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Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 2198-5855

Uniform estimate of the relative free energy by the dissipation rate for finite volume discretized reaction-diffusion systems

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submitted: March 18, 2014

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No. 1934
Berlin 2014

2010 *Mathematics Subject Classification.* 65M08, 46E39, 35B40, 35K57, 35R05.

Key words and phrases. Admissible finite volume mesh, reaction-diffusion system, free energy, discrete Poincaré and Sobolev-Poincaré inequality.

The work was partially supported by the European Commission within the 7th Framework Programme MD^3 "Material Development for Double Exposure and Double Patterning" and by the DFG Research Center MATHEON *Mathematics for Key Technologies* within project D22 "Modeling of Electronic Properties of Interfaces in Solar Cells".

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Abstract

We prove a uniform Poincaré-like estimate of the relative free energy by the dissipation rate for implicit Euler, finite volume discretized reaction-diffusion systems. This result is proven indirectly and ensures the exponential decay of the relative free energy with a unified decay rate for admissible finite volume meshes.

1 Introduction

In a heterostructured domain $\Omega \subset \mathbb{R}^N$, we consider m diffusing species X_i with initial densities U_i which undergo a finite number of reversible chemical reactions. Besides the densities u_i of the species X_i we introduce their (dimensionless) chemical potentials v_i and chemical activities a_i. According to Boltzmann statistics we have $u_i = \overline{u}_i \mathrm{e}^{v_i} = \overline{u}_i a_i$, $i = 1, \ldots, m$, where the reference densities $\overline{u}_i$ express the heterogeneity of the system. For the fluxes j_i of the species X_i we make the ansatz $j_i = -d_i u_i \nabla v_i = -d_i \overline{u}_i \mathrm{e}^{v_i} \nabla v_i = -d_i \overline{u}_i \nabla a_i$, $i = 1, \ldots, m$, with diffusion coefficients d_i. Let $\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$ be a finite subset. Each pair $(\alpha, \beta) \in \mathcal{R}$ represents the vectors of stoichiometric coefficients of a reversible reaction

$$\alpha_1 \mathsf{X}_1 + \cdots + \alpha_m \mathsf{X}_m \rightleftharpoons \beta_1 \mathsf{X}_1 + \cdots + \beta_m \mathsf{X}_m.$$

According to the mass action law, the net rate of this pair of reactions is of the form $k_{\alpha\beta}(a^\alpha - a^\beta)$, where $k_{\alpha\beta}$ is a reaction rate coefficient and $a^\alpha := \prod_{i=1}^m a_i^{\alpha_i}$. The net production rate of species X_i resulting from all reactions taking place is

$$R_i := \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(a^\alpha - a^\beta)(\beta_i - \alpha_i).$$

The problem under consideration consists of the m continuity equations

$$\left.\begin{aligned} \frac{\partial u_i}{\partial t} + \nabla \cdot j_i = R_i \text{ in } \mathbb{R}_+ \times \Omega, \quad \nu \cdot j_i = 0 \text{ on } \mathbb{R}_+ \times \partial\Omega, \\ u_i(0) = U_i \text{ in } \Omega, \quad i = 1, \ldots, m. \end{aligned}\right\} \tag{P}$$

The set $\mathcal{S} := \operatorname{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}\} \subset \mathbb{R}^m$ represents the stoichiometric subspace defined by the reaction system. Our essential assumptions on the data are

(A1) Ω is an open, bounded, polyhedral domain in $\mathbb{R}^N$, $N = 2, 3$;
$\overline{u}_i, U_i \in L_+^\infty(\Omega)$, $\overline{u}_i, U_i \geq \delta > 0$, $i = 1, \ldots, m$, $\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$ finite subset,
$k_{\alpha\beta}, d_i : \Omega \times \mathbb{R}_+^m \to \mathbb{R}_+$ Carathéodory functions satisfying
$d_i(x, a) \geq \delta$, $c \geq k_{\alpha\beta}(x, a) \geq b_{\alpha\beta}(x)$ f.a.a. $x \in \Omega$, and all $a \in \mathbb{R}_+^m$,
where $\|b_{\alpha\beta}\|_{L^1} > 0$ for all $(\alpha, \beta) \in \mathcal{R}$.
If $N = 3$ then $\max_{(\alpha,\beta)\in\mathcal{R}} \max\left\{ \sum_{i=1}^m \alpha_i, \sum_{i=1}^m \beta_i \right\} \leq 3$,
$\mathcal{A} \cap \partial\mathbb{R}_+^m = \emptyset$, where
$\mathcal{A} := \left\{ a \in \mathbb{R}_+^m : \ a^\alpha = a^\beta \text{ for all } (\alpha, \beta) \in \mathcal{R}, \ \int_\Omega (\bar{u}a - U) \,\mathrm{d}x \in \mathcal{S} \right\}.$

These assumptions allow us to handle a general class of reaction-diffusion systems, including heterogeneous materials, reactions occurring in subdomains and diffusion and reaction rate coefficients depending on the state variables, see [3, Remark 1].

