rate of degradation and production, respectively. This equation is easily discretized and the resulting discrete chemical concentration field may be inserted into the transition rate (19) allowing a straightforward scheme for integration of the cell density.

IV. FINE-TUNING THE MED ALGORITHM

From numerical investigations (see the next section) we have found that the MED is generally far more accurate than both the LCD and upwind schemes. In regions where the velocity function has strong spatial variation, the MED does an excellent job in predicting the correct density even for grid scales approaching the scale of variation of the velocity. However, in the ‘‘simpler case’’ when dynamics are dominated by advection in a region of quasi-constant velocity, the MED fares less well. This problem can be traced back to the exponential weights yielding, in regions of constant velocity, an over-estimated drift velocity. In terms of a hopping process, the bias in hopping rates between neighboring sites is proportional to $\sinh(\gamma \delta \phi)$, whereas the correct drift velocity is simply proportional to $\gamma \delta \phi$.

We discuss here two straightforward extensions to MED which alleviate this problem, but also lead to slightly less accurate algorithms in the ‘‘non-trivial’’ regions where the velocity is strongly varying. Both extensions amount to a renormalization of the hopping rates. An ideal algorithm would be a hybrid, using the original MED and either of the following extensions in appropriate regions. We will not discuss such hybrid schemes here since their form will be strongly dependent on actual applications.

For simplicity let us consider again the one-dimensional ADE given in Eq. (2). The MED scheme for this case is given in Eq. (7), where the transition rate from site i to neighboring site j has the explicit form

$$W_{i \rightarrow j} = (D_0/h^2) \exp[-\gamma(\phi_i - \phi_j)]. \quad (22)$$

It is clear from (22) that the effective drift velocity arising from the bias in hopping rates between i and j is

$$v_{\text{eff}} = h(W_{i \rightarrow j} - W_{j \rightarrow i}) = (2D_0/h) \sinh[\alpha(\phi_j - \phi_i)/2D_0], \quad (23)$$

where we have reinstated $\gamma = \alpha/2D_0$ for clarity. The correct drift velocity between these two points is simply $\alpha(\phi_j - \phi_i)/h$ which is recovered if the grid scale is small (or else the velocity potential is slowly varying).

In order to correct the MED algorithm one may either renormalize the effective diffusion coefficient (which is the pre-factor of the exponential weight) or else renormalize the

parameter γ which appears in the argument of the exponential. In the former case one has, on fitting the drift velocity to its correct value, the effective diffusion coefficient

$$D_{\text{eff}} = D_0 \frac{\alpha \delta \phi / 2D_0}{\sinh(\alpha \delta \phi / 2D_0)}, \quad (24)$$

which leads to the MED transition weight taking the ‘‘Fermi-Dirac’’ (FD) form

$$W_{i \rightarrow j} = \left(\frac{D_0}{h^2} \right) \frac{\alpha(\phi_i - \phi_j)/D_0}{\exp[\alpha(\phi_i - \phi_j)/D_0] - 1}. \quad (25)$$

The alternative is to correct the drift velocity by adjusting γ , which leads to

$$\gamma_{\text{eff}} = \frac{1}{\delta \phi} \sinh^{-1} \left(\frac{\alpha \delta \phi}{2D_0} \right). \quad (26)$$

Writing the inverse hyperbolic function in terms of a logarithm leads to the MED transition rate taking the ‘‘square root’’ (SR) form

$$W_{i \rightarrow j} = (D_0/h^2) \left\{ \left[1 + \left(\frac{\alpha(\phi_i - \phi_j)}{2D_0} \right)^2 \right]^{1/2} - \left(\frac{\alpha(\phi_i - \phi_j)}{2D_0} \right) \right\}. \quad (27)$$

Numerically one finds that the FD form (25) is generally more accurate than the SR form (27), and that both are superior to the LCD and upwind schemes. As already mentioned, the original MED scheme defined by Eq. (22) is the best of all the schemes described when the velocity field is strongly varying, and/or during asymptotic relaxation of the density field to its steady-state.

