Some free-boundary problems and their control

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Outline

Free-boundary problem = differential system with unknown function(s) and domain(s)
A part of the boundary? An internal curve or surface? etc.

Many motivations sharing transitions or changes of state:
buying to selling actions in finance, active to inactive transition in biology, phase transition in physics, etc.

The free boundary indicates the points where transition occurs

Figure: Buying to selling change process

The free boundary indicates: change of trade activity (e.g. buy to sell)

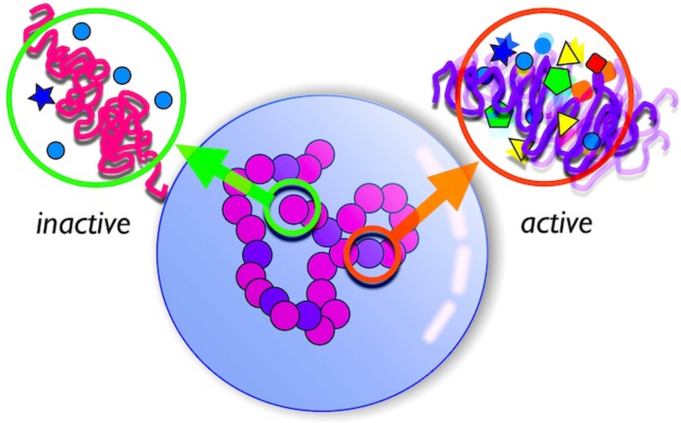

Figure: Active to inactive biological change

The free boundary indicates: change of biological role (e.g. active to inactive)

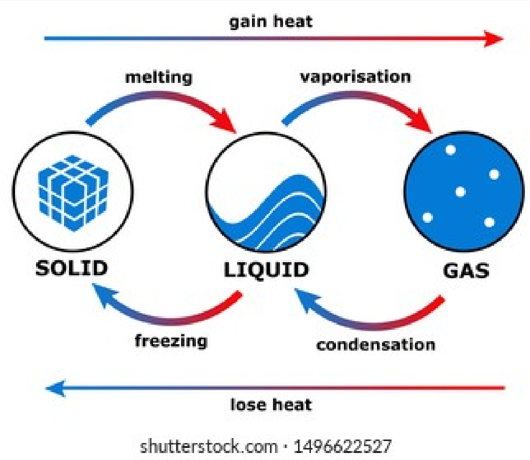

Figure: Phase transition

The free boundary indicates: change of state (e.g. solid to liquid)
Interesting question: can we act to control the free boundary evolution?

Usually: ODE's and/or PDE's and complements + additional laws

$$\left\{ \begin{array}{l} E(y) = 0 \ \text{ in } \ \Omega \ + \dots \\ \text{Additional laws} \end{array} \right.$$

Many works on the theory: since [Caffarelli 1976, Friedman 1978, Monakhov 1983, Crank 1987, Vázquez 1987, Texeira 2007, . . .]

Not so many on the numerics: [Proc. Workshops in Jyvaskyla 1990, Kyoto 1991; Chen 2016, . . .]

Example 1: The obstacle problem

Data: Ω_0, $f = f(x)$, $\varphi = \varphi(x)$ and $\psi = \psi(x)$
Unknowns: Ω and u

$$\begin{cases} u \geq \varphi \ \text{ in } \ \Omega_0 \\ -\Delta u = f(x) \ \text{ in } \ \Omega := \{x \in \Omega_0 : u(x) > \varphi(x)\} \\ u = \psi \ \text{ on } \ \partial\Omega_0 \end{cases}$$

The solution to the obstacle problem

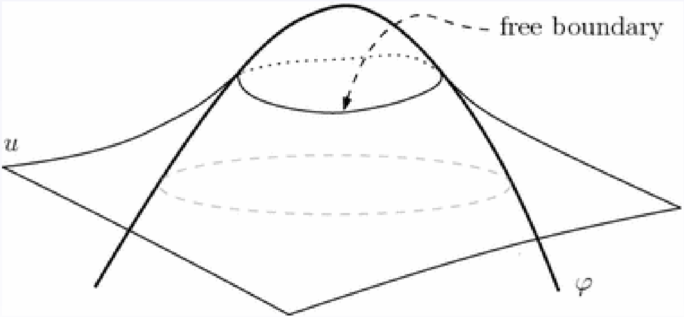

Figure: The obstacle problem

The solution to the obstacle problem

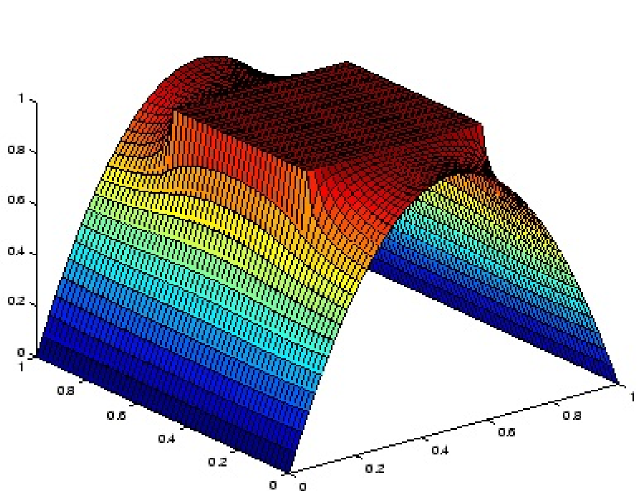

Figure: An obstacle problem for a nonregular obstacle. Numerical solution

The obstacle problem

Data: Ω_0, $f = f(x)$, $\varphi = \varphi(x)$ and $\psi = \psi(x)$

$$\left\{ \begin{array}{l} u \geq \varphi \ \text{ in } \ \Omega_0 \\ -\Delta u = f(x) \ \text{ in } \ \Omega := \{x \in \Omega_0 : u(x) > \varphi(x)\} \\ u = \psi \ \text{ on } \ \partial\Omega_0 \end{array} \right.$$

Unknowns: Ω and u

Many theoretical results: reformulation as a variational inequality

$$\left\{ \begin{array}{l} \int \nabla u \cdot (\nabla v - \nabla u)\, dx \geq \int f(v - u)\, dx \\ \forall v \in K := \{z \in H^1(\Omega_0) : z \geq \varphi, \ \ z = \psi \ \text{ on } \ \partial\Omega_0\}, \ \ u \in K \end{array} \right.$$

Existence, uniqueness, regularity, . . . [Friedman 1988, Caffarelli 1998, . . .]

