

Fast solvers for partial differential equations subject to inequalities

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Many Traditions One Alaska



Outline: *Fast solvers for PDEs subject to inequalities*

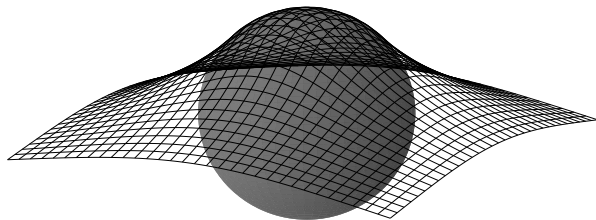
- 1 variational inequalities (VIs)
- 2 nonlinear multigrid for PDEs
- 3 multigrid for VIs
- 4 results

MATH 692 Finite Element Seminar in Spring 2024 (Thursdays 3:30–4:30pm)

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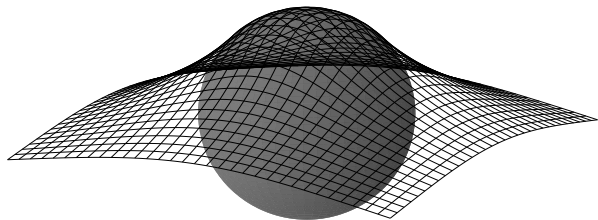
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- *problem.* on a domain $\Omega \subset \mathbb{R}^2$, find the displacement $u(x)$ of a membrane, with fixed value $u = g$ on $\partial\Omega$, above an *obstacle* $\psi(x)$, which minimizes elastic (plus some potential) energy

$$J(v) = \int_{\Omega} \frac{1}{2} |\nabla v|^2 - f v$$

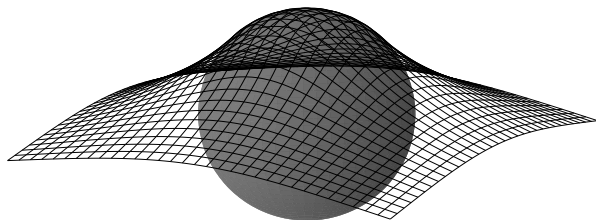
- shown above: Ω a square, $\psi(x)$ a hemisphere
- Q. how to solve this as a PDE with boundary conditions?



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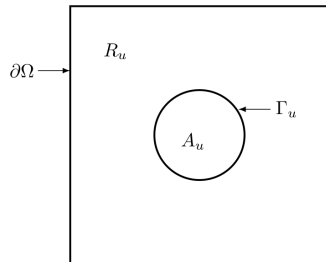
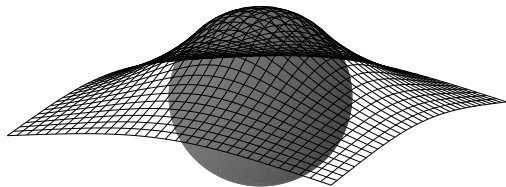
- this is constrained optimization over an infinite-dimensional *admissible set*

$$\mathcal{K} = \left\{ v \in H^1(\Omega) : v|_{\partial\Omega} = g \text{ and } v \geq \psi \right\}$$

- \mathcal{K} is a closed and convex subset of the Sobolev space

$$H^1(\Omega) = \left\{ v : \int_{\Omega} |v|^2 + |\nabla v|^2 < \infty \right\}$$

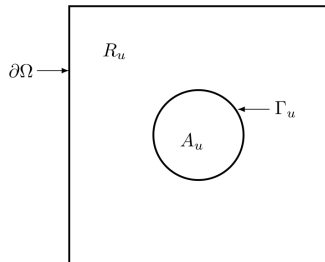
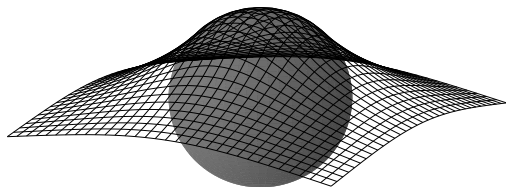
example: classical obstacle problem



- the solution defines subsets of Ω :

- *active set* $A_u = \{u = \psi\}$
- *inactive set* $R_u = \{u > \psi\}$
- *free boundary* $\Gamma_u = \partial R_u \cap \Omega$

example: classical obstacle problem

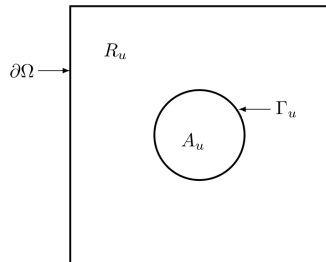
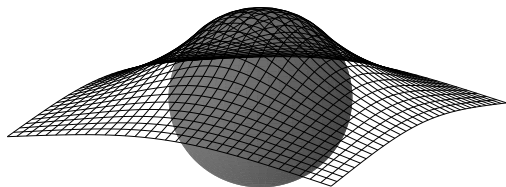


- a naive strong form would pose the problem in terms of its solution:

$$\begin{aligned} -\nabla^2 u &= f & \text{on } R_u \\ u &= \psi & \text{on } A_u \end{aligned}$$

- Poisson equation $-\nabla^2 u = f$ is “ $J'(u) = 0$ ” on R_u
- using the solution u to define the set R_u on which to solve the PDE $-\nabla^2 u = f$ **does not lead to solution algorithms**

example: classical obstacle problem



- the *complementarity problem* (CP) is a meaningful strong form:

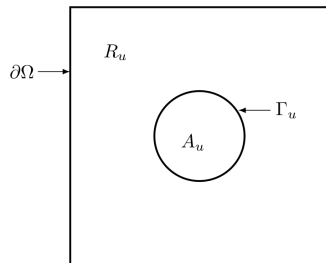
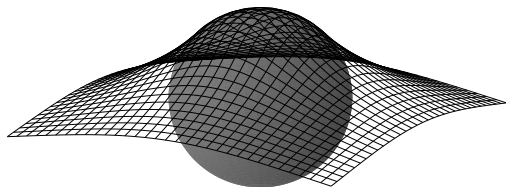
$$u - \psi \geq 0$$

$$-\nabla^2 u - f \geq 0$$

$$(u - \psi)(-\nabla^2 u - f) = 0$$

- CP = KKT conditions
 - but in ∞ -dimensions

example: classical obstacle problem



- the weak form is a *variational inequality (VI)*, which says that $J'(u)$ points directly into \mathcal{K} :

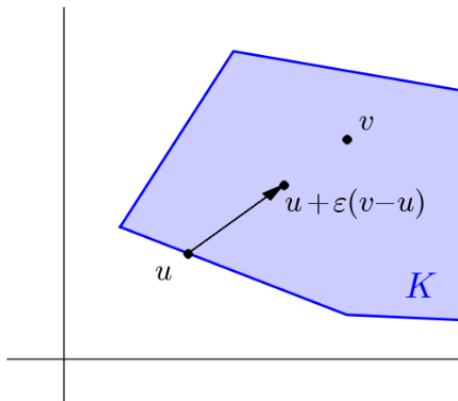
$$\langle J'(u), v - u \rangle = \int_{\Omega} \nabla u \cdot \nabla (v - u) - f(v - u) \geq 0$$

for all $v \in \mathcal{K}$

VI = weak form

- for problems of optimization type, the VI is the weak form, with $v - u$ as the test function:

$$J(u) \leq J(v) \quad \forall v \in \mathcal{K} \quad \iff \quad \langle J'(u), v - u \rangle \geq 0 \quad \forall v \in \mathcal{K}$$



- let \mathcal{K} be a closed and convex subset of a Banach space \mathcal{V}
- suppose $F : \mathcal{K} \rightarrow \mathcal{V}'$ is a continuous operator
 - F is generally nonlinear
 - F may be defined *only* on \mathcal{K}
 - F may *not* be the derivative of an objective function J
 - $F = J'$, a linear operator, in classical obstacle problem
- the general variational inequality $\text{VI}(F, \mathcal{K})$ is

$$\langle F(u), v - u \rangle \geq 0 \quad \text{for all } v \in \mathcal{K}$$

- when \mathcal{K} is nontrivial the problem $\text{VI}(F, \mathcal{K})$ is nonlinear *even when* F is a linear operator

VI = constrained “system of equations”

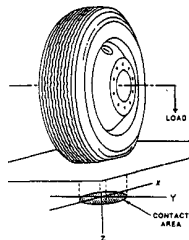
	unconstrained	constrained
optimization	$\min_{u \in \mathcal{V}} J(u)$	$\min_{u \in \mathcal{K} \subset \mathcal{V}} J(u)$
equations	<p>find $u \in \mathcal{V}$:</p> $F(u) = 0$	<p>find $u \in \mathcal{K} \subset \mathcal{V}$:</p> $\langle F(u), v - u \rangle \geq 0 \quad \forall v \in \mathcal{K}$

VI = constrained “system of equations”

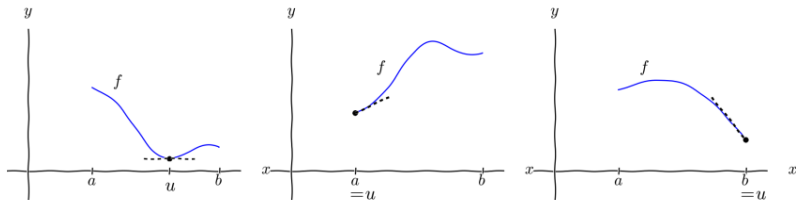
	unconstrained	constrained
optimization	$\min_{u \in \mathcal{V}} J(u)$	$\min_{u \in \mathcal{K} \subset \mathcal{V}} J(u)$
weak form equations	<p>find $u \in \mathcal{V}$:</p> $\langle F(u), v \rangle = 0 \quad \forall v \in \mathcal{V}$	<p>find $u \in \mathcal{K} \subset \mathcal{V}$:</p> $\langle F(u), v - u \rangle \geq 0 \quad \forall v \in \mathcal{K}$

applications of VIs

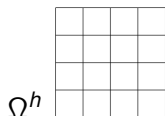
- elastic contact
 - car tires, for example
- pricing of American options
 - inequality-constrained Black-Scholes model
- the geometry of glaciers
- first-semester calculus:



$$u \leftarrow \min_{x \in [a, b]} f(x) \iff f'(u)(v - u) \geq 0 \quad \forall v \in [a, b]$$



