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Finite volumes for simulation of large molecules

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Finite volumes for simulation of large molecules

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Abstract

We study a finite volume scheme for simulating the evolution of large molecules within their reduced state space. The finite volume scheme under consideration is the SQRA scheme developed by Lie, Weber and Fackeldey. We study convergence of a more general family of FV schemes in up to 3 dimensions and provide a convergence result for the SQRA-scheme in arbitrary space dimensions.

1 Smoluchovski equation in high dimension

The evolution of a large molecule over time can be modelled using the Smoluchovski equation where the state of the molecule is described by its position in the state space. While the true state space consists of the positions and velocities of all atoms of the molecule, for large molecules we can often identify several critical degrees of freedom that dominate the behavior and the state of the molecule, which can be used to reduce the dimension of the state space. Considering e.g. a critical bond within the molecule, which can vary its angles $(\theta,\phi)\in[0,\pi)\times[0,2\pi)$. If the molecule has 3 such bonds, this leads to a polygonal subset $\mathbf{Q}$ of a $d=6$ dimensional state space $\mathbb{X}$. The variable $u(t,\cdot):\mathbf{Q}\to\mathbb{R}$ will henceforth be indicating the probability distribution to find the molecule in the state $x\in\mathbf{Q}$ at time t and $u_0=u(0,\cdot)$ is the initial distribution (or initial state $u_0=\delta_{x_0}$, in case this is known precisely). The evolution of u over time is described by the Smoluchovski equation with mobility κ and chemical potential V

$$\dot{u}=\nabla\cdot(\kappa\nabla u)+\nabla\cdot(\kappa u\nabla V)\quad\text{on }[0,T]\times\mathbf{Q}$$

Without going into details but refering to [5] we claim that the major point for the understandig of long-term evolution of the molecule is the understanding of the right hand side linear operator, i.e. its eigenvalues and eigenvectors.

From the numerical point of view, this results in the necessity to discretize the following elliptic equation:

$$-\nabla\cdot(\kappa\nabla u)-\nabla\cdot(\kappa u\nabla V)=f\qquad\text{on }\mathbf{Q}\tag{1.1}$$

and to study the convergence behavior of the discretization. For simplicity we assume in the following that $\kappa,V\in C^2(\overline{\mathbf{Q}})$, $f\in L^2(\mathbf{Q})$ are real-valued functions.

The assumption $V\in C^2(\overline{\mathbf{Q}})$ implies strict positivity of $\pi:=\exp(-V)$. Using a transformation $U=u/\pi$ we find that (1.1) is equivalent with

$$-\nabla\cdot(\pi\kappa\nabla U)=f.\tag{1.2}$$

The particular challenges we address are, first, the choice of discretization approach for π, as addressed in [3], and second the issues that arise from high dimensionality of the problem, i.e. the curse of dimensionality, and the issue arising from $V(x)\to+\infty$ as $x\to\partial\mathbf{Q}$ at least for some models, addressed in [4].

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1.1 Discretization

Discretizing (1.2) on an admissible mesh in the sense of Definition 10.1 in Chapter 3 of [1] or in [2] we write $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ for the mesh consisting of convex polytope control volumes $\mathcal{V} := \{\Omega_i, i = 1, \dots, N\}$ with mass m_i,$(d-1)$-dimensional flat interfaces $\mathcal{E}_{\mathbf{Q}} = \{\sigma_{i,j}\}$ with measure $m_{i,j}$ and points $\mathcal{P}_{\mathbf{Q}} = \{x_i, i = 1, \dots, N\}$ which we sometimes call the cell centers. Two cells Ω_i, Ω_j are neighbors if $\sigma_{i,j} := \partial\Omega_i \cap \partial\Omega_j$ has positive measure and we write $i \sim j$. If $i \sim j$, the distance of the cell centers is $h_{i,j} := |x_i - x_j|$.

