High order conservative difference methods
for 2D drift-diffusion model
on non-uniform grid

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Abstract

A new accurate compact finite difference scheme for solving the 2D drift-diffusion
system is introduced. The scheme is based on the computation on staggered grids
of the current densities given by advection-dominated equations. Conservativity is
preserved and the compactness of the scheme leads to a good treatment of boundary
conditions. The discretization is realized on uniform and non-uniform grids. This
last grid is analytically defined using mapping techniques (spline functions). Several
numerical tests show the robustness of the method.

1 Introduction

This work describes high-order compact finite difference schemes used to solve
the coupled system of nonlinear elliptic partial differential equations, which
models semiconductor devices. The most popular and effective methods are
based on the Scharfetter-Gummel method [10] which is interpreted as a mixed
finite element method in [11,12]. Recently there has been a great deal of interest
in using high-order compact schemes. Many papers are devoted to the
construction of such schemes [1,3–5]. For the sake of clarity, we restrict our
attention to the bidimensional steady-state problems. We consider the nonlinear
drift-diffusion equations in dimensionless form given in [9]. The dependant
unknowns of the problem are the electrostatic potential \( \psi \), the electron density
\( n \) and the hole density \( p \). In a bounded domain \( \Omega \) in \( \mathbb{R}^2 \). \( \psi \), \( n \), \( p \) satisfy the
following system of partial differential equation:

\[
\begin{align*}
\text{div} \ J_n &= GR, & (x, y) \in \Omega, \text{ electron continuity equation.} \\
\text{div} \ J_p &= -GR, & (x, y) \in \Omega, \text{ hole continuity equation.} \\
\lambda^2 \Delta \psi - n + p + C &= 0, & (x, y) \in \Omega, \text{ Poisson’s equation.}
\end{align*}
\]

Preprint submitted to Elsevier Preprint 4 November 1995
where \( J_n = (J_{nx}, J_{ny}) \), \( J_p = (J_{px}, J_{py}) \) are the current densities given by the drift-diffusion form:

\[
\begin{align*}
J_n &= -D_n \nabla n + \mu_n n \nabla \psi, \\
J_p &= D_p \nabla p + \mu_p p \nabla \psi.
\end{align*}
\tag{2}
\]

The quantities \( \psi, n, p \) satisfy the mixed Neumann and Dirichlet boundary conditions:

\[
\begin{align*}
\psi &= \psi_D, \quad n = n_D, \quad p = p_D, \quad \text{on } \Gamma_D, \\
\frac{\partial \psi}{\partial n} &= J_n \cdot \nu - J_p \cdot \nu = 0, \quad \text{on } \Gamma_N = \partial \Omega \setminus \Gamma_D.
\end{align*}
\]

where \( \nu \) represents the unit outgoing vector of the domain. The constants \( \mu_n, \mu_p, D_n, D_p \) are respectively the mobility and diffusivity coefficients, \( C(x, y) \) is the doping profile, and \( GR(x, y) \) is the generation-recombination rate.

From a numerical point of view, difficulties arise in the discretization of current density equations due to the advection-dominated character of these equations. Indeed, \( \nabla \psi \) can take large values in a significant part of the domain. Accurate computation of the currents is of major importance, and the continuity equations must be discretized in a conservative way.

This paper is organized as follows. In section 2, we explicitly compute the current densities of the problem \( \{1\} \) formulated on uniform staggered grids, using a fourth-order compact finite difference scheme. The technique presented by Abarbanel and Kumar \( \{2\} \) for steady state Euler equations is used, however.

particular approximation of the currents is required to preserve the conservativity and the compactness character of the whole discretization. We consider the other equations and present the treatment of boundary conditions based on the elimination (without loss of accuracy) of fictitious points. In section 3, we extend our results on a non-uniform grid. Mesh refinement is mandatory because strong variations of the solutions do exist in some regions of the device (nearby interfaces and junctions), although no boundary layers occur at ohmic contacts and insulating segments. The derivation of an efficient scheme on this kind of grids is based on mapping techniques which have been previously used, in particular for convection-diffusion problems by Spotz and Carey \( \{13\} \). For a given class of discretizations (control of the refinement regions), we present a simple and efficient construction of the mapping functions based on interpolation spline, which do not introduce numerical error in the resulting scheme. In section 4, we discuss some numerical results, and show that our scheme is computationally efficient and stable.