Numerical resolution: [Scholz 1984, Cheng et al 2021, . . .]

Example 2: Navier-Stokes + free boundaries

Motivation: Rotating fluids [Ciuperca, 1996]

Fluid rotating around a flexible cylindrical structure (a gas container)

Two actions:
• $y_B = \omega \times x$ on the fixed external boundary
• p_F on the unknown internal boundary

The free boundary is the internal boundary

2D Navier-Stokes and free boundaries

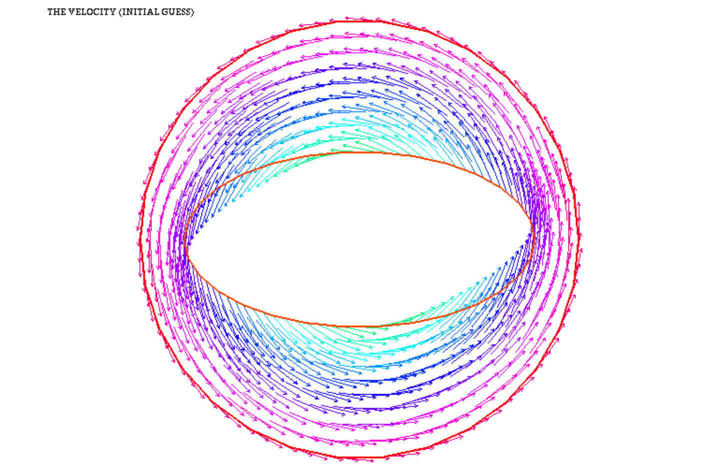

Figure: A fluid rotating around a flexible structure

2D Navier-Stokes and free boundaries

Data: $\Omega_0 \subset \mathbf{R}^2$, $\partial\Omega_0 = S_B \cup S_{F,0}$ (the circle of radius 1 and a closed interior curve);
$\mathbf{k}$ (Gravity force); y_B and p_F (boundary data)

Unknowns: $\Omega = \Omega(t) \subset \mathbf{R}^2$ for $t \in [0, T]$, y, p with

$$\left\{\begin{array}{l}
\partial\Omega(t) = S_B \cup S_F(t) \\
\\
-\nu\Delta y + (y\cdot\nabla)y + \nabla p = \mathbf{k}, \quad x \in \Omega(t),\ t \in (0,T) \\
\nabla \cdot y = 0, \quad x \in \Omega(t),\ t \in (0,T) \\
y = y_B, \quad x \in S_B,\ t \in (0,T) \\
(-\nu D(y) + p\mathrm{Id.}) \cdot \mathbf{n} = p_F\, \mathbf{n}, \quad x \in S_F(t),\ t \in (0,T) \\
\\
\Omega(0) = \Omega_0
\end{array}\right.$$