In order to formulate discrete Dirichlet conditions, we follow [2] and enrich the mesh with finitely many points $\mathcal{P}_{\partial\mathbf{Q}} = (y_k)_k \subset \partial\mathbf{Q}$ and virtual interfaces $\mathcal{E}_{\partial\mathbf{Q}} = \{\sigma_{i,k} \text{ flat} : \exists i \text{ with } \sigma_{i,k} \subset \partial\mathbf{Q} \cap \partial\Omega_i\}$ i.e., for every flat segment $\sigma_{i,k} \subset \partial\mathbf{Q} \cap \partial\Omega_i$ we chose $y_k \in \sigma_{i,k}$ such that $(y_k - x_i) \perp \sigma_{i,k}$ and denote $m_{i,k} := |\sigma_{i,k}|$ with $h_{i,k} := |y_k - x_i|$. We further generalize the notation $i \sim j$ if $\sigma_{i,j} \subset \partial\Omega_i$ or $\sigma_{i,j} \subset \partial\Omega_j$. Then, when summing up over the interfaces in the calculations below, we do not have to distinguish between inner interface of type $\partial\Omega_i \cap \partial\Omega_j$ and outer interfaces of type $\partial\mathbf{Q} \cap \partial\Omega_i$.

We finally denote $\mathcal{P} = \mathcal{P}_{\mathbf{Q}} \cup \mathcal{P}_{\partial\mathbf{Q}}$ and $\mathcal{E} = \mathcal{E}_{\mathbf{Q}} \cup \mathcal{E}_{\partial\mathbf{Q}}$ and write $\sum_{j:\, j\sim i}$ for the sum over all interfaces belonging to Ω_i and $\sum_{j\sim i}$ for the sum over all interfaces $\mathcal{E}$.

Given a family of admissible meshes $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ we denote for $\Omega_i \in \mathcal{V}_h$ the diameter $h_i = \mathrm{diam}\Omega_i$. The family of meshes is called *quasi uniform* if for every $x_i, x_j \in \mathcal{P}_h$, $i \sim j$, it holds $h_{i,j} < h$ and if there exists $R, r > 0$ independent from $\mathcal{T}_h$ such that the following holds: For every $\Omega_i \in \mathcal{V}_h$ there exists $x \in \Omega_i$ such that $\mathbb{B}_{rh_i}(x) \subset \Omega_i \subset \mathbb{B}_{Rh_i}(x)$.

We make the following proposal for a discretization of (1.2)

$$\forall x_i \in \mathcal{P}_{\mathbf{Q}} \qquad -\sum_{j:\, j\sim i} \frac{m_{i,j}}{h_{i,j}} S_{i,j} \left(U_{\mathcal{T},j} - U_{\mathcal{T},i}\right) = m_i f_{\mathcal{T},i}, \tag{1.3}$$

where $f_{\mathcal{T},i} = \fint_{\Omega_i} f$ is the average of f over Ω_i and $S_{i,j} = S_{\alpha,\beta}\left(\pi_i, \pi_j\right)$ is a Stolarsky mean of π_i and π_j [6], $\pi_i = \mathrm{e}^{-V_i}$, $V_i = V(x_i)$ resp. $V_i = V(y_i)$ and

$$S_{\alpha,\beta}\left(x, y\right) = \left(\frac{\beta\left(x^\alpha - y^\alpha\right)}{\alpha\left(x^\beta - y^\beta\right)}\right)^{\frac{1}{\alpha-\beta}}, \qquad \alpha \neq 0,\, \beta \neq 0,\, \alpha \neq \beta,\, x \neq y \tag{1.4}$$

Stolarsky means can be extended to the critical points $\alpha = 0,\ \beta = 0,\ \alpha = \beta,\ x = y$ in a continuous way and generalize the logarithmic mean and other means. Interestingly, for a choice $\alpha = 0$ $\beta = -1$ one obtains the Scharfetter–Gummel scheme with $S_{0,-1}(x, y) = xy(x - y)^{-1} \log \frac{x}{y}$. While we do not want to go into detail on this aspect, we mention that $\alpha = 1, \beta = -1$ yields $S_{1,-1}(x, y) = \sqrt{xy}$, which is the SQRA scheme and refer for more information on motivation and background to [3].

