Adaptive Discontinuous Galerkin Methods for Nonlinear Diffusion-Convection-Reaction Equations

Bulent Karasözen, Murat Uzunca, and Murat Manguoğlu

Abstract In this work, we apply the adaptive discontinuous Galerkin method (DGAFEM) to the convection dominated nonlinear, quasi-steady state convection diffusion reaction equations. We propose an efficient algorithm to solve the sparse linear systems iteratively arising from the discretized nonlinear equations. Numerical examples demonstrate the effectiveness of the DGAFEM to damp the spurious oscillations for the convection dominated nonlinear equations.

1 Introduction

Many engineering problems such as chemical reaction processes, heat conduction, nuclear reactors, population dynamics are governed by coupled convection-diffusion-reaction partial differential equations (PDEs) with nonlinear source or sink terms. It is a significant challenge to solve such PDEs numerically when they are convection/reaction-dominated, which is the case in our study. As a model problem, we consider the coupled quasi-stationary model arising from the time discretization of the time dependent nonlinear diffusion-convection-reaction equations

$$\alpha u_i - \epsilon_i \Delta u_i + \mathbf{b}_i \cdot \nabla u_i + r_i(\mathbf{u}) = f_i \quad \text{in } \Omega, \quad u_i = g_i \quad \text{on } \Gamma, \quad i = 1, \ldots, m \tag{1}$$

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with Ω is a bounded, open, convex domain in $\mathbb{R}^2$ with boundary $\partial\Omega = \Gamma$, $0 < \epsilon_i \ll 1$ are the diffusivity constants, $f_i \in L^2(\Omega)$ are the source functions, $\mathbf{b}_i \in \left(W^{1,\infty}(\Omega)\right)^2$ are the velocity fields, $g_i \in H^{1/2}(\Gamma_D)$ are the Dirichlet boundary conditions and $\mathbf{u}(x,t) = (u_1, \ldots, u_m)^T$ denotes the vector of unknown solutions. The coefficients of the linear reaction terms, $\alpha > 0$, stand for the temporal discretization, corresponding to $1/\Delta t$, where Δt is the discrete time step. For the uniqueness of the solution of (2), we assume that the nonlinear reaction terms are bounded, locally Lipschitz continuous and monotone, i.e. satisfy the following conditions [3]

$$r_i \in C^1(\mathbb{R}_0^+), \quad r_i(0) = 0, \quad r_i'(s) \geq 0, \quad \forall s \geq 0, \quad s \in \mathbb{R}$$

Such models describe chemical processes and they are strongly coupled as an inaccuracy in one unknown affects all the others. Hence, an efficient numerical approximation of these systems is needed. For the convection/reaction-dominated problems, the standard Galerkin finite element methods are known to produce spurious oscillations, especially in the presence of sharp fronts in the solution, on boundary and interior layers. In contrast to standard Galerkin conforming finite element methods, DG methods produce stable discretizations without the need for stabilization strategies, and overcome the spurious oscillations due to the convection domination. For linear convection dominated problems, the streamline upwind Petrov-Galerkin(SUPG) method is capable of stabilizing the unphysical oscillations [3, 4]. Nevertheless, in nonlinear convection dominated problems, spurious oscillations are still present in crosswind direction. Therefore, SUPG is used with the anisotropic shock capturing technique (SUPG-SC) for reactive transport problems [3,4].

Similar to the stabilized conforming finite elements, discontinuous Galerkin finite element methods (DGFEMs) damp the unphysical oscillations for linear convection dominated problems. In [9], several nonlinear convection dominated problems of type (1) are solved with DGFEM and DG-SC, discontinuous Galerkin method with the shock-capturing technique. The main advantages of DGFEMs are the flexibility in handling non-matching grids and in designing hp-refinement strategies. An important drawback is that the resulting linear systems are more dense than the ones in continuous finite elements and ill-conditioned. The condition number grows rapidly with the number of elements and with the penalty parameter. Therefore, efficient solution strategies such as preconditioning are required to solve the linear systems. In this paper, an adaptive discontinuous Galerkin method (DGAFEM) is developed for the convection dominated nonlinear problems of type (1) using the modification of a posteriori error estimates for linear convection dominated problems in [6]. We show the effectiveness and accuracy of DGAFEM capturing boundary and internal layers very sharply and without significant oscillations.

