A finite-volume approximation for a degenerate Keller-Segel system

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International Workshop on Mathematical Fluid Dynamics
Waseda University March 11, 2010

Keller-Segel system (E. F. Keller & L. A. Segel 1970)

$$\begin{cases} u_t = \nabla \cdot (D_u \nabla u - u \nabla g(v)) & \text{in} \quad \Omega \times (0, T), \\ k v_t = D_v \Delta v + k_1 v - k_2 u & \text{in} \quad \Omega \times (0, T), \\ \dfrac{\partial u}{\partial \nu} = 0, \quad \dfrac{\partial v}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0, T), \\ u\big|_{t=0} = u_0, \quad v\big|_{t=0} = v_0 & \text{on} \quad \Omega \end{cases} \tag{KS}$$

- Ω: bounded domain in $\mathbb{R}^d$ $(d = 2, 3)$
- Mathematical model for aggregation phenomenon of slime molds resulting from their chemotactic features
  - u density of the cellular slime molds;
  - v concentration of the chemical substance secreted by molds;
  - D_u, D_v diffusion coefficients, k relaxation time (≥ 0) and $k_1 v - k_2 u$ ratio of generation/extinction.
  - $g(v)$ sensitive function ($g : \mathbb{R} \to \mathbb{R}$ smooth and non-deceasing),
- Conservation laws: positivity and total mass; $\|u(t)\|_{L^1} = \|u_0\|_{L^1}$.
- The solution may blow up. (It depends on $\|u_0\|_{L^1}$ and d.)

Degenerate Keller-Segel system

$$\begin{cases} u_t = \nabla \cdot (\nabla f(u) - u \nabla g(v)) & \text{in} \quad \Omega \times (0, T), \\ k v_t = D_v \Delta v + k_1 v - k_2 u & \text{in} \quad \Omega \times (0, T), \\ \dfrac{\partial}{\partial \nu} f(u) - u \dfrac{\partial}{\partial \nu} g(v) = 0, \quad \dfrac{\partial v}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0, T), \\ u\big|_{t=0} = u_0, \quad v\big|_{t=0} = v_0 & \text{on} \quad \Omega \end{cases} \tag{DKS}$$

- $f : \mathbb{R} \to \mathbb{R}$, non-decreasing, continuous, $f(0) = 0$,
- See Sugiyama (2005, 2006, 2007) and Sugiyama & Kunii (2006) for the definition of weak solutions and the wellposedness.

Contents

§1. Remark on the positivity conservation for convection-diffusion equations

Convection-diffusion equation in S^1

Model problem: $u(x,t),\ b(x,t) \geq 0$: 1-periodic functions in x

$$u_t = u_{xx} - (b(x,t)u)_x \qquad (x \in [0,1),\ 0 < t < T)$$

Positivity $u(x,0) \geq 0, \not\equiv 0 \quad \Rightarrow \quad u(x,t) > 0\ (t > 0)$

Finite difference method:

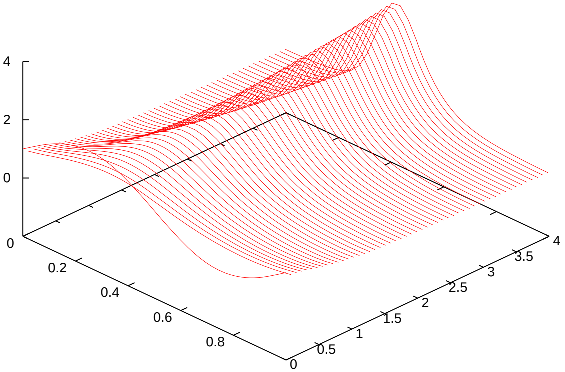
- $x_i = ih\ (h = 1/N)$, $t_n = \tau_1 + \tau_2 + \cdots + \tau_n$: Grid points;
- $b_i^n = b(x_i, t_n)$;
- $u_i^n \approx u(x_i, t_n)$: finite difference approximation.