From a discrete solution $U_{\mathcal{T}}$ one can obtain a discrete $u_{\mathcal{T}}$ reversing the above transformation $U = u/\pi$. One obtains that $u_{\mathcal{T},i} := U_{\mathcal{T},i}\pi_i$ solves the discrete Smoluchovski

$$\forall x_i \in \mathcal{P}_{\mathbf{Q}} \qquad -\sum_{j:\, j\sim i} \frac{m_{i,j}}{h_{i,j}} S_{i,j} \left(\frac{u_{\mathcal{T},j}}{\pi_j} - \frac{u_{\mathcal{T},i}}{\pi_i}\right) = m_i f_{\mathcal{T},i}, \tag{1.5}$$

In what follows we will provide convergence results for the above discretizations in low dimensions, i.e. $d \leq 3$ and in high dimensions for (1.3) only.

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1.2 Results and challenges

Our results are centered around two different questions that arise from the convergence analysis of (1.3) and (1.5) in high dimensions: The first results in Section 2 deal with the convergence of (1.3) and (1.5) in low dimensions up to $d = 3$. We will see that all schemes converge with the same rate for U but that there is a different convergence behavior in u: The classical Scharfetter-Gummel scheme has a better convergence behavior than the other schemes for high gradients of V. From the analytical point of view, it is interesting that for any choice of the Stolarsky mean, the rate of convergence is not worse than the consistency of the mesh for the ordinary Laplace operator, i.e. $\kappa = \pi = 1$.

The results of Section 3 are centered around the convergence of a general finite volume scheme of type (1.3) in high dimensions when the resolution of the underlying grid is not homogeneous: In particular, we assume that the expected solution is almost constant in some regions, where the resolution is chosen rough, while the resolution is fine in regions of strong oscillations of the solution or the coefficients κ and π. We will see that this can lead to good results by simultaneously bypassing the curse of dimensionality to some extend. Furthermore, we deal with the case that the elliptic parameter degenerates locally close to the boundary. This scenario is relevant in chemistry as the potential V might tend to $+\infty$ in some regions of the state space.

The mathematical challenge in the second case is that one cannot rely on the "classical"pointwise evaluation of the limit function, but one has to compare the discrete solution with a locally averaged continuous solution. In particular, Taylor arguments have to be carried out in an averaged sense and one needs to be very careful that averaged lower order terms really cancel each other out. Furthermore, also the proof of the Poincaré inequality has to rely on dimensionless averaging arguments.

2 Convergence results based on consistency, [3]

In this section, we assume $\kappa = 1$ for simplicity of notation, but mention that the results in [3] hold more general. We then denote

$$L^2(\mathcal{P}) := \{U : \mathcal{P}_\mathbf{Q} \to \mathbb{R}\} \qquad H_\mathcal{T} := \left\{U : \mathcal{P} \to \mathbb{R} \mid U|_{\mathcal{P}_{\partial\mathbf{Q}}} \equiv 0\right\}$$

with the embedding $H_\mathcal{T} \hookrightarrow L^2(\mathcal{P})$ and for $\tilde{v} \in L^2(\mathcal{P}),\ v \in H_{:\mathcal{T}}$ we introduce

$$\|v\|^2_{H_\mathcal{T}} := \sum_{i\sim j} \frac{m_{i,j}}{h_{i,j}} \left(v_j - v_i\right)^2 , \quad \|\tilde{v}\|^2_{L^2(\mathcal{P})} := \sum_{\Omega_i} m_i \tilde{v}_i^2 . \tag{2.1}$$

Definition 2.1 (inf-sup stability)**.** Let $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ be a quasi uniform family of admissible meshes. A family of bilinear forms a_h on $H_{\mathcal{T}_h}$ is called *uniformly inf-sup stable* with respect to two norms $\|\cdot\|_{h,1}$, $\|\cdot\|_{h,2}$ if there exists $\gamma > 0$ (independent from h) such that

$$\forall u \in H_{\mathcal{T}_h} : \quad \gamma \|u\|_{h,1} \leq \sup_{v\in H_{\mathcal{T}_h}} \frac{a_h(u,v)}{\|v\|_{h,2}} .$$

