Adaptive Mesh Refinement for Obstacle Problems

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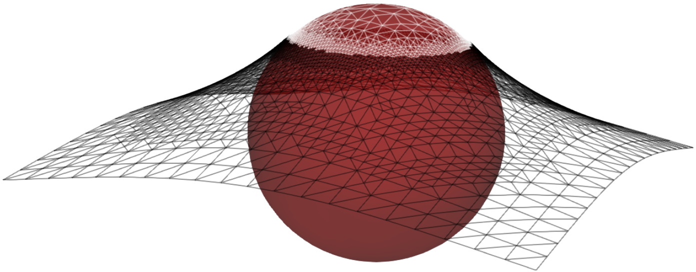
Overview

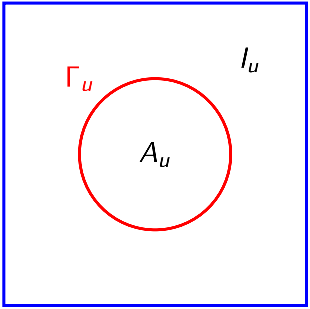
Variational Inequalities: Classical Obstacle Problem



Problem: Solve for the displacement of an elastic membrane $u(x, y)$ over a region Ω which minimizes elastic potential energy, subject to a distributed load $f(x, y)$, $u|_{\partial\Omega} = g$ and $u \geq \psi$.

Variational Inequalities: Classical Obstacle Problem

- The solution u defines the following subsets of Ω
  - Active Set $A_u = \{u = \psi\}$
  - Inactive Set $I_u = \{u > \psi\}$ on which u satisfies a PDE (Poisson equation)
  - Free Boundary $\Gamma_u = \partial I_u \cap \Omega$
- What is true on the free boundary?
  - $u = \psi$ on Γ_u
  - $u' = \psi'$ on Γ_u



Variational Inequalities: Equivalent Formulations

Theorem (FTVI; Kinderlehrer & Stampacchia 2000)

Fix $g, f \in C^\infty(\Omega)$ *with* $g_D \in C(\overline{\Omega})$, $\psi \in C(\overline{\Omega})$, $g_D \leq \psi$ *and*

$$K_\psi = \{v \in H^1_{g_D}(\Omega) | v \geq \psi\}$$

Then the following are equivalent:

(a) *u is a solution to the energy minimization formulation,*

$$\underset{u \in K_\psi}{\text{minimize:}}\ I(u) = \int_\Omega \frac{1}{2} |\nabla u|^2 - fu$$

(b) *u is a solution to the variational inequality formulation,*

$$\int_\Omega \nabla u \cdot \nabla(v - u) \geq \int_\Omega f(v - u), \qquad \text{for all } v \in K_\psi.$$

Variational Inequalities: Complimentarity Problem

Theorem (FTVI)

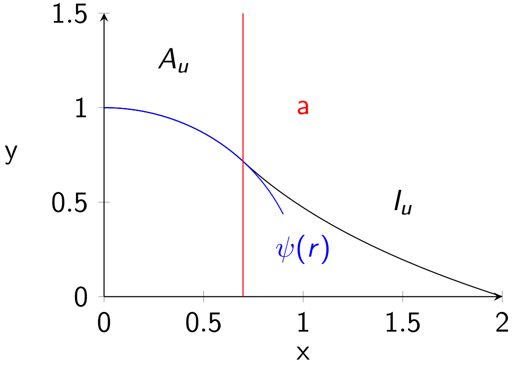
If $u \in C(\overline{\Omega}) \cap C^2(\Omega)$, then (a) or (b) implies:

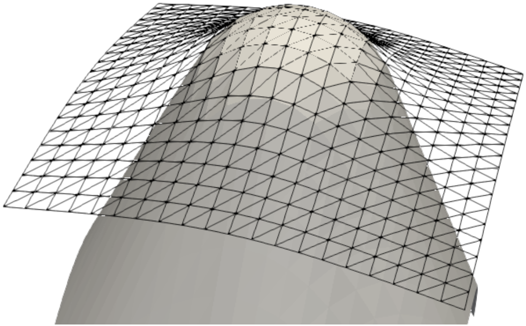
(c) *u is a solution to the complementarity problem (CP) formulation, for which the following hold over Ω a.e.*

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

Variational Inequalities: Ball Obstacle Reference

- Exact solutions in 1d and 2d for ball obstacles. (Bueler 2021)





Variational Inequalities: Active Set Newton's Method

- This problem is nonlinear so ...
  - VI-adapted Newton Solver with Reduced Space Line Search.
    - `vinewtonrsls` in PETSc
    - (Benson & Munson 2006)
  - Solves finite nonlinear complementarity problems(NCP) with the form,

$$F(w) \geq 0, \quad w \geq 0, \quad F(w)w = 0.$$

- To write the obstacle problem as an NCP:

$$\underbrace{\begin{aligned} -\nabla^2 u - f &\geq 0 \\ u - \psi &\geq 0 \\ (-\nabla^2 u - f)(u - \psi) &= 0 \end{aligned}}_{\text{Continuum CP}} \quad \underset{\substack{\text{Discretize} \\ \& \\ \text{Substitute}}}{\Longrightarrow} \quad \underbrace{\begin{aligned} F(w) &\geq 0 \\ w &\geq 0 \\ F(w)w &= 0 \end{aligned}}_{\text{Finite Dimensional NCP}}$$