2 Discretization on uniform grids

The problem \( \{1\} \) can be formulated in a mixed form on staggered grids by considering the current densities \( J_n \) and \( J_p \) as independent unknowns. Such
grids are displayed in Fig. 1. We approximate the problem on uniform spatial grids with step $h$ in $x$-direction and $k$ in $y$-direction. We denote by $f_{i,j}$ the approximation of a function $f$ at the mesh points $(x_i, y_j)$. 

$$J_{nx}, J_{px} \leftrightarrow \Delta \leftrightarrow (i, j + \frac{1}{2})$$

$$J_{ny}, J_{py} \leftrightarrow \subset \leftrightarrow (i + \frac{1}{2}, j)$$

$$\psi, n, p \leftrightarrow \sqcup \leftrightarrow (i + \frac{1}{2}, j + \frac{1}{2})$$

Figure 1 - The staggered grids: dark marks denote the grid points used to compute $J_{nx}$ and $J_{px}$ at $(i, j + \frac{1}{2})$ node.

2.1 Discretization of the current densities on uniform grid

We describe the construction of a fourth-order scheme on the $\Delta$ grid for $J_{nx}$. The value of $J_{nx}$ at the grid point $(i, j + \frac{1}{2})$ depends on those of $\psi, n, p$ at the grid points $(i - \frac{1}{2}, j)$, $(i + \frac{1}{2}, j - 1)$, $(i, j)$, $(i - \frac{1}{2}, j + 1)$, $(i, j + 1)$, $(i, j)$. Contrary to usual compact discretization using 5 points, the computation of $J_{nx}$ is achieved using 6 points making our work more intricate.

To approximate $J_{nx}$ at the $\Delta$ nodes, we use the central difference formula,

$$\left( \frac{\partial n}{\partial x} \right)_{i, j + \frac{1}{2}} = \frac{n_{i + \frac{1}{2}, j + \frac{1}{2}} - n_{i - \frac{1}{2}, j + \frac{1}{2}}}{h} - \frac{h^2}{12} \left( \frac{\partial^3 n}{\partial x^3} \right)_{i, j + \frac{1}{2}} + O(h^4). \quad (3)$$

A fourth-order truncation error is obtained by using a second-order approximation of the third derivative on the $\Delta$ nodes. Moreover, to preserve the compactness character of our discretization, we use the differential equations (1) and the equations deduced by differentiation as additional relations to handle $\left( \frac{\partial^3 n}{\partial x^3} \right)$, at the $(i, j + \frac{1}{2})$ node. Writing,

$$\frac{\partial^3 n}{\partial x^3} \cdot \partial \left( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} \right) - \frac{\partial^3 n}{\partial x \partial y^2}, \quad (4)$$
we note that the term \( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} \) can be deduced from the electron continuity equation,

\[
D_n \left( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} \right) = -GR + \mu_n n \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \mu_n \left( \frac{\partial n}{\partial x} \frac{\partial \psi}{\partial y} + \frac{\partial n}{\partial y} \frac{\partial \psi}{\partial x} \right) .
\]

(5)

Using Poisson's equation (1c), we substitute \( \left( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} \right) \) in (5), and obtain after differentiating with respect to \( x \) and rearranging.

\[
\frac{\partial^3 n}{\partial x^3} = -\frac{1}{D_n} \frac{\partial GR}{\partial x} + \frac{\mu_n}{D_n} \frac{\partial n}{\partial x} \left( n - p - C \right) + \mu_n \left( n + \frac{h^2 \partial^2 n}{24 \partial x^2 \partial y^2} \right) \left( \frac{\partial^3 n}{\partial x^3} \right) + \mu_n \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right) + \mu_n \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right).
\]

(6)

Injecting (6) in (3), the expression of \( J_{nx} \) at the node \( \left( i, j+\frac{1}{2} \right) \) is given by,

\[
\left( J_{nx} \right)_{i,j+\frac{1}{2}} = -\frac{D_n}{h} \left( \frac{\partial n}{\partial x} \right)_{i+\frac{1}{2},j+\frac{1}{2}} - h^2 \left( \frac{\partial GR}{\partial x} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + \mu_n \left( \frac{\partial^3 n}{\partial x^3} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + \mu_n \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + \mu_n \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + \mu_n \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + n \left( \frac{\partial n}{\partial x} \right)_{i+\frac{1}{2},j+\frac{1}{2}} + O(h^4).
\]

(7)

Hereafter, our attention is focused on the fourth-order approximation of \( (\mu_n(\frac{\partial \psi}{\partial x}))(n+\frac{h^2 \partial^2 n}{24 \partial x^2 \partial y^2}) \). The treatment of the remaining terms is detailed in appendix A.

