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Energy estimates for space and time discretized electro-reaction-diffusion systems

Outline

- ▷ Model equations
- ▷ Weak formulation and energy functionals
- ▷ Energy estimates for the continuous problem
- ▷ Results for discrete time problems
- ▷ Results for space and time discrete problems

Model equations

X_i	species, $i = 1, \dots, m$	$\zeta_i = v_i + q_i v_0$	electrochemical potentials
v_i	chemical potentials	$u_i = \overline{u}_i \mathrm{e}^{v_i}$	densities
q_i	charge numbers	$\overline{u}_i$	reference densities
v_0	electrostatic potential	$u_0 = \sum_{i=1}^m q_i u_i$	charge density

reversible reactions of mass action type

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m, \quad (\alpha, \beta) \in \mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$$

net rate $\quad k_{\alpha\beta}(\mathrm{e}^{\zeta\cdot\alpha} - \mathrm{e}^{\zeta\cdot\beta}), \quad \zeta = (\zeta_1, \dots, \zeta_m)$

net production rate of species X_i

$$R_i := \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\mathrm{e}^{\zeta\cdot\alpha} - \mathrm{e}^{\zeta\cdot\beta})(\beta_i - \alpha_i)$$

stoichiometric subspace $\quad \mathcal{S} := \mathrm{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}\}$

Model equations

anisotropies

- mass fluxes $j_i = -u_i \mathbf{S}_i(\cdot)\nabla\zeta_i, \quad i = 1,\dots,m,$

$$\mathbf{S}_i(x) = Q_i^T(x)\text{diag}\big(\mu_i^1(x), \mu_i^2(x)\big)Q_i(x) \quad \text{(Lades/Wachutka'97)}$$

- dielectric permittivity matrix $\mathbf{S}_0(x) = Q_0^T(x)\text{diag}(\varepsilon^1(x), \varepsilon^2(x))Q_0(x),$

continuity equations

$$\frac{\partial u_i}{\partial t} + \nabla\cdot j_i = R_i \text{ in } \mathbb{R}_+ \times \Omega, \quad \nu\cdot j_i = 0 \text{ on } \mathbb{R}_+ \times \Gamma,$$

$$u_i(0) = U_i \text{ in } \Omega, \quad i = 1,\dots,m.$$

Poisson equation

$$-\nabla\cdot(\mathbf{S}_0\nabla v_0) = f + \sum_{i=1}^m q_i u_i \quad \text{in } \mathbb{R}_+ \times \Omega, \quad \nu\cdot(\mathbf{S}_0 v_0) + \tau v_0 = f^\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma,$$

Assumptions (A)

$\Omega \subset \mathbb{R}^2$ bounded Lipschitzian domain, $\Gamma = \partial\Omega$;

$f \in L^\infty(\Omega),\ f^\Gamma \in L^\infty(\Gamma),\ \tau \in L^\infty_+(\Gamma),\ \int_\Gamma \tau \, \mathrm{d}\Gamma > 0,$
$\varepsilon^k \in L^\infty_+(\Omega),$ ess $\inf_\Omega \varepsilon^k \geq \delta,\ k = 1, 2;$

$\mu_i^k \in L^\infty_+(\Omega),$ ess $\inf_\Omega \mu_i^k \geq \delta,\ k = 1, 2,\ i = 1, \ldots, m;$

$\overline{u}_i \in L^\infty_+(\Omega),\ \overline{u}_i \geq \delta, U_i \in L^\infty_+(\Omega),\ q_i \in \mathbb{Z},\ i = 1, \ldots, m;$

$\mathcal{R} \subset \mathbb{Z}^m_+ \times \mathbb{Z}^m_+$ finite subset, $k_{\alpha\beta} \in L^\infty_+(\Omega),\ \int_\Omega k_{\alpha\beta} \, \mathrm{d}x > 0$ for $(\alpha, \beta) \in \mathcal{R}$,
$\int_\Omega \sum_{i=1}^m U_i \kappa_i \, \mathrm{d}x > 0 \quad \forall \kappa \in \mathcal{S}^\perp,\ \kappa \geq 0,\ \kappa \neq 0,$
there are no “false” equilibria in the sense of Prigogin & Defay’54.