forward Euler = central difference + central difference

$$\frac{u_i^n - u_i^{n-1}}{\tau_n} = \frac{u_{i-1}^{n-1} - 2u_i^{n-1} + u_{i+1}^{n-1}}{h^2} - \frac{b_{i+1}^{n-1}u_{i+1}^{n-1} - b_{i-1}^{n-1}u_{i-1}^{n-1}}{2h}$$

Numerical example

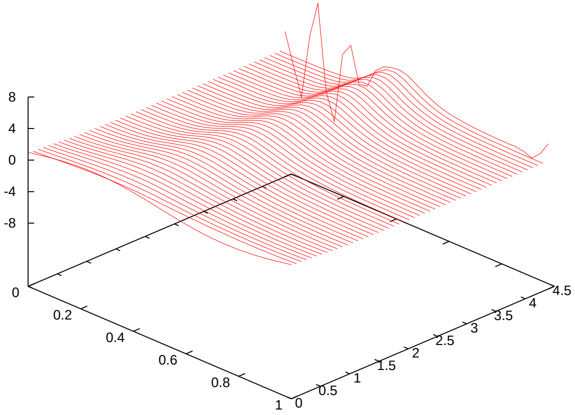
$$b(x,t) = 4(1+\cos 2\pi x)(1+t)^2, \; h = 2^{-5}, \; \tau_j = 0.4 \cdot h^2$$



$$0 \le t_n \le 4.0$$

Numerical example

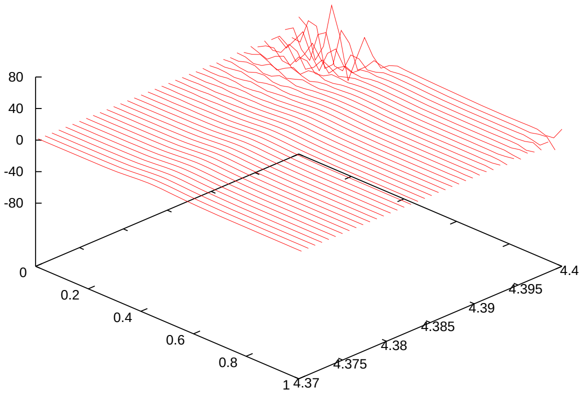
$$b(x,t) = 4(1+\cos 2\pi x)(1+t)^2\text{,}\;\; h = 2^{-5}\text{,}\;\; \tau_j = 0.4\cdot h^2$$



$$0 \le t_n \le 4.4$$

Numerical example

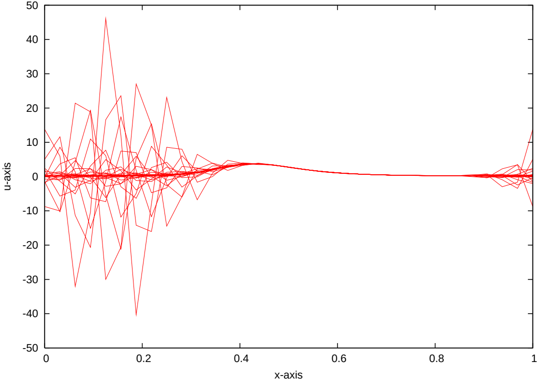
$$b(x,t) = 4(1+\cos 2\pi x)(1+t)^2\,,\;\; h = 2^{-5}\,,\;\; \tau_j = 0.4 \cdot h^2$$



$$4.37 \le t_n \le 4.4$$

Numerical example

$$b(x,t) = 4(1+\cos 2\pi x)(1+t)^2, \; h = 2^{-5}, \; \tau_j = 0.4 \cdot h^2$$



$4.37 \le t_n \le 4.4$ (another view-point)

Consideration

Finite difference scheme $\left(\lambda_n = \tau_n/h^2\right) \Leftrightarrow$

$$u_i^n = (1-2\lambda_n)u_i^{n-1} + \left(\lambda_n + \frac{\tau_n}{2h} b_{i-1}^{n-1}\right) u_{i-1}^{n-1} + \left(\lambda_n - \frac{\tau_n}{2h} b_{i+1}^{n-1}\right) u_{i+1}^{n-1}$$

