A C^0 interior penalty discontinuous Galerkin method for fourth-order total variation flow. I: Derivation of the method and numerical results

Chandi Bhandari[1] **Ronald H.W. Hoppe**[1,2] **Rahul Kumar**[3]

[1]Department of Mathematics, University of Houston, Houston, Texas
[2]Department of Mathematics, University of Augsburg, Augsburg, Germany
[3]Basque Center for Applied Mathematics, Bilbao, Spain

Correspondence
Ronald H. W. Hoppe, Department of Mathematics, University of Houston, 651 P.G. Hoffman, Houston, TX 77204.
Email: rohop@math.uh.edu

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We consider the numerical solution of a fourth-order total variation flow problem representing surface relaxation below the roughening temperature. Based on a regularization and scaling of the nonlinear fourth-order parabolic equation, we perform an implicit discretization in time and a C^0 Interior Penalty Discontinuous Galerkin (C^0IPDG) discretization in space. The C^0IPDG approximation can be derived from a mixed formulation involving numerical flux functions where an appropriate choice of the flux functions allows to eliminate the discrete dual variable. The fully discrete problem can be interpreted as a parameter dependent nonlinear system with the discrete time as a parameter. It is solved by a predictor corrector continuation strategy featuring an adaptive choice of the time step sizes. A documentation of numerical results is provided illustrating the performance of the C^0IPDG method and the predictor corrector continuation strategy. The existence and uniqueness of a solution of the C^0IPDG method will be shown in the second part of this paper.

KEYWORDS

C^0 interior penalty discontinuous Galerkin method, fourth-order total variation flow, surface relaxation

1 | INTRODUCTION

Surface relaxation by surface diffusion is about the relaxation of a high symmetry crystalline surface on which a particular profile has been imprinted such that the typical length scale of the imposed profile is much larger than the lattice constant (dimension of unit cells in the crystal lattice). Therefore, surface relaxation is an important process in material sciences, in particular in the production of nanotechnology devices. The problem is to understand along which route the initial profile relaxes to a completely flat surface. One distinguishes between relaxation above and below the roughening temperature. Below the roughening temperature, the surface free energy has a cusp singularity. Several authors have suggested to model the dynamics by a total variation H^{-1} flow problem that can be formulated as a fourth-order total variation flow (TVF) problem (cf., e.g., [1–8]).

Given a bounded domain $\widehat{\Omega} \subset \mathbb{R}^2$ with boundary $\widehat{\Gamma} = \partial\widehat{\Omega}$, the total variation-$H^{-1}$ (TV-H^{-1}) minimization of the energy functional

$$E(w) = \beta \int_{\widehat{\Omega}} |\nabla w| \; dx, \quad \beta > 0, \tag{1.1}$$

leads to the following fourth-order TVF problem

$$\frac{\partial w}{\partial \hat{t}} + \beta \Delta \nabla \cdot \frac{\nabla w}{|\nabla w|} = 0 \quad \text{in } \widehat{Q} := \widehat{\Omega} \times (0, \widehat{T}), \tag{1.2a}$$

$$\mathbf{n}_{\widehat{\Gamma}} \cdot \beta \frac{\nabla w}{|\nabla w|} = \mathbf{n}_{\widehat{\Gamma}} \cdot \nabla \nabla \left(\nabla \cdot \frac{\nabla w}{|\nabla w|} \right) = 0 \quad \text{on } \widehat{\Sigma} := \widehat{\Gamma} \times (0, \widehat{T}), \tag{1.2b}$$

$$w(\cdot, 0) = w^0 \quad \text{in } \widehat{\Omega}, \tag{1.2c}$$

where $\beta > 0$ is related to the mobility, $\widehat{T} > 0$ is the final time, $\mathbf{n}_{\widehat{\Gamma}}$ stands for the exterior unit normal at $\widehat{\Gamma}$, and $w^0 \in L^2(\widehat{\Omega})$ is some given initial data. The fourth-order Equation (1.2a) has to be interpreted as follows: On $H^{-1}(\widehat{\Omega})$ we introduce an inner product according to

$$(w, z)_{-1,\widehat{\Omega}} := (\nabla(-\Delta^{-1} w), \nabla(-\Delta^{-1} z))_{0,\widehat{\Omega}},$$

where Δ^{-1} stands for the inverse of the Laplacian. For $E(w) = \beta \int_{\widehat{\Omega}} |\nabla w| \; dx$, $w \in H^{-1}(\widehat{\Omega})$, with $D(E) = \{w \in H^{-1}(\widehat{\Omega}) \mid E(w) < \infty\}$, the subdifferential

$$\partial_{H^{-1}} E(w) = \{v \in H^{-1}(\widehat{\Omega}) \mid (v, z - w)_{-1,\Omega} \le E(z) - E(w) \text{ for all } z \in H^{-1}(\widehat{\Omega})\}$$

is given by (cf., e.g., [9])

$$\partial_{H^{-1}} E(w) = \{\Delta \nabla \cdot \boldsymbol{\xi} \mid \boldsymbol{\xi}(\hat{x}) \in \partial \Phi(\nabla w(\hat{x}))\},$$

where $\Phi(|\boldsymbol{\eta}|)$ and $\partial\Phi(|\boldsymbol{\eta}|)$ are given by

$$\Phi(\boldsymbol{\eta}) = \beta |\boldsymbol{\eta}|, \quad \partial \Phi(\boldsymbol{\eta}) = \begin{cases} \beta \boldsymbol{\eta}/|\boldsymbol{\eta}| & \text{if } \boldsymbol{\eta} \neq \mathbf{0} \\ \{\boldsymbol{\tau} \in \mathbb{R}^2 \mid |\boldsymbol{\tau}| \le \beta\} & \text{if } \boldsymbol{\eta} = \mathbf{0} \end{cases}. \tag{1.3}$$

We thus obtain

$$-\frac{\partial w}{\partial \hat{t}} \in \partial E_{H^{-1}}(w).$$

Initial-boundary value problems for fourth-order TVF problems have been considered mainly from an analytical point of view (cf., e.g., [9–13]).

Here, we consider the regularized TV-H^{-1} energy functional

$$E_{reg}(w) = \beta \int_{\widehat{\Omega}} (\delta^2 + |\nabla w|^2)^{1/2} \; dx, \quad w \in H^{-1}(\widehat{\Omega}),$$

where $\delta > 0$ is a regularization parameter. This leads to the regularized fourth-order TVF problem

$$\frac{\partial w}{\partial \hat{t}} + \beta \Delta \nabla \cdot ((\delta^2 + |\nabla w|^2)^{-1/2} \nabla w) = 0 \quad \text{in } \widehat{Q}, \tag{1.4a}$$

$$\mathbf{n}_{\widehat{\Gamma}} \cdot \beta(\delta^2 + |\nabla w|^2)^{-1/2}\nabla w = 0 \quad \text{on } \widehat{\Sigma}, \tag{1.4b}$$

$$\mathbf{n}_{\widehat{\Gamma}} \cdot \beta\nabla(\nabla \cdot (\delta^2 + |\nabla w|^2)^{-1/2}\nabla w) = 0 \quad \text{on } \widehat{\Sigma},$$

$$w(\cdot, 0) = w^0 \quad \text{in } \widehat{\Omega}. \tag{1.4c}$$

We further consider a scaling in both the time variable and the spatial variables according to

$$t = \delta\widehat{t}, \quad x_i = \delta\widehat{x}_i, \;\; 1 \le i \le 2. \tag{1.5}$$

Setting $T := \delta\widehat{T}, \Omega := \delta\widehat{\Omega}, \Gamma := \partial\Omega, Q := \Omega\times(0,T), \Sigma := \Gamma\times(0,T)$, and $u^0(x) = w^0(\delta^{-1}x)$, as well as

$$\omega(\nabla u) := 1 + |\nabla u|^2, \tag{1.6}$$

the scaled regularized fourth-order TVF problem reads as follows

$$\frac{\partial u}{\partial t} + \beta\delta^2\Delta\nabla \cdot (\omega(\nabla u)^{-1/2}\nabla u) = 0 \quad \text{in } Q, \tag{1.7a}$$

$$\mathbf{n}_\Gamma \cdot \beta\delta^2(\omega(\nabla u)^{-1/2}\nabla u) = \mathbf{n}_\Gamma \cdot \beta\delta^2\nabla(\nabla \cdot (\omega(\nabla u)^{-1/2}\nabla u)) = 0 \quad \text{on } \Sigma, \tag{1.7b}$$

$$u(\cdot, 0) = u^0 \quad \text{in } \Omega. \tag{1.7c}$$

The numerical solution of the regularized fourth-order TVF problem with periodic boundary conditions has been considered in Kohn and Versieux [3] based on a mixed formulation of the implicitly in time discretized problem. At each time-step, this amounts to the solution of two second-order elliptic partial differential equations (PDEs) by standard Lagrangian finite elements with respect to a triangulation of the computational domain Ω [14]. On the other hand, Interior Penalty Discontinuous Galerkin (IPDG) methods for fourth-order elliptic boundary value problems, fourth-order and higher-order polyharmonic parabolic initial-boundary value problems have been studied in [15–28]. The advantage of the C^0IPDG approach is that it directly applies to the fourth-order problem and thus only requires the numerical solution of one equation by using the same Lagrangian finite elements as in the mixed method.

