Regularization and adaptivity in the approximation of quasilinear PDE.

Solving nonlinear PDE to reduce variational crime.

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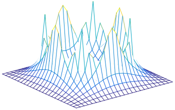
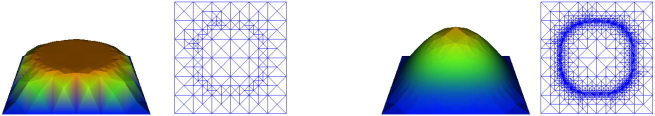
Motivation and main points



Finite element approximation: $-\mathrm{div}(\kappa(u)\nabla u) - f = 0.$ $\kappa(u) \Rightarrow$

- **Nonmonotone** problems with *steep gradients* and *internal layers* in the solution-dependent coefficients:
  - The coarse mesh problem is *wrong*.
  - Standard methods: (Damped) Newton, Picard iterations may not converge.
  - Fully solving on a coarse mesh is not useful.
- The coarse mesh problem may not satisfy coercivity or discrete inf-sup conditions.
- From a coarse mesh, adaptively refining for local features **can** be sufficient!
  - *If* the problem features can be uncovered from the unstable coarse mesh problem.
  - *Which can be done!*
  - **Method:** auto-regulated strategy using **partial solves** of **regularized problems** and **adaptive mesh refinement**.



- The regularized iteration can be derived from the original PDE in terms of **minimizing an appropriate energy** functional.

Quasilinear Diffusion Problem

$$-\operatorname{div}(\kappa(x,u,\nabla u)\nabla u) = f, \text{ in } \Omega \subset \mathbb{R}^d,\ d = 2,3 \quad + \quad \text{Boundary Conditions (BC)}$$

Applications and Examples

Engineering, Materials science, Mathematics

Concentration-dependent diffusion

$$-\operatorname{div}(\kappa(u)\nabla u) = f$$

Steady state solutions of:

- Heat conduction*
- Groundwater flow
- Diffusion of contaminants*
- Flow in porous media, *e.g.*, $\kappa(u) = c_0 + c_1 \frac{u^2(1-u^2)}{(u^3+c_2(1-u^3))}$
- Diffusion in polymers*
- Hydration of legumes(!!)

Gradient-dependent diffusion

$$-\operatorname{div}(\kappa(|\nabla u|)\nabla u) = f$$

- P-Laplacian $\kappa(|\nabla u|) = \|\nabla u\|^{p-2}$
- Prescribed mean curvature $\kappa(|\nabla u|) = (1 + \|\nabla u\|^2)^{-1/2}$
- Stationary conservation laws
- Perona-Malik equation, $\partial_t u = \operatorname{div}(\kappa \nabla u)$ (image deblurring): *e.g.*, $\kappa(s^2) = (1 + s^2/\lambda^2)^{-1},\ \lambda > 0$

* Convection-diffusion Problem: $-\operatorname{div}(\kappa(u)\nabla u) + b \cdot \nabla u = f$

Weak solutions for $F(u) = -\mathrm{div}(\kappa \nabla u) - f,\ F : \mathcal{U} \to \mathcal{V}^*$.

Quasilinear stationary diffusion with solution-dependent $\kappa(u)$.

$$-\mathrm{div}(\kappa(u)\nabla u) = f(x) \ \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega \Longrightarrow \int_\Omega -\mathrm{div}(\kappa(u)\nabla u)v = \int_\Omega fv$$

and integrate by parts to obtain the *weak form*: Find $u \in \mathcal{U}$ such that

$$B(u;u,v) := \int_\Omega \kappa(u)\nabla u \cdot \nabla v = \int fv, \text{ for all } v \in \mathcal{V}.$$

Usually, we think of $\mathcal{U} = \mathcal{V} = H_0^1(\Omega)$.

Technicality: for this problem $\mathcal{U} = W_0^{1,p},\ \mathcal{V} = W_0^{1,q}, p > 2$ and $\frac{1}{p} + \frac{1}{q} = 1$, for $F(u) = -\mathrm{div}(\kappa(u)\nabla u) - f(x)$ to be a C^1 map (Caloz, Rappaz, 1994).

Under the assumptions that $\kappa(s)$ is sufficiently smooth bounded and bounded away from zero, the PDE has a unique solution.