Non-negativity (*) $\quad u_i^{n-1} \geq 0 \ (\forall i) \quad \Rightarrow \quad u_i^n \geq 0 \ (\forall i)$

A sufficient condition:

- $(\cdots) \geq 0$, $(\cdots) \geq 0$, $(\cdots) \geq 0 \Rightarrow (*)$
- $h \leq \dfrac{1}{2\beta^{n-1}} \Rightarrow (*)$. $\quad \left(\beta^n = \max\limits_{1\leq i\leq N} b_i^n\right)$

Issue before computation, we have to choose h satisfying:

$$h \leq \frac{1}{2\beta_T}, \qquad \beta_T = \max_{0\leq t_n\leq T} \beta^n.$$

Upwind finite difference scheme

forward Euler = central difference + upwind difference

$$\frac{u_i^n - u_i^{n-1}}{\tau_n} = \frac{u_{i-1}^{n-1} - 2u_i^{n-1} + u_{i+1}^{n-1}}{h^2} - \frac{b_i^{n-1} u_i^{n-1} - b_{i-1}^{n-1} u_{i-1}^{n-1}}{h}$$

$\Leftrightarrow$

$$u_i^n = \left(1 - 2\lambda_n - \frac{\tau_n}{h} b_i^{n-1}\right) u_i^{n-1} + \left(\lambda_n + \frac{\tau_n}{h} b_{i-1}^{n-1}\right) u_{i-1}^{n-1} + \lambda_n u_{i+1}^{n-1}$$

A sufficient condition : $\tau_n \leq \dfrac{h^2}{2 + h\beta_{n-1}} \Rightarrow (*)$.

- In each time step, we re-choose τ_n to satisfy the above condition.
- Extension to $d \geq 2$ and arbitrary Ω
  - FEM; Tabata (1977), Heinrich et al. (1977) $\rightarrow$ flow problems.
  - In general, the upwind FEM destroys the conservation of mass.
- Conservative numerical schemes;
  - FEM;   Baba-Tabata upwinding (1981),
  - Finite volume method (FVM), ... $\leftarrow$ **main topic of this talk!**

§2. FVM for convection-diffusion equations

Convection-diffusion problem (model problem)

Find a function $u = u(x,t)$ of $(x,t) \in \overline{\Omega} \times [0, T]$ satisfying

$$\begin{cases} u_t - \nabla \cdot (\nabla u - \mathbf{b} u) = 0 \quad \text{in} \quad \Omega \times (0,T), \\ \dfrac{\partial u}{\partial \nu} = 0 \quad \text{on} \quad \partial\Omega \times (0,T), \quad u|_{t=0} = u_0 \quad \text{on} \quad \Omega, \end{cases}$$

- $\Omega \subset \mathbb{R}^2$: polygonal domain, T: positive constant
- $\mathbf{b} : \Omega \times (0,T) \to \mathbb{R}^2$, $\mathbf{b} \cdot \nu = 0$ on $\partial\Omega$ (given flow)
- $u_0 : \Omega \to \mathbb{R}$ (initial value)

Conservation properties:

- **Total mass:** $\displaystyle\int_\Omega u(x,t)\ dx = \int_\Omega u_0(x)\ dx;$
- **Positivity:** $u_0 \geq 0,\ u_0 \not\equiv 0 \quad \Rightarrow \quad u(x,t) > 0\ (t > 0).$

Admissible mesh: definition [Eymard et al. 2000]

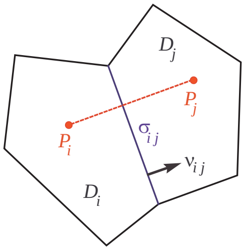
$\mathscr{D} = \{D_i\}_{i\in\Lambda}$: <u>*admissible mesh*</u> $\Leftrightarrow$