The aim of the paper is to show for finite volume discretized versions of Problem (P) a Poincaré-like estimate of the discrete relative free energy by the discrete dissipation rate uniformly for all meshes with (A2), see Theorem 1. The essential new result is that our proof works without any restriction on the mesh size which is needed in [4, Theorem 3.2]. Using discrete functional inequalities from [1] instead of results in [5] the estimate is generalized from Voronoi meshes to admissible finite volume meshes. More general reaction rate and diffusion coefficients are treated, too. Finally, for Euler backward in time and finite volume in space discretization schemes, the discretized free energy along the discrete solutions decays exponentially to its equilibrium value with a uniform decay rate for all discretizations fulfilling (A2), see Theorem 2. This gives the discrete counterpart to the behavior in the continuous case characterized by [6, Theorem 4.3] in a more general setting.

2 Discretization scheme and main result

An admissible mesh of Ω (see [2]) denoted by $\mathcal{M} = (\mathcal{P}, \mathcal{T}, \mathcal{E})$ is formed by a family of grid points $\mathcal{P}$ in $\bar{\Omega}$, a family $\mathcal{T}$ of control volumes and a family $\mathcal{E}$ of parts of hyperplanes in $\mathbb{R}^N$ (which represent the faces of the boxes). Let M be the number of grid points $x_K \in \mathcal{P}$, $M = \#\mathcal{P}$. $|K|$ denotes the measure of the box $K \in \mathcal{T}$. For $K, L \in \mathcal{T}$ with $K \neq L$ either the $(N-1)$ dimensional Lebesgue measure of $\bar{K} \cap \bar{L}$ is zero or $\bar{K} \cap \bar{L} = \bar{\sigma}$ for some $\sigma \in \mathcal{E}$. The symbol $\sigma = K|L$ denotes the surface between K and L. The set of interior surfaces is called $\mathcal{E}_{int} \subset \mathcal{E}$. Moreover, for $\sigma \in \mathcal{E}$ we denote by m_σ the $(N-1)$ dimensional Lebesgue measure of the face σ. For $\sigma = K|L \in \mathcal{E}_{int}$ let d_σ be the Euclidean distance of x_K and x_L and σ is assumed to be orthogonal to the line connecting x_K and x_L. $\mathcal{E}_K$ is the subset of $\mathcal{E}$ such that $\partial K = \bar{K} \setminus K = \cup_{\sigma \in \mathcal{E}_K} \bar{\sigma}$. Concerning the discretization we suppose

(A2) Let $\mathcal{M}$ be an admissible finite volume mesh with
$\operatorname{dist}(x_K, \sigma) \geq \theta d_\sigma \ \ \forall K \in \mathcal{T} \ \ \forall \sigma \in \mathcal{E}_K \cap \mathcal{E}_{int} \ (\theta > 0)$.
Let $\mathcal{Z} = \{t_0, t_1, \dots, t_n, \dots\}$ be a partition of $\mathbb{R}_+$ with $t_0 = 0$, $t_n \in \mathbb{R}_+$, $t_{n-1} < t_n$, $n \in \mathbb{N}$, $t_n \to +\infty$ as $n \to \infty$, $\sup_{n\in\mathbb{N}}(t_n - t_{n-1}) \leq \tau < \infty$.

$X(\mathcal{M})$ represents the set of functions from Ω to $\mathbb{R}$ which are constant on each box of the mesh. For $w_h \in X(\mathcal{M})$ the value at the box $K \in \mathcal{T}$ is called w_K. For $w_h \in X(\mathcal{M})$ the discrete H^1 seminorm $|w_h|_{1,\mathcal{M}}$ and H^1 norm $\|w_h\|_{1,\mathcal{M}}$ are defined by

$$|w_h|_{1,\mathcal{M}}^2 = \sum_{\sigma = K|L \in \mathcal{E}_{int}} \frac{m_\sigma}{d_\sigma} |w_K - w_L|^2, \quad \|w_h\|_{1,\mathcal{M}}^2 = |w_h|_{1,\mathcal{M}}^2 + \|w_h\|_{L^2}^2. \tag{1}$$