and

$$V(x,t) = y(x,t), \quad x \in S_F(t),\ t \in (0,T)$$

The free boundary: $\{(x,t) : x \in S_F(t),\ t \in (0,T)\}$

2D Navier-Stokes and free boundaries

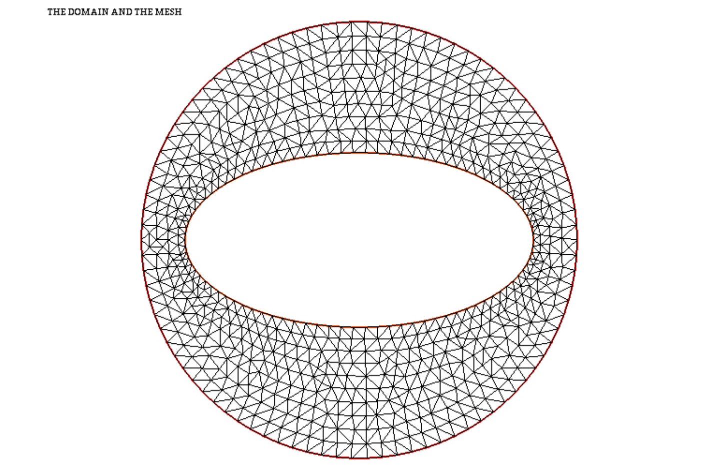

Figure: Initial state: free boundary and mesh

2D Navier-Stokes and free boundaries

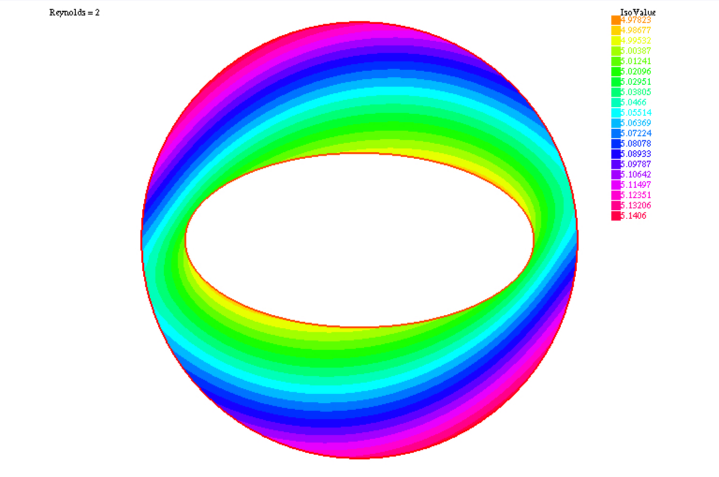

Figure: Initial state: pressure

2D Navier-Stokes and free boundaries

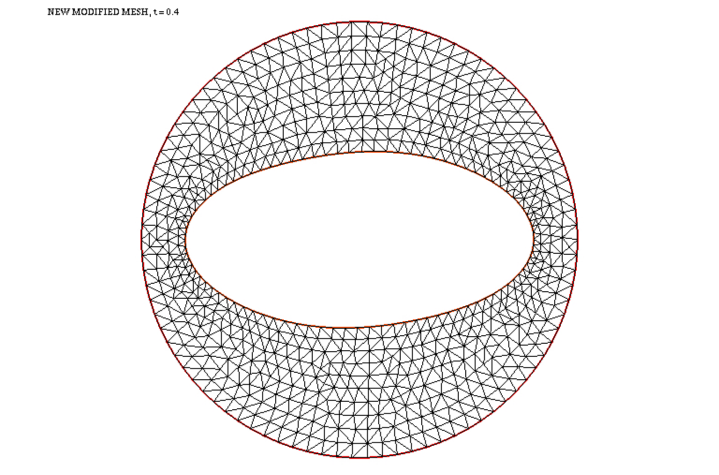

Figure: State at $t = 0.5$: free boundary and mesh

2D Navier-Stokes and free boundaries

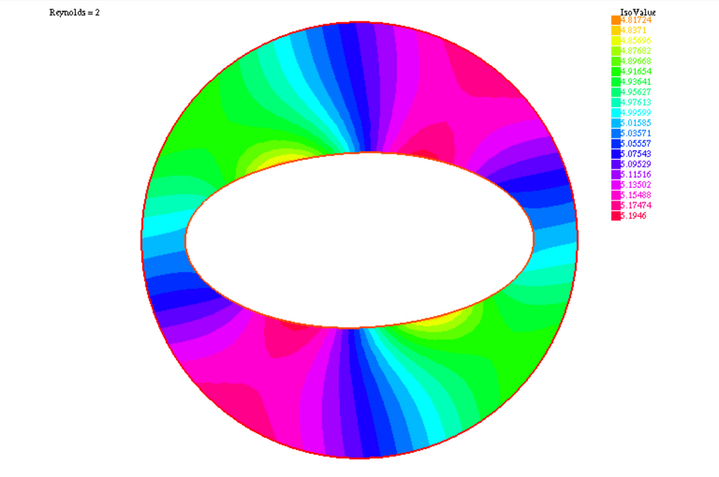

Figure: State at $t = 0.5$: pressure

2D Navier-Stokes and free boundaries

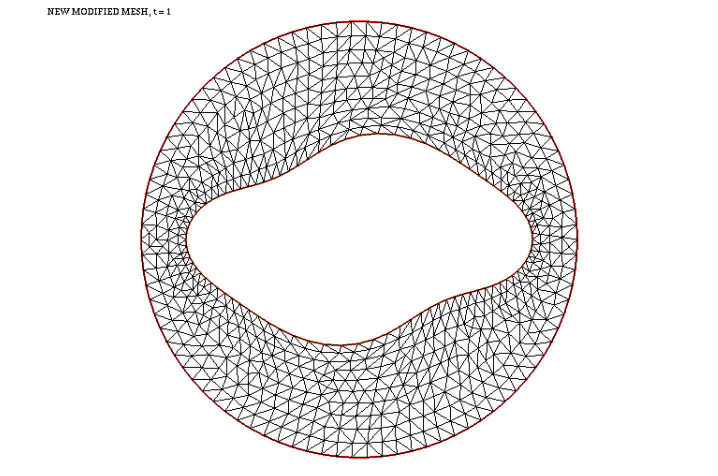

Figure: Final state: free boundary and mesh

2D Navier-Stokes and free boundaries

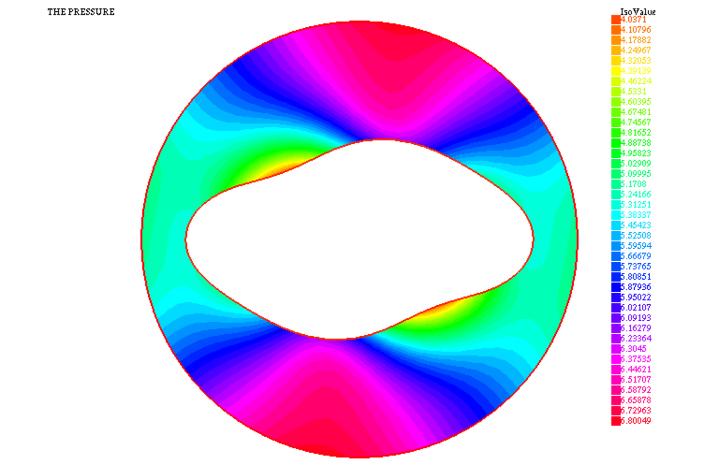

Figure: Final state: pressure

2D Navier-Stokes and free boundaries
A related control question

Question: Is it possible to choose p_F to get desired $\Omega(T)$, $y(\cdot\,,T)$ and $p(\cdot\,,T)$?

$$\left\{\begin{array}{l} \partial\Omega(t) = S_B \cup S_F(t) \\ \\ -\nu\Delta y + (y\cdot\nabla)y + \nabla p = \mathbf{k}, \quad x\in\Omega(t),\ t\in(0,T) \\ \nabla\cdot y = 0, \quad x\in\Omega(t),\ t\in(0,T) \\ y = y_B, \quad x\in S_B,\ t\in(0,T) \\ (-\nu D(y) + p\mathrm{Id.})\cdot\mathbf{n} = p_F\,\mathbf{n}, \quad x\in S_F(t),\ t\in(0,T) \\ \\ \Omega(0) = \Omega_0 \end{array}\right.$$

and

$$V(x,t) = y(x,t), \quad x\in S_F(t),\ t\in(0,T)$$

Example 3: The one-phase Stefan problem

Motivation: melting of ice and similar phenomena
In a simple situation (1D, one-phase):

- Heat equation on the left, $x < \ell(t)$, $t \in (0, T)$
- Initial and boundary conditions at $t = 0$, on the left and on the right
- Stefan condition on $x = \ell(t)$, $t \in (0, T)$

The free boundary is $x = \ell(t)$, controlled dynamically by y
Water for $x < \ell(t)$, Ice for $x > \ell(t)$

Motivation of Stefan problems: melting of ice

Figure: Ice and water

Motivation of Stefan problems: melting of ice

Figure: Ice and water

Figure: Jozef Stefan (1835–1893)

Discovered the power law: $j^* = \sigma T^4$ – Advisor of Boltzmann

The Stefan problem

Motivation: melting of ice and similar phenomena
In a simple situation (1D, one-phase), with data f, $k > 0$, $\ell_0 > 0$, $y_0 \geq 0$:

$$\left\{ \begin{array}{l} y_t - y_{xx} = f(x,t), \quad x \in (0, \ell(t)), \quad t \in (0,T) \\ y(0,t) = y(\ell(t),t) = 0, \quad t \in (0,T) \\ \ell(0) = \ell_0, \quad y(x,0) = y_0(x), \quad x \in (0, \ell_0) \end{array} \right. \qquad \text{and} \quad y_x(\ell(t),t) = -k\ell'(t), \quad t \in (0,T)$$

The free boundary is $x = \ell(t)$, controlled dynamically by y.
Also motivated by other applications:

- Solidification processes, tumor growth models and others [Friedman, . . .]
- Gas flow through porous media [Aronson, Fasano, Vazquez, . . .]
- Finances [Salsa, . . .]