(A1) D_i: (open) convex polygonal domain; $\overline{\Omega} = \cup\{\overline{D_i} \mid i \in \Lambda\}$

(A2) $\overline{D_i} \cap \overline{D_j} =$ entire common side σ_{ij} / vertex / empty set $\quad (i \neq j)$

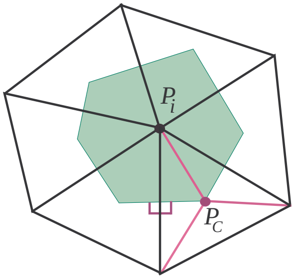
(A3) $\exists\{P_i\}_{i\in\overline{\Lambda}}$ such that $P_i \in \overline{D}_i$ and that the line segment connecting P_i with P_j is orthogonal to the line including σ_{ij}, if $\overline{D_i}$ and $\overline{D_j}$ share a common side σ_{ij}.

(A4) $\exists$ side σ of D_i: $\sigma \subset \partial\Omega \quad \Rightarrow \quad P_i \in \overline{\sigma}$.

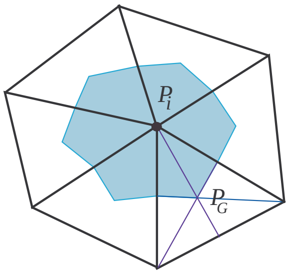


- $h = h_{\mathscr{D}} = \max\{\mathrm{diam}\,(D_i) \mid i \in \Lambda\}$
- D_i: *control volume*
- $\Lambda \subset \mathbb{N}$: index set of control volumes

Circumcentric and barycentric domains

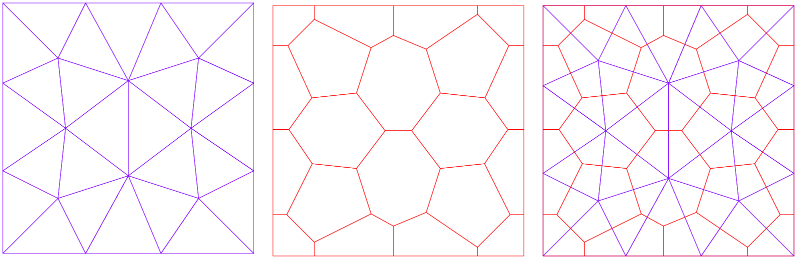


circumcentric domain
(P_C = circumcenter)



barycentric domain
(P_G = barycenter)

Admissible mesh: examples (acute triangulations)



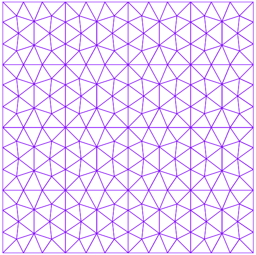
acute triangulation   admissible mesh

Lemma: The circumcentric dual mesh of an acute triangulation is an admissible mesh.

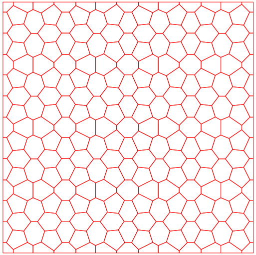
Remark: The barycentric dual mesh does not imply an admissible mesh in general.

Remark: acute = nonobtuse

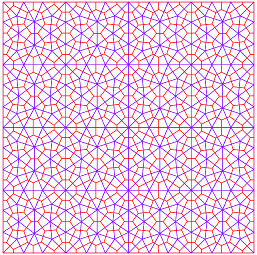
Admissible mesh: examples (acute triangulations)



acute triangulation



admissible mesh

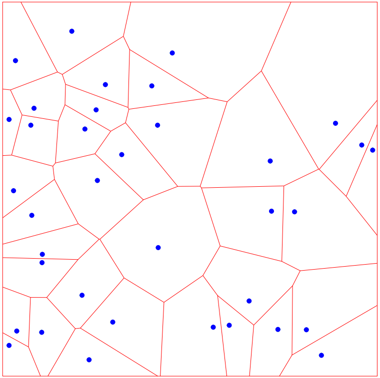


Lemma: The circumcentric dual mesh of an acute triangulation is an admissible mesh.