In the same way, a fourth-order approximation of \( (\mu_n(\frac{\partial \psi}{\partial x})) \) at the node \( \left( i, j+\frac{1}{2} \right) \) is given by:

\[
\left( \frac{\partial \psi}{\partial x} \right)_{i,j+\frac{1}{2}} = \frac{\psi_{i+\frac{1}{2},j+\frac{1}{2}} - \psi_{i-\frac{1}{2},j+\frac{1}{2}}}{h} - h^2 \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right)_{i,j+\frac{1}{2}} + \frac{h^2}{24} \left( \frac{\partial^3 \psi}{\partial x^2 \partial y^2} \right)_{i,j+\frac{1}{2}} + O(h^4),
\]

(8)

By Taylor developments, we obtain the following fourth-order approximation:

\[
\left( \frac{\partial \psi}{\partial x} \right)_{i,j+\frac{1}{2}} = H_1 \frac{h^2}{24} \left( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} \right)_{i,j+\frac{1}{2}} + O(h^4),
\]

(9)
where \( R_1 \) is given by
\[
\frac{h^2}{24k^2} \left( n_{i+\frac{1}{2},j-\frac{1}{2}} + n_{i-\frac{1}{2},j-\frac{1}{2}} + n_{i+\frac{1}{2},j+\frac{1}{2}} + n_{i-\frac{1}{2},j+\frac{1}{2}} \right) \\
+ \frac{6k^2 - h^2}{12k^2} \left( n_{i+\frac{1}{2},j+\frac{1}{2}} + n_{i-\frac{1}{2},j+\frac{1}{2}} \right).
\]

Equations (9) and (5) yield:
\[
n_{i,j+\frac{1}{2}} + \frac{h^2}{24} \left( \frac{\partial^2 n}{\partial x^2} \right)_{i,j+\frac{1}{2}} = -\frac{h^2}{12} \frac{\mu_n}{D_n} \left( \frac{n}{\lambda^2} (n - p - C) + \left( \frac{\partial n}{\partial x} \frac{\partial \psi}{\partial x} - \frac{\partial n}{\partial y} \frac{\partial \psi}{\partial y} \right) \right)_{i,j+\frac{1}{2}} \\
+ R_1 + \frac{h^2}{12} \frac{GR}{D_n} + O(h^4 + k^4).
\]

Finally, we substitute (10) and (8) in (7) (using the approximations presented in appendix A) to obtain the discretization of the current \( J_{nx} \) on the \( \Lambda \) grid. We obtain analogous schemes for \( J_{ny} \), \( J_{px} \), \( J_{py} \).

The discretizations of the continuity equation and the Poisson’s equation on the uniform grids \( \Lambda \) are realized using respectively a central difference approximation of order 2, and the classical fourth-order compact (9 points) scheme [20]. In the discretization of the continuity equation, we can recover the fourth-order and preserve the compactness and the conservativity using a suggestion of Kreiss. We refer to the works of Hirsch [15], Ciment and al. [18], and Tolsykh [16]. This approach leads to a non profitable inversion of a system, so we do not give more details.

### 2.2 Treatment of boundary conditions

We shall discuss the discretization of the boundary conditions. The Neumann boundary conditions on the current densities are taken into account in the interior schemes (due to the compactness of the discretization). Elsewhere we use fictitious points outside the domain which are replaced by grid points by using extrapolation formulas. The loss of accuracy in the discretization of the boundary conditions must be at most of order one so as to preserve the global accuracy. So for a first order equation discretized with an order \( n \) (continuity equation or current equations), we use extrapolation formulas of order \((n+1)\), and for a second order equation (Poisson’s equation) discretized at the same order \( n \), we use the order \((n+2)\). The extrapolation formulas are obtained by Taylor expansions. We search some constants \( \alpha_i \) \((i = 0, \cdots, 6)\) given in Table 1, such that a function \( u \) satisfies (with an order \( p \)),
\[
u_{i-\frac{1}{2},j} = \alpha_0 u_{i,j} + \alpha_1 u_{i+\frac{1}{2},j} + \alpha_2 u_{i+\frac{3}{2},j} + \alpha_3 u_{i+3,2,j} + \alpha_4 u_{i+3,2,j} + \alpha_5 u_{i+3,2,j} + \alpha_6 u_{i+3,2,j} + O(h^p).
\]
<table>
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Table 1 - Extrapolation formulas.

