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RANDOM WALK MODEL IN CASE OF ISO- AND DIAPYCNAL DIFFUSION

Daria Spivakovskaya*, Eric Deleersnijder†1 and Arnold W. Heemink††

*Delft University of Technology, Delft Institute of Applied Mathematics
Mekelweg 4, 2628 CD, The Netherlands
e-mail: D.Spivakovskaya@ewi.tudelft.nl

†Universite catholique de Louvain,
G. Lemaitre Institute of Astronomy and Geophysics (ASTR) & Centre for Systems Engineering and Applied Mechanics (CESAME),
Avenue G. Lemaitre 4, 1348 Louvain-la-Neuve, Belgium
e-mail: ericd@uclouvain.be

††Delft University of Technology, Delft Institute of Applied Mathematics
Mekelweg 4, 2628 CD, The Netherlands
e-mail: A.W.Heemink@ewi.tudelft.nl

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Abstract. *In order to efficiently simulate the advection-diffusion processes along and across density surfaces, we need to deal with the diffusivity tensor containing off-diagonal elements [16]. However, an application of Eulerian approach may lead to serious problems. In the present paper the Lagrangian model in case of a space-varying, general positive definite diffusivity matrix is developed. This random walk model is applied for two idealized test cases for which the analytical solutions are known.*

1 INTRODUCTION

It is common knowledge that large-scale diffusion processes in the ocean occur mostly along isopycnal surfaces, i.e. surfaces of equal density. There is also some diapycnal diffusion. The latter is associated with a diffusion flux orthogonal to isopycnal diffusion. The diapycnal and isopycnal diffusion fluxes are commonly parameterized *a la Fourier-Fick*, a formulation involving a diffusion tensor that is not isotropic [16]. As was seen by Beckers et. al. [2] many Eulerian discretizations of the isopycnal diffusion term yield discrete operators that are not monotonic - a problem which is particularly annoying. So, the Eulerian approach may not always be the best option.

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There are two basic approaches to solve the advection-diffusion problems usually called Eulerian and Lagrangian approaches. The first way describes what happens at a fixed point (or region) and is connected with the numerical solution (for instance, with the help of finite difference method) of partial differential equations. However, this method can lead to severe problems, for example, such as positiveness and mass conservation [12, 20]. The Lagrangian approach follows the particle through space at every time step. The movement of particle is modeled with the help of stochastic differential equation, which is consistent with the advection-diffusion equation. By simulating the positions of many particles the diffusion processes can be described. These random walk models allow to avoid a lot of problems, connected with the Eulerian approach, and this makes them very attractive in a number of applications (see, for instance, [9, 15, 19, 24]).

In most of the random walk models the diffusion matrix is diagonal (see, for instance, [25]). However for many realistic applications the diffusion matrix is not a diagonal [6, 10, 22]. In this paper, the random walk schemes associated with non-diagonal diffusivity tensors whose components vary in space are established. They are applied to test problems for which the analytical solution is known and to problems for which essential properties of the solution can be derived.

2 Lagrangian model for space varying diffusivity

2.1 Stochastic differential equations

To introduce the random walk model for the modelling of diffusion processes close to pycnoclines we will need some basic facts from the theory of stochastic differential equations. The stochastic differential equation in Îto sense has the following form (see,for instance, [1, 7, 14])

$$\begin{aligned} &d\boldsymbol{X}(t) = \boldsymbol{a}(t, \boldsymbol{X}(t))dt + \boldsymbol{\sigma}(t, \boldsymbol{X}(t))d\boldsymbol{W}(t) \\ &\boldsymbol{X}(0) = \boldsymbol{0} \end{aligned} \tag{1}$$

where $\boldsymbol{X} \in \mathbb{R}^d$ is a d-dimensional stochastic process, $\boldsymbol{a}$ is a d-dimensional vector function and $\boldsymbol{\sigma}$ is $d \times m$-matrix function and m-dimensional Brownian motion process $\boldsymbol{W}$ has the following statistics

$$\begin{aligned} &E(\boldsymbol{W}(t_2) - \boldsymbol{W}(t_1)) = 0 \\ &E((\boldsymbol{W}(t_4) - \boldsymbol{W}(t_3))(\boldsymbol{W}(t_2) - \boldsymbol{W}(t_1))) = 0, \quad t_4 \geq t_3 \geq t_2 \geq t_1 \\ &E((\boldsymbol{W}(t_2) - \boldsymbol{W}(t_1))(\boldsymbol{W}(t_2) - \boldsymbol{W}(t_1))) = (t_2 - t_1)\boldsymbol{I}_m, \quad t_2 \geq t_1, \end{aligned} \tag{2}$$

where $\boldsymbol{I}_m$ is $m \times m$ identity matrix.

Furthermore we will assume that the functions $\boldsymbol{a}$ and $\boldsymbol{\sigma}$ are continuous differentiable and the matrix $\boldsymbol{b} := \boldsymbol{\sigma}'\boldsymbol{\sigma}$ is of full of rank for every $(t, \boldsymbol{x}) \in [0, T] \times \mathbb{R}^d$. This particularly implies the existence and uniqness of the solution of (1).

The transition density $p(t, \boldsymbol{x})$ $(0 \leq t \leq T)$ to find a particle at position $\boldsymbol{y}$ at time s given that it was released at time $t = 0$ at location $\boldsymbol{0}$ can be obtained by solving the Fokker-Planck equation (the forward Kolmogorov equation) [1, 7, 14]:

$$\begin{aligned} &\frac{\partial p}{\partial t} + \sum_{i=1}^{d} \frac{\partial}{x_i}(a_i(t,\boldsymbol{x})p) - \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j}(b_{ij}(t,\boldsymbol{x})p) = 0, \\ &[p(t,\boldsymbol{x})]_{t=0} = \delta(\boldsymbol{x}-\boldsymbol{0}), \end{aligned} \tag{3}$$

where $\delta(\boldsymbol{x})$ denotes the Dirac function.

In the general case it is impossible to find the analytical solution of the SDE (2) and we have to use one of the numerical schemes. The simplest and more often used method is the Euler scheme [11, 13], that is an one-step approximation method of following form

$$\begin{aligned} &\overline{\boldsymbol{X}}_{i+1}^{\Delta t} = \overline{\boldsymbol{X}}_{i}^{\Delta t} + \boldsymbol{a}(t,\overline{\boldsymbol{X}}_{i}^{\Delta t})\Delta t + \boldsymbol{\sigma}(t,\overline{\boldsymbol{X}}_{i}^{\Delta t})\Delta \boldsymbol{W}_i, \\ &\overline{\boldsymbol{X}}_{0}^{\Delta t} = \boldsymbol{0}, \end{aligned} \tag{4}$$

where $i = 0,\ldots,L-1$, $\overline{\boldsymbol{X}}_{i}^{\Delta t} := \overline{\boldsymbol{X}}^{\Delta t}(t_i)$ is the numerical approximation of the position $\boldsymbol{X}(t_i)$, $t_i = i\Delta t$, $\Delta t = t/L$ is the time step of numerical integration and $\Delta \boldsymbol{W}_i$ are mutually independent Gaussian variable with zero mean and covariance matrix $\Delta t \boldsymbol{I}_m$.