For $K \in \mathcal{T}$ we denote by $u_{iK}(t_n)$ the constant density on K at t_n. Associated to the grid points we have chemical potentials $v_{iK}(t_n)$ and chemical activities $a_{iK}(t_n)$, $i = 1, \dots, m$. Moreover we work with the vectors $\vec{u}$, $\vec{v}$, $\vec{a} \in \mathbb{R}^{Mm}$ and the vectors on a box $\vec{u}_K$, $\vec{v}_K$, $\vec{a}_K \in \mathbb{R}^m$. We introduce the mean values on the control volumes $K \in \mathcal{T}$,

$$\overline{u}_{iK} = \frac{1}{|K|} \int_K \overline{u}_i(x)\, \mathrm{d}x, \quad k_{\alpha\beta K}(\cdot) = \frac{1}{|K|} \int_K k_{\alpha\beta}(x, \cdot)\, \mathrm{d}x$$

and the corresponding piecewise constant functions $\bar{u}_{ih}$ and $k_{\alpha\beta\,h}$. The discrete version of Problem (P) is

$$\left.\begin{aligned} \frac{u_{iK}(t_n) - u_{iK}(t_{n-1})}{t_n - t_{n-1}}|K| - \sum_{\sigma=K|L\in\mathcal{E}_K} Y_i^\sigma(t_n)\big(a_{iL}(t_n) - a_{iK}(t_n)\big)\frac{m_\sigma}{d_\sigma} = R_i^K(t_n),\\ u_{iK}(t_n) = \overline{u}_{iK}\,\mathrm{e}^{v_{iK}(t_n)} = \overline{u}_{iK}\,a_{iK}(t_n), \quad i = 1,\dots,m,\ n \ge 1,\\ u_{iK}(0) = U_{iK} := \tfrac{1}{|K|}\int_\Omega U_i\,\mathrm{d}x, \quad i = 1,\dots,m, \quad K \in \mathcal{T}, \end{aligned}\right\} \qquad (\mathrm{P}_\mathcal{M})$$

where $Y_i^\sigma = Y_i^\sigma(\vec{a})$ is a mean of $d_i(x,a)\overline{u}_i(x)$ on the face σ and R_i^K are given by

$$R_i^K = R_i^K(\vec{a}_K) = \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i)k_{\alpha\beta K}(\vec{a}_K)\Big(\vec{a}_K^{\,\alpha} - \vec{a}_K^{\,\beta}\Big)|K|.$$

We introduce the operator $\widehat{E}: \mathbb{R}^{Mm} \to \mathbb{R}^{Mm}$, $\widehat{E}\vec{v} = \big((\overline{u}_{iK}\mathrm{e}^{v_{iK}})_{K\in\mathcal{T}}\big)_{i=1,\dots,m}$ and

$$\widehat{\mathcal{U}} = \Big\{\vec{u} \in \mathbb{R}^{Mm} : \big(\sum_{K\in\mathcal{T}} u_{1K}|K|, \dots, \sum_{K\in\mathcal{T}} u_{mK}|K|\big) \in \mathcal{S}\Big\}.$$

The discrete dissipation rate $\widehat{D} : \mathbb{R}^{Mm} \to \mathbb{R}$ corresponding to Problem $(\mathrm{P}_\mathcal{M})$ and the discrete free energy $\widehat{F} : \mathbb{R}^{Mm} \to \overline{\mathbb{R}}$ take the form

$$\begin{aligned} \widehat{D}(\vec{v}) =& \sum_{i=1}^m \sum_{\sigma=K|L\in\mathcal{E}_{int}} Y_i^\sigma\,(\mathrm{e}^{v_{iK}} - \mathrm{e}^{v_{iL}})(v_{iK} - v_{iL})\frac{m_\sigma}{d_\sigma}\\ &+ \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{K\in\mathcal{T}} k_{\alpha\beta K}\Big(\mathrm{e}^{\alpha\cdot\vec{v}_K} - \mathrm{e}^{\beta\cdot\vec{v}_K}\Big)(\alpha - \beta)\cdot\vec{v}_K|K|,\\ \widehat{F}(\vec{u}) =& \sum_{i=1}^m \sum_{K\in\mathcal{T}} \Big(u_{iK}\ln\frac{u_{iK}}{\overline{u}_{iK}} - u_{iK} + \overline{u}_{iK}\Big)|K|. \end{aligned}$$

