Part 1:

Monotonic data fitting and interpolation

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Monotonic regression

Given a vector $\bar{u} \in R^n$ and a matrix $M \in R^{m \times n}$, find $u_M \in R^n$ that solves the problem

$$\begin{array}{ll} \text{min} & \frac{1}{2}\|u - \bar{u}\|^2 \\ \text{s.t.} & Mu \geq 0. \qquad \text{(monotonicity constraints)} \end{array}$$

The inequalities in $Mu \geq 0$ are of the form $u_j \geq u_i$.

Monotonic regression test problems

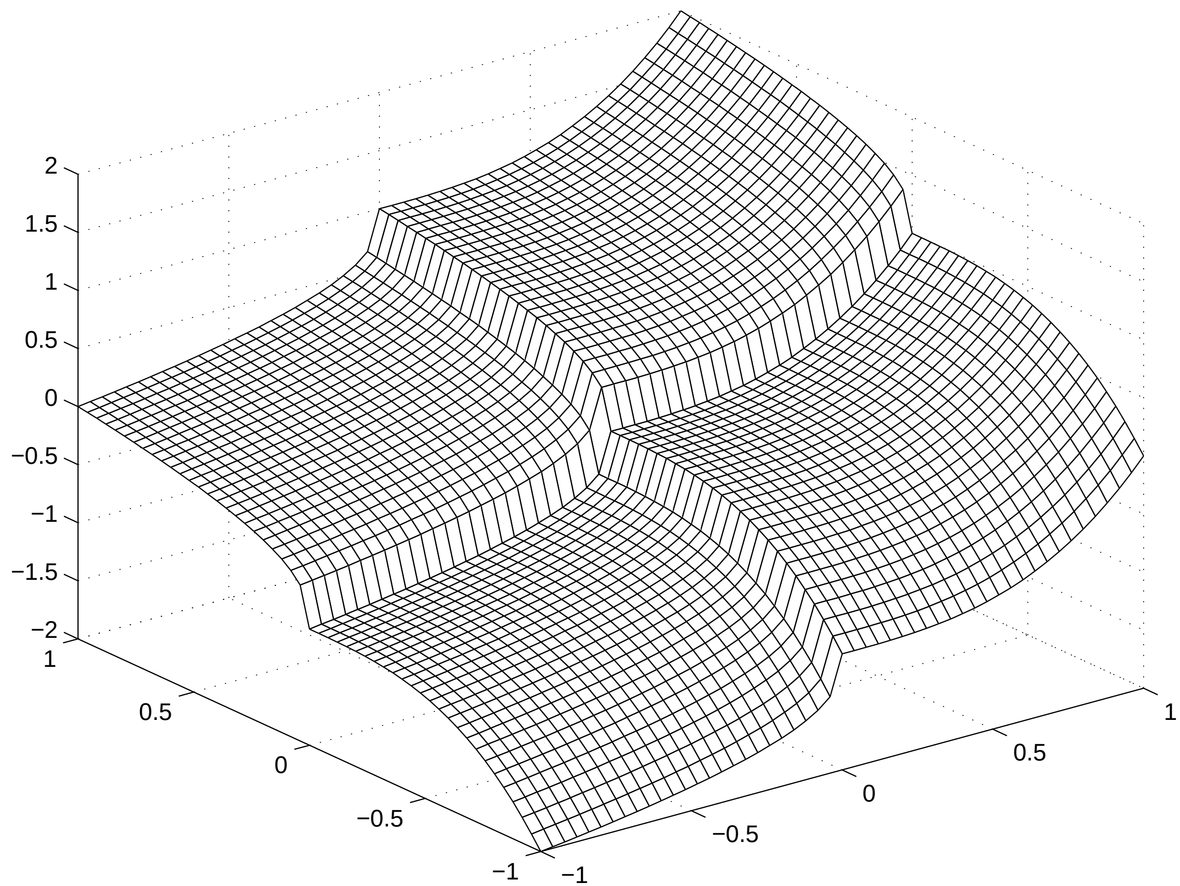
- Independent uniform distribution of the explanatory variables $x \in R^2$ in the interval $[-2, 2]$.
- Samples of $n = 10^2$, $n = 10^3$ and $n = 10^4$ observations.
- Independent normally distributed error terms ε_i with mean 0 and variance 1 in observations $\bar{u}_i = y(X_i) + \varepsilon_i$.
- Three test functions:

$$y(x) = 0.1x_1 + 0.1x_2 \quad (\text{lin1})$$

$$y(x) = x_1 + x_2 \quad (\text{lin2})$$

Monotonic regression test problems (cont.)

$$y(x) = f(x_1) - f(-x_2) \quad \text{where} \quad f(t) = \begin{cases} \sqrt[3]{t}, & t \leq 0, \\ t^3, & t > 0. \end{cases} \quad (\text{nonlin})$$



Relative error

algorithm	model	$n = 10^2$ #constr. = 322	$n = 10^3$ #constr. = 5497	$n = 10^4$ #constr. = 78170
GPAV	lin1	0.98	0.77	0.47
	lin2	2.79	2.43	2.02
	nonlin	3.27	5.66	11.56
GPAVR	lin1	0.01	0.07	0.09
	lin2	0.08	0.12	0.24
	nonlin	0.00	0.17	0.46

$$r.e._A = \frac{F_A - F_*}{F_*} \cdot 100\%$$

Computational time

algorithm	model	$n = 10^2$	$n = 10^3$	$n = 10^4$
GPAV	lin1	0.02	0.76	89.37
	lin2	0.01	0.71	93.76
	nonlin	0.01	0.67	87.51
GPAVR	lin1	0.05	1.67	234.31
	lin2	0.05	1.60	197.06
	nonlin	0.04	1.58	192.08
NEW	lin1	0.54	19.92	2135.03
	lin2	0.51	4.03	294.29
	nonlin	0.43	4.13	360.14
IBCR	lin1	0.21	129.74	—
	lin2	0.09	5.07	2203.10
	nonlin	0.08	6.68	3448.94

Part 2:

