NUMERICAL SIMULATIONS OF DIFFUSION IN CELLULAR FLOWS AT HIGH PÉCLET NUMBERS

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Abstract. We study numerically the solutions of the steady advection-diffusion problem in bounded domains with prescribed boundary conditions when the Péclet number $Pe$ is large. We approximate the solution at high, but finite Péclet numbers by the solution to a certain asymptotic problem in the limit $Pe \to \infty$. The asymptotic problem is a system of coupled 1-dimensional heat equations on the graph of streamline-separatrices of the cellular flow, that was developed in [21]. This asymptotic model is implemented numerically using a finite volume scheme with exponential grids. We conclude that the asymptotic model provides for a good approximation of the solutions of the steady advection-diffusion problem at large Péclet numbers, and even when $Pe$ is not too large.

1. Introduction. In the simply connected, bounded domain $\Omega \subset \mathbb{R}^2$ consider the steady advection-diffusion problem

$$\varepsilon \Delta \phi^\varepsilon - \mathbf{v} \cdot \nabla \phi^\varepsilon = 0,$$

where $\phi^\varepsilon$ is a temperature. We assume here that the time-independent flow $\mathbf{v}$ is incompressible: $\nabla \cdot \mathbf{v} = 0$, and it does not penetrate through the boundary of $\Omega$: $\mathbf{v} \cdot \mathbf{n} = 0$ at $\partial \Omega$. The small parameter $\varepsilon = Pe^{-1} \ll 1$ is the inverse of the Péclet number, the relative strength of the advection, compared to the diffusion. Since the flow $\mathbf{v}$ is assumed to be incompressible, there is a stream function $\Psi(x, y)$ such that

$$\mathbf{v} = \nabla^\perp \Psi = \left( \frac{\partial \Psi}{\partial y} - \frac{\partial \Psi}{\partial x} \right).$$

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Equation (1) is supplemented by the Dirichlet boundary data:
\[ \phi^\varepsilon(x, y) = T_0(x, y), \quad (x, y) \in \partial \Omega, \] (3)
where \( T_0 \) is a given temperature. We also will consider the Neumann boundary conditions on a part of the boundary of \( \Omega \):
\[ \phi^\varepsilon(x, y) = T_0(x, y), \quad \text{if} \quad (x, y) \in \Gamma_1, \quad \frac{\partial \phi^\varepsilon}{\partial n}(x, y) = 0, \quad \text{if} \quad (x, y) \in \Gamma_2, \] (4)
where \( \partial \Omega = \Gamma_1 \cup \Gamma_2 \). Boundary conditions (4) arise naturally in periodic homogenization theory [8].

Condition \( \mathbf{v} \cdot \mathbf{n} = 0 \) at \( \partial \Omega \) implies that \( \partial \Omega \) belongs to a level-set of \( \Psi \). Without loss of generality we may assume that \( \Psi(x, y) = 0, \quad \text{if} \quad (x, y) \in \partial \Omega \). The level set \( \{(x, y) | \Psi(x, y) = 0\} \) decomposes \( \Omega \) into a union of cells, separated by separatrices, as depicted on Figure 2. This decomposition is the characteristic property of cellular flows, that we study here.

Advection-diffusion at high Péclet numbers is one of the classical fundamental problems in physics, mathematics and engineering, see e.g. [24, 21] and references therein. The two-dimensional flows are used extensively in models of ocean and atmospheric circulation [4], because density variation leads to vertical stratification of flows. In particular, streamline diffusion models [20, 22] are similar to the model discussed in this paper. These streamline diffusion models are used to assess circulation of chemicals, temperature, and migration of plankton (see, e.g. [27, 12, 13] and references therein). Significant effort was put to evaluate the effective diffusivity of cellular flows at large Péclet numbers, because it characterizes the rate of diffusive transport in turbulence [2, 8]. In particular, [8, 9, 14, 17] are concerned with finding bounds on the effective diffusivity. In [23, 26] the boundary layer analysis is used to show the asymptotic behavior of the effective diffusivity in the special case of symmetric square cells.

A number of numerical methods for advection-diffusion problem at high Péclet numbers have been also proposed and developed. There are two classes of common approaches to deal with this problem. One of them is local mesh refinement [18, 1]. The main idea of this class is to set more grid points where they are required, and hence adaptive grid generating methods based on a posteriori error estimates are used. The other class is obtained by modifying the discrete operator. The upwind method [16], the streamline-diffusion method [15, 6] and other artificial viscosity methods fall into this class. The key weaknesses of these methods are that they become less accurate and/or less stable as \( \text{Pe} \to \infty \) (see e.g. [10, 19, 5]).

We present here a numerical method which accuracy improves as \( \text{Pe} \to \infty \). Moreover, its computational complexity is independent of the Péclet number. The reason for these two facts is simple, and it is as follows. The numerical method is based on an asymptotic model proposed in [21]. This model arises as \( \text{Pe} \to \infty \). It was shown [21] that the solution of (1)-(3) converges to the solution of a certain system of the one-dimensional heat equations on a graph as \( \text{Pe} \to \infty \). Thus the solution of the system of the heat equations becomes more and more accurate as \( \text{Pe} \to \infty \). Further, since any numerical method for the asymptotic system of heat equations is independent of the Péclet number, we conclude that its computational complexity is independent of \( \text{Pe} \).

The analysis of [21] implies that their asymptotic model is accurate at very large Péclet numbers. The main motivation for our work here is to assess numerically the accuracy of this model at intermediate Péclet numbers. We therefore compare the
solutions of the asymptotic model of [21] with numerical simulations, obtained in the MATLAB PDE Toolbox™. We observe that the asymptotic model approximates well the solution of (1)-(3) even when the Péclet number is about 10^2.

