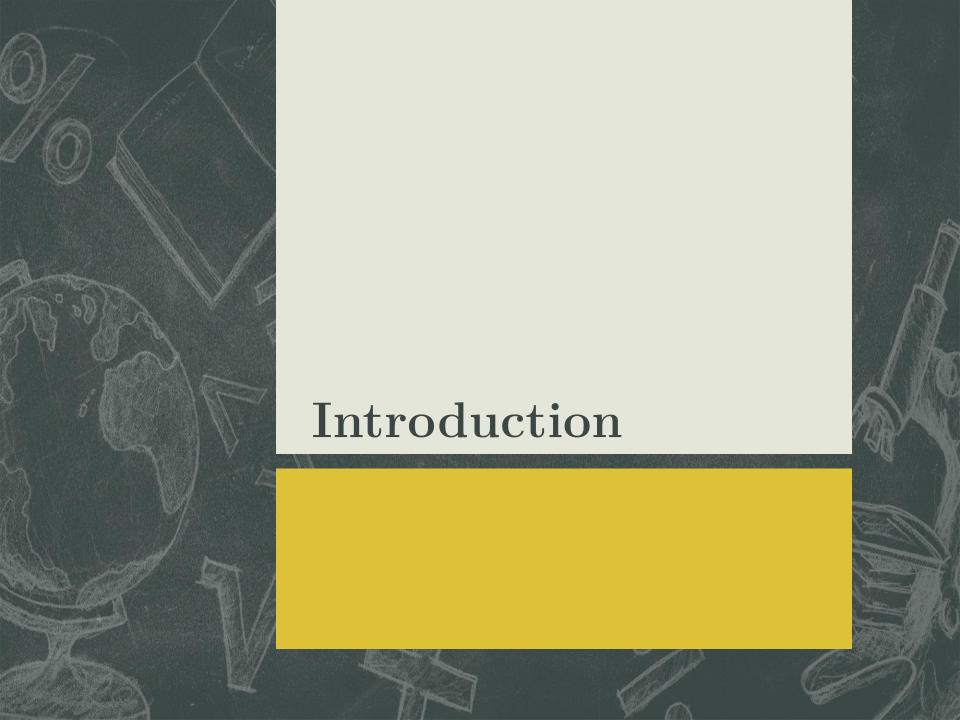


Outline

- Introduction
- Some motivating examples
- A strong boundary maximum-minimum principle
- The number of the L-level points and the number of the local extremizers the continuous case
- The discrete case



Preservation of qualitative properties

The real-life problem to be modelled

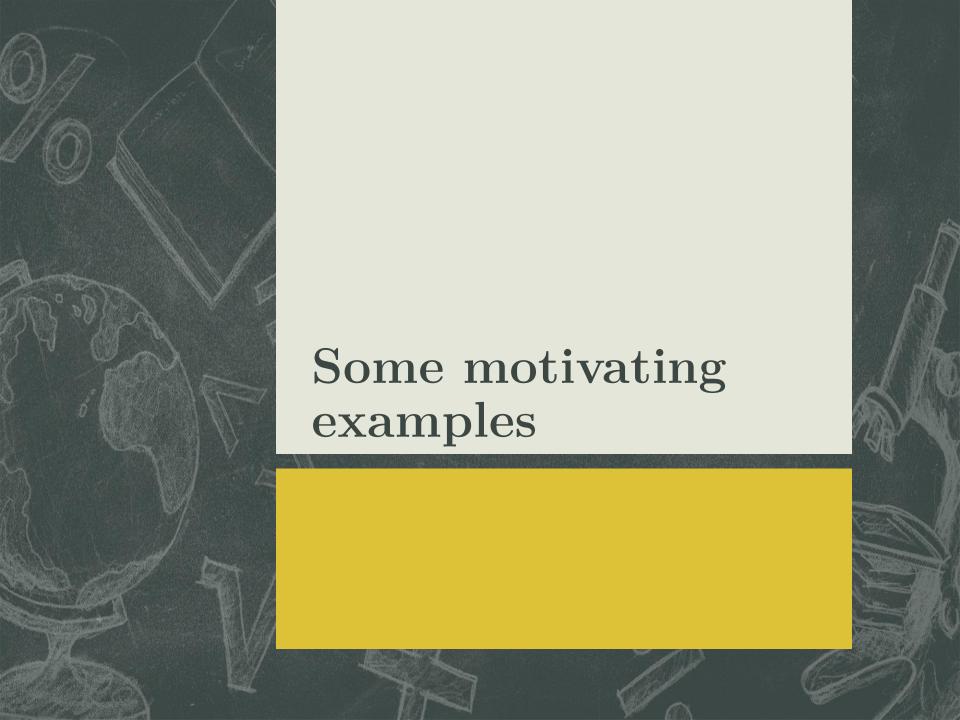
Mathematical model

Numerical model

Preservation of qualitative properties

Problems

- What are the qualitative properties of the original phenomenon?
- What are the qualitative properties of the mathematical model?
- What are the discrete equivalents of the above qualitative properties?
- What are the relations of them?
- Sufficient conditions (mesh, time-step) for the qualitative properties in the discrete models.