In the next two sections, we give the DGFEMs discretization and describe the residual based adaptivity for nonlinear diffusion-convection-reaction problems.

Section 4 deals with an efficient solution technique to handle the linear systems arising from the DGAFEM. In Sect. 5, we demonstrate on two examples the efficiency of the adaptivity for handling the sharp layers.

2 DG Discretization

The weak formulation of the scalar equation ($m = 1$) of (1) reads as

$$\int_\Omega (\epsilon \nabla u \cdot \nabla v + \mathbf{b} \cdot \nabla u v + \alpha u v) dx + \int_\Omega r(u) v dx = \int_\Omega f v dx \quad \forall v \in V \tag{2}$$

where the solution space U and the test function space V are given by

$$U = \{u \in H^1(\Omega) \,:\, u = g \text{ on } \Gamma\}, \quad V = \{v \in H^1(\Omega) \,:\, v = 0 \text{ on } \Gamma\}$$

The variational form of the scalar equation (1) is discretized by the symmetric discontinuous interior penalty Galerkin (SIPG) method with upwinding for the convection part [1, 2]

$$a_h(u_h, v_h) + b_h(u_h, v_h) = l_h(v_h)\,, \qquad \forall v_h \in V_h \subset H^1(\Omega) \tag{3}$$

$$\begin{aligned}
a_h(u_h, v_h) = & \sum_{K \in \xi_h} \int_K \epsilon \nabla u_h \cdot \nabla v_h dx + \sum_{K \in \xi_h} \int_K (\mathbf{b} \cdot \nabla u_h + \alpha u_h) v_h dx \\
& - \sum_{e \in \Gamma_0 \cup \Gamma} \int_e \{\epsilon \nabla v_h\} \cdot [u_h] ds - \sum_{e \in \Gamma_0 \cup \Gamma} \int_e \{\epsilon \nabla u_h\} \cdot [v_h] ds \\
& + \sum_{K \in \xi_h} \int_{\partial K^- \setminus \Gamma} \mathbf{b} \cdot \mathbf{n} (u_h^{out} - u_h^{in}) v_h ds - \sum_{K \in \xi_h} \int_{\partial K^- \cap \Gamma^-} \mathbf{b} \cdot \mathbf{n} u_h^{in} v_h ds \\
& + \sum_{e \in \Gamma_0 \cup \Gamma} \frac{\sigma \epsilon}{h_e} \int_e [u_h] \cdot [v_h] ds, \\
b_h(u_h, v_h) = & \sum_{K \in \xi_h} \int_K r(u_h) v_h dx, \\
l_h(v_h) = & \sum_{K \in \xi_h} \int_K f v_h dx + \sum_{e \in \Gamma} \int_e g \left(\frac{\sigma \epsilon}{h_e} v_h - \epsilon \nabla v_h \cdot \mathbf{n} \right) ds \\
& - \sum_{K \in \xi_h} \int_{\partial K^- \cap \Gamma^-} \mathbf{b} \cdot \mathbf{n} g v_h ds,
\end{aligned}$$

where the finite dimensional solution and test function spaces are the same. ∂K^- and Γ^- denote the inflow parts to an element boundary ∂K and the domain boundary Γ, respectively. The jump and average terms for u_h and v_h across the edges are denoted by $[\cdot]$ and $\{\cdot\}$, respectively. The parameter $\sigma \in \mathbb{R}_0^+$ is called the penalty parameter which should be sufficiently large for SIPG [6].

