Adaptive inexact semi smooth Newton methods for a contact between two membranes

Jad Dabaghi, Vincent Martin, Martin Vohralík

Inria Paris & Université Paris-Est

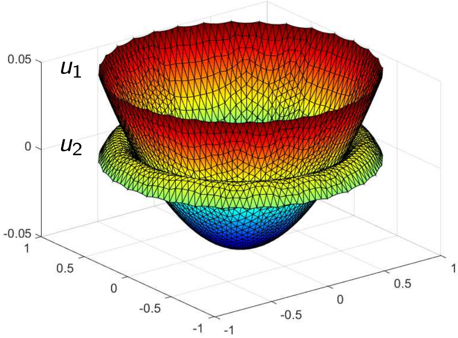
Milan, May 26-27 2017

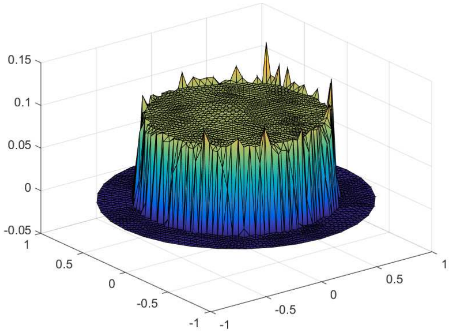
Outline

System of variational inequalities:

Find u_1, u_2, λ such that

$$\begin{cases} -\mu_1 \Delta u_1 - \lambda = f_1 & \text{in} \quad \Omega, \\ -\mu_2 \Delta u_2 + \lambda = f_2 & \text{in} \quad \Omega, \\ (u_1 - u_2)\lambda = 0, \quad u_1 - u_2 \geq 0, \quad \lambda \geq 0 & \text{in} \quad \Omega, \\ u_1 = g > 0 & \text{on} \quad \partial\Omega, \\ u_2 = 0 & \text{on} \quad \partial\Omega. \end{cases}$$





Continuous model problem and setting

Notation

- $H^1_g(\Omega)=\{u \in H^1(\Omega),\ u = g \text{ on } \partial\Omega\}$
- $\Lambda = \{\chi \in L^2(\Omega),\ \chi \geq 0 \text{ on } \Omega\}$
- $\mathcal{K}_g = \{(v_1, v_2) \in H^1_g(\Omega) \times H^1_0(\Omega),\ v_1 - v_2 \geq 0 \ \text{ on } \Omega\}$

Variational formulation: For $(f_1, f_2) \in L^2(\Omega) \times L^2(\Omega)$ and $g > 0$ find $(u_1, u_2, \lambda) \in H^1_g(\Omega) \times H^1_0(\Omega) \times \Lambda$ such that

$$\begin{cases} \sum_{i=1}^{2} \mu_i (\nabla u_i, \nabla v_i)_\Omega - (\lambda, v_1 - v_2)_\Omega = \sum_{i=1}^{2} (f_i, v_i)_\Omega \quad \forall (v_1, v_2) \in H^1_0(\Omega) \times H^1_0(\Omega) \\ (\chi - \lambda, u_1 - u_2)_\Omega \geq 0 \quad \forall \chi \in \Lambda. \end{cases}$$

Existence and uniqueness: Lions-Stamppachia Theorem

Faker Ben Belgacem, Christine Bernardi, Adel Blouza, and Martin Vohralík.
A finite element discretization of the contact between two membranes.
M2AN Math. Model. Numer. Anal., 43(1):33–52, 2008.

Discretization by finite elements

Notation:

- $\mathcal{T}_h$: conforming mesh, $\omega_{\boldsymbol{a}}$: patch of elements of $\mathcal{T}_h$ that share $\boldsymbol{a}$

Conforming spaces for the discretization:

- $\mathbb{X}_{gh} = \left\{ v_h \in \mathcal{C}^0(\overline{\Omega}), \forall K \in \mathcal{T}_h, v_{h|K} \in \mathbb{P}_1(K), \quad v_h = g \text{ on } \partial\Omega \right\}$
- $\mathcal{K}_{gh} = \{(v_{1h}, v_{2h}) \in \mathbb{X}_{gh} \times \mathbb{X}_{0h}, \quad v_{1h} - v_{2h} \geq 0 \text{ on } \Omega\}$
- $\Lambda_h = \left\{ \lambda_h \in \mathbb{X}_{0h}; \ \lambda_h(\boldsymbol{a}) \geq 0 \quad \forall \boldsymbol{a} \in \mathcal{V}_h^{\text{int}} \right\}$.