In many cases we do not need to know the realization of the stochastic process $\boldsymbol{X}$, but the value of the functional

$$U = Eg(\boldsymbol{X}(t)). \tag{5}$$

To find this functional one can use the extrapolation method of second order which is based on the Euler method. First one can apply the Euler approximation $\overline{\boldsymbol{X}}^{\Delta t}$ generated by (4) with time step Δt to simulate the functional $\overline{U}^{\Delta t} = Eg(\overline{\boldsymbol{X}}^{\Delta t}(t))$. The one can simulate the functional $\overline{U}^{2\Delta t} = Eg(\overline{\boldsymbol{X}}^{2\Delta t}(t))$ for the double time step $2\Delta t$, and finally two results are combined to yield the approximation of (1)

$$\overline{U} = 2\overline{U}^{\Delta t} - \overline{U}^{2\Delta t}. \tag{6}$$

This method was proposed by Talay and Tubaro [23].

2.2 The random walk model for space varying diffusivity

Let us consider the following the following boundary value problem on $[0,T]\times\Omega$ ($\Omega \subset \mathbb{R}^d$ is domain of interest and Γ is its boundary)

$$\begin{aligned} &\text{in } \Omega \begin{cases} \dfrac{\partial C}{\partial t} = -\nabla \bullet (\boldsymbol{u}C - \boldsymbol{K} \bullet \nabla C) \\ \nabla \bullet \boldsymbol{u} = 0, \end{cases} \\ &\text{on } \Gamma \begin{cases} \boldsymbol{u} \bullet \boldsymbol{n} = 0 \\ (-\boldsymbol{K} \bullet \nabla C) \bullet \boldsymbol{n} = 0, \end{cases} \\ &[C(t,\boldsymbol{x})]_{t=0} = f(\boldsymbol{x}). \end{aligned} \tag{7}$$

Here $\boldsymbol{n}$ denotes the outward unit vector to Γ, $\boldsymbol{K}$ is the diffusivity tensor that is symmetric and positive definite (e..g [5]), function $f(\boldsymbol{x})$ represents the initial concentration and d is

the number of space dimensions. In practice $d = 1, 2, 3$, however the present Lagrangian approach can be applied for any integer value of d. Further we will assume that $f(\boldsymbol{x})$, where δ denotes the Dirac function. If we interpret the partial differential equation (7) as Fokker-Planck equation (3) than the concentration can be found with the help of the following stochastic differential equation

$$\begin{cases} d\boldsymbol{X}(t) = (\boldsymbol{u} + \nabla \bullet \boldsymbol{K})dt + \sqrt{2}\boldsymbol{V}d\boldsymbol{W}(t) \\ \boldsymbol{X}(0) = \boldsymbol{0}, \end{cases} \tag{8}$$

where $d\boldsymbol{X}(t) = \boldsymbol{X}(t+dt) - \boldsymbol{X}(t)$ is a displacement of vector $\boldsymbol{X}$, $\boldsymbol{K} = \boldsymbol{V}\boldsymbol{V}^T$. The density function $p(t, \boldsymbol{x})$ of the stochastic process $\boldsymbol{X}$ is the solution of the partial differential equation (7).

2.3 The kernel estimator

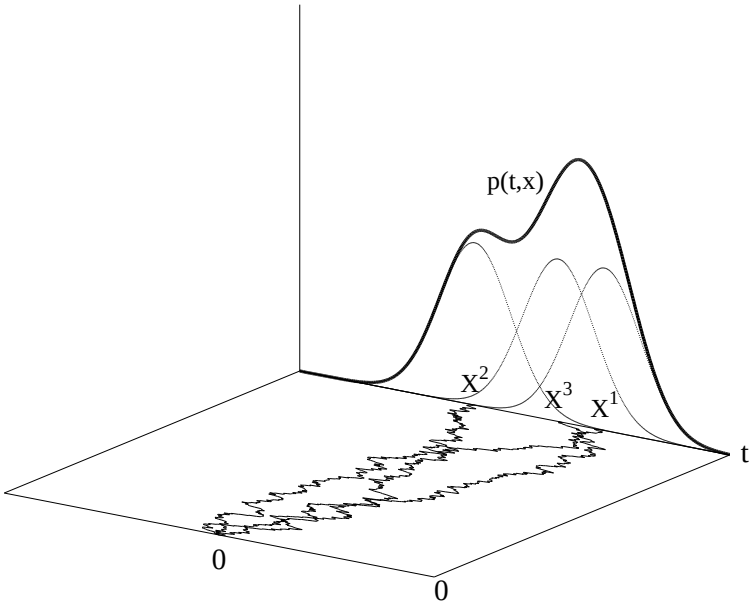


Figure 1: The kernel estimator

The main idea of the random walk model is to simulate the movement of many particles with the help of the numerical solution of the system of the stochastic differential equations (8) and then, from the obtained sample, construct the probability density function using the methods of non-parametric statistics called the kernel estimator(see Figure 1)

$$\widehat{p}(t, \boldsymbol{x}) = \frac{1}{N\lambda^d} \sum_{n=1}^{N} K\left(\frac{\overline{\boldsymbol{X}}^{(n)}(t) - \boldsymbol{x}}{\lambda}\right). \tag{9}$$

Here $K(\boldsymbol{u})$ is a kernel function (any function which satisfies the condition $\int K(\boldsymbol{u})d\boldsymbol{u} = 1$), λ is a positive number, usually called bandwidth and $\overline{\boldsymbol{X}}^{(n)}(T)$, $n = 1, \dots N$ is a sample from the approximation $\overline{\boldsymbol{X}}$ of the process $\boldsymbol{X}$. One can think of the kernel estimator as spreading of a "probability mass" of size $1/N$ associated with each data point about its neighborhood. Combining contributions from each data point means that in regions where there are many observations the density has a relatively large value and opposite in regions with only few observations.

Usually the kernel function is chosen to be a probability density function that is symmetric about zero, for instance Gaussian

$$K(\boldsymbol{u}) = (2\pi)^{-d/2} exp\left(-\frac{1}{2}\boldsymbol{u}^T\boldsymbol{u}\right), \tag{10}$$

or Epanechnikov function

$$K(\boldsymbol{u}) = \frac{1}{2}\nu_d^{-1}(d+2)(1-\boldsymbol{u}^T\boldsymbol{u})1_{\boldsymbol{u}^T\boldsymbol{u}\leq 1} \tag{11}$$

where $\nu_d = 2\pi^{d/2}/\{d\Gamma(d/2)\}$ is the volume of the unit d-dimensional sphere. This ensures that $\widehat{p}(t, \boldsymbol{x})$ is itself also a density. For example, constructing the kernel estimator, shown on figure 1, we used the 1-dimensional Gaussian kernel.