Various "Conforming" Admissibility

Definition (FE VI Solution)

Let $\mathcal{K}_h = \{v_h \in H^1_{g_D}(\Omega) | v_h \geq \psi_h\}$ be the feasible set.
Our FE method seeks $u_h \in \mathcal{K}_h$ which satisfies

$$\int_\Omega \nabla u_h \cdot \nabla(v_h - u_h) \geq \int_\Omega f(v_h - u_h), \quad \text{for all } v_h \in \mathcal{K}_h.$$

There are levels of conformity,

1. $\mathcal{K}_h \not\subset \mathcal{K}$ (e.g. ψ_h is a P1 interpolant)
2. $\mathcal{K}_h \subset \mathcal{K}$ (e.g. ψ_h is a P1 interpolant + monotone injection operator (Bueler & Farrell 2024))
3. $\mathcal{K}_h = \mathcal{K} \cap \mathcal{X}_h$ (ψ exactly representable in FE space)

Definition (Preferred Approximation)

Let u_h be the FE solution to the VI problem with computed active set A_u^h. The preferred approximation $\tilde{u}_h$ as the measurable function,

$$\tilde{u}_h(x) = \begin{cases} \psi(x), & x \in A_u^h \\ u_h(x), & \text{otherwise.} \end{cases} \tag{1}$$

The error decomposes into active and inactive set contributions,

$$\|u - \tilde{u}_h\|_2^2 = \int_{A_u \cap A_u^h} |\psi - \psi|^2 + \int_{A_u \setminus A_u^h} |\psi - u_h|^2 + \int_{A_u^h \setminus A_u} |u - \psi|^2 + \int_{I_u \cap I_u^h} |u - u_h|^2.$$

- Accurate free boundary approximation minimizes the middle two terms.
- PDE error estimators only control the last term.

Active Set Residual Measure

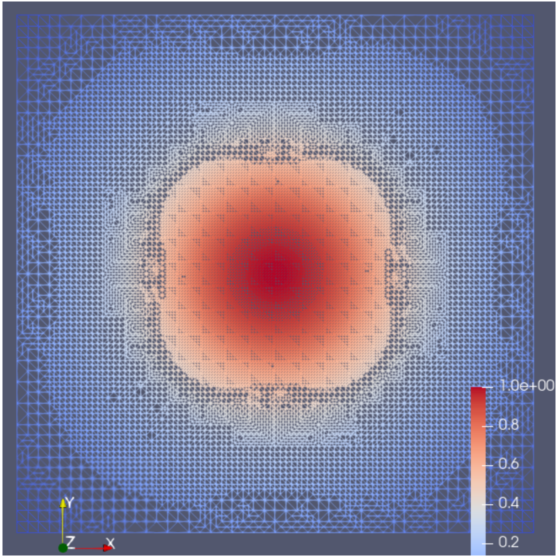
Definition

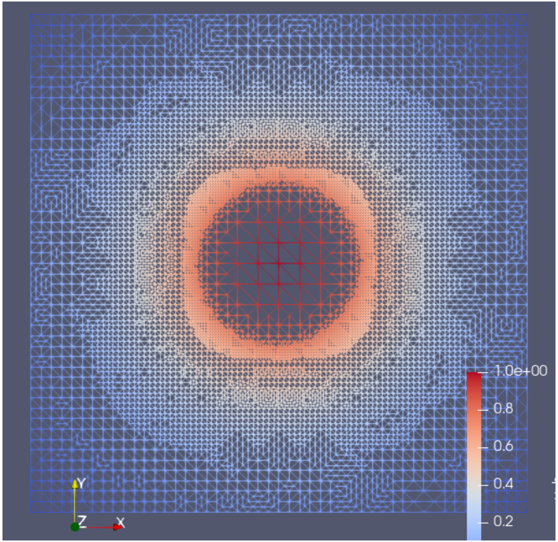
Suppose $u \in \mathcal{K}$ solves the continuum VI. Then $F(u) - \ell = d\mu_u$ is a positive Radon measure supported in A_u. Thus for $w \in \mathcal{X}$ we have

$$(F(u) - \ell)[w] = \int_{A_u} w \, d\mu_u. \tag{2}$$

Why Regular PDE Error Estimators Won't Work

- For a VI solution u the active set residual is very different from a PDE residual.





Variational Inequalities: A Priori Error

Corollary (2.5 (Fochesatto & Bueler))

Suppose $u \in \mathcal{K}$ solves the continuum VI and $u_h \in \mathcal{K}_h$ solves the FE VI and $\psi \in C^1(\Omega)$.

$$\|u - u_h\|^2 \lesssim \inf_{v \in \mathcal{K}} \int_{A_u} (v - u_h)\, d\mu_u + \inf_{v_h \in \mathcal{K}_h} \int_{A_u} (v_h - \psi)\, d\mu_u + \inf_{v_h \in \mathcal{K}_h} \left(\int_{A_u} |\nabla v_h - \nabla \psi|^2\, dx + \int_{I_u} |\nabla v_h - \nabla u|^2\, dx \right)$$

As long as $\Gamma_h \approx \Gamma$ the first three terms don't require mesh refinement to improve the FE solution.

QoI: Free Boundary Location?

- Simulation goal is locating the free boundary.
- Active Set dominated problems.
- Apply correct type of AMR on Inactive Set. (Possible DWR and admissable P-adaptivity etc.)
- Many methods (FASCD and VINEWTON) benefit from Free Boundary aware AMR.