V. NUMERICAL WORK

We have made a careful numerical analysis of the simple one-dimensional ADE given in Eq. (2), along with its two-dimensional extension. Since we wish to gauge the accuracy of our new scheme, we have compared the MED scheme (7), and its variants [the MED(FD) given in (25), the MED(SR) given in (27), and the linearized MED, denoted by MED(LIN), given in (9)], with both the LCD and upwind schemes [12]. In one dimension we use a static velocity potential given by $\phi(x) = [1 + \cos(2\pi nx/L)]/2$ with $n=16$ and $L=12.8$. The initial density function is taken to be uniform in the region $x \in (-3, 3)$ and zero otherwise. The density is normalized to unity and periodic boundary conditions are enforced. This set-up provides a challenging test of all the schemes since the velocity field is a strongly varying function of position. Furthermore, we challenge the methods by using the parameter values $D_0=1.0$ and $\alpha=5.0$ (Fig. 1) and $\alpha=20.0$ (Fig. 2), which correspond to moderate to high grid Peclet numbers [1] at the grid scales of interest. Here, the largest Peclet numbers are approximately given by $2\alpha h$ and so vary between 0.25 and 8 for the data shown in Figs. 1 and 2. The dynamics consists of a rapid transient phase where the density field adapts to the periodic structure of the velocity field, followed by a slower relaxation toward the steady state. Thus, the numerical analysis probes each scheme’s ability to

track rapid advective motion and diffusive relaxation around maxima and minima of the velocity field.

In order to assess the accuracy of the methods we first run all schemes at a very small grid size of $h=0.00625$, using an explicit temporal scheme with $\delta t=10^{-6}$. Very good agreement is found among all the schemes and the solution is denoted ‘‘exact.’’ We then run all the schemes at larger grid scales using $\delta t=10^{-4}$, and dynamically compare the approximate solutions with the exact one. This is gauged using the relative error, which is defined via

$$E(t) = \frac{\sum_i [\rho_i(t) - \rho_{i,\text{exact}}(t)]^2}{\sum_i \rho_{i,\text{exact}}(t)^2}. \quad (28)$$

Note that δt is chosen small enough such that any differences between our first-order temporal discretization for LCD and second-order schemes (in the temporal dimension) such as Crank-Nicholson or Lax-Wendroff are negligible. Figures 1(a)–1(e) show $E(t)$ for grid scales $h=0.025, 0.05, 0.1, 0.2,$ and 0.4 , respectively, for $\alpha=5.0$. The entire dynamical evolution up to the steady state is shown. In the first four panels we clearly see that the MED and its (nonlinear) variants give a relative error approximately 10 times less than the LCD and UW schemes. [Note UW does not appear in Fig. 1(a) since its error is too large to be usefully included.] The relative errors of all the schemes increases roughly by a factor of 10 as the grid scale is doubled. Figure 1(e) shows the breakdown of all the schemes at the scale $h=0.4$ which is comparable to the period of the velocity field. By ‘‘breakdown’’ we mean a relative error of 10% or more. To give an idea of the spatial form of the density field near the steady state we show in Fig. 1(f) the exact density profile in a peripheral region, along with the LCD and MED (FD) at a grid scale of $h=0.2$ for comparison. Note the LCD fails to capture the magnitude of the maximum density, and also becomes negative at some grid points.

In a similar fashion, Figs. 2(a)–2(d) show $E(t)$ for $h=0.025, 0.05, 0.1,$ and 0.2 , respectively, for $\alpha=20.0$. As before the non-linear MED schemes perform far better than the LCD and UW, meaning the relative error is roughly 10 times smaller for a given grid scale. Note also that the MED(FD) and MED(SR) algorithms perform better than MED during the transient period, as expected. All schemes break down for $h=0.2$. In Fig. 2(e) we show the exact density profile close to the steady state, compared with the MED and LCD schemes for $h=0.1$. Again, the LCD shows negative values and fails in the vicinity of the density peaks. Figure 2(f) is the same except the UW scheme is compared to the MED. The UW scheme is designed to give non-negative densities, but has high (artificial) ‘‘numerical diffusion’’ which inflates the width of the density peaks.

We have performed an exactly analogous numerical examination in two dimensions (2D). We integrated the 2D generalization of Eq. (2) using the potential $\phi(x,y) = [1 + \cos(2\pi nx/L)][1 + \cos(2\pi ny/L)]/4$ with $n=16$ and $L=12.8$. We take $D_0=1.0$ and $\alpha=10.0$. The initial density function is uniform in a disk of radius 3.0 and zero otherwise, and again normalized to unity. The ‘‘exact’’ density profile is evaluated