3 Adaptivity

We apply the residual based adaptive strategy in [6] which is robust, i.e. independent of the Péclet number, for linear diffusion-convection equations. We include in the a posteriori error estimates the nonlinear reaction terms as local contributions to the cell residuals and not to the interior/boundary edge residuals [Chp. 5.1.4, [8]]. Let the constant $\kappa \geq 0$ satisfies

$$\alpha(x) - \frac{1}{2}\nabla \cdot \mathbf{b}(x) \geq \kappa \,, \qquad \| - \nabla \cdot \mathbf{b} + \alpha\|_{L^\infty(\Omega)} \leq \kappa^* \kappa$$

for a non-negative κ^*, to easily have the efficiency of the a posteriori error estimator. We define the local error indicator for each element $K \in \xi_h$

$$\eta_K^2 = \eta_{R_K}^2 + \eta_{E_K^0}^2 + \eta_{E_K^D}^2,$$

$$\eta_{R_K}^2 = \rho_K^2 \| f - \alpha u_h + \epsilon \Delta u_h - \mathbf{b} \cdot \nabla u_h - r(u_h)\|_{L^2(K)}^2,$$

$$\eta_{E_K^0}^2 = \sum_{e \in \partial K \cap \Gamma_0} \left(\frac{1}{2} \epsilon^{-\frac{1}{2}} \rho_e \| [\epsilon \nabla u_h] \|_{L^2(e)}^2 + \frac{1}{2} (\frac{\epsilon \sigma}{h_e} + \kappa h_e + \frac{h_e}{\epsilon}) \| [u_h] \|_{L^2(e)}^2 \right),$$

$$\eta_{E_K^D}^2 = \sum_{e \in \partial K \cap \Gamma} (\frac{\epsilon \sigma}{h_e} + \kappa h_e + \frac{h_e}{\epsilon}) \| g - u_h \|_{L^2(e)}^2,$$

with the weights ρ_K and ρ_e on an element K are defined for $\kappa \neq 0$

$$\rho_K = \min\{h_K \epsilon^{-\frac{1}{2}}, \kappa^{-\frac{1}{2}}\}, \ \rho_e = \min\{h_e \epsilon^{-\frac{1}{2}}, \kappa^{-\frac{1}{2}}\}.$$

When $\kappa = 0$, we set $\rho_K = h_K \epsilon^{-\frac{1}{2}}$ and $\rho_e = h_e \epsilon^{-\frac{1}{2}}$. Our adaptive algorithm is based on the standard adaptive finite element (AFEM) iterative loop: SOLVE $\rightarrow$ ESTIMATE $\rightarrow$ MARK $\rightarrow$ REFINE. The mesh is marked at each iteration using the Dörfler strategy and refined using the longest edge bisection method [5]. For coupled problems, the elements in the set of union of each component are refined.

4 Efficient Solution of Linear Systems

Because the stiffness matrices obtained by DGFEM become ill-conditioned and more dense with increasing polynomial degree [2], several preconditioners are developed for an efficient and accurate solution of linear diffusion-convection equations under DG discretization. Here we apply the matrix reordering and partitioning technique in [7], which uses the largest eigenvalue and corresponding eigenvector of the Laplacian matrix. This reordering reflects very well the block structure of the underlying sparse matrix.

The solution to (3) has the form $u_h = \sum_{i=1}^{dof} U_i \phi_i$ where ϕ_i's are the basis functions spanning the DGFEM space V_h, and U_i's are the unknown coefficients. Then, the discrete residual of (3) can be given as