Under the assuption of a **sufficiently small meshsize** the linear Lagrange finite elment solution $u_h \to u$ (Caloz, Rappaz, 1994); and Holst, Tsogterel, Zhu, 2008)

- Problem 1: The theory does not suggest how to *compute* the finite element solution, only that it exists.
- **Problem 2:** Assuming the initial maximum meshsize is sufficiently small potentially makes the method totally impractical!

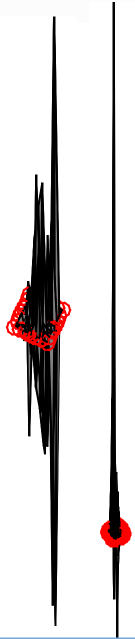
$F(u) := -\mathrm{div}(\kappa(x,u,|\nabla u|)\nabla u) - f = 0$

Newton Iterations: Do not always converge.

They may massively fail, if κ contains thin layers and steep gradients, *e.g.*, $\kappa(u) = 1 + 1/(\varepsilon + (u-0.5)^2)$.

- Newton iterations are only guaranteed to converge locally: near the solution, and under Lipschitz assumptions on the Jacobian.
  - A **Damped** or globalized Newton method: $u^{n+1} = u^n + \alpha w$ $\alpha = 2^{-j}$ chosen to reduce the residual, also fails $\sim \varepsilon = 10^{-3}$.
- Existence and (local) uniqueness of $F(u) = 0$ does **not** necessarily carry over to the coarse mesh problem.

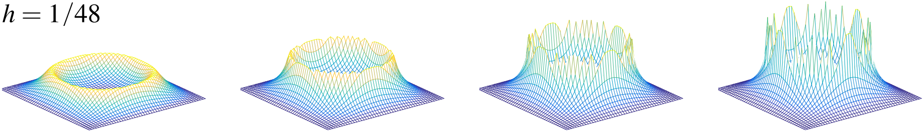
- The coarse mesh problem may be considered a **noisy** (inaccurate) representation of the PDE.
- It may be **ill-posed**: unstable, with multiple or no solutions.
- Coarse mesh **Jacobians** are ***ill-conditioned*** and sometimes ***indefinite***.
  - **Picard iterations**: Solve $A(U;U) = F$ by iterating $A(U^n;U^{n+1}) = F$. Fails $\sim \varepsilon = 10^{-2}$.
- **The diffusion term is not resolved!**



Visualization of $\kappa(u) = 1 + 1/(\varepsilon + (u-0.5)^2),\ u = \sin(\pi x)\sin(\pi y)$

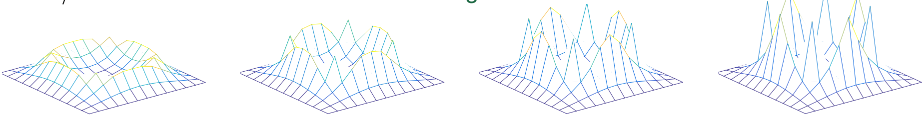
$\Uparrow\Uparrow$ finer mesh $\Uparrow\Uparrow$ (log scale)

$h = 1/48$



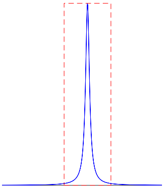
$h = 1/12$

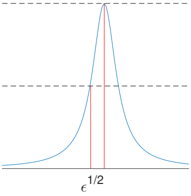
Quadrature error is high even for exact u!



$\varepsilon = 10^{-2}$ $\varepsilon = 10^{-3}$ $\varepsilon = 10^{-4}$ $\varepsilon = 10^{-5}$