The paper is organized as follows. In the next section, the summary of the asymptotic model [21] is presented. The asymptotic system of heat equations is solved numerically using a finite volume method on exponential grids. We discuss its numerical implementation in Section 3. We then perform numerical tests in order to determine accuracy of the asymptotic model. The numerical results are presented in Section 4.

2. Asymptotic model. At high Péclet numbers the numerical solution to (1) becomes expensive if a discretization method does not take into account diffusive boundary layers. These boundary layers arise where the stream function \( \Psi(x, y) \) for the incompressible flow \( \mathbf{v} \) (see (2)) vanishes: \( \Psi(x, y) = 0^2 \). We propose here to use a detailed analysis of boundary layers for (1) developed in [21] as \( \varepsilon = 1/\text{Pe} \to 0 \).

Let us summarize some results obtained in [21]. As \( \varepsilon \) tends to zero, the solution to (1) converges to a solution of a coupled one-dimensional heat equations on a graph. The edges of the graph, that arise in this diffusion on the graph model, are associated with the separatrices between different flow cells, and the vertices of this graph are associated with saddle-points of the stream function \( \Psi(x, y) \). See e.g. the two-cell case on Figure 1.

The diffusion on the graph model is independent of Péclet number, and the relative \( H^1 \) error between the solution to (1) and the solution to the diffusion on the graph model was estimated a priori as \( O(\varepsilon^{1/2}) \) (Theorem 6.1 in [21]). Let us first describe the simplest case, when we have just two vertices.

2.1. The two-cell case. We describe the asymptotic problem first on the simplest example of a domain \( \Omega \) that consists of two cells \( C_1 \) and \( C_2 \) depicted in the left figure of Figure 1. We denote by \( e_{\theta_0} = \partial \Omega \cap \partial C_j, \ j = 1, 2 \), the part of the boundary of \( \Omega \) along the cell \( C_j \) and by \( e_{12} \) the common edge of the two cells. We also introduce the boundary layer coordinates \( h \) and \( \theta_{12}, \theta_{\theta_0}, j = 1, 2 \). The coordinate \( h = \Psi/\sqrt{\varepsilon} \), and it represents the (rescaled) distance to the level-set \( \{(x, y) | \Psi(x, y) = 0\} \). The coordinate \( \theta_{12} \) represents parametrization along the edge \( e_{12} = \{h = 0\} \cap \{0 \leq \theta_{12} \leq l_{12}\} \), while the coordinates \( \theta_{\theta_0} \) parameterize along the boundaries \( e_{\theta_0} = \{h = 0\} \cap \{l_{12} \leq \theta_{\theta_0} \leq l_{\theta_0}\} \). We first solve the heat equation “along \( e_{12}^2 \): 

\[
\frac{\partial f_{12}}{\partial \theta_{12}} = \frac{\partial^2 f_{12}}{\partial h^2}, \quad h \in (R), \quad 0 \leq \theta_{12} \leq l_{12}
\]  

Recall that \( \Psi(x, y) = 0 \), if \( (x, y) \in \partial \Omega \). Thus there are boundary layers near \( \partial \Omega \).
with a prescribed initial data \( f_{12}^0 \) and
\[
  f_{12}(h, \theta) \to C^\pm, \quad \text{as } h \to \pm \infty. \tag{6}
\]
A natural way to impose this decay to constants is to prescribe homogeneous Neumann boundary conditions:
\[
  \lim_{h \to \pm \infty} \frac{\partial f_{12}(h, \theta_{12})}{\partial h} = 0. \tag{7}
\]
Then we solve two half-space problems “along the outer boundaries \( e_{j0} \)” with the prescribed Dirichlet data that comes from (3):
\[
  \frac{\partial f_{10}}{\partial \theta_{10}} = \frac{\partial^2 f_{10}}{\partial h^2}, \quad -\infty < h \leq 0, \quad l_{12} \leq \theta_{10} \leq l_{12} + l_{10} \tag{8}
\]
and
\[
  \frac{\partial f_{20}}{\partial \theta_{20}} = \frac{\partial^2 f_{20}}{\partial h^2}, \quad 0 \leq h < \infty, \quad l_{12} \leq \theta_{20} \leq l_{12} + l_{20} \tag{9}
\]
with (7) \( h = \pm \infty \), and with the Dirichlet data \( f_{j0}(0, \theta_{j0}) = T_0(\theta_{j0}) \) at \( h = 0 \). The initial data for (8) and (9) comes from (5):
\[
  f_{10}(h, l_{12}) = f_{12}(h, l_{12}), \quad -\infty < h \leq 0, \tag{10}
\]
\[
  f_{20}(h, l_{12}) = f_{12}(h, l_{12}), \quad 0 \leq h < \infty.
\]
Finally we glue together the functions \( f_{10}(h, l_{10}), h \leq 0 \) and \( f_{20}(h, l_{20}), h \geq 0 \):
\[
  f_{12}^g(h) = \begin{cases} f_{10}(h, l_{10}), & -\infty < h \leq 0 \\ f_{20}(h, l_{20}), & 0 \leq h < \infty \end{cases} \tag{11}
\]
The asymptotic problem is to construct a periodic solution of the above, that is, find a function \( f_{12}^g(h) \) so that \( f_{12}^g(h) = f_{12}(h), \quad h \in \mathbb{R} \). This problem is described schematically in the right figure of Figure 1. There exists a unique function \( f_{12}^g \in L^2(\mathbb{R}) \) such that \( f_{12}^g = f_{12}^g \) (Proposition 5.1 in [21]).