Assuming (A1), Problem (P) has exactly one weak stationary solution (u^*, v^*) fulfilling $\int_\Omega (u^* - U)\,\mathrm{d}x \in \mathcal{S}$, see [6, Theorem 3.2]. It is the thermodynamic equilibrium and the corresponding constant vector of chemical activities a^* lies in $\mathcal{A}$. Also the discrete Problem $(\mathrm{P}_\mathcal{M})$ has a unique stationary solution $(\vec{u}^*, \vec{v}^*)$ with $\vec{u}^* - \vec{U} \in \widehat{\mathcal{U}}$ which again represents the thermodynamic equilibrium of the discrete problem $(\mathrm{P}_\mathcal{M})$, see [4, Theorem 3.1]. Let u_h^*, v_h^*, $a_h^* \in X(\mathcal{M})$ be the piecewise constant functions corresponding to $\vec{u}^*$, $\vec{v}^*$, $\vec{a}^*$. According to [4, Corollary 3.1] we have

$$u_{ih}^* = u_i^*\,\frac{\overline{u}_{ih}}{\overline{u}_i}, \quad i = 1,\dots,m, \quad v_h^* = v^*, \quad a_h^* = a^*.$$

Both results from [4] hold true for admissible meshes, too.

We now prove a Poincaré type inequality (similar to [6, Theorem 4.2] for the continuous case) which gives for the discretized situation a uniform estimate of the relative free energy $\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*)$ by the dissipation rate $\widehat{D}$ being independent on the underlying mesh $\mathcal{M}$. [4, Theorem 3.2] contains a proof for Voronoi meshes with mesh sizes less than some constant depending on the data of the problem. Here we establish a uniform estimate for all admissible finite volume meshes fulfilling (A2).

Theorem 2.1 *We assume* (A1) *and* (A2). *Let* $(\vec{u}^*, \vec{v}^*)$ *be the thermodynamic equilibrium of* $(\mathrm{P}_{\mathcal{M}})$. *Then for every* $\rho > 0$ *there is a constant* $c_\rho > 0$ *such that*

$$\widehat{F}(\widehat{E}\vec{v}) - \widehat{F}(\vec{u}^*) \le c_\rho \widehat{D}(\vec{v}) \tag{2}$$

for all $\vec{v} \in \widehat{\mathcal{N}}_\rho := \Big\{\vec{v} \in \mathbb{R}^{Mm} : \ \widehat{F}(\widehat{E}\vec{v}) - \widehat{F}(\vec{u}^*) \le \rho, \ \vec{u} = \widehat{E}\vec{v} \in \vec{U} + \widehat{\mathcal{U}}\Big\}$, *uniformly for all admissible finite volume meshes.*

Proof. In this proof we denote by c (possibly different) positive constants depending only on the data but not depending on the mesh. Let $\rho > 0$ be arbitrarily given.

1. Let $\vec{u} = \widehat{E}\vec{v} \in \vec{U} + \widehat{\mathcal{U}}$. By [4, Lemma 3.1] there exist constants c_1, $c_2 > 0$ not depending on the mesh $\mathcal{M}$ such that

$$c_1 \sum_{i=1}^{m} \|\sqrt{u_{ih}} - \sqrt{u_{ih}^*}\|_{L^2}^2 \le \widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \le c_2 \sum_{i=1}^{m} \|u_{ih} - u_{ih}^*\|_{L^2}^2. \tag{3}$$

Using (A1) and the inequality $(x-y)\ln\frac{x}{y} \ge |\sqrt{x} - \sqrt{y}|^2$ for $x, y > 0$, we estimate

$$\begin{aligned}\widehat{D}(\vec{v}) \ge{}& c\sum_{i=1}^{m} \sum_{\sigma\in\mathcal{E}_{int}} |\sqrt{\mathrm{e}^{v_{iK}}} - \sqrt{\mathrm{e}^{v_{iL}}}|^2 \frac{m_\sigma}{d_\sigma} \\ &+ c \sum_{(\alpha,\beta)\in\mathcal{R}} \int_\Omega b_{\alpha\beta h}\Big(\mathrm{e}^{v_h\cdot\alpha/2} - \mathrm{e}^{v_h\cdot\beta/2}\Big)^2 \mathrm{d}x =: D_1(\vec{v}), \quad \vec{v} \in \mathbb{R}^{Mm}.\end{aligned}$$

Therefore it suffices to prove the inequality

$$\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \le C D_1(\vec{v}) \quad \forall \vec{v} \in \widehat{\mathcal{N}}_\rho \tag{4}$$

with some constant $C > 0$ not depending on the mesh $\mathcal{M}$.