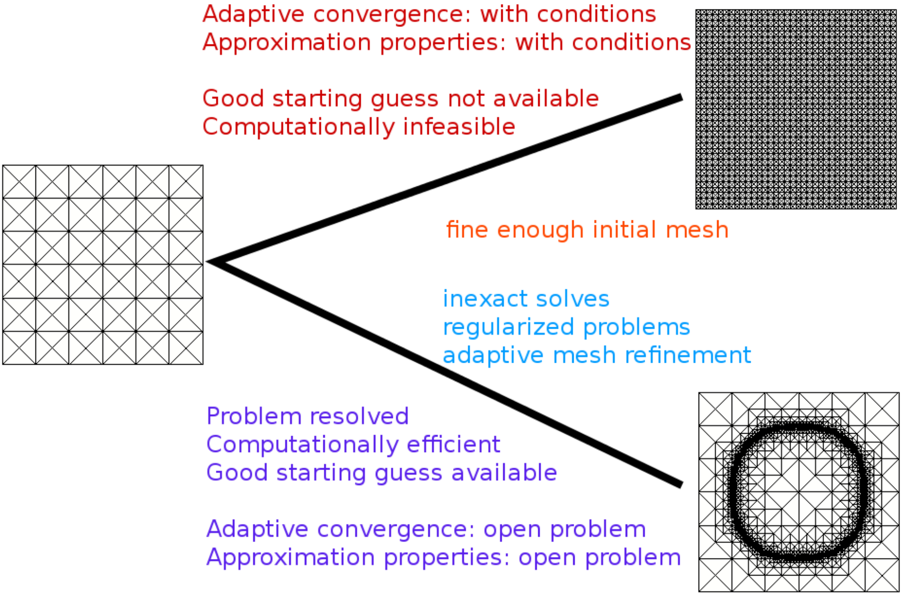
Profile of $u = \sin(\pi x)$ vs. $\kappa(u) \Rightarrow$





Solution u must be accurate to within $\sqrt{\varepsilon}$ to resolve diffusion coefficient near peak!

How do we solve the discrete problem?



Related methods

- Pseudo-transient continuation (Kelley, Keyes, *et al.,*). Addresses convergence of the pseudo-time stabilization of the Jacobian for nonlinear elliptic problems using a scaled identity preconditioner, on a given mesh. (Coffey, Kelley, Keyes) for differential-algebraic problems with positive pseudo-time stabilization applied to part of the system.

- Adaptive framework for balancing linearization and discretization errors for quasilinear problems (El Alaoui, Ern, Vohralík) and (Ern, Vohralík). Assumes discrete problem is well-posed, and solve does not fail. Coarse mesh and preasymptotic regimes are not considered.

- Standard technique: Kirchhoff transform $\theta = \int^u \kappa(s)\, ds$ transforms $-\mathrm{div}(\kappa(u)\nabla u) = f$, to $-\mathrm{div}(\nabla\theta) = f$. Problem 1: nonlinear inverse transform is nontrivial for $\kappa(s)$ other than exponential or linear or quadratic polynomial. Problem 2: Does not generalize to handle $\kappa = \kappa(x,u)$ or lower order terms, *e.g.,* convection or reaction. Boundary terms are also difficult. Recent discussion: (Vadasz).

Main idea: inexact solves of regularized problems

Coarse mesh (*ill-posed*) $\longrightarrow$ Preasymptotic $\longrightarrow$ Asymptotic(*well-posed*)

- Coarse mesh regime: Solve minimally, and refine mesh adaptively.
  - Extract information from inexact regularized problem for mesh refinement.
  - Goal of regularization: *stability* not *accuracy*
  - Even regularized problem may be ill-posed.
- Preasymptotic regime: reduce regularization, and refine mesh adaptively.
  - Increase the accuracy of each solve: construct a better initial guess for the next refinement.
  - Update the regularization parameters adaptively to increase both accuracy and efficiency.

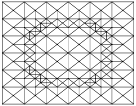
  For convergence of the method:
  - Stopping criteria for inexact nonlinear solves.
  - Update criteria for regularization parameters.
- Asymptotic regime: Solve to tolerance, and refine mesh adaptively.
  - Reduction to a standard Newton method.

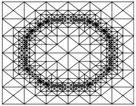
Recent publications: $-\mathrm{div}(\kappa(u,|\nabla u|)\nabla u) + b(u)\cdot\nabla u = f$

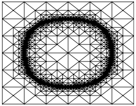
- SP, A regularized Newton-like method for nonlinear PDE.
  Numer. Func. Anal. Opt., 36 (11), p 1493-1511, 2015.

- SP, An improved method for solving quasilinear convection diffusion problems on a coarse mesh.
  SIAM J. Sci. Comput., 32 (2), p A1121-A1145, 2016.

- SP, Stabilized and inexact adaptive methods for capturing internal layers in quasilinear PDE.
  J. Comput. Appl. Math., 302, p 243-262, 2016.