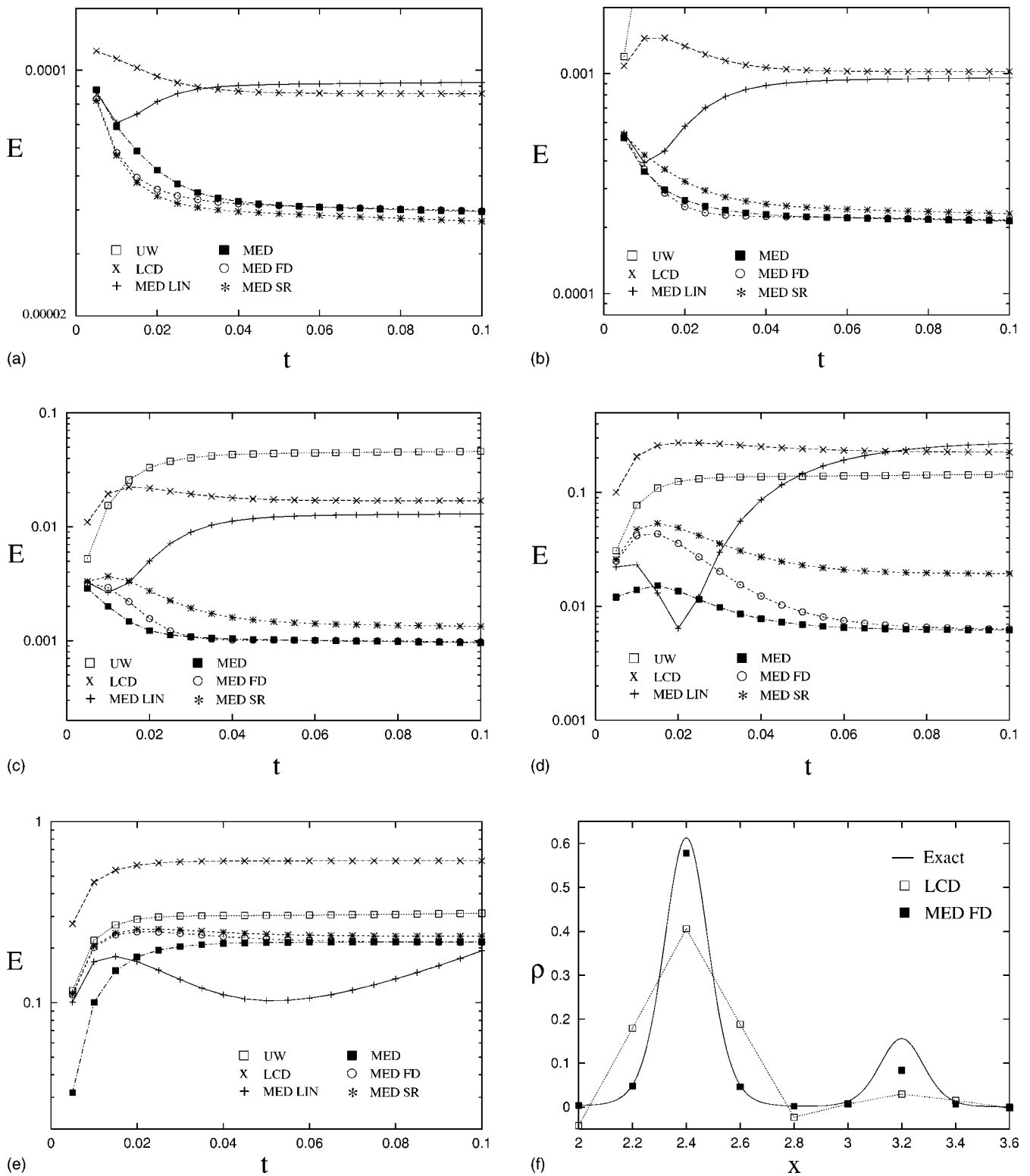


FIG. 1. Data from numerical integration of Eq. (2) using various schemes in one dimension, with $D_0=1.0$ and $\alpha=5.0$. The particular form of the velocity potential and the initial density profile are described in Sec. V. The time step is $\delta t=10^{-4}$. (a), (b), (c), (d), and (e): The relative error (28) as a function of time for grid scales of $h=0.025, 0.05, 0.1, 0.2,$ and 0.4 , respectively. The methods used are upwind (UW), LCD (4), linearized MED (9), MED (7), “Fermi-Dirac” version of MED (25), and “square-root” version of MED (27). (f) Comparison of the exact density profile in the peripheral region $x \in (2, 3.6)$ with both the MED(FD) scheme and the LCD scheme at time $t=0.1$ using $h=0.2$. In Figs. 1–3, time is measured in units of δt , space in units of h , and the density in dimensionless units.