The solution to the 1D one-phase Stefan problem

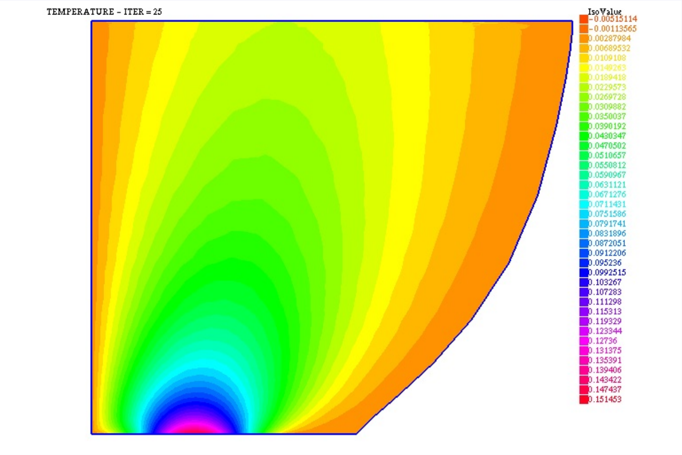

Figure: The iso-regions $y = \text{Const.}$ and the free boundary $x = \ell(t)$

The solution to the 1D one-phase Stefan problem

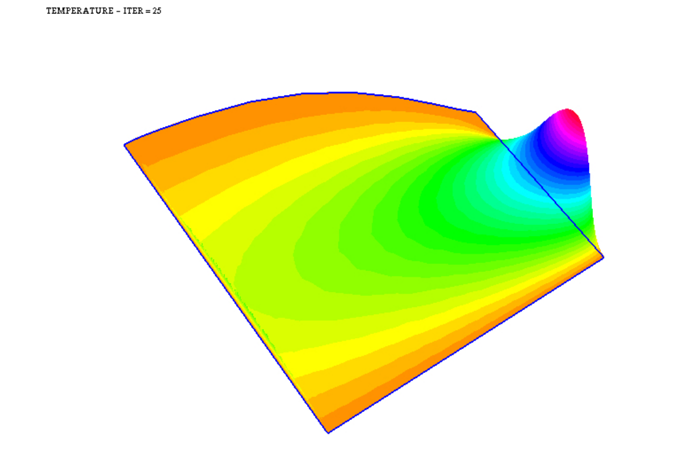

Figure: The iso-regions $y =$ Const. and the free boundary $x = \ell(t)$

Analysis of the Stefan problem
Main questions and results

- Reformulation as a parabolic variational inequality, weak solution:

$$\text{New (working) variable: } w(x,t) = \int_0^t (1_{\{y>0\}} y)(x,s)\, ds$$

Formulation (for some f, ψ and Q):

$$\left\{ \begin{array}{l} \int (w_t(v-w) + w_x(v_x - w_x))\, dx \geq \int f(v-w)\, dx \\ \forall v \in K := \{z \in H^1(Q) : z \geq 0, \;\; z = \psi \;\text{ on }\; \partial_p Q\}, \;\; w \in K \end{array} \right.$$

- Existence, uniqueness
- Regularity of the free boundary

Contributions by Duvaut, Friedman, Kinderlherer, Caffarelli, . . .

Controllability
NC of 1D one-phase Stefan

Find $v \in L^2(\omega \times (0,T))$, $\ell = \ell(t) > 0$ and $y = y(x,t)$ with

$$(NC)_1 \quad \left\{ \begin{array}{l} y_t - y_{xx} = v 1_\omega, \quad x \in (0, \ell(t)), \ t \in (0,T) \\ y(0,t) = y(\ell(t),t) = 0, \quad t \in (0,T) \\ \ell(0) = \ell_0, \quad y(x,0) = y_0(x), \quad x \in (0, \ell_0) \end{array} \right. \qquad y_x(\ell(t),t) = -k\ell'(t), \ t \in (0,T)$$

and

$$(NC)_2 \qquad y(x,T) = 0, \quad x \in (0, \ell(T))$$

Here: $\ell_0 > 0$, $y_0 \geq 0$, $\omega = (a,b) \subset (0, \ell_0)$ (small)

Theorem (Local NC, EFC-Limaco-Menezes 2016)

$\exists \varepsilon > 0$ *such that* $\|y_0\|_{H_0^1} \leq \varepsilon \ \Rightarrow \exists v, \ell, y$ *satisfying* $(NC)_1, (NC)_2$

Recall: Heat flux proportional to free boundary speed
Note: Also NC with Dirichlet or Neumann boundary controls . . .

Formulation as a fixed-point equation
1D one-phase Stefan

For the proof:

1. $\left[y_x(\ell(t), t) \equiv -k\ell'(t),\ \ \ell(0) = \ell_0\right] \ \Leftrightarrow\ \ell(t) \equiv \ell_0 - \int_0^t y_x(\ell(s), s)\, ds$
2. The good formulation: $\ell = \Lambda(\ell),\ \ \ell \in \mathcal{M} \subset C^1([0, T])$, with

$$L = \Lambda(\ell) \ \Leftrightarrow\ L(t) = \ell_0 - k \int_0^t y_x(\ell(s), s)\, ds \ \ \forall t \quad \text{where}$$

$$\begin{cases} y_t - y_{xx} = v 1_\omega, & x \in (0, \ell(t)),\ t \in (0, T) \\ y(0, t) = y(\ell(t), t) = 0, & t \in (0, T) \\ y(x, 0) = y_0(x), & x \in (0, \ell_0) \end{cases}$$

and

$$y(x, T) = 0, \ \ x \in (0, \ell(T))$$

(a NC problem for a fixed boundary)

3. Schauder's Theorem $\Rightarrow \exists$ fixed-points of Λ

The method: $\ell^{n+1} = \Lambda(\ell^n)$ for $n \geq 0$

For the numerical solution for prescribed ℓ:
Fursikov-Imanuvilov reformulation + finite element approx.