Discretization: find $(u_{1h}, u_{2h}, \lambda_h) \in \mathbb{X}_{gh} \times \mathbb{X}_{0h} \times \Lambda_h$ such that $\forall (v_{1h}, v_{2h}, \chi_h) \in \mathbb{X}_{0h} \times \mathbb{X}_{0h} \times \Lambda_h$

$$\left\{ \begin{array}{l} \displaystyle\sum_{i=1}^{2} \mu_i \left(\nabla u_{ih}, \nabla v_{ih}\right)_\Omega - \sum_{\boldsymbol{a} \in \mathcal{V}_h^{\text{int}}} \lambda_h(\boldsymbol{a})(v_{1h} - v_{2h})(\boldsymbol{a})(\psi_{h,\boldsymbol{a}}, 1)_{\omega_{\boldsymbol{a}}} = \sum_{i=1}^{2} (f_i, v_{ih})_\Omega, \\ (u_{1h} - u_{2h})(\boldsymbol{a}) \geq 0, \ \lambda_h(\boldsymbol{a}) \geq 0, \ \lambda_h(\boldsymbol{a})(u_{1h} - u_{2h})(\boldsymbol{a}) = 0. \end{array} \right.$$

Discrete complementarity problem

To reformulate the discrete constraints:

Definition

A function $f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ is a C-function if

$$\forall(\boldsymbol{a}, \boldsymbol{b}) \in \mathbb{R}^n \times \mathbb{R}^n \quad f(\boldsymbol{a}, \boldsymbol{b}) = 0 \quad \iff \quad \boldsymbol{a} \geq 0, \quad \boldsymbol{b} \geq 0, \quad \boldsymbol{ab} = 0.$$

Example: $\min(a, b) = 0 \iff a \geq 0, \ b \geq 0, \ ab = 0.$

For any C-function $\mathbf{C}$, the discrete formulation reads

$$\begin{cases} \mathbb{E}\mathbf{X}_h & = \boldsymbol{F} \\ \mathbf{C}(\mathbf{X}_h) & = 0. \end{cases}$$

C is not Fréchet differentiable!

The vector of unknowns has the following block structure

$$\mathbf{X}_h^T = (\boldsymbol{X}_{1h}, \boldsymbol{X}_{2h}, \boldsymbol{X}_{3h})^T \in \mathcal{M}_{3N_{\boldsymbol{h}},1}(\mathbb{R})$$

Semi-smooth Newton method

For $\mathbf{X}_h^0$ given, the semi-smooth Newton method reads

$$\mathbb{A}^{k-1}\mathbf{X}_h^k = \boldsymbol{B}^{k-1} \quad \forall k \geq 1$$

The Clark Jacobian matrix and the right-hand side vector are defined by

$$\mathbb{A}^{k-1} = \begin{cases} \mathbb{E} \\ \mathbf{J_C}(\mathbf{X}_h^{k-1}) \end{cases} \quad \text{and} \quad \boldsymbol{B}^{k-1} = \begin{cases} \boldsymbol{F} \\ \mathbf{J_C}(\mathbf{X}_h^{k-1})\mathbf{X}_h^{k-1} - \mathbf{C}(\mathbf{X}_h^{k-1}) \end{cases} \quad \forall k \geq 1.$$

Example: semi-smooth "min" function

$$\boldsymbol{C}(\mathbf{X}_h) = \min\left(\boldsymbol{X}_{1h} - \boldsymbol{X}_{2h}, \boldsymbol{X}_{3h}\right)$$

Example: semi-smooth "Fischer-Burmeister" function

$$\boldsymbol{C}(\mathbf{X}_h) = \sqrt{(\boldsymbol{X}_{1h} - \boldsymbol{X}_{2h})^2 + \boldsymbol{X}_{3h}^2} - (\boldsymbol{X}_{1h} - \boldsymbol{X}_{2h} + \boldsymbol{X}_{3h})$$

Algebraic resolution in semi-smooth Newton method

Any iterative algebraic solver yields on step $i \geq 0$:

$$\mathbb{A}^{k-1}\mathbf{X}_h^{k,i} + \boldsymbol{R}_h^{k,i} = \boldsymbol{B}^{k-1}$$

with $\boldsymbol{R}_h^{k,i} = (\boldsymbol{R}_{1h}^{k,i}, \boldsymbol{R}_{2h}^{k,i}, \boldsymbol{R}_{3h}^{k,i})^T$ the algebraic residual block vector.

