Toward nonlinear multigrid for nonlinear and nonlocal variational inequalities

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Outline

- variational inequalities (VIs)
- 2 full approximation scheme (FAS) multigrid for PDEs
- 3 the nonlinear and nonlocal VI for a fluid layer in a climate
- 4 multigrid approaches for VIs
- 5 FAS multigrid for VIs?



problem. on a domain Ω ⊂ ℝ², find the displacement u(x) of a membrane, with fixed value u = g on ∂Ω, above an *obstacle* ψ(x), which minimizes the elastic energy

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

• shown above: $\Omega = (-2,2)^2$, $\psi(x)$ a hemisphere, f(x) = 0



i.e. constrained optimization over a convex admissible set

$$\mathcal{K} = \left\{ oldsymbol{v} \in \mathcal{H}^1(\Omega) \, : \, oldsymbol{v} \Big|_{\partial\Omega} = oldsymbol{g} ext{ and } oldsymbol{v} \geq \psi
ight\}$$

• J'(u) points directly into \mathcal{K} , the *variational inequality* (VI):

$$\langle J'(u), v - u \rangle = \int_{\Omega} \nabla u \cdot \nabla (v - u) - f(v - u) \ge 0$$
 for all $v \in \mathcal{K}$



- the solution defines active A_u = {u = ψ} and inactive R_u = {u > ψ} subsets of Ω, and a free boundary Γ_u = ∂R_u ∩ Ω
- naive strong form would pose the problem in terms of its solution:

$$-\nabla^2 u = f \quad \text{on } R_u$$

 $u = \psi \quad \text{on } A_u$



• the complementarity problem (CP) is meaningful as a strong form:

$$egin{aligned} & u-\psi \geq 0 \ & -
abla^2 u-f \geq 0 \ & (u-\psi)(-
abla^2 u-f) = 0 \end{aligned}$$

 \circ for optimization problems: CP = KKT conditions

 $\bullet~$ let ${\cal K}$ be a closed and convex subset of a Banach space ${\cal V}$

- suppose $F : \mathcal{K} \to \mathcal{V}'$ is a continuous, generally nonlinear operator
 - $\circ~\textit{F}$ may be defined only on $\mathcal K$
 - \circ F may not be the derivative of an objective function J
- the general problem VI(F,K) is

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

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

unconstrained optimization:	constrained optimization:		
$\min_{u\in\mathcal{V}}J(u)$	$\min_{u\in\mathcal{K}}J(u)$		
equation for $u \in \mathcal{V}$:	VI for $u \in \mathcal{K}$:		
F(u) = 0	$\langle F(u), v - u \rangle \geq 0 \forall v \in \mathcal{K}$		

applications of VIs

- elastic contact, Signorini problems (e.g. Kikuchi & Oden 1988)
- viscous contact problems (de Diego et al. 2022)
- pricing of American options in the Black-Scholes model
- the geometry of glaciers \leftarrow more soon
- first-semester calculus



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• consider a nonlinear elliptic PDE problem:

$$F(u) = \ell$$

• for example, $F : \mathcal{V} \to \mathcal{V}'$ for $\mathcal{V} = H^1(\Omega)$, with $\ell \in \mathcal{V}'$

discretization gives algebraic system on fine grid Ω^h:

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

• suppose w^h yields residual norm $\|\ell^h - F^h(w^h)\| > \text{TOL}$



- how can we improve w^h without globally linearizing F^h?
 (are there alternatives to Newton's method?)
- note the *residual* $r^h(w^h) = \ell^h F^h(w^h)$ is computable, while the *error* $e^h = w^h u^h$ is unknown
- the residual definition can be rewritten

$$F^h(u^h) - F^h(w^h) \stackrel{*}{=} r^h(w^h)$$

• for F^h linear, try to solve this *error equation* $F^h(e^h) = -r^h(w^h)$ for \tilde{e}^h , and correct $w^h \leftarrow w^h - \tilde{e}^h$ to improve w^h ?