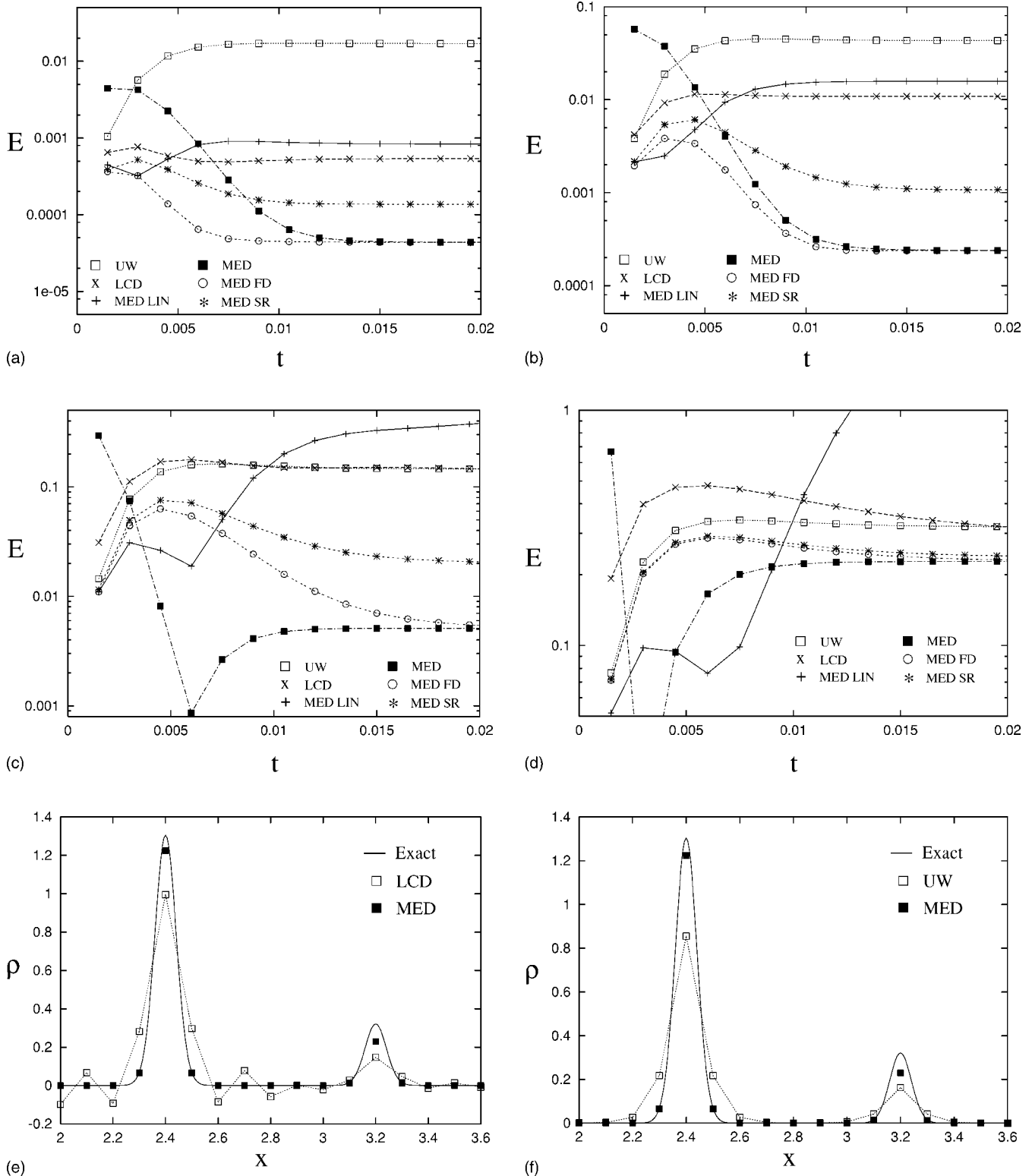


FIG. 2. Same as Fig. 1, but with $\alpha=20.0$. (a), (b), (c), and (d): The relative error (28) as a function of time for grid scales of $h=0.025, 0.05, 0.1$, and 0.2 , respectively. (e) Comparison of the exact density profile in the peripheral region $x \in (2, 3.6)$ with both the MED scheme and the LCD scheme at time $t=0.02$ using $h=0.1$. (f) The same as (e) but compares the exact profile with both MED and UW.