Weak formulation

$$v = (v_0, \dots, v_m) \in V = H^1(\Omega; \mathbb{R}^{m+1}), \quad u = (u_0, \dots, u_m) \in V^*$$

operators:

$A: V \cap L^\infty(\Omega, \mathbb{R}^{m+1}) \to V^*$, $E = (E_0, \dots, E_m): V \to V^*$

$$\langle A\, v, \overline{v} \rangle_V := \int_\Omega \Big\{ \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i} \mathbf{S}_i \nabla \zeta_i \cdot \nabla \overline{\zeta}_i + \sum_{(\alpha,\, \beta) \in \mathcal{R}} k_{\alpha\beta} \Big(\mathrm{e}^{\alpha \cdot \zeta} - \mathrm{e}^{\beta \cdot \zeta} \Big) (\alpha - \beta) \cdot \overline{\zeta} \Big\} \, \mathrm{d}x$$

$$\langle E v, \overline{v} \rangle_V := \langle E_0 v_0, \overline{v}_0 \rangle + \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i} \overline{v}_i \, \mathrm{d}x, \quad \overline{v} \in V,$$

$$\langle E_0 v_0, \overline{v}_0 \rangle_{H^1} := \int_\Omega (\mathbf{S}_0 \nabla v_0 \cdot \nabla \overline{v}_0 - f v_0) \, \mathrm{d}x + \int_\Gamma (\tau v_0 - f^\Gamma) \overline{v}_0 \, \mathrm{d}\Gamma$$

Weak formulation

Problem (P)

$$\left.\begin{array}{l} u'(t) + Av(t) = 0,\ u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+,\ \ u(0) = U, \\ u \in H^1_{\mathrm{loc}}(\mathbb{R}_+; V^*),\ v \in L^2_{\mathrm{loc}}(\mathbb{R}_+; V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+; L^\infty(\Omega)^{m+1}) \end{array}\right\} \qquad \text{(P)}$$

dissipation rate

$$\begin{aligned} D(v) :=& \langle Av, v\rangle \\ =& \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i}\, \mathbf{S}_i\, \nabla\zeta_i \cdot \nabla\zeta_i \, \mathrm{d}x \\ &+ \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(e^{\zeta\cdot\alpha} - e^{\zeta\cdot\beta})(\alpha-\beta)\cdot\zeta \, \mathrm{d}x \end{aligned}$$

$$D(v) \geq 0 \quad \forall v \in V \cap L^\infty(\Omega, \mathbb{R}^{m+1})$$

Energy functionals

E strictly monotone potential operator, $Ev = \partial G(v)$, $G : V \to \mathbb{R}$,

$$G(v) = \int_\Omega \Big\{ \sum_{i=1}^{m} \overline{u}_i(\mathrm{e}^{v_i} - 1) + \frac{1}{2}\mathbf{S}_0 \nabla v_0 \cdot \nabla v_0 - f v_0 \Big\} \,\mathrm{d}x + \int_\Gamma (\frac{\tau}{2}\, v_0^2 - f^\Gamma v_0) \,\mathrm{d}\Gamma$$

free energy $F : V^* \to \overline{\mathbb{R}}$, $F(u) := G^*(u) = \sup_{v \in V} \Big\{ \langle u, v \rangle - G(v) \Big\}$

G, F proper, convex, lower semi-continuous, $u \in H^1(\Omega)^* \times L^2_+(\Omega, \mathbb{R}^m) \Longrightarrow$

$$F(u) = \int_\Omega \Big\{ \sum_{i=1}^{m} \big(u_i(\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i\big) + \frac{1}{2}\mathbf{S}_0 \nabla v_0 \cdot \nabla v_0 \Big\} \,\mathrm{d}x + \int_\Gamma \frac{\tau}{2}\, v_0^2 \,\mathrm{d}\Gamma$$

where $u_0 = E_0 v_0$

Results for the continuous problem (G./Hünlich'97, G./Gärtner'07)

- Invariants: (u, v) solution to (P) $\Longrightarrow \quad u(t) - U \in \mathcal{U} \quad \forall\, t > 0$ where

$$\mathcal{U} := \Big\{ u \in V^* : \ u_0 = \sum_{i=1}^{m} q_i u_i, \ (\langle u_1, 1\rangle, \ldots, \langle u_m, 1\rangle) \in \mathcal{S} \Big\}.$$

- Thermodynamic equilibrium: There exists a unique solution (u^*, v^*) to

$$Av^* = 0, \quad u^* = Ev^*, \quad u^* - U \in \mathcal{U}. \qquad \text{(S)}$$

It holds $v^* \in V \cap L^\infty(\Omega)^{m+1}$, $\nabla\zeta^* = 0$ and $\zeta^* \in \mathcal{S}^\perp$.