A simple example in Matlab (pdetool)

$$\frac{\partial u}{\partial t} = \Delta u, \text{ in } (0, T) \times \Omega, \quad \Omega = (0, 1) \times (0, 1),$$

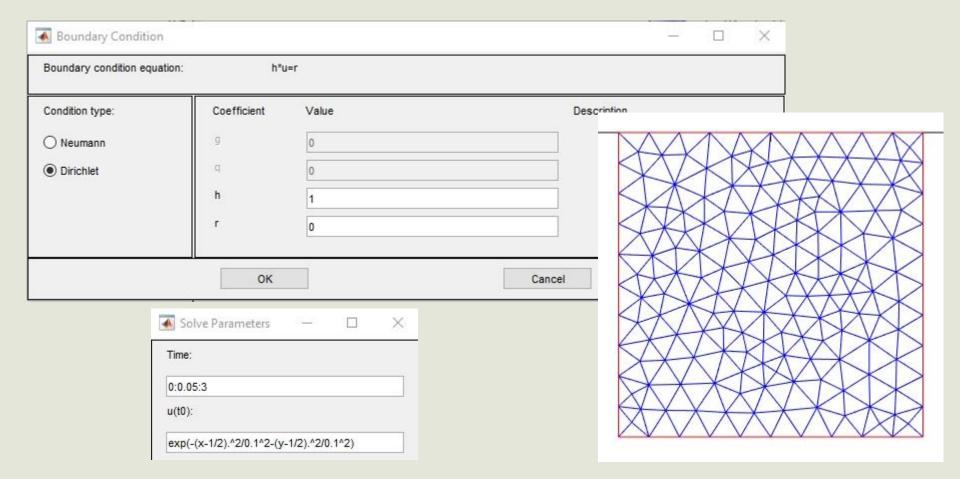
$$u(t, x) = 0, \ x \in \partial \Omega$$

$$u(0, x) = \exp(-(x - 1/2)^2 / 0.1^2 - (y - 1/2)^2 / 0.1^2)$$

PDE Specification	on		- C X
Equation:	d*u'-div(c*grad(u))+a*u=f		
Type of PDE:	Coefficient	Value	
○ Elliptic	c	1.0	Definition
Parabolic	a	0.0	of the model
O Hyperbolic	f	0	parameters
Eigenmodes	d	1.0	
	ОК		Cancel

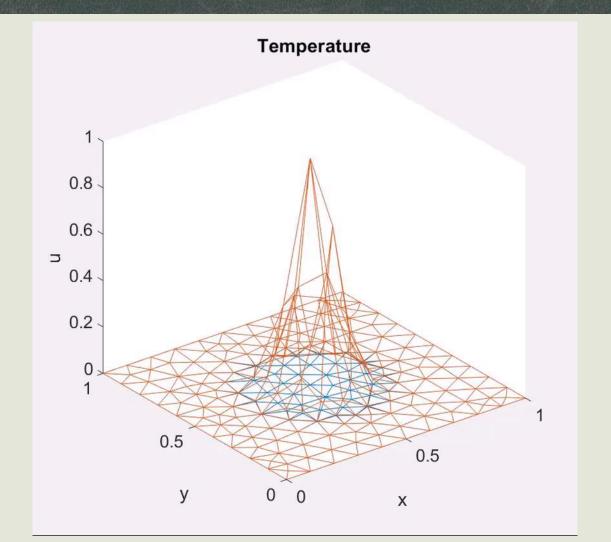
A simple example in Matlab (pdetool)

The mesh and the boundary and initial conditions



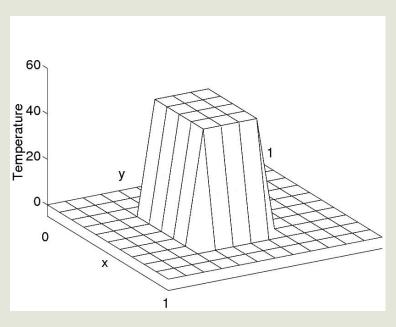
A simple example in Matlab (pdetool)

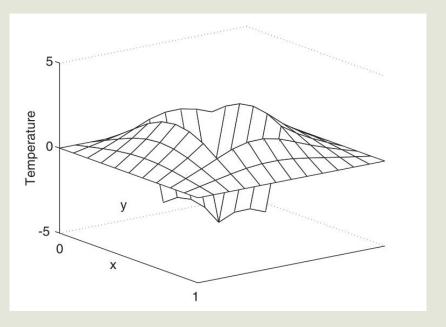
The result



Another finite element example

We solve the previous problem with FEM (θ -method, $\theta = 0.9$) and bilinear elements. (I. Faragó, R.H., SIAM J. Sci. Comput., 2006)

