An Exponentially Fitted Finite Element Scheme for Diffusion Process Simulation on Coarse Grids

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Abstract

A new finite element scheme for diffusion process simulation, which allows coarse grid spacings in the areas of exponentially varying concentrations and fluxes, is proposed. It employs a nonlinear test function obtained from local divergence free conditions. Two-dimensional test computations show clear superiority of the exponentially fitted finite element scheme over the standard approach, as well as its robustness regarding irregular grid geometry.

1. Introduction

The gradually increasing complexity of the multiparticle diffusion models and necessity to simulate in higher dimensions persistently challenge computational efficiency of the modern process simulators. An obvious guideline to cope with the efficiency problems in the discretization phase is to make a grid structure as coarse as possible for a given tolerance of the discrete solution accuracy. To this end, considerable effort has been directed to the development of advanced adaptive grid generation techniques for both the finite difference (FD) and finite element (FE) methods. On the other hand, the discretization fitting to the particular features of the solution is much less exploited in the diffusion process simulation as an additional grid coarsening technique. The FD scheme that exploits the exponential flux behavior to allow the coarse grid spacings in diffusion process simulation, has been proposed by Lowther [1]. The main intention of this paper is to propose a corresponding FE scheme, which could be also robust for irregular element geometry.

2. Problem formulation

The transport of the particles (impurities or point-defects) involved in the diffusion process is commonly modeled by the diffusion equations in the form:

$$\frac{\partial C}{\partial t} - \nabla \cdot (D \nabla C + Z \mu C \nabla \varphi) = r. \tag{1}$$

C and Z are the concentration and charge state of the particle. r, D, μ and φ are concentration dependent reaction term, diffusion coefficient, mobility and built-in

electric potential, which govern various interactions among particles. Introducing the normalized chemical potential $u = \log C$ and making use of the Einstein relation ($D/\mu = V_T$, with V_T representing the thermal voltage), the diffusion equation (1) can be expressed as

$$-\nabla \cdot \boldsymbol{F} + R = 0 \text{ with } \boldsymbol{F} = De^u \nabla v. \tag{2}$$

Here $v = u + Z\varphi/V_T$ is the normalized particle electrochemical potential, while the zero-order term $R = \partial e^u/\partial t - r$ consists of the time-derivative and reaction terms. In (2), we consider both u and v (actually, u and φ) as well behaved quantities, which is consistent with the basic assumption that the components of the flux $\boldsymbol{F}$ are exponentially varying quantities.

The diffusion equation (2) is defined in a bounded domain $\Omega \subseteq \boldsymbol{R}^n$ with piecewise smooth boundary $\partial\Omega$. An initial state $u = u_0$ at $t = 0$ is defined in $\bar{\Omega} = \Omega \cup \partial\Omega$. Let the boundary $\partial\Omega$ consists of Dirichlet ($\partial\Omega_d$) and Neumann ($\partial\Omega_n$) segments with boundary conditions: $u = u_0$ on $\partial\Omega_d$ and $\boldsymbol{F} \cdot \boldsymbol{n} = 0$ on $\partial\Omega_n$, where $\boldsymbol{n}$ denotes the normal vector to the boundary. Without any loss of generality we consider the discretization of $\bar{\Omega}$ into N_e nonoverlapping elements Ω_e constructed over N_n nodes as simplexes, i.e., intervals, triangles or tetrahedra for $n = 1, 2$ or 3.

3. Exponentially fitted FE scheme

A class of generalized FE methods [2] is used to derive the FE discretization of (2). As a weak integral statement we consider

$$\int_\Omega \boldsymbol{F} \cdot \nabla\psi_i d\Omega + \int_\Omega R\psi_i dx = 0 \ , \tag{3}$$

where ψ_i represents an exponentially fitted test function which satisfies the local divergence free problems

$$\nabla \cdot (De^u \nabla\psi_i) = 0 \quad \text{in } \Omega_e \ni i \text{ with } \psi_i(k) = \delta_{ik}. \tag{4}$$

Here i and k denote grid nodes while δ_{ik} is the Kronecker delta. Although the local divergence free problems (4) cannot be solved in a closed form, it seems appropriate to assume that $De^u \nabla\psi_i$ varies at least linearly in Ω_e to achieve first order accuracy. With this assumption, ψ_i is given by

$$\psi_i = (\phi_i - \alpha I_{\Omega_e}(e^u)) \cdot e^{u_i - u} + \alpha e^{u_i} \text{ and } \alpha = \frac{\nabla\phi_i \cdot \nabla u}{\nabla I_{\Omega_e}(e^u) \cdot \nabla u}, \tag{5}$$

where ϕ_i is the standard linear test function and $I_{\Omega_e}(\cdot)$ represents a linear interpolation from the nodal values in the element Ω_e. In the special case of the piecewise constant u, we have $\psi_i = \phi_i$. The exponentially fitted FE scheme is obtained from (3) and (5), using ϕ_i as a finite element basis for u and v and approximating D as a piecewise constant discrete function.