An alternative approach to the proof of existence of a periodic solution of (5)-(11), that is somewhat less transparent in the two-cell case but is easier to generalize to the case of multiple cells is as follows. Let us define the operator \( L_{12} : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \) by \( L_{12} : f_{12}^0 \to f_{12}(l_{12}) \), that is, the solution operator of (5). We also let \( L_{10} \) and \( L_{20} \) be solution operators for (8) and (9), respectively with homogeneous boundary data \( T_0 = 0 \). We introduce an operator \( \mathcal{L} = L_{12} \otimes L_{10} \otimes L_{20} \) defined on \( L^2(\mathbb{R}) \times L^2(\mathbb{R}_-) \times L^2(\mathbb{R}_+) \) as
\[
  \mathcal{L} \begin{pmatrix} f_{12}^0 \\ f_{10} \\ f_{20} \end{pmatrix} = \begin{pmatrix} L_{12} f_{12}^0 \\ L_{10} f_{10} \\ L_{20} f_{20} \end{pmatrix}.
\]
We also define a redistribution operator \( \mathcal{R} \) on the same space \( L^2(\mathbb{R}) \times L^2(\mathbb{R}_-) \times L^2(\mathbb{R}_+) \) as
\[
  \mathcal{R} \begin{pmatrix} f_{12} \\ f_{10} \\ f_{20} \end{pmatrix} = \begin{pmatrix} \mathcal{G}[f_{10}, f_{20}] \\ \mathcal{R}_- f_{12} \\ \mathcal{R}_+ f_{12} \end{pmatrix}, \tag{12}
\]
Above the operators \( \mathcal{R}_\pm \) restrict a function defined on \( \mathbb{R} \) to the positive and negative semi-axes, respectively, while the gluing operator \( \mathcal{G} \) glues together two functions defined on those axes:
\[
  \mathcal{G}[f_-, f_+](h) = \begin{cases} f_-(h), & h \leq 0, \\ f_+(h), & h > 0, \end{cases}
\]
(13)
as in (11). Then the existence of a unique function \( f_{12}^0 \in L^2(\mathbb{R}) \) such that \( f_{12}^0 = f_{12}^g \) means

\[
\mathcal{R}L \begin{pmatrix} f_{12}^0(h) \\ f_{10}(h, l_{12}) \\ f_{20}(h, l_{12}) \end{pmatrix} + \begin{pmatrix} g(h) \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} f_{12}^0(h) \\ f_{10}(h, l_{12}) \\ f_{20}(h, l_{12}) \end{pmatrix},
\]

where the function \( g(h) \) is obtained by solving (5)-(11) with \( f_{12}^0 = 0 \) and inhomogeneous boundary conditions.

### 2.2. The general multiple-cell case.

Equation (14) has a straightforward generalization to the case of more than two cells. Suppose the domain \( \Omega \) consists of a finite number of cells. The asymptotic model is described in terms of an oriented graph constructed using the stream function \( \Psi \) as shown on Figures 2. The vertices of this graph are associated with the saddle points of \( \Psi \). The edges \( e_{ij} \) of the graph are associated with the separatrices of the the stream function. The direction of an edge is determined by the direction of the velocity field on the corresponding separatrix. The length of an edge is determined by the length of the separatrix in the boundary layer coordinate \( \theta \) associated with \( \Psi \). The boundary edges are those that are associated with the separatrices at the boundary of the domain. The cells \( C_i \) are quadrangles bounded by minimal cycles of the graph. The interior edges (drawn as solid arrows on the right figure of Figure 2) are indexed so that a common edge of two cells \( C_i \) and \( C_j \) is denoted by \( e_{ij} \). The boundary edges (drawn as dotted arrows on the right figure of Figure 2) are indexed so that the outer part of a boundary cell \( C_i \) is denoted by \( e_{i0} \). The boundary value problem is:

- [ii] Given the values of the temperature \( T_0 \) on the boundary edges \( e_{i0} \), determine the values of the temperature \( f_{ij} \) on all the edges. Note that the value of \( f_{ij} \) may vary along each edge.
- [iii] Given the values of \( f_{ik} \) on all the edges, find the solutions \( f_i \) of the Childress' problem [3] for each cell \( C_i \):

\[
\begin{cases}
\frac{\partial^2 f_i}{\partial h^2} - \frac{\partial f_i}{\partial \theta} = 0, \\
h \in [0, \infty), \quad \theta \in [-\infty, +\infty[,
\end{cases}
\]

\[
f_i(h = 0, \theta) = f_{ik}(\theta),
\]

\[
\lim_{h \to \infty} \frac{\partial f_i}{\partial h}(h, \theta) = 0,
\]

\[
f_i(h, \theta + l_i) = f_i(h, \theta) + l_i,
\]

where the index \( k \) takes four values of the adjacent cells, \( l_i = l_{ik_1} + \cdots + l_{ik_4} \) is the length in \( \theta \) of the four edges \( e_{ik_1}, \ldots, e_{ik_4} \), bounding \( C_i \), and \( f_{ik}(\theta) = f_{ik}(\theta), \ldots, f_{ik}(\theta) = f_{ik}(\theta) \) are the values of the temperature on respective edges.
• [iii] When any two cells $C_i$ and $C_j$ share a common edge, the normal derivatives from the left and from the right match point-wise on this edge:

$$\frac{\partial f_i}{\partial h}\big|_{h=0} + \frac{\partial f_j}{\partial h}\big|_{h=0} = 0 \text{ on } e_{ij}.$$  

There exists a unique solution of the boundary value problem [i], [ii], [iii] (Theorem 5.2 in [21]). A generalization of the method in [21] allows to treat other boundary conditions. For example, the case where on a part of $\partial \Omega$ homogeneous boundary conditions are prescribed, and we use Dirichlet boundary conditions on the other part of $\partial \Omega$.