We do not give the explicit expressions after substitution in the discrete equations. These manipulations require very intricate algebraic manipulations which are realized using symbolic computations [4]. To preserve the compactness of the scheme, third-order extrapolation formulas have to be used, but in this case, the accuracy is altered. The stability of the complete numerical scheme, including boundary conditions, must be determined by an appropriate eigenvalue analysis (for the linearized problem). We refer to the article of Lele [6] where the treatment of boundaries in the basic schemes approximating the first and second derivatives and the effect on the overall scheme are discussed. Since the local accuracy of the boundary scheme increases, we expect a loss of stability, however. Lele proves an unexpected stability. The same behaviour is observed in many numerical tests presented in section 4 (using Table 1). For steady state problems, the stability issues of such boundary conditions were presented in 7,8 to control error growth in time caused by the way the mathematical boundary conditions were imposed.

## 3 Discretization on non-uniform grids

We can transform by mapping a problem $(P)$ formulated on a rectangular domain $\Omega$ (coordinates $(x, y)$), decomposed with non-uniform mesh $NU$ into a new problem $(\bar{P})$ on the domain $\Omega$ (coordinates $(\zeta, \eta)$), with uniform grids $U$ (and $k$ represent the discretization steps in each direction). This approach was developed by Spotz and Carey [13] for special transformations adjusted to boundary layers. In this paper, we define a refinement zone near junctions, inside the domain. We present an analytical construction of such transformations based on spline functions which do not introduce numerical errors. The definition of analytical maps and construction of the schemes are realized with symbolic software (note that this is quite impossible by hand).
We consider the regular and non-degenerate transformations \( x, y \) and their inverses \( \zeta, \eta \),

\[
\begin{align*}
&x : \zeta \rightarrow x(\zeta') = x, \\
y : \eta \rightarrow y(\eta) = y,
\end{align*}
\]

These transformations are chosen in order to generate orthogonal and independent grids. We define \( \tilde{u}(\zeta, \eta) = u(x(\zeta), y(\eta)) \). The problem (1') is transformed into the new problem (11), formulated with the unknowns \( \tilde{\psi}, \tilde{n}, \tilde{p}, \tilde{C} \),

\[
\begin{align*}
\tilde{J}_{nx} &= a(\zeta) \left( -D_n \frac{\partial \tilde{n}}{\partial \zeta} + \mu_n \tilde{n} \frac{\partial \tilde{\psi}}{\partial \zeta} \right), \\
\tilde{J}_{ny} &= b(\eta) \left( -D_n \frac{\partial \tilde{n}}{\partial \eta} + \mu_n \tilde{n} \frac{\partial \tilde{\psi}}{\partial \eta} \right), \\
a(\zeta) \frac{\partial \tilde{J}_{nx}}{\partial \zeta} + b(\eta) \frac{\partial \tilde{J}_{ny}}{\partial \eta} = \tilde{G}_R, \\
\lambda^2 \left( a^2(\zeta) \frac{\partial^2 \tilde{\psi}}{\partial \zeta^2} + b^2(\eta) \frac{\partial^2 \tilde{\psi}}{\partial \eta^2} + c(\zeta) \frac{\partial \tilde{\psi}}{\partial \zeta} + d(\eta) \frac{\partial \tilde{\psi}}{\partial \eta} \right) - \tilde{n} + \tilde{p} + \tilde{C} = 0,
\end{align*}
\]

where \( a(\zeta), b(\eta), c(\zeta) \) and \( d(\eta) \) should be computed at the uniform grid point \( U \), using,

\[
\begin{align*}
a(\zeta) &= \zeta'(x) - \frac{1}{x'(\zeta)} , \\
b(\eta) &= \eta'(y) - \frac{1}{y'(\eta)} , \\
c(\zeta) &= \zeta''(x) - \frac{x''(\zeta)}{(x'(\zeta))^3} , \\
d(\eta) &= \eta''(y) - \frac{y''(\eta)}{(y'(\eta))^3}.
\end{align*}
\]

For more general mapping functions depending on \( \zeta \) and \( \eta \), similar problem (where appear some cross derivatives of high-order) can be defined on non-cartesian grid and the same technique than (8-9) must be investigated in detail to obtain compact discretization (future work).