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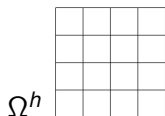
- consider a nonlinear elliptic PDE problem:

$$F(u) = \ell$$

- $u \in \mathcal{V} = H^1(\Omega)$
- $\ell \in \mathcal{V}'$
- $F : \mathcal{V} \rightarrow \mathcal{V}'$ continuous and one-to-one
- for example, the Liouville-Bratu problem: $-\nabla^2 u - e^u = f$
- discretization gives algebraic system on fine mesh Ω^h :

$$F^h(u^h) = \ell^h$$

- u^h denotes exact (algebraic) solution



- *goal*: to solve $F^h(u^h) = \ell^h$ on Ω^h
- suppose w^h is a not-yet-converged iterate:

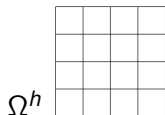
$$r^h = \ell^h - F^h(w^h), \quad \|r^h\| > \text{TOL}$$

- how can we improve w^h *without* globally linearizing F^h ?
 - are there alternatives to Newton's method?

- notes:

- the *residual* $r^h = \ell^h - F^h(w^h)$ is computable
- the *error* $e^h = u^h - w^h$ is unknown
- our equation can be rewritten

$$F^h(u^h) - F^h(w^h) = r^h$$



- *updated goal*: from iterate w^h , to solve

$$F^h(u^h) - F^h(w^h) = r^h$$

- **for F^h linear**, convert this to the *error equation*

$$F^h(e^h) = r^h$$

- an approximation solution \tilde{e}^h would improve our iterate:

$$w^h \leftarrow w^h + \tilde{e}^h$$

- but F^h is not linear!



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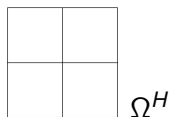
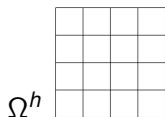
$$F^h(e^h) = r^h$$

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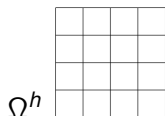
nonlinear 2-mesh scheme



- *updated goal*: use a coarser mesh Ω^H to somehow estimate the solution u^h in the nonlinear *correction equation*

$$F^h(u^h) - F^h(w^h) = r^h$$

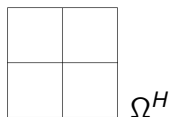
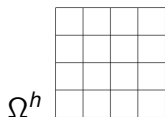
- basic multigrid idea: there are algorithms (**smoothers**) which “improve” w^h ... use them a little first ... then correct from the coarser mesh
 - “improve” means they remove high-frequency error components efficiently



- *nodewise problem*: for ψ_i^h a hat function or dof, solve for $c \in \mathbb{R}$ to make the residual at that location zero:

$$\phi_i(\mathbf{c}) = r^h(\mathbf{w}^h + \mathbf{c}\psi_i^h)[\psi_i^h] = 0$$

- sweeping through and solving nodewise problems is a **smoother**
 - Fourier analysis shows smoothing property
 - after smoothing, e^h and r^h have smaller high-frequencies
- after smoothing, the correction equation on Ω^h should be accurately approximate-able on the coarser mesh Ω^H



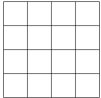
- *updated goal*: use a coarser mesh Ω^H to somehow estimate the solution u^h in $F^h(u^h) - F^h(w^h) = r^h(w^h)$
- Brandt's (1977) *full approximation scheme* (FAS) equation:


$$F^H(u^H) - F^H(R^\bullet w^h) = R r^h(w^h)$$

- $R^\bullet : \mathcal{V}^h \rightarrow \mathcal{V}^H$ is *node-wise injection*
 - $R : (\mathcal{V}^h)' \rightarrow (\mathcal{V}^H)'$ is *canonical restriction*
 - note: if $w^h = u^h$ exactly then $u^H = R^\bullet w^h$ since F^H injective
- rewritten FAS equation: let $\ell^H = F^H(R^\bullet w^h) + R r^h(w^h)$ then

$$F^H(u^H) = \ell^H$$

full approximation scheme (FAS) 2-mesh solver

fine mesh = Ω^h 

 $\Omega^H =$ coarse mesh

pre-smooth over fine:

[smoother updates w^h]

restrict:

$$\ell^H = F^H(R^\bullet w^h) + R r^h(w^h)$$

solve coarse:

$$F^H(w^H) = \ell^H$$

correct:

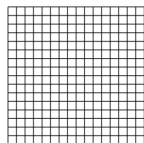
$$w^h \leftarrow w^h + P(w^H - R^\bullet w^h)$$

post-smooth over fine:

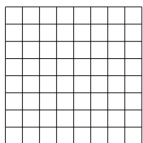
[smoother updates w^h]

- $P : \mathcal{V}^H \rightarrow \mathcal{V}^h$ is *canonical prolongation*
- **restrict+(solve coarse)+correct** = *FAS coarse grid correction*

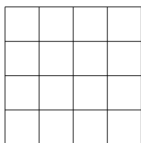
nonlinear multigrid by FAS: V-cycle



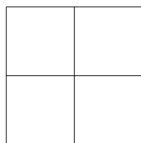
$J = 3$



$j = 2$



$j = 1$



$j = 0$

FAS-VCYCLE($\ell^J; w^J$):

for $j = J$ **downto** $j = 1$

SMOOTH^{down}($\ell^j; w^j$)

$w^{j-1} = R \bullet w^j$

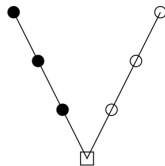
$\ell^{j-1} = F^{j-1}(w^{j-1}) + R(\ell^j - F^j(w^j))$

SOLVE($\ell^0; w^0$)

for $j = 1$ **to** $j = J$

$w^j \leftarrow w^j + P(w^{j-1} - R \bullet w^j)$

SMOOTH^{up}($\ell^j; w^j$)



does it work?