3. Numerical implementation. For simplicity of comparison with MATLAB™ we focus on the case where the domain $\Omega$ of the problem (1) is the square $(0, \pi) \times (0, \pi)$ in $\mathbb{R}^2$. We choose $\Psi(x, y) = \sin(k_1 \pi x) \sin(k_2 \pi y)$ with integer $k_1$ and $k_2$. The domain $\Omega$ will contain either one ($k_1 = 1, k_2 = 1$), two ($k_1 = 2, k_2 = 1$), or four flow cells ($k_1 = 2, k_2 = 2$). The second boundary layer coordinate is defined as before: $h = \Psi/\bar{\epsilon}$.

In the case of two cells the only interior separatrix is the line $x = \frac{\pi}{2}$ (as on the left plot of Figure 5). For the four-cell problem the interior separatrices are the lines $x = \frac{\pi}{2}$ and $y = \frac{\pi}{2}$ (as on the right plot of Figure 5).

With a slight abuse of notation we use $f$ for the periodic solutions of (15) as well as for the numerical approximations of (15) in the rest of this paper.

For the spatial discretization we use a finite volume method [7], and we assume that the solution is piecewise constant. The finite difference backward Euler method is used for the temporal discretization.

3.1. Boundary layer coordinates. It was shown in e.g. [3, 8, 21] that the solution of (1)-(4) can be well-approximated by the stretched asymptotic boundary layer solution $f^*(x, y) = f(h(x, y), \theta(x, y))$, where $f(h, \theta)$ is the unique solution of the Childress’ problem (15). In this section we briefly discuss the construction of the local coordinates $(h, \theta)$. We concentrate on the 2-cell case (see the left plot in Fig. 5), because the one-cell case is discussed in [8, p.349], and the four-cell case is similar to the one-cell case.

Here, we consider a cellular flow in the domain $\Omega = \{(x, y) : x \in [0, \pi], \ y \in [0, \pi]\}$ with the stream function $\Psi(x, y) = \sin 2x \sin y$, for which the level lines $\Psi = 0$ are separatrices. We introduce a new coordinate system $(x, y) \rightarrow (\Psi, \theta)$ from the square $[0, \pi] \times [0, \pi]$ to the region $\Psi \in \mathbb{R}$, $0 \leq \theta \leq 10$, so that $\nabla \Psi \cdot \nabla \theta = 0$ near the boundary of the square and $|\nabla \Psi| = |\nabla \theta|$ on the boundary of the square. The pair $(h, \theta) = \left(\frac{\Psi}{\sqrt{\epsilon}}, \theta\right)$ is called the boundary layer coordinates. The variable $h$ is simply $h(x, y) = \Psi(x, y)/\sqrt{\epsilon}$. The circulation or the angle variable $\theta$ is defined from two conditions: a) for any $(x, y)$ we have $\nabla \theta(x, y) \perp \nabla \Psi(x, y)$, and b) if $(x, y)$ is a point on a separatrix, then $|\nabla \theta(x, y)| = |\nabla \Psi(x, y)|$. Note that $\theta$ is not the arclength parameter. In our two-cell case we obtain the following values of $\theta$. For $x = \pi/2$, $0 < y < \pi$ we have

$$\frac{\partial \Psi}{\partial x}\left(\frac{\pi}{2}, y\right) = -2 \sin y, \quad \frac{\partial \Psi}{\partial y}\left(\frac{\pi}{2}, y\right) = 0,$$

so one obtains $|\nabla \theta| = |2 \sin y|$. Thus,

$$\theta\left(\frac{\pi}{2}, y\right) = 2 \int_0^y \sin t \ dt = 2 - 2 \cos y, \quad \text{and} \quad 0 \leq \theta \leq 4.$$
When \( y = \pi, 0 < x < \pi/2 \) we have \( |\nabla \theta| = |\sin 2x| \). On the separatrix defined as \( y = \pi, \pi/2 < x < \pi \) we also have \( |\nabla \theta| = |\sin 2x| \). Thus we have for these two separatrices the circulation parameter is the same:

\[
\theta(x) = 5 - \int_0^x \sin 2t \, dt = 5 - \sin^2 x, \quad \text{and} \quad 4 \leq \theta \leq 5.
\]

When \( x = 0, 0 < y < \pi \) we have \( |\nabla \theta| = |2 \sin y| \). On the separatrix defined as \( x = \pi, 0 < y < \pi \) we also have \( |\nabla \theta| = |2 \sin y| \). For these two separatrices

\[
\theta(y) = 9 - 2 \int_0^y \sin t \, dt = 7 + 2 \cos y, \quad \text{and} \quad 5 \leq \theta \leq 9.
\]

For separatrices \( y = 0, 0 < x < \pi/2 \) and \( y = 0, 0 < x < \pi/2 \) we have \( |\nabla \theta| = |\sin 2x| \). Thus

\[
\theta(x) = 9 + \int_0^x \sin 2t \, dt = 9 + \sin^2 x, \quad \text{and} \quad 9 \leq \theta \leq 10.
\]

### 3.2. Exponential grids.

We restrict the infinite and the semi-infinite domains \((-\infty, \infty), (0, \infty)\) to \([-M, M]\) and \((0, M)\) for sufficiently large \( M > 0 \), respectively. Observe that the solutions of (15) converge to constants exponentially fast in \( h \). Thus we use a standard exponential grid [25, 11] to obtain a numerical discretization of (15).