Adaptive Mesh Refinement: Tagging Methods

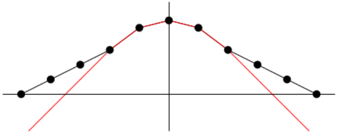
- Refinement Loop:
  1. **Solve**: Compute the solution on the current mesh.
  2. **Estimate**: Estimate error for each element.
  3. **Tag**: Tag elements for refinement based on estimate.
  4. **Refine**: Refine mesh while maintaining minimum angle criteria.

  Implementation: `github.com/StefanoFochesatto/viamr`
- Firedrake will address the Solve step.
- PETSc/Netgen (Zerbinati et al. 2024) integration will address the Refine step.

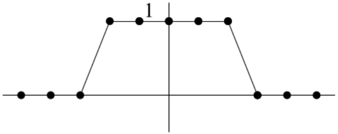
- The goal is to tag elements near the free boundary for refinement.

1. Variable Coefficient Diffusion (VCD).
2. Unstructured Dilation Operator (UDO).
3. Averaged-metric Method (AVM).

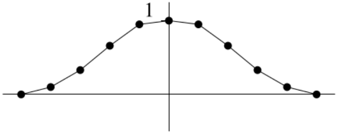
Variable Coefficient Diffusion (VCD)



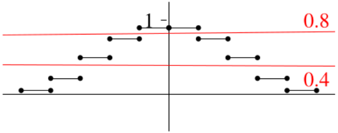
(1) Iterate u^k(black) and obstacle ψ(red).



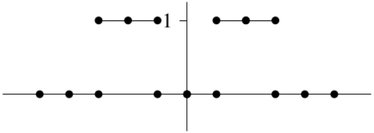
(2) Nodal active set indicator s_0.



(3) Smoothed s_1.



(4) $interpolate(s_1, W)$. Threshold values in red.



(5) Refinement indicator function I.

Algorithm VCD Element Tagging for VIs

Require: mesh $\mathcal{T}_h$, solution $u_h \in \mathcal{K}_h$, obstacle $\psi_h \in \mathcal{X}_h$, tolerance tol > 0, and threshold interval $0 < \alpha < \beta < 1$.

1: Compute nodal active set indicator $\nu_h \in \mathcal{X}_h$ for u_h.

2: For h_K the element diameter, let $D = 0.5 h_K^2 \in \mathrm{DG}_0(\mathcal{T}_h)$.

3: Approximately solve for $s_h \in \mathcal{X}_h$, with natural boundary conditions:

$$s_h - \nabla \cdot (D \nabla s_h) = \nu_h \tag{3}$$

4: **return** marking $1_h \in \mathrm{DG}_0(\mathcal{T}_h)$ of all elements such that $s_h(x_k) \in (\alpha, \beta)$.

- D is set so diffusion range $\propto$ element diameter
- Solve Eq.(3) with 4 iterations of Incomplete Cholesky-preconditioned CG ($O(V)$ complexity).

Unstructured Dilation Operator

Definition (Neighborhood Depth Parameter)

Let T be a triangulation of Ω. We define the function $N(\triangle)$ as follows:

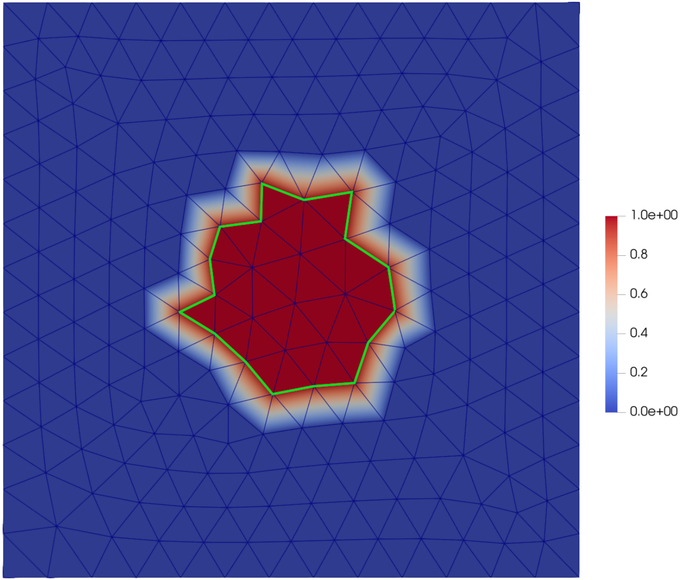
$$N(\triangle) = \{\triangle_i \in T : \triangle \text{ shares at least 1 vertex with } \triangle_i\}.$$

We define the n composition of N as follows:

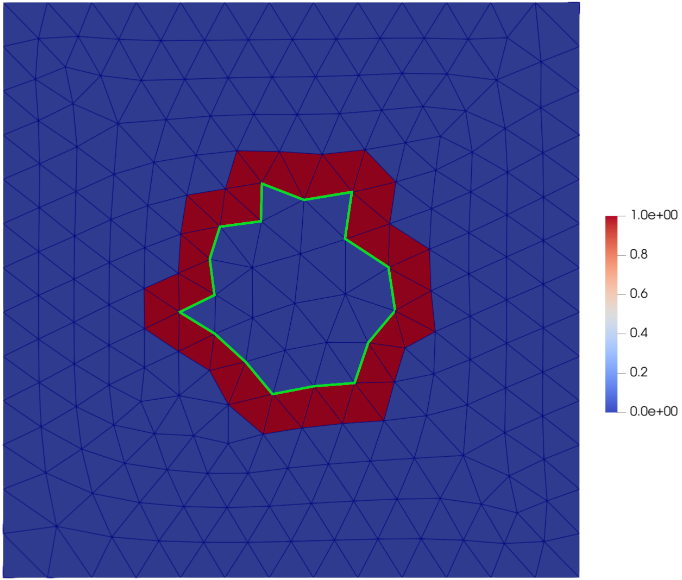
$$N^n(\triangle) = \underbrace{N(...N(\triangle))}_{n \text{ times}}.$$

We will refer to n as the neighborhood depth parameter.