Fursikov-Imanuvilov reformulation and approximation

Task: NC for prescribed ℓ (noncylindrical domain)

With appropriate $\rho = \rho(x,t)$ ($\rho|_{t=T} = +\infty$) and $\rho_0 = \rho_0(x,t)$

$$\begin{cases} \text{Minimize } \iint [\rho^2 |y|^2 + 1_\omega \rho_0^2 |v|^2] \\ \text{Subject to } v \in L^2(\omega \times (0,T)), \quad y : \text{asssociated state} \end{cases}$$

Then:

- Automatically: $y(\cdot\,,T) = 0$
- The solution: $y = \rho^{-2} L^* p$, $v = -\rho_0^{-2} p|_{\omega \times (0,T)}$ (Lagrange)

$$\begin{cases} \iint \left(\rho^{-2} L^* p \, L^* q + \rho_0^{-2} 1_\omega p \, q \right) = \int_\Omega y_0(x)\, q(x,0)\, dx \\ \forall q \in P, \quad p \in P \end{cases}$$

for $L^* p := -p_t - p_{xx}$, appropriate P ...
Essentially, $p \in P \Leftrightarrow \iint \left(\rho^{-2} |L^* p|^2 + \rho_0^{-2} 1_\omega |p|^2 \right) < +\infty$

Computation of a null control for prescribed ℓ
A Lax-Milgram problem

$$\left\{\begin{array}{l}\iint \left(\rho^{-2}L^*p\,L^*q+\rho_0^{-2}1_\omega p\,q\right)=\int_\Omega y_0(x)\,q(x,0)\,dx\\ \forall q\in P,\quad p\in P\end{array}\right.$$

Numerical approximation (I): finite dimensional $P_h\subset P$

$$\left\{\begin{array}{l}\iint_{\Omega\times(0,T)}\left(\rho^{-2}L^*p_h\,L^*q_h+\rho_0^{-2}1_\omega p_h,q_h\right)=\int_\Omega y_0(x)\,q_h(x,0)\,dx\\ \forall q_h\in P_h,\quad p_h\in P_h\end{array}\right.$$

Numerical approximation (II): mixed reformulation in $Z\times\Lambda$ (multipliers)
+ finite dimensional approx. ($Z_h\subset Z$, $\Lambda_h\subset\Lambda$)

$$\left\{\begin{array}{l}\iint (y_h\,z_h+1_\omega f_h,g_h)+\langle z_h-\rho^{-2}L^*(\rho_0^2g_h),\lambda_h\rangle=\int_\Omega \rho_0(x,0)y_0(x)\,g_h(x,0)\,dx\\ \langle\left(y_h-\rho^{-2}L^*(\rho_0^2f_h)\right),\mu_h\rangle=0\\ \forall(z,g)\in Z,\quad\forall\mu\in\Lambda;\quad (y,f)\in Z,\quad \lambda\in\Lambda\end{array}\right.$$

The strategy:

a) Fix ℓ^0

b) For given $n \geq 0$, ℓ^n:

   b.1) NC with $\ell^n \to v^n$ and y^n with $y^n(x, T) \equiv 0$
   (Fursikov-Imanuvilov, $P_h \subset P$, etc.)

   b.2) $v^n, \ell^n, y^n \to \ell^{n+1}$

Numerical experiments

All experiments with FreeFem++ (http://www.freefem.org//ff++)
To appear soon, [EFC-Souza]

A first numerical experiment: one-phase Stefan

- $\ell_0 = 5$, $y_0(x) \equiv 2.5 \sin^2(\pi x/\ell_0)$.
- $d_0 = 2.15$, $\omega = (0, 3)$, $k = 0.06$, $T = 10$.

Stopping criterion: $\|y^{n+1} - y^n\|_{L^2}/\|y^{n+1}\|_{L^2} \leq 10^{-5}$
Starting from $y^0 \equiv y_0$: convergence after 19 iterates

One-phase Stefan problem

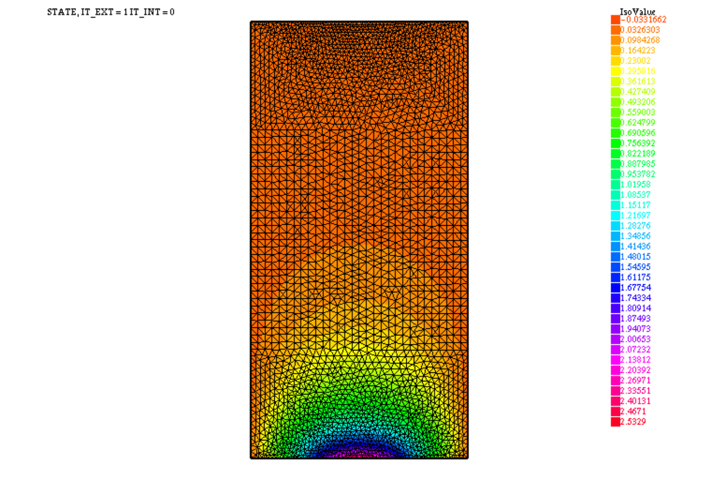

Figure: Initial mesh and first controlled solution

One-phase Stefan problem

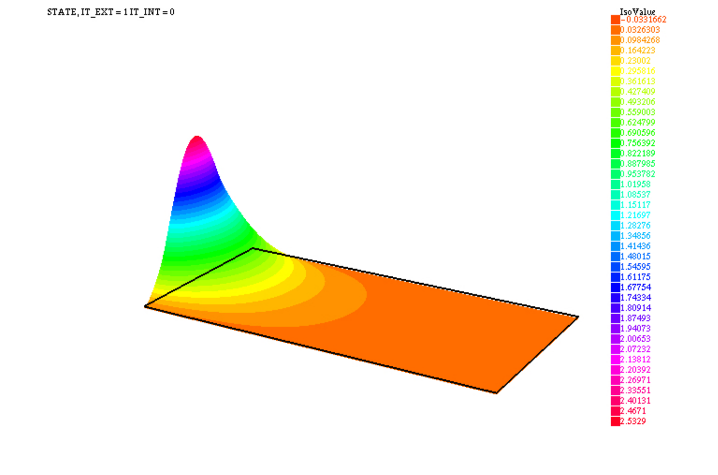

Figure: First controlled solution

One-phase Stefan problem

Th: NV = 2912 NT = 5582

Iter = 1	Error = 0.197536
Iter = 2	Error = 0.00468906
Iter = 3	Error = 0.00400187
Iter = 4	Error = 0.00344997
Iter = 5	Error = 0.00299561
Iter = 6	Error = 0.00261805
Iter = 7	Error = 0.00230164
Iter = 8	Error = 0.00203722
Iter = 9	Error = 0.00181725
Iter = 10	Error = 0.0016362
Iter = 11	Error = 0.00149084
Iter = 12	Error = 0.00137592
Iter = 13	Error = 0.00129143
Iter = 14	Error = 0.00123042
Iter = 15	Error = 0.00119376
Iter = 16	Error = 0.00128955
Iter = 17	Error = 0.00134318
Iter = 18	Error = 0.00100526
Iter = 19	Error = 0.000977661