The error of the estimator (9) can be split into two parts: the error due to the numerical approximation (4) of the system (1) and the error due to kernel estimator. The first error depends on the choice of timestep Δt, while the second error depends on the number of particles. It is well known [17, 26] that the optimal bandwidth is given by

$$\lambda_{opt} \sim N^{-\frac{1}{d+4}}$$

provides the error due to kernel estimator of the following order

$$\epsilon(p) \sim N^{-\frac{2}{d+4}}. \tag{12}$$

It should be noticed that it is a little of sense to choose the very small timestep while the number of particles stays relatively small or opposite to start the numerical simulation for a lot of particles, while the timestep is not sufficient small. The further discussion and practical suggestions concerning the choice of parameters Δt and N can be found in [18].

2.4 The simulation of movement of particles near the boundaries

One should be careful simulating particles movement close to the boundaries. The diffusion tensor converges to zero in the neighbourhood of the boundary, therefore, the particle cannot theoretically cross the boundary. However, because of the discretizations of the stochastic system (1) particles can occur outside domain. To prevent this we need to take a time step that is sufficiently small. This procedure is described in [21]. The original

step time step is split in two, letting the particle travel two short time steps instead of a single big one. This process is repeated until the particle does not pass the boundary anymore. The result is that the particle trjectory bends along a certain boundary, but never crosses it.

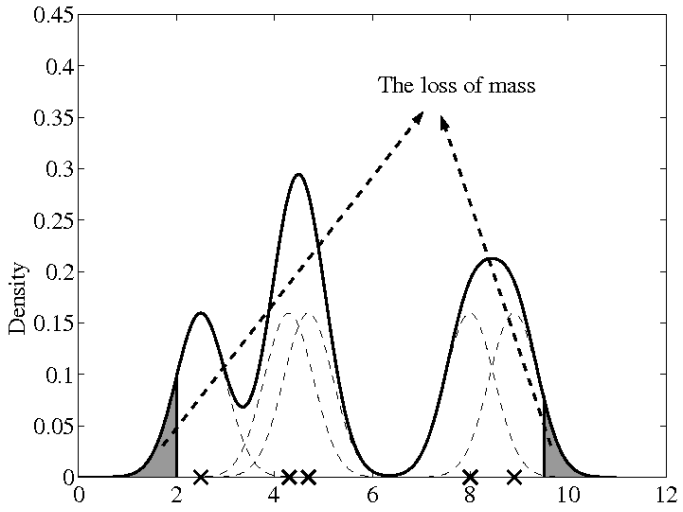


Figure 2: The loss of mass due to kernel estimator

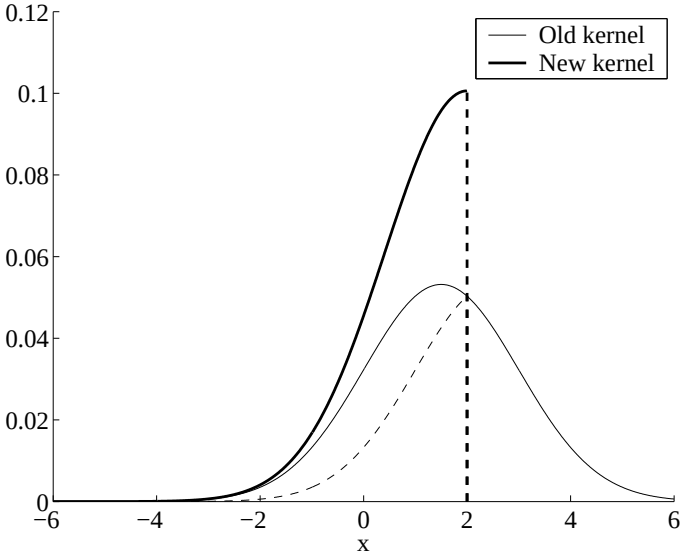


Figure 3: The transformation of the kernel function

Another potential risk connected with using of random walk is is that it may lead to the loss of total mass, if the particles are close to the boundary (see figure 2). To avoid

this problem we can use the following method, called box estimator: the space of interest is divided in a number of boxes and the estimation of the concentration is then obtained by multiplying the number of particles in each box with their mass and dividing the total mass by the size of the box. However this method is much less effective as compared with the kernel estimator method [8].

With the kernel estimator this problem can be also easily solved. When the particle is close to the boundary it is necessary to transform the kernel function in order to prevent the loss of mass. One kernel function transformation is shown on the figure 3. The main idea of this method is that, to prevent mass from being lost, we reflect the kernel function with regard to the boundary. The resulting function is the sum of the original kernel and this symmetric reflected function.

3 Test problem 1: Linear three-dimension iso- and diapycnal diffusion problem

First we discuss the Lagrangian method described above for linear iso and dia-pycnal diffusion problem that can be solved analytically. We consider a following three-dimensional problem for the concentration $C(t, \boldsymbol{x})$ (we suppose that the advection process can be neglected and $\boldsymbol{u} = \boldsymbol{0}$)

$$\frac{\partial C}{\partial t} = \nabla \bullet (\boldsymbol{K} \bullet \nabla C). \tag{13}$$

For a large-scale ocean model the formulation of diffusion model resorts to two diffusivity coefficients, K^i and K^d , which are the isopycnal and diapycnal dissusivities, respectively. In the principal axes, the diffusivity tensor reads

$$\boldsymbol{K} = \begin{pmatrix} K^i & 0 & 0 \\ 0 & K^i & 0 \\ 0 & 0 & K^d \end{pmatrix} \tag{14}$$

The z-principal axe is perpendicular to the isopycnal plane. To rotate the coordinate system associated with the isopycnal surface into the geodesic (x, y, z)-system we need two angles θ and γ ([16]) and the diffusivity tensor takes the form

$$\boldsymbol{K} = \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix}, \tag{15}$$

where

$$\begin{aligned}
K_{xx} &= K^i \cos^2\theta + \sin^2\theta(K^i \sin^2\gamma + K^d \cos^2\gamma) \\
K_{xy} &= K_{yx} = -\cos\gamma \sin\gamma \sin^2\theta(K^i - K^d) \\
K_{xz} &= K_{zx} = \cos\gamma \sin\theta \cos\theta(K^i - K^d) \\
K_{yy} &= K^i \cos^2\theta + \sin^2\theta(K^i \cos^2\gamma + K^d \sin^2\gamma) \\
K_{yz} &= K_{zy} = \sin\gamma \sin\theta \cos\theta(K^i - K^d) \\
K_{zz} &= K^i \sin^2\theta + K^d \cos^2\theta.
\end{aligned}$$

The domain of interest is assumed to be infinite,

$$-\infty < x < \infty, \quad -\infty < y < \infty, \quad -\infty < z < \infty,$$

and the initial concentration is a Dirac impulse, i.e.

$$C(0.\boldsymbol{x}) = \delta(\boldsymbol{x} - \mathbf{0}) = \delta(x-0)\delta(y-0)\delta(z-0).$$