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- goal: use a coarser mesh to estimate the error in *
- *nodewise problem*: for ψ_i^h a hat function or dof, solve for $c \in \mathbb{R}$:

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

- sweeping through and solving nodewise problems is a *smoother*
 - Fourier analysis on linear PDEs shows smoothing property
 - post-smoothing, e^h and $r^h(w^h)$ have smaller high-frequencies
- Brandt (1977): after smoothing, F^h(u^h) F^h(w^h) = r^h(w^h) should be accurately approximate-able on a coarser grid



- goal: use a coarser mesh to estimate the error in *
- full approximation storage (FAS) equation:

$$F^{H}(w^{H}) - F^{H}(R^{\bullet}w^{h}) = Rr^{h}(w^{h})$$

R•: *V*^h → *V*^H is injection *R*: (*V*^h)' → (*V*^H)' is canonical restriction
if w^h = u^h exactly then w^H = R•w^h by well-posedness
rewritten: F^H(w^H) = ℓ^H where ℓ^H = F^H(R•w^h) + Rr^h(w^h)

smooth by sweeps over grid: restrict:

solve coarse:

correct :

smooth by sweeps over grid:

 $w^{h} \leftarrow [\phi_{i}(c) = 0 \forall i]$ $\ell^{H} = F^{H}(R^{\bullet}w^{h}) + R r^{h}(w^{h})$ $F^{H}(w^{H}) = \ell^{H}$ $w^{h} \leftarrow w^{h} + P(w^{H} - R^{\bullet}w^{h})$ $w^{h} \leftarrow [\phi_{i}(c) = 0 \forall i]$

• $P: \mathcal{V}^H \to \mathcal{V}^h$ is prolongation

- recall: $\phi_i(\mathbf{c}) = \mathbf{r}^h(\mathbf{w}^h + \mathbf{c}\psi_i^h)[\psi_i^h]$
- restrict+(solve coarse)+correct = coarse grid correction

nonlinear multigrid by FAS V-cycle or F-cycle



-	-	-	-		
			1		



$$\begin{aligned} \mathsf{FAS-VCYCLE}(\ell^{J}; w^{J}) &: \\ & \mathsf{for} \; j = J \; \mathsf{downto} \; j = 1 \\ & \mathsf{SMOOTH}^{\mathsf{down}}(\ell^{j}; w^{j}) \\ & w^{j-1} \leftarrow R^{\bullet} w^{j} \\ & \ell^{j-1} = F^{j-1}(w^{j-1}) + R\left(\ell^{j} - F^{j}(w^{j})\right) \\ & \mathsf{SOLVE}(\ell^{0}; w^{0}) \\ & \mathsf{for} \; j = 1 \; \mathsf{to} \; j = J \\ & w^{j} \leftarrow w^{j} + P(w^{j-1} - R^{\bullet} w^{j}) \\ & \mathsf{SMOOTH}^{\mathrm{up}}(\ell^{j}; w^{j}) \end{aligned}$$

nonlinear multigrid by FAS V-cycle or F-cycle



- FAS multigrid works well on the right nonlinear PDE problem
- example: Liouville-Bratu equation¹

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

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

- implement with minimal problem-specific code:
 - 1. residual evaluation on grid level: $F^{j}(\cdot)$
 - 2. pointwise smoother: $\phi_i(c) = 0 \forall i$
 - o e.g. nonlinear Jacobi or Gauss-Seidel iteration
 - 3. coarse solve can be same as smoother, or use Newton etc.

¹exact solution by Liouville (1853) makes a nice test case

multigrid solver composition in PETSc

- implemented here using an FD discretization and PETSc:²
 - multigrid solvers in PETSc are *composed* from smoothers on each level, and a coarse-level solver . . . here these are nonlinear GS
 - FAS multigrid is a nonlinear solver (SNES) type
 - \circ PETSc = C/Fortran/python

FAS multigrid F-cycle:

```
./bratu -da_grid_x 5 -da_grid_y 5 -da_refine J \
    -snes_rtol 1.0e-12 \
    -snes_type fas \
    -snes_fas_type full \
    -fas_levels_snes_ngs_sweeps 2 \
    -fas_levels_snes_ngs_max_it 1 \
    -fas_levels_snes_norm_schedule none \
    -fas_coarse_snes_max_it 1 \
    -fas_coarse_snes_max_it 1 \
    -fas_coarse_snes_max_it 1 \
    -fas_coarse_snes_ngs_sweeps 4 \
    -fas_coarse_snes_ngs_max_it 1
```

²Portable Extensible Toolkit for Scientific computing petsc.org **EPETSc**

Multigrid for nonlinear and nonlocal VIs

observed optimality:

flops = $O(N^1)$ exp evaluations = $O(N^1)$ processor time = $O(N^1)$

- up to $N \approx 10^8$ dofs
 - J = 11 refinements
 laptop is memory-limited
- compare $\approx 20 \,\mu \,s/N$ for Poisson equation using Firedrake P_1 elements and geometric multigrid



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• benefits of FAS multigrid?

- 1. minimal code, esp. in from-scratch implementations
 - o just write residual plus pointwise smoother!
- 2. composition with nonlinear preconditioners (Brune et al. 2015)

o disadvantages?