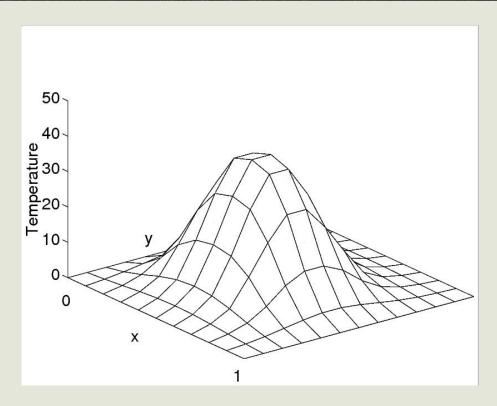




$$t = 0$$
 $\Delta x = 1/10, \ \Delta y = 1/12$

$$t = 0.5, \ \Delta t = 0.5$$

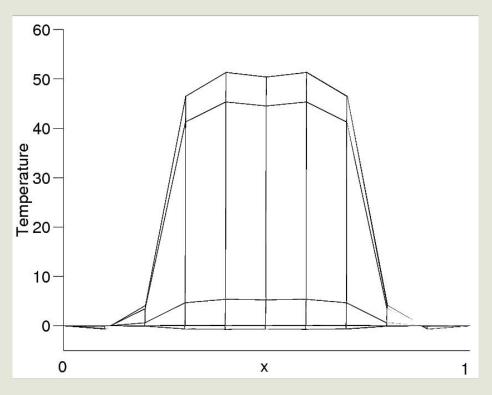
Another finite element example



$$t = 0.0005, \ \Delta t = 0.0005$$

$$\Delta x = 1/10, \, \Delta y = 1/12$$

Another finite element example



The numerical solution does not satisfy:

- the maximum-minimum principle
- the nonnegativity preservation property

$$t = 0.0001, \ \Delta t = 0.0001$$

$$\Delta x = 1/10, \, \Delta y = 1/12$$

Cut-off methods

The remedy can be the so-called cut-off method:

Changna Lu et al, The cutoff method for the numerical computation of nonnegative solutions of parabolic PDEs with application to anisotropic diffusion and Lubrication-type equations, J. Comp. Phys., 242, (2013), pp. 24-36

Christian Kreuzer, A note on why enforcing discrete maximum principles by a simple a posterori cutoff is a good idea, Numerical methods of PDEs, 30, (2014), pp. 994-1002

Cut-off methods

The numerical scheme

$$\mathbf{X}_1 \mathbf{u}^{n+1} = \mathbf{X}_2 \mathbf{u}^n + \mathbf{f}^n$$

is changed to

$$\mathbf{X}_1\mathbf{v}^{n+1} = \mathbf{X}_2(\mathbf{v}^n)^+ + \mathbf{f}^n.$$

$$\mathbf{X}_1(\mathbf{v}^{n+1} - \mathbf{U}^{n+1}) = \mathbf{X}_2((\mathbf{v}^n)^+ - \mathbf{U}^n) - \boldsymbol{\tau}^n,$$

thus

$$\|\mathbf{v}^{n+1} - \mathbf{U}^{n+1}\| = \|\mathbf{X}_1^{-1}\mathbf{X}_2((\mathbf{v}^n)^+ - \mathbf{U}^n) - \mathbf{X}_1^{-1}\boldsymbol{\tau}^n\|$$

$$\leq (1 + K\Delta t)\|(\mathbf{v}^n)^+ - \mathbf{U}^n\| + K_1\|\boldsymbol{\tau}^n\|$$

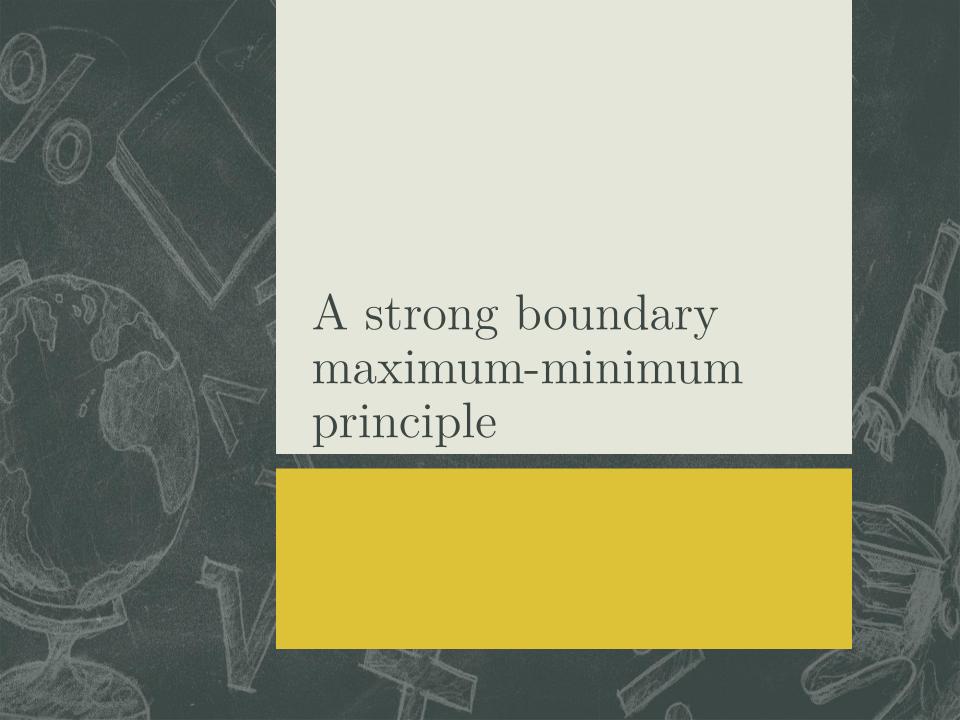
and

$$\|(\mathbf{v}^{n+1})^+ - \mathbf{U}^{n+1}\| \le (1 + K\Delta t)\|(\mathbf{v}^n)^+ - \mathbf{U}^n\| + K_1\|\boldsymbol{\tau}^n\|.$$

Cut-off methods

Problems with this approach:

- The convergence is guaranteed, but is the numerical solution reliable on a fixed mesh?
- We have to check the nonnegativity in each iteration step. A priori conditions are better.
- It is difficult to extend the method to other qualitative properties



A strong boundary maximumminimum principle

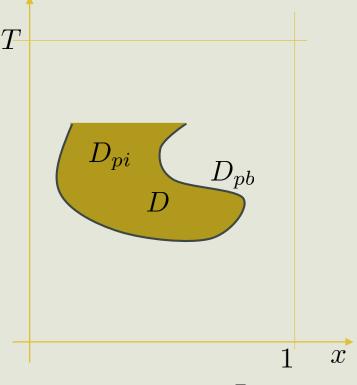
K. Nickel, Gestaltaussagen über Lösungen parabolischer Differentialgleichungen, Journal für die reine und angewandte Mathematik, 211 (1962), pp. 78–94

J. D. Logan, Introduction to nonlinear partial differential equations, T John Wiley & Sons, 2008

Protter, Weinberger, Maximum principles in differential equations, Prentice-Hall, 1967

$$L[u] := u_t - f(t, x, u, u_x, u_{xx}) = 0 \text{ in } Q_{\bar{T}}$$

Thm. Assume that f(t, x, z, p, r) is non-decreasing in r and $f(t, x, z, 0, 0) \equiv 0$ (L[const.] = 0). Assume that $u \in C(\bar{Q}_T) \cap C^{1,2}(Q_{\bar{T}})$ is a solution of the equation. Then $m \leq u \leq M$ on D_{pb} implies $m \leq u \leq M$ on \bar{D} .



$$D_{pb} \cup D_{pi} = \bar{D}$$

A strong boundary maximumminimum principle

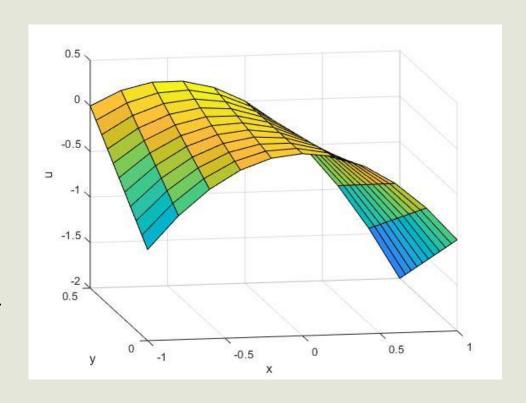
An example:

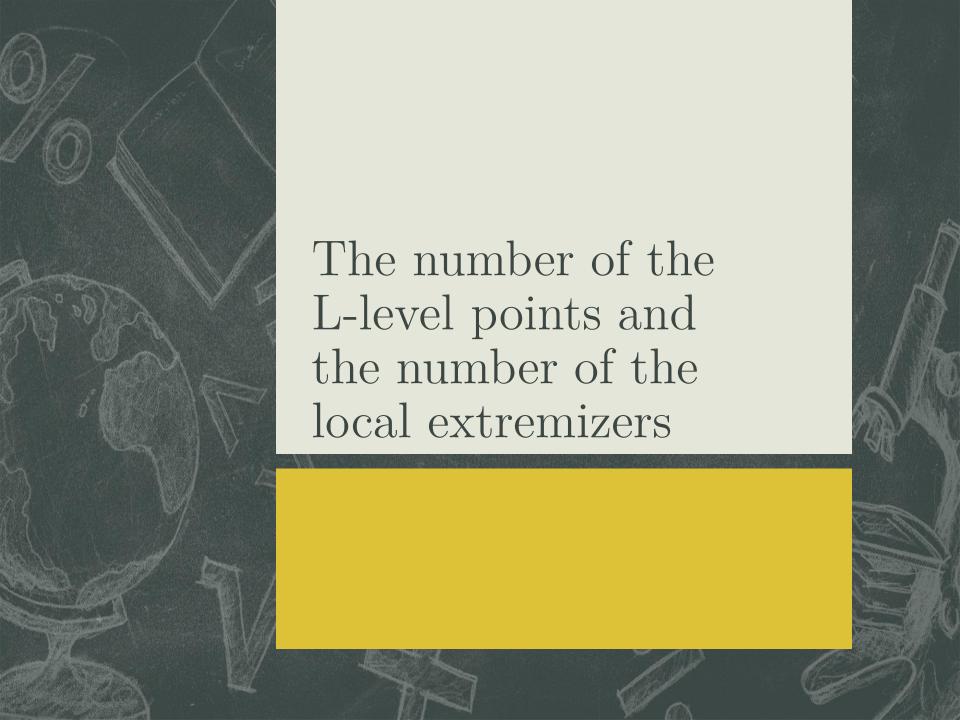
$$u_t - xu_{xx} = 0$$

The solution is

$$u(t,x) = -x^2 - 2xt.$$

f(t, x, z, p, r) = xr, which decreases in r if x < 0.

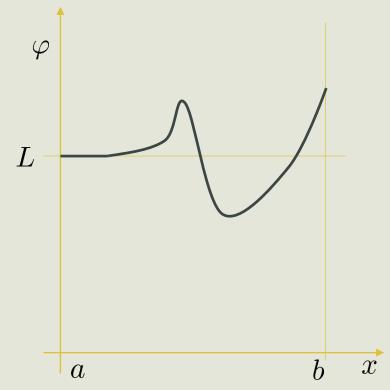




L-level points, local extremizers

Def. $\varphi:[a,b]\to\mathbb{R}$ is a continuous function. $L\in\mathbb{R}$ is a fixed level value. The number of the L-level points is denoted by $\zeta_{\phi|_{[a,b]}}^L$.