### 3.1 Analytical construction of the maps

We present a simple way to construct the map transformation \( x \) (or \( y \)). The appropriate transformation \( x \) for a grid \( NU \) is obtained by interpolation. To avoid possible oscillations, \( x \) is considered to be equal to a B-spline function of class \( C^2([0,1]) \). This regularity results from relations (12). The analytical expression of \( x \) is obtained by an appropriate choice of the interpolation points and of the values of the derivative \( x'(\zeta) \) in these points. We choose \( n \) points \( P_j = (\zeta_j, x_j), j = 1, \cdots, n \) and \( \bar{n} \) values of the derivatives of \( x \) in \( \bar{P}_j = (\bar{\zeta}_j, \bar{x}_j), j = 1, \cdots, \bar{n} \). The number of constraints on \( x \) is also equal to \( n + \bar{n} \).
then \( x \) is searched under the form.

\[
x(\zeta) = \sum_{i=1}^{n+n} a_i N_i^4(\zeta),
\]

where \((N_i^4)^n_{i=1} \) is a family of basis B-spline functions. We refer to [21] for a recurrence definition of such a basis. The coefficients \( a_i, i = 1, \cdots, (n + n) \) are obtained by solving the linear system resulting from the constraints on \( x \).

For the following numerical simulations, we give an example of B-spline function \( x \) drawn on Fig. 2b. We choose, \( P'_j = \tilde{P}_j \ (j = 1, \cdots, 5) \), defined by \( P_1 = (0.0, 0.0), P_2 = (0.25, 0.3), P_3 = (0.5, 0.5), P_4 = (0.75, 0.7) \) and \( P_5 = (1.0, 1.0) \). We impose \( x' \) to be equal to \( 1.0 \) at points \( P_1, P_2 \) and \( x' \) to be equal to \( 0.2 \) at points \( P_3, P_4 \). If we consider the same transformation to define \( y \), a uniform grid represented by the Fig. 2a is transformed via \( (x, y) \) into a non-uniform grid given by the Fig. 2c.

![Fig. 2- (a) Uniform grid 50x50 - (b) Transformations x, y - (c) Non-uniform grid 50x50](image)

3.2 Discretization of the current densities on non-uniform grids

The problem (11) presents the same characteristics as (1), and its discretization is similar. So we only present the formula which corresponds to (9) for the computation of \( \tilde{J}_{n_v} \). Noting \( R_2 = \frac{\partial^2 n}{\partial \zeta^2} + (\frac{h q}{n \zeta})^2 \frac{\partial^2 n}{\partial \eta^2} \) and \( R_3 = (\frac{h q}{n \zeta})^2 - 3 \), we have:

\[
n_{i,j+rac{1}{2}} \frac{h^2}{24} \left( \frac{\partial^2 n}{\partial \zeta^2} \right)_{i,j+rac{1}{2}} = -\frac{h^2}{48k^2} \left( n_{i+rac{1}{2},j-rac{1}{2}} + n_{i-rac{1}{2},j-rac{1}{2}} + n_{i+rac{1}{2},j+rac{1}{2}} + n_{i-rac{1}{2},j+rac{1}{2}} \right) (R_3)_{i,j+rac{1}{2}} \\
+ \left( \frac{1}{2} + \frac{h^2}{24k^2} (R_3)_{i,j+rac{1}{2}} \right) \left( n_{i+rac{1}{2},j+rac{1}{2}} + n_{i-rac{1}{2},j+rac{1}{2}} \right) - \frac{h^2}{12} (R_2)_{i,j+rac{1}{2}} + O(h^4 + k^4). \tag{13}
\]
4 Numerical tests

The objective of this section is to prove the robustness of this new method. The discretization yields a system of nonlinear equations linearized by a Newton iteration [17] and inverted using the solver BMRFS [19]. The Newton iteration requires the definition of the associated Jacobian matrix. Its computation and the implementation of the discretized problem are realized using the symbolic system AXIOM [14]. The geometry of the device, a silicon pn-diode, is shown in Fig. 3, where $\Gamma_D = \{AB\} \cup \{CD\}$ and $\Gamma_N = \partial \Omega \setminus \Gamma_D$. The numerical values of the physical parameters at room temperature $T = 300K$ are given in Table 2 with $U_T = kT/q$ ($k$: Boltzmann constant), $D_n = \mu_n U_T$ and $D_p = \mu_p U_T$.