- 1. Firedrake/FENiCs *do* automatically provide linearizations from UFL statements of weak forms
- 2. small literature of convergence or descriptive performance for FAS (Trottenberg et al. (2001), Reusken (1987))
- 3. not enough tutorial literature?

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- Iet's not get stuck on textbook example problems!
- multigrid for a real-world VI problem?
- consider an incompressible, viscous layer with surface elevation s(x, y), flowing with velocity $\mathbf{u}(x, y, z)$, driven by gravity, over fixed bed topography with elevation b(x, y), in a *climate* which adds or removes fluid at a signed rate a(x, y) [m s⁻¹]

 \circ data *a*, *b* defined on domain $\Omega \subset \mathbb{R}^2$

• geophysical examples: glaciers and ice sheets, sea ice, lakes



example: glacier ice coverage of the Alps in prior climates



Sequinot et al. (2018)

more ice sheet modeling at my Math. Geosci. Seminar tomorrow 2pm L5

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• naive strong form of the steady model:

 $s \ge b$ everywhere in Ω $-\mathbf{u}|_s \cdot \mathbf{n}_s = a$ where s(x, y) > b(x, y)

- \circ surface velocity $\mathbf{u}|_s$ is determined by fluid domain geometry s
- \circ **n**_s = $\langle -\nabla s, 1 \rangle$ is upward surface normal
- ∘ generally: $-\mathbf{u}|_{s} \cdot \mathbf{n}_{s}$ is a *non-local* function of *s*
- the inequality constraint $s \ge b$ generates a free boundary if an ablative climate a < 0 forces surface down to bed



how to evaluate $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$ for glacier ice?

Stokes model

solve the Stokes problem, then evaluate velocity at surface:

$$\int_{\Lambda(s)=\{b < z < s\}} 2\nu(D\mathbf{u})D\mathbf{u} : D\mathbf{v} - p\nabla \cdot \mathbf{v} - (\nabla \cdot \mathbf{u})q - \rho_{i}\mathbf{g} \cdot \mathbf{v} = 0 \quad \forall \mathbf{v}, q$$

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

- assuming incompressibility and non-Newtonian viscosity: $\nu(D\mathbf{u}) = \frac{1}{2}\Gamma|D\mathbf{u}|^{p-2}$ with $p = \frac{4}{3}$
- ∘ given *s*, this is a well-posed problem for velocity $\mathbf{u} \in \mathbf{W}^{1,p}$ and pressure $p \in L^q$ on domain $\Lambda(s)$
- near-optimal solvers available (Isaac et al 2015)

how to evaluate $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$ for glacier ice?

 Iubrication approximation³ model apply a nonlinear elliptic differential operator to s:

$$\Phi(s) = -rac{\gamma}{\mathsf{q}}(s-b)^{\mathsf{q}}|
abla s|^{\mathsf{q}} -
abla \cdot \left(rac{\gamma}{\mathsf{q}+\mathsf{1}}(s-b)^{\mathsf{q}+\mathsf{1}}|
abla s|^{\mathsf{q}-2}
abla s
ight)$$

- q = 4
- ∇ is in *x*, *y* only
- Φ(s) is a nonlinear differential operator in this model because membrane stresses are *not* balanced
- Φ(s) is doubly-degenerate

³also known as the *shallow ice approximation*

admissible surface elevations:

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

 $\circ \mathcal{V}$ to be determined by viscous fluid model⁴

• VI problem for surface elevation $s \in \mathcal{K}$:

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

where

$$\Phi(\boldsymbol{s}) = -\mathbf{u}|_{\boldsymbol{s}} \cdot \mathbf{n}_{\boldsymbol{s}},$$

with extension by 0 to all of Ω , and **u** is the velocity solution on

$$\Lambda(s) = \{(x, y, z) : b(x, y) < z < s(x, y)\}$$

⁴in shallow ice approximation, $(s - b)^{8/3} \in W^{1,4}(\Omega)$ (Jouvet & Bueler, 2012)