Optimization methods for postprocessing finite element solutions

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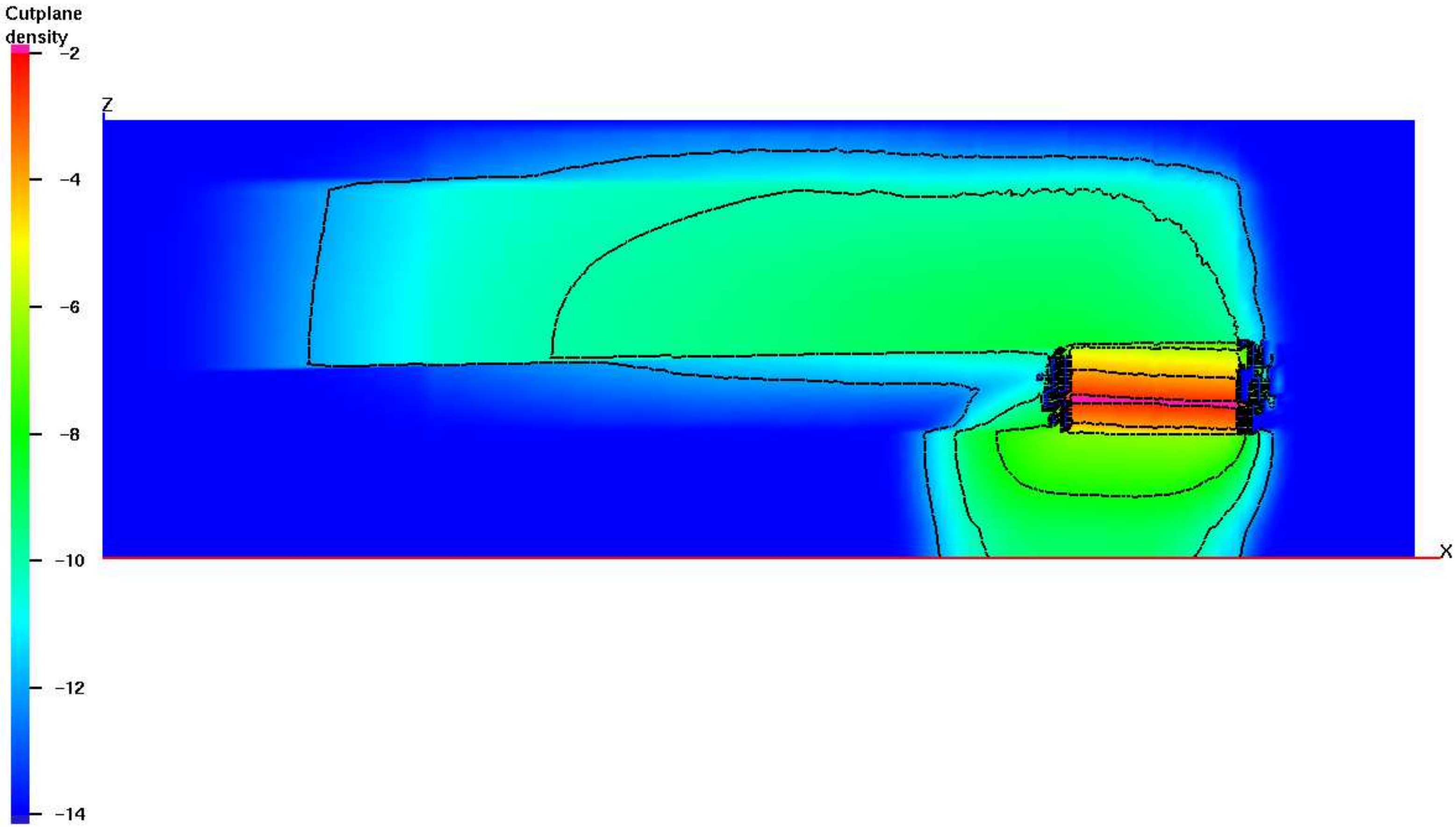
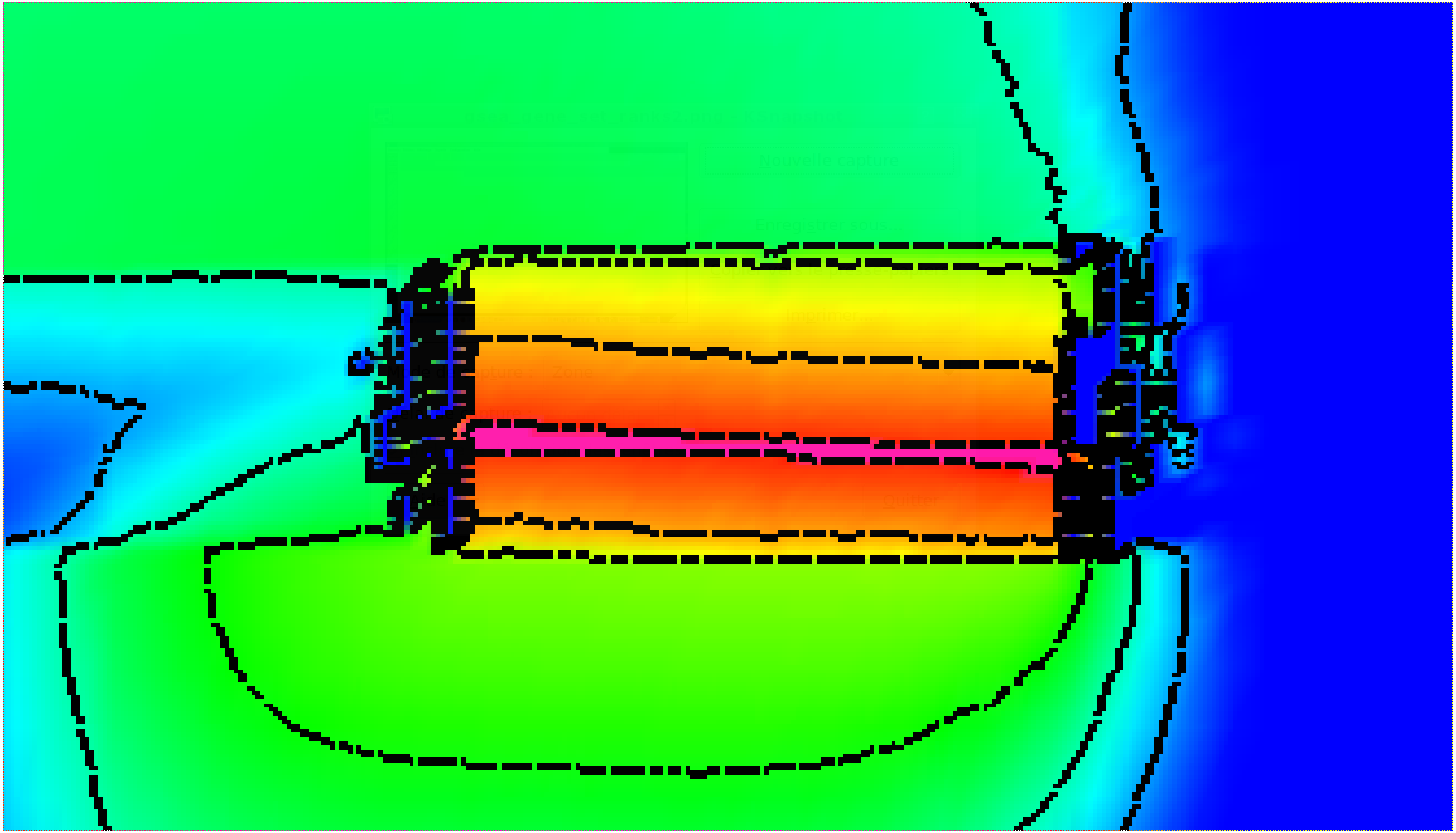
Origin



Non-negativity and non-monotonicity in nuclear waste transport simulation (Couplex1 test case simulation for ANDRA, the French Agency for Nuclear Waste Depositing, T=50500 years, 25000m$\times$700m)

Couplex1 zoomed



Non-negativity and non-monotonitity

Sources of troubles:

- Anisotropy and heterogeneity in the diffusion tensor.
- Distorted meshes.