- FAS multigrid works **very well** on nice nonlinear PDE problems
- example: Liouville-Bratu equation

$$-\nabla^2 u - e^u = 0$$

with Dirichlet boundary conditions on $\Omega = (0, 1)^2$

- discretize by (straightforward) finite differences
- minimal problem-specific code:
 1. residual evaluation on grid level: $F^j(\cdot)$
 2. pointwise smoother: $\phi_i(c) = 0 \forall i$
 - nonlinear Gauss-Seidel iteration
 3. coarsest-level solve can be same as smoother, or more sophisticated (e.g. Newton iteration)

the meaning of “fast solver”

- what does “very well” on the previous slide mean?

definition

a solver is *optimal* if work in flops, and/or run-time, is $O(N)$ for N unknowns

- since ~ 1980 : optimality can be achieved by multigrid for PDE problems with reasonably-smooth solutions
- in fact, multigrid people get greedy

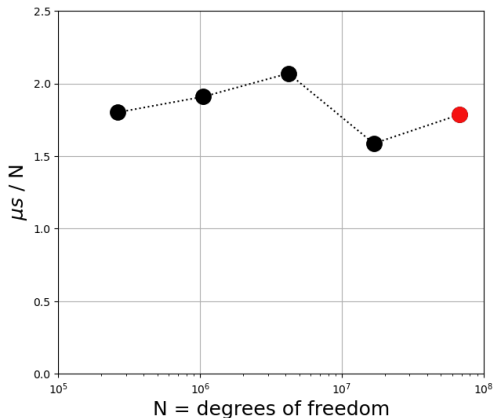
definition

a solver shows *textbook multigrid efficiency* if it does total work less than 10 times that of a single smoother sweep

- TME \implies optimal

Bratu model problem: TME

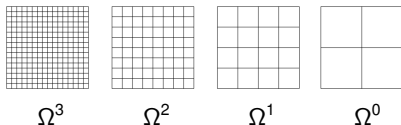
- `bratu.c`
- observed optimality:
 $\text{flops} = O(N^1)$
 $\text{processor time} = O(N^1)$
- highest-resolution **12-level V-cycle** has $N \approx 10^8$ unknowns
- compare $\approx 20 \mu\text{s}/N$ for Poisson using Firedrake (P_1 , geometric multigrid)



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- new algorithm (Bueler & Farrell 2023):
FASCD = full approximation scheme constraint decomposition
- what is “constraint decomposition” in FASCD?

subspace decomposition



- start with subspace decomposition over nested meshes:

$$\Omega^j \subset \Omega^{j+1}$$

- the FE function spaces \mathcal{V}^j over Ω^j are also nested:

$$\mathcal{V}^j \subset \mathcal{V}^{j+1}$$

definition

$\mathcal{V}^J = \sum_{i=0}^J \mathcal{V}^i$ is called a *subspace decomposition* (Xu 1992)

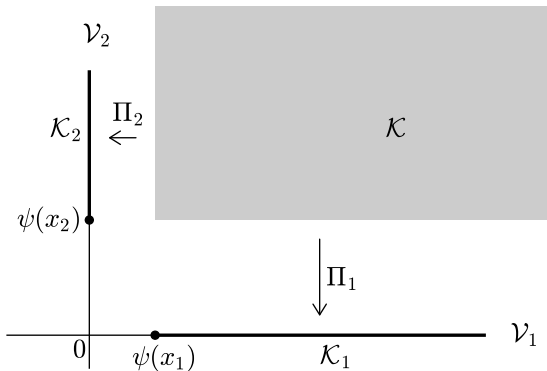
- *non-unique* vector space sum
- Xu's paper explains how to analyze linear multigrid for PDEs via subspace decomposition

- Tai's (2003) constraint decomposition *non-trivially* extends a subspace decomposition $\mathcal{V}^J = \sum_i \mathcal{V}^i$ to convex subsets
- suppose $\mathcal{K}^J \subset \mathcal{V}^J$ is a closed and convex subset

definition

$\mathcal{K}^J = \sum_{i=0}^J \mathcal{K}^i$ is a *constraint decomposition* (CD) if there are closed and convex subsets $\mathcal{K}^i \subset \mathcal{V}^i$, and (nonlinear) projections $\Pi_i : \mathcal{K}^J \rightarrow \mathcal{K}^i$, so that $v = \sum_{i=0}^J \Pi_i v$ and a stability condition applies (not shown)

- observation: generally $\mathcal{K}^i \not\subset \mathcal{K}^j$



obstacle problem on a two-point mesh with $\mathcal{V} \cong \mathbb{R}^2$

- Tai proposed abstract iterations for solving $VI(F, \ell, \mathcal{K})$ over a CD
 $\mathcal{K}^J = \sum_{i=0}^J \mathcal{K}^i$

