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A new Control Volume Finite Element Method for the stable and accurate solution of the drift–diffusion equations on general unstructured grids

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ABSTRACT

We present a new Control Volume Finite Element Method with multi-dimensional Scharfetter–Gummel upwinding (CVFEM-SG) for the drift–diffusion equations. The method combines a conservative formulation of the carrier density continuity equations with an edge element lifting of the one-dimensional Scharfetter–Gummel edge currents into curl-conforming elemental currents. These elemental currents combine the upwind effect from all element edges and enable accurate computation of the flux on arbitrary surfaces inside the elements. In so doing, we obtain a formulation that is stable and accurate on general unstructured finite element grids. This approach sets our formulation apart from other methods, which require the control volumes to be topologically dual to the primal grid. Numerical studies of the CVFEM-SG for a suite of scalar advection–diffusion test problems confirm the accuracy and the robustness of the new formulation. Simulations of a PN diode and an n-channel MOSFET device demonstrate the performance of the method for the fully coupled drift–diffusion system.

1. Introduction

The drift–diffusion equations are a coupled system of nonlinear Partial Differential Equations (PDE's) [26,24], which model the motion of electrons and holes in semiconductor materials. Predictive simulation of semiconductor devices depends on the robust, accurate and efficient numerical solution of these equations. Two desirable properties of numerical schemes for the drift–diffusion equations are (a) stability in the strong drift regime, i.e., when carriers drift velocities dominate their diffusivity, and (b) local conservation of electron and hole current densities.

The development of the exponentially fitted Scharfetter–Gummel (SG) scheme [30] was a major breakthrough that enabled stable and accurate numerical solution of the drift–diffusion equations in one-dimension. Extension of SG to multiple dimensions [20,14,31] typically relies on topologically dual grids[2]; see the right plot in Fig. 1. For such grids, the area of the dual (control volume) face times the SG edge current on the primal edge crossing that face gives an accurate approximation of the current density flux through the boundary of the dual cell. The resulting conservative finite volume method[3] with SG upwinding (FVM-SG) has excellent stability and is the workhorse in most modern device simulators [9,19,14].

Insofar as the conservation of current density is concerned, finite volume and finite element methods follow different paths. The former integrate the continuity equation on the (topologically dual) control volumes and apply the Divergence Theorem to transform the volume integrals into surface integrals. This ensures conservation of current density with respect to the dual control volumes. On the other hand, conservative finite elements approximate the current density by div-conforming *face elements* [6]. The resulting mixed finite element methods [5] have indefinite systems

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[2] We recall that two grids in d-dimensions are topologically dual if there is one-to-one correspondence between their k and $d-k$-dimensional entities. For example, in three dimensions ($d=3$) every primal vertex ($k=0$) corresponds to a unique dual cell ($3-0=3$); every primal edge ($k=1$) corresponds to a unique dual face ($3-1=2$), every primal face ($k=2$) corresponds to a unique dual edge ($3-2=1$), and every primal cell ($k=3$) corresponds to a unique dual vertex ($3-3=0$). In two dimensions ($d=2$) the correspondence is between primal vertices ($k=0$) and dual cells ($2-0=2$), primal edges ($k=1$) and dual edges ($2-1=1$) and primal cells ($k=2$) and dual vertices ($2-2=0$).

[3] This scheme is often referred to as the Box Integration Method, or the Finite Boxes approach.

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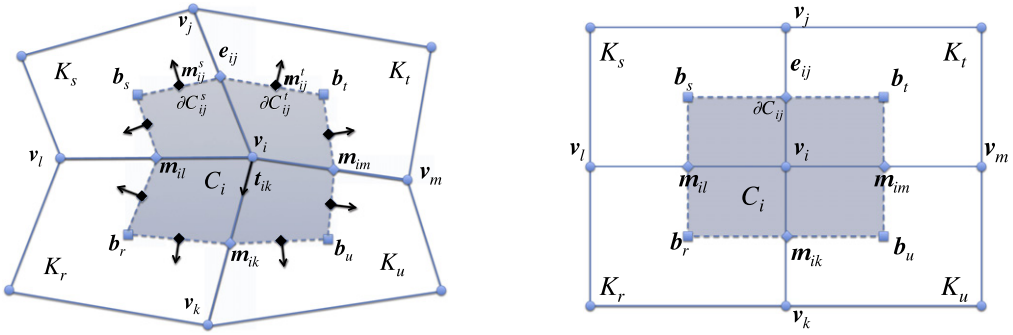

Fig. 1. On quadrilateral grids we connect the barycenter $\boldsymbol{b}_r$ of every $K_r \in K(\boldsymbol{v}_i)$ with the centers $\boldsymbol{m}_{ik}, \boldsymbol{m}_{il}$ of its two faces sharing the vertex $\boldsymbol{v}_i$. The resulting control volume C_i is an octagon. The two facets ∂C^s_{ij} and ∂C^t_{ij} of this octagon, connected to $\boldsymbol{m}_{ij}$, form the *control volume face* ∂C_{ij} that is dual to edge $\boldsymbol{e}_{ij} : \partial C_{ij} = \partial C^s_{ij} \cup \partial C^t_{ij}$. On Cartesian grids (right panel) the control volumes C_i form a topologically dual grid and the unit normals to ∂C^s_{ij} and ∂C^t_{ij} are parallel to $\boldsymbol{e}_{ij}$. On nonuniform grids (left panel) these normals are not parallel to $\boldsymbol{e}_{ij}$ and C_i are not topologically dual to the elements on the primal mesh.

with more variables than primal Galerkin methods, which approximate only the carrier densities. However, primal Galerkin methods do not conserve current density and so, they lack one of the two desirable properties for device simulations.