Approaches for avoiding the troubles:

- Special meshes (Delaunay meshes, meshes oriented along the principal diffusion axis).
- Larger time steps (increase the main diagonal of approximation matrix), different time steps for advection and diffusion for the transport problem.
- Special schemes preserving non-negativity of solution for a wide class of meshes and diffusion tensors.
- Postprocessing of solution, least-change corrections recovering monotonicity and non-negativity, and preserving the accuracy.

Postprocessing as an optimization problem

Given a FE solution $\bar{u} \in R^n$, find $u_* \in R^n$ that solves the problem

$$
\begin{array}{lll}
\min & \frac{1}{2}\|u-\bar{u}\|^2 & \\
\text{s.t.} & Mu \geq 0, & (\text{monotonicity } u_j \geq u_i) \\
 & \alpha e \leq u \leq \beta e, & (\text{generalized non-negativity } \alpha \leq u_i \leq \beta) \\
 & e^T u = m, & (\text{conservativity } u_1 + \ldots + u_n = m)
\end{array}
$$

where

- the inequalities in $Mu \geq 0$ are of the form $u_j \geq u_i$ (adjacent FE cells)
- $e = (1, 1, \ldots, 1)^T \in R^n$
- the scalars $\alpha < \beta$ (originate, e.g., from the maximum principle)
- m is a scalar (e.g., the total mass $m > 0$)

Monotonic regression

Let $u_{\mathrm{M}} \in R^n$ solve the problem

$$\begin{array}{ll} \min & \frac{1}{2}\|u - \bar{u}\|^2 \\ \text{s.t.} & Mu \geq 0. \end{array}$$

Remarks

- there exist efficient methods for solving large-scale monotonic regression problems
- $e^T u_{\mathrm{M}} = e^T \bar{u}$
- $e^T \bar{u} = m \;\Rightarrow\; e^T u_{\mathrm{M}} = m$
- $\alpha e \leq u_{\mathrm{M}} \leq \beta e$ is not guaranteed

Box-constrained monotonic regression

Let $u_{\text{MB}} \in R^n$ solve the problem

$$\begin{array}{ll} \min & \frac{1}{2}\|u - \bar{u}\|^2 \\ \text{s.t.} & Mu \geq 0, \\ & \alpha e \leq u \leq \beta e. \end{array}$$

Remarks

- u_{MB} is the orthogonal projection of u_{M} on the box
- $e^T u_{\text{MB}} = e^T \bar{u}$ is not guaranteed

Lagrangian relaxation

Lagrangian function:

$$L(u,\lambda) = \frac{1}{2}\|u - \bar{u}\|^2 + \lambda(m - e^T u)$$

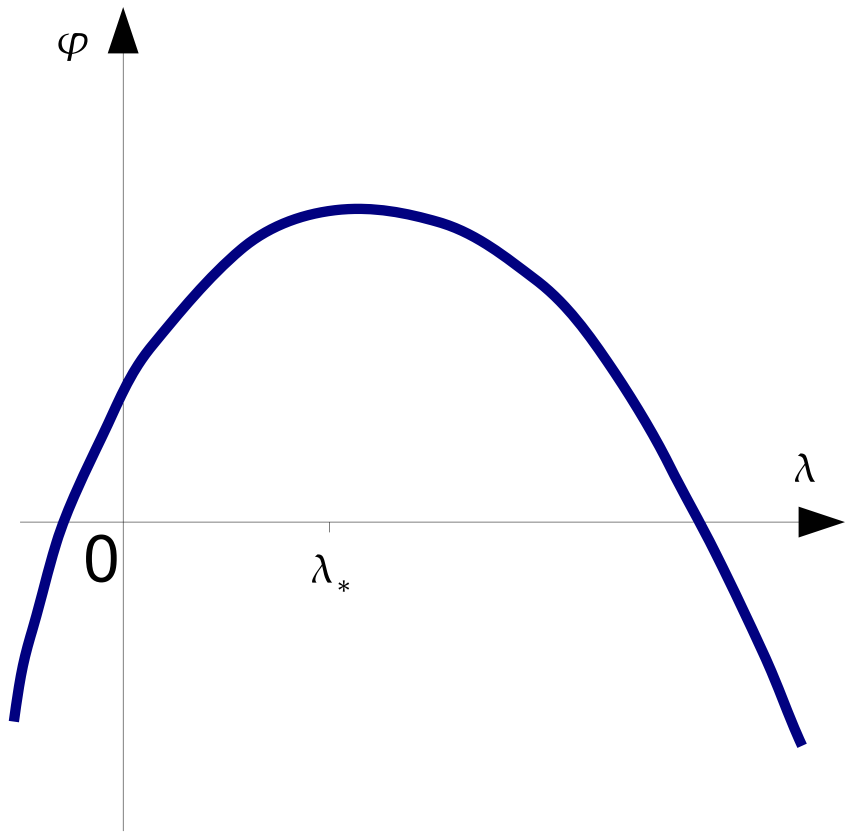
The dual function:

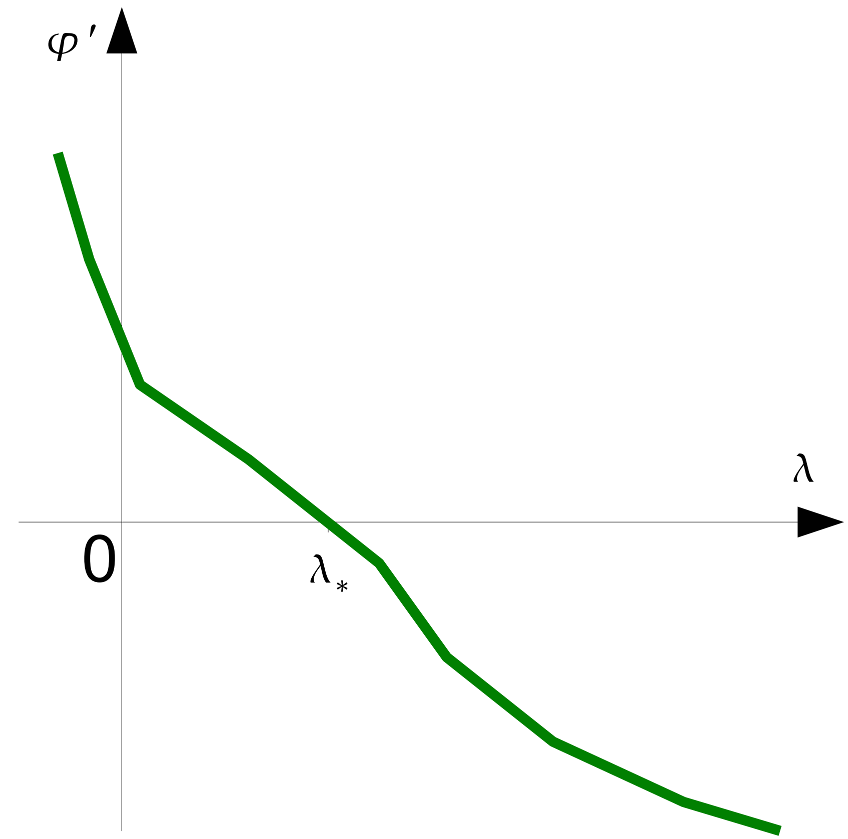
$$\begin{aligned} \varphi(\lambda) = \text{min} \quad & L(u,\lambda) \\ \text{s.t.} \quad & Mu \geq 0, \\ & \alpha e \leq u \leq \beta e. \end{aligned}$$

