Efficient solver for a large class of convection-diffusion problems

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(Dated: September 19, 2018)

We describe an exact and highly efficient numerical algorithm for solving a broad class of convection-diffusion equations. These equations occur in many problems in physics, chemistry, or biology, and they are usually hard to treat due to the presence of a convection term, represented by a first order derivative in the spatial co-ordinate. Our algorithm reduces the convection-diffusion equation to a pure diffusion problem within a complex-valued potential which can be solved efficiently and accurately using conventional parabolic partial differential equation solvers.

PACS numbers: 42.25.Fx, 42.50.Pq, 78.67.Bf

I. INTRODUCTION

Convection-diffusion processes play an important role in physics, chemistry and biology. They are described by the convection-diffusion partial differential equation which models the transport of particles, heat, energy or other quantities in space over time, involving both directed transport (convection) as well as diffusive, stochastically driven transport. In statistical physics and probability theory, convection-diffusion equations are also known as Fokker-Planck equations and describe the spatio-temporal transport of a probability density within an external force field (convection). Thus, convection-diffusion equations are omnipresent, and their numerical solution is of great importance in diverse fields of science.

However, accurate numerical integration of convection-diffusion equations is a challenging task, due to the presence of the convection term. Many sophisticated procedures and algorithms have been developed in the past, such as finite-difference methods [1], lattice Boltzmann methods [2], or relating the problem to a Smoluchowski-Langevin stochastic differential equation [3], for which powerful numerical solvers are available. In a recent paper [4] we developed an approximate solution to this kind of equation by using path-integral approach. From this effort, we have found that one can efficiently eliminate the convective term in the equation by representing the solution as

\[ \frac{\partial c(r, t)}{\partial t} = D \Delta c(r, t) - v(x) \partial_r c(r, t) \]  \hspace{0.5cm} (1)

where \( c(r, t) \) is the local concentration of the transported diffusing quantity at position \( r \) and time \( t \), \( D \) is the diffusion coefficient, and \( v(x) \) is a flow along the \( x \)-direction which depends only on the coordinates \( r_\perp \) perpendicular to \( x \). This is the case for all laminar flows along straight channels with arbitrary cross-section and with arbitrary boundary conditions. Two important examples of this kind which will be discussed in this paper are (i) convection-diffusion in a shear-flow over a surface, and (ii) convection-diffusion in a capillary flow. As already mentioned, the numerically difficult term is the convection term which involves spatial derivatives of the first order. In a recent paper [4] we developed an approximate solution to this kind of equation by using path-integral approach. From this effort, we have found that one can efficiently eliminate the convective term in the equation by representing the solution \( c(r, t) \) in integral form as

\[ c(r, t) = \int \frac{dk}{2\pi} \tilde{w}(k, r_\perp, t) \exp(ikx - Dk^2t) \]  \hspace{0.5cm} (2)

where we have introduced the auxiliary function \( \tilde{w}(k, r_\perp, t) \). After inserting this expression into eq. (1), we find that this function has to obey the differential equation

\[ \frac{\partial \tilde{w}}{\partial t} = D \Delta_\perp \tilde{w} - ikv(r_\perp) \tilde{w} \]  \hspace{0.5cm} (3)

where the operator \( \Delta_\perp \) is the Laplacian along the transversal co-ordinates \( r_\perp \). The initial conditions for \( \tilde{w} \) are

\[ \tilde{w}(k, r_\perp, t = 0) = \tilde{c}_0(k, r_\perp) \]  \hspace{0.5cm} (4)

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where \( \hat{c}_0(k, r_\perp) \) is the Fourier transform along the \( x \)-coordinate of the initial concentration distribution \( c_0(r) \):

\[
\hat{c}_0(k, r_\perp) = \int_{-\infty}^{\infty} dx c_0(x, r_\perp) \exp(-ikx)
\]  

(5)

The differential equation (3) describes a diffusion process within a complex-valued potential \( ik\varphi(r_\perp) \). Such equations can be numerically solved in a very efficient way. First, one discretizes the lateral coordinates into an \( N \times M \) grid, \( r_\perp \rightarrow \{y_j, z_k\} \) with \( 1 \leq j \leq N \) and \( 1 \leq k \leq M \), and one sorts the corresponding values \( \tilde{w}_{j,k} = \tilde{w}(y_j, z_k, t) \) into a linear vector \( \tilde{w} \). Then, the discrete solution of eq. (6) is given by the matrix equation

\[
\tilde{w}(k, r_\perp, t) = \exp \left[ t \left(D\Delta - ik\hat{\varphi}\right) \right] \cdot \tilde{w}_0(k, r_\perp)
\]  