Remark 1.1 We note that another example for a TV-H^{-1} minimization problem is the minimization of the energy functional

$$E(w, \widehat{g}) = \int_{\widehat{\Omega}} |\nabla w| \;\, dx + \frac{\lambda}{2}\|w - \widehat{g}\|^2_{H^{-1}(\widehat{\Omega})}$$

which occurs in image recovery where w represents a true image, $\widehat{g}$ describes a blurred and/or noisy image, and $\lambda > 0$ is a fidelity parameter (cf., [29–32]). The associated fourth-order TVF problem is given by the initial-boundary value problem

$$\frac{\partial w}{\partial \widehat{t}} + \lambda^{-1}\Delta\nabla \cdot \frac{\nabla w}{|\nabla w|} + w - \widehat{g} = 0 \quad \text{in } \widehat{Q}, \tag{1.8a}$$

$$\mathbf{n}_{\widehat{\Gamma}} \cdot \frac{\nabla w}{|\nabla w|} = \mathbf{n}_{\widehat{\Gamma}} \cdot \nabla\left(\nabla \cdot \frac{\nabla w}{|\nabla w|}\right) = 0 \quad \text{on } \widehat{\Sigma}, \tag{1.8b}$$

$$w(\cdot, 0) = w^0 \quad \text{in } \widehat{\Omega}. \tag{1.8c}$$

The paper is organized as follows: In Section 2, we will perform a discretization in time of the regularized and scaled fourth-order TVF problem and consider a reformulation in terms of the matrix of second-order partial derivatives of the unknown. Section 3 is devoted to the derivation of the C^0IPDG approximation based on an appropriate choice of numerical flux functions. In Section 4, we will show that the fully discrete system can be written as a parameter-dependent nonlinear system with the discrete time as a parameter. Since the choice of the time steps is crucial for the convergence of Newton's method, we suggest a predictor corrector continuation strategy with constant continuation as a predictor and Newton's method as a corrector featuring an adaptive choice of the time step sizes. This avoids a breakdown of Newton's method due to convergence failure because of too large time steps. Finally, in Section 5 we present numerical results illustrating the performance of the C^0IPDG method and the predictor corrector continuation strategy.

Throughout the paper we will use the following notations and basic results. For vectors $\underline{\mathbf{x}} = (x_1, \cdots, x_n)^T, \underline{\mathbf{y}} = (y_1, \cdots, y_n)^T \in \mathbb{R}^n$ and for matrices $\underline{\underline{\mathbf{A}}} = (a_{ij})_{i,j=1}^n, \underline{\underline{\mathbf{B}}} = (b_{ij})_{i,j=1}^n \in \mathbb{R}^{n\times n}$ we denote by $\underline{\mathbf{x}} \cdot \underline{\mathbf{y}}$ and $\underline{\underline{\mathbf{A}}} : \underline{\underline{\mathbf{B}}}$ the Euclidean inner product $\underline{\mathbf{x}} \cdot \underline{\mathbf{y}} = \sum_{i=1}^n x_i y_i$ and the Frobenius inner product $\underline{\underline{\mathbf{A}}} : \underline{\underline{\mathbf{B}}} = \sum_{i,j=1}^n a_{ij} b_{ij}$. In particular, $|\underline{\mathbf{x}}| := (\underline{\mathbf{x}} \cdot \underline{\mathbf{x}})^{1/2}$ and $|\underline{\underline{\mathbf{A}}}| := (\underline{\underline{\mathbf{A}}} : \underline{\underline{\mathbf{A}}})^{1/2}$ refer to the Euclidean norm and the Frobenius norm, respectively.

We will further use standard notation from Lebesgue and Sobolev space theory (cf., e.g., [33]). In particular, for a bounded domain $D \subset \mathbb{R}^d$, $d \in \mathbb{N}$, we refer to $L^2(D)$ as the Hilbert space of square integrable functions on D with inner product $(\cdot,\cdot)_{0,D}$ and norm $\|\cdot\|_{0,D}$. Moreover, we denote by $H^m(D)$, $m \in \mathbb{N}$, the Sobolev space with inner product $(\cdot,\cdot)_{m,D}$ and norm $\|\cdot\|_{m,D}$.

2 | IMPLICIT TIME-DISCRETIZATION

For the numerical solution of the regularized fourth-order TVF problem (Equation (1.7)) we perform a discretization in time with respect to a partition of the time interval $[0, T]$ into subintervals $[t_{m-1}, t_m]$ of length $\tau_m := t_m - t_{m-1}$. Denoting by u^m some approximation of u at time t_m, for $1 \le m \le M$ we have to solve the problems

$$u^m - u^{m-1} + \tau_m \beta \delta^2 \Delta \nabla \cdot (\omega(\nabla u^m)^{-1/2} \nabla u^m) = 0 \quad \text{in } \Omega, \tag{2.1a}$$

$$\mathbf{n}_\Gamma \cdot \beta \delta^2 (\omega(\nabla u^m)^{-1/2} \nabla u^m) = \mathbf{n}_\Gamma \cdot \beta \delta^2 \nabla (\nabla \cdot (\omega(\nabla u^m)^{-1/2} \nabla u^m)) = 0 \quad \text{on } \Gamma. \tag{2.1b}$$

Introducing the objective functional

$$J(v) := \frac{1}{2} \|v - u^{m-1}\|_{-1,\Omega}^2 + \tau_m \beta \delta^2 \int_\Omega (1 + |\nabla v|^2)^{1/2} \, dx, \tag{2.2}$$

it is easy to see that Equation (2.1) is related to the necessary and sufficient optimality condition for the minimization problem

$$J(u^m) = \inf_{v \in H^{-1}(\Omega)} J(v), \tag{2.3}$$

which has a unique solution, since the objective functional J is strictly convex, coercive, and lower semicontinuous. The fourth-order Equation (2.1a) can be reformulated in terms of the 2×2 matrix

$$D^2 u^m = \begin{pmatrix} \frac{\partial^2 u^m}{\partial x_1^2} & \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \\ \frac{\partial^2 u^m}{\partial x_1 \partial x_2} & \frac{\partial^2 u^m}{\partial x_2^2} \end{pmatrix}.$$

of second partial derivatives of u^m. We note that the divergence of a matrix-valued function $\underline{\underline{\mathbf{q}}} = (q_{ij})_{i,j=1}^2$ with row vectors $\underline{\mathbf{q}}^{(i)} = (q_{i1}, q_{i2})^T$, $1 \le i \le 2$, is defined by means of

$$\nabla \cdot \underline{\underline{\mathbf{q}}} := (\nabla \cdot \underline{\mathbf{q}}^{(1)}, \nabla \cdot \underline{\mathbf{q}}^{(2)})^T. \tag{2.4}$$

Theorem 2.1 *The fourth-order Equation* (2.1a) *is equivalent to*

$$u^m - u^{m-1} + \tau_m \beta \delta^2 \nabla \cdot \nabla \cdot (\omega(\nabla u^m)^{-3/2} \underline{\underline{\mathbf{M}}}(u^m) D^2 u^m) = 0, \tag{2.5}$$

where $\underline{\underline{\mathbf{M}}}(v)$ *stands for the matrix-valued function*

$$\underline{\underline{\mathbf{M}}}(v) := \begin{pmatrix} 1 + \left(\frac{\partial v}{\partial x_2}\right)^2 & -\frac{\partial v}{\partial x_1}\frac{\partial v}{\partial x_2} \\ -\frac{\partial v}{\partial x_1}\frac{\partial v}{\partial x_2} & 1 + \left(\frac{\partial v}{\partial x_2}\right)^2 \end{pmatrix}. \tag{2.6}$$

Proof. We reformulate the second term on the left-hand side of Equation (2.1a) according to

$$\begin{aligned} \Delta \nabla \cdot (\omega(\nabla u^m)^{-1/2} \nabla u^m) &= \nabla \cdot \nabla (\nabla \cdot (\omega(\nabla u^m)^{-1/2} \nabla u^m)) \\ &= \nabla \cdot \nabla \cdot \nabla (\omega(\nabla u^m)^{-1/2} \nabla u^m). \end{aligned} \tag{2.7}$$

Obviously, we have

$$\nabla(\omega(\nabla u^m)^{-1/2} \nabla u^m) = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \end{pmatrix} \left(\omega(\nabla u^m)^{-1/2} \begin{pmatrix} \frac{\partial u^m}{\partial x_1} \\ \frac{\partial u^m}{\partial x_2} \end{pmatrix} \right). \tag{2.8}$$