The dual problem:

$$\max_{\lambda} \varphi(\lambda)$$

The dual function and its derivative





The key observation

$$L(u,\lambda) = \frac{1}{2}\|u - \bar{u} - \lambda e\|^2 - \frac{1}{2}\lambda^2 + \lambda(m - e^T\bar{u})$$

Implication:

$$\begin{aligned} \varphi(\lambda) = q(\lambda) + \min \quad & \tfrac{1}{2}\|u - \bar{u}_\lambda\|^2 \\ \text{s.t.} \quad & Mu \geq 0, \\ & \alpha e \leq u \leq \beta e, \end{aligned}$$

where

$$q(\lambda) = -\frac{1}{2}\lambda^2 + \lambda(m - e^T\bar{u}), \qquad \bar{u}_\lambda = \bar{u} + \lambda e.$$

The key observation (cont.)

If u_{M} solves the problem

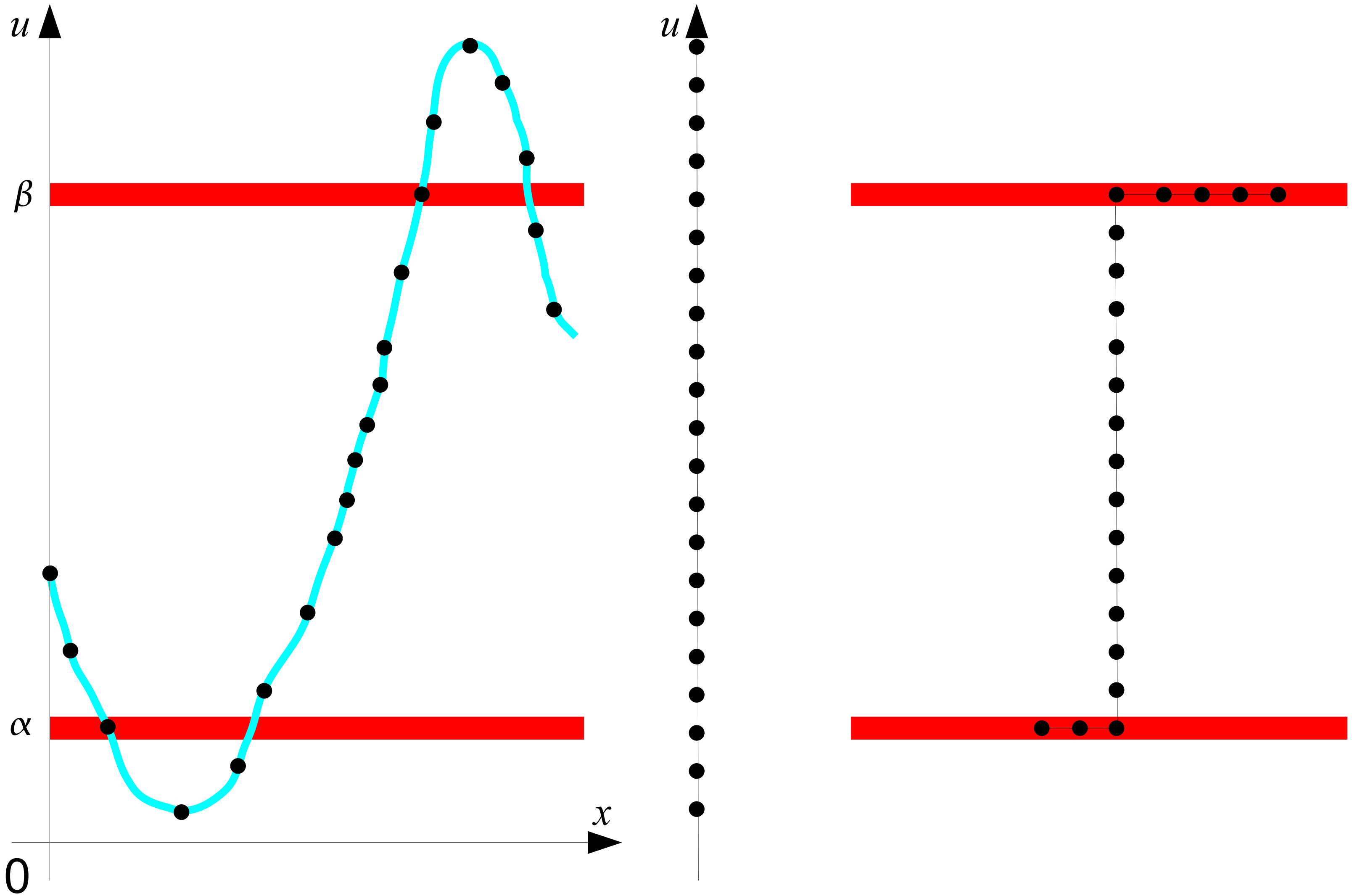
$$\begin{array}{ll} \min & \frac{1}{2}\|u - \bar{u}\|^2 \\ \text{s.t.} & Mu \geq 0, \end{array}$$

then $u_{\mathrm{M}} + \lambda e$ solves the problem

$$\begin{array}{ll} \min & \frac{1}{2}\|u - \bar{u}_\lambda\|^2 \\ \text{s.t.} & Mu \geq 0. \end{array}$$

Reformulation of the postprocessing problem: find the shift λ_* such that $u_*^T e = m$ for u_*, which is the projection of the shifted solution $u_{\mathrm{M}} + \lambda_* e$ on the box.