It is useful to introduce dimensionless variables. The time and space coordinate are transformed as follows:

$$t' = \frac{t}{T}, \quad x' = \frac{x}{L_h}, \quad y' = \frac{y}{L_h}, \quad z' = \frac{z}{L_\nu}, \tag{16}$$

where T, L_h and L_ν denote the appropriate timescale, horizontal length scale and vertical length scale. It is convenient to define the latter in such a way that

$$T = \frac{L_h^2}{K^i} = \frac{L_\nu^2}{K^d}. \tag{17}$$

The ratio of the vertical length scale to the horizontal one, i.e. the aspect ratio, is

$$\alpha = \frac{L_\nu}{L_h}. \tag{18}$$

The concentration is scaled as follows:

$$C' = \frac{C}{1/(L_h^2 L_\nu)}. \tag{19}$$

The equation to be solved now reads

$$\begin{aligned} \frac{\partial C'}{\partial t'} = \quad & \frac{\partial}{\partial x'}\left(K'_{xx}\frac{\partial C'}{\partial x'} + K'_{xy}\frac{\partial C'}{\partial y'} + K'_{xz}\frac{\partial C'}{\partial z'}\right) + \\ & \frac{\partial}{\partial y'}\left(K'_{yx}\frac{\partial C'}{\partial x'} + K'_{yy}\frac{\partial C'}{\partial y'} + K'_{yz}\frac{\partial C'}{\partial z'}\right) + \\ & \frac{\partial}{\partial z'}\left(K'_{zx}\frac{\partial C'}{\partial x'} + K'_{zy}\frac{\partial C'}{\partial y'} + K'_{zz}\frac{\partial C'}{\partial z'}\right) \end{aligned} \tag{20}$$

with

$$\begin{aligned} K'_{xx} &= \frac{K_{xx}}{L_h^2/T} = \cos^2\theta + \sin^2\theta(\sin^2\gamma + \alpha^2\cos^2\gamma), \\ K'_{xy} = K'_{yx} &= \frac{K_{xy}}{L_h^2/T} = -\sin^2\theta\cos\gamma\sin\gamma(1-\alpha^2), \\ K'_{xz} = K'_{zx} &= \frac{K_{xz}}{L_h L_\nu/T} = \cos\theta\sin\theta\cos\gamma(\alpha^{-1} - \alpha), \\ K'_{yy} &= \frac{K_{yy}}{L_h^2/T} = \cos^2\theta + \sin^2\theta(\cos^2\gamma + \alpha^2\sin^2\gamma), \\ K'_{yz} = K'_{zy} &= \frac{K_{yz}}{L_h L_\nu/T} = \cos\theta\sin\theta\sin\gamma(\alpha^{-1} - \alpha), \\ K'_{zz} &= \frac{K_{zz}}{L_\nu^2/T} = \cos^2\theta + \alpha^{-2}\sin^2\theta. \end{aligned} \tag{21}$$

The initial condition is

$$C'(0, \boldsymbol{x}') = \delta(\boldsymbol{x}' - \mathbf{0}) = \delta(x' - 0)\delta(y' - 0)\delta(z' - 0). \tag{22}$$

From here on, only dimensionless variables quantities will be dealt with. So, for the sake of simplicity, the primes will be dropped.

The general form of the solution to the differential problem (20), (22) is

$$C(t, \boldsymbol{x}) = \frac{1}{(4\pi t)^{3/2}\sqrt{\det \boldsymbol{K}}} \exp\left[-\frac{\boldsymbol{x} \bullet \boldsymbol{K}^{-1} \bullet \boldsymbol{x}}{4t}\right]. \tag{23}$$

It is easily can be shown that

$$det(\boldsymbol{K}) = 1,$$

and the inverse matrix

$$K^{-1} = \begin{pmatrix} \tilde{K}_{xx} & \tilde{K}_{xy} & \tilde{K}_{xz} \\ \tilde{K}_{yx} & \tilde{K}_{yy} & \tilde{K}_{yz} \\ \tilde{K}_{zx} & \tilde{K}_{zy} & \tilde{K}_{zz}, \end{pmatrix}$$

where

$$\begin{aligned} \tilde{K}_{xx} &= \cos^2\theta + \sin^2\theta(\sin^2\gamma + \alpha^{-2}\cos^2\gamma), \\ \tilde{K}_{xy} &= -\sin^2\theta\cos\gamma\sin\gamma(1 - \alpha^{-2}), \\ \tilde{K}_{xz} &= \tilde{K}_{zx} = -\cos\theta\sin\theta\cos\gamma(\alpha^{-1} - \alpha), \\ \tilde{K}_{yy} &= \cos^2\theta + \sin^2\theta(\cos^2\gamma + \alpha^{-2}\sin^2\gamma), \\ \tilde{K}_{yz} &= \tilde{K}_{zy} = -\cos\theta\sin\theta\sin\gamma(\alpha^{-1} - \alpha), \\ \tilde{K}_{zz} &= \cos^2\theta + \alpha^2\sin^2\theta. \end{aligned} \tag{24}$$

Then, the solution may be rewritten as follows:

$$\begin{aligned} &C(t, x, y, z) = \frac{1}{(4\pi t)^{3/2}} \exp\{-\frac{1}{4t} \times [\\ &(z\cos\theta - \alpha^{-1}(y\sin\theta\sin\gamma + x\sin\theta\cos\gamma))^2 + \\ &(z\alpha\sin\theta + x\cos\theta\cos\gamma + y\cos\theta\sin\gamma)^2 + \\ &(x\sin\gamma - y\cos\gamma)^2]\} \end{aligned} \tag{25}$$

In the ocean, the slope of the isopycnal surfaces and the aspect ratio is usually small - which is why [3] suggested a simplified version of the isopycnal diffusivity tensor. For numerical experiments, the following values can be used [12]

$$\theta \approx 10^{-3} \approx \alpha. \tag{26}$$

The random walk model (8) has the form

$$\begin{aligned} dX &= \sqrt{2}V_{xx}dW_1 \\ dY &= \sqrt{2}V_{yx}dW_1 + \sqrt{2}V_{yy}dW_2 \\ dZ &= \sqrt{2}V_{zx}dW_1 + \sqrt{2}V_{zy}dW_2 + \sqrt{2}V_{zz}dW_3 \\ X(0) &= Y(0) = Z(0) = 0, \end{aligned} \tag{27}$$

where $\boldsymbol{K} = \boldsymbol{V}\boldsymbol{V}^T$ and the matrix $\boldsymbol{V}$ has the following form

$$\boldsymbol{V} = \begin{pmatrix} V_{xx} & 0 & 0 \\ V_{yx} & V_{yy} & 0 \\ V_{zx} & V_{zy} & V_{zz} \end{pmatrix}.$$