2. If (4) would be false, then there would be a sequence of admissible meshes $\mathcal{M}_n$ and corresponding $\vec{v}_n \in \widehat{\mathcal{N}}_\rho$, $\vec{u}_n = \widehat{E}\vec{v}_n \in \vec{U}_n + \widehat{\mathcal{U}}$, $n \in \mathbb{N}$, such that

$$\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}_n^*) = C_n D_1(\vec{v}_n) > 0, \tag{5}$$

and $\lim_{n\to\infty} C_n = +\infty$. Clearly, for each $\mathcal{M}_n$ we have to use the corresponding quantities M, $\widehat{E}$, $\widehat{F}$, D_1,... and sets $\mathcal{E}_{int}$, $\widehat{\mathcal{U}}$, $\widehat{\mathcal{N}}_\rho$. But we don't write them with an index $\mathcal{M}_n$. Let $a_{niK} = \mathrm{e}^{v_{niK}}$, $K \in \mathcal{T}_n$. By $u_{nih}, v_{nih}, a_{nih},... \in X(\mathcal{M}_n)$, $i = 1, \dots, m$, we denote the corresponding piecewise constant functions. From (3) we obtain

$$\|\sqrt{a_{nih}} - \sqrt{a_{nih}^*}\|_{L^2}^2 \le c\|\sqrt{u_{nih}} - \sqrt{u_{nih}^*}\|_{L^2}^2 \le \frac{c}{c_1}\big(\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}_n^*)\big) \le c(\rho). \tag{6}$$

Thus by assumption and because of $a_{nih}^* = a_i^*$ we find a suitable $\tilde{c}(\rho) < \infty$ with

$$\|\sqrt{a_{nih}}\|_{L^2} \le \tilde{c}(\rho), \quad i = 1, \dots, m, \text{ for all } n. \tag{7}$$

3. The definition of D_1 and (4) gives $\sum_{i=1}^m |\sqrt{a_{nih}}|_{1,\mathcal{M}_n}^2 \le cD_1(\vec{v}_n) \to 0$. Applying the discrete Poincaré inequality for functions with general boundary values (see [1, Theorem 5]) we find for $\sqrt{a_{nih}} \in X(\mathcal{M}_n)$, $i = 1, \dots, m$,

$$\sqrt{a_{nih}} - m_\Omega(\sqrt{a_{nih}}) \to 0 \quad \text{in} \quad L^2(\Omega), \quad \text{where} \quad m_\Omega(\sqrt{a_{nih}}) := \frac{1}{|\Omega|}\int_\Omega \sqrt{a_{nih}}\,\mathrm{d}x.$$

The discrete Sobolev-Poincaré inequality (see [1, Theorem 3]) gives for $q \in [1, \infty)$ if $N = 2$ and for $q \in [1, 6]$ if $N = 3$ the estimate

$$\begin{aligned}\|\sqrt{a_{nih}} - m_\Omega(\sqrt{a_{nih}})\|_{L^q} &\le c_q \|\sqrt{a_{nih}} - m_\Omega(\sqrt{a_{nih}})\|_{1,\mathcal{M}_n} \\ &\le \tilde{c}_q(|\sqrt{a_{nih}}|_{1,\mathcal{M}_n} + \|\sqrt{a_{nih}} - m_\Omega(\sqrt{a_{nih}})\|_{L^2}) \to 0.\end{aligned}$$

Since $m_\Omega(\sqrt{a_{nih}})\,|\Omega| = \|\sqrt{a_{nih}}\|_{L^1} \le c\|\sqrt{a_{nih}}\|_{L^2} \le c(\rho)$ by (7) for all $\mathcal{M}_n$ we find (for a subsequence, and we restrict our further investigations to this subsequence) $m_\Omega(\sqrt{a_{nih}}) \to \sqrt{\widehat{a}_i}$ in $\mathbb{R}$. Using that

$$|\sqrt{a_{nih}} - \sqrt{\widehat{a}_i}| \le |\sqrt{a_{nih}} - m_\Omega(\sqrt{a_{nih}})| + |m_\Omega(\sqrt{a_{nih}}) - \sqrt{\widehat{a}_i}|$$

we conclude

$$\sqrt{a_{nih}} \to \sqrt{\widehat{a}_i} \quad \text{in} \quad L^q(\Omega), \quad i = 1, \ldots, m, \tag{8}$$

for $q \in [1, \infty)$ if $N = 2$ and for $q \in [1, 6]$ if $N = 3$. From

$$a_{nih} - \widehat{a}_i = (\sqrt{a_{nih}} - \sqrt{\widehat{a}_i})(\sqrt{a_{nih}} + \sqrt{\widehat{a}_i}) = (\sqrt{a_{nih}} - \sqrt{\widehat{a}_i})^2 + 2\sqrt{\widehat{a}_i}(\sqrt{a_{nih}} - \sqrt{\widehat{a}_i})$$

we find that

$$\|a_{nih} - \widehat{a}_i\|_{L^2} \le \|\sqrt{a_{nih}} - \sqrt{\widehat{a}_i}\|_{L^4}^2 + 2\sqrt{\widehat{a}_i}\|\sqrt{a_{nih}} - \sqrt{\widehat{a}_i}\|_{L^2} \to 0. \tag{9}$$