We write $(\mathcal{R}_h u)_i := (\mathcal{R}_{\mathcal{T}_h} u)_i := u(x_i)$ on Ω_i. For a continuous and coercive bilinear form a : $H^1_0(\mathbf{Q}) \times H^1_0(\mathbf{Q}) \to mathbbR$, the associated linear operator $A :\ H^2(\mathbf{Q}) \to L^2(\mathbf{Q})$ is defined by

$$\forall u \in H^2(\mathbf{Q}) \cap H^1_0(\mathbf{Q}),\ v \in H^1_0(\mathbf{Q}) : \quad a(u,v) = \int_\mathbf{Q} v\, Au\, . \tag{2.2}$$

Definition 2.2 (Consistency)**.** Let $a\,:\,H^1_0(\mathbf{Q})\times H^1_0(\mathbf{Q})\to\mathbb{R}$ be bilinear and continuous with linear operator A such that (2.2) holds and let $\mathcal{T}_h=(\mathcal{V}_h,\mathcal{E}_h,\mathcal{P}_h)$ be a family of admissible meshes with $a_h\,:\,H_{\mathcal{T}_h}\times H_{\mathcal{T}_h}\to\mathbb{R}$ continuous bilinear forms. The *variational consistency error* of a_h in $u\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ is the linear form $E_h\left(u;\cdot\right):\,H_{\mathcal{T}_h}\to\mathbb{R}$ where

$$\forall v\in H_{\mathcal{T}_h}:\quad E_h\left(u;v\right):=\sum_i v_i\int_{\Omega_i}Au-a_h\left(\mathcal{R}_hu,\,v\right)\,. \tag{2.3}$$

We say *consistency* holds for $\|\cdot\|_{h,2}$ on $H_{\mathcal{T}_h}$ and $u\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ if

$$\left\|E_h\left(u;\cdot\right)\right\|_{h,2,*}:=\sup_{v\in H_{\mathcal{T}_h}\setminus\{0\}}\frac{\left|E_h\left(u;v\right)\right|}{\|v\|_{h,2}}\to0\quad\text{as}\quad h\to0\,.$$

A special role is played by

$$a_{\mathrm{D}}\left(u,v\right)=\int_{\mathbf{Q}}\nabla u\cdot\nabla v\,,\qquad a_{h,\mathrm{D}}\left(u,v\right)=\sum_{i\sim j}\frac{m_{i,j}}{h_{i,j}}\left(u_j-u_i\right)\left(v_j-v_i\right)\,,$$

with the corresponding consistency error $E_{h,\mathrm{D}}$. This is the underlying concept of the following definition:

Definition 2.3 (φ-consistency)**.** Let $\mathcal{T}_h=(\mathcal{V}_h,\mathcal{E}_h,\mathcal{P}_h)$ be a quasi uniform family of admissible meshes. We say that $\mathcal{T}_h$ is *φ-consistent* for a continuous monotone increasing φ with $\varphi(0)=0$ if for every $u\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ there exists $C\geq0$ such that for every $h>0$

$$\left\|E_{h,\mathrm{D}}\left(u;\cdot\right)\right\|_{H^*_{\mathcal{T}_h}}\leq C\left\|u\right\|_{H^2}\varphi\left(h\right)\,.$$

Our main results are formulated in terms of φ-consistency as follows:

Theorem 2.4 ([3], Theorem 1.4)**.** *Let $d\leq3$ and $\mathcal{T}_h=(\mathcal{V}_h,\mathcal{E}_h,\mathcal{P}_h)$ be a quasi uniform family of admissible meshes and let the above assumptions on κ,V and f hold. Moreover, let $\mathcal{T}_h$ be φ-consistent (Def. 2.3). If $U\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ is the solution of (1.2) and $U_{\mathcal{T}_h}$ the solution of (1.3) with discrete homogeneous Dirichlet boundary conditions then*

$$\left\|U_{\mathcal{T}_h}-\mathcal{R}_{\mathcal{T}_h}U\right\|^2_{H_{\mathcal{T}_h}}\leq C_1\left\|\pi\right\|^2_\infty\varphi(h)^2+C_2h^k\,,$$

where $k=2$ in general and $k=4$ if the grid is cubic or $d=1$. Here, C_1 and C_2 depend only on d and $\mathbf{Q}$, r and R.