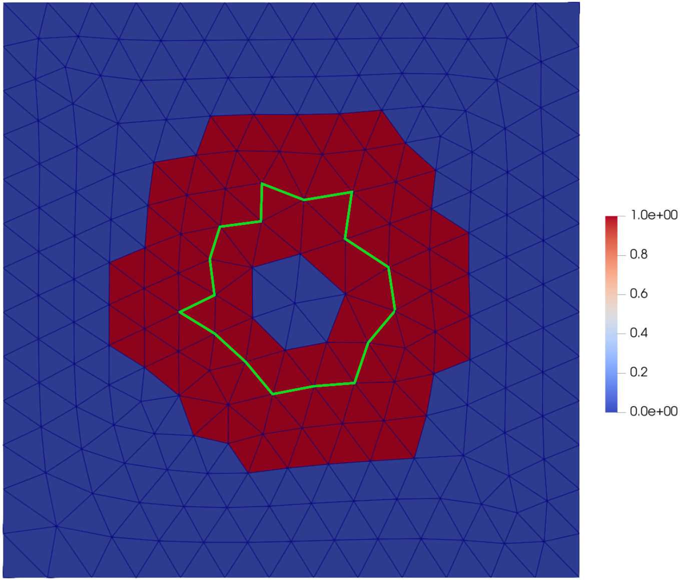
Unstructured Dilation Operator



Unstructured Dilation Operator



Unstructured Dilation Operator



Algorithm UDO Element Tagging for VIs

Require: mesh $\mathcal{T}_h$, solution $u_h \in \mathcal{K}_h$, obstacle $\psi_h \in \mathcal{X}_h$, tolerance tol > 0, and expansion parameter $n \geq 1$.

Compute nodal active set indicator $\nu_h \in \mathcal{X}_h$ for u_h.

Find initial element index set S_0: $k \in S_0$ if $\nu_h(x_k) \in (0, 1)$.

Use DMPlex to facilitate construction of $S_n = N^n(S_0)$.

return marking $1_h \in \mathrm{DG}_0(\mathcal{T}_h)$ of all elements with indices in S_n.

Algorithm Averaged-metric (AVM) mesh adaptation

Require: mesh $\mathcal{T}_h$, solution $u_h \in \mathcal{K}_h$, obstacle $\psi_h \in \mathcal{X}_h$, target complexity N, element diameter bounds $0 < h_{\mathrm{min}} < h_{\mathrm{max}}$, and averaging weight $0 \leq \gamma \leq 1$

1: Compute $s_h \in \mathcal{X}_h$ from VCD, using u_h and ψ_h.

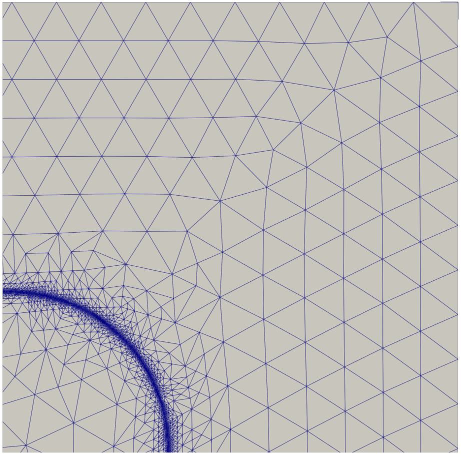
2: Compute normalized isotropic free-boundary metric:
$M_1(x) = c_1 |\nabla s_h(x)| I_{d\times d}$.

3: Compute normalized anisotropic metric from Hessian:
$M_2(x) = c_2 |Hu_h(x)|$.

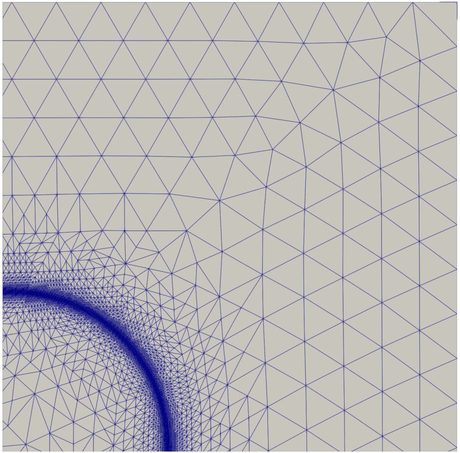
4: Average the metrics: $M(x) = \gamma M_1(x) + (1-\gamma) M_2(x)$.

5: **return** new mesh $\tilde{\mathcal{T}}_h$ which is unit with respect to $M(x)$.