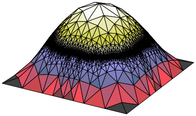


Right: Adaptive meshes for $-\mathrm{div}(\kappa(u)\nabla u) = f$,

$\kappa(u) = 1 + \{\varepsilon + (u-0.5)^2\}^{-1}, \quad \varepsilon = 10^{-5}$,

using inexact regularized iteration:

$$\left\{\alpha R + \gamma_{10}A_1'(u^n;u^n) + \gamma_{01}A_2'(u^n)\right\} w = -A(u^n;u^n) + \delta(f+\psi).$$



Regularization term: R.

Parameters from pseudo-time integrator: $\alpha, \gamma_{10}, \gamma_{01}, \delta$.

Pictured: Solution with 10706 dof. Runtime to residual convergence: < 3 min

Main ideas developed

- **Jacobian stabilization** via Tikhonov regularization and related pseudo-time stepping.
  - Pseudo-time stepping (pseudo-transient continuation)
    $F(x,u) = 0 \implies R\dot{u} + F(x,u) = 0$
  - Tikhonov regularization: minimize $G_\alpha(w) = \|F'(x,u^n)w + F(x,u^n)\|^2_{L_2} + \alpha_n\|Rw\|^2_{L_2}$ for positive semidefinite R.
  - Example: Replace positive definite R by χR, to regularize degrees of freedom *selectively*.
- Pseudo-time integrator: replace standard backward Euler discretization with Newmark update for increased numerical dissipation

$$u^{n+1} - u^n = \Delta t_n\{(1-\gamma)R\dot{u}^n + \gamma R\dot{u}^{n+1}\}, \quad R\dot{u} = \partial(Ru)/\partial t.$$

- **Stopping criteria** for partial solves.
- Definition and analysis of regularization parameters.
  - **Convergence** of the inexact iteration to the exact iteration with asymptotically quadratic convergence.
- Next: Generalize the pseudo-time stepping by seeking a solution with an approximate time-derivative *of minimum energy*, $\mathcal{E}(\dot{u}) = \min!$ rather than $\dot{u} = 0$.

Pseudo-time regularization

PDE with homogeneous Dirichlet or mixed BC

$$\text{Strong form: } -\operatorname{div}(\kappa(u)\nabla u) = f \quad \text{in } \Omega, \quad u = 0 \text{ on } \Gamma_D,$$
$$\kappa(u)\nabla u \cdot n = \psi \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D.$$

Weak form: find $u \in \mathcal{V}$:

$$B(u;u,v) := \int_\Omega \kappa(u)\nabla u \nabla v = \int_\Omega f v + \int_{\Gamma_N} \psi v, \text{ for all } v \in \mathcal{V}.$$

Pseudo-time regularization: $u = u(t), \quad \dot{u} = \mathrm{FD}(\partial u/\partial t). \quad \mathcal{E}(w) = \frac{1}{2}\phi(w,w),\ w \in \mathcal{V}$
Seek a minimum energy solution: $\mathcal{E}(\dot{u}) = \min!, \implies \mathcal{E}'(\dot{u})v = 0$ for all $v \in \mathcal{V}$.

Energy. For $\mathcal{V} \subseteq H^1_{0,\Gamma_D}(\Omega)$.
For $u = 0$ on $\partial\Omega$, minimize in H^1_0

$$\mathcal{E}(\dot{u}) = \frac{1}{2}\int_\Omega |\nabla \dot{u}|^2.$$

For $u = 0$ on Γ_D, $\kappa(u)\nabla u \cdot n = \psi$ on Γ_N, minimize in H^1_{0,Γ_D}

$$\mathcal{E}(\dot{u}) = \frac{1}{2}\left\{ c_D \int_\Omega |\nabla \dot{u}|^2 + (1 - c_D)\int_{\Gamma_N} \dot{u}^2 \right\},\ 0 < c_D \leq 1.$$

(Auchmuty, 2004) on $\int_{\partial\Omega} v^2$ rather than $\int_\Omega v^2$ in norm $\|\cdot\|_{H^1}$.