In particular,

$$\begin{aligned} \frac{\partial}{\partial x_1} \left(\omega(\nabla u^m)^{-1/2} \begin{pmatrix} \frac{\partial u^m}{\partial x_1} \\ \frac{\partial u^m}{\partial x_2} \end{pmatrix} \right) &= -\omega(\nabla u^m)^{-3/2} \left(\frac{\partial u^m}{\partial x_1} \frac{\partial^2 u^m}{\partial x_1^2} + \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \right) \begin{pmatrix} \frac{\partial u^m}{\partial x_1} \\ \frac{\partial u^m}{\partial x_2} \end{pmatrix} \\ + \omega(\nabla u^m)^{-1/2} \begin{pmatrix} \frac{\partial^2 u^m}{\partial x_1^2} \\ \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \end{pmatrix} &= \omega(\nabla u^m)^{-3/2} \begin{pmatrix} (1 + \left(\frac{\partial u^m}{\partial x_2}\right)^2 \frac{\partial^2 u^m}{\partial x_1^2} - \frac{\partial u^m}{\partial x_1} \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \\ (1 + \left(\frac{\partial u^m}{\partial x_1}\right)^2 \frac{\partial^2 u^m}{\partial x_1 \partial x_2} - \frac{\partial u^m}{\partial x_1} \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_1^2} \end{pmatrix}, \end{aligned} \tag{2.9}$$

and

$$\begin{aligned} \frac{\partial}{\partial x_2} \left(\omega(\nabla u^m)^{-1/2} \begin{pmatrix} \frac{\partial u^m}{\partial x_1} \\ \frac{\partial u^m}{\partial x_2} \end{pmatrix} \right) &= -\omega(\nabla u^m)^{-3/2} \left(\frac{\partial u^m}{\partial x_1} \frac{\partial^2 u^m}{\partial x_1 \partial x_2} + \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_2^2} \right) \begin{pmatrix} \frac{\partial u^m}{\partial x_1} \\ \frac{\partial u^m}{\partial x_2} \end{pmatrix} \\ + \omega(\nabla u^m)^{-1/2} \begin{pmatrix} \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \\ \frac{\partial^2 u^m}{\partial x_2^2} \end{pmatrix} &= \omega(\nabla u^m)^{-3/2} \begin{pmatrix} (1 + \left(\frac{\partial u^m}{\partial x_2}\right)^2 \frac{\partial^2 u^m}{\partial x_1 \partial x_2} - \frac{\partial u^m}{\partial x_1} \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_1^2} \\ (1 + \left(\frac{\partial u^m}{\partial x_1}\right)^2 \frac{\partial^2 u^m}{\partial x_2^2} - \frac{\partial u^m}{\partial x_1} \frac{\partial u^m}{\partial x_2} \frac{\partial^2 u^m}{\partial x_1 \partial x_2} \end{pmatrix}. \end{aligned} \tag{2.10}$$

Using Equations (2.9) and (2.10) in Equation (2.8), it follows that

$$\nabla(\omega(\nabla u^m)^{-1/2} \nabla u^m) = \omega(\nabla u^m)^{-3/2} \begin{pmatrix} 1 + \left(\frac{\partial u^m}{\partial x_2}\right)^2 & -\frac{\partial u^m}{\partial x_1}\frac{\partial u^m}{\partial x_2} \\ -\frac{\partial u^m}{\partial x_1}\frac{\partial u^m}{\partial x_2} & 1 + \left(\frac{\partial u^m}{\partial x_2}\right)^2 \end{pmatrix} D^2 u^m, \tag{2.11}$$

which can be written as

$$\nabla(\omega(\nabla u^m)^{-1/2}\nabla u^m) = \omega(\nabla u^m)^{-3/2}\underline{\underline{\mathbf{M}}}(u^m)D^2u^m. \tag{2.12}$$

■

Remark 2.1 The matrix $\underline{\underline{\mathbf{M}}}(v)$ is symmetric positive definite with the eigenvalues

$$\lambda_{min}(\underline{\underline{\mathbf{M}}}(v)) = 1, \quad \lambda_{max}(\underline{\underline{\mathbf{M}}}(v)) = 1 + |\nabla v|^2. \tag{2.13}$$

For notational convenience we set

$$\underline{\underline{\mathbf{A}}}_1(v) := \omega(\nabla v)^{-3/2}\underline{\underline{\mathbf{M}}}(v). \tag{2.14}$$

The weak formulation of Equation (2.5) reads: Find

$$u^m \in V := \{v \in H^2(\Omega) \ | \ \mathbf{n}_\Gamma \cdot \beta\delta^2\omega(\nabla v)^{-1/2}\nabla v = 0 \ \text{ on } \Gamma\}$$

such that for all $v \in V$ it holds

$$(u^m - u^{m-1}, v)_{0,\Omega} + \tau_m\beta\delta^2 \int_\Omega (\underline{\underline{\mathbf{A}}}_1(u^m)D^2u^m) : D^2v \ dx = 0. \tag{2.15}$$

Finally, we provide a mixed formulation of Equation (2.5), because the derivation of the C^{0}IPDG method will be based on the discrete analogue of that mixed formulation. Introducing the matrix-valued function

$$\underline{\underline{\mathbf{p}}}^m := \omega(\nabla u^m)^{-1/4}D^2u^m, \tag{2.16}$$

and the matrix

$$\underline{\underline{\mathbf{A}}}_2(v) := \omega(\nabla v)^{-5/4}\underline{\underline{\mathbf{M}}}(v). \tag{2.17}$$

the mixed formulation of Equations (2.1a) and (2.1b) reads as follows

$$\underline{\underline{\mathbf{p}}}^m - \omega(\nabla u^m)^{-1/4}D^2u^m = 0 \ \text{ in } \Omega, \tag{2.18a}$$

$$u^m - u^{m-1} + \tau_m\beta\delta^2\nabla\cdot\nabla\cdot\underline{\underline{\mathbf{A}}}_2(u^m)\underline{\underline{\mathbf{p}}}(u^m) = 0 \ \text{ in } \Omega, \tag{2.18b}$$

$$\mathbf{n}_\Gamma \cdot \beta\delta^2\omega(\nabla u^m)^{-1/2}\nabla u^m = 0 \ \text{ on } \Gamma, \tag{2.18c}$$

$$\mathbf{n}_\Gamma \cdot \beta\delta^2\nabla\cdot\underline{\underline{\mathbf{A}}}_2(u^m)\underline{\underline{\mathbf{p}}}^m = 0 \ \text{ on } \Gamma. \tag{2.18d}$$

3 | C^0 INTERIOR PENALTY DISCONTINUOUS GALERKIN APPROXIMATION

Let $\mathcal{T}_h$ be a geometrically conforming, uniform simplicial triangulation of Ω. We denote by $\mathcal{E}_h(\Omega)$ and $\mathcal{E}_h(\Gamma)$ the set of edges of $\mathcal{T}_h$ in the interior of Ω and on the boundary Γ, respectively, and set $\mathcal{E}_h := \mathcal{E}_h(\Omega) \cup \mathcal{E}_h(\Gamma)$. For $K \in \mathcal{T}_h$ and $E \in \mathcal{E}_h$ we denote by h_K and h_E the diameter of K and the length of E, and we set $h := \max(h_K \ | \ K \in \mathcal{T}_h)$. Due to the assumptions on $\mathcal{T}_h$ there exist constants $0 < c_R \le C_R$, $0 < c_Q \le C_Q$, and $0 < c_S \le C_S$ such that for all $K \in \mathcal{T}_h$ it holds

$$c_R h_K \le h_E \le C_R h_K, \quad E \in \mathcal{E}_h(\partial K), \tag{3.1a}$$

$$c_Q h \le h_K \le C_Q h, \tag{3.1b}$$

$$c_S h_K^2 \le \text{meas}(K) \le C_S h_K^2. \tag{3.1c}$$

For two quantities A and B we write $A \lesssim B$, if there exists a constant $C > 0$ independent of h such that $A \leq CB$.

Denoting by $P_k(T)$, $k \in \mathbb{N}$, the linear space of polynomials of degree $\leq k$ on T, for $k \in \mathbb{N}$ we define

$$V_h := \{v_h \in C^0(\Omega) | v_h|_T \in P_k(T), \ \ T \in \mathcal{T}_h\} \tag{3.2}$$

and note that $V_h \subset H^1(\Omega)$, but $V_h \not\subset H^2(\Omega)$. Further, we introduce

$$\underline{\underline{\mathbf{M}}}_h := \{\underline{\underline{\mathbf{q}}}_h \in L^2(\Omega)^{2\times 2} | \underline{\underline{\mathbf{q}}}_h|_K \in P_k(K)^{2\times 2}, \ \ K \in \mathcal{T}_h\} \tag{3.3}$$

as the space of element-wise polynomial moment tensors.

For interior edges $E \in \mathcal{E}_h(\Omega)$ such that $E = K_+ \cap K_-, K_\pm \in \mathcal{T}_h$ and boundary edges on Γ we introduce the average and jump of ∇v_h according to

$$\{\nabla v_h\}_E := \begin{cases} \frac{1}{2}(\nabla v_h|_{E\cap K_+} + \nabla v_h|_{E\cap K_-}) & E \in \mathcal{E}_h(\Omega) \\ \nabla v_h|_E & E \in \mathcal{E}_h(\Gamma) \end{cases}, \tag{3.4a}$$

$$[\nabla v_h]_E := \begin{cases} \nabla v_h|_{E\cap K_+} - \nabla v_h|_{E\cap K_-} & E \in \mathcal{E}_h(\Omega) \\ \nabla v_h|_E & E \in \mathcal{E}_h(\Gamma) \end{cases}. \tag{3.4b}$$

The average $\{\Delta v_h\}_E$ and jump $[\Delta v_h]_E$ are defined analogously. We further denote by $\mathbf{n}_E$ the unit normal vector on E pointing in the direction from K_+ to K_-.