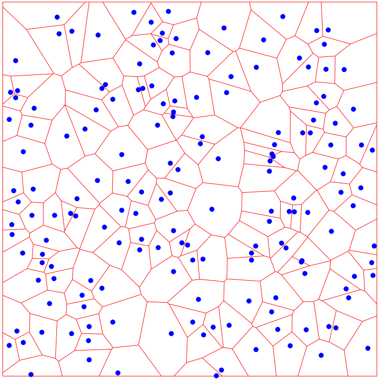
Remark: The barycentric dual mesh does not imply an admissible mesh in general.

Remark: acute = nonobtuse

Admissible mesh: examples (Voronoi diagram)

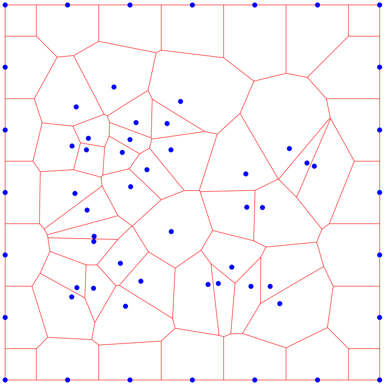


Voronoi diagram

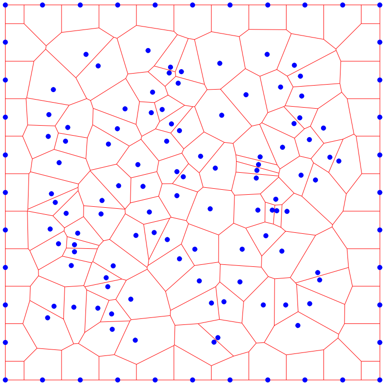


Voronoi diagram

Admissible mesh: examples (Voronoi diagram)



admissible mesh



admissible mesh

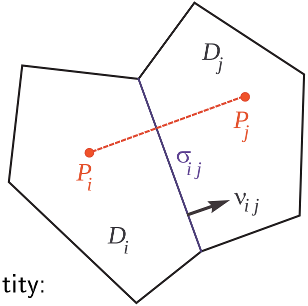
Lemma: A Voronoi diagram implies an admissible mesh if the number of points $\{P_i\}$ which are located on $\partial\Omega$ is large enough.

Definitions

- Piecewise constant functions:

$$V_h = \text{span}\,\{\overline{\phi}_{hi}\}_{i\in\Lambda} = \{v_h \in L^\infty(\Omega) \mid v_h|_{D_i} = \text{Const.}\ (i\in\Lambda)\}$$

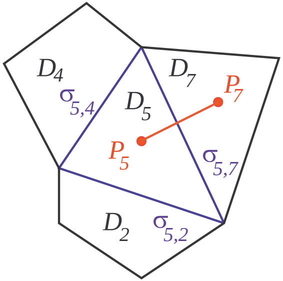
- $\gamma_{ij} = \dfrac{m_{ij}}{d_{ij}}$ *transmissibility*
- $m_{ij} =$ length of σ_{ij}
- $d_{ij} = |P_i - P_j|$
- $m_i =$ area of D_i



Remark: FVM is based on the identity:

$$\int_{D_i} u_t\ dx + \int_{D_i} (-\Delta u)\ dx + \int_{D_i} \nabla\cdot(\mathbf{b}u)\ dx = 0 \quad (i\in\Lambda).$$

Approximation of the diffusion part



$$
\begin{aligned}
\int_{D_i} (-\Delta u)\, dx &= -\int_{\partial D_i} \nabla u \cdot \nu_i \; dS \\
&= -\sum_{j \in \Lambda_i} \int_{\sigma_{ij}} \nabla u \cdot \nu_{ij} \; dS \\
&\approx -\sum_{j \in \Lambda_i} \int_{\sigma_{ij}} \frac{u(P_j) - u(P_i)}{d_{ij}} \; dS \\
&= -\sum_{j \in \Lambda_i} \gamma_{ij} (u(P_i) - u(P_j)).
\end{aligned}
$$