Pseudo-time regularized equation

Discrete regularized problem: find $u_k \in \mathcal{V}_k \subset \mathcal{V}$ such that

$$\mathcal{E}'(\dot{u}_k, v) = -B_k(u_k; u_k, v) + (f, v) + (\psi, v)_{\partial\Omega}, \quad \text{for all } v \in \mathcal{V}_k.$$

Discretize in time: (generalized) Newmark time integration strategy ($u^n := u^n_k$, $B := B_k$)

$$\mathcal{E}'\left(\frac{1}{\Delta t^n}(u^{n+1} - u^n), v\right) = -\tilde{\gamma}_{00} B(u^n; u^n, v) - \tilde{\gamma}_{10} B(u^{n+1}; u^n, v) - \tilde{\gamma}_{01} B(u^n; u^{n+1}, v) + (f, v) + (\psi, v)_\Gamma.$$

Linearized equation for $w = u^{n+1} - u^n$, $\alpha^n = 1/(\Delta t^n \cdot (\gamma_{00} + \gamma_{01} + \gamma_{10}))$

$$\alpha^n \mathcal{E}'(w, v) + \gamma_{10} B'(u^n; u^n, v)(w) + \gamma_{01} B(u^n; w, v) = B(u^n; u^n, v) + \delta((f, v) + (\psi, v)_\Gamma).$$

Assembled linearized matrix equation (with some abuse of notation):

$$\left\{\alpha R + \gamma_{10} A_1'(u^n; u^n) + \gamma_{01} A_2'(u^n)\right\} w = -A(u^n; u^n) + \delta(f + \psi).$$

$$\begin{aligned}
Rw &= \text{ASSEMBLE}\left\{\mathcal{E}'(w, v) = (\nabla w, \nabla v) + (w, v)_\Gamma\right\} \\
A_1'(u^n; u^n) w &= \text{ASSEMBLE}\left\{B_1'(u^n; u^n, v)(w) = (\kappa'(u^n) w \nabla u^n, v)\right\} \\
A_2'(u^n) w &= \text{ASSEMBLE}\left\{B_2'(u^n; u^n, v)(w) = B(u^n; w, v) = (\kappa(u^n) \nabla w, \nabla v)\right\}
\end{aligned}$$

Quadrature error introduced in assembly may be nontrivial!

Error representation and conditions for convergence

Linear convergence rate: For $r^n = -A(u^n;u^n) + \delta(f+\psi)$

$$r^{n+1} = \left(1 - \frac{1}{\gamma_{10}}\right) r^n + \frac{1}{\gamma_{10}}\alpha^n R w^n + \left(\overbrace{\frac{\gamma_{01}}{\gamma_{10}} - 1}^{\sigma^n}\right) A(u^n;w^n) - A_1'(u^n;w^n,w^n) + O(\|r^n\|^2).$$

Linear residual convergence rate: $1 - 1/\gamma_{10}$ used to predict stability, and send $\gamma_{10} \to 1$ to recover quadratic convergence rate.

- $\gamma_{01} = \gamma_{10}$: Newmark-type time integration. $\gamma_{01} = \gamma_{10} = 1$: Backward-Euler.
- $\delta = 1$: Consistent!
- $\sigma^n \geq 0$ adds additional diffusion to balance out error from linearization, adding a Picard-like term to a Newton iteration!

Updated every iteration: α^n, σ^n. Conditions for convergence

- $\alpha^n \leq \|r^n\|$. Example: $\alpha^n = \frac{\gamma_{10}}{\|Rw^{n-1}\|} \cdot \min\{\|A_1'(u^n;w)w\|, c\|r^n\|\}$
- $\sigma^n := \left(\frac{\gamma_{01}}{\gamma_{10}} - 1\right)$ satisfies: $\sigma^n \|A(u^n;w^n)\| \leq \|A_1'(u^n,w^n)w^n\|$

$$\text{Example: } \sigma^n = \frac{\langle A(u^n;w^{n-1}), A_1'(u^n,w^{n-1})w^{n-1}\rangle}{\|A(u^n,w^{n-1})\|^2}$$

Efficiency: Parameter computations are Euclidean products in $\mathbb{R}^n$.