using $h=0.0125$ and $\delta t=0.25 \times 10^{-4}$. The two-dimensional extensions of all six schemes are integrated for grid scales of $h=0.025, 0.05, 0.1$, and 0.2 using $\delta t=10^{-4}$. The relative error $E(t)$ for these cases is shown in Figs. 3(a)–3(d), for a time

period encompassing the initial rapid adaptation to the potential followed by the early stages of relaxation to the steady-state. As with one dimension, the MED and its (non-linear) variants perform far better than the LCD and UW,

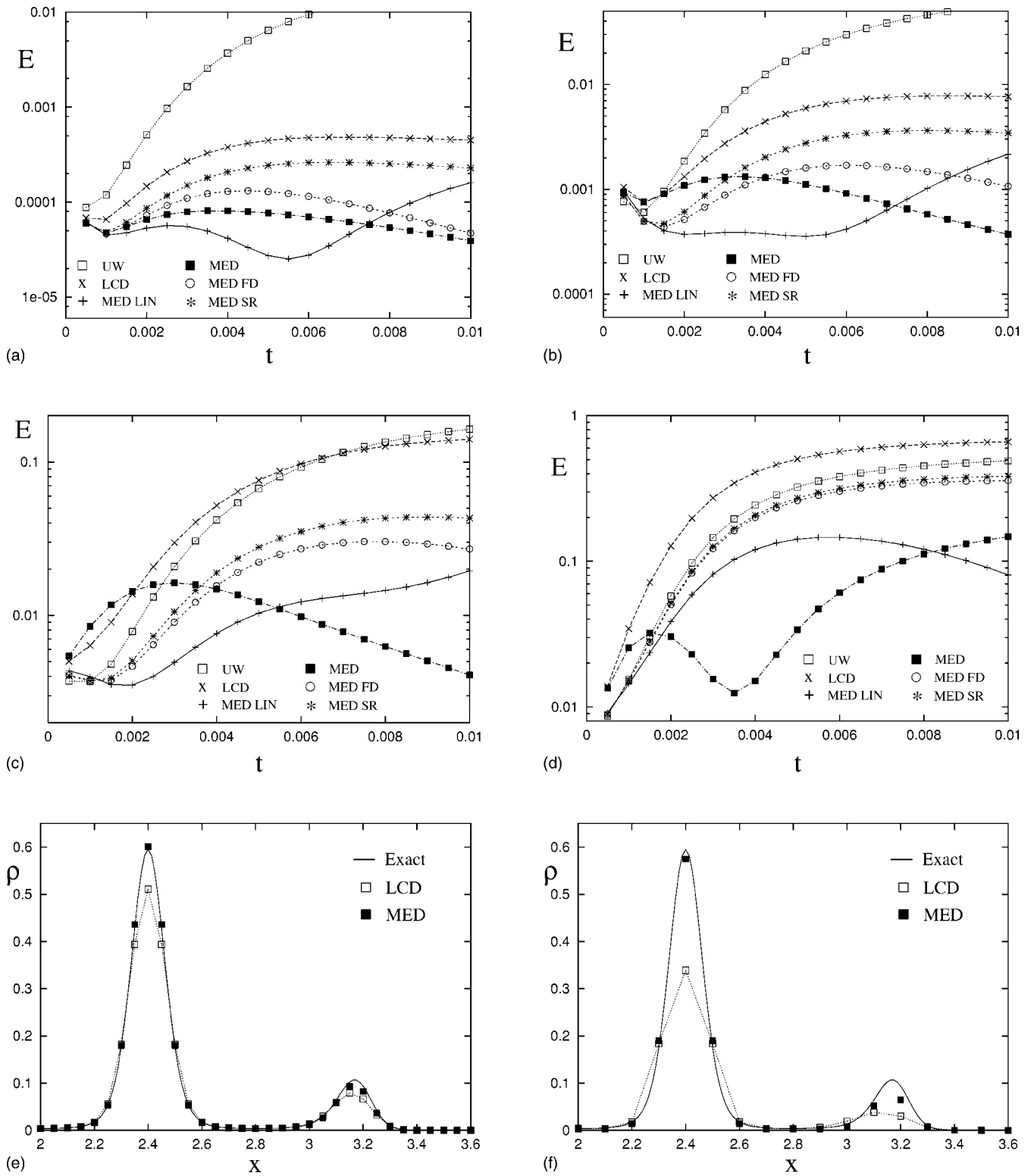


FIG. 3. Data from numerical integration of the two-dimensional generalization of Eq. (2) using various schemes, with $D_0=1.0$ and $\alpha=10.0$. The particular form of the velocity potential and the initial density profile are described in Sec. V. The time step is $\delta t=10^{-4}$. (a), (b), (c), and (d): The relative error (28) as a function of time for grid scales of $h=0.025, 0.05, 0.1$, and 0.2 , respectively. The methods used are two-dimensional generalizations of upwind (UW), LCD (4), linearized MED (9), MED (7), “Fermi-Dirac” version of MED (25), and “square-root” version of MED (27). (e) Comparison of the exact density profile along a cut ($y=0$) in the peripheral region $x \in (2, 3.6)$ with both the MED scheme and the LCD scheme at time $t=0.01$ using $h=0.05$. (f) The same as (e) except that a larger grid scale of $h=0.1$ is used.