Convergence Error = 0.000977661

One-phase Stefan problem

Figure: Final computed state y

One-phase Stefan problem

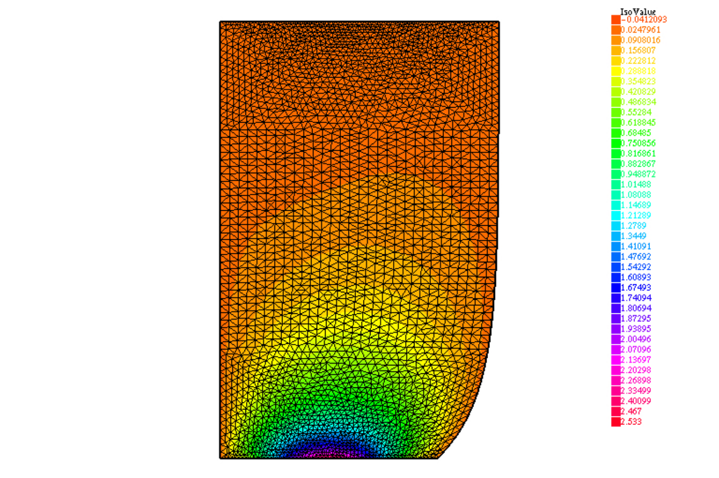

Figure: Final mesh and solution

One-phase Stefan problem

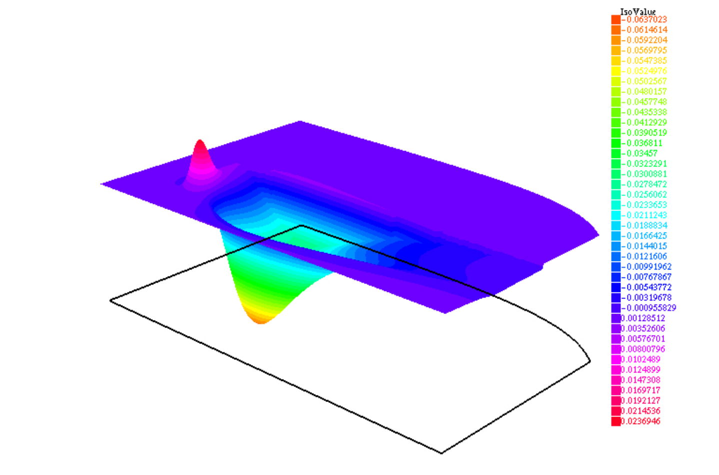

Figure: Final computed control v

One-phase Stefan problem

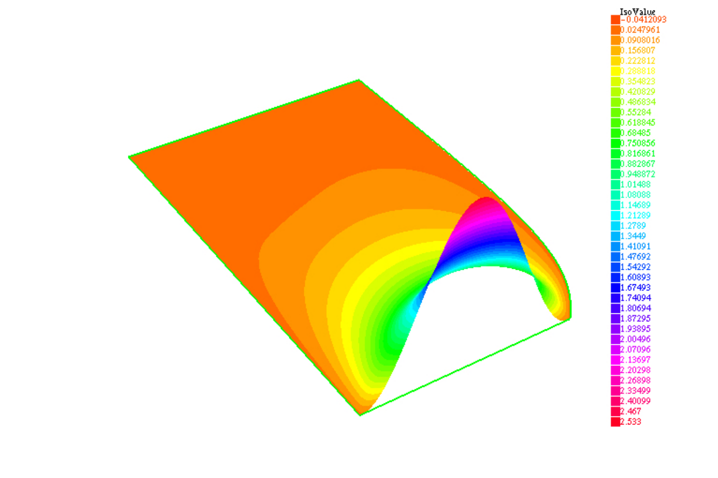

Figure: Final computed state y

Controllability and Stefan problems
An improvement: controlling y and ℓ at time T

Find $v \in L^2(\omega \times (0,T))$, $\ell = \ell(t) > 0$ and $y = y(x,t)$ with

$$(NC)_1 \quad \begin{cases} y_t - y_{xx} = v 1_\omega, \quad x \in (0,\ell(t)), \ t \in (0,T) \\ y(0,t) = y(\ell(t),t) = 0, \quad t \in (0,T) \qquad\qquad y_x(\ell(t),t) = -k\ell'(t), \ t \in (0,T) \\ \ell(0) = \ell_0, \quad y(x,0) = y_0(x), \quad x \in (0,\ell_0) \end{cases}$$

and

$$(NC)_3 \qquad y(x,T) = 0, \quad x \in (0,\ell(T)), \quad \ell(T) = \ell_T$$

Here: $\ell_0 > 0$, $y_0 \geq 0$, $\omega = (a,b) \subset (0,\ell_0)$ (small)

Theorem (Local NC)

$\exists \varepsilon > 0$ *such that* $\|y_0\|_{H_0^1} + |\ell_0 - \ell_T| \leq \varepsilon \;\Rightarrow \exists v, \ell, y$ *satisfying* $(NC)_1, (NC)_3$

Controllability and Stefan problems
NC of 1D two-phase Stefan

Same motivation: melting of ice and similar phenomena

1D, two-phase:

- Heat equation for y on the left, $x < \ell(t)$, $t \in (0, T)$
- Heat equation for z on the right, $x > \ell(t)$, $t \in (0, T)$
- Initial and boundary conditions at $t = 0$, on the left and the right
- Stefan condition on $x = \ell(t)$, $t \in (0, T)$