Update criteria for γ_{10} and δ

Update γ_{10} on sufficiently stable rate of residual reduction near predicted rate.

$$\left| \frac{\|r^{n+1}\|}{\|r^n\|} - \left(1 - \frac{1}{\gamma_{10}^n}\right) \right| < \varepsilon_T, \quad \text{and} \quad \left| \frac{\|r^{n+1}\|}{\|r^n\|} - \frac{\|r^n\|}{\|r^{n-1}\|} \right| < \varepsilon_T.$$

By:

$$\tilde{\gamma}_{10}^{n+1} = q \cdot \frac{\langle r^n, r^n \rangle}{\langle r^n, A(u^{n+1}, u^{n+1}) - A(u^n, u^n) \rangle}, \quad \gamma_{10}^{n+1} = \max\left\{1\ , \tilde{\gamma}_{10}^{n+1}\right\}.$$

Update δ and **Exit iteration** on sufficient decrease *and* convergence rate.
By:

$$\tilde{\delta}_{k+1} = \frac{\langle f, \gamma_{10}(A(u^{n+1}; u^{n+1}) - A(u^n; u^n)) + \left\{(\gamma_{01} - \gamma_{10})A_2'(u^{n+1}) + \alpha R\right\} w^n + A(u^n; u^n) \rangle}{q_k \|f + \psi\|^2}$$

$$\delta_{k+1} = \min\{1\ , \tilde{\delta}_{k+1}\},$$

Convergence of $\gamma_{10} \to 1$ from above and $\delta \to 1$ from below are established.

Adaptive algorithm for nonlinear diffusion

Set the parameters $q_\gamma,\ \gamma_{\text{MAX}}$. Start with initial $u^0(=0),\ \gamma_{10}^0$. On partition $\mathcal{T}_k,\ k=0,1,2,\ldots$

1. Compute R_k and $r^0 = -A(u^n;u^n)+\delta_k(f_k+\psi_k)$.
2. Set $\alpha_0 = \|r^0\|$ and $\sigma^0 = 0$.
3. While the Exit Criteria are not met on iteration $n-1$:
   - (a) **Solve** $\{\alpha^n R_k + \gamma_{10}A_1'(u^n;u^n)+\gamma_{01}A_2'(u^n)\}w^n = r^n$, for w^n.
   - (b) **Update** $u^{n+1} = u^n + w^n$, and $r^{n+1} = -A(u^n;u^n)+\delta_k(f_k+\psi_k)$.
   - (c) If Criteria to update γ are satisfied, update γ_{10}^{n+1}.
   - (d) Update α^n and σ^n.
4. If Criteria to update δ are satisfied, update δ_{k+1} for partition $\mathcal{T}_{k+1}$, with $q_\delta = \max\{q_\gamma,(q_\gamma)^P\},\ P = \{$ Number of times γ_{10} is updated on refinement $k\}$.
5. Compute the error indicators to determine the next mesh refinement.

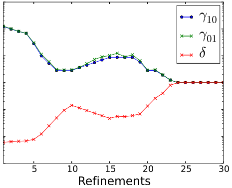
Take-home message: The algorithm adjusts the mesh *and* the regularization parameters: *The user is not involved once the computation starts.*

Model problem with steep layers

Quasilinear diffusion problem on $\Omega = (0,1)^2$.

$$-\mathrm{div}(\kappa(u)\nabla u) = f \text{ in } \Omega\,, \quad u = 0 \text{ on } \partial\Omega.$$

$$\kappa(s) = k + \frac{1}{((\varepsilon + (s-a)^2)} \quad \varepsilon = 4\times 10^{-5},\ a = 0.5,\ \text{ and } k = 1.$$



$f(x,y)$ and $\psi(x,y)$ chosen so the exact solution $u(x,y) = \sin(\pi x)\sin(\pi y)$.

Regularization: $\mathcal{E}(\dot u) = \int_\Omega |\nabla \dot u|^2$.

The initial mesh has 144 elements. $\gamma_{\mathrm{MAX}} = 180,\ q = 0.8$.

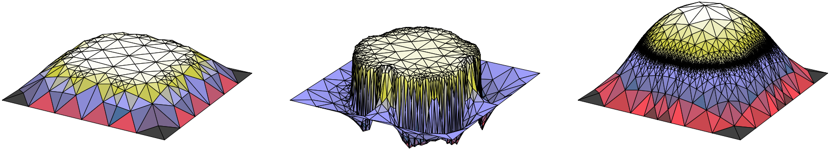


Figure: Three phases of the solution process: Level 5 with 166 dof; Level 15 with 827 dof; Level 25 with 3802 dof. Runtime to residual convergence: < 1min.