- Monotone decay of the free energy: Let (u, v) be a solution to Problem (P). Then

$$F(u(t_2)) \le F(u(t_1)) \le F(U) \quad \text{for } t_2 \ge t_1 \ge 0.$$

Results for the continuous problem (G./Hünlich'97, G./Gärtner'07)

- Exponential decay of the free energy: Let (u,v) be a solution to Problem (P), and let (u^*,v^*) be the thermodynamic equilibrium. Then there exists a constant $\lambda > 0$ such that

$$F(u(t)) - F(u^*) \le \mathrm{e}^{-\lambda t}(F(U) - F(u^*)) \quad \forall\, t \ge 0.$$

- Nonlinear Poincaré type inequality: Let (u^*,v^*) be the thermodynamic equilibrium. Then for every $\rho > 0$ there exists a constant $c_\rho > 0$ such that

$$F(u) - F(u^*) \le c_\rho D(v) \qquad \forall v \in \mathcal{N}_\rho$$

where

$$\mathcal{N}_\rho = \{v \in V :\; Ev - U \in \mathcal{U},\; F(Ev) - F(u^*) \le \rho\}.$$

Results for discrete time problems

(B) $\mathcal{Z} = \{0, t_1, \ldots, t_n, \ldots\}$ partition of $\mathbb{R}_+$, $t_n \in \mathbb{R}_+,\ t_{n-1} < t_n,\ n \in \mathbb{N},$

$t_n \to \infty$ as $n \to \infty,\ h_n = t_n - t_{n-1},\ \sup_{n\in\mathbb{N}} h_n < \infty$

Monotone and exponential decay of the free energy: Let (u^*, v^*) be the thermodynamic equilibrium. Then the fully implicit time discretization scheme

$$u(t_n) - u(t_{n-1}) + h_n A v(t_n) = 0, \quad u(t_n) = E v(t_n), \quad n \geq 1,$$
$$u(0) = U, \quad v(t_n) \in V, \quad n \geq 0$$

is dissipative. Moreover, there exists a constant $\lambda > 0$ such that

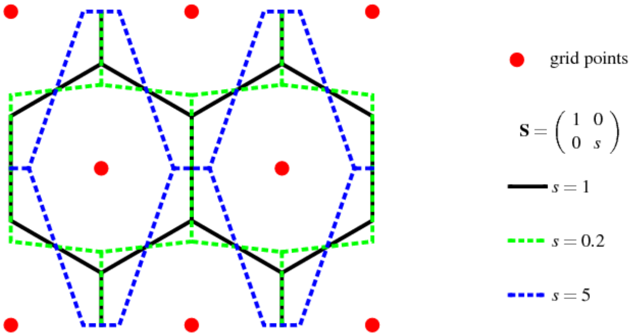
$$F\big(u(t_n)\big) - F(u^*) \leq \mathrm{e}^{-\lambda t_n}\big(F(U) - F(u^*)\big) \quad \forall n \geq 1.$$

Space and time discretized problems

fixed set of grid points x^k, $k \in K$, for each species anisotropic Voronoi boxes

$$V_i^k = \{x \in \overline{\Omega} : \ d_i(x, x^k) \leq d_i(x, x^l) \quad \forall l \in K\}, \ i = 0, \ldots, m, \ k \in K$$

$$d_i(x, y)^2 := (x - y)^T \mathbf{S}_i^{-1} (x - y)$$



Space and time discretized problems

(C) $\overline{u}_i = \text{const},\ i = 1, \dots, m,\ k_{\alpha\beta} = \text{const}\ (\alpha, \beta) \in \mathcal{R},\ \tau = \text{const}$

$\mathbf{S}_i$ constant, symmetric, positive definite 2×2 matrices

- u_i^k mass of species X_i in V_i^k, $U_i^k = \int_{V_i^k} U_i \, \mathrm{d}x, \quad k \in K, i = 1, \dots, m$

$$u_0^k = \sum_{i=1}^m q_i \sum_{l \in K} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} u_i^l, \quad U_0^k = \dots, \quad k \in K$$