The Control Volume Finite Element Method (CVFEM) [3] is an alternative approach that combines the simplicity of the primal Galerkin method with the local conservation properties of finite volume methods, *without requiring topologically dual grids*. The CVFEM approximates carrier densities using the same nodal shape functions as the primal Galerkin method. However, the "weak" CVFEM equations result from the application of the Divergence Theorem to control volumes surrounding the element vertices, i.e., they resemble finite volume equations.

While the CVFEM is conservative, it still needs some form of stabilization for advection-dominated problems [25,33,34]. In this paper we present a new CVFEM for the drift–diffusion equations, which combines a conservative formulation of the carrier density continuity equations with an edge element lifting of the one-dimensional Scharfetter–Gummel edge currents into curl-conforming elemental currents. In a nutshell, we solve one-dimensional drift–diffusion equations on the edges of the finite element mesh and then use $H(curl,\Omega)$-conforming edge elements [28] to expand the resulting edge current densities into an elemental current density. The latter combines the upwind effect from all element edges and enables accurate computation of the current density flux on arbitrary surfaces inside the elements. In so doing we obtain a truly multidimensional extension of the Scharfetter–Gummel approach to general unstructured grids and a numerical method that merges the exceptional stability of the FVM-SG with the greater flexibility of CVFEM. Accordingly, we term the new method CVFEM-SG. The new method is computationally equivalent to FVM-SG on topologically dual grids, yet because the elemental current density can be integrated accurately on arbitrary surfaces inside the elements, it remains robust and accurate in the absence of this property.

To motivate our approach we examine the nodal CVFEM current in the pure diffusion limit. Using that nodal and edge elements belong to an exact sequence we prove that in the absence of carrier drift the nodal current is the lifting of one-dimensional purely diffusive currents by $H(curl,\Omega)$-conforming edge basis functions. Therefore, the $H(curl,\Omega)$-conforming lifting of the Scharfetter–Gummel edge currents represents a consistent extension of the nodal current density.

Application of $H(curl,\Omega)$-conforming elements to lift edge currents into an elemental current density, and independence from explicit stabilization parameters set apart the CVFEM-SG from the existing stabilized CVFEM formulations [34,33], which rely on the same perturbation functions as the Streamline Upwind Petrov–Galerkin (SUPG) method [8]. The quality of their solutions can depend on the choice of the stabilization parameter. Finding the optimal stabilization parameter for a given PDE and simulation setting remains an open problem. Some of the parameters that enter its definition are not known exactly [15], and different solution features, such as internal layers and boundary layers, require different definitions of this parameter [18].

Our brief survey deliberately omits approaches that use the primal Galerkin formulation of the drift–diffusion equations because they lack the second desirable property, i.e., the local current conservation. We refer the interested readers to [32] (extension of SUPG to drift–diffusion), [1,29,37,36] (exponentially fitted conforming finite elements), [17,13,12] (multiscale finite elements), and [35] (stabilized Generalized Finite Element) for examples and further details. Likewise, we skip mixed methods for drift–diffusion because of their more complicated computational structure, which does not allow simple reuse of an existing primal Galerkin code infrastructure. We refer to [6,7] for more information about these methods.

The rest of this section reviews the relevant notation and the governing drift–diffusion equations. Section 2 motivates and presents the semi-discrete in space CVFEM-SG formulation using a stand-alone version of the electron continuity equation. Section 3 defines the fully discrete CVFEM-SG and discusses its implementation for the coupled drift–diffusion system in Sandia's semiconductor device simulation code Charon. Section 4 presents numerical studies of the new method in two different simulation settings. The first study compares and contrasts the CVFEM-SG with FVM-SG and a stabilized CVFEM for a suite of stationary and transient scalar advection test problems. The second study uses simulations of a PN diode and a MOSFET device to examine the performance of the CVFEM-SG for the fully coupled drift–diffusion system. Section 5 summarizes our conclusions and Appendix A sheds some additional light on the key distinctions between CVFEM-SG and FVM-SG by comparing their stencils on a uniform grid.

1.1. Notation

In this paper Ω is a bounded region in $\Re^n,\ n = 2, 3$ with Lipschitz-continuous boundary $\partial\Omega$. The Neumann and Dirichlet parts of the boundary are Γ_N and Γ_D, respectively. We use the standard notation $H^1(\Omega)$ for the Sobolev space of order one, $L^2(\Omega)$ for the space of all square integrable functions, and $H(curl,\Omega)$ for the space of all square integrable vector fields whose curl is also square integrable. Lower case Roman and Greek letters denote scalar quantities and bold face symbols are vector quantities. The meaning of the symbol $|\cdot|$ varies with the context and can be Euclidean length, domain measure, or cardinality of a finite set.

Throughout the paper $K_h(\Omega)$ is a conforming finite element partition of Ω into elements K_s with sizes h_s and barycenters $\boldsymbol{b}_s$. The