Mesh Refinement Examples: 7 iterations of VCD

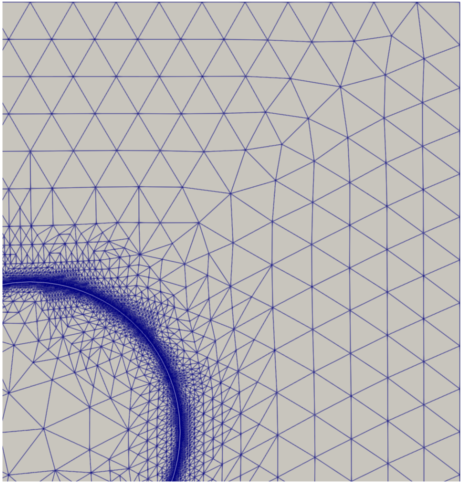


$(\alpha, \beta) = (.45, .65)$.

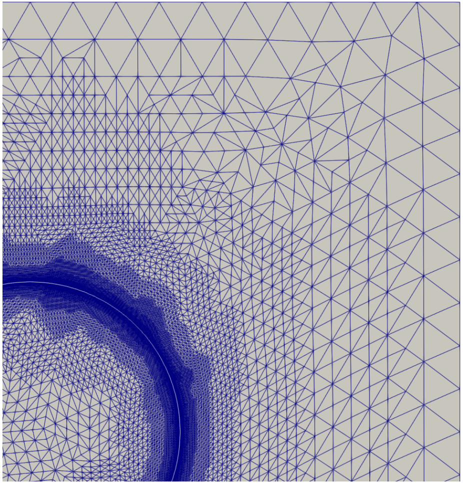


$(\alpha, \beta) = (.1, .9)$.

Mesh Refinement Examples: 7 iterations of UDO



$n = 1$



$n = 5$

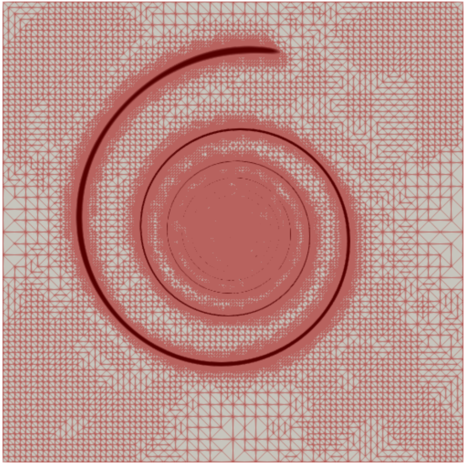


Figure: A spiral obstacle example with 2×10^5 elements, 7x UDO+BR with initial mesh of 200 elements. Element diameter (resolution) is $h \approx 10^{-3}$ along the free boundary.

Quality Metric for Free Boundary Approximation

Definition (Jaccard distance)

The Jaccard distance between measurable sets $S, T \subset \Omega$ is

$$d(S,T) = 1 - \frac{|S \cap T|}{|S \cup T|}$$

where $|\cdot|$ is the Lebesgue measure, with $d(S,T) = 0$ by definition if $|S \cup T| = 0$.

- `viamr.jaccard()` parallel implementation works for DG0 and UFL indicator functions.

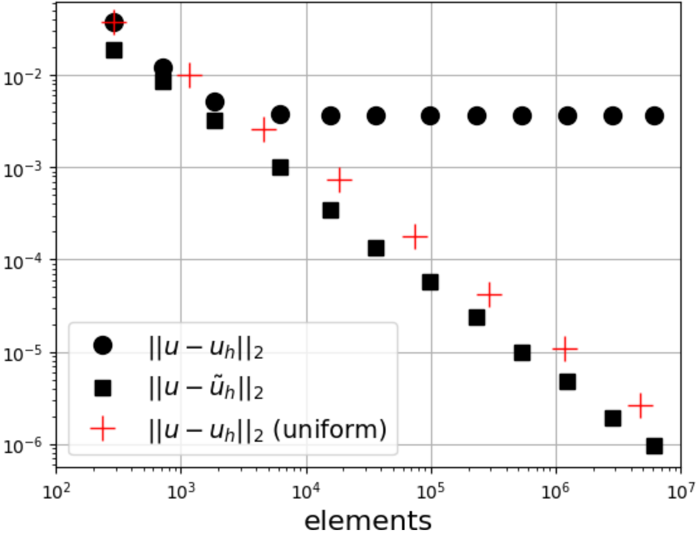


Figure: L^2 norm errors for the UDO+BR versus uniform on mostly active set problem with preferred solution $\tilde{u}_h$

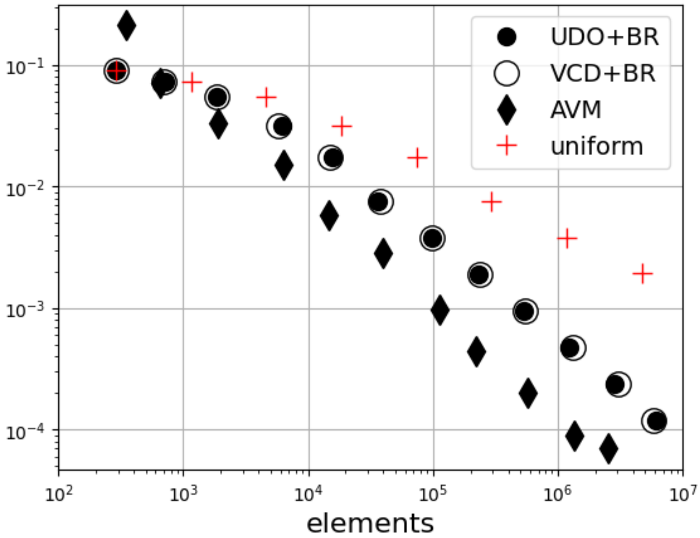


Figure: Active set Jaccard distances $d(A_u^h, A_u)$.