- potentials $v_0^k,\ v_i^k,\ \zeta_i^k$ associated to grid points x^k

$$\zeta_i^k = v_i^k + q_i \sum_{l \in K} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l, \quad i = 1, \dots, m$$

- discrete state equations $\quad u_i^k = \overline{u}_i \mathrm{e}^{v_i^k} |V_i^k|, \quad k \in K,\ i = 1, \dots, m$
- notation $\quad \vec{u}_i = (u_i^k)_{k \in K}, \quad \vec{v}_i = (v_i^k)_{k \in K}$

Space and time discretized problems

discretized Poisson equation

$$-\sum_{l\in K}\frac{v_0^l-v_0^k}{|x^l-x^k|}|\mathbf{S}_0\nu_0^{kl}||\partial V_0^k\cap\partial V_0^l|+\tau v_0^k|\partial V_0^k\cap\Gamma|-f^k=u_0^k,\quad k\in K,$$

where

$$f^k=\int_{V_0^k}f\,\mathrm{d}x+\int_{\partial V_0^k\cap\Gamma}f^\Gamma\,\mathrm{d}\Gamma,$$

$$u_0^k=\sum_{i=1}^m q_i\sum_{l\in K}\frac{|V_0^k\cap V_i^l|}{|V_i^l|}u_i^l,$$

ν_0^{kl} outer unit normal of V_0^k on $\partial V_0^k\cap\partial V_0^l$,

$$\vec{v}_0=(v_0^k)_{k\in K},\ \vec{f}=(f^k)_{k\in K},\ \vec{u}_0=(u_0^k)_{k\in K}$$

discretized Poisson equation reads as $\quad P\vec{v}_0-\vec{f}=\vec{u}_0$

Space and time discretized problems

Discretization scheme

$$\left.\begin{aligned} &P\vec{v}_0(t_n) - \vec{f} = \vec{u}_0(t_n), \quad n \geq 0, \\ &\frac{u_i^k(t_n)-u_i^k(t_{n-1})}{h_n} = -\sum_{l\in K} J_i^{kl}(t_n)|\partial V_i^k \cap \partial V_i^l| + R_i^k(t_n), \\ &k \in K,\ n \geq 1,\ i = 1,\dots,m, \\ &u_i^k(0) = U_i^k, \quad k \in K,\ i = 0,\dots,m. \end{aligned}\right\} \qquad \text{(PD)}$$

discretized fluxes

$$J_i^{kl} = -\overline{u}_i\, Z_i^{kl}\, \frac{\zeta_i^l - \zeta_i^k}{|x^l - x^k|}\, |\mathbf{S}_i \nu_i^{kl}|, \qquad Z_i^{kl} = \frac{1}{2}(\mathrm{e}^{v_i^k} + \mathrm{e}^{v_i^l})$$

source terms from reactions

$$R_i^k = \sum_{\alpha,\beta\in\mathcal{R}} (\beta_i - \alpha_i) \sum_{k_1\in K} \cdots \sum_{k_{i-1}\in K} \sum_{k_{i+1}\in K} \cdots \sum_{k_m\in K} R_{\alpha\beta}[\zeta_1^{k_1},\dots,\zeta_{i-1}^{k_{i-1}},\zeta_i^k,\zeta_{i+1}^{k_{i+1}},\dots,\zeta_m^{k_m}]$$
$$\times\, |V_1^{k_1} \cap \dots \cap V_{i-1}^{k_{i-1}} \cap V_i^k \cap V_{i+1}^{k_{i+1}} \cap \dots \cap V_m^{k_m}|,$$

$$R_{\alpha\beta}[\zeta_1^{k_1},\dots,\zeta_m^{k_m}] = k_{\alpha\beta}\left(\mathrm{e}^{\sum_{i=1}^m \alpha_i \zeta_i^{k_i}} - \mathrm{e}^{\sum_{i=1}^m \beta_i \zeta_i^{k_i}}\right)$$