Shifting and projecting procedure



2D Test 1: $\delta(x,y)$ as the source function

Problem:

$$-\nabla\mathcal{D}\nabla C = \delta(x,y) \quad \text{in } \Omega = (-\infty;+\infty)^2 \text{— plane (x,y),}$$

where

$$\mathcal{D} = QDQ^T,$$

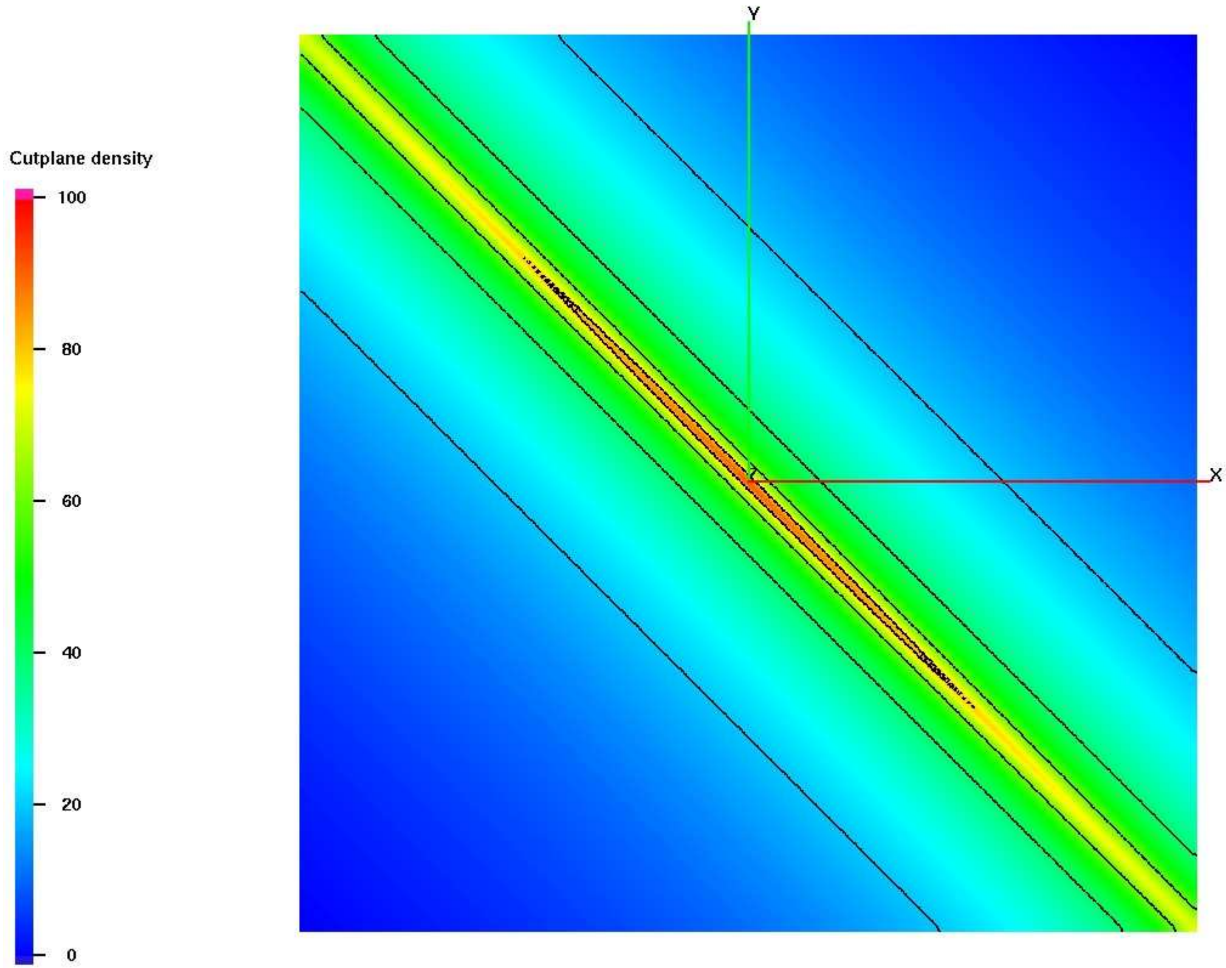
$$Q = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \text{ and } D = \begin{pmatrix} K_1 & 0 \\ 0 & K_2 \end{pmatrix}$$

Exact solution:

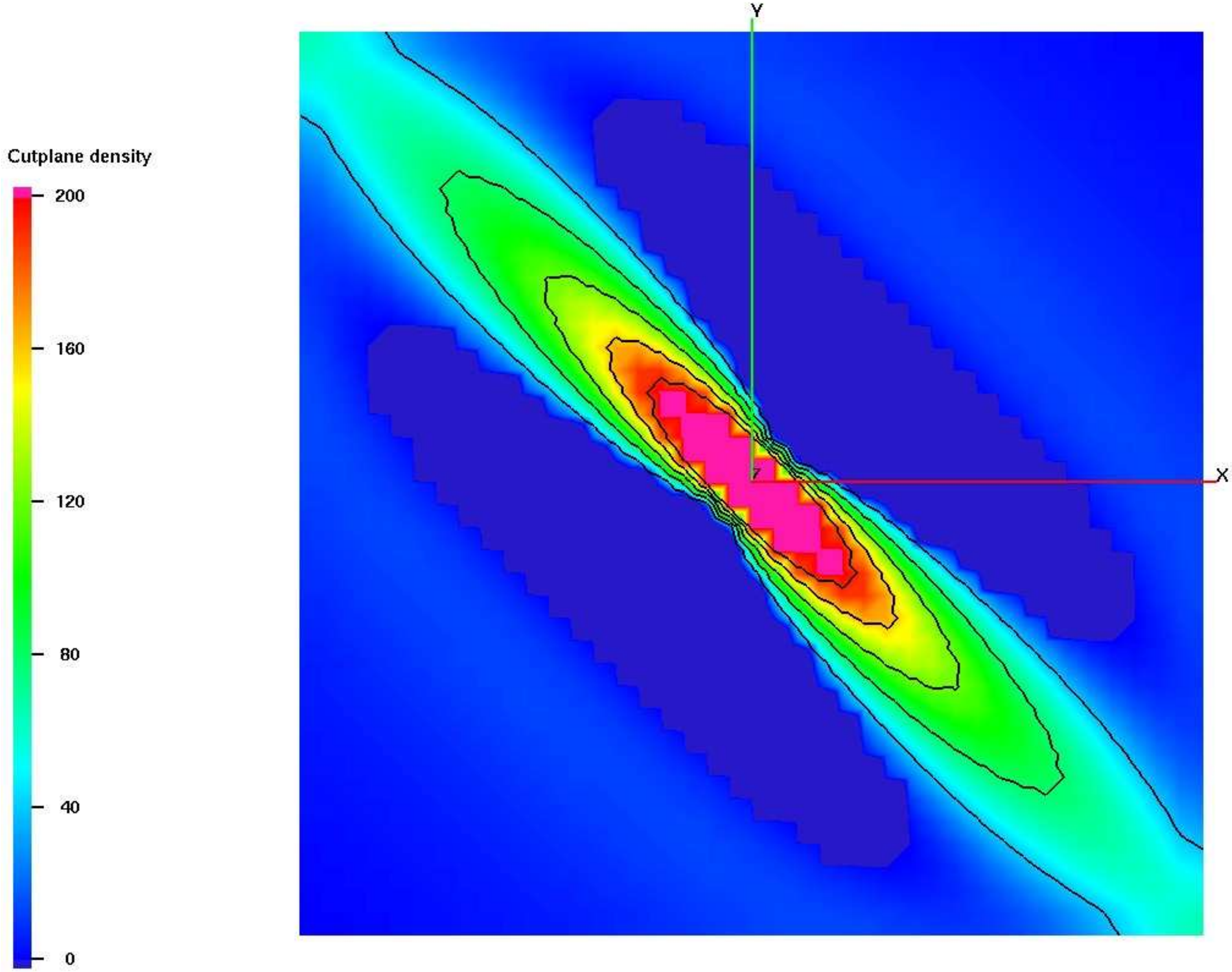
$$C = -\frac{1}{2\pi\sqrt{K_1 K_2}} \ln\sqrt{\frac{(x\cos\alpha - y\sin\alpha)^2}{K_1} + \frac{(x\sin\alpha + y\cos\alpha)^2}{K_2}}$$