- $\gamma_{ij} = \dfrac{m_{ij}}{d_{ij}}$, $m_{ij} =$ length of σ_{ij} , $d_{ij} = |P_i - P_j|$
- $\Lambda_i = \{j \in \Lambda \mid P_i$ and P_j share the entire common side $\sigma_{ij}\}$ $(\Lambda_5 = \{2, 4, 7\})$

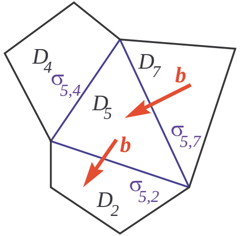
Approximation of the convection part

$$\begin{aligned}
\int_{D_i} \nabla \cdot (\mathbf{b}u)\ dx &= \sum_{j\in\Lambda_i} \int_{\sigma_{ij}} u\ (\mathbf{b}\cdot\nu_i)\ dS \\
&\approx \sum_{j\in\Lambda_i} \int_{\sigma_{ij}} [(1-r_{ij})u(P_j) + r_{ij}u(P_i)]\ (\mathbf{b}\cdot\nu_i)\ dS \\
&= \sum_{j\in\Lambda_i} [(1-r_{ij})u(P_j) + r_{ij}u(P_i)]\,\beta_{ij}.
\end{aligned}$$

- $0 \le r_{ij} \le 1$: the weighting parameter;

$$r_{ij} = \begin{cases} \frac{1}{2}(\text{sign } \beta_{ij} + 1) & \text{(Baba-Tabata upwinding)} \\ \ldots\ldots & \end{cases}$$

- $\beta_{ij} = \int_{\sigma_{ij}} \mathbf{b}\cdot\nu_{ij}\ dS$



Finite volume scheme (implicit scheme)

Find $\{u_h^n\}_{n=0}^{\overline{n}} \subset V_h$ satisfying

$$\begin{cases} \dfrac{u_i^n - u_i^{n-1}}{\Delta t} m_i - \displaystyle\sum_{j \in \Lambda_i} \gamma_{ij} (u_j^n - u_i^n) \\ \qquad + \displaystyle\sum_{j \in \Lambda_i} \beta_{ij}^n \left[(1 - r_{ij}^n) u_j^n + r_{ij}^n u_i^n \right] = 0 \\ \qquad\qquad\qquad\qquad (i \in \Lambda,\ 1 \le n \le \overline{n}), \\ u_i^0 = u_{0,i} \quad (i \in \Lambda), \end{cases}$$

- $u_i^n = u_h^n(P_i), \quad t_n = n\Delta t, \quad \Delta t = T/\overline{n}.$
- $u_{0,i} = (1/m_i) \displaystyle\int_{D_i} u_0(x)\ dx$ or $u_{0,i} = u_0(P_i).$
- Mass conservation: $\displaystyle\sum_{i \in \Lambda} u_i^n m_i = \sum_{i \in \Lambda} u_{0,i} m_i.$
- Positivity: $u_{0h} \ge 0,\ \Delta t \le \dfrac{1}{2\|\mathbf{b}\|_\infty} \min_{\sigma_{ij}} \mathrm{dist}\,(\sigma_{ij}, P_i) \Rightarrow u_h^n \ge 0$

§3. FVM for a degenerate Keller-Segel system

FVM for (DKS) with $k = 0$; explicit scheme

Find $\{u_h^n\}_{n\geq 0}$ and $\{v_h^n\}_{n\geq 0} \subset V_h$ satisfying

$$\begin{cases} \dfrac{u_i^{n+1} - u_i^n}{\tau_{n+1}} m_i - \displaystyle\sum_{j\in\Lambda_i} \gamma_{ij}[f(u_j^n) - f(u_i^n)] \\ \qquad + \displaystyle\sum_{j\in\Lambda_i} \left[(1 - r_{ij}^n)u_j^n + r_{ij}^n u_i^n\right] \gamma_{ij} \left[g(v_j^n) - g(v_i^n)\right] = 0, \\ -D_v \displaystyle\sum_{j\in\Lambda_i} \gamma_{ij}(v_j^n - v_i^n) + k_1 v_i^n m_i = k_2 u_i^n m_i, \qquad (i \in \Lambda), \\ u_i^0 = u_{0,i} \quad (i \in \Lambda), \end{cases}$$