The free boundary: $x = \ell(t)$, controlled dynamically by y and z

Nonconstant temperature water for $x < \ell(t)$ and ice for $x > \ell(t)$

Controllability and Stefan problems
NC of 1D two-phase Stefan

Find $v_l \in L^2(\omega_l \times (0,T))$, $v_r \in L^2(\omega_r \times (0,T))$, ℓ, y and z with

$$(NC)_1 \quad \left\{ \begin{array}{l} y_t - d_l y_{xx} = v_l 1_\omega, \; x \in (0, \ell(t)), \; t \in (0,T) \\ z_t - d_r z_{xx} = v_r 1_\omega, \; x \in (\ell(t), L), \; t \in (0,T) \\ y|_{x=0} = y|_{x=\ell(t)} = z|_{x=\ell(t)} = z|_{x=L} = 0, \; t \in (0,T) \\ \ell(0) = \ell_0; \; y|_{t=0} = y_0, \;\; x \in (0, \ell_0); \; z|_{t=0} = z_0, \;\; x \in (\ell_0, L) \\ (d_l y_x - d_r z_x)|_{x=\ell(t)} = -k\ell'(t), \;\; t \in (0,T) \end{array} \right.$$

and

$$(NC)_4 \quad \left\{ \begin{array}{l} y(x,T) = 0, \;\; x \in (0, \ell(T)), \quad z(x,T) = 0, \;\; x \in (\ell(T), L) \\ \ell(T) = \ell_T \end{array} \right.$$

Now: $\ell_0 > 0$, $y_0 \geq 0$, $z_0 \leq 0$, $\omega_l = (a_l, b_l) \subset (0, \ell_0)$, $\omega_r = (a_r, b_r) \subset (\ell_0, L)$ (small)

Theorem (Local NC, Araujo-EFC-Limaco-Souza 2021)

$\exists \varepsilon > 0$ *such that* $\|y_0\|_{H_0^1} + \|z_0\|_{H_0^1} + |\ell_0 - \ell_T| \leq \varepsilon \Rightarrow \exists v_l, v_r, \ell, y, z$ *satisfying* $(NC)_1, (NC)_4$

Numerical experiments

A second numerical experiment: two-phase Stefan
To appear soon, [EFC-Souza]

- $\ell_0 = 5$, $L = 15$, $y_0(x) \equiv 3\,\sin(\pi x/\ell_0)$, $z_0(x) \equiv -2\,sin(\pi(x-\ell_0)/(L-\ell_0))$.
- $d_l = d_r = 2.15$, $\omega_l = (0,3)$, $\omega_r = (12,15)$, $k = 0.06$, $T = 10$.

Stopping criterion: $\|y^{n+1} - y^n\|_{L^2}/\|y^{n+1}\|_{L^2} \leq 10^{-5}$
Starting from $y^0 \equiv y_0$, $z^0 \equiv z_0$: convergence after 13 iterates

Two-phase Stefan problem

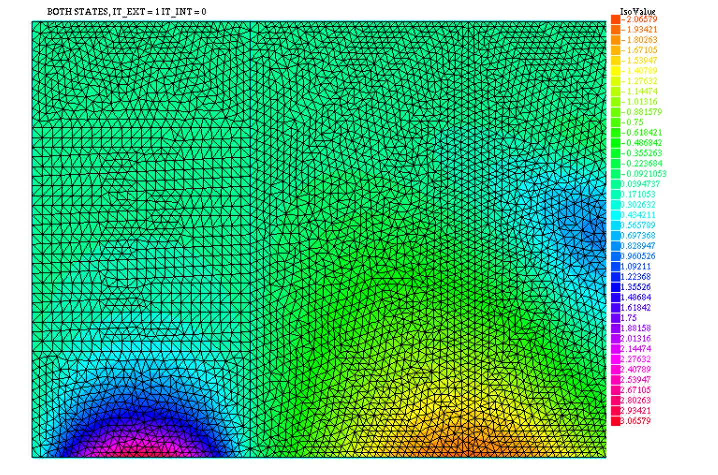

Figure: Initial mesh and first controlled solution

Two-phase Stefan problem

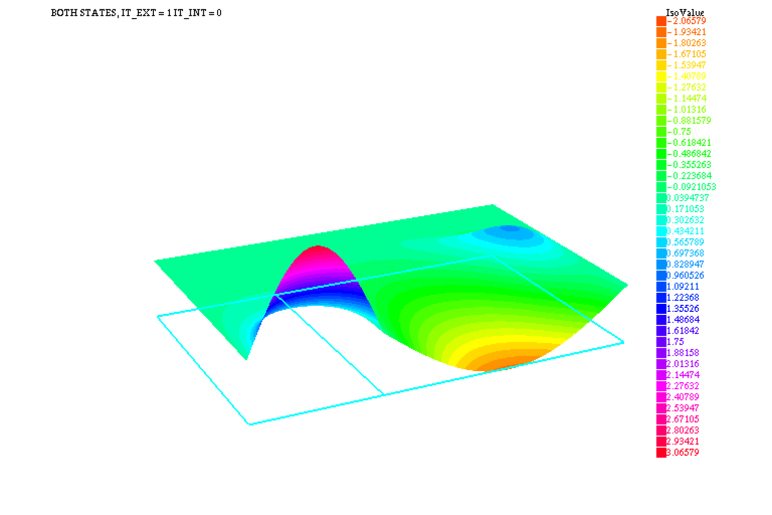

Figure: First controlled solution

Two-phase Stefan problem

Th1: NV = 1407 NT = 2662 - Th2: NV = 3421 NT = 6630

Iter = 1	Error = 0.0934006
Iter = 2	Error = 0.015046
Iter = 3	Error = 0.030527
Iter = 4	Error = 0.0292835
Iter = 5	Error = 0.0205314
Iter = 6	Error = 0.0141885
Iter = 7	Error = 0.0110615
Iter = 8	Error = 0.00850354
Iter = 9	Error = 0.00567204
Iter = 10	Error = 0.00692685
Iter = 11	Error = 0.00506353
Iter = 12	Error = 0.00125576
Iter = 13	Error = 0.000849974