$$R(U) = SU + h(U) - L \tag{4}$$

where $U = (U_1, U_2, \ldots, U_{dof})^T$ is the vector of unknown coefficients, $S \in \mathbb{R}^{dof \times dof}$ is the stiffness matrix with the entries $S_{ij} = a_h(\phi_j, \phi_i)$, $h \in \mathbb{R}^{dof}$ is the vector function of U with the entries $h_i = b_h(u_h, \phi_i)$ and $L \in \mathbb{R}^{dof}$ is the vector to the linear form with $L_i = l_h(\phi_i)$, $i, j = 1, 2, \ldots, dof$. We start with a non-zero initial vector U^0. The nonlinear system of equations (4) are solved by Newton-Raphson method. The linear system arising from ith-Newton-Raphson iteration step has the form $Jw^i = -R^i$, where J is the Jacobian matrix to $R(U^0)$ (i.e. $J = S + h'(U^0)$ and it remains unchanged among the iteration steps), $w^i = U^{i+1} - U^i$ is the Newton correction, and R^i denotes the residual of the system at U^i ($R^i = R(U^i)$). Next, we construct a permutation matrix P for the Jacobian matrix J as described in [7]. Then, we apply the permutation matrix P to obtain the permuted system $Nw = b$ where $N = PJP^T$, $w = Pw^i$ and $b = -PR^i$. After solving the permuted system, the solution of the unpermuted linear system can be obtained by applying the inverse permutation, $w^i = P^T w$. The permuted and partitioned linear system can be solved via the block LU factorization in which the coefficient matrix has the form

$$N = \begin{bmatrix} A & B \\ C^T & D \end{bmatrix} = \begin{bmatrix} A & 0 \\ C^T & S \end{bmatrix} \begin{bmatrix} I & U \\ 0 & I \end{bmatrix}$$

where $U = A^{-1}B$ and S is the Schur complement matrix: $S = D - C^T U$. For the right hand side vector $b = (b_1, b_2)^T$ and the reordered solution $w = (w_1, w_2)^T$, solution of the block LU factorized system can be obtained in three steps as follows

$$Az = b_1, \quad Sw_2 = b_2 - C^T z, \quad w_1 = z - Uw_2 \tag{5}$$

with both the matrices A and S are well-conditioned compared to the coefficient matrix of the unpermuted system shown in Table 1.

Table 1 Condition numbers of the stiffness matrices corresponding to the systems obtained by the model in Example 5.1 on a uniform mesh

Degree	1	2	3	4
dof	24,576	49,152	81,192	122,880
J	299.1	660.8	1,596.2	3,399.0
S	139.9	279.1	911.7	1,485.7
A	5.3	18.3	37.7	79.7

5 Numerical Results

Example 5.1 We consider the problem in [3] on $\Omega = (0,1)^2$ with $\epsilon = 10^{-6}$, $\mathbf{b} = \frac{1}{\sqrt{5}}(1,2)^T$, $\alpha = 1$ and $r(u) = u^2$. The source function f and the Dirichlet boundary condition are chosen so that $u(x,y) = \frac{1}{2}\left(1 - \tanh\frac{2x_1 - x_2 - 0.25}{\sqrt{5\epsilon}}\right)$ is the exact solution. The problem is characterized by an internal layer of thickness $\mathcal{O}(\sqrt{\epsilon} \mid \ln\epsilon \mid)$ around $2x_1 - x_2 = \frac{1}{4}$. This problem was solved using SUPG-SC in [3] and SIPG-SC in [9]. Similar to those results, the mesh is locally refined by DGAFEM around the interior layer and the spurious solutions are damped out in Fig. 1, right similar to [3] using SUPG-SC, in [9] with SIPG-SC. On adaptively and uniformly refined meshes, from the Fig. 2, left, it is evident that the adaptive meshes save substantial computing time. On uniform meshes, the SIPG is slightly more accurate than the SUPG-SC in [3]. The error reduction by increasing the degree of the polynomials is remarkable on finer adaptive meshes (Fig. 2, right). For solving the sparse linear systems, we present the results for the *BiCGStab* iterative method of MATLAB with the stopping criterion as $\|r_k\|_2/\|r_0\|_2 \leq tol$ for $tol = 10^{-4}$ (r_i is the residual of the corresponding linear system at the ith iteration) applied to the original unpermuted system and Schur complement system with and without preconditioner. As a preconditioner, the incomplete LU factorization of the Schur complement matrix S (ILU(S)) is used. The linear systems with the coefficient matrix A are solved directly. Table 2 shows that solving the problem by block LU factorization where the Schur complement system is solved iteratively using the preconditioner ILU(S) is the fastest and has the least number of iterations. We use an adaptive mesh by quadratic elements with dof 85,488 at the final refinement level of the 16 refinement levels. The time to obtain the reordered matrix N and computing the permutation in sum among the refinement levels takes 45.18 s, whereas, it takes 1.42 s to compute the Schur complement matrix S and ILU(S), on a PC with Intel Core-i7 processor and 8 GB 1066 MHz DDR3 RAM.