Def. $\varphi:[a,b]\to\mathbb{R}$ is a continuous function. The number of the local maximizers (minimizers) of ϕ is denoted by $\mu_{\phi|_{[a,b]}}$.



Pólya's and Sturm's result

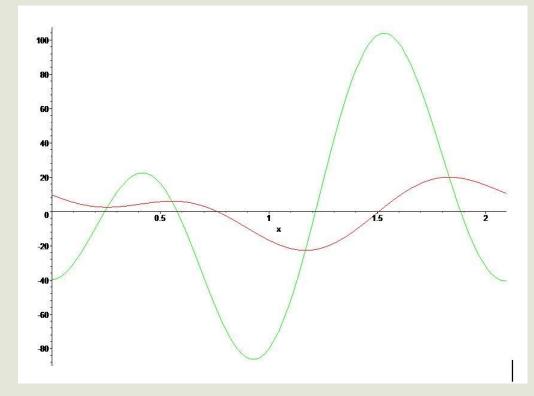
$$u_t - u_{xx} = 0$$
, in Q_T ,
 $u = 0$, $(t, x) \in (0, T) \times \{0, 1\}$,
 $u = u_0$, $(t, x) \in \{0\} \times [0, 1]$.

Thm. [Gy. Pólya (1933), Ch. Sturm (1936)] The number of the roots of the functions $x \to u(x, t)$ does not increase in time t.

Pólya's proof

Lemma. If f is a differentiable periodic function (p > 0) and $f(a) \neq 0$ then the function $\alpha f + f'$ ($\alpha \neq 0$) has not less roots than that of f on

the interval [a, a + p].



Pólya's proof

$$u(x,t) = A_0 + \sum_{i=1}^{\infty} (A_i \cos(ix) + B_i \sin(ix)) \cdot e^{-i^2 t}$$

Let $t_2 > t_1 \ge 0$ be two different time levels $(\Delta t = t_2 - t_1)$. Then

$$u(x, t_2) = a_0 + \sum_{i=1}^{\infty} (a_i \cos(ix) + b_i \sin(ix)),$$

ahol
$$a_0 = A_0$$
, $a_i = A_i \cdot e^{-i^2 t_2}$, $b_i = B_i \cdot e^{-i^2 t_2}$.

Pólya's proof

Let us apply the lemma 2k times $(\alpha = \pm \sqrt[2(k-1)]{k})$:

$$a_0 + \sum_{i=1}^{\infty} (a_i \cos(ix) + b_i \sin(ix)) \cdot \left(1 + \frac{i^2 \Delta t}{k}\right)^k$$

$$\downarrow \quad (k \to \infty)$$

$$a_0 + \sum_{i=1}^{\infty} (a_i \cos(ix) + b_i \sin(ix)) \cdot e^{i^2 \Delta t} = v(x, t_1).$$

This completes the proof.

L-level points, local extremizers

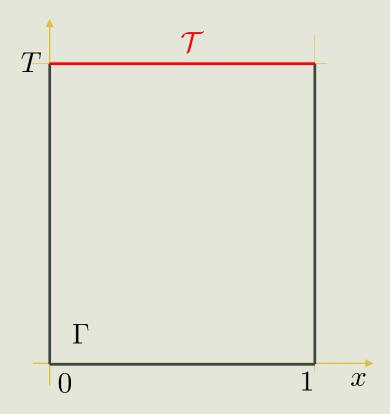
Thm. [Nickel 1962] Under the above conditions for the equation L[u] = 0 and for any fixed real number L we have

$$\zeta_{u|_{\mathcal{T}}}^{L} \le \zeta_{u|_{\Gamma}}^{L}$$

for the L-level points, moreover,

$$\mu_{u|_{\mathcal{T}}} \le \mu_{u|_{\Gamma}}$$

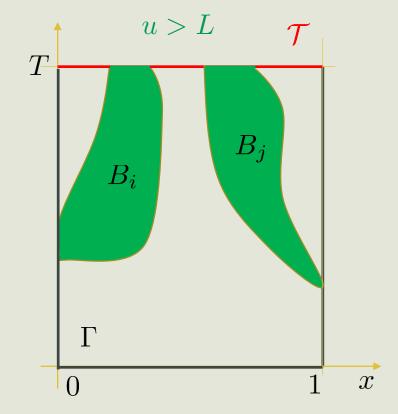
is valid for the local maximizers (minimizers) of the solution u.