The grid is defined as follows. Let \( \{0 = y_0, y_1, \ldots, y_N = 1\} \) be the uniformly distributed points in the interval \([0, 1]\). Then for an appropriate positive constant \( C \) which is a stretching parameter, the positive part of the exponential grid points are defined by

\[
t_j = -C \ln y_j, \quad \text{for each} \quad j = 1, \ldots, N.
\]

The negative part of the exponential grid points is obtained by reflecting the points \( \{t_j\}_{j=1}^N \) about the origin. All the grid points \( \{x_i\}_{i=1}^{2N-1} \) can be obtained by merging those two parts

\[
x_1 = -t_1, x_2 = -t_2, \ldots, x_N = -t_N, \quad x_{N+1} = t_{N-1}, \ldots, x_{2N-1} = t_1.
\]

### 3.3. Discretization of the heat equations.

As described in Section 2.1, the Childress’ problem consists of solving the heat equations along the common edges of the two cells (e.g. see equation (5)) and along the exterior boundaries (e.g. see equations (8), (9)).

Consider an interior edge. We impose the Neumann boundary conditions (7) at the endpoints of the interval as

\[
\frac{\partial f}{\partial h}(h = x_1, \theta) = \frac{\partial f}{\partial h}(h = x_{2N-1}, \theta) = 0.
\]

Integrating the equation over each subinterval \([x_i, x_{i+1}]\), \( i = 1, \ldots, 2N-2 \) we obtain

\[
\int_{x_i}^{x_{i+1}} \frac{\partial f}{\partial h} \, dh = \int_{x_i}^{x_{i+1}} \frac{\partial^2 f}{\partial h^2} \, dh,
\]

\[
\frac{\partial f}{\partial \theta} \Delta x = \frac{\partial f}{\partial h}(x_{i+1}) - \frac{\partial f}{\partial h}(x_i),
\]

where \( \Delta x = x_{i+1} - x_i \). Since \( f \) is piecewise constant we denote its value on the subinterval \((x_i, x_{i+1})\) by \( f_{i+1/2} \). Then (18) is

\[
\frac{\partial f_{i+1/2}}{\partial \theta} \Delta x = \frac{\partial f}{\partial h}(x_{i+1}) - \frac{\partial f}{\partial h}(x_i).
\]
Using the backward Euler method with the step size $\Delta \theta$, we obtain the difference equation at the $(n+1)$th time step:

$$
\frac{f_{i+1}^{n+1} - f_i^N}{\Delta \theta} \Delta x = \frac{f_{i+1}^{n+1} - f_{i+\frac{1}{2}}^{n+1}}{x_{i+\frac{1}{2}} - x_{i+\frac{1}{2}}} - \frac{f_{i+\frac{1}{2}}^{n+1} - f_i^{n+1}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \tag{19}
$$

for $i = 2, \ldots, 2N - 3$. For $i = 1, 2N - 2$ we impose Neumann boundary conditions at end points to obtain:

$$
\left(1 + \frac{\Delta \theta}{\Delta x} \frac{1}{x_{\frac{N}{2}} - x_{\frac{1}{2}}}ight) f_{\frac{N}{2}}^{n+1} - \frac{\Delta \theta}{\Delta x} \frac{1}{x_{\frac{N}{2}} - x_{\frac{1}{2}}} f_{\frac{N}{2}}^{n+1} = f_N^{n+1}, \tag{20}
$$

for $i = N - 1$. For the Dirichlet boundary conditions we use

$$
f_{\frac{N}{2}}^{n+1} - \frac{\Delta \theta}{\Delta x} \left( \frac{f_{\frac{N}{2}+\frac{1}{2}}^{n+1} - f_{\frac{N}{2}+\frac{1}{2}}^{n+1}}{x_{\frac{N}{2}+\frac{1}{2}} - x_{\frac{N}{2}+\frac{1}{2}}} - \frac{f_{\frac{N}{2}-\frac{1}{2}}^{n+1} - f_{\frac{N}{2}-\frac{1}{2}}^{n+1}}{x_{\frac{N}{2}-\frac{1}{2}} - x_{\frac{N}{2}-\frac{1}{2}}} \right) = f_{\frac{N}{2}}^{n} + \frac{\Delta \theta}{\Delta x} \frac{f_{\frac{N}{2}}^{n+1}}{x_{\frac{N}{2}} - x_{\frac{N}{2}}} \tag{23}
$$

where for $i = N - 1$, and $f_{\frac{N}{2}}^{n+1}$ are the known values which are Dirichlet data.