Remark *We note that since the Jacobian matrix does not change during the nonlinear iterations, the permutation, the Schur complement matrix and ILU(S) are computed only once for each adaptive refinement level. In Table 2, we give the number of Newton-Raphson iterations, the average number of BiCGStab iterations for each adaptive mesh refinement level and the total time to solve the problem*

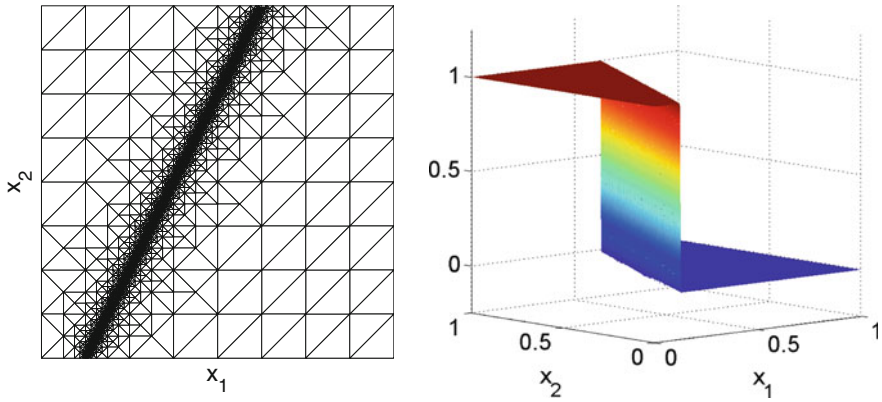

Fig. 1 Example 5.1, Adaptive mesh (*left*) and adaptive solution (*right*), quadratic elements with dof 85,488

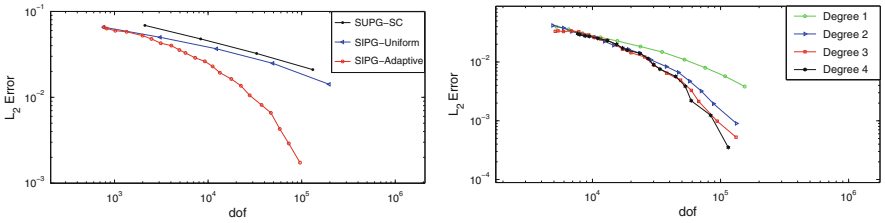

Fig. 2 Example 5.1, Global errors: comparison of the methods by quadratic elements (*left*), adaptive DG for polynomial degrees 1–4 (*right*)

Table 2 Example 5.1, Efficiency results for the sparse linear solver technique for adaptive mesh refinement levels

Linear solver	# Newton its.	# BiCGStab its.	Time (s)
BiCGStab w/o prec. (Unpermuted)	10–11	49–1,143	879.6
Block LU + (BiCGStab w/o prec.)	10–12	33–1,162	454.4
Block LU + (BiCGStab w/ prec. ilu(S))	10–14	4–82	144.9

just including the computation time for the reordered matrix N, the permutation P, Schur complement matrix S, ILU(S) and solving the linear systems among all adaptive mesh refinement levels.

Example 5.2 We consider the two component quasi-steady problem from [4]

$$u_i + \mathbf{b} \cdot \nabla u_i - \nabla \cdot (\epsilon \nabla u_i) + u_1 u_2 = f_i \qquad i = 1, 2$$