Discrete energy functionals

discrete version of E $\quad \widehat{E}\colon \mathbb{R}^{M(m+1)} \to \mathbb{R}^{M(m+1)}$, $\qquad (M = \#K)$

$$\widehat{E}\vec{v} = \Big(P\vec{v}_0 - \vec{f}, \Big(\big(\overline{u}_i \mathrm{e}^{v_i^k}|V_i^k|\big)_{k\in K}\Big)_{i=1,\dots,m}\Big)$$

corresponding discrete potential $\widehat{G}\colon \mathbb{R}^{M(m+1)} \to \mathbb{R}$,

$$\widehat{G}(\vec{v}) = \frac{1}{2}(P\vec{v}_0, \vec{v}_0) - (\vec{f}, \vec{v}_0) + \sum_{i=1}^{m}\sum_{k\in K} \overline{u}_i |V_i^k| (\mathrm{e}^{v_i^k} - 1)$$

discrete free energy $\widehat{F}$ as conjugate functional

$$\widehat{F}(\vec{u}) = \sup_{\vec{v}\in\mathbb{R}^{M(m+1)}} \big\{(\vec{u}, \vec{v}) - \widehat{G}(\vec{v})\big\}$$

Invariants and steady states

$$\widehat{\mathcal{U}} = \Big\{\vec{u} \in \mathbb{R}^{M(m+1)} : u_0^k = \sum_{i=1}^{m} q_i \sum_{l\in K} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} u_i^l,\ k \in K,\ \big(\sum_{k\in K} u_1^k, \ldots, \sum_{k\in K} u_m^k\big) \in \mathcal{S}\Big\}$$

Invariants: $(\vec{u}, \vec{v})$ solution to the discretized problem (PD) $\Longrightarrow$

$$\vec{u}(t_n) - \vec{U} \in \widehat{\mathcal{U}} \quad \forall n \in \mathbb{N}$$

Discretized stationary problem

$$\left.\begin{aligned} &\textstyle\sum_{l\in K} J_i^{kl} |\partial V_i^k \cap \partial V_i^l| - R_i^k = 0,\ k \in K,\ i = 1, \ldots, m, \\ &\vec{u} = \widehat{E}\vec{v}, \quad \vec{u} - \vec{U} \in \widehat{\mathcal{U}}. \end{aligned}\right\} \qquad \text{(SD)}$$

Steady states of the discretized problem

Theorem 1. [Thermodynamic equilibrium] (Glitzky'08)
We assume (A) and (C). Then there is a unique solution $(\vec{u}^*, \vec{v}^*)$ to Problem (SD). This solution satisfies $\vec{v}^* \in \widehat{\mathcal{U}}^\perp$.

Idea of the proof

- introduce $\widehat{G}_0 : \mathbb{R}^{M(m+1)} \to \overline{\mathbb{R}}$,

$$\widehat{G}_0(\vec{v}) := \widehat{G}(\vec{v}) + I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) - \langle \vec{U}, \vec{v} \rangle, \quad \vec{v} \in \mathbb{R}^{M(m+1)},$$

  ($I_{\widehat{\mathcal{U}}^\perp}$characteristic function of $\widehat{\mathcal{U}}^\perp$). $\widehat{G}_0$ is proper, lower semicontinuous, and strictly convex, Moreau-Rockafellar theorem $\Longrightarrow$

$$\partial \widehat{G}_0(\vec{v}) = \widehat{E}\vec{v} + \partial I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) - \vec{U}, \quad \vec{v} \in \mathbb{R}^{M(m+1)}.$$

- If $(\vec{u}, \vec{v})$ is a solution to (SD) then $\vec{v}$ is the unique minimizer of $\widehat{G}_0$. If $\vec{v}$ is a minimizer of $\widehat{G}_0$ then $(\widehat{E}\vec{v}, \vec{v})$ is a solution to (SD).
- suffices to show that $\widehat{G}_0(\vec{v}) \to \infty$ if $\|\vec{v}\| \to \infty$ (indirect proof).