In order to motivate the C^0IPDG approximation, we will follow the approach taken in Arnold and co-workers [34] for second-order elliptic boundary value problems. For $\underline{\underline{\mathbf{p}}}_h^m \in \underline{\underline{\mathbf{M}}}_h$ and $u_h^m \in V_h$ we consider Equations (2.18a) and (2.18b) element-wise and Equations (2.18c) and (2.18d) edgewise, that is,

$$\underline{\underline{\mathbf{p}}}_h^m - \omega(\nabla u_h^m)^{-1/4} D^2 u_h^m = 0 \quad \text{in } K \in \mathcal{T}_h, \tag{3.5a}$$

$$u_h^m - u_h^{m-1} + \tau_m \beta\delta^2 \nabla\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m = 0 \quad \text{in } K \in \mathcal{T}_h, \tag{3.5b}$$

$$\mathbf{n}_E \cdot \beta\delta^2 \omega(\nabla u_h^m)^{-1/4} \nabla u_h^m = 0 \quad \text{on } E \in \mathcal{E}_h(\Gamma), \tag{3.5c}$$

$$\mathbf{n}_E \cdot \beta\delta^2 \nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m = 0 \quad \text{on } E \in \mathcal{E}_h(\Gamma), \tag{3.5d}$$

with $u_h^0 = Q_h u^0$, where $Q_h : L^2(\Omega) \to V_h$ denotes the L^2 projection onto V_h. We multiply Equation (3.5a) by $\underline{\underline{\mathbf{q}}}_h \in \underline{\underline{\mathbf{M}}}_h$ and integrate over K:

$$\int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{q}}}_h \ dx = \int_K (\omega(\nabla u_h^m)^{-1/4} D^2 u_h^m) : \underline{\underline{\mathbf{q}}}_h \ dx. \tag{3.6}$$

In view of Equation (2.11) Green's formula yields

$$\int_K (\omega(\nabla u_h^m)^{-1/4} D^2 u_h^m) : \underline{\underline{\mathbf{q}}}_h \ dx = \int_K D^2 u_h^m : (\omega(\nabla u_h^m)^{-1/4} \underline{\underline{\mathbf{q}}}_h) \ dx \tag{3.7}$$

$$= -\int_K \nabla u_h^m \cdot \nabla\cdot (\omega(\nabla u_h^m)^{-1/4} \underline{\underline{\mathbf{q}}}_h) \ dx + \int_{\partial K} \omega(\nabla u_h^m)^{-1/4} \nabla u_h^m \cdot \underline{\underline{\mathbf{q}}}_h \mathbf{n}_{\partial K} \ ds.$$

On the other hand, we multiply Equation (3.5b) by $v_h \in V_h$ and integrate over K:

$$\int_K (u_h^m - u_h^{m-1}) v_h \ dx + \tau_m \beta\delta^2 \int_K \nabla\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h \ dx = 0. \tag{3.8}$$

Applying Green's formula twice, we obtain

$$\int_K \nabla\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h\ dx = -\int_K \nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m \cdot \nabla v_h\ dx \tag{3.9}$$

$$+\int_{\partial K} \mathbf{n}_{\partial K}\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h\ ds = \int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{A}}}_2(u_h^m) D^2 v_h\ dx$$

$$-\int_{\partial K} \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m \mathbf{n}_{\partial k}\cdot\nabla v_h\ ds + \int_{\partial K} \mathbf{n}_{\partial K}\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h\ ds.$$

Summing over all $K\in\mathcal{T}_h$ in Equations (3.7) and (3.9), we obtain the weak formulation of the mixed formulation Equations (3.5a)–(3.5d): Find $(u_h^m, \underline{\underline{\mathbf{p}}}_h^m) \in V_h \times \underline{\underline{\mathbf{M}}}_h$ such that for all $(v_h, \underline{\underline{\mathbf{q}}}_h) \in V_h \times \underline{\underline{\mathbf{M}}}_h$ it holds

$$\sum_{K\in\mathcal{T}_h} \int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{q}}}_h\ dx + \sum_{K\in\mathcal{T}_h} \int_K \nabla u_h^m \cdot \nabla\cdot(\omega(\nabla u_h^m)^{-1/4}\underline{\underline{\mathbf{q}}}_h)\ dx$$

$$-\sum_{K\in\mathcal{T}_h} \int_{\partial K} \omega(\nabla u_h^m)^{-1/4}\nabla u_h^m \cdot \underline{\underline{\mathbf{q}}}_h \mathbf{n}_{\partial K}\ ds = 0, \tag{3.10a}$$

$$\sum_{K\in\mathcal{T}_h} \int_K u_h^m v_h\ dx + \tau_m\beta\delta^2\Bigg(\sum_{K\in\mathcal{T}_h} \int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{A}}}_2(u_h^m) D^2 v_h\ dx$$

$$-\sum_{K\in\mathcal{T}_h} \int_{\partial K} \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m \mathbf{n}_{\partial K}\cdot\nabla v_h\ ds + \sum_{K\in\mathcal{T}_h} \int_{\partial K} \mathbf{n}_{\partial K}\cdot\nabla\cdot \underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h\ ds\Bigg)$$

$$= \sum_{K\in\mathcal{T}_h} \int_K u_h^{m-1} v_h\ dx. \tag{3.10b}$$

A general C^0DG approximation of Equations (2.1b) and (2.1b) is based on the mixed formulation Equations (3.10a) and (3.10b) and characterized by numerical flux functions $\widehat{\underline{\mathbf{u}}}_{\partial K}^m$, $\widehat{\underline{\mathbf{p}}}_{\partial K}^m$, and $\widehat{\underline{\mathbf{s}}}_{\partial K}^m$ that are single-valued on $E\in\mathcal{E}_h(\Omega)$, that is, $\widehat{\underline{\mathbf{u}}}_{\partial K}^m|_{E_+} = \widehat{\underline{\mathbf{u}}}_{\partial K}^m|_{E_-}$, $\widehat{\underline{\mathbf{p}}}_{\partial K}^m|_{E_+} = \widehat{\underline{\mathbf{p}}}_{\partial K}^m|_{E_-}$, and $\widehat{\underline{\mathbf{s}}}_{\partial K}^m|_{E_+} = \widehat{\underline{\mathbf{s}}}_{\partial K}^m|_{E_-}$. We replace $\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m \cdot \underline{\underline{\mathbf{q}}}_h \mathbf{n}_{\partial K}$ in Equation (3.10a) by $\widehat{\underline{\mathbf{u}}}_{\partial K}^m \cdot \underline{\underline{\mathbf{q}}}_h \mathbf{n}_{\partial K}$ and $\underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m \mathbf{n}_{\partial K}\cdot\nabla v_h = \underline{\underline{\mathbf{A}}}_2(u_h^m) D^2(u_h^m)\mathbf{n}_{\partial K}\cdot\omega(\nabla u_h^m)^{-1/4}\nabla v_h$ as well as $\mathbf{n}_{\partial K}\cdot\nabla\cdot\underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m v_h$ in Equation (3.10b) by $\widehat{\underline{\mathbf{p}}}_{\partial K}^m \cdot \omega(\nabla u_h^m)^{-1/4}\nabla v_h$ and $\mathbf{n}_{\partial K}\cdot\widehat{\underline{\mathbf{s}}}_{\partial K}^m v_h$. In view of Equation (3.5d) we choose $\widehat{\underline{\mathbf{s}}}_{\partial K}^m|_E = \mathbf{n}_E\cdot\nabla\cdot\underline{\underline{\mathbf{A}}}_2(u_h^m)\underline{\underline{\mathbf{p}}}_h^m = 0, E\in\mathcal{E}_h(\Gamma)$, Then, no matter how we choose $\widehat{\underline{\mathbf{s}}}_{\partial K}^m|_E$ on $E\in\mathcal{E}_h(\Omega)$, due to $[\widehat{\underline{\mathbf{s}}}_{\partial K}^m]_E = 0, E\in\mathcal{E}_h(\Omega)$, and $v_h\in C^0(\Omega)$ we have

$$\sum_{K\in\mathcal{T}_h} \int_{\partial K} \mathbf{n}_{\partial K}\cdot\widehat{\underline{\mathbf{s}}}_{\partial K}^m v_h\ ds = \sum_{E\in\mathcal{E}_h(\Omega)} \mathbf{n}_E\cdot[\widehat{\underline{\mathbf{s}}}_{\partial K}^m]_E v_h\ ds = 0. \tag{3.11}$$

Consequently, observing Equation (3.11), in a general C^0DG approximation, we are looking for a pair $(u_h^m, \underline{\underline{\mathbf{p}}}_h^m) \in V_h \times \underline{\underline{\mathbf{M}}}_h$ such that for all $(v_h, \underline{\underline{\mathbf{q}}}_h) \in V_h \times \underline{\underline{\mathbf{M}}}_h$ it holds

$$\sum_{K\in\mathcal{T}_h} \int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{q}}}_h\ dx + \sum_{K\in\mathcal{T}_h} \int_K \nabla u_h^m \cdot \nabla\cdot(\omega(\nabla u_h^m)^{-1/4}\underline{\underline{\mathbf{q}}}_h)\ dx$$

$$-\sum_{K\in\mathcal{T}_h} \int_{\partial K} \widehat{\underline{\mathbf{u}}}_{\partial K}^m \cdot \underline{\underline{\mathbf{q}}}_h \mathbf{n}_{\partial K}\ ds = 0, \tag{3.12a}$$

$$\sum_{K\in\mathcal{T}_h} \int_K u_h^m v_h\ dx + \tau_m\beta\delta^2(\sum_{K\in\mathcal{T}_h} \int_K \underline{\underline{\mathbf{p}}}_h^m : \underline{\underline{\mathbf{A}}}_2(u_h^m) D^2 v_h\ dx$$

$$-\sum_{K\in\mathcal{T}_h}\int_{\partial K}\widehat{\underline{\mathbf{p}}}^m_{\partial K}\cdot(\omega(\nabla u_h^m)^{-1/4}\nabla v_h\ \ ds)=\sum_{K\in\mathcal{T}_h}\int_K u_h^{m-1}v_h\ \ dx. \tag{3.12b}$$

In particular, for the C^{0}IPDG approximation the numerical flux functions $\widehat{\underline{\mathbf{u}}}^m_{\partial K}$ and $\widehat{\underline{\mathbf{p}}}^m_{\partial K}$ are given by

$$\widehat{\underline{\mathbf{u}}}^m_{\partial K}|_E := \begin{cases}\{\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m\}_E & E\in\mathcal{E}_h(\Omega)\\ \mathbf{0} & E\in\mathcal{E}_h(\Gamma)\end{cases}, \tag{3.13a}$$

$$\widehat{\underline{\mathbf{p}}}^m_{\partial K}|_E := \ \{\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2u_h^m\}_E\mathbf{n}_E-\alpha h_E^{-1}[\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m]_E,\ \ E\in\mathcal{E}_h, \tag{3.13b}$$

where $\alpha>0$ is a penalty parameter.