4. Let $r_{\alpha\beta}(a_h) := (a_h^{\alpha/2} - a_h^{\beta/2})^2$. Using $\|b_{\alpha\beta}\|_{L^1} = \|b_{\alpha\beta\,h}\|_{L^1}$, taking into account the restriction of the reaction order if $N = 3$ and (8) we have for all $(\alpha, \beta) \in \mathcal{R}$

$$\begin{aligned}0 &\le \|b_{\alpha\beta} r_{\alpha\beta}(\widehat{a})\|_{L^1} = \|b_{\alpha\beta\,h} r_{\alpha\beta}(\widehat{a})\|_{L^1} \\ &\le \|b_{\alpha\beta\,h} r_{\alpha\beta}(a_{nh}) - b_{\alpha\beta\,h} r_{\alpha\beta}(\widehat{a})\|_{L^1} + \|b_{\alpha\beta\,h} r_{\alpha\beta}(a_{nh})\|_{L^1} \\ &\le \|b_{\alpha\beta\,h}\|_{L^\infty} \|r_{\alpha\beta}(a_{nh}) - r_{\alpha\beta}(\widehat{a})\|_{L^1} + cD_1(\vec{v}_n) \to 0.\end{aligned}$$

Therefore, with $\|b_{\alpha\beta}\|_{L^1} > 0$ we find necessarily that

$$\widehat{a}^\alpha = \widehat{a}^\beta \quad \forall(\alpha, \beta) \in \mathcal{R}. \tag{10}$$

5. We introduce $\widehat{u} := (\widehat{u}_1, \ldots, \widehat{u}_m)$, $\widehat{u}_i := \overline{u}_i\,\widehat{a}_i$, and show $\int_\Omega(\widehat{u} - U)\,\mathrm{d}x \in \mathcal{S}$. Let $\gamma \in \mathcal{S}^\perp$ (orthogonal complement of $\mathcal{S}$ in $\mathbb{R}^m$) be arbitrarily given. Then

$$|\gamma \cdot \int_\Omega (\overline{u}\widehat{a} - U)\,\mathrm{d}x| \le |\gamma \cdot \int_\Omega (\widehat{a} - a_{nh})\overline{u}_{nh}\,\mathrm{d}x| + |\gamma \cdot \int_\Omega (a_{nh}\overline{u}_{nh} - U_{nh})\,\mathrm{d}x|.$$

By (9) the first integral on the right hand side tends to zero, the second is zero since $\vec{u}_n - \vec{U}_n \in \widehat{\mathcal{U}}$. Thus, together with (10) we find $\widehat{a} \in \mathcal{A}$, and according to (A1) we obtain that $\widehat{a} = a^*$. By the definition of $\widehat{u}$ this yields $\widehat{u} = u^*$.

6. Because of (3) and (9) we have

$$\lambda_n^2 := \widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}_n^*) \le c_2 \sum_{i=1}^m \|\overline{u}_i\|_{L^\infty} \|a_{nih} - a_{nih}^*\|_{L^2}^2 \to 0 \tag{11}$$

as $n \to \infty$. Additionally (according to (5)) we find

$$\frac{1}{C_n} = \frac{1}{\lambda_n^2} D_1(\vec{v}_n) \to 0 \text{ as } n \to \infty. \tag{12}$$

7. For all n we introduce

$$b_{nih} := \frac{1}{\lambda_n}\Big(\sqrt{\frac{a_{nih}}{\widehat{a}_i}} - 1\Big) \in X(\mathcal{M}_n), \quad i = 1, \dots, m.$$

Because of $(b_{niK} - b_{niL})^2 \le \frac{1}{\lambda_n^2 \widehat{a}_i}(\sqrt{a_{niK}} - \sqrt{a_{niL}})^2$ for all $\sigma = K|L \in \mathcal{E}_{int}$ it results

$$\sum_{i=1}^m |b_{nih}|^2_{1,\mathcal{M}_n} \le c\frac{D_1(\vec{v}_n)}{\lambda_n^2} \to 0.$$