Discrete Poincaré like inequality

Theorem 2. [Estimate of the free energy by the dissipation rate] (Glitzky'08)
Let (A) and (C) be fulfilled. Moreover, let $(\vec{u}^*, \vec{v}^*)$ be the thermodynamic equilibrium according to Theorem 1. Then for every $\rho > 0$ there exists a constant $c_\rho > 0$ such that

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

for all $\vec{v} \in \widehat{\mathcal{N}}_\rho := \Big\{ \vec{v} \in \mathbb{R}^{M(m+1)} : \ \widehat{F}(\widehat{E}\vec{v}) - \widehat{F}(\vec{u}^*) \le \rho, \ \vec{u} = \widehat{E}\vec{v} \in \vec{U} + \widehat{\mathcal{U}} \Big\}$.

$$\widehat{D}(\vec{v}) = \sum_{i=1}^{m} \sum_{k,l \in K,\, l<k} \overline{u}_i \, Z_i^{kl} \frac{(\zeta_i^l - \zeta_i^k)^2}{|x^l - x^k|} |\mathbf{S}_i \nu_i^{kl}| |\partial V_i^k \cap \partial V_i^l|$$

$$+ \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{k_1 \in K} \cdots \sum_{k_m \in K} R_{\alpha\beta}\big[\zeta_1^{k_1}, \dots, \zeta_m^{k_m}\big] \sum_{i=1}^{m} (\alpha_i - \beta_i) \zeta_i^{k_i} \, |V_1^{k_1} \cap \dots \cap V_m^{k_m}| \ge 0.$$

Energy estimates for (PD)

Theorem 3. [Monotone and exponential decay of the free energy] (Glitzky'08)
We assume (A), (B) and (C). Then the (fully implicit in time) discretization scheme (PD) is dissipative, i.e. solutions $(\vec{u}, \vec{v})$ to (PD) fulfil

$$\widehat{F}(\vec{u}(t_{n_2})) \le \widehat{F}(\vec{u}(t_{n_1})) \le \widehat{F}(\vec{U}) \quad \text{for all } t_{n_1} < t_{n_2}.$$

Moreover, there exists a $\lambda > 0$ such that

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

Proof

- $\widehat{F} : \mathbb{R}^{M(m+1)} \to \overline{\mathbb{R}}$ is convex, lower semicontinuous, differentiable in arguments $\vec{u}$ with $\vec{u}_i > 0$, $i = 1, \dots, m$. If $\vec{u} = \widehat{E}\vec{v} \Longrightarrow$
  $\vec{u} = \widehat{G}'(\vec{v}), \quad \vec{v} = \widehat{F}'(\vec{u}), \quad \widehat{F}(\vec{u}) - \widehat{F}(\vec{w}) \le \widehat{F}'(\vec{u}) \cdot (\vec{u} - \vec{w}) \quad \forall \vec{w} \in \mathbb{R}^{M(m+1)}$
- $\widehat{F}(u(\vec{t_l})) - \widehat{F}(\vec{u}(t_{l-1})) \le \big(\vec{u}(t_l) - \vec{u}(t_{l-1})\big) \cdot \vec{v}(t_l) = \sum_{i=1}^{m} \sum_{k \in K} \big(u_i^k(t_l) - u_i^k(t_{l-1})\big)\zeta_i^k$

Proof of Theorem 3

- let $n_2 > n_1 \geq 0$, $\lambda \geq 0$

$$
\begin{aligned}
&\mathrm{e}^{\lambda t_{n_2}}\left(\widehat{F}(\vec{u}(t_{n_2})) - \widehat{F}(\vec{u}^*)\right) - \mathrm{e}^{\lambda t_{n_1}}\left(\widehat{F}(\vec{u}(t_{n_1})) - \widehat{F}(\vec{u}^*)\right) \\
&\quad = \sum_{l=n_1+1}^{n_2} \mathrm{e}^{\lambda t_l}\left(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*)\right) - \mathrm{e}^{\lambda t_{l-1}}\left(\widehat{F}(\vec{u}(t_{l-1})) - \widehat{F}(\vec{u}^*)\right) \\
&\quad = \sum_{l=n_1+1}^{n_2} \mathrm{e}^{\lambda t_{l-1}}\Big\{(\mathrm{e}^{\lambda h_l} - 1)\big(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*)\big) + \big(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}(t_{l-1}))\big)\Big\} \\
&\quad \leq \sum_{l=n_1+1}^{n_2} \mathrm{e}^{\lambda t_{l-1}}\Big\{\mathrm{e}^{\lambda h_l}\lambda h_l\big(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*)\big) + \langle \vec{u}(t_l) - \vec{u}(t_{l-1}), \vec{v}(t_l)\rangle\Big\} \\
&\quad \leq \sum_{l=n_1+1}^{n_2} h_l\, \mathrm{e}^{\lambda t_{l-1}}\Big\{\mathrm{e}^{\lambda h_l}\lambda\big(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*)\big) - \widehat{D}(\vec{v}(t_l))\Big\}
\end{aligned}
$$