Test 1: Exact solution

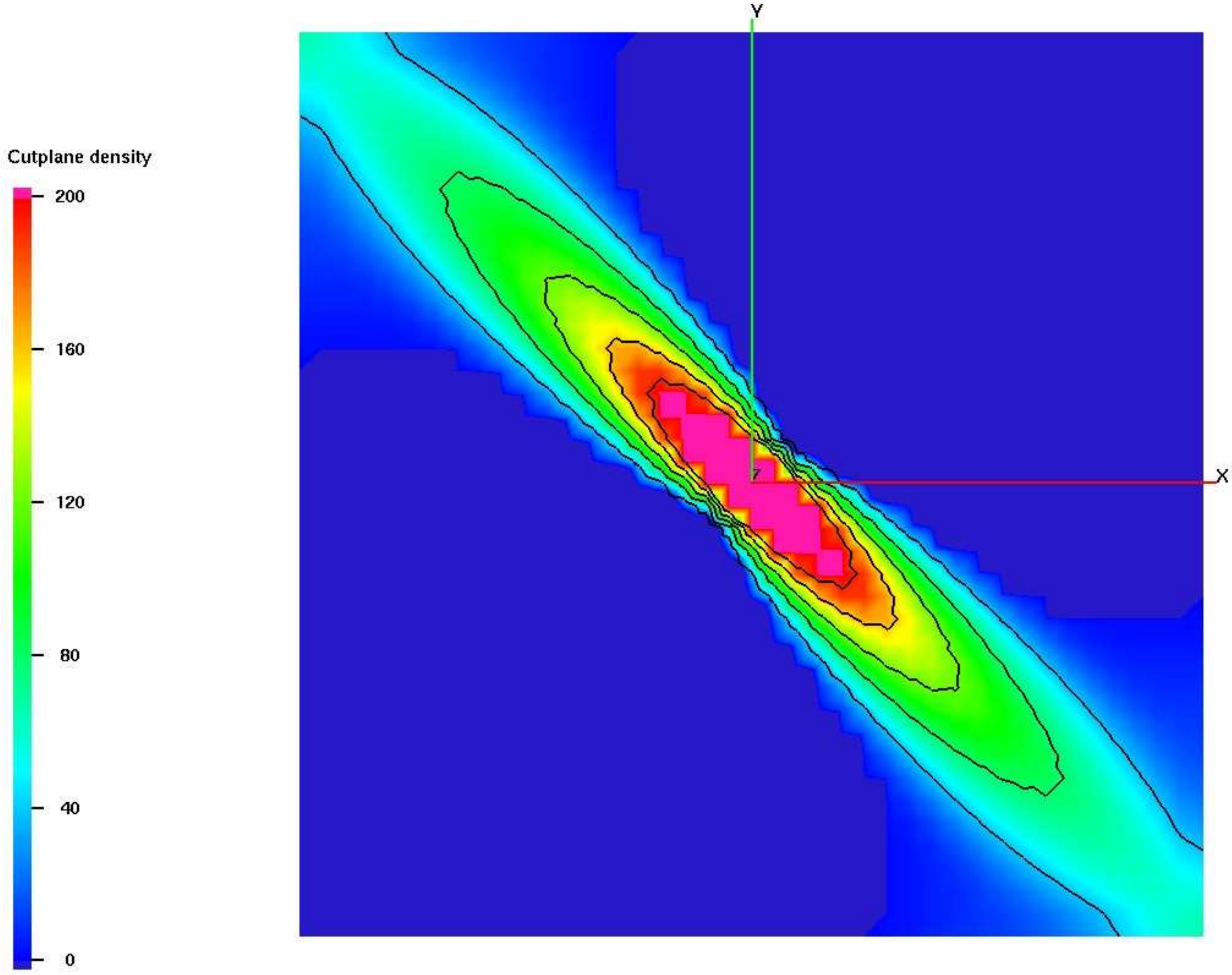
$$D = \begin{pmatrix} 1 & 0 \\ 0 & 10^{-4} \end{pmatrix}, \qquad \alpha = -\frac{\pi}{4} \text{—rotation angle}$$