Here

$$\begin{aligned}
V_{xx} &= \sqrt{K_{xx}} \\
V_{yx} &= K_{xy}/\sqrt{K_{xx}} \\
V_{zx} &= K_{xz}/\sqrt{K_{xx}} \\
V_{yy} &= \sqrt{\frac{K_{yy}K_{xx} - K_{xy}^2}{K_{xx}}} \\
V_{zy} &= \frac{K_{yz}K_{xx} - K_{xy}K_{xz}}{\sqrt{K_{xx}(K_{xx}K_{yy} - K_{xy}^2)}} \\
V_{zz} &= \frac{K_{zz}K_{yy}K_{xx} + 2K_{xy}K_{xz}K_{yz} - K_{xz}^2K_{yy} - K_{yz}^2K_{xx} - K_{xy}^2K_{zz}}{\sqrt{K_{yy}K_{xx} - K_{xy}^2}}.
\end{aligned}$$

To calculate the concentration the extrapolation method (6) has been used with following parameters

$$\alpha = 10^{-3}, \quad \gamma = \pi/6, \quad T = 1.$$

Two cases were consideredwith with two different values of angle $\theta = 10^{-3}$ (the figures 4, 5) and $\theta = 5 \cdot 10^{-3}$ (the figures **??**, 6). From the figures it can be easily seen that the random walk model gives a good approximation of the exact solution in both cases.

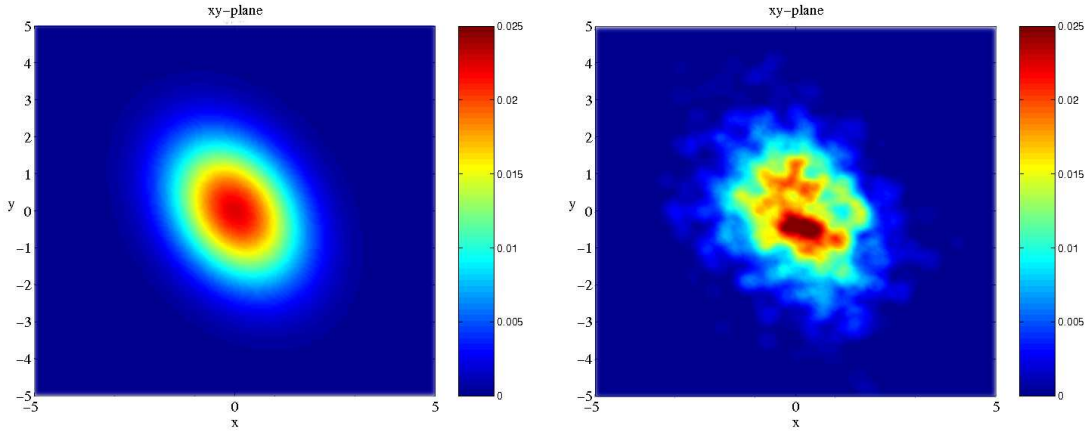
In table 1 the results of estimation of the concentration $C(t, \boldsymbol{x})$ ($\theta = 10^{-3}$) at given point $\boldsymbol{x} = (-1, 1.5, 0)$ are shown. For fixed value N of particle we calculate the statistical error using the formula

$$\epsilon_{\text{statistical}} = \frac{1}{M-1}\sqrt{\sum_{m=1}^{M}\left(C^{(m)}(t,\boldsymbol{x}) - \overline{C}(t,\boldsymbol{x})\right)^2}, \tag{28}$$

where M is a number of experiments (in our case the value $M = 30$ was taken), $C^{(m)}$, $m = 1, \ldots, M$ is the concentration obtained in the mth simulation and

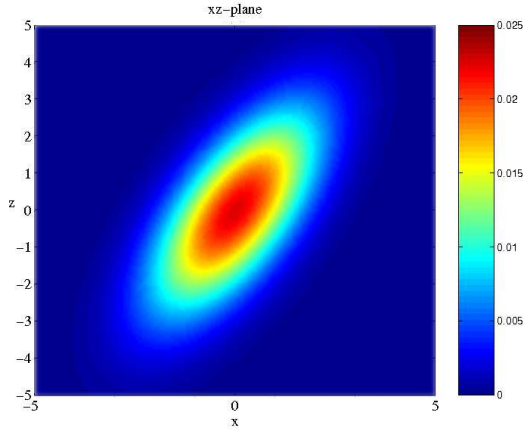
$$\overline{C}(t,\boldsymbol{x}) = \frac{1}{M}\sum_{m=1}^{M} C^{(m)}(T,\boldsymbol{x}). \tag{29}$$

The theoretical rate of the convergence of statistical error $\epsilon_{\text{statistical}}$ is $\mathcal{O}(N^{-2/7})$ (see the formula (12) for $d = 3$). From the figure 7 it can be seen that the statistical error agrees with the theoretical one.