3.4. Discretization of the boundary conditions on the outer edges. As mentioned earlier, the homogeneous Neumann conditions and the Dirichlet conditions have been imposed on the outer edges. For the Neumann boundary conditions we use

$$
\left(1 + \frac{\Delta \theta}{\Delta x} \frac{1}{x_{\frac{N}{2}} - x_{\frac{1}{2}}}ight) f_{\frac{N}{2}}^{n+1} - \frac{\Delta \theta}{\Delta x} \frac{1}{x_{\frac{N}{2}} - x_{\frac{1}{2}}} f_{\frac{N}{2}}^{n+1} = f_{\frac{N}{2}}^{n}, \tag{22}
$$

for $i = N - 1$. For the Dirichlet boundary conditions we use

$$
f_{\frac{N}{2}}^{n+1} - \frac{\Delta \theta}{\Delta x} \left( \frac{f_{\frac{N}{2}+\frac{1}{2}}^{n+1} - f_{\frac{N}{2}+\frac{1}{2}}^{n+1}}{x_{\frac{N}{2}+\frac{1}{2}} - x_{\frac{N}{2}+\frac{1}{2}}} - \frac{f_{\frac{N}{2}-\frac{1}{2}}^{n+1} - f_{\frac{N}{2}-\frac{1}{2}}^{n+1}}{x_{\frac{N}{2}-\frac{1}{2}} - x_{\frac{N}{2}-\frac{1}{2}}} \right) = f_{\frac{N}{2}}^{n} + \frac{\Delta \theta}{\Delta x} \frac{f_{\frac{N}{2}}^{n+1}}{x_{\frac{N}{2}} - x_{\frac{N}{2}}} \tag{23}
$$

where for $i = N - 1$, and $f_{\frac{N}{2}}^{n+1}$ are the known values which are Dirichlet data.

4. Numerical results. In this section, we present some numerical results, and compare them with simulations obtained in the MATLAB PDE Toolbox$^\text{TM}$. We start with the reduced Childress’ problem (15) for the one-cell case, $\Psi(x, y) = \sin x \sin y$. Figure 3 illustrates the agreement between the initial condition $(\theta = 0)$, and the solution after one period $(\theta = 8)$. The $L_2$-norms of the difference between the initial function and the function on $[4M\pi, 4(M+1)\pi]$ are computed for $M = 0, 1, 2, 3$:

| $M$ | $L_2$-norm |
|-----|------------|
| 0   | $7.2721\times 10^{-15}$ |
| 1   | $2.8771\times 10^{-15}$ |
| 2   | $1.1075\times 10^{-14}$ |
| 3   | $3.6108\times 10^{-15}$ |
which shows that we can find the periodic solution with our numerical scheme.

In Figure 4 we plot this periodic solution. The left plot represents the solution of the asymptotic Childress’ problem (15) in the boundary layer coordinates $h > 0$, $0 \leq \theta \leq 8$. The right plot shows the same solution with $\varepsilon = 10^{-3}$ in the Cartesian coordinates.

**Figure 3.** The asymptotic solution for the one-cell problem is periodic with period 8.

**Figure 4.** The asymptotic solution for the 1-cell problem in the boundary layer coordinates (left), and the same solution in the Cartesian coordinates (right).

### 4.1. The case of the mixed Dirichlet-Neumann boundary conditions.

The domain for the two-cell case with $\Psi(x, y) = \sin 2x \sin y$ is shown on the left part of Figure 5. In the boundary layer coordinate system, as $\varepsilon \to 0$, the problem for the two-cell case becomes the following system of equations over the rectangular region $h \in \mathbb{R}$, $0 < \theta < 10$. First, for $0 < \theta < 4$:

$$
\frac{\partial^2 f}{\partial h^2} - \frac{\partial f}{\partial \theta} = 0, \quad h \in \mathbb{R},
$$

(24)

with the homogeneous Neumann boundary conditions at $\pm \infty$ and an unknown initial data $f^0(h)$ which will be determined below in (27).
Figure 5. The set up for the 2-cell problem (left), and for the 4-cell problem (right).

Figure 6. The asymptotic solution for the 2-cell problem with mixed BC is periodic with period 10 (left), and the comparison of this asymptotic solution with the 2-D solution of (1) at $\theta = 0$ with $\varepsilon = 10^{-3}$ (right).

Figure 7. Comparison of the asymptotic solution with the 2-D solution of (1) for the 4-cell case at $\theta = 0$ with $\varepsilon = 10^{-3}$ (left), the 2-D solution (right).

For $4 < \theta < 5$ we solve two problems for $h > 0$ and $h < 0$, respectively:
\[
\frac{\partial f^+}{\partial n} - \frac{\partial^2 f^+}{\partial h^2} = 0, \quad h > 0, \quad 4 < \theta < 10, \\
\frac{\partial f^+}{\partial h}(0, \theta) = 0, \quad 4 < \theta < 5, \\
f^+(0, \theta) = \pi, \quad 5 < \theta < 9, \\
\frac{\partial f^+}{\partial h}(0, \theta) = 0, \quad 9 < \theta < 10,
\]

and

\[
\frac{\partial f^-}{\partial n} - \frac{\partial^2 f^-}{\partial h^2} = 0, \quad h < 0, \quad 4 < \theta < 10, \\
\frac{\partial f^-}{\partial h}(0, \theta) = 0, \quad 4 < \theta < 5, \\
f^-(0, \theta) = 0, \quad 5 < \theta < 9, \\
\frac{\partial f^-}{\partial h}(0, \theta) = 0, \quad 9 < \theta < 10,
\]

with the initial data

\[
f^+(h, 4) = f(h, 4), \quad h > 0, \\
f^-(h, 4) = f(h, 4), \quad h < 0,
\]

where \(f\) solves (24), and the homogeneous Neumann boundary conditions at \(\pm\infty\).

Hence due to the periodicity we have

\[
f^0(h) = \begin{cases} 
  f^+(h, 10), & h > 0, \\
  f^-(h, 10), & h < 0.
\end{cases}
\]

The stretching parameter \(C\ (16)\) for the exponential grid was chosen to be 5. In Figure 6 we present the asymptotic solution for the two-cell problem (24)-(26). The left plot shows that we indeed obtain a periodic solution. The right plot shows a comparison with the solution of (1) with \(\varepsilon = 10^{-3}\).