Theorem 2.5 ([3], Theorem 1.5)**.** *Let $d\leq3$ and $\mathcal{T}_h=(\mathcal{V}_h,\mathcal{E}_h,\mathcal{P}_h)$ be a quasi uniform family of admissible meshes and let the above assumptions on κ,V and f hold. Moreover, let $\mathcal{T}_h$ be φ-consistent (Def. 2.3). If $u\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ is the solution of (1.1) and $u_{\mathcal{T}_h}$ the solution of (1.5) with discrete homogeneous Dirichlet boundary conditions then*

$$\left\|u_{\mathcal{T}_h}-\mathcal{R}_{\mathcal{T}_h}u\right\|^2_{H_{\mathcal{T}_h}}\leq C_1\left(\|u\|^2_{H^2}+\|u\|^2_\infty\|V\|^2_{H^2}\right)\varphi(h)^2+C_2h^k\,,$$

where $k=2$ in general and $k=4$ if $\alpha+\beta=-1$ and where C_1 depends on $\mathbf{Q}$,d, r and R and C_2 additionally depends on $\|V\|_{C^2}$ and $\|u\|_{H^2}$.

On cubic grids, the above estimates further simplify.

Theorem 2.6 ([3], Theorem 1.7)**.** *Let $d\leq3$ and $\mathcal{T}_h=(\mathcal{V}_h,\mathcal{E}_h,\mathcal{P}_h)$ be a sequence of cubic grids $h\mathbb{Z}^d$ and let the above assumptions on κ,V and f hold. If $u\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ is the solution of (1.1) and $u_{\mathcal{T}_h}$ the solution of (1.5) with discrete homogeneous Dirichlet boundary conditions then*

$$\left\|u_{\mathcal{T}_h}-\mathcal{R}_{\mathcal{T}_h}u\right\|^2_{H_{\mathcal{T}_h}}\leq Ch^k\,,$$

where $k=2$ in general and $k=4$ if $\alpha+\beta=-1$ and where C depends on on $\mathbf{Q}$,d, $\|V\|_{C^2}$ and $\|u\|_{H^2}$.

3 Finite volume in high dimension, [4]

We will now focus on (1.2) with $\kappa = 1$. When we speak of periodic boundary conditions below, we assume that $\mathbf{Q}$ is a cube. We further assume $\pi \in C^2(\mathbf{Q})$. **Since molecules could face non self-penetrating conditions, the event $V(x) \to +\infty$ as $x \to x_0 \in \mathbf{Q}$, i.e. $\pi(x_0) = 0$ is a plausible scenario.** However, we will be very general on our assumptions on π. For every $\Omega_i \in \mathcal{T}$ we take a value π_i and for every $\sigma \in \mathcal{E}_\mathbf{Q}$ we take a value π_σ. It may or may not hold for $\sigma = \sigma_{ij}$ that $\pi_{ij} = \pi_{\sigma_{ij}} = S_{\alpha,\beta}(\pi_i, \pi_j)$ but we always assume that the discretization is such that $\pi_i, \pi_j, \pi_{ij} > 0$ for every $i \sim k$. Finally, for every cell Ω_i we assume that there exist positive constants $R_i > r_i$ such that

$$\mathbb{B}_{r_i}(x_i) \subset \Omega_i \subset \mathbb{B}_{R_i}(x_i)\,.$$

Since we are in high dimension and want to break the curse of dimensionality by using a high resolution (i.e. small R_i) only in a region as small as possible, we will replace the typically used upper bound for R_i by a distribution of R_i.

In what follows, we write $H^2_0(\mathbf{Q}) := H^2(\mathbf{Q}) \cap H^1_0(\mathbf{Q})$ as well as $H^2_{per}(\mathbf{Q})$ for periodic $H^2(\mathbf{Q})$ functions with mean value 0 and

$$H^2_{(0)}(\mathbf{Q}) := \left\{ U \in H^2(\mathbf{Q}) \,|\, \int_\mathbf{Q} U = 0,\ \partial_\nu U = 0 \text{ on } \partial\mathbf{Q} \right\}\,.$$

These spaces clearly correspond to homogeneous Dirichlet boundary conditions (BC), periodic or homogeneous Neumann boundary conditions.