with the pure MED scheme performing best at later times. All schemes break down for $h=0.2$. Direct comparison of the exact density profile, MED, and LCD is given in Figs. 3(e) and 3(f), for $h=0.05$ and $h=0.1$, respectively, along a one-dimensional cut ($y=0$) in a peripheral region of the density. The MED shows excellent agreement, especially in the vicinity of the density peaks. The LCD fails in the vicinity of the density peaks as expected.

From this and similar numerical work we have concluded that the MED and its (non-linear) extensions are superior spatial discretization schemes compared to the LCD and up-wind schemes. The MED works especially well in regions of large variation in the velocity potential. Generally speaking, for a given error tolerance, the MED and variants allow one to use grid scales at least two times larger than traditional schemes, which translates into a saving of *at least* a factor of 4 and 8 in computational cost for two- and three-dimensional numerical analyses.

VI. DISCUSSION AND CONCLUSIONS

We end with some remarks on the non-linear transition rates of the MED. In most applications the ADEs represent processes for which there is no underlying lattice (e.g., cosmic ray diffusion [3] or chemotactically moving cells [9]). When one discretizes the continuum ADE one must therefore not regard the lattice version as “more fundamental” or “more microscopic.” It is simply a mathematical analog of the original equation and identical in the limit of the lattice spacing being taken to zero. This is a different situation to that found for many models arising from solid state physics in which there is an underlying crystal lattice, and for which the discrete equation can often be regarded as more fundamental (or, at least, more microscopic) than continuum models. Although the hopping process encapsulated by the MED cannot be viewed as the underlying microscopic dynamics, it is interesting that ADEs can be accurately modeled by a process in which diffusion and advection are non-linearly combined in Arrhenius transition rates. Figure 4 summarizes our understanding of the algorithmic connections between ADE and the MED discretization, in which a given ADE typically arises from a mean-field approximation of a microscopic stochastic process which is not constrained by a lattice.

Pragmatically one wishes to impose a “large” lattice scale for numerical efficiency, while avoiding the loss of accuracy. Algorithms which remain accurate for larger lattice scales

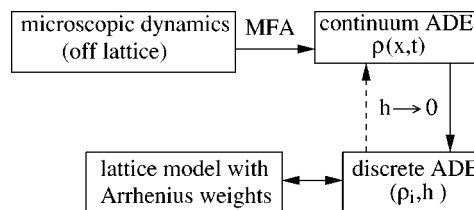


FIG. 4. A schematic diagram summarizing the relationships between various descriptions of advection-diffusion processes. The MED is a useful mesoscopic description in terms of Arrhenius hopping rates, rather than a reflection of the underlying dynamics.

yield great computational speed-up in higher dimensions, since the number of required grid points (and hence computer operations) scales as h^{-d} . We find that our new scheme typically allows grid scales between two and four times larger than traditional schemes, which in three dimensions allows a potential speed-up in computation of one or two orders of magnitude. Naturally, our improved spatial discretizations can be used in more advanced algorithms which use implicit temporal methods and/or adaptive spatial grids.

In conclusion we have shown that a wide class of advection-diffusion equations can be exactly rewritten in a form which immediately allows a direct and simple spatial discretization in all dimensions. Our new discrete forms contain important non-linear terms, which when linearized are seen to be related to the curvature of the velocity potential, such terms being absent in commonly used discretization schemes. We have shown explicitly that these curvature effects are essential for accurate integration of ADEs, both in one and two dimensions, and allow simple algorithms to be constructed which are accurate for grid scales up to the size of spatial variation in the velocity field. We estimate that our new algorithm may allow a speed-up of ADE computation by factors of 10 or more in three dimensions due to the increased grid scale one can impose. The fact that ADE can be recast as master equations also yields interesting physical insight into their dynamics—namely that at mesoscopic scales the processes of diffusion and advection may be modeled as a non-linear combination within Arrhenius-like transition rates.

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