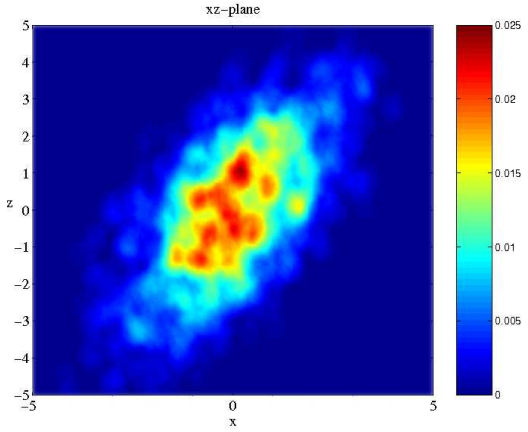


(a) (x, y)-plane

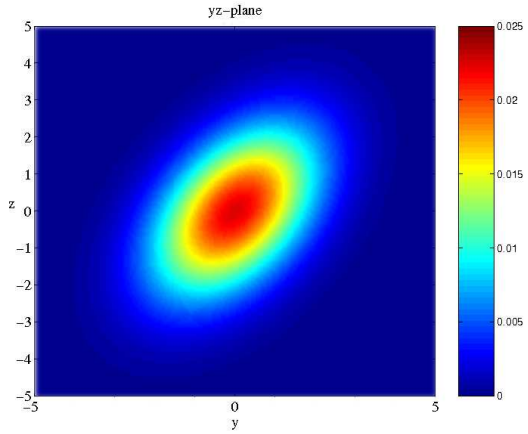
(b) (x, y)-plane



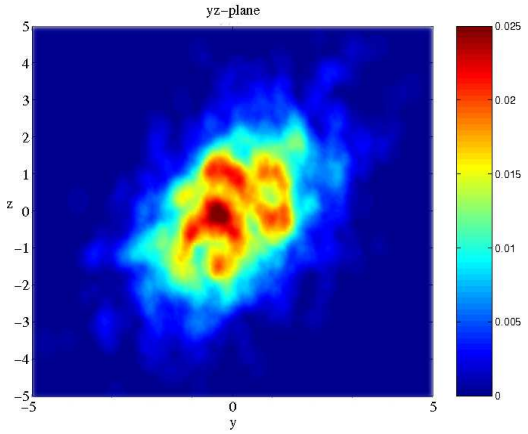
(c) (x, z)-plane



(d) (x, z)-plane

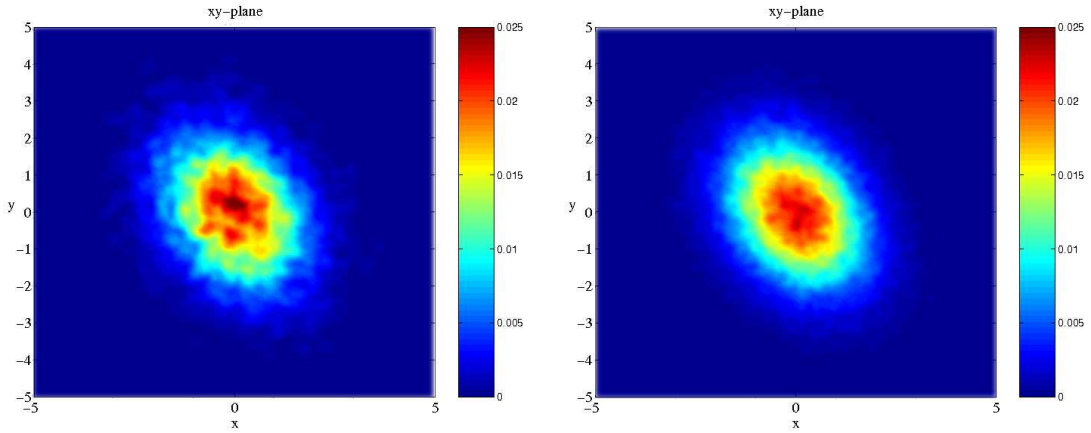


(e) (y, z)-plane



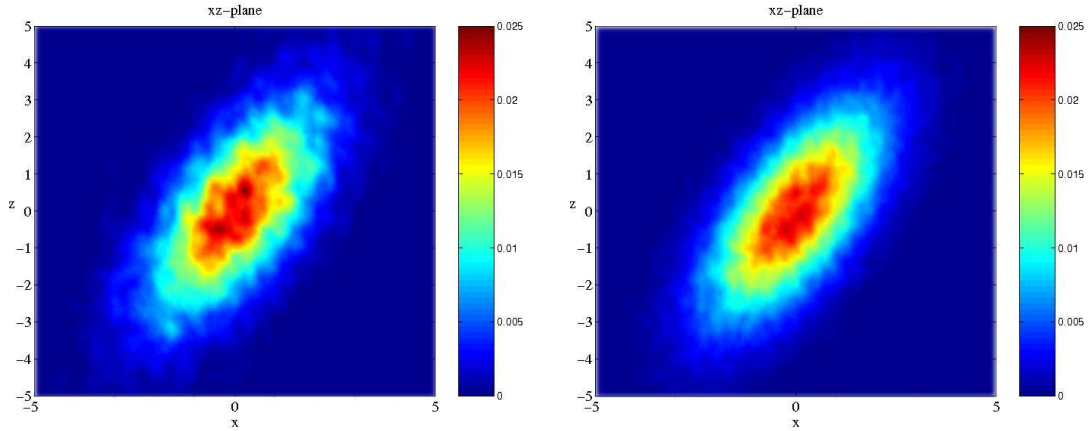
(f) (y, z)-plane

Figure 4: The exact and numerical (for $N = 10^4$) solutions



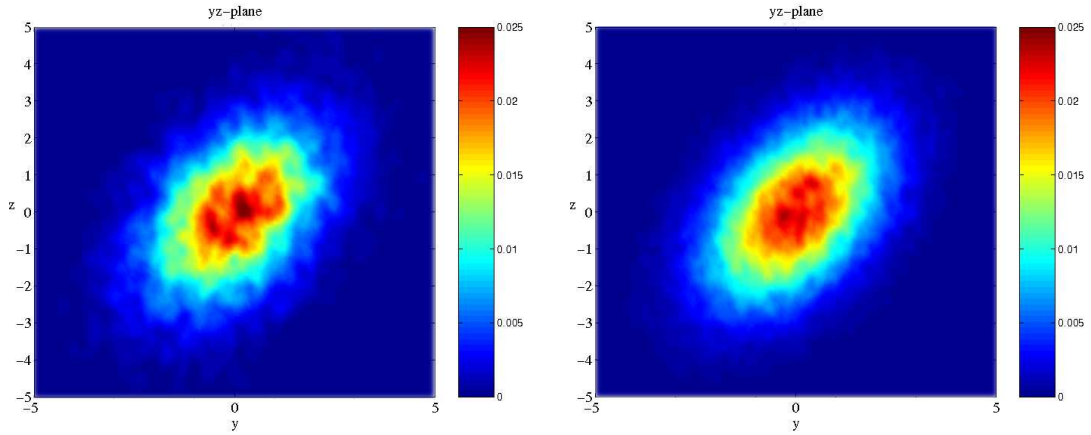
(a) (x, y)-plane

(b) (x, y)-plane



(c) (x, z)-plane

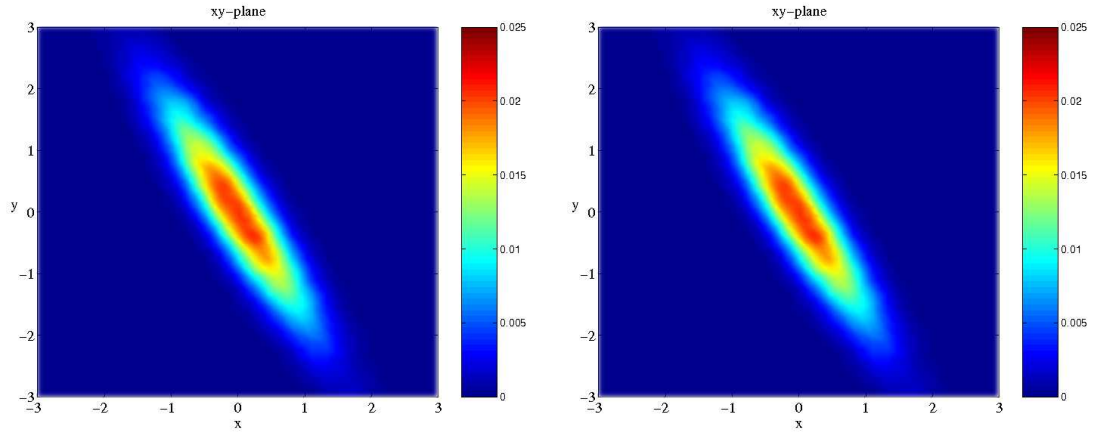
(d) (x, z)-plane



(e) (y, z)-plane

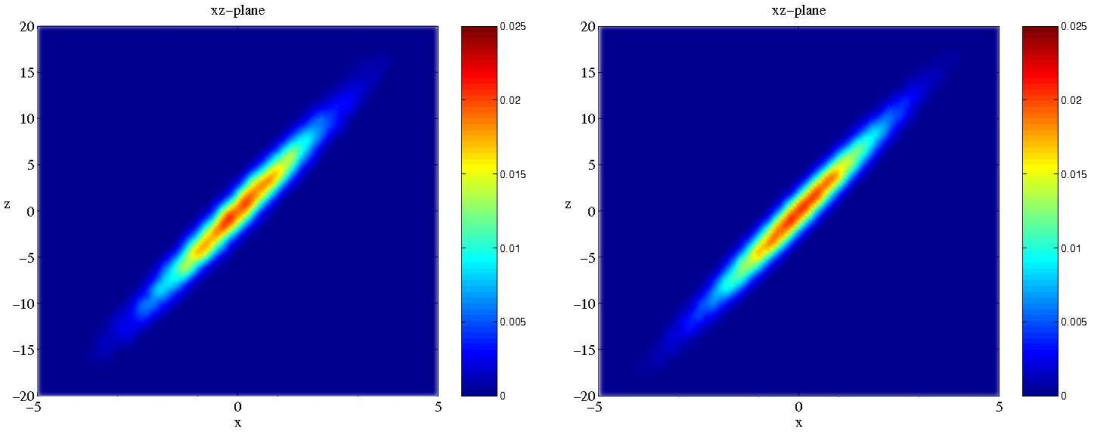
(f) (y, z)-plane

Figure 5: The numerical solutions for $N = 10^5$ particles (a), (c), (e) and for $N = 10^6$ particles (b), (c), (e)



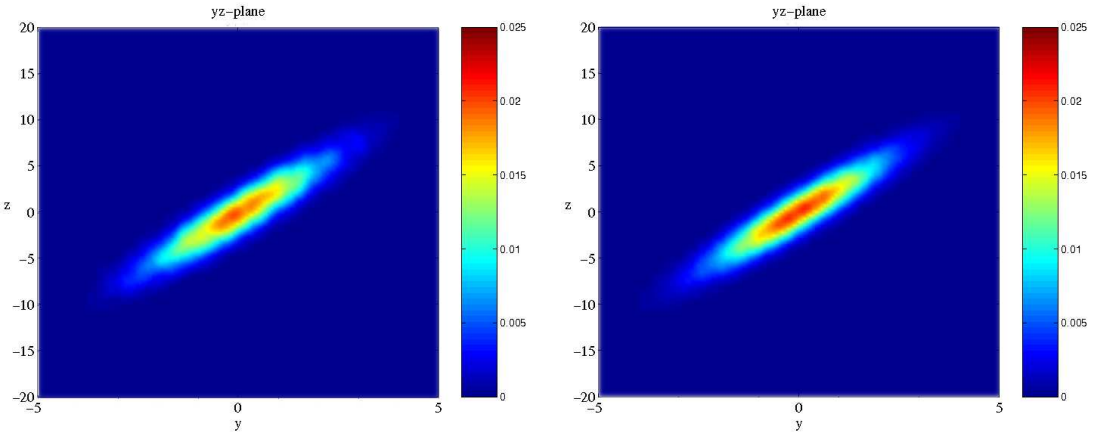
(a) (x, y)-plane

(b) (x, y)-plane



(c) (x, z)-plane

(d) (x, z)-plane



(e) (y, z)-plane

(f) (y, z)-plane

Figure 6: The numerical solutions for $N = 10^5$ particles (a), (c), (e) and for $N = 10^6$ particles (b), (c), (e)