In what follows, we write $\mathcal{E}_i = \{\sigma_{ij} \,:\, i \sim j\}$ and for $\sigma = \sigma_{ij} \in \mathcal{E}_i$ we write $\partial_{i,\sigma_{ij}} = \frac{1}{h_{ij}}(U_j - U_i)$. If $\sigma \subset \partial\mathbf{Q} \cap \partial\Omega_i$ exists, we write $\mathcal{E}_{i,\partial}$ for the set of all such piecewise flat subsets σ and include $\mathcal{E}_{i,\partial}$ into $\mathcal{E}_i$ and write $\partial_{i,\sigma}$ accordingly.

We then define discrete spaces incorporating discrete boundary conditions (DBC) as follows:

- Dirichlet: $H_{\mathcal{T},0} := \{U : \mathcal{P} \to \mathbb{R} \,|\, \forall \sigma \in \mathcal{E}_\partial\ U_\sigma = 0\}$
- Neumann: $H_{\mathcal{T},(0)} := \{U : \mathcal{P} \to \mathbb{R} \,|\, \forall i,\, \sigma \in \mathcal{E}_{i,\partial} :\ \partial_{K,\sigma} U = 0\,,\ \sum_K m_k U_K = 0\}$
- Periodic: we periodize the discretization, consider discrete functions on the full space and require identical values on "periodically shifted"cells. The corresponding space will be called $H_{\mathcal{T},per}$

In the following, we always match discrete with the corresponding continuous BC. When there is no need to distinguish between the cases, we simply write $H^2_{\mathrm{BC}}(\mathbf{Q})$ and $H_{\mathcal{T},\mathrm{BC}}$ and use the index BC accordingly throughout this work. We study the discrete equation (3.1) i.e.,

$$\forall i : \quad \sum_{\sigma \in \mathcal{E}_i} m_\sigma \pi_\sigma \partial_{i,\sigma} U_\mathcal{T} = m_i f_i\,, \tag{3.1}$$

in either one of the spaces $H_{\mathcal{T},0}$, $H_{\mathcal{T},(0)}$ or $H_{\mathcal{T},per}$ and with the additional condition $\int_\mathbf{Q} \pi U = 0$ in case of Neumann or periodic boundary conditions (BC) i.e. $\sum_i m_i U_{\mathcal{T},i} = 0$.

Defining $L^2(\mathcal{T}) := \{v |\, \mathcal{P}_\mathbf{Q} \to \mathbb{R}\}$ and

$$\|v\|^2_{L^2(\mathcal{T})} := \sum_{i \in \mathcal{V}} m_i v_i^2\,, \qquad \|v\|^2_{H_{\mathcal{T},\pi}} := \sum_{\sigma \in \mathcal{E}} m_\sigma h_\sigma \pi_\sigma \left|\partial_\sigma v\right|^2\,, \tag{3.2}$$

as well as the pair of operators

$$\tilde{\mathcal{R}}_{\mathcal{T}}:\ L^2(\mathbf{Q}) \ \to\ L^2(\mathcal{T})\,, \left(\tilde{\mathcal{R}}_{\mathcal{T}}U\right)_i := \fint_{\mathbb{B}_{r_i}(x_i)} U\,, \tag{3.3}$$

$$\mathcal{R}^*_{\mathcal{T}}:\ L^2(\mathcal{T}) \ \to\ L^2(\mathbf{Q})\,, \left(\mathcal{R}^*_{\mathcal{T}}U\right)(x) := U_i \text{ if } x\in\Omega_i \tag{3.4}$$