(6)

where \( \Delta \) is the \( MN \times MN \) matrix of the discretized transversal Laplace operator corresponding to the ordering of the elements in \( \tilde{w} \) and encoding also the correct boundary conditions, and \( \hat{\varphi} \) is an \( MN \times MN \) diagonal matrix with elements \( v(y_j, z_k) \). The exponential function on the r.h.s. in eq. (6) is understood as matrix exponentiation. Numerically, eq. (6) is efficiently evaluated using programs such as MATLAB\textsuperscript{®} with built-in sparse matrix exponentiation capabilities. In this way, one solves eq. (6) for a discrete set of \( k \)-values and then calculates the final result for \( c(r, t) \) via a discrete version of eq. (2).

\[
c(x, r_\perp, t) = \delta k \sum_l \tilde{w}(k_l, r_\perp, t) \exp(ik_l x - Dk_l^2 t)
\]  

(7)

where the \( k_l \) are evenly spaced discrete values of \( k \) (with spacing \( \delta k \)), and the summation runs over a suitably chosen finite set of \( k \)-values. In the following, we will demonstrate this approach on two important examples.

### III. SHEAR FLOW

First, we consider a linear shear flow above an impermeable planar surface. The flow direction is the \( x \)-axis and the \( y \)-axis is oriented perpendicular to the surface. We consider initial conditions that are independent of the third axis (\( z \)-axis), so that the solution will also be independent of \( z \). We renormalize the coordinates in such a way that the flow profile has the simple form \( v(y) = y \). As initial concentration distribution we consider a symmetric Gaussian distribution,

\[
c_0(r, t) = \exp \left(-\frac{|r-r_0|^2}{2\sigma^2}\right)
\]  

(8)

within the range \(-20 < x < 80 \) and \( 0 < y < 20 \). Two different boundary conditions are considered at \( y = 0 \): A reflecting boundary, i.e. \( c'(x, y = 0, t) = \tilde{w}'(k, y = 0, t) \), where a prime denotes differentiation after \( y \); and a perfectly absorbing boundary, i.e. \( c(x, y = 0, t) = \tilde{w}(k, y = 0, t) = 0 \). For all other domain boundaries, we kept the concentration zero for all times (which is, of course, physically acceptable only for sufficiently small integration times). For each considered time value, we first find the discrete vector \( \tilde{w} \) via eq. (6) for 200 discrete values of \( k \) given by \( k_l = (\Delta k/200 - 0.5, 1 \leq l \leq 200 \), with \( \Delta k = \sqrt{20}/(0.1 + t) \). Using a discrete \( k \)-vector on a domain that scales with the inverse square root of time assures that the \( k \)-vector domain adopts to the diffusive spreading of the concentration profile along the \( z \)-axis. The number and spacing of the discrete \( k \)-values were chosen in such a way that at zero time the absolute difference between the exact initial concentration distribution \( c_0 \), eq. (8), and its discrete representation as given by eq. (7) was everywhere less than \( 2 \cdot 10^{-15} \) over the whole considered spatial domain.

After having found \( \tilde{w} \), we calculate \( c(r, t) \) using eq. (7) with the index \( l \) running from \(-200 \) to \( 200 \) and using the fact that due to the special initial conditions we have \( \tilde{w}(-k, r_\perp, t) = \tilde{w}(k, r_\perp, t) \). The computational results for both reflecting and absorbing boundary conditions for time values \( t = 2, 4, 6, 8 \) are shown in Fig. 1. One computation for one time value takes less than three seconds on a state-of-the-art desktop computer (Intel\textsuperscript{®} Xeon\textsuperscript{®} CPU ES-1650 v4 @ 3.6 GHz). Using the computed result for the absorbing boundary conditions allows us also to compute the relative absorption rate, \(-[\partial c(x, y = 0, t)/\partial y]/C_0 \), as a function of lateral coordinate \( x \) and time \( t \), where \( C_0 = \int dr c_0(r) \) is the initial total amount of matter. This relative absorption rate for the diffusion-convection process from Fig. 1 is shown in Fig. 2.

### IV. TAYLOR-ARIS DISPERSION

Taylor-Aris dispersion \[5, 7\] is an important diffusion-convection effect of great importance in microfluidics \[8, 9\]. It relates to the enhanced diffusive spreading of matter in a flow with an inhomogeneous flow profile. The classical example is the diffusion-convection in a cylindrical capillary with parabolic flow profile \( v(y) \),

\[
v(y) = 2\bar{v} \left(1 - \frac{y^2}{a^2}\right),
\]  

(9)

where \( y \) is now the radial coordinate (distance from capillary axis), \( \bar{v} \) the mean flow velocity, and \( a \) the capillary radius. For numerical purposes, it is best to write the cylindrical diffusion-convection equation in the form
FIG. 1. Numerical results for the solution of the diffusion-convection for an initially \((t = 0)\) Gaussian-distributed concentration. Horizontal axis is the \(x\)-axis, vertical axis is the \(y\)-axis. Flow direction is from left to right, with flow profile \(v = y\). The numerical value of the diffusion coefficient \(D\) is one. Upper half planes show the results for a reflecting surface, lower half planes for a perfectly absorbing surface.

\[
\frac{\partial (\sqrt{y}c)}{\partial t} = \left[ D \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{1}{4}y^2 \right) - v(y) \frac{\partial}{\partial x} \right] (\sqrt{y}c) \tag{10}
\]

so that the second-order differential operator on the r.h.s looks similar to the Laplace operator in Cartesian coordinates, which is most convenient for discretization.