Convergence Error = 0.000849974

Two-phase Stefan problem

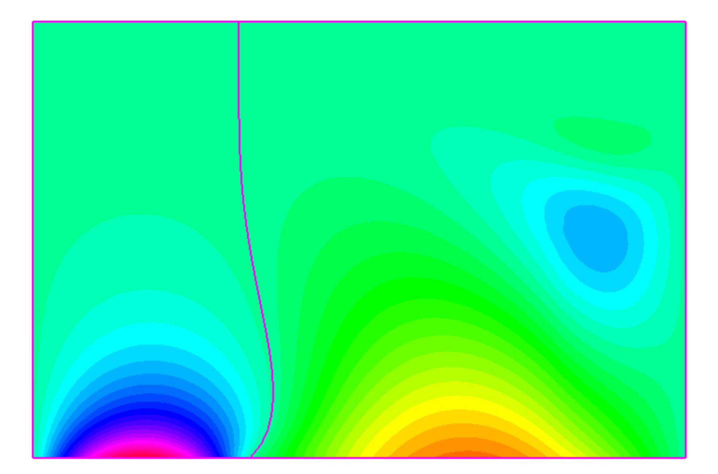

Figure: Final computed states y and z

Two-phase Stefan problem

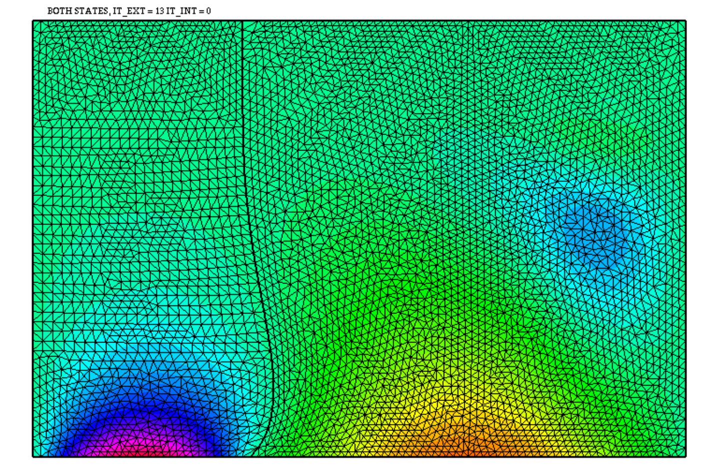

Figure: Final mesh and solution

Two-phase Stefan problem

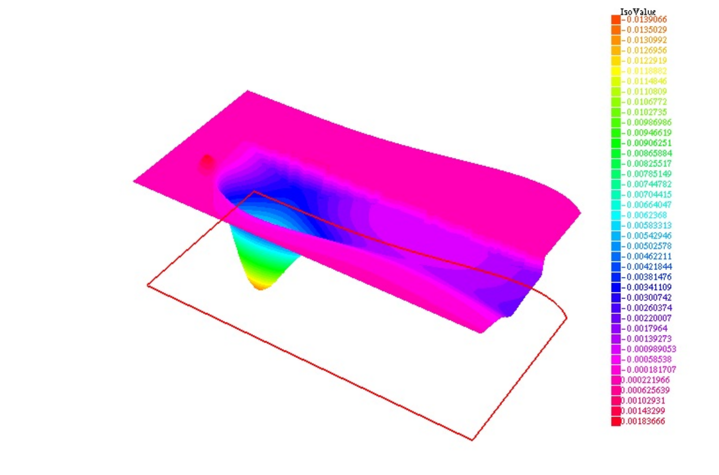

Figure: Computed control v_l

Two-phase Stefan problem

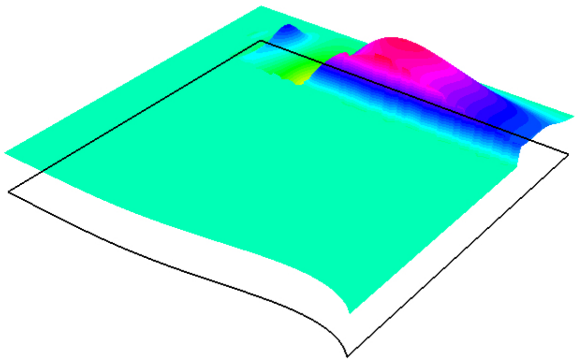

Figure: Computed control v_r

Two-phase Stefan problem

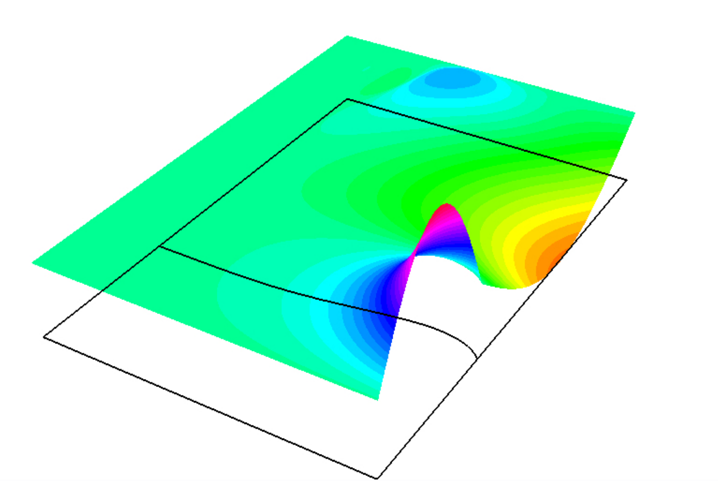

Figure: Final solution

Other results and related questions

- 1D Stefan + semilinear heat PDEs, Burgers and others: similar results [EFC-Triburtino 2016]
- 2D one-phase Stefan?
  Unknown. Star-shaped and Stokes-Stefan, [Demarque-EFC 2017]:

$$(-\varepsilon \Delta V + V) \cdot n = \frac{\partial y}{\partial n} \quad \text{on} \quad \Gamma$$

- Controlling 2D Navier-Stokes + free boundary?
- A new AC result for the two-phase problem, Neumann control, [Barbu 2021]:

$$\forall \text{ meas. } \omega^* \subset (0, L) \ \exists u \ \text{ such that } \ \{|y(x,T)| + |z(x,T)| \leq \varepsilon\} \supset \omega^*$$

- Stabilization, again Neumann control, [Krstic 2020]

Future work (and work in progress)

- Other algorithms? Maybe a least-squares approach (like [Lemoine-Münch]) . . .
  More numerical experiments?
- Exact control to trajectories? (in progress, with JA Barcena and DA Souza)

THANK YOU VERY MUCH . . .