CD-MULT(u):

for $i = 0, \dots, m - 1$:

find $w_i \in \mathcal{K}_i$ **s.t.**

$$\left\langle F\left(\sum_{j<i} w_j + w_i + \sum_{j>i} \Pi_j u\right), v_i - w_i \right\rangle \geq \langle \ell, v_i - w_i \rangle \quad \forall v_i \in \mathcal{K}_i$$

return $w = \sum_i w_i \in \mathcal{K}$

- Tai's iterations are not practical because you compute on the finest level in fact
- we added two techniques: *defect obstacles* on each level, and *FAS coarse corrections*

- recall $\mathcal{K} = \{v \geq \psi\}$ in an obstacle problem

definition

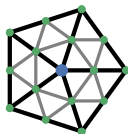
for finest-level admissible set $\mathcal{K}^J = \{v^J \geq \psi^J\} \subset \mathcal{V}^J$ and an iterate $w^J \in \mathcal{K}^J$, the *defect obstacle* (Gräser & Kornhuber 2009) is

$$\chi^J = \psi^J - w^J \in \mathcal{V}^J$$

- note $\chi^J \leq 0$
- we generate the CD through defect obstacles χ^j on each level via *monotone restriction*:

$$\chi^j = R^\oplus \chi^{j+1}$$

- a *nonlinear* operator
- also due to (Gräser & Kornhuber 2009)



- coarse mesh node
- fine mesh node

up and down sets

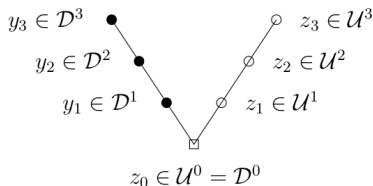
- upward part in the FASCD V-cycle uses large admissible sets:

$$\mathcal{U}^j = \{z^j \geq \chi^j\}$$

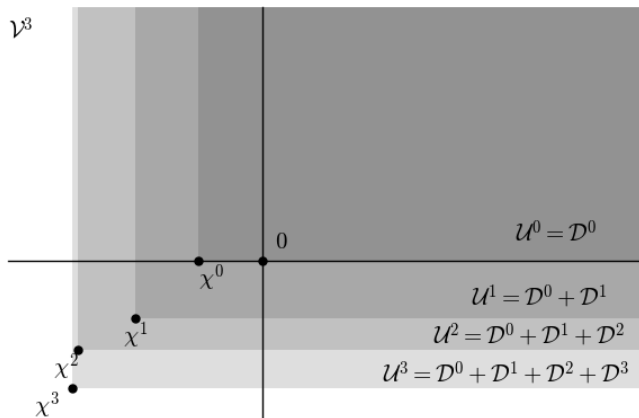
- downward sets are smaller to guarantee admissibility of the upcoming coarse correction:

$$\mathcal{D}^j = \{y^j \geq \phi^j = \chi^j - \chi^{j-1}\}$$

- $\mathcal{U}^j = \sum_{i=0}^j \mathcal{D}^i$ is a CD of the j th-level admissible set



multilevel constraint decomposition in FASCD



full approximation scheme constraint decomposition

FASCD-VCYCLE($J, \ell^J, \psi^J; w^J$):

$$\chi^J = \psi^J - w^J$$

for $j = J$ downto $j = 1$

$$\chi^{j-1} = R^\oplus \chi^j$$

$$\phi^j = \chi^j - P\chi^{j-1}$$

$$y^j = 0$$

SMOOTH^{down}($\ell^j, \phi^j, w^j; y^j$)

$$w^{j-1} = R^\bullet(w^j + y^j)$$

$$\ell^{j-1} = f^{j-1}(w^{j-1}) + R(\ell^j - f^j(w^j + y^j))$$

$$z^0 = 0$$

SOLVE($\ell^0, \chi^0, w^0; z^0$)

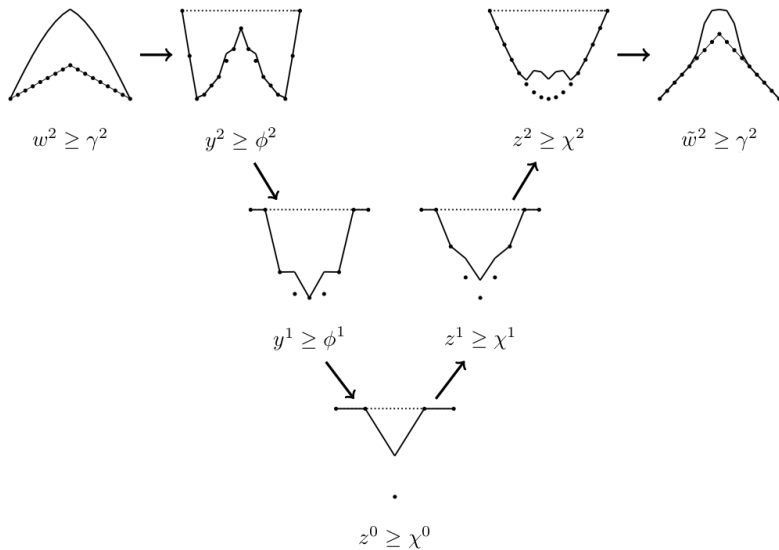
for $j = 1$ to $j = J$

$$z^j = y^j + Pz^{j-1}$$

SMOOTH^{up}($\ell^j, \chi^j, w^j; z^j$)

return $w^J + z^J$

FASCD V-cycle: visualization on a 1D problem



see paper (Bueler & Farrell 2023) for:

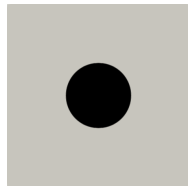
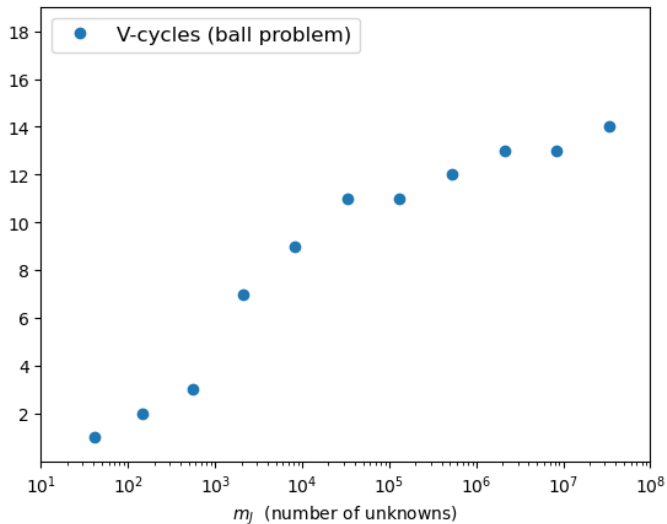
- generalization to upper and lower obstacles:

$$\mathcal{K}^J = \{\underline{\psi}^J \leq v^J \leq \overline{\psi}^J\}$$

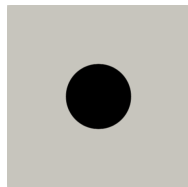
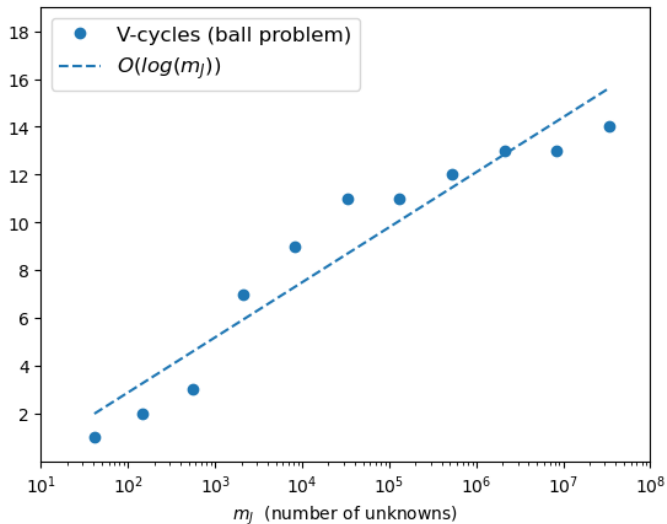
- stopping criteria
 - evaluate whether CP/KKT conditions are satisfied
- FMG cycle
- details of $O(m_J)$ smoother

- 1 variational inequalities (VIs)
- 2 nonlinear multigrid for PDEs
 - full approximation scheme (FAS)
- 3 multigrid for VIs
 - full approximation scheme constraint decomposition (FASCD)
- 4 **results**
 - **classical obstacle problem**
 - **advection-diffusion of a concentration**
 - **glacier surface elevations**

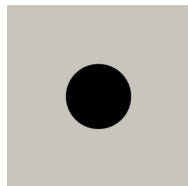
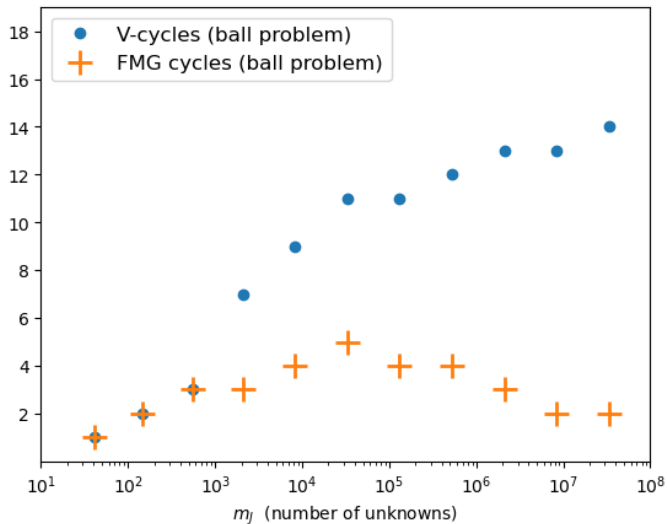
classical obstacle problem by FASCD