The test function (5) produces an upwinding effect, that is similar to the streamline Petrov-Galerkin methods, but with no need for an external adjustment of the numerical dissipation. To avoid any occurrence of the singular and counter upwinding effects, we propose to perform $I_{\Omega_e}(\cdot)$ in obtuse elements as one-dimensional linear interpolation between nodes X_1 and X_{n+1}; here X_k, $(k = 1, \ldots, n+1)$ denote coordinates of the element Ω_e nodes in ascending order along the X axis, that is aligned with ∇u. In this way, $\nabla I_{\Omega_e}(e^u) \cdot \nabla u > 0$ is guaranteed for $|\nabla u| > 0$.

4. Test computations

As a model problem we employ here the two-dimensional diffusion equation (2) in a rectangular domain ($0.4\mu m \times 0.4\mu m$), with $v = u$, $r = 0$ and assuming constant $D = 5 \cdot 10^{-15} cm^{-2}/s$. It is useful for the practical analysis of discretization schemes since the exact differential solution is available [3] for 2-D Gaussian initial state (here $R_p = 0.063\mu m$, $\Delta R_p = 0.021\mu m$, $\Delta R_{pl} = 0.018\mu m$ and $C_{max} = 10^{20} cm^{-3}$). The grid structure is selected as extremely coarse with $N_e = 106$ and $N_n = 70$. The exact solution at $t = 300s$ is shown in Figure 1. The gray and white areas denote the concentration ranges $10^i < C < 10^{i+1}$ starting from $i = 12$ at the bottom. The discrete solutions obtained with the standard FE scheme (test LIN-FE) [4] and a new exponentially fitted FE scheme (test EXP-FE) are shown in Figure 2 and Figure 3, respectively. The result of the third test (EXP-FE(o)), that employs the grid structure consisting exclusively of obtuse triangles ($N_e = 318$ and $N_n = 176$), is shown in Figure 4. For the more quantitative examination of the test computations, the relative error in the junction depth is analyzed for all above tests including also the exponentially fitted FD scheme (test EXP-FD) [1]. The progression of the junction depth error during diffusion and the dependence of the junction depth error on the substrate concentration are shown in Figure 5 and Figure 6, respectively.

It could be observed that the standard FE scheme tends to significantly overestimate the amount of diffusion and the junction depth. On the other hand, with the exponentially fitted FE scheme, besides substantial improvements of the solution accuracy, the junction depth error shows a stable accumulation during diffusion, as well as uniform distribution in the wide range of the substrate concentrations.

5. Conclusion

The efficiency of the diffusion process simulation could be significantly improved with exponentially fitted FE schemes that allow coarser grid spacings then standard approaches. A new FE scheme has combined properties of the streamline Petrov-Galerkin and the divergence free upwinding methods. The superiority of a new FE scheme over its standard counterpart is demonstrated in the test computations with the known exact analytical solution. Unlike the exponentially fitted FD scheme [1], a new exponentially fitted FE scheme appears to be robust on grid structures with obtuse triangles.

References

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Figure 1: The exact solution.

Figure 2: The discrete solution in the test LIN-FE.

Figure 3: The discrete solution in the test EXP-FE.

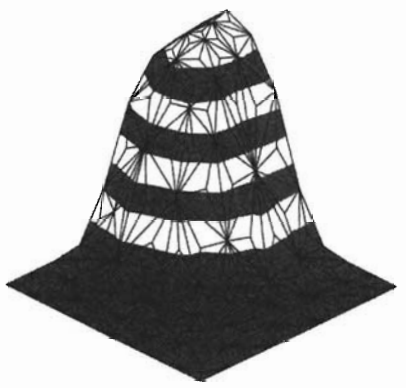

Figure 4: The discrete solution in the test EXP-FE(o).

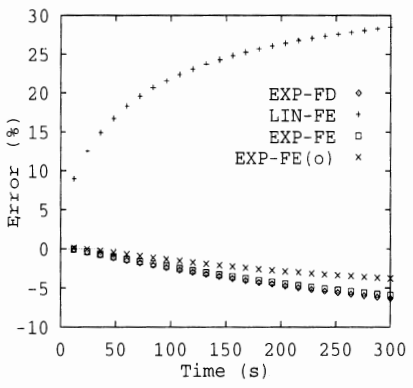

Figure 5: The progression of the junction depth error during diffusion.

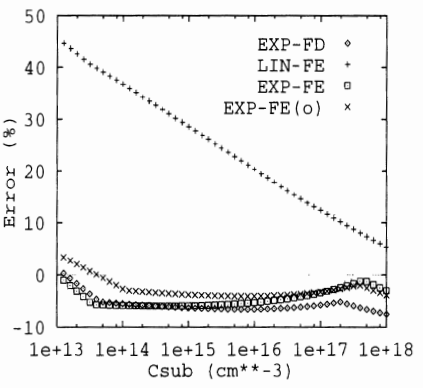

Figure 6: The dependence of the junction depth error on the substrate concentration.