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<th>Numerical value</th>
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</table>

Table 2. Physical parameters.

In a care of simplicity, we neglect recombination-generation effects ($GR = 0$). We consider a reverse biased diode with an applied bias of $U = -5V$, defined as the difference of the applied potential at the contacts of the $n$-region and the $p$-region. We choose a doping profile equal to $C(x, y) = -10^{15}$cm$^{-3}$ in the $p$-region and $C(x, y) = 10^{15}$cm$^{-3}$ in the $n$-region which generates an abrupt junction. The device is assumed to be a square of size $10^{-3}$cm$\times$10$^{-3}$cm. The squared scaled Debye length is equal to $\lambda^2 = \frac{U_T \varepsilon}{\varepsilon_0 q C_{\max}} = 1.67153 \times 10^{-5}$, where $C_{\max} = \max\{C(x, y)\}$ and $\varepsilon_0$ a typical length of the device. The Figures 4-5-6a and 4-5-6b represent the solution $\psi$, $u$, $p$, computed using respectively a $50 \times 50$ uniform and non-uniform grid presented in section 3.1 (Fig. 2).
We notice that this scheme eliminates spurious numerical oscillations which often arise using central differencing of second-order when the cell Reynolds number is greater than 2. This behaviour was already observed by Spotz [5] and can be compared to the stability of an exponential scheme [11,12] which corresponds to an adaptive upwind scheme (comparative studies are presented in [22]). Using non-uniform grids, we obtain a better approximation of the solution in the depletion zone. The presence of few grid points within the junction leads to an easier resolution of the discretized problem. If we push up voltage bias, a threshold equal to 1.3V is observed (the Newton iteration does not converge).

5 Conclusions

In this work we have developed a new finite difference scheme for drift-diffusion model. We have used a fourth-order compact scheme (using 6 points) to compute the current densities using a formulation of the problem on staggered grids. The current conservation is preserved. We have extended this formulation on non-uniform grids by mapping. These maps and the corresponding tedious manipulations have been determined using symbolic manipulations.
which not allow to introduce numerical errors. The scheme gives a good treatment of abrupt junctions, and eliminates nonphysical oscillations. We are not limited by the algebra, then we can imagine the construction of more general non-uniform grids. Successful tests are in preparation for more general models like Energy Transport where the equations are strongly coupled.

Acknowledgments. I am very grateful to P. Pietra for her assistance with the computing work and to F. BenBelgacem and A. Rigel for many discussions.

Appendix A. This appendix contains approximations of order 2 used in the discretization of $J_{xx}$ at the node $(i, j+\frac{1}{2})$. We give in Table 3, the values of the constants $\alpha_i$ ($i = 1, \cdots, 6$), $\mu$ and $\gamma$ in $u_0 u_1 + \alpha_1 u_{-\frac{1}{2}} u_{-\frac{1}{2}} + \alpha_2 u_{-\frac{1}{2}} u_{\frac{1}{2}} + \alpha_3 u_{\frac{1}{2}} u_{\frac{1}{2}} + \alpha_4 u_{-\frac{1}{2}} u_{\frac{1}{2}} + \alpha_5 u_{-\frac{1}{2}} u_{\frac{1}{2}} + \alpha_6 u_{-\frac{1}{2}} u_{\frac{1}{2}} + O(h^2 + k^2)$, which define approximations of $u$, $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial y}$, $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^2 u}{\partial y^2}$ and $\frac{\partial^2 \psi}{\partial y^2}$ ($\psi$ solution of (1c)), only using the neighbouring nodes of $(i, j+\frac{1}{2})$, (see Fig. 1. dark marks).

<table>
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<th></th>
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Table 3. Finite difference approximations.

References