More Mesh Refinement Examples

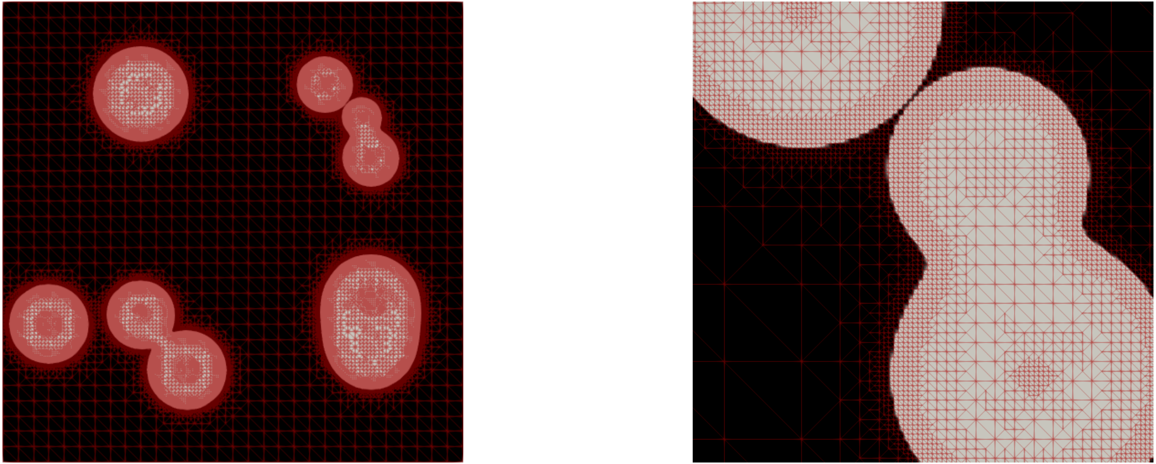


Figure: A mesh for active set dominated problem of 4.7×10^5 elements, with resolution $h \approx 10^{-3}$ along the free boundary, from four levels of the VCD+BR approach, starting from a uniform mesh of 1800 elements.

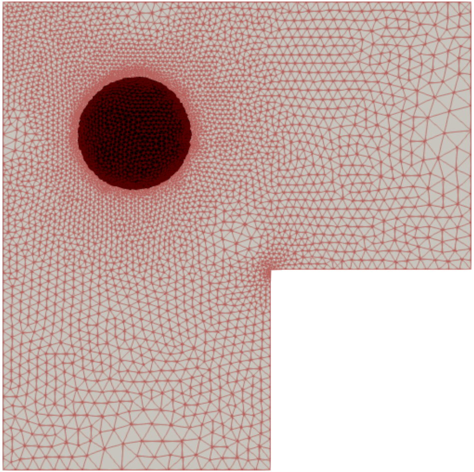


Figure: A refined mesh from three iterations of AVM Algorithm an L-Shaped domain problem, showing a well-resolved free boundary and refinement in the interior corner.

Application: Determining Glaciated Land Areas

Goal

Solve for the area of land covered by ice, also known as the **glaciated area**.

The model uses the **shallow ice approximation** with a standard shear-thinning flow law for ice. This results in a VI based on a "tilted" variation of the p-Laplacian operator.

Application: Determining Glaciated Land Areas

Variational Inequality Formulation

Find $u \in \mathcal{K}$ such that for all $v \in \mathcal{K}$:

$$\int_\Omega \Gamma |\nabla u + \beta(u)|^2 (\nabla u + \beta(u)) \cdot \nabla(v - u) - \tilde{a}(u)(v - u)\, dx \geq 0$$

Function Spaces & Physical Variables

We solve for a transformed ice thickness u:

- **Physical ice thickness**: $H = u^{3/8}$
- **Ice surface elevation**: $s = u^{3/8} + b$
- **Bedrock elevation**: $b(x, y)$
- **Surface mass-balance**: $a(x, y, s)$
- **Ice softness**: $\Gamma > 0$
- **Tilt term**: $\beta(u) = \frac{8}{3} u^{5/8} \nabla b$
- $\tilde{a}(u) = a(x, y, s)$
- $u \in \mathcal{K} = \{u \in W^{1,4}(\Omega) : u \geq 0 \text{ and } u|_{\partial\Omega} = 0\}$

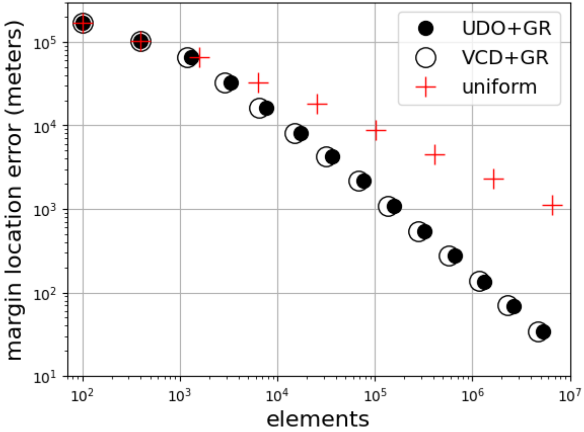
- Generally $|\nabla s| \to \infty$ at the glacier margin.