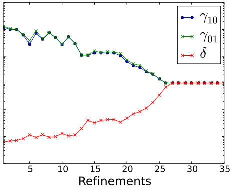
Model problem with steep layers and mixed BC

Quasilinear diffusion problem on $\Omega = (0,1)^2$.

$$-\mathrm{div}(\kappa(u)\nabla u) = f \ \text{ in } \Omega\,, \quad u = 0 \ \text{ on } \Gamma_D = \{(x,y) \in \partial\Omega \,|\, y = 1\},$$
$$\kappa(u)\nabla u \cdot n = \psi \ \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D.$$

$$\kappa(s) = k + \frac{1}{((\varepsilon + (s-a)^2)} \quad \varepsilon = 4\times 10^{-5},\ a = 0.5,\ \text{ and } k = 1.$$

$f(x,y)$ and $\psi(x,y)$ chosen so the exact solution $u(x,y) = \sin(\pi x)\sin(\pi y)$.



Regularization: $\mathcal{E}(\dot u) = \frac{1}{4}\cdot\int_\Omega |\nabla \dot u|^2 + \frac{3}{4}\cdot\int_{\Gamma_N} \dot u^2.$

The initial mesh has 144 elements. $\gamma_{\mathrm{MAX}} = 180,\ q = 0.8.$

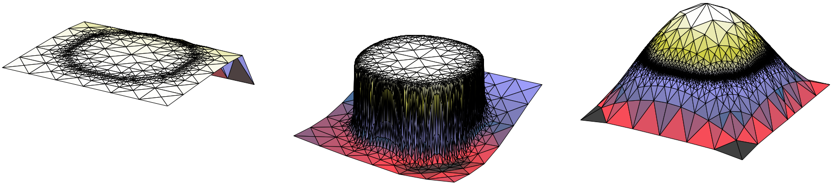


Figure: Three phases of the solution process: Level 12 with 498 dof; Level 20 with 1771 dof; Level 27 with 7266 dof. Runtime to residual convergence: $\approx$ 1.5 min.

Model problem with steep layers and mixed BC

Quasilinear diffusion problem on $\Omega = (0,1)^2$.

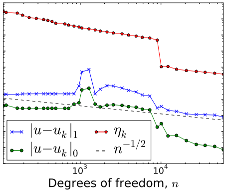
$$-\mathrm{div}(\kappa(u)\nabla u) = f \text{ in } \Omega\,, \quad u = 0 \text{ on } \Gamma_D = \{(x,y) \in \partial\Omega \,|\, y = 1\},$$
$$\kappa(u)\nabla u \cdot n = \psi \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D.$$

$$\kappa(s) = k + \frac{1}{((\varepsilon + (s-a)^2)} \quad \varepsilon = 4 \times 10^{-5},\ a = 0.5, \text{ and } k = 1.$$

$f(x,y)$ and $\psi(x,y)$ chosen so the exact solution $u(x,y) = \sin(\pi x)\sin(\pi y)$.

Regularization: $\mathcal{E}(\dot{u}) = \frac{1}{4} \cdot \int_\Omega |\nabla \dot{u}|^2 + \frac{3}{4} \cdot \int_{\Gamma_N} \dot{u}^2$.

The initial mesh has 144 elements. $\gamma_{\text{MAX}} = 180,\ q = 0.8$.



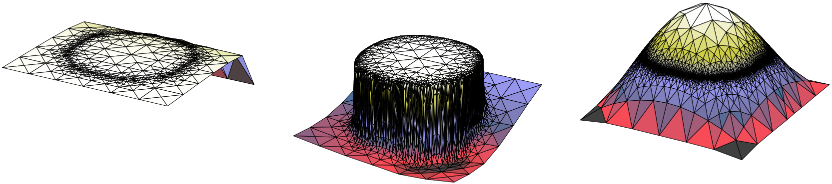


Figure: Three phases of the solution process: Level 12 with 498 dof; Level 20 with 1771 dof; Level 27 with 7266 dof. Runtime to residual convergence: $\approx$ 1.5 min.

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thank you!

Main references

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