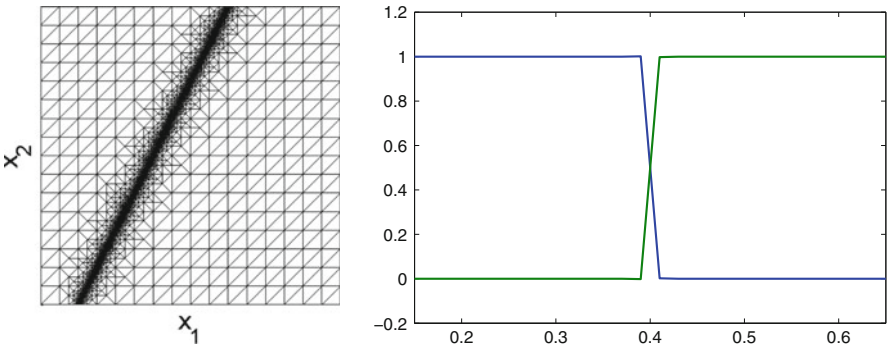

Fig. 3 Example 5.2, Adaptive mesh (*left*) and the cross-section plot (*right*) in the crosswind direction $x_1 + 2x_2 = 1.5$, quadratic elements with dof 144678

on $\Omega = (0,1)^2$ with $\epsilon = 10^{-8}$, $\mathbf{b} = \frac{1}{\sqrt{5}}(1,2)^T$. The source functions f_i and the Dirichlet boundary conditions are chosen with the exact solutions $u_{1,2}(x_1,x_2) = \frac{1}{2}\left(1 \pm \tanh \frac{2x_1 - x_2 - 0.25}{\sqrt{5\epsilon}}\right)$. The equations are coupled by the lowest order terms of the unknowns through $r_i(u,x)$. This problem was solved in [4] with SUPG and SUPG-SC and it was shown that unphysical oscillations are damped using SUPG-SC with fourth order finite elements. Our results in Fig. 3 show that the sharp fronts are very well detected and preserved with the adaptive DG using second order elements. As a results, there is no over or under prediction, and artificial mixing due to discretization will not occur.

We have shown that DGAFEM with the sparse linear solver is an efficient method for solving nonlinear convection dominated problems accurately and avoids the design of the parameters in the shock capturing technique as for the SUPG-SC and DG-SC. The MATLAB programs can be obtained from `http://www.ceng.metu.edu.tr/m̃anguoglu/MatLab.zip`.

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References

1. D. Arnold, F. Brezzi, B. Cockburn, L. Marini, Unified analysis of discontinuous Galerkin methods for elliptic problems. SIAM J. Numer. Anal. **39**, 1749–1779 (2002)

2. B. Ayuso, L.D. Marini, Discontinuous Galerkin methods for advection-diffusion-reaction problems. SIAM J. Numer. Anal. **47**, 1391–1420 (2009)
3. M. Bause, Stabilized finite element methods with shock-capturing for nonlinear convection-diffusion-reaction models, in *Numerical Mathematics and Advanced Applications*, ed. by G. Kreiss, P. Lötstedt, A. Møalqvist, M. Neytcheva (Springer, Berlin, 2010), pp. 125–134
4. M. Bause, K. Schwegler, Higher order finite element approximation of systems of convection-diffusion-reaction equations with small diffusion. J. Comput. Appl. Math. **246**, 52–64 (2013)
5. L. Chen, *i*FEM: an innovative finite element method package in MATLAB. Technical report, Department of Mathematics, University of California, Irvine, 2008
6. D. Schötzau, L. Zhu, A robust a-posteriori error estimator for discontinuous Galerkin methods for convection-diffusion equations. Appl. Numer. Math. **59**, 2236–2255 (2009)
7. O. Tarı, M. Manguoğlu, A new sparse matrix reordering scheme using the largest eigenvector of the graph Laplacian. Numerical Linear Algebra with Applications, in review. http://people.maths.ox.ac.uk/ekertl/PRECON13/talks/Talk_Tari_Manguoglu.pdf
8. R. Verfürth, *A Posteriori Error Estimation Techniques for Finite Element Methods* (Oxford University Press, Oxford, 2013)
9. H. Yücel, M. Stoll, P. Benner, Discontinuous Galerkin finite element methods with schock-capturing for nonlinear convection dominated models. Comput. Chem. Eng. **58**, 278–287 (2013)