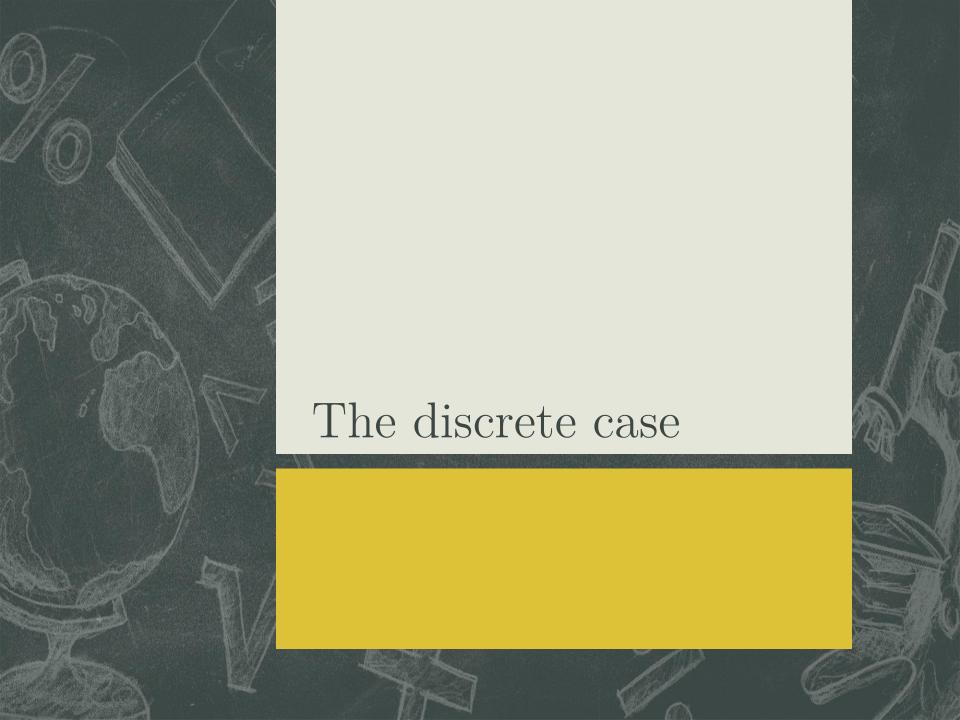


The sketch of the proof

Proof. The proof is based on the following properties of the sets B_i :

- i) $B_k \cap \Gamma \neq \emptyset$,
- ii) $B_i \cap B_j = \emptyset$.





We solve

$$u_{t} = (u_{xx})^{3}, (t, x) \in Q_{\bar{T}},$$

$$u(0, x) = u_{0}(x) = \sin(\pi x) \cdot \left(1 + \left(19e^{-\frac{(x-1/2)^{2}}{2 \cdot 0.01^{2}}}\right)\right), x \in [0, 1],$$

$$u(t, 0) = u(t, 1) = 0, t \in [0, T],$$

with the explicit Euler method

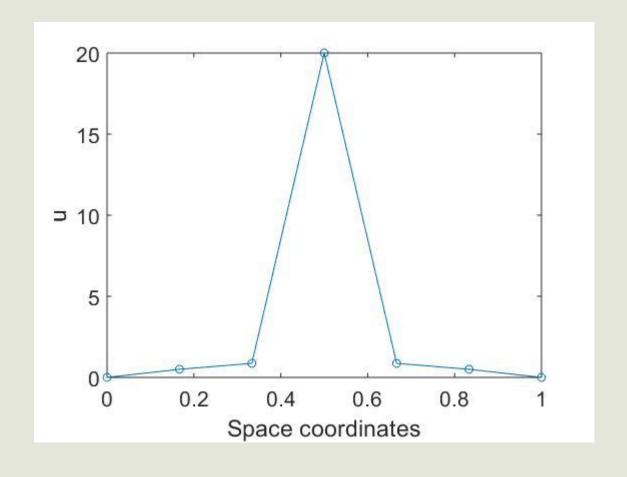
$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = f\left(t_k, x_i, u_i^k, \frac{u_{i+1}^k - u_{i-1}^k}{2\Delta x}, \frac{u_{i-1}^k - 2u_i^k + u_{i+1}^k}{\Delta x^2}\right), \quad \underset{k=0,\dots,n_T-1}{\overset{i=1,\dots,n}{\Delta x^2}},$$

$$u_i^0 = u_0(x_i), \quad i = 0, \dots, n+1,$$

$$u_0^k = u_{n+1}^k = 0, \quad k = 0, \dots, n_T.$$

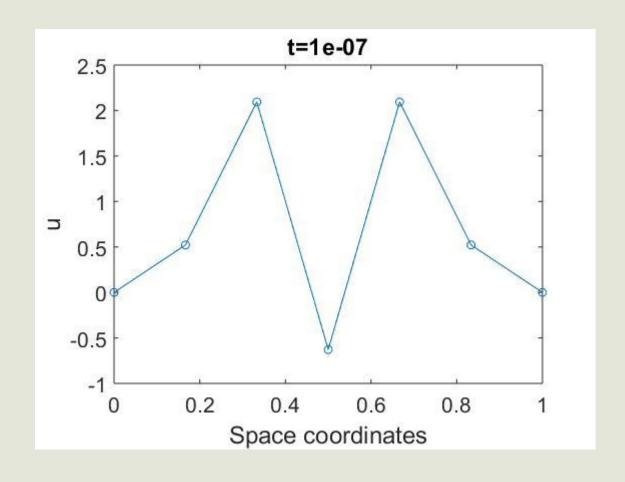
Approximation of the initial function with $\Delta x = 1/6$.

 $\zeta_{p|\Gamma}^0 = 2$ and for the local maximizers (minimizers) we have $\mu_{p|\Gamma} = 1(2)$.