The boundary conditions are: \(\partial_y c(x, y) = 0\) at \(y = a\), the capillary’s radius; \(\partial_y yc(x, y) = 0\) at \(y = 0\); and at the left and right boundary of the integration domain, we keep the concentration zero. Now, we can apply the same approach as described before, with the only difference that in the exponential on the r.h.s. of eq. \([6]\) appears an additional diagonal matrix with elements \(Dt/4y^2 \equiv -Dty^{-1/2}\partial_y y^{1/2}\), where we have used the last expression for discretization. For numerical integration, we discretize the \(\{x, y\}\)-domain into square elements of edge length 0.1 within the range \(-20 < x < 80\) and \(0 < y < 15\). As initial concentration distribution we consider a transversally homogeneous Gaussian distribution with unit variance, i.e. \(c_0(x, y) = \exp(-x^2/2)\). For each time value \(t\), we first use again eq. \([6]\) for finding the vectors \(\tilde{w}\) for a discrete set of \(k\)-values, and then compute the final solution \(c(x, y, t)\) via eq. \([7]\). For the actual example, we use the same set of discrete \(k\)-values as in the previous shear flow example. And as before, the calculation of the concentration distribution for one time value takes less than 2.5 seconds. The computational results for four time values \(t = 2, 4, 6, 8\) are shown in Fig. 3.

Taylor and Aris worked out an approximate solution for the concentration profile along the \(z\)-direction averaged over the capillary’s cross-section. For our initial distribution, this solution reads

\[
C(x, t) = \frac{1}{\sqrt{2D_{\text{eff}}t + 1}} \exp \left[ -\frac{(x - \bar{v}t)^2}{4D_{\text{eff}}t + 2} \right] \tag{11}
\]

where \(C(x, t)\) is the concentration integrated over the capillary’s cross section, and \(D_{\text{eff}}\) is an efficient diffusion coefficient given by

\[
D_{\text{eff}} = D + \bar{v}^2a^2\frac{1}{48D} = D \left( 1 + \frac{Pe^2}{192} \right), \tag{12}
\]

where \(Pe = 2\bar{v}a/D\) is the Péclet number for the diffusion in the capillary flow. A comparison between this approximate result and the exact one as calculated from our numerical solution of the convection-diffusion equation is shown in Fig. 4. The approximate result (bottom half of figure) strongly differs from the exact numerical result (top figure), which is to be expected for the large value of the Péclet number (\(Pe = 60\)) in our example.

FIG. 2. Absorption rate \(-[\partial c(x, y = 0, t)/\partial y]/C_0\) as a function of lateral coordinate \(x\) and time \(t\) for the solution shown in the bottom half planes of Fig. 1.
FIG. 3. Numerical results for the solution of the diffusion-convection equation for a parabolic flow in a cylindrical capillary of radius \( a = 15 \) with an initially Gaussian-distributed concentration along the horizontal \( z \)-axis. The vertical axis is the radial coordinate \( r \) (negative and positive values are identical radial positions). Flow direction is from left to right, mean flow speed \( \bar{v} \) is 3.375, and the numerical value of the diffusion coefficient \( D \) is again one.

V. DISCUSSION AND CONCLUSION

In summary, we have presented a numerical solver for a broad class of convection-diffusion problems. The importance of our approach is its extreme efficiency: using a standard desktop computer, one can solve complex diffusion-convection problems within seconds, which becomes particularly important when fitting parameters such as flow characteristics of diffusion coefficients against experimental data which requires the frequent repetition of computations for varying parameter sets.

In the future, it will be interesting to study whether our approach can be generalized to non-Cartesian geometries, for example to a flow along curved pipes. At the moment, our approach is restricted to geometries where we can split the Laplace operator into a transversal part independent on the coordinate of the flow direction, and the remaining part along the flow direction.

FIG. 4. Axial dispersion of matter along the capillary’s axis. Shown is the concentration integrated over the cross section, \( C(x, t) = 2\pi \int dy c(x, y, t) \). The top half of the image shows the exact result obtained from the numerical solution of the convection-diffusion equation, whereas the bottom half of the image shows the result of the Taylor-Aris approximation. Contour lines are at values 0.001, 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2 and 0.5.

ACKNOWLEDGMENTS

Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged (SFB 937, project A5). We thank Marcus Müller for many fruitful discussions.

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