As demonstrated in Step 3 (for $\sqrt{a_{nih}}$), the discrete Poincaré and Sobolev-Poincaré inequality ensure for b_{nih} the convergence $\|b_{nih} - m_\Omega(b_{nih})\|_{L^q} \to 0$, $i = 1, \dots, m$, for $q \in [1, \infty)$ if $N = 2$ and for $q \in [1, 6]$ if $N = 3$. Using $\widehat{a}_i = a_i^* = a^*_{nih}$, (6) and (11) we obtain

$$\begin{aligned}|m_\Omega(b_{nih})|\,|\Omega| &\le \frac{1}{\lambda_n\sqrt{\widehat{a}_i}}\int_\Omega |\sqrt{a_{nih}} - \sqrt{\widehat{a}_i}|\,\mathrm{d}x \le \frac{1}{\lambda_n\sqrt{a_i^*}}\|\sqrt{a_{nih}} - \sqrt{a^*_{nih}}\|_{L^1} \\ &\le \frac{c}{\lambda_n}\|\sqrt{a_{nih}} - \sqrt{a^*_{nih}}\|_{L^2} \le \frac{c}{\lambda_n}(\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*_n))^{1/2} \le \frac{c}{\lambda_n}\lambda_n = c\end{aligned}$$

for all $\mathcal{M}_n$. Thus we find (for a subsequence) $m_\Omega(b_{nih}) \to \widehat{b}_i$ in $\mathbb{R}$. By $|b_{nih} - \widehat{b}_i| \le |b_{nih} - m_\Omega(b_{nih})| + |m_\Omega(b_{nih}) - \widehat{b}_i|$ we conclude for $i = 1, \dots, m$ that

$$b_{nih} \to \widehat{b}_i \quad \text{in} \quad L^q(\Omega) \text{ for } q \in [1, \infty) \text{ if } N = 2 \text{ and for } q \in [1, 6] \text{ if } N = 3. \tag{13}$$

8. We define $\widehat{y} = (\widehat{y}_1, \dots, \widehat{y}_m)$, $\widehat{y}_i := 2\widehat{b}_i u_i^* = 2\widehat{b}_i\widehat{a}_i\overline{u}_i$ and show $\int_\Omega \widehat{y}\,\mathrm{d}x \in \mathcal{S}$. Let $\gamma \in \mathcal{S}^\perp$. Since $2b_{nih}\widehat{a}_i\overline{u}_{nih} = (u_{nih} - u^*_{nih})/\lambda_n + b_{nih}(\sqrt{\widehat{a}_i} - \sqrt{a_{nih}})\sqrt{\widehat{a}_i}\,\overline{u}_{nih}$ it results

$$\begin{aligned}\Big|\gamma\cdot\int_\Omega \widehat{y}\,\mathrm{d}x\Big| &= 2\Big|\sum_{i=1}^m\int_\Omega \widehat{b}_i\widehat{a}_i\overline{u}_{nih}\gamma_i\,\mathrm{d}x\Big| = 2\Big|\sum_{i=1}^m\int_\Omega\big(b_{nih}\widehat{a}_i\overline{u}_{nih}\gamma_i + (\widehat{b}_i - b_{nih})\widehat{a}_i\overline{u}_{nih}\gamma_i\big)\mathrm{d}x\Big| \\ &\le \Big|\gamma\cdot\int_\Omega \tfrac{u_{nh} - u^*_{nh}}{\lambda_n}\,\mathrm{d}x\Big| + c\|b_{nh}\|_{L^2}\|\sqrt{\widehat{a}_h} - \sqrt{a_{nh}}\|_{L^2} + c\|b_{nh} - \widehat{b}\|_{L^2}\|\widehat{a}\|_{L^2},\end{aligned}$$

where the first term on the last line is zero since $\vec{u}_n$, $\vec{u}^*_n \in \widehat{\mathcal{U}} + \vec{U}_n$ and the last two terms tend to zero as $n \to \infty$ by (8) and (13), respectively. This leads to $\int_\Omega \widehat{y}\,\mathrm{d}x \in \mathcal{S}$.

9. By the definition of $r_{\alpha\beta}(a_{nh})$ and b_{nih} we obtain for all $(\alpha, \beta) \in \mathcal{R}$,

$$\begin{aligned}\widehat{a}^{-\alpha} r_{\alpha\beta}(a_{nh}) &= \Big(\prod_{i=1}^m(\lambda_n b_{nih} + 1)^{\alpha_i} - \prod_{i=1}^m(\lambda_n b_{nih} + 1)^{\beta_i}\Big)^2 \\ &= \Big(\lambda_n\sum_{i=1}^m b_{nih}(\alpha_i - \beta_i)\Big)^2 + Q_n,\end{aligned} \tag{14}$$

where

$$|Q_n| \le c\lambda_n^3(|b_{nh}|+1)^{p_0} \qquad \text{with} \qquad 0 \le p_0 \le 2 \max_{(\alpha,\beta)\in\mathcal{R}} \max\Big\{\sum_{i=1}^m \alpha_i, \sum_{i=1}^m \beta_i\Big\}.$$