Theorem 3.1 *The particular choice (Equations (3.13a) and (3.13b)) of the numerical flux functions allows to eliminate the dual variable $\underline{\underline{\mathbf{p}}}_h^m$ from the system (Equations (3.12a) and (3.12b)). We thus obtain the C^{0}IPDG approximation: Find $u_h^m\in V_h$ such that for all $v_h\in V_h$ it holds*

$$(u_h^m,v_h)_{0,\Omega}+\tau_m\beta\delta^2a_h^{IP}(u_h^m,v_h;u_h^m)=(u_h^{m-1},v_h)_{0,\Omega}, \tag{3.14}$$

where for $z_h\in V_h$ the mesh-dependent C^{0}IPDG form $a_h^{IP}(\cdot,\cdot;z_h):V_h\times V_h$ is given by

$$\begin{aligned}a_h^{IP}(u_h,v_h;z_h) :=& \sum_{K\in\mathcal{T}_h}(\underline{\underline{\mathbf{A}}}_1(z_h)D^2u_h,D^2v_h)_{0,K}\\ &-\sum_{E\in\mathcal{E}_h}(\mathbf{n}_E\cdot\{\underline{\underline{\mathbf{A}}}_2(z_h)D^2u_h\}_E\mathbf{n}_E,\mathbf{n}_E\cdot[\omega(\nabla z_h)^{-1/4}\nabla v_h]_E)_{0,E}\\ &-\sum_{E\in\mathcal{E}_h}(\mathbf{n}_E\cdot\{\underline{\underline{\mathbf{A}}}_2(z_h)D^2v_h\}_E\mathbf{n}_E,\mathbf{n}_E\cdot[\omega(\nabla z_h)^{-1/4}\nabla u_h]_E)_{0,E}\\ &+\alpha\sum_{E\in\mathcal{E}_h}h_E^{-1}(\mathbf{n}_E\cdot[\omega(\nabla z_h)^{-1/4}\nabla u_h]_E,\mathbf{n}_E\cdot[\omega(\nabla z_h)^{-1/4}\nabla v_h]_E)_{0,E}.\end{aligned} \tag{3.15}$$

Proof. If we choose $\underline{\underline{\mathbf{q}}}_h=\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h$ in Equations (3.12a) and use (3.13a), we obtain

$$\begin{aligned}&\sum_{K\in\mathcal{T}_h}\int_K\underline{\underline{\mathbf{p}}}_h^m:\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\ \ dx\\ &+\sum_{K\in\mathcal{T}_h}\int_K\nabla u_h^m\cdot\nabla\cdot(\omega(\nabla u_h^m)^{-1/4}\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h)\ \ dx\\ &-\sum_{E\in\mathcal{E}_h(\Omega)}\int_E\{\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m\}_E\cdot[\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h]_E\mathbf{n}_E\ \ ds=0.\end{aligned} \tag{3.16}$$

For the second term on the left-hand side of Equation (3.16), applying Green's formula element-wise and observing Equations (2.14) and (2.17) yields

$$\begin{aligned}&\sum_{K\in\mathcal{T}_h}\int_K\nabla u_h^m\cdot\nabla\cdot(\omega(\nabla u_h^m)^{-1/4}\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h)\ \ dx\\ &=-\sum_{K\in\mathcal{T}_h}\int_K D^2u_h^m:\underline{\underline{\mathbf{A}}}_1(u_h^m)D^2v_h\ \ dx\\ &\quad+\sum_{K\in\mathcal{T}_h}\int_{\partial K}\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m\cdot\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\mathbf{n}_{\partial K}\ \ ds.\end{aligned} \tag{3.17}$$

Now, taking advantage of

$$\sum_{K\in\mathcal{T}_h}\int_{\partial K}\underline{\mathbf{p}}\cdot\underline{\underline{\mathbf{q}}}\ \mathbf{n}_{\partial K}\ ds$$

$$=\sum_{E\in\mathcal{E}_h}\int_E\ [\underline{\mathbf{p}}]_E\cdot\{\underline{\underline{\mathbf{q}}}\}_E\mathbf{n}_E\ ds+\sum_{E\in\mathcal{E}_h(\Omega)}\int_E\{\underline{\mathbf{p}}\}_E\cdot[\underline{\underline{\mathbf{q}}}]_E\mathbf{n}_E\ ds \tag{3.18}$$

with $\underline{\mathbf{p}}=\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m$ and $\underline{\underline{\mathbf{q}}}=\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h$, we get

$$\sum_{K\in\mathcal{T}_h}\int_{\partial K}\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m\cdot\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\mathbf{n}_{\partial K}\ ds$$

$$=\sum_{E\in\mathcal{E}_h}\int_E\ [\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m]_E\cdot\{\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\}_E\mathbf{n}_E\ ds$$

$$+\sum_{E\in\mathcal{E}_h(\Omega)}\int_E\{\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m\}_E\cdot[\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h]_E\mathbf{n}_E\ ds. \tag{3.19}$$

Using Equations (3.17) and (3.19) in Equation (3.16) it follows that

$$\sum_{K\in\mathcal{T}_h}\int_K\underline{\underline{\mathbf{p}}}_h^m\ :\ \underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\ dx$$

$$=\sum_{K\in\mathcal{T}_h}\int_K D^2u_h^m\ :\ \underline{\underline{\mathbf{A}}}_1(u_h^m)D^2v_h\ dx$$

$$-\sum_{E\in\mathcal{E}_h}\int_E\ [\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m]_E\cdot\{\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\}_E\mathbf{n}_E\ ds \tag{3.20}$$

On the other hand, inserting Equation (3.13b) into Equation (3.12b) and applying again Equation (3.18), we obtain

$$\sum_{K\in\mathcal{T}_h}\int_K u_h^m v_h\ dx+\tau_m\beta\delta^2\Bigg(\sum_{K\in\mathcal{T}_h}\int_K\underline{\underline{\mathbf{p}}}_h^m\ :\ \underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\ dx$$

$$-\sum_{K\in\mathcal{T}_h}\int_{\partial K}\widehat{\underline{\mathbf{p}}}_{\partial K}^m\cdot\nabla v_h\ ds\Bigg)=\sum_{K\in\mathcal{T}_h}\int_K u_h^m v_h\ dx$$

$$+\tau_m\beta\delta^2\Bigg(\sum_{K\in\mathcal{T}_h}\int_K\underline{\underline{\mathbf{p}}}_h^m\ :\ \underline{\underline{\mathbf{A}}}_2(u_h^m)D^2v_h\ dx$$

$$-\sum_{E\in\mathcal{E}_h}\int_E\{\underline{\underline{\mathbf{A}}}_2(u_h^m)D^2u_h^m\}_E\mathbf{n}_E\cdot[\omega(\nabla u_h^m)^{-1/4}\nabla v_h]_E\ ds$$

$$+\alpha\sum_{E\in\mathcal{E}_h}h_E^{-1}\int_E\ [\omega(\nabla u_h^m)^{-1/4}\nabla u_h^m]_E\cdot[\omega(\nabla u_h^m)^{-1/4}\nabla v_h]_E\ ds\Bigg)$$

$$=\sum_{K\in\mathcal{T}_h}\int_K u_h^{m-1}v_h\ dx. \tag{3.21}$$

The assertion follows from using Equations (3.20) in (3.21). ■

Remark 3.1 We note that the C^0IPDG approximation (Equation (3.14)) can be derived from the boundary value problem (2.1a),(2.1b) (cf., e.g., [20] for a fourth-order boundary value problem related to the biharmonic problem). However, we have chosen the approach via the mixed formulation, since the C^0DG approximation (3.10a),(3.10b) is more general in so far as another choice of the numerical flux functions than (3.13a),(3.13b) may lead to a different C^0DG approach as, for instance, a C^0 Local Discontinuous Galerkin (C^0LDG) method.

4 | A PREDICTOR CORRECTOR CONTINUATION STRATEGY FOR THE NUMERICAL SOLUTION OF THE C^0IPDG APPROXIMATION

The solution $u(x,t)$, $(x,t) \in Q$, of the fourth-order TVF problem (1.2) is characterized by

- the formation of facets around local extrema of the initial data with steep gradients at the interfaces,
- a finite extinction time $t_{ext} > 0$, that is, $u(x,t) = 0$, $x \in \Omega$, for $t \geq t_{ext}$.