Proof of Theorem 3

- $\widehat{D}(\vec{v}(t_l)) \geq 0 \quad \forall l \geq 1,$ setting $\lambda = 0 \Longrightarrow$

$$\widehat{F}(\vec{u}(t_{n_2})) \leq \widehat{F}(\vec{u}(t_{n_1})) \leq \widehat{F}(\vec{U}) \quad \forall t_{n_2} > t_{n_1} \geq 0$$

- $\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*) \leq \widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*) =: \rho, \quad \vec{u}(t_l) = \widehat{E}\vec{v}(t_l) \in \vec{U} + \widehat{\mathcal{U}}, l \geq 1 \quad \Longrightarrow$ $\vec{v}(t_l) \in \widehat{N}_\rho$, $l \geq 1$, and Theorem 2 supplies $c_\rho > 0$ s.t.

$$\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*) \leq c_\rho \widehat{D}(\vec{v}(t_l)) \quad \forall l$$

- choose $\lambda > 0$ such that $\lambda e^{\lambda \bar{h}} c_\rho < 1$, $n_1 = 0$

□

Theorem 2: very short sketch of the proof

- $$c_1\left(\|\vec{v}_0-\vec{v}_0^*\|^2+\sum_{i=1}^{m}\sum_{k\in K}|\sqrt{u_i^k}-\sqrt{u_i^{*k}}|^2\right)\le \widehat{F}(\vec{u})-\widehat{F}(\vec{u}^*)$$
$$\le c_2\left(\|\vec{v}_0-\vec{v}_0^*\|^2+\sum_{i=1}^{m}\sum_{k\in K}|u_i^k-u_i^{*k}|^2\right)$$

- indirect proof: assume sequences $\vec{v}_n\in\mathcal{N}_\rho$, $C_n\to+\infty$ such that
$$\vec{u}_n=\widehat{E}\vec{v}_n,\quad \rho\ge\widehat{F}(\vec{u}_n)-\widehat{F}(\vec{u}^*)=C_n\widehat{D}(\vec{v}_n)$$

- derive convergence properties for subsequences of $\vec{u}_n$, $\vec{v}_{n0}$, $a_{ni}^k=\mathrm{e}^{\zeta_{ni}^k}$

Theorem 2: very short sketch of the proof

- for subsequences, $v_{n0}^k \to v_0^k, \quad a_{ni}^k \to a_i^k = a_i,\, k \in K, \quad a^\alpha = a^\beta\ \forall(\alpha,\beta) \in \mathcal{R},$ $\vec{u}_n \to \vec{u}, \quad P\vec{v}_0 - \vec{f} = \vec{u}_0, \quad \vec{u} - \vec{U} \in \widehat{\mathcal{U}}$
- (a, v_0) characterizes equilibrium, exist no "false" equilibria $\Longrightarrow a_i > 0,\ i = 1, ..., m,$ define

$$\zeta_i := \ln a_i, \quad v_i^k = \zeta_i - q_i \sum_{l\in K} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l,\ k \in K,\ i = 1, \dots, m,$$

$\Longrightarrow (\vec{u}, \vec{v}) = (\vec{u}^*, \vec{v}^*)$ thermodynamic equilibrium

- $\lambda_n^2 := \widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*)$

$$\frac{1}{\lambda_n}\Big(\sqrt{\frac{a_{ni}^k}{a_i^*}} - 1\Big) \to 0,\ k \in K, \quad \frac{\vec{u}_n - \vec{u}^*}{\lambda_n} \to 0, \quad \frac{\vec{v}_{n0} - \vec{v}_0^*}{\lambda_n} \to 0$$

- $1 = \dfrac{\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*)}{\lambda_n^2} \le c_2\Big(\Big\|\dfrac{\vec{v}_{n0} - \vec{v}_0^*}{\lambda_n}\Big\|^2 + \sum_{i=1}^m \sum_{k\in K} \Big|\dfrac{\vec{u}_{ni}^k - \vec{u}_i^{*k}}{\lambda_n}\Big|^2\Big) \to 0$ contradiction

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