In the four-cell case the structure of the separatrices is as in Figure 5. In the right plot of Figure 7 we show the 2-D solution of (1) in the Cartesian coordinates. In the left plot of Figure 7 we compare this 2-D solution with our asymptotic solution of the Childress’ problem in the boundary layer variables and at fixed \(\theta = 0\).

4.2. The two-cell problem with Dirichlet boundary conditions. Finally, we consider another two-cell problem with Dirichlet boundary conditions

\[f(x, y) = x, \quad \text{on} \ \partial \Omega.\]
For these boundary conditions, the system of the heat equations (24)-(26) is changed slightly, and it is as follows. For $0 < \theta < 4$ the equation is as before (24). For $4 < \theta < 5$ we consider splitting for positive and negative half spaces:

$$\begin{align*}
\frac{\partial f^+}{\partial \theta} - \frac{\partial^2 f^+}{\partial h^2} &= 0, \\
h > 0, & \quad 4 < \theta < 10, \\
f^+(0, \theta) &= \pi - \arcsin(\sqrt{5 - \theta}), \quad 4 < \theta < 5, \\
f^+(0, \theta) &= \pi, & \quad 5 < \theta < 9, \\
f^+(0, \theta) &= \pi - \arcsin(\sqrt{\theta - 9}), & \quad 9 < \theta < 10,
\end{align*}$$

(28)
Asymptotic solution at $\theta = 0$

$2-D$ solution

$\frac{\partial f^-}{\partial \theta} - \frac{\partial^2 f^-}{\partial \theta^2} = 0, \quad h < 0, \quad 4 < \theta < 10,$

$f^-(0, \theta) = \arcsin(\sqrt{5 - \theta}), \quad 4 < \theta < 5,$

$f^-(0, \theta) = 0, \quad 5 < \theta < 9,$

$f^-(0, \theta) = \arcsin(\sqrt{\theta - 9}), \quad 9 < \theta < 10.$

(29)

with homogeneous Neumann boundary conditions at $h = \pm \infty$. Figures 8-11 show the solution of the system of the heat equations (24), (28), (29). In particular, the curve in the left plot in the Figure 8 is the periodic initial condition which is obtained by solving the Childress’ problem for the two-cell case. Finally, in Figure 12 we compare our solution (solid curve from the left plot of Figure 8) with the corresponding solution of (1) with $\varepsilon = 10^{-3}$.

4.3. Numerical convergence. In this section we present the numerical convergence of the asymptotic problem on the graph given by (15). The convergence tests are presented in Tables 1-3 for each of the three cases discussed in Subsections 4.1, 4.2. In these tables, $N$ denotes the number of grid points of the exponential grid in the spatial domain $[-30, 30]$, and $T$ is chosen so that $1/T$ is the “time-step” size in the circulation variable $\theta$ to solve the heat equations. The solution for the case of $N = 800$ and $T = 400$ is used as a reference to calculate the errors of solutions over coarser grids and with bigger “time-step” sizes.

| Table 1. | 2-cell problem with mixed boundary conditions |
|----------|---------------------------------------------|
|          | $N=50$ | $N=100$ | $N=200$ | $N=400$ |
| $T=25$   | 0.131157 | 0.129614 | 0.127467 | 0.128123 |
| $T=50$   | 0.066336 | 0.061471 | 0.059312 | 0.059709 |
| $T=100$  | 0.039639 | 0.029570 | 0.026201 | 0.026088 |
| $T=200$  | 0.031560 | 0.017017 | 0.011255 | 0.009711 |
| $T=400$  | 0.030213 | 0.014553 | 0.007907 | 0.004221 |

As it is expected from our first-order discretization, we observe the $O(1/N, 1/T)$ numerical convergence. Higher order methods can be used to solve (15), but we
Table 2. 4-cell problem with mixed boundary conditions

|   | N=50    | N=100   | N=200   | N=400   |
|---|---------|---------|---------|---------|
| T=25 | 0.279972 | 0.275604 | 0.274103 | 0.273977 |
| T=50 | 0.134366 | 0.125462 | 0.122572 | 0.122057 |
| T=100 | 0.077413 | 0.060403 | 0.053852 | 0.052497 |
| T=200 | 0.060425 | 0.035495 | 0.022400 | 0.018742 |
| T=400 | 0.058223 | 0.031341 | 0.014927 | 0.007730 |

Table 3. 2-cell problem with Dirichlet boundary conditions

|   | N=50    | N=100   | N=200   | N=400   |
|---|---------|---------|---------|---------|
| T=25 | 0.267840 | 0.245369 | 0.251492 | 0.254067 |
| T=50 | 0.131058 | 0.093376 | 0.093452 | 0.094881 |
| T=100 | 0.102930 | 0.059813 | 0.045032 | 0.044711 |
| T=200 | 0.094386 | 0.052409 | 0.027989 | 0.019835 |
| T=400 | 0.091749 | 0.052745 | 0.024072 | 0.011315 |

did not implement them because our main objective to investigate how well (15) approximates (1) for large Péclét numbers. We emphasize that unlike other numerical schemes for advection-diffusion problems (such as e.g. upwind methods which are not suited for problems with high Péclét number) our numerical scheme was developed for the asymptotic problem (15), which is independent of the Péclét number [21]. Thus it provides an effective numerical tool to solve the problem at high Péclét numbers. We now turn to assessing the accuracy of the numerical scheme. In the next section we discuss the convergence of our method in terms of $\varepsilon = \text{Pe}^{-1} \ll 1$.