The same behavior can be expected from the solution of the C^0IPDG approximation (3.14). In particular, the appropriate choice of the time step is a crucial issue when solving the nonlinear system resulting from (3.14). Therefore, it is more advantageous to work with a variable time step $\tau_m = t_m - t_{m-1}$, $1 \leq m \leq M$, instead of a uniform time step $\Delta t = T/M$, $M \in \mathbb{N}$ and to choose τ_m such that convergence of a Newton-type method is guaranteed. This can be achieved by viewing (3.14) as a parameter dependent nonlinear system with the time as the parameter and to apply a predictor corrector continuation strategy featuring an adaptive choice of the time step sizes τ_m (cf., e.g., [35, 36]).

We assume $V_h = \text{span}\{\varphi_1, \cdots, \varphi_{N_h}\}, N_h \in \mathbb{N}$, such that

$$u_h^m = \sum_{j=1}^{N_h} u_j^m \varphi_j.$$

Setting $\mathbf{u}^m := (u_1^m, \cdots, u_{N_h}^m)^T$, the algebraic formulation of (3.14) leads to the nonlinear system

$$\mathbf{F}(\mathbf{u}^m, t_m) = \mathbf{0}, \tag{4.1}$$

where the components $\mathbf{F}_i$, $1 \leq i \leq N_h$, are given by

$$\begin{aligned}\mathbf{F}_i(\mathbf{u}^m, t_m) = &\sum_{j=1}^{N_h} u_j^m \ (\varphi_j, \varphi_i)_{0,\Omega} \\ &+ \tau_m \beta \delta^2 a_h^{DG}\left(\sum_{j=1}^{N_h} u_j^m \varphi_j, \varphi_i; \sum_{j=1}^{N_h} u_j^m \varphi_j\right) - \sum_{j=1}^{N_h} u_j^{m-1} \ (\varphi_j, \varphi_i)_{0,\Omega}.\end{aligned}$$

Given $\mathbf{u}^{m-1}$, the time step size $\tau_{m-1,0} = \tau_{m-1}$, and setting $k = 0$, where k is a counter for the predictor corrector steps, the predictor step for (4.1) consists of constant continuation leading to the initial guess

$$\mathbf{u}^{(m,k)} = \mathbf{u}^{m-1}, \quad t_m = t_{m-1} + \tau_{m-1,k}. \tag{4.2}$$

Setting $\nu = 0$ and $\mathbf{u}^{(m,k,\nu_1)} = \mathbf{u}^{(m,k)}$, for $\nu \leq \nu_{max}$, where $\nu_{max} > 0$ is a pre-specified maximal number, the Newton iteration

$$\mathbf{F}'(\mathbf{u}^{(m,k,\nu)}, t_m)\Delta\mathbf{u}^{(m,k,\nu)} = -\mathbf{F}(\mathbf{u}^{(m,k,\nu)}, t_m), \tag{4.3}$$

serves as a corrector whose convergence is monitored by the contraction factor

$$\Lambda^{(m,k,\nu)} = \frac{\|\overline{\Delta u^{(m,k,\nu)}}\|}{\|\Delta u^{(m,k,\nu)}\|}, \tag{4.4}$$

where $\overline{\Delta u^{(m,k,\nu)}}$ is the solution of the auxiliary Newton step

$$\mathbf{F}'(\mathbf{u}^{(m,k,\nu)}, t_m)\overline{\Delta u^{(m,k,\nu)}} = -\mathbf{F}(\mathbf{u}^{(m,k,\nu+1)}, t_m). \tag{4.5}$$

If the contraction factor satisfies

$$\Lambda^{(m,k,\nu)} < \frac{1}{2}, \tag{4.6}$$

we set $\nu = \nu + 1$. If $\nu > \nu_{max}$, both the Newton iteration and the predictor corrector continuation strategy are terminated indicating non-convergence. Otherwise, we continue the Newton iteration (4.3). If (4.6) does not hold true, we set $k = k + 1$ and the time step is reduced according to

$$\tau_{m,k} = \max\left(\frac{\sqrt{2}-1}{\sqrt{4\Lambda^{(m,\nu)}+1}-1}\ \tau_{m,k-1}, \tau_{min}\right), \tag{4.7}$$

where $\tau_{min} > 0$ is some pre-specified minimal time step. If $\tau_{m,\,k} \geq \tau_{min}$, we go back to the prediction step (Equation (4.2)). Otherwise, the predictor corrector strategy is stopped indicating nonconvergence. The Newton iteration is terminated successfully, if for some $\nu^* > 0$ the relative error of two subsequent Newton iterates satisfies

$$\frac{\|\mathbf{u}^{(m,k,\nu^*)} - \mathbf{u}^{(m,k,\nu^*-1)}\|}{\|\mathbf{u}^{(m,k,\nu^*)}\|} < \varepsilon \tag{4.8}$$

for some prespecified accuracy $\varepsilon > 0$. In this case, we set

$$\mathbf{u}^m = \mathbf{u}^{(m,k,\nu_1^*)} \tag{4.9}$$

and predict a new time step according to

$$\tau_m = \min\left(\frac{(\sqrt{2}-1)\ \ \|\Delta u^{(m,k,0)}\|}{2\Lambda^{(m,k,0)}\ \ \|\mathbf{u}^{(m,k,0)} - \mathbf{u}^m\|}, \mathrm{amp}\right)\ \tau_{m,k}, \tag{4.10}$$

where amp > 0 is a prespecified amplification factor for the time step sizes. We set $m = m + 1$ and begin new predictor corrector iterations for the time interval $[t_m, t_{m+1}]$. The choice of the contraction factor (Equation (4.6)), the choice of the reduced time step (Equation (4.7)), and the choice of the enlarged time step (Equation (4.10)) are motivated by the affine covariant convergence theory of Newton's method (cf., e.g., [35, 36]).

5 | NUMERICAL RESULTS

We have implemented the C^0IPDG method of Section 3 along with the predictor corrector continuation strategy of Section 5 for two examples. In both cases, we have chosen $\Omega = (0,1)^2$, $\beta = 1.0 \cdot 10^{-7}$, polynomial degree $k = 2$ and penalization parameter $\alpha = 200.0$ in the C^0IPDG method, and $\nu_{\max} = 50$, $\varepsilon = 1.0 \cdot 10^{-3}$, and $\tau_{\min} = 1.0 \cdot 10^{-8}$ for the predictor corrector continuation strategy.

Example 1 The first example is the same as in Kohn and Versieux [3], where the initial data u^0 has been chosen according to

$$u^0(x_1, x_2) = x_1(x_1 - 1)x_2(x_2 - 1) - \frac{1}{36}.$$

The C^0IPDG approximation u_h^m has been computed for various regularization parameters δ and finite element mesh sizes h.

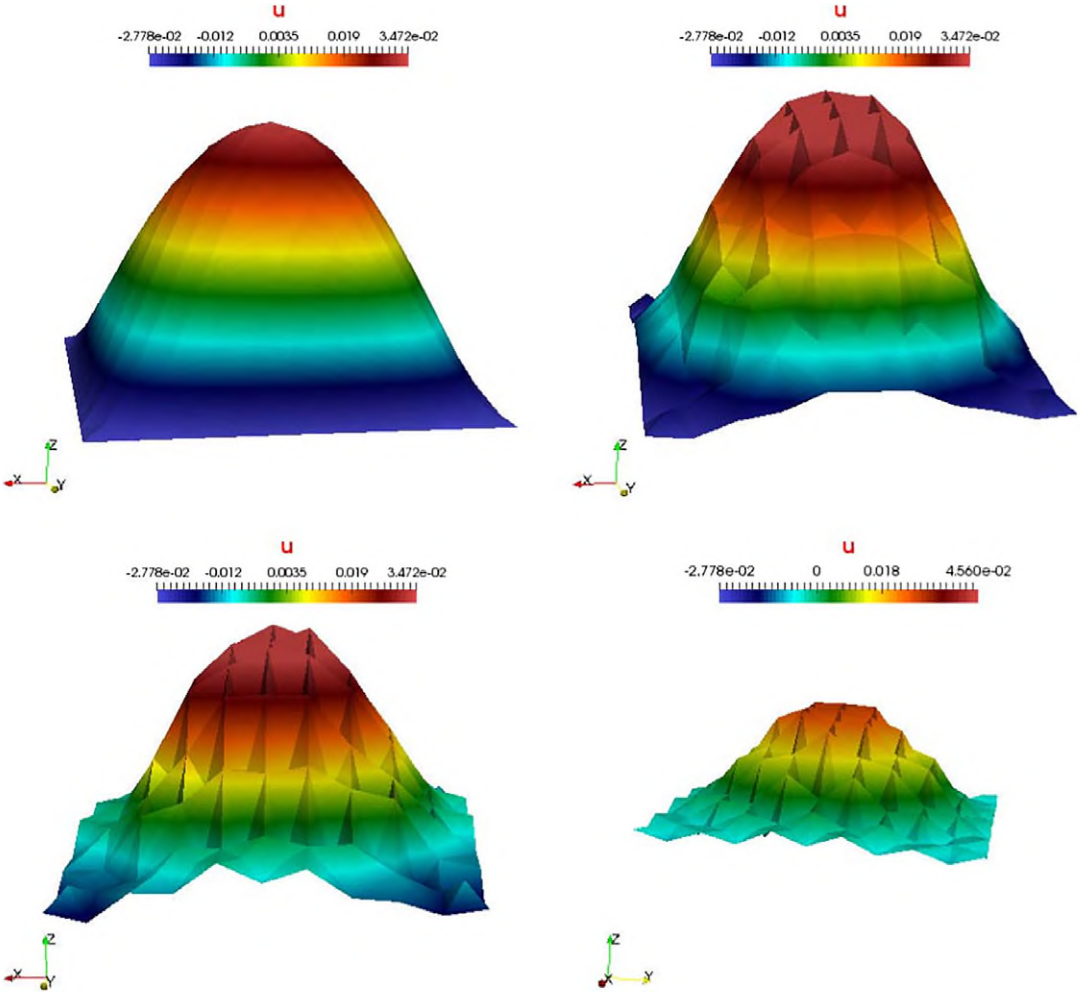

FIGURE 1 Example 1: Computed solution for $h = 1/10$ and $\delta = 2.5 \cdot 10^{-4}$ at initial time $t = 0$ s (top left), at time $t = 4.6 \cdot 10^{-5}$ s (top right), at time $t = 2.6 \cdot 10^{-3}$ s, and at time $t = 1.2 \cdot 10^{-2}$ s (bottom right) [Color figure can be viewed at wileyonlinelibrary.com]