(A1) ensures $p_0 \le 6$ if $N=3$. Since $\lambda_n \to 0$ as $n \to \infty$ (see (11)), we find

$$\frac{1}{\lambda_n^2}\|Q_n\|_{L^1} \le c\lambda_n \int_\Omega (|b_{nh}|+1)^{p_0}\,\mathrm{d}x \to 0 \text{ as } n \to \infty.$$

This together with (12) and (14) gives

$$\lim_{n\to\infty} \int_\Omega b_{\alpha\beta h}\Big(\sum_{i=1}^m b_{nih}(\alpha_i-\beta_i)\Big)^2\,\mathrm{d}x = 0 \quad \forall(\alpha,\beta)\in\mathcal{R}.$$

Therefore, from (A1) we conclude $\widehat{b} = (\widehat{b}_1,\dots,\widehat{b}_m) \in \mathcal{S}^\perp$. This together with the definition of $\widehat{y}$ and $\int_\Omega \widehat{y}\,\mathrm{d}x \in \mathcal{S}$ (see Step 8) leads to

$$\widehat{b}\cdot\int_\Omega \widehat{y}\,\mathrm{d}x = \sum_{i=1}^m \int_\Omega 2u_i^*\widehat{b}_i^2\,\mathrm{d}x = 0$$

which ensures $\widehat{b}=0$ and $\widehat{y}=0$.

10. Using the definition of λ_n (see (11)), (3), $b_{nih}\to 0$ in $L^4(\Omega)$ and (8) we find

$$\begin{aligned}
1 &= \tfrac{1}{\lambda_n^2}\Big(\widehat{F}(\vec{u}_n)-\widehat{F}(\vec{u}_n^*)\Big) \le c\sum_{i=1}^m \|\overline{u}_{nih}\|_{L^\infty}\|\tfrac{a_{nih}-\widehat{a}_i}{\lambda_n}\|_{L^2}^2 \\
&\le c\sum_{i=1}^m \int_\Omega \tfrac{(\sqrt{a_{nih}}-\sqrt{\widehat{a}_i})^2}{\lambda_n^2}\Big(\sqrt{a_{nih}}+\sqrt{\widehat{a}_i}\Big)^2\,\mathrm{d}x \le c\sum_{i=1}^m b_{nih}^2\widehat{a}_i\Big(\widehat{a}_i+|\sqrt{a_{nih}}-\sqrt{\widehat{a}_i}|^2\Big)\,\mathrm{d}x \\
&\le c\sum_{i=1}^m \|b_{nih}\|_{L^4}^2\Big(1+\|\sqrt{a_{nih}}-\sqrt{\widehat{a}_i}\|_{L^4}^2\Big) \to 0.
\end{aligned}$$

This contradiction shows that the assumption made at the beginning of Step 2 of the proof was wrong, i.e., (4) holds, and the proof is complete. □

3 Conclusions

Since $\widehat{F}(\vec{U})-\widehat{F}(\vec{u}^*) \le c(U,u^*,\overline{u}) =: \rho$ uniformly for all discretizations we have $\vec{v}(t_n)\in\widehat{\mathcal{N}}_\rho$ for $n\ge 1$ for solutions $(\vec{u},\vec{v})$ to $(\mathrm{P}_\mathcal{M})$. Following the proof of [4, Theorem 3.3], but now using the improved result of our Theorem 1, we can choose in step 3 of that proof one $\lambda>0$ such that $\lambda \mathrm{e}^{\lambda\tau}c_\rho < 1$ uniform for all $\mathcal{M}$, see (A2), too. Especially we do not have any upper restriction on the mesh size, can use admissible finite volume meshes, and obtain

Theorem 3.1 *We assume* (A1) *and* (A2)*. Then there exists a universal* $\lambda > 0$ *such that for all solutions* $(\vec{u}, \vec{v})$ *to* $(\mathrm{P}_{\mathcal{M}})$ *the estimate*

$$\widehat{F}(\vec{u}(t_n)) - \widehat{F}(\vec{u}^*) \leq \mathrm{e}^{-\lambda t_n}\big(\widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*)\big) \quad \forall n \geq 1$$

holds uniformly for all discretizations, especially the scheme $(\mathrm{P}_{\mathcal{M}})$ *is dissipative.*

Theorem 2 (as discrete version of [6, Theorem 4.3]) enables us to provide uniform positive lower bounds for the particle densities for the solutions of $(\mathrm{P}_{\mathcal{M}})$ if the order of all reactions is less or equal to two and $N = 2$, see [3, Lemma 4, Theorem 4].

Acknowledgment The authors were partially supported by the European Commission within the 7th Framework Programme MD^3 "Material Development for Double Exposure and Double Patterning" and by the DFG Research Center MATHEON *Mathematics for Key Technologies* within the project D22 "Modeling of Electronic Properties of Interfaces in Solar Cells".

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