Application: Determining Glaciated Land Areas

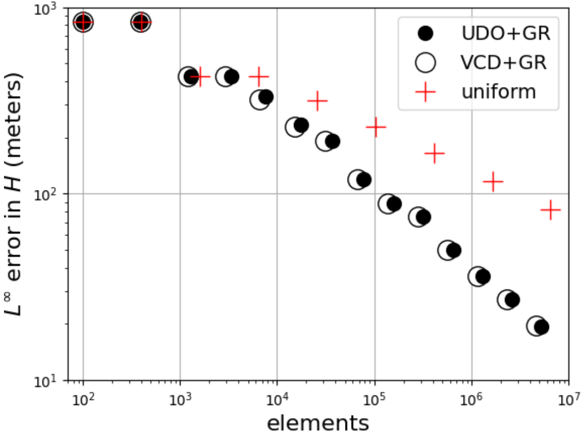
Let $\Omega = (0, L)^2$ with $L = 1800$ kilometers. With flat bed, elevation-independent source, and a known exact solution (Bueler 2016)

Simulation Setup

- **Refinement Strategy:** 13 levels of adaptive mesh refinement (AMR).
- **Initial Mesh:** Uniform grid with element size $h_0 = 360$ km.
- **Final Resolution:** High resolution at the glacier margin, $h_{13} \approx 30$ m.
- **AMR Algorithms:** Both UDO+GR and VCD+GR methods were applied with similar results.



Maximum radial error of the glacier margin.



Max error in the ice thickness H.

Conclusion

- Stabilizing Active/Inactive Sets is important.
  - Efficiency in computation on Active Set.
  - Correct type of PDE AMR on Inactive Set.
  - Preferred Approximation uses data and is generally admissible.

- Parallel Firedrake implementation with examples in 2d and 3d
  `github.com/StefanoFochesatto/viamr`
- Associated Paper

Conclusion

- Question?

Acknowledgements

- Travel support provided by the University of Colorado Boulder

Example: A Classical Obstacle Problem

Solving Ainsworth, Oden & Lee (1993) with viamr + Firedrake

We solve a classical obstacle problem with a known exact solution ($\psi = 0$). The algorithm proceeds in three steps:

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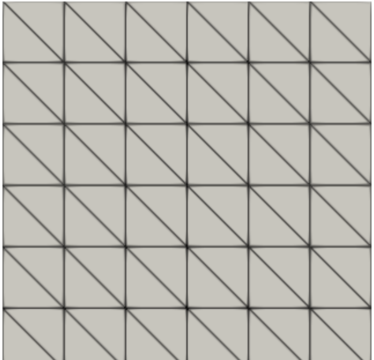
- Start with a uniform coarse mesh.

Initial Mesh



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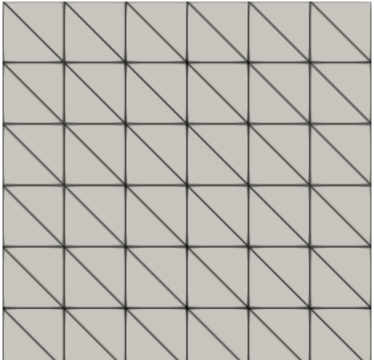
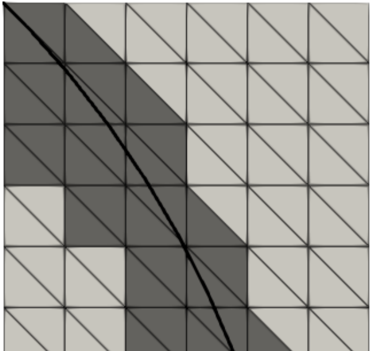
- Apply VCD marking to identify cells near the free boundary.

Initial Mesh



Marked Cells (VCD)



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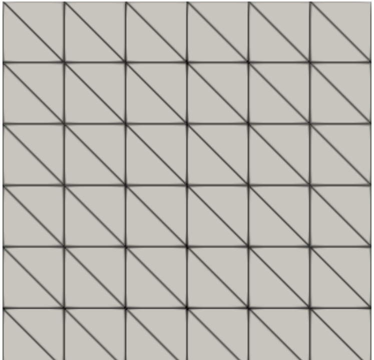
- Apply VCD marking to identify cells near the free boundary.
- Refine only the marked cells to generate the new mesh.