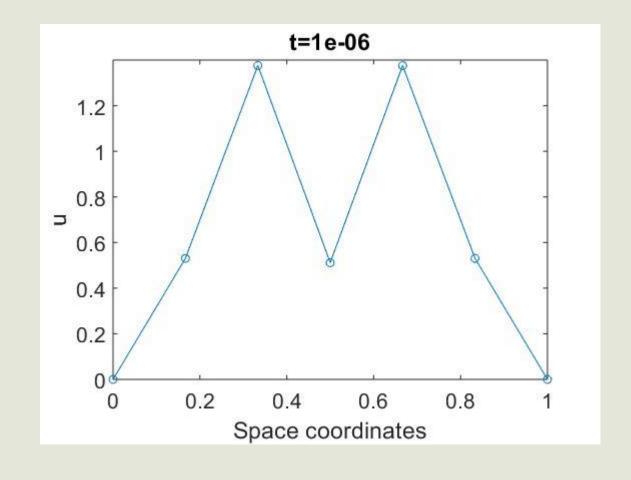
Approximation of the solution at $t = 10^{-7}$ (10th time level) with the time step $\Delta t = 10^{-8}$.

 $\zeta_{p|\tau}^0 = 4$ and for the local maximizers (minimizers) we have $\mu_{p|\tau} = 2(3)$.

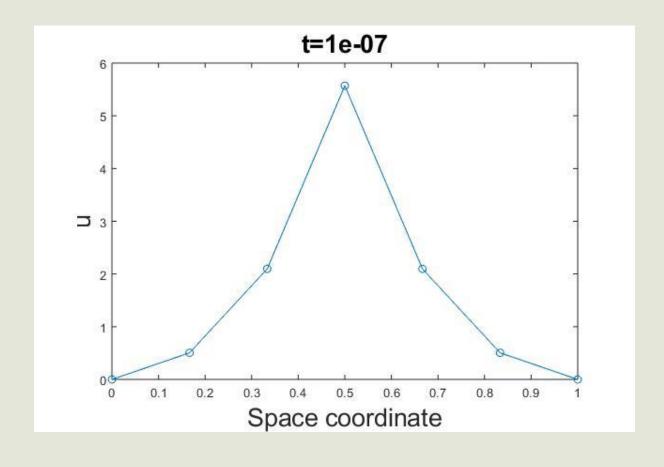


Approximation of the solution at $t = 10^{-6}$ (100th time level) with the time step $\Delta t = 10^{-8}$.

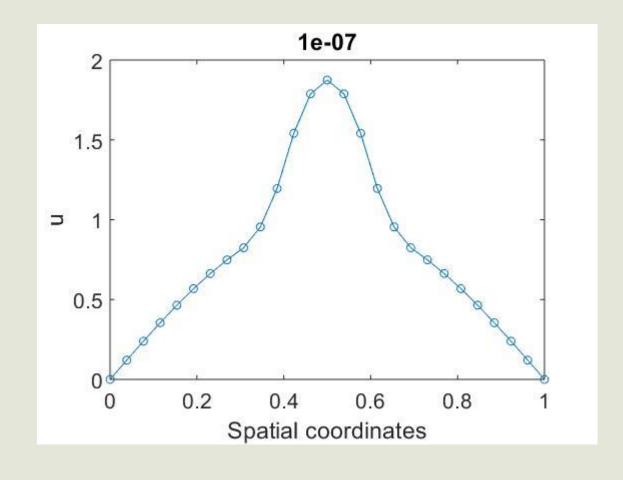
 $\zeta_{p|\tau}^0 = 2$ and for the local maximizers (minimizers) we have $\mu_{p|\tau} = 2(3)$.



With a smaller time step (10^{-9}) we get a correct solution at the same time level (100th time level).



On a finer mesh we obtain the approximation seen in the figure. $\Delta x = 1/26$, $\Delta t = 10^{-12}$ (10⁵th time step) (stability!)



Investigation of the IE-method

The scheme of the implicit Euler method.

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = f\left(t_{k+1}, x_i, u_i^{k+1}, \frac{u_{i+1}^{k+1} - u_{i-1}^{k+1}}{2\Delta x}, \frac{u_{i-1}^{k+1} - 2u_i^{k+1} + u_{i+1}^{k+1}}{\Delta x^2}\right), \quad \sum_{k=0,\dots,n_T-1}^{i=1,\dots,n} u_i^0 = u_0(x_i), \quad i = 0,\dots,n+1, \\
u_0^k = \nu_0(t_k), \quad u_{n+1}^k = \nu_1(t_k), \quad k = 0,\dots,n_T.$$

Investigation of the IE-method

Thm. Assume that

- f(t, x, z, p, r) is nondecreasing in r and
- $f(t, x, z, 0, 0) \equiv 0 \ (L[\text{const.}] = 0) \ \text{and}$
- f(t, x, z, p, r) is independent of p.

Then, if the implicit Euler finite difference numerical solution of the problem exists, then it satisfies the relations

$$\zeta_{p|_{\mathcal{T}}}^L \le \zeta_{p|_{\Gamma}}^L, \quad \mu_{p|_{\mathcal{T}}} \le \mu_{p|_{\Gamma}}$$

for the number of L-level points (L is a fixed real number) and for the number of the local maximizers (minimizers).

Proof. Paper submitted to J. Comp. Appl. Math.