N	Average value	Statistical error	Exact value
10^3	0.0103	0.0044	0.0099
$5 \cdot 10^3$	0.0091	0.0028	0.0099
10^4	0.0102	0.0023	0.0099
$5 \cdot 10^4$	0.0100	0.0011	0.0099
10^5	0.0098	0.0011	0.0099
$5 \cdot 10^5$	0.0099	0.0006	0.0099
10^6	0.0097	0.0005	0.0099

Table 1: The concentration at the location $\boldsymbol{x} = (-1, 1.5, 0)$

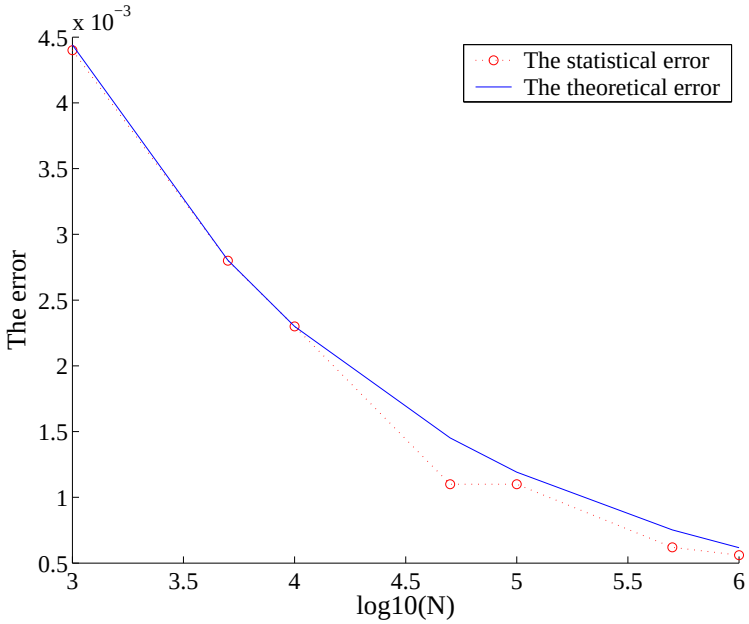


Figure 7: The comparison of the statistical error with the theoretical error

4 Test problem 2: The residence time in case of settling and diffusion problem

In the test case considered in the previous section the area of interest is assumed infinite. However, in the most applications we have to deal with the bounded area. That is the reason why it is important to test the random walk scheme for the model with space-varying diffusivity in the presence of boundaries. The example comsidered in this section, the model of settling and diffusion of sinking material (see Figure 8) has the solid and open boundaries. This model has been introduced and investigated in [4].