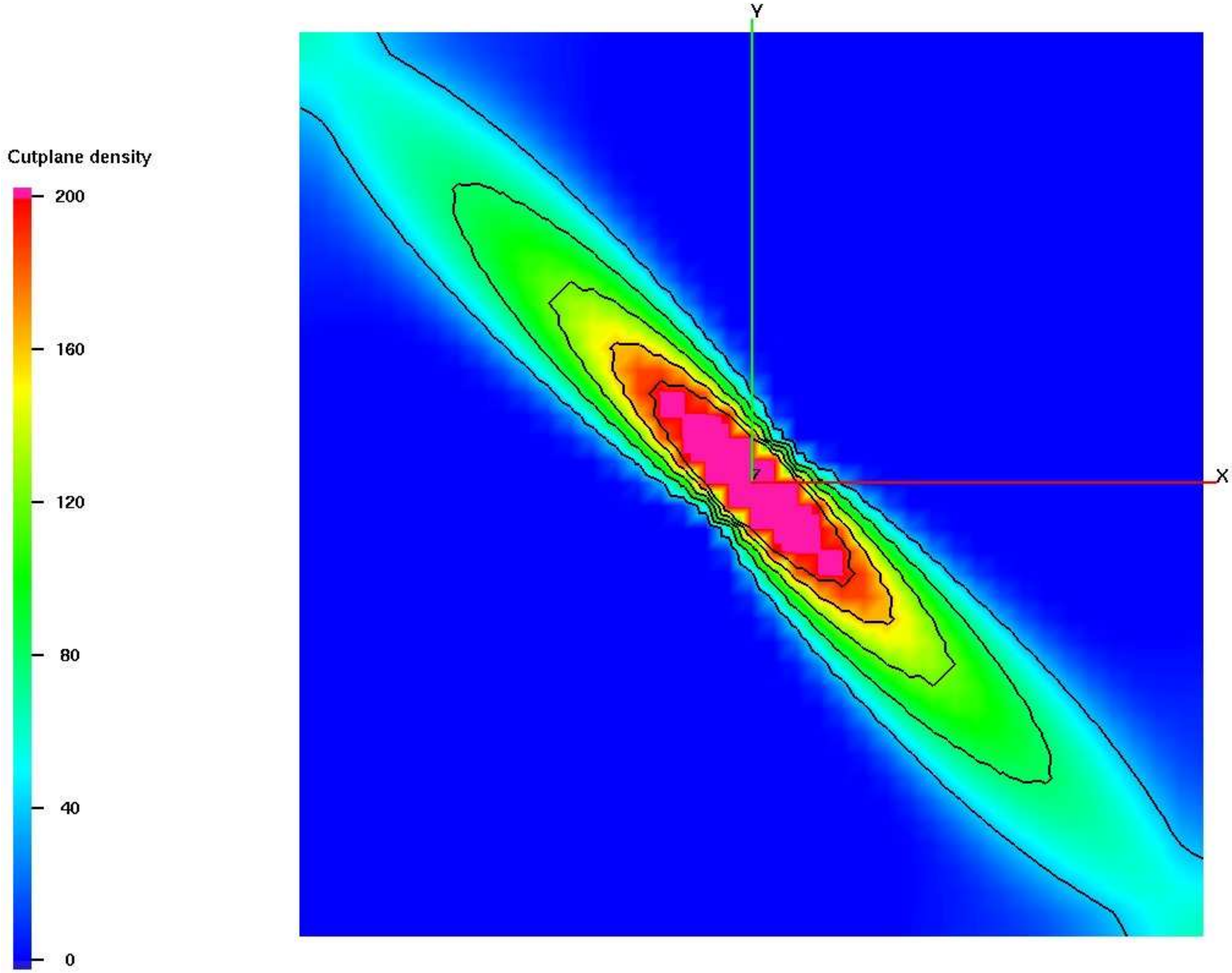
Test 1: Numerical solution



Test 1: Monotonicity recovering solution



Test 1: Final postprocessed solution



Test 1: CPU time

Number of unknowns	Solving time	Postprocessing time
3200	0.53	0.35
12800	5.33	6.14
51200	68.4	78.04

2D Test 2:

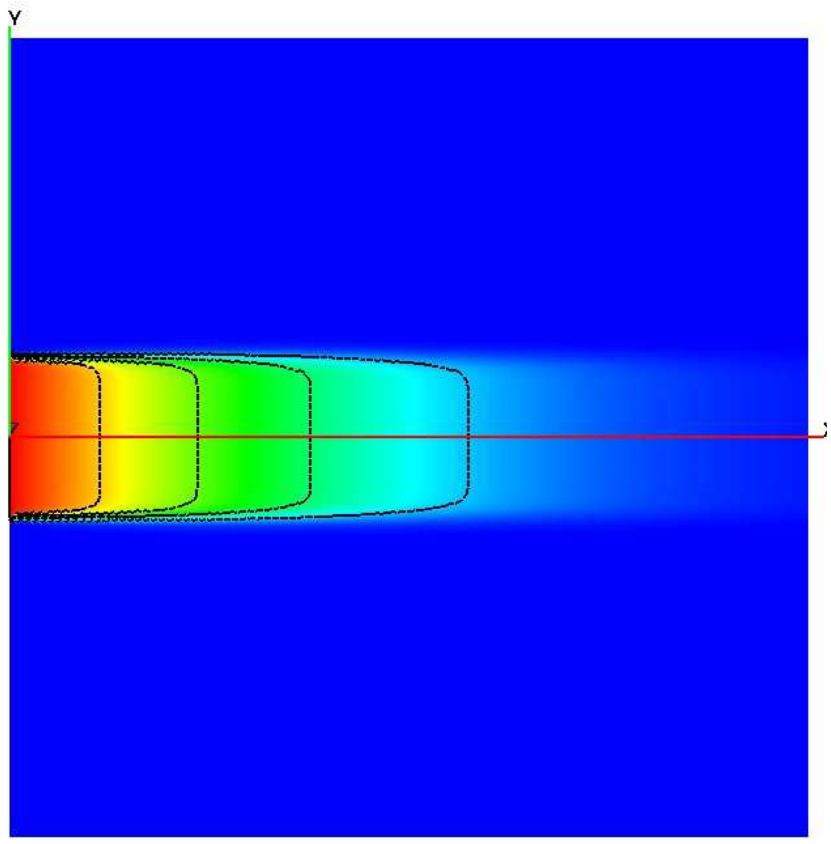
Non-homogeneous Dirichlet boundary conditions

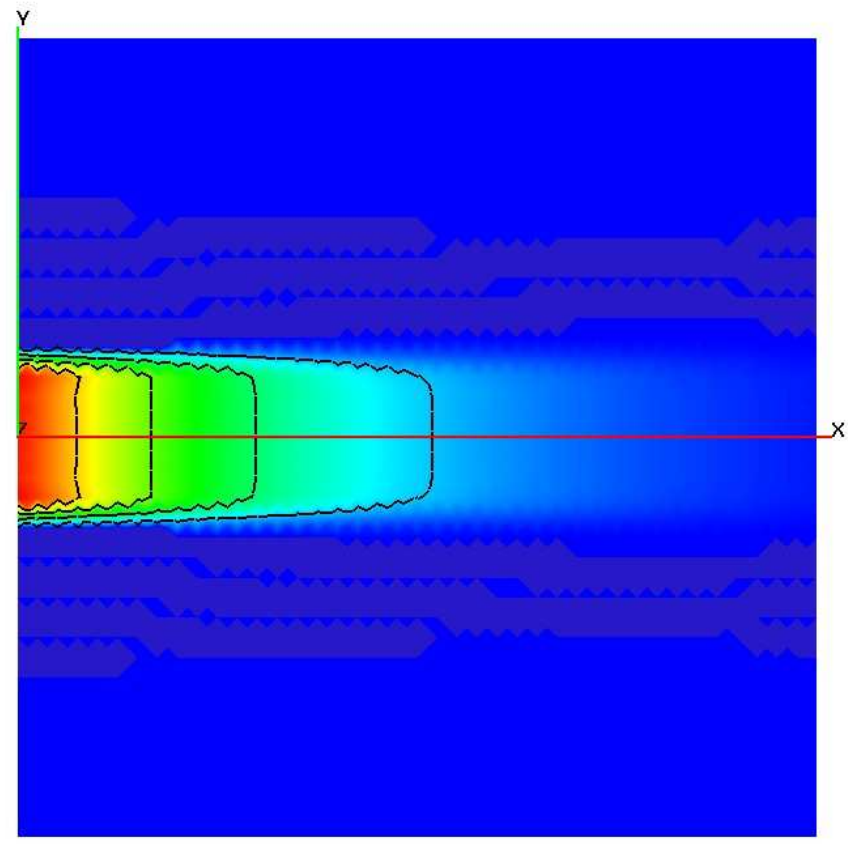
Problem:

$$
\begin{aligned}
\frac{\partial C}{\partial t} - \nabla \mathcal{D} \nabla C &= 0 \quad \text{in } \Omega \times [0;T], \quad \Omega = (0;+\infty) \times (-\infty;+\infty), \\
C(x,y,0) &= 0 \quad \text{in } \Omega \text{ — initial conditions}, \\
\left.\frac{\partial C}{\partial x}\right|_{x \to +\infty} &= 0 \quad y \in (-\infty;+\infty),\ t > 0 \text{ and} \\
\left.\frac{\partial C}{\partial y}\right|_{y \to \pm\infty} &= 0 \quad x \in (0;+\infty),\ t > 0 \text{ — Neumann b.c.} \\
C(0,y,t) &= \begin{cases} 1 & \text{if } |y| < 0.1, \\ 0 & \text{elsewhere.} \end{cases} \quad \text{— Dirichlet b.c.}
\end{aligned}
$$

Anisotropic diffusion tensor: $\mathcal{D} = \begin{pmatrix} 10^{-3} & 0 \\ 0 & 1 \end{pmatrix}$

2D Test 2: Exact and numerical solutions

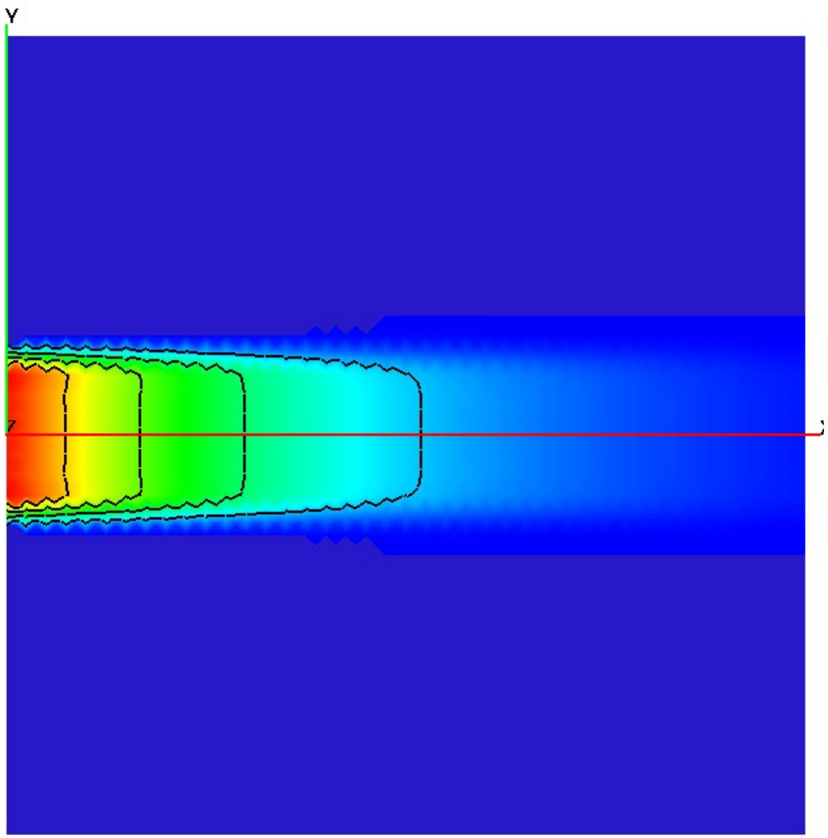




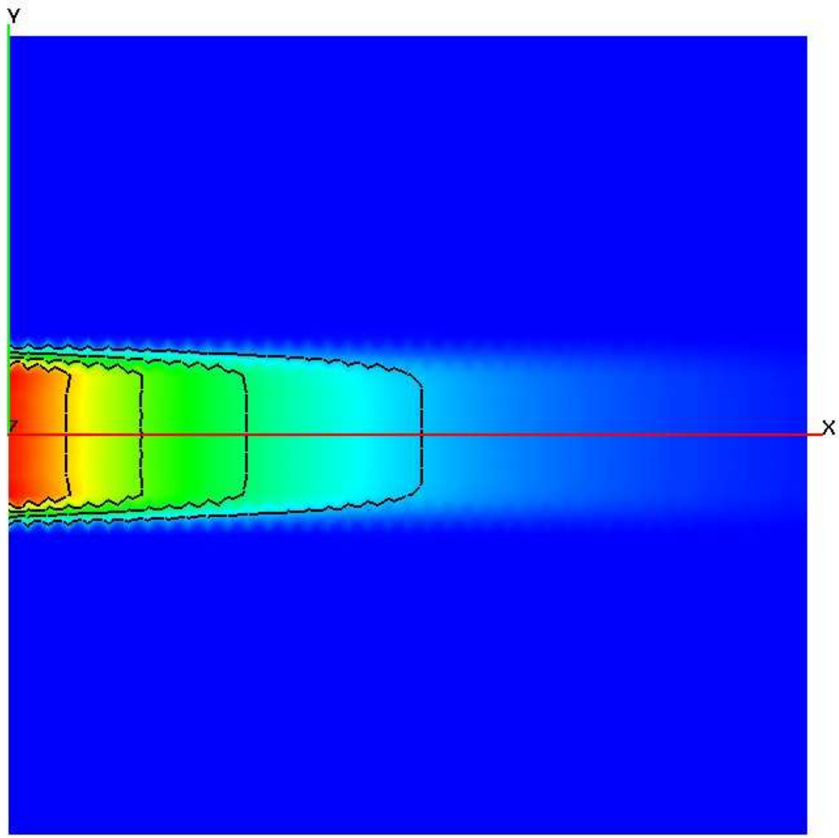
Exact solution

Numerical solution

2D Test 2: Postprocessing



Monotonicity recovering solution



Final postprocessed solution

Future plans

$$
\begin{aligned}
\text{min} \quad & \|Au - b\| \\
\text{s.t.} \quad & Mu \geq 0, && \text{(monotonicity)} \\
& \alpha e \leq u \leq \beta e, && \text{(generalized non-negativity)} \\
& e^T u = m. && \text{(conservativity)}
\end{aligned}
$$