- The weighting parameter is defined by

$$r_{ij}^n = \begin{cases} 1 & \text{if } g(v_i^n) \leq g(v_j^n), \\ 0 & \text{if } g(v_i^n) > g(v_j^n). \end{cases}$$

- The uniqueness existence of a solution (u_h^n, v_h^n) is trivial, since this is an explicit scheme.

Conservation properties

- Mass conservation: $\sum_{i\in\Lambda} u_i^n m_i = \sum_{i\in\Lambda} u_{0,i} m_i$.
- Positivity conservation: Let $\varepsilon \in (0,1]$ and $\tau > 0$. If

$$\tau_{n+1} = \min\left\{\tau,\ \frac{\varepsilon\kappa_h}{\lambda_n + \mu_n}\right\},$$

then we have $u_h^{n+1} \geq 0$ and $\|u_h^{n+1}\|_{L^1} = \|u_h^n\|_{L^1} = \cdots = \|u_{0h}\|_{L^1}$.

Here,

$$\kappa_h = \min_{i\in\Lambda}\left(\sum_{j\in\Lambda_i} \frac{m_{ij}}{\gamma_{ij}}\right)^{-1} m_i,$$

$$\lambda_n = \sup_{M_n' \leq z, w \leq M_n} \frac{f(z) - f(w)}{z - w}, \qquad M_n' = \min u_h^n, M_n = \max u_h^n$$

$$\mu_n = \max_{\sigma_{ij}}\left\{0,\ g(v_j^n) - g(v_i^n)\right\}.$$

- It is applicable to the fast diffusion case $f(u) = u|u|^{m-1}$, $0 < m < 1$.

Convergence; the case $f(u) = D_u u$ (linear diffusion)

- F. Filbet (2006) [$k = 0$, fully implicit scheme]
  - general admissible mesh
  - $\|u_0\|_{L^1} \ll 1 \Rightarrow u_h^n \to u$ in $L^2(0, T : L^2(\Omega))$, ...
  - fixed point theorem and several a priori estimates
- S (2007), (2010) [$k \geq 0$, semi-implicit, explicit schemes]
  - admissible meshes are associated with acute triangulations of FEM
  - with some suitable $p > d$,

$$\sup_{0 \leq t_n \leq T} \left(\|u(t_n) - u_h^n\|_{L^p} + \|v(t_n) - \hat{v}_h^n\|_{W^{1,\infty}} \right) \leq C(h + \tau)$$

    for arbitrary $\|u_0\|_{L^1}$.
  - discrete version of analytical semigroup theory in L^p.
  - rational approximation of analytical semigroup.
  - finite volume element method in 3D.

Convergence; the case $g(v) = 0$

- S (201X) [semidiscrete (in time) scheme for $u_t = \Delta f(u)$]
  - $A_h : V_h \to V_h$

$$(A_h v_h)(P_i) = -\sum_{j\in\Lambda_i} \gamma_{ij}[f(v_j) - f(v_i)] \qquad (v_h \in V_h,\ v_i = v_h(P_i)).$$

  - A_h: L^1 contraction and order-preserving properties

$$\|[v_h - w_h]_+\|_{L^1} \le \|[v_h - w_h + \lambda A_h v_h - \lambda A_h w_h]_+\|_{L^1} \quad (\lambda > 0)$$

    $\Rightarrow -A_h$ is m-dissipative in V_h
    $\Rightarrow$ By Crandall & Liggett, $\exists! u_h(t)$: sol. of $du_h(t)/dt + A_h u_h(t) = 0$.