We extend $\tilde{\mathcal{R}}_{\mathcal{T}}$ to account for discrete Dirichlet BC by $\left(\mathcal{R}_{\mathcal{T},0}U\right)_i := \left(\tilde{\mathcal{R}}_{\mathcal{T}}U\right)_i$ and

$$\forall\sigma\in\mathcal{E}_\partial:\quad \left(\mathcal{R}_{\mathcal{T},0}U\right)_\sigma := 0\,, \tag{3.5}$$

and for Neumann BC by $\mathcal{R}_{\mathcal{T},(0)}U := \tilde{\mathcal{R}}_{\mathcal{T}}U - \left(\sum_i m_i\left(\tilde{\mathcal{R}}_{\mathcal{T}_h}U\right)_i\right)$ and

$$\forall\sigma\in\mathcal{E}_\partial:\quad \left(\mathcal{R}_{\mathcal{T},(0)}U\right)_\sigma := \left(\mathcal{R}_{\mathcal{T}}U\right)_K\,,\quad K\in\mathcal{V}_\sigma\,. \tag{3.6}$$

For periodic BC, we set $\mathcal{R}_{\mathcal{T},per}U := \tilde{\mathcal{R}}_{\mathcal{T}}U - \left(\sum_K m_K\left(\tilde{\mathcal{R}}_{\mathcal{T}_h}U\right)_K\right)$ and find the general relation $\mathcal{R}_{\mathcal{T},\mathrm{BC}}:\ H^2_{\mathrm{BC}}(\mathbf{Q})\to H_{\mathcal{T},\mathrm{BC}}$.

Theorem 3.1 ([4] Theorem 2.5)**.** *Given a polygonal bounded domain $\mathbf{Q}\subset\mathbb{R}^d$ and $U\in H^2(\mathbf{Q})$ a solution to (1.2) with $f\in L^2(\mathbf{Q})$ satisfying the boundary conditions BC then for every admissible mesh $\mathcal{T}$ it holds: there exists a unique solution $U_{\mathcal{T}}$ to (3.1) for $f_{\mathcal{T}}$ given by (3.1) satisfying the discrete boundary conditions BC. Furthermore*

$$\begin{aligned} \left\|U_{\mathcal{T}}-\mathcal{R}_{\mathcal{T},\mathrm{BC}}U\right\|_{H_{\mathcal{T},\pi}} &\le \left(I_{1,\mathcal{T}}(U)+I_{2,\mathcal{T}}(U)\right)\,, \\ I_{1,\mathcal{T}}(U) &= \left(\sum_{\sigma\in\mathcal{E}} h_\sigma m_\sigma \pi_\sigma^{-1}\left(\fint_\sigma |\pi-\pi_\sigma|\,|\nabla U|\right)^2\right)^{\frac12}\,, \\ I_{2,\mathcal{T}}(U) &= \left(\sum_{\sigma\in\mathcal{E}} m_\sigma\pi_\sigma h_\sigma\left(\fint_\sigma \nabla U\cdot\nu_{\sigma,K}-\partial_{\sigma,K}\mathcal{R}_{\mathcal{T}}U\right)^2\right)^{\frac12}\,. \end{aligned} \tag{3.7}$$

Furthermore, there exists a constant $C>0$ depending only on d such that for every $U\in H^2(\mathbf{Q})\cap H^1_0(\mathbf{Q})$ the following holds:

$$|I_{1,\mathcal{T}}(U)|^2 \le C\left(\sum_i \frac{R_i^3}{r_i^3}R_i^2\left\|\sqrt{\pi}\nabla U\right\|^2_{H^1(\Omega_i)}\|\nabla\pi\|^2_{L^\infty(\Omega_i)}\sum_{\sigma\in\mathcal{E}_i}\fint_\sigma\frac{1}{\pi\kappa_\sigma}\right)\,, \tag{3.8}$$

$$|I_{1,\mathcal{T}}(U)|^2 \le C\left(\sum_i \frac{R_i^3}{r_i^3}R_i^2\left\|\nabla U\right\|^2_{H^1(\Omega_i)}\|\nabla\pi\|^2_{L^\infty(\Omega_i)}\sum_{\sigma\in\mathcal{E}_i}\frac{1}{\pi_\sigma}\right)\,, \tag{3.9}$$

$$|I_{2,\mathcal{T}}(U)|^2 \le C\left(\sum_i R_i^2\left(\frac{R_i}{r_i}\right)^{d+1}\left\|\nabla^2 U\right\|^2_{L^2(\Omega_i)}\sum_{\sigma\in\mathcal{E}_i}\pi_\sigma\right)\,. \tag{3.10}$$