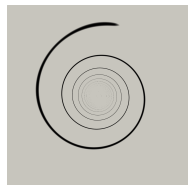
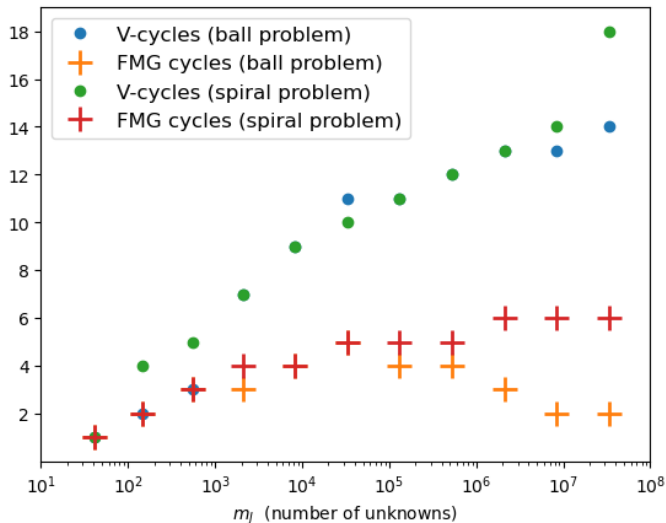
classical obstacle problem by FASCD



classical obstacle problem by FASCD



classical obstacle problem by FASCD



advection-diffusion of a concentration

- suppose $u(x)$ is a concentration in $\Omega \subset \mathbb{R}^d$: $0 \leq u \leq 1$
- suppose it moves by combination of diffusion, advection by wind $\mathbf{X}(x)$, and source function $\phi(x)$:

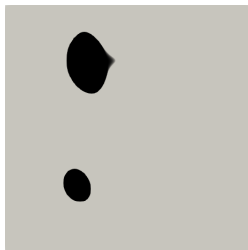
$$-\epsilon \nabla^2 u + \mathbf{X} \cdot \nabla u = \phi$$

- two active sets ($d = 2$ case):

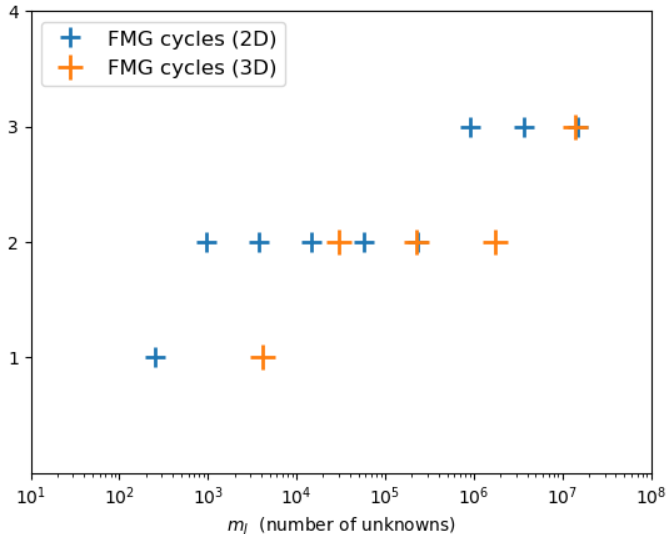
$$\underline{A}_u = \{u(x) = 0\}$$



$$\overline{A}_u = \{u(x) = 1\}$$



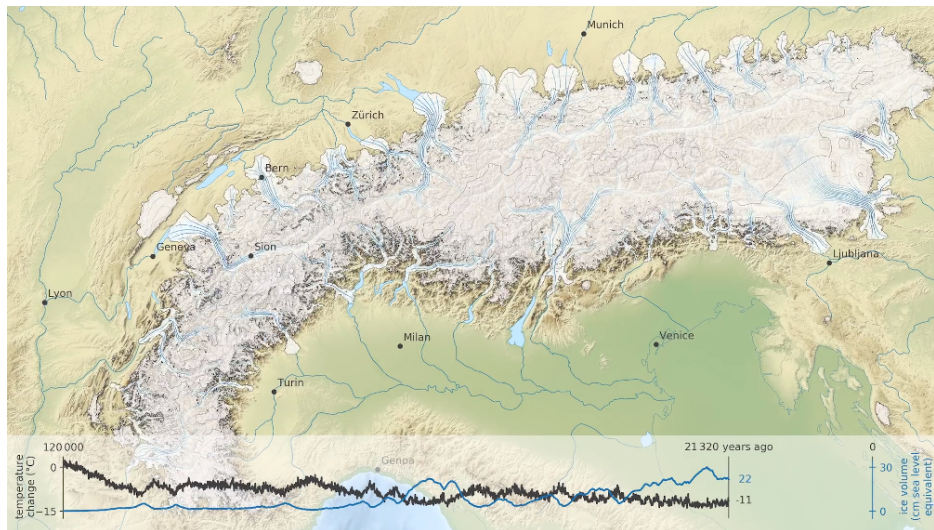
advection-diffusion of a concentration



compare: linear programming (Klee-Minty cube?), spatial correlations

problem: geometry of flowing glacier ice in a climate

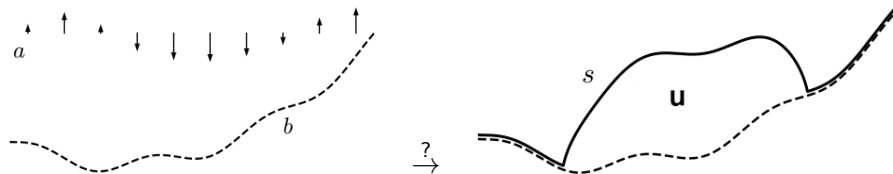
- “where are there glaciers?” is a free-boundary problem