For $\delta = 2.5 \cdot 10^{-4}$ and $h = 1/10$, Figure 1 displays the initial data u_h^0 at time $t = 0.0$ (top left), and the computed solutions at times $t = 4.6 \cdot 10^{-6}$ (top right), $t = 2.6 \cdot 10^{-3}$ (bottom left), and $t = 1.2 \cdot 10^{-3}$ (bottom right). We see that the solution develops facets around local extrema of the initial data with a narrow interface featuring steep gradients in between. The extinction time, that is, the time when the initial profile gets completely flat, is $t_{ext} = 1.1 \cdot 10^{-2}$.

For $\delta = 7.5 \cdot 10^{-3}$, and $h = 1/64$, Figure 2 shows the same behavior of the solution. However, due to the significantly smaller mesh size h the interface between the upper and lower facets is much better resolved. In this case, the extinction time turned out to be $t_{ext} = 2.2 \cdot 10^{-2}$.

The performance of the predictor corrector continuation strategy for $h = 1/10$ and $\delta = 2.5 \cdot 10^{-4}$ is shown in Figure 3 where the adaptive choice of the time steps τ_m is shown as a function of the iterations. We see that the time step sizes are gradually increasing in a step-like way where the individual steps correspond to the formation of the interface between the upper and the lower facets.

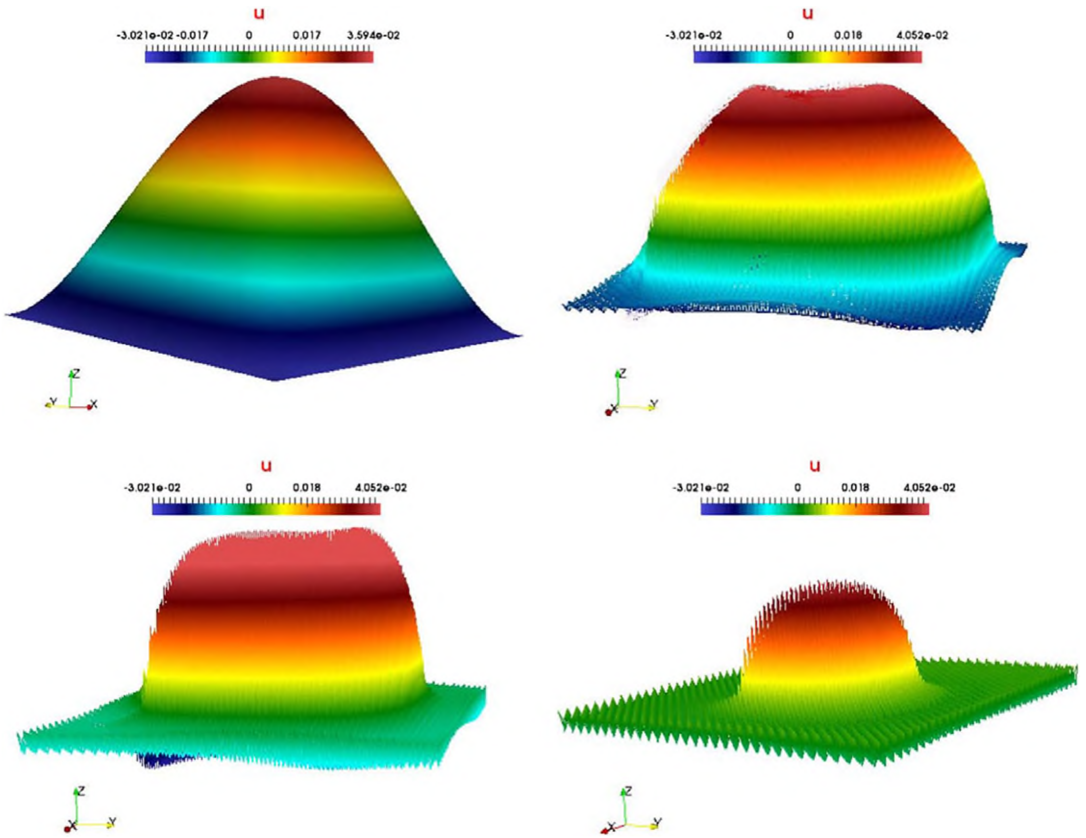

FIGURE 2 Example 1: Computed solution for $h = 1/64$ and $\delta = 7.5 \cdot 10^{-3}$ at initial time $t = 0$ s (top left), at time $t = 6.9 \cdot 10^{-7}$ s (top right), at time $t = 9.5 \cdot 10^{-5}$ s, and at time $t = 1.3 \cdot 10^{-3}$ s (bottom right) [Color figure can be viewed at wileyonlinelibrary.com]

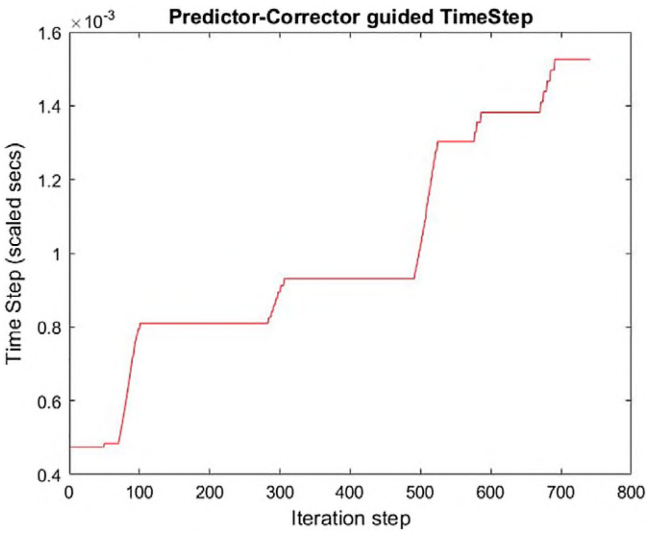

FIGURE 3 Example 1: Performance of the predictor corrector continuation strategy for $h = 1/10$ and $\delta = 2.5 \cdot 10^{-4}$. Adaptive choice of time steps τ_m [Color figure can be viewed at wileyonlinelibrary.com]

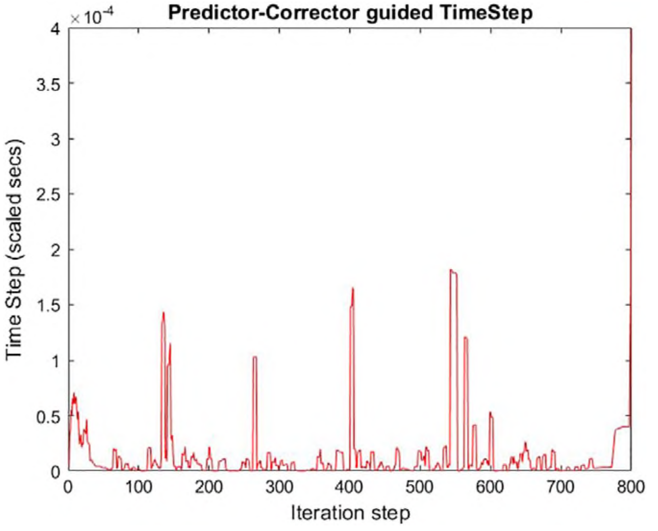

FIGURE 4 Example 1: Performance of the predictor corrector continuation strategy for $h = 1/64$ and $\delta = 7.5 \cdot 10^{-3}$. Adaptive choice of time steps τ_m [Color figure can be viewed at wileyonlinelibrary.com]

Figure 4 shows the corresponding results for the predictor corrector continuation strategy in case $h = 1/64$ and $\delta = 7.5 \cdot 10^{-3}$. The convergence is expected to become a tougher issue for smaller mesh width h which is reflected by Figure 4.