Theorem 3.1 provides only an estimate on the $H_{\mathcal{T},\pi}$-norm while we seek convergence also in $L^2(\mathcal{T})$. For this it is convenient to derive a Poincaré inequality. As the above discussion suggests, we will seek for such an inequality with respect to the weighted norms. In what follows, we assume that $\mathbf{Q}$ has the following structure, even though there are more general possible structures:

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Definition 3.2. Let $\mathbf{Q}$ be simply connected, let $\omega \subset \mathbf{Q}$ be open convex and let $\pi : \overline{\mathbf{Q}} \to \mathbb{R}$ be a simple piecewise constant function. Let $\omega(\pi,\pi_0) := \{x \in \omega |\, \pi(x) \geq \pi_0\}$. Given $\pi_0 \geq \pi_1 > 0$ we say that π is pseudo monotone on ω w.r.t π_0, π_1 and an open ball $\mathbb{B} \subset \omega(\pi,\pi_0)$ if for every $x \in \omega \backslash \omega(\pi,\pi_0)$ and every $y \in \mathbb{B}$ there exists $z \in \partial\omega(\pi,\pi_0)$ such that $t \mapsto \pi(x + t(z-x))$ is monotone increasing on $[0,1]$ and if π restricted to the closed convex hull of $\omega(\pi,\pi_0)$ is bigger or equal to π_1.

Definition 3.3. Using

$$\mathcal{E}_{\mathcal{T},x,y} := \{\sigma \in \mathcal{E} |\ [x,y] \cap \sigma \neq \emptyset\} \ .$$

we define $\pi_{\mathcal{T}}(x) := \left(\mathcal{R}^*_{\mathcal{T}}\pi_{\mathcal{T}}\right)(x)$ and the following function for $x \in \omega_i$ and corresponding $\mathbb{B}_{ij} \subset \omega_i$:

$$a_{\pi,\mathcal{T}}(x) := \min\left\{ \left(\mathcal{R}^*_{\mathcal{T}}\pi_{\mathcal{T}}\right)(x) \,,\ \inf_{y\in\mathbb{B}_{ij}} \inf_{\sigma\in\mathcal{E}_{\mathcal{T},x,y}} \pi_\sigma \right\} \,,$$
$$\tilde{\pi}_{\mathcal{T}}(x) := \begin{cases} \left(\mathcal{R}^*_{\mathcal{T}}\pi_{\mathcal{T}}\right)(x) & \text{if } \left(\mathcal{R}^*_{\mathcal{T}}\pi_{\mathcal{T}}\right)(x) \geq \pi_0 \text{ and } a_{\pi,\mathcal{T}}(x) \geq \pi_1 \\ a_{\pi,\mathcal{T}}(x) & \text{else} \end{cases} \ .$$

Next, we introduce the notation $\tilde{\pi}_{\mathcal{T},K} := m_K^{-1} \int_K \tilde{\pi}_{\mathcal{T}}$. Based on this we write for $U \in L^2(\mathcal{T})$:

$$\overline{\pi}^{\mathcal{V}} := \int_{\mathbf{Q}} \tilde{\pi}_{\mathcal{T}}(x) \,, \qquad \overline{U}^{\tilde{\pi}} := \frac{1}{\overline{\pi}^{\mathcal{V}}} \int_{\mathbf{Q}} \tilde{\pi}_{\mathcal{T}} \mathcal{R}^*_{\mathcal{T}} U \ .$$

Theorem 3.4 ([4] Theorem 2.14)**.** *Under the above assumptions on $\mathbf{Q}$ and π and $\mathcal{T}$ exists a constant C depending only on d, $\tilde{\mathbf{Q}}$, $C(\mathcal{T},\pi_0)$, π_0 and $\|\pi\|_\infty$ such that*

$$\sum_K \tilde{\pi}_{\mathcal{T},K} m_K \left(U_K - \overline{U}^{\tilde{\pi}}\right)^2 \leq C \left\|U\right\|^2_{H_{\mathcal{T},\pi}} \ . \tag{3.11}$$

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