CP form of viscous fluid layer in a climate

- VI form on previous slide is too abstracted for clarity
- the strong form of the same problem is a complementarity problem (CP) coupled to a Stokes problem:

$$\begin{split} s-b &\geq 0 & \text{in } \Omega \subset \mathbb{R}^2 \\ -\mathbf{u}|_s \cdot \mathbf{n}_s - a &\geq 0 & \text{"} \\ (s-b)(-\mathbf{u}|_s \cdot \mathbf{n}_s - a) &= 0 & \text{"} \\ -\nabla \cdot (2\nu(D\mathbf{u}) D\mathbf{u}) + \nabla p - \rho_i \mathbf{g} &= \mathbf{0} & \text{in } \Lambda(s) \subset \mathbb{R}^3 \\ \nabla \cdot \mathbf{u} &= 0 & \text{"} \\ (2\nu(D\mathbf{u}) D\mathbf{u} - pl) \mathbf{n} &= \mathbf{0} & \{z = s\} \subset \partial \Lambda(s) \\ \mathbf{u} &= \mathbf{0} & \{z = b\} \subset \partial \Lambda(s) \end{split}$$

 solve this for s on Ω, and simultaneously for u, p on Λ(s) = {b < z < s}

a non-local VI problem

- in the Stokes case, the residual r(s) = a − Φ(s) = a + u|_s · n_s depends non-locally on s
- for example, consider u_(s+ψ) u_(s) from surface perturbation (hat function) ψ



Bueler and Farrell

what's needed for multigrid to work here?

viscous fluid layer geometry problem

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

where

- $\mathcal{K} = \{r \in \mathcal{V} : r \geq b\}$
- $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$
- *s* is solution surface elevation
- u is Stokes solution on Λ(s) = {b < z < s}
- *a* (climate) and *b* (bed elevation) are the input data

 $\circ~$ for more on this problem class see (Bueler, 2021)

- what is needed for scalable multilevel solutions?
 - 1. iterates must be admissible
 - 2. global linearization of $\Phi(s)$ must be avoided
 - 3. smoother cost must be comparable to one residual

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Newton-multigrid for the classical obstacle problem

- VIs are nonlinear problems, even for linear operators like $-\nabla^2$
- Newton-multigrid is straightforward in PETSc:

```
./obstacle -da_grid_x 3 -da_grid_y 3 \
    -snes_type vinewtonrsls -ksp_type cg -pc_type mg \
    -da_refine J
```

linear solver applies to inactive variables

rsls = reduced space line search

- Newton step equations solved by CG with GMG V-cycles
- issue: the outer Newton iteration must converge on the active set before multigrid can provide effective preconditioning
 - o grid-dependent (growing) Newton iterations



• applying nested iteration (nonlinear F-cycle) resolves this:

./obstacle -da_grid_x 3 -da_grid_y 3 \
 -snes_type vinewtonrsls -ksp_type cg -pc_type mg \
 -snes_grid_sequence J

- grid-independent Newton iterations
 optimal O(N¹) flops and time
- Chapter 12 example in my new book





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- o grid-independent Newton iterations
- optimal $O(N^1)$ flops and time
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- semi-smooth Newton also yields mesh-independent iterations
 - o penalty scaling argument (Farrell et al. 2020)
- other VI multilevel strategies:
 - projected FAS multigrid for linear CPs (Brandt & Cryer, 1983)
 - monotone multigrid (Kornhuber, 1994)
 - \circ multilevel constraint decomposition (Tai, 2003) \leftarrow more below

multigrid strategies for VIs: feature table

	admissible iterates	mesh-indep. rates	no global linearization	PETSc or Firedrake
RS NM	\checkmark			\checkmark
+ NI	\checkmark	\checkmark		\checkmark
SS NM		\checkmark		\checkmark
FASCD	\checkmark	?	\checkmark	

RS = reduced space, SS = semi-smooth, NM = Newton-multigrid, NI = nested iteration

- o for the non-local fluid layer VI problem we need all 4 checked
- we are trying-out a new algorithm, FASCD = full approximation storage constraint decomposition
 - Firedrake implementation

multigrid strategies for VIs: feature table

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 FASCD = full approximation storage constraint decomposition
 - Firedrake implementation ... as of yesterday

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constraint decomposition

- Tai's (2003) constraint decomposition (CD) for VIs follows the subspace decomposition idea (Xu 1992)
- $\bullet~$ suppose $\mathcal{K} \subset \mathcal{V}$ is a closed and convex admissible subset
- for a subspace decomposition $\mathcal{V} = \sum_i \mathcal{V}_i$, write the admissible subset as a sum

$$\mathcal{K} = \sum_{i} \mathcal{K}_{i}$$

where $\mathcal{K}^i \subset \mathcal{V}^i$, with projections $\Pi_i : \mathcal{K} \to \mathcal{K}_i$

CD additive and multiplicative iterations exist for VI(F, ℓ, K)