  - L^∞ stability: $\|u_h(t)\|_{L^\infty} \le C\|u_{0h}\|_{L^\infty}$.
  - if f is strictly increasing and admissible meshes are obtained from acute triangulations of FEM, we have the L^1 (strong) convergence

$$\lim_{h\to 0} \sup_{0\le t\le T} \|u_h(t) - u(t)\|_{L^1} = 0.$$

- We follow the method of Mizutani, S & Suzuki (2005)

§4. Display of numerical results

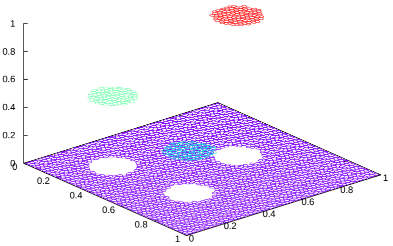
Numerical examples

$f(u) = u^m$, $g(v) = k_0 v^l$

$$\begin{cases} u_t = \nabla \cdot \left(\nabla u^m - k_0 u \nabla v^l\right) & \text{in} \quad \Omega \times (0, T), \\ 0 = \Delta v + v - u & \text{in} \quad \Omega \times (0, T), \\ \dfrac{\partial}{\partial \nu} u^m - k_0 u \dfrac{\partial}{\partial \nu} v^l = 0, \quad \dfrac{\partial v}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0, T), \\ u|_{t=0} = u_0 & \text{on} \quad \Omega, \end{cases}$$

Numerical example (A): $\Omega = (0,1)^2$

	m	$\|u_0\|_{L^1}$
d0209-1	1.0	20.0
d0209-2	1.2	20.0
d0209-3	1.4	20.0



u_{0h}

- $\Omega = (0,1)^2$ square
- $f(u) = u^m$, $g(v) = k_0 v$
- $k_1 = k_2 = 1.0$, $k_0 = 5.0$
- $\|u_{0h}\|_{L^1} = 20 > 4\pi > 2\pi$

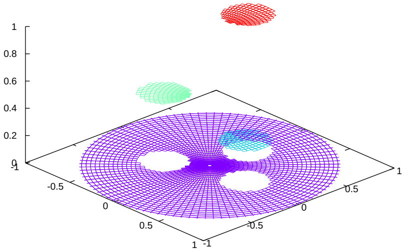
  If $m = 1$, the boundary/corner blow up may occur.

left figure	right figure
u_h^n	$u_h^n / \|u_h^n\|_{L^\infty}$

Numerical example (B): $\Omega = B(0,1)$

	m	$\|\|u_0\|\|_{L^1}$
d0221-1	1.0	20.0
d0221-2	1.2	20.0
d0221-3	1.4	20.0

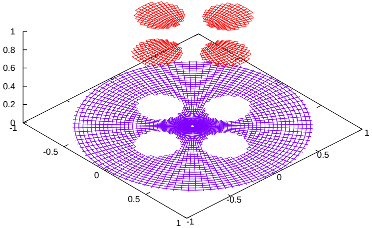
- $\Omega = B(0,1)$ disk
- $f(u) = u^m$, $g(v) = k_0 v$
- $k_1 = k_2 = 1.0$, $k_0 = 2.0$
- The smooth boundary is exactly discretized.



left figure	right figure
u_h^n	$u_h^n / \|\|u_h^n\|\|_{L^\infty}$

Numerical example (C): $\Omega = B(0,1)$

	m	l	$\|\|u_0\|\|_{L^1}$
d0225-6	1.0	1.0	80.0
d0225-8	1.0	2.0	80.0
d0301-6	1.2	1.0	80.0
d0301-8	1.2	2.0	80.0



- $\Omega = B(0,1)$ disk
- $f(u) = u^m$, $g(v) = k_0 v^l$
- $k_1 = k_2 = 1.0$, $k_0 = 1.0$
- The smooth boundary is exactly discretized.

left figure	right figure
u_h^n	$u_h^n / \|\|u_h^n\|\|_{L^\infty}$

Thank you for your attention!

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