Sequinot et al. (2018)

free-boundary problem: flowing glacier ice in a climate

- glacier = incompressible, viscous fluid driven by gravity
- to find: ice surface elevation $s(t, x, y)$ and velocity $\mathbf{u}(t, x, y, z)$
- over fixed bed topography with elevation $b(x, y)$
 - $s(t, x, y) \geq b(x, y)$
- in a *climate* which adds or removes ice at a signed rate $a(t, x, y)$
 - data a, b is defined on domain $\Omega \subset \mathbb{R}^2$



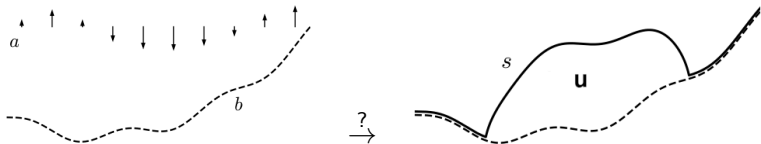
glacier free-boundary problem: naive strong form

- is this an adequate description?:

$$\begin{aligned} s &\geq b && \text{everywhere in } \Omega \\ \frac{\partial s}{\partial t} &= a + \mathbf{u}|_s \cdot \mathbf{n}_s && \text{where } s(t, x, y) > b(x, y) \end{aligned}$$

- notes:

- surface velocity $\mathbf{u}|_s$ is, **in some manner**, determined by s
 - $\mathbf{u}|_s$ is generally a *non-local* function of s
- $\mathbf{n}_s = \langle -\nabla s, 1 \rangle$ is upward surface normal



- admissible surface elevations:¹

$$\mathcal{K} = \{r \in \mathcal{V} : r \geq b\}$$

- steady ($\frac{\partial s}{\partial t} = 0$) VI problem for surface elevation $s \in \mathcal{K}$:

$$\langle \Phi(s) - a, r - s \rangle \geq 0 \quad \text{for all } r \in \mathcal{K}$$

where

$$\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$$

with extension by 0 to all of Ω

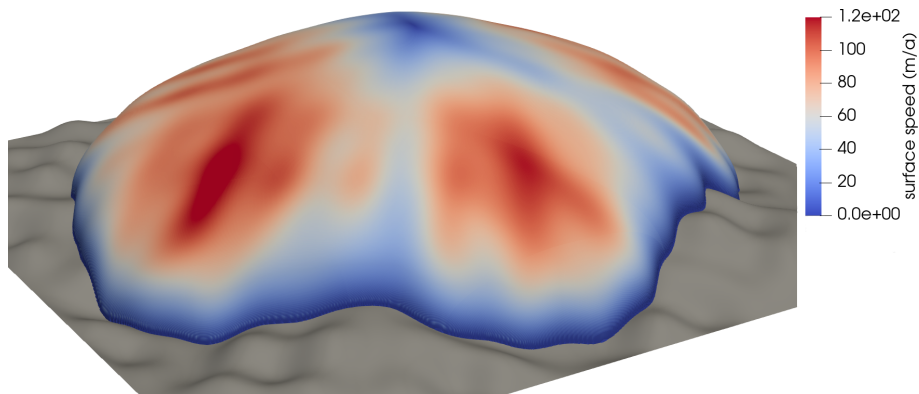
¹ $(s - b)^{8/3} \in W^{1,4}(\Omega)$ so $\mathcal{V} \stackrel{?}{=} (W^{1,4})^{3/8} \dots$ see (Jouvet & Bueler, 2012)

- the *shallow ice approximation* is a highly-simplified view of conservation of momentum
- isothermal, nonsliding case:

$$\begin{aligned}\Phi(s) &= -\mathbf{u}|_s \cdot \mathbf{n}_s \\ &= -\frac{\gamma}{4}(s-b)^4 |\nabla s|^4 - \nabla \cdot \left(\frac{\gamma}{5}(s-b)^5 |\nabla s|^2 \nabla s \right)\end{aligned}$$

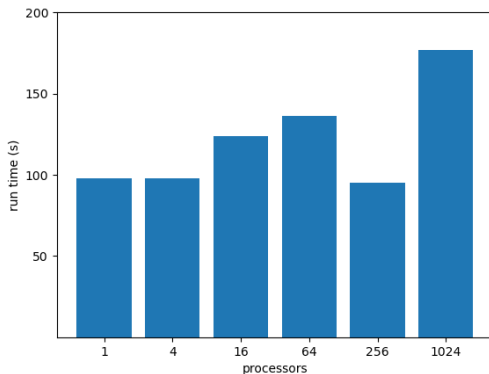
FASCD test case: simplified ice sheet the size of Greenland

- *ice sheet* = big glacier



FASCD: parallel weak scaling

- observed optimality of FMG solver
- good parallel *weak scaling* as well
 - each processor owns 641×641 (sub) mesh
 - $P = 1024$ run had $20481^2 = 4.1 \times 10^8$ unknowns
... and 88 meter resolution



- FASCD = new multilevel solver for VI (free-boundary) problems
 - implemented in Python Firedrake (over PETSc)
- observed optimality, even TME, in many cases
 - actually fast

to do:

- add mesh adaptivity to free boundary (Stefano)
- implement in C inside PETSc
- apply to space-time (*parabolic*) VI problems
- prove convergence
- identify smoothers for problems like elastic contact
- include membrane stresses in glacier case

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