CD-ADD(*u*):
for
$$i \in \{0, ..., m-1\}$$
:
find $\hat{w}_i \in \mathcal{K}_i$ so that for all $v_i \in \mathcal{K}_i$,
 $\left[\langle F(u - \Pi_i u + \hat{w}_i), v_i - \hat{w}_i \rangle \ge \langle \ell, v_i - \hat{w}_i \rangle \right]$
 $\hat{w} = \sum_i \hat{w}_i \in \mathcal{K}$
return $w = (1 - \alpha)u + \alpha \hat{w}$

• recall $\mathcal{K} = \{ \mathbf{v} \ge \psi \}$ in classical obstacle problem

• define **defect obstacle** for a fine-level iterate w^{J} :

$$\chi^J = \psi^J - \mathbf{W}^J$$

• monotone restriction generates obstacles on each level:

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

• let
$$\mathcal{U}^j = \{ z \ge \chi^j \}, \ \mathcal{D}^j = \{ y \ge \chi^j - \chi^{j-1} \}$$

• get CD of fine-level constraint set:

$$\mathcal{U}^{J} = \sum_{i=0}^{J} \mathcal{D}^{i} \qquad \qquad \begin{array}{c} y_{3} \in \mathcal{D}^{3} \\ y_{2} \in \mathcal{D}^{2} \\ y_{1} \in \mathcal{D}^{1} \end{array} \qquad \begin{array}{c} \varphi \quad z_{3} \in \mathcal{U}^{3} \\ z_{2} \in \mathcal{U}^{2} \\ z_{1} \in \mathcal{U}^{1} \end{array}$$

iteration \rightarrow V-cycle $z_{0} \in \mathcal{U}^{0} = \mathcal{D}^{0}$

• multiplicative CD iteration \rightarrow V-cycle

as decomposition of the fluid layer

- again this is too abstract
- what does it look like for the fluid layer?
 - o coarse grids have admissible pieces of the fine-grid iterate



full approximation storage constraint decomposition

$$\begin{aligned} & \mathsf{FASCD-VCYCLE}(\ell^J, \psi^J; w^J) \mathbf{:} \\ & \chi^J = \psi^J - w^J \\ & \mathsf{for} \ j = J \ \mathsf{downto} \ j = 1 \\ & \chi^{j-1} = R^{\oplus} \chi^j \\ & \phi^j = \chi^j - P\chi^{j-1} \\ & y^j = 0 \\ & \mathsf{SMOOTH}^{\operatorname{down}}(\ell^j, \phi^j, w^j; y^j) \qquad (\textit{smoothing in } \mathcal{D}^j) \\ & w^{j-1} = R^{\bullet}(w^j + y^j) \\ & \ell^{j-1} = f^{j-1}(w^{j-1}) + R\left(\ell^j - f^j(w^j + y^j)\right) \\ & z^0 = 0 \\ & \mathsf{SOLVE}(\ell^0, \chi^0, w^0; z^0) \qquad (\textit{coarse solve in } \mathcal{U}^0) \\ & \mathsf{for} \ j = 1 \ \mathsf{to} \ j = J \\ & z^j = y^j + Pz^{j-1} \\ & \mathsf{SMOOTH}^{\operatorname{up}}(\ell^j, \chi^j, w^j; z^j) \qquad (\textit{smoothing in } \mathcal{U}^j) \\ & w^J \leftarrow w^J + z^J \end{aligned}$$

- preliminary results
- dome test case in lubrication approximation
 - \circ here Φ(s) is a differential operator \circ note $s^{8/3} \in W^{1,4}(Ω)$ but not in C^2
- FASCD algorithm result
 - Firedrake P₁ elements
 - strong smoother (vinewtonrsls)



evidence of mesh independence

- same lubrication approximation, but in 1D
- FASCD V-cycles with NGS and NJacobi smoothers
- up-smoothing preferred: V(0,2) beats V(1,1)
- evidence of mesh independence of factors $||r^{(k+1)}|| / ||r^{(k)}||$



summary and outlook

- the variational inequality (VI) problem class is good to know
- Iikewise full approximation storage (FAS) multigrid
 - $\circ~$ need for better support and documentation in PETSc/Firedrake
- multigrid treatment of nonlinear and nonlocal VIs?
 - smoothers not obvious in nonlocal cases
 - $\circ~$ seeking practical evidence of mesh-independent convergence
- glacier evolution, as fluid-layer-in-climate problems, needs attention from applied mathematicians and numerical analysts
 - VI form not widely recognized
 - $\circ~$ current state of the art = explicit time stepping of surface
 - ▷ slow for science, intrinsically *not* scalable
 - to do: steady-state and implicit step VI problems
 - $\circ~$ more on this view in my Math. Geosci. seminar tomorrow 2pm L5

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