Initial Mesh



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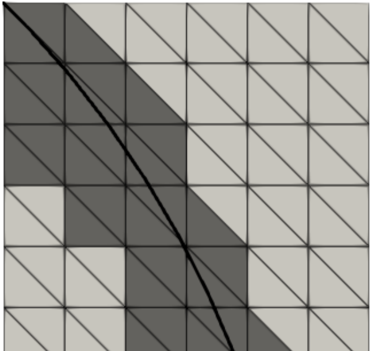
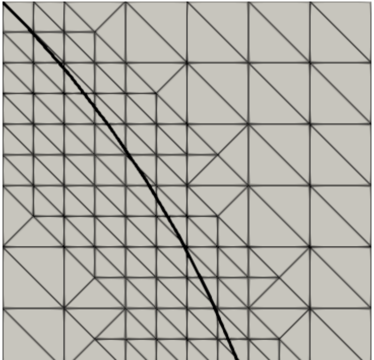


Refined Mesh



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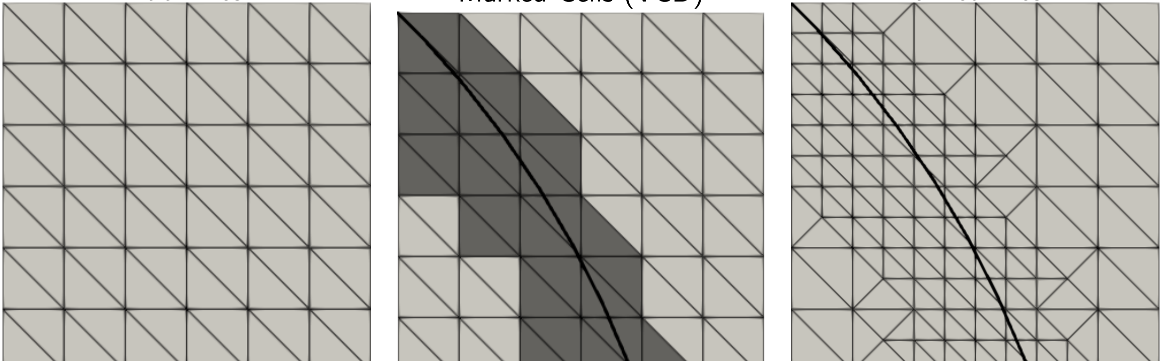
Initial Mesh | Marked Cells (VCD) | Refined Mesh



```python
from firedrake import *
from viamr import VIAMR

mesh = RectangleMesh(6, 12, 0.5, 1.0)
x, y = SpatialCoordinate(mesh)
r = (x + 1.0) ** 2 + y ** 2
uexact = conditional(r < 2.0, 0.25 * r - 0.5 - 0.5 * ln(0.5 * r), 0.0)

V = FunctionSpace(mesh, "CG", 1)
uh, vh = Function(V), TestFunction(V)
F = inner(grad(uh), grad(vh)) * dx - Constant(-1) * vh * dx
bcs = DirichletBC(V, Function(V).interpolate(uexact), "on_boundary")
problem = NonlinearVariationalProblem(F, uh, bcs)

sp = {"snes_type": "vinewtonrsls"}
solver = NonlinearVariationalSolver(problem, solver_parameters=sp)
psih = Function(V).interpolate(0.0)
INF = Function(V).interpolate(Constant(PETSc.INFINITY))
solver.solve(bounds=(psih, INF))

amr = VIAMR()
mark = amr.vcdmark(uh, psih)
VTKFile("mesh.pvd").write(uh, mark)

refinedmesh = amr.refinemarkedelements(mesh, mark)
VTKFile("refinedmesh.pvd").write(refinedmesh)
```

Appendix: Active Set Newton's Method Formulas

- Define new residual,

$$\hat{F}_i(w) = \begin{cases} F_i(w) & \text{if } w_i > 0, \\ \min\{F_i(w), 0\} & \text{if } w_i = 0. \end{cases}$$

- Define iterate's Active and Inactive sets,

$$A(w^k) = \{i \in \{1, ..., N\} | w_i^k = 0 \text{ and } F_i(w^k) > 0\},$$
$$I(w^k) = \{i \in \{1, ..., N\} | w_i^k > 0 \text{ or } F_i(w^k) \leq 0\}.$$

- Reduced Space Newton Step,

$$J(w^k)_{I^k, I^k} d_{I_k} = -F(w^k)_{I^k}.$$

- Projected Line Search,

$$\pi(w)_i = \begin{cases} w_i & \text{if } w_i > 0, \\ 0 & \text{if } w_i \leq 0. \end{cases}$$

Inactive Set A Posteriori Error: Gradient Recovery

Definition (Gradient Recovery)

Suppose $\mathcal{X}_h = \mathrm{CG}_k$, $u_h \in \mathcal{X}_h$. Define $\mathcal{Y}_h = \mathrm{DG}_{k-1}$ and note that $\nabla u_h \in \mathcal{Y}_h^d$ (vector-valued). Let $G : \mathcal{X}_h \to \mathcal{X}_h^d$ be a linear operator called *gradient recovery* (GR) so that $G(u_h) \approx \nabla u_h$ in some sense. Over an element $K \in \mathcal{T}_h$, the corresponding error indicator $\eta_K \geq 0$ is then

$$\eta_K^2 = \int_K |G(u_h) - \nabla u_h|^2 \,. \tag{4}$$

Inactive Set A Posteriori Error: Babuška–Rheinboldt

Definition (Babuška–Rheinboldt)

Let $u \in H^1(\Omega)$ and $u_h \in \mathcal{X}_h = \mathrm{CG}_1$ be analytic and FE solutions to the Poisson problem. Given the (strong) residual $r(u_h) = -\nabla^2 u_h - f$ of the Poisson equation, well-defined within each element K, the Babuška–Rheinboldt (BR) error estimator is

$$\eta_K^2 = h_K^2 \int_K |r(u_h)|^2 \, dx + \frac{h_K}{2} \sum_{\gamma \in \partial K \setminus \partial\Omega} \int_\gamma [\![\nabla u_h \cdot n]\!]^2 \, dS, \tag{5}$$