![Figure 13](image_url)

**Figure 13.** Comparison of the asymptotic solution at $\theta = 0$ or $(x, y) = (\pi/2, 0)$ with the solution of (1) with various $\varepsilon$ (left), a magnified region (right).

4.4. **Convergence as $\varepsilon \to 0$.** Our final set of results concerns the comparison of the solutions obtained by the developed combined asymptotic/numerical scheme with the solutions to advection-diffusion problem computed using the MATLAB
Figure 14. Comparison of the asymptotic solution at $\theta = 2$ or $(x, y) = (\pi/2, \pi/2)$ with the solution of (1) with various $\varepsilon$ (left), a magnified region (right).

PDE Toolbox$^\text{TM}$ for various $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}$. For smaller $\varepsilon$ the MATLAB's solution becomes unreliable.

The comparison results are shown for the two-cell case (24)-(27) at two different values of $\theta$: for $\theta = 0$ in Figure 13, and for $\theta = \pi/2$ in Figure 14. In order to put all four functions on the same graph we rescaled the solutions of (1) obtained with MATLAB$^\text{TM}$. As it is evident from these plots the asymptotic model is reliable for $\varepsilon$ as large as $10^{-2}$. For $\varepsilon = 10^{-1}$ shows less fidelity, but the approximate solution is still fairly close to the solution of (1).

Numerically the convergence can be estimated as the $L^\infty$-error between the two solutions at the points $\theta = 0$ and $\theta = 2$ (which correspond to $(x, y) = (\pi/2, 0)$ and $(x, y) = (\pi/2, \pi/2)$ in the original system of coordinate, respectively) in Tables 4, 5.

Table 4. $L^\infty$-error for the 2-cell problem with mixed boundary conditions

| $\varepsilon$ | $\theta = 0$ | $\theta = 2$ |
|--------------|--------------|--------------|
| $10^{-3}$    | 0.0211       | 0.0052       |
| $10^{-2}$    | 0.5805       | 0.0109       |
| $10^{-1}$    | 0.9398       | 0.0601       |

Table 5. $L^\infty$-error for the 2-cell problem with Dirichlet boundary conditions

| $\varepsilon$ | $\theta = 0$ | $\theta = 2$ |
|--------------|--------------|--------------|
| $10^{-3}$    | 0.0280       | 0.0043       |
| $10^{-2}$    | 0.0549       | 0.0101       |
| $10^{-1}$    | 0.0858       | 0.0380       |

5. Concluding remarks. We have presented here a numerical implementation of the asymptotic model [21]. This model allows to find a numerical solution of the convection-diffusion equation in cellular flows at large Péclet numbers. This method is independent of the Péclet, therefore it is attractive for simulations at very large Péclet numbers. We have also demonstrated that the asymptotic solution agrees well with the solution of (1) even at intermediate Péclet numbers around 100.
We used a finite volume method with exponential grid to discretize the asymptotic system of the heat equations (15). It turns out that piecewise constant functions in our finite volume method allow us to handle complicated restriction and gluing transformations easily. By imposing homogeneous Neumann conditions at end points of the restricted domains (17), we can capture the constant states (6) automatically.

Figure 15. Approximate solutions by the “water-pipe network”.

Spectral methods, e.g. Galerkin approach [25, 11] are used for the problems on unbounded domains because spectral approach has lower computational cost and higher accuracy. It is, however, difficult to implement for our problem, because complicated gluing conditions, described in Section 3, need to be explicitly specified for Galerkin basis functions, i.e. Laguerre and Hermite polynomials. We are currently implementing a spectral method with Laguerre polynomials for advection-diffusion at high Péclet numbers.

It was shown in [21] that it was also possible to approximate the solutions of (1) by the “water-pipe network”. Namely, restrict the domain to the region of width $K\sqrt{\varepsilon}$ near the separatrices for some positive fixed number $K$, and denote it by $\Omega_K = \Omega \cap \{|\Psi(x)| \leq K\sqrt{\varepsilon}\}$. The boundary of $\Omega_K$ consists of $\partial \Omega$ and the level curves $l_K = \{x \in \Omega : \Psi(x) = K\sqrt{\varepsilon}\}$. Then we approximate the solution of (1) by the solution

$$\varepsilon \Delta \phi_K^\varepsilon - u \cdot \nabla \phi_K^\varepsilon = 0, \quad x \in \Omega_K^\varepsilon,$$

with the boundary conditions

$$\phi_K^\varepsilon |_{\partial \Omega} = T_0, \quad \frac{\partial \phi_K^\varepsilon}{\partial n} |_{l_K} = 0.$$

We performed numerical tests for the “water-pipe network” using MATLAB PDE Toolbox™. We focused on the one-cell and four-cell cases in these tests. The square $(0, 1) \times (0, 1)$ and $(-1, 1) \times (-1, 1)$ in $\mathbb{R}^2$ are considered as the domains for one-cell and four-cell cases, respectively. The stream function $\Psi(x)$ by $\Psi(x, y) = \sin(\pi x) \sin(\pi y) / \sqrt{2}$, and the small molecular diffusivity by $\varepsilon = 10^{-2}$ and $\varepsilon = 10^{-3}$ for one-cell and four-cell case, respectively. The positive number $K$ was chosen by 5 in both cases. The results of numerical simulations are depicted in Figure 15. For such relatively large $\varepsilon$ the “water-pipe network” approximates well the solution of (1). It turns out, however, that this method is not accurate enough for smaller $\varepsilon$ due to difficulty in mesh generation in the narrow pipes.
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