In case when the settling velocity w is nonzero, the analytical solution cannot be obtained. However, the exact solution for the adjoint problem of finding the residence time $\theta(z_0)$ is known [4]. To obtain the residence time $\theta(z_0)$, a unit amount of tracer is

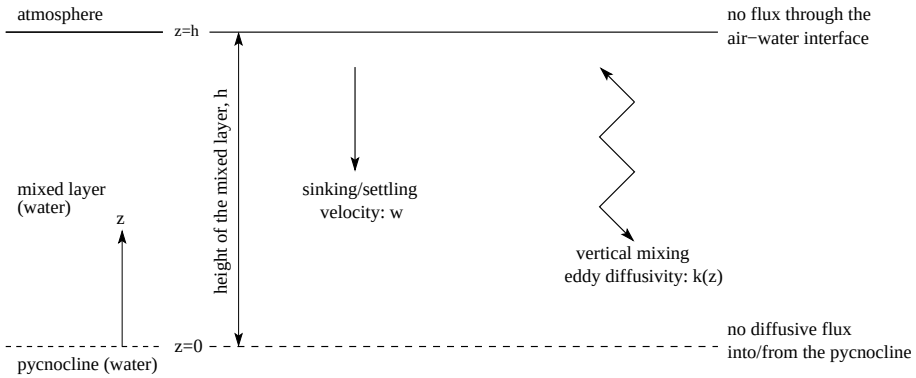


Figure 8: Sinking-diffusion model: illustration of its geometry, parameters and boundary conditions.Source: [4]

released at the initial time at a distance z_0 to the pycnocline. In other words, the initial condition reads

$$C(0, z) = \delta(z - z_0). \tag{30}$$

For the sake of generality, it is convenient to reformulate the problem above using dimensionless variables. The latter are defined to be

$$t' = \frac{t}{h/w}, \quad (z', z_0') = \frac{(z, z_0)}{h}, \quad k' = \frac{k}{\overline{k}}, \quad \theta' = \frac{\theta}{h/w}. \tag{31}$$

Finally, the Peclet number is defined to be

$$Pe = \frac{wh}{\overline{k}} \tag{32}$$

and because only the dimensionless variables will be used from now on we will drop all primes. Accordingly, the domain of the interest is now defined as $0 \leq 0$ and $0 \leq z \leq 1$.

As an example of the diffusivity profile the following function may be chosen

$$k(z) = 6z(1 - z). \tag{33}$$

This choice is consistent with the diffusion processes in the upper mixed layer. The diffusivity profile $k(z)$ should lead to zero in the neigboorhood of the bottom of the mixed layer and the maximum of the diffusivity should not occur at surface. It is clear that the diffusivity function (33) satisfies these conditions.

In this test problem the random walk model is presented by the equation

$$\begin{aligned} dZ &= \left(w + \frac{\partial k}{\partial z} \right) dt + \sqrt{2k(z)} dW(t) \\ Z(0) &= z_0 \end{aligned} \tag{34}$$

We release the bunch of particles at the position z_0 and model the movement of particles using the Euler scheme analogously to (34). For each realization of the particle track we calculate the residence time, i.e. how much time the particle needs to leave the domain. By averaging the results, the average residence time can be obtained. The numerical results for $N = 10^3$, $N = 10^4$ and $N = 10^5$ are shown on the figure 10 (b)-(d). For this numerical simulation the following parameters were used

Timestep	Δt	10^{-4}
Peclet number	Pe	5.

Comparing the exact solution (figure 10 (a)) with the numerical solutions (figure 10 (b)-(d)) it is clear that already the numerical solution for $N = 10^3$ particles provides a good approximation of the exact solution.

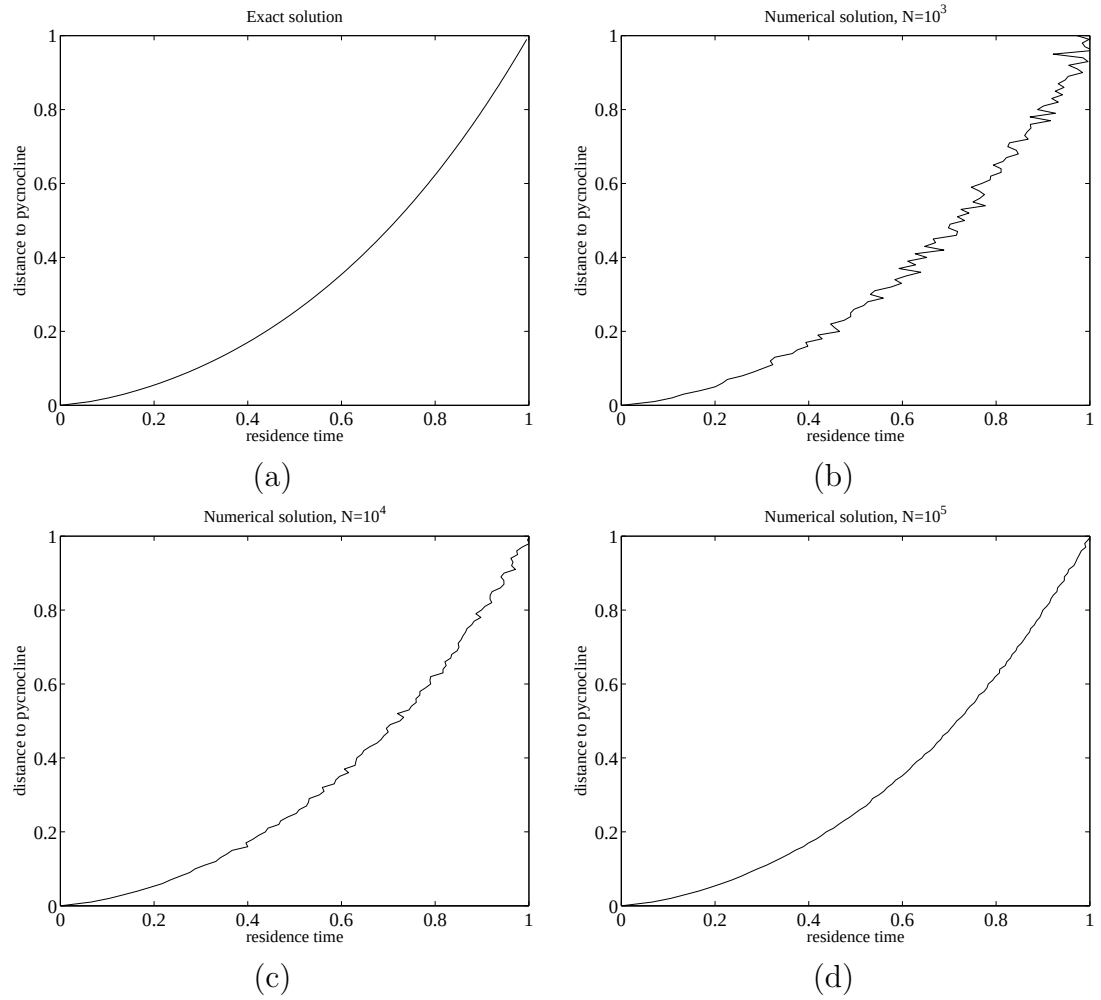


Figure 9: The residence time (a) exact (b) $N = 10^3$ (c) $N = 10^4$ (d) $N = 10^5$

5 Conclusion

In this paper the random walk model for the simulation of diffusion processes with space-varying, general positive definite diffusivity, particularly for iso and dia-pycnal diffusion, is introduced and analyzed. The Lagrangian approach is applied for linear idealised test problems, for which the exact solution is known. The random walk model is also tested for a sinking-diffusion model and it is shown that the Lagrangian approach can also be used for the solution of the adjoint problem. i.e. computing the residence time. The results obtained show that this random walk model may be a good alternative to commonly-used Eulerian models.

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