As far as the convergence of the C^{0}IPDG approximations u_h^m to the solution u^m, $m \geq 1$, of Equation (2.1) is concerned, we have computed an experimental convergence rate, since the exact solutions u^m are not explicitly known. The experimental convergence rate is given by

$$\mathrm{err}(t_m) := \mathrm{err}_2 \frac{|||u_h^m - u_{2h}^m|||}{|||u_{h/2}^m - u_h^m|||}, \tag{5.1}$$

where $|||\cdot|||$ stands for the norm

$$|||z_h^m||| := \left(\|z_h^m\|_{0,\Omega}^2 + \sum_{\ell=1}^{m} \tau_\ell \|z_h^\ell\|_{2,h/2,\Omega}^2 \right)^{1/2}. \tag{5.2}$$

Figure 5 displays the experimental convergence rate as a function of time for $h = 1/64$. Taking into account that the initial data is smooth, at the very beginning the rate drops significantly due to the formation of facets with sharp interfaces between the upper and the lower facet. Afterwards it stabilizes around 0.5.

Forthcoming work will be devoted to provide an a priori error estimate in the $|||\cdot|||$-norm.

Example 2 The initial profile u^0 has been chosen according to

$$u^0(x_1,x_2) = \begin{cases} x_1\left(\frac{1}{2}-x_1\right)(1-x_1)x_2\left(\frac{1}{2}-x_2\right)(1-x_2)-\frac{1}{32} & 0 \leq x_1 < \frac{1}{2}, 0 \leq x_2 < \frac{1}{2} \\ x_1\left(x_1-\frac{1}{2}\right)(1-x_1)x_2\left(\frac{1}{2}-x_2\right)(1-x_2)-\frac{1}{32} & \frac{1}{2} \leq x_1 \leq 1, 0 \leq x_2 < \frac{1}{2} \\ x_1\left(\frac{1}{2}-x_1\right)(1-x_1)x_2\left(x_2-\frac{1}{2}\right)(1-x_2)-\frac{1}{32} & 0 \leq x_1 < \frac{1}{2}, \frac{1}{2} \leq x_2 \leq 1 \\ x_1\left(x_1-\frac{1}{2}\right)(1-x_1)x_2\left(x_2-\frac{1}{2}\right)(1-x_2)-\frac{1}{32} & \frac{1}{2} \leq x_1 \leq 1, \frac{1}{2} \leq x_2 \leq 1 \end{cases}.$$

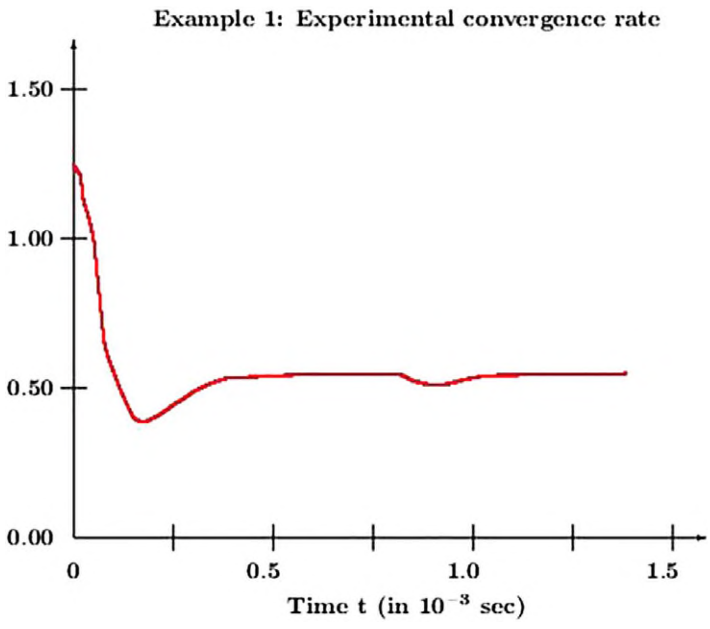

FIGURE 5 Example 1: Experimental convergence rate err(t_m) for $h = 1/64$ [Color figure can be viewed at wileyonlinelibrary.com]

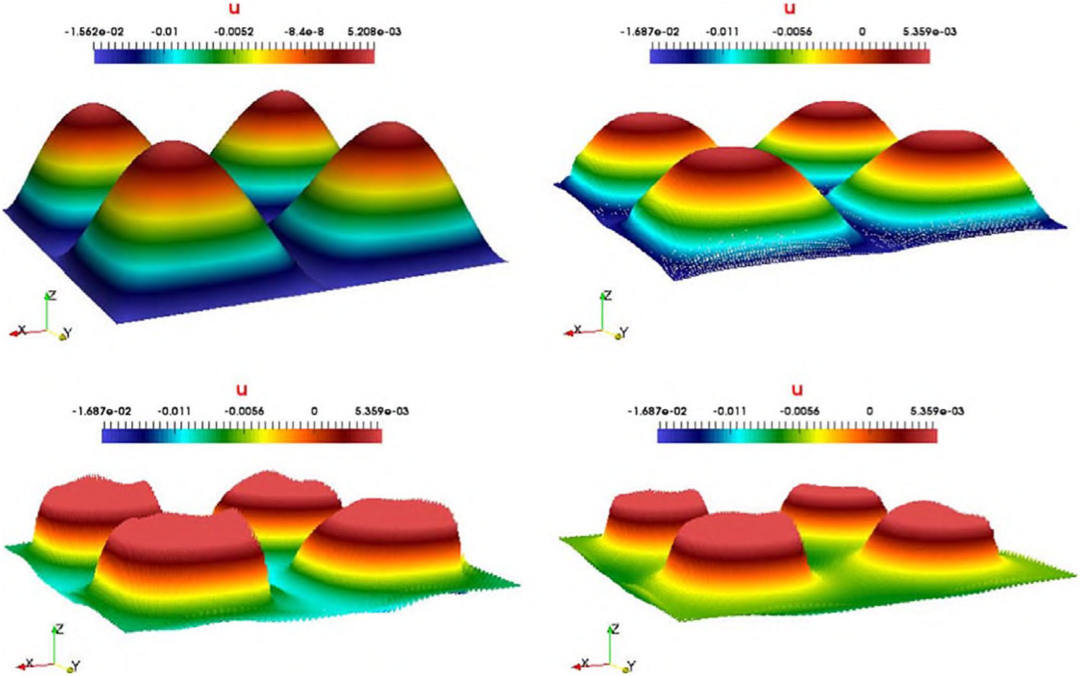

FIGURE 6 Example 2: Computed solution for $h = 1/128$ and $\delta = 4.5 \cdot 10^{-3}$ at initial time $t = 0$ s (top left), at time $t = 3.4 \cdot 10^{-5}$ s (top right), at time $t = 9.7 \cdot 10^{-3}$ s (bottom left), and at time $t = 7.1 \cdot 10^{-2}$ s (bottom right) [Color figure can be viewed at wileyonlinelibrary.com]

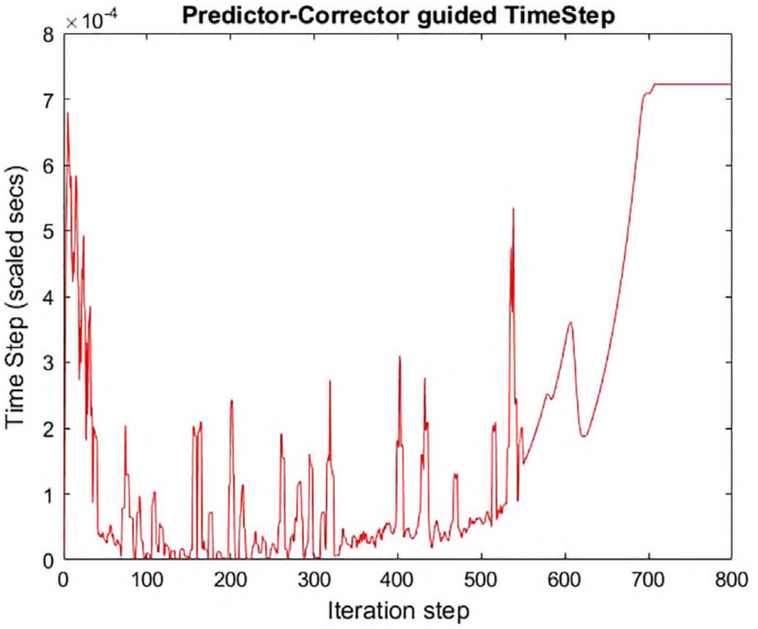

FIGURE 7 Example 2: Performance of the predictor corrector continuation strategy for $h = 1/128$ and $\delta = 4.5 \cdot 10^{-3}$. Adaptive choice of time steps τ_m [Color figure can be viewed at wileyonlinelibrary.com]

For $\delta = 4.5 \cdot 10^{-3}$ and $h = 1/128$, Figure 6 shows the route along which the initial profile becomes completely flat. We observe the development of four upper facets around the four maxima of the initial data and lower facets around the minima. Due to the small mesh size h, the formation of narrow interfaces with steep gradients between the upper and lower facets happens quickly. The extinction time is $t_{ext} = 1.2 \cdot 10^{-2}$.

Figure 7 displays the adaptive choice of the time steps. We see a similar behavior as in Example 1 for $h = 1/64$ and $\delta = 7.5 \cdot 10^{-3}$.

6 | CONCLUSION

We have derived a C^0IPDG approximation of an implicitly in time discretized, regularized and scaled fourth-order TVF problem describing surface relaxation below the roughening temperature. We have further developed a predictor corrector continuation strategy for the numerical solution of the fully discretized problem featuring an adaptive choice of the time steps. Numerical results have been presented that illustrate the performance of the approach.

The existence and uniqueness of a solution of the C^0IPDG method will be shown in part II of the paper.

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ORCID

Ronald H.W. Hoppe https://orcid.org/0000-0003-2287-6102

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