An example

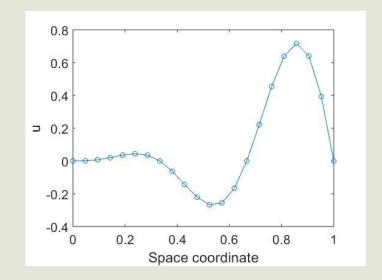
We solve problem

$$u'_{t} = (1 + u^{2})(u''_{xx})^{3}, (t, x) \in Q_{\bar{T}},$$

$$u(0, x) = x^{2} \sin(3\pi x), x \in [0, 1],$$

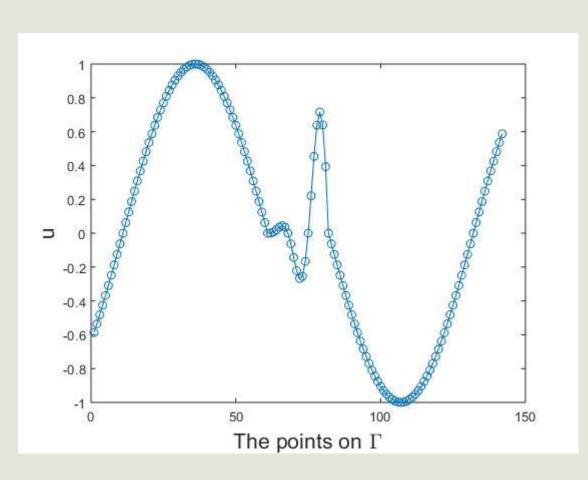
$$u(t, 0) = \sin(2\pi t), u(t, 1) = -\sin(2\pi t), t \in [0, T],$$

with the IE method. $T = 0.51, n = 20 \ (\Delta x = 1/21), \Delta t = 1/100.$

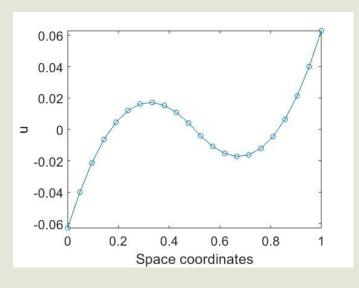


$$t = 0$$

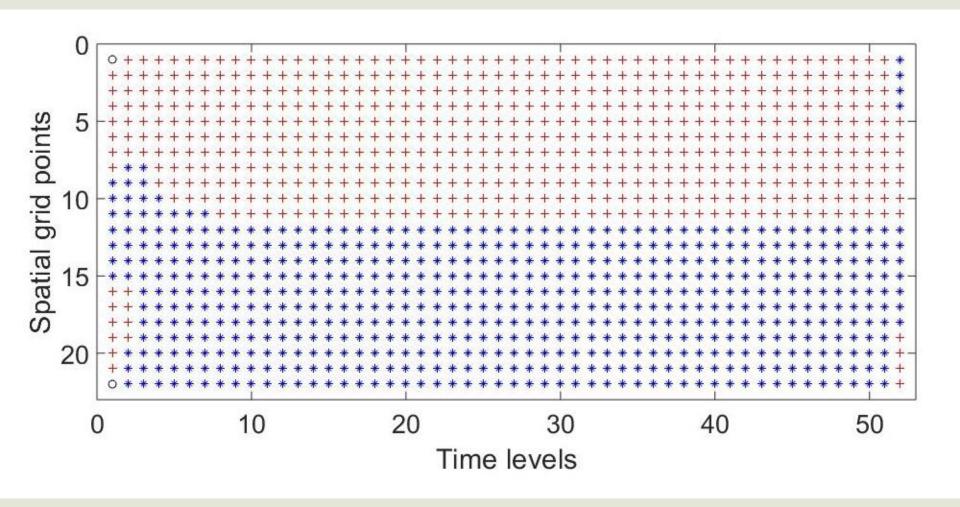
An example



$$t = T = 0.51$$



An example



Some related work

Masahisa Tabata, A finite difference approach to the number of peaks of solutions for semilinear parabolic problems, J. Math. Soc. Japan Vol. 32, No. 1, (1980), pp. 171-192.

$$u_t = a(t, x)u_{xx} + b(t, x)u_x + f(t, u), |\partial f/\partial u| \le M_0$$

Homogeneous Dirichlet boundary — The EE solution (provided that Δt sufficiently small) does not increase the number of the peaks in time.

Horváth R, On the Sign-Stability of Finite Difference Solutions of Semilinear Parabolic Problems, LECT NOTES COMPUT SC 5434: 305-313 (2009).

$$\begin{bmatrix} -1\\2\\-3\\5\\10 \end{bmatrix}, S=3, \begin{bmatrix} 1\\0\\-1\\2\\0 \end{bmatrix} \longrightarrow \begin{bmatrix} 1\\\emptyset\\-1\\2\\\emptyset \end{bmatrix}, S=2$$

 $\begin{bmatrix} -1 \\ 2 \\ -3 \\ 5 \\ 10 \end{bmatrix}, S=3, \begin{bmatrix} 1 \\ 0 \\ -1 \\ 2 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ \emptyset \\ -1 \\ 2 \\ \emptyset \end{bmatrix}, S=2$ If Δt is sufficiently small then the EE scheme does not increase the number of the sign changes.

Future work

- How to handle the explicit Euler case or generally the θ -method?
- Conditions for the time step and the spatial grid that guarantee the validity of the investigated properties.
- More general f functions (now terms like cu were excluded)

Thank you for your attention