Definition

We define discontinous $\mathbb{P}_1$ polynomials $r_{1h}^{k,i}$ and $r_{2h}^{k,i}$

- $(r_{1h}^{k,i}, \psi_{h,\boldsymbol{a}_l})_K = \dfrac{(\boldsymbol{R}_{1h}^{k,i})_l}{N_{h,\boldsymbol{a}}}, \; r_{1h}^{k,i}{}_{|\partial K \cap \partial\Omega} = 0 \qquad \forall 1 \leq l \leq N_h$
- $(r_{2h}^{k,i}, \psi_{h,\boldsymbol{a}_l})_K = \dfrac{(\boldsymbol{R}_{2h}^{k,i})_l}{N_{h,\boldsymbol{a}}}, \; r_{2h}^{k,i}{}_{|\partial K \cap \partial\Omega} = 0 \qquad \forall 1 \leq l \leq N_h$

Equivalent form of the $2N_h$ first equations

$$\mu_1 \left(\boldsymbol{\nabla} u_{1h}^{k,i}, \boldsymbol{\nabla}\psi_{h,\boldsymbol{a}_l}\right)_\Omega = \left(f_1 + \lambda_h^{k,i}(\boldsymbol{a}_l) - r_{1h}^{k,i}, \psi_{h,\boldsymbol{a}_l}\right)_\Omega,$$

$$\mu_2 \left(\boldsymbol{\nabla} u_{2h}^{k,i}, \boldsymbol{\nabla}\psi_{h,\boldsymbol{a}_l}\right)_\Omega = \left(f_2 - \lambda_h^{k,i}(\boldsymbol{a}_l) - r_{2h}^{k,i}, \psi_{h,\boldsymbol{a}_l}\right)_\Omega.$$

A posteriori analysis and preliminary study

A posteriori error estimates: $|||\boldsymbol{u} - \boldsymbol{u}_h^{k,i}||| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_K(\boldsymbol{u}_h^{k,i})^2 \right\}^{1/2}.$

Sergey Repin.
A posteriori estimates for partial differential equations.
Walter de Gruyter GmbH & Co. KG, Berlin, 2008.

Goal: $\left\{ \begin{array}{l} \boldsymbol{\sigma}_{1h}^{k,i} \in \mathbf{H}(\mathrm{div}, \Omega) \text{ such that } (\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{1h}^{k,i}, 1)_K = (f_1 + \lambda_h^{k,i}, 1)_K \ \forall K \in \mathcal{T}_h, \\ \boldsymbol{\sigma}_{2h}^{k,i} \in \mathbf{H}(\mathrm{div}, \Omega) \text{ such that } (\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{2h}^{k,i}, 1)_K = (f_2 - \lambda_h^{k,i}, 1)_K \ \forall K \in \mathcal{T}_h. \end{array} \right.$

- $\boldsymbol{\sigma}_{1h}^{k,i} = \boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i} + \boldsymbol{\sigma}_{1,h,\mathrm{alg}}^{k,i}$ and $\boldsymbol{\sigma}_{2h}^{k,i} = \boldsymbol{\sigma}_{2,h,\mathrm{disc}}^{k,i} + \boldsymbol{\sigma}_{2,h,\mathrm{alg}}^{k,i}$

Algebraic fluxes reconstruction:

- $\left\{ \boldsymbol{\sigma}_{1,h,\mathrm{alg}}^{k,i}, \boldsymbol{\sigma}_{2,h,\mathrm{alg}}^{k,i} \right\} \in \mathbf{H}(\mathrm{div}, \Omega), \quad \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{1,h,\mathrm{alg}}^{k,i} = r_{1h}^{k,i}, \quad \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{2,h,\mathrm{alg}}^{k,i} = r_{2h}^{k,i}$

Papez Jan, Rüde Ulrich, Vohralík Martin, and Wohlmuth Barbara.
Sharp algebraic and total a posteriori error bounds via a multilevel approach.
In preparation, 2017.

Discretization fluxes reconstruction

$\boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i,\boldsymbol{a}}$ and $\boldsymbol{\sigma}_{2h,\mathrm{disc}}^{k,i,\boldsymbol{a}}$ are the solution of mixed system on patches

$$\begin{cases} (\boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i,\boldsymbol{a}}, \boldsymbol{v}_{1h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} - (\gamma_{1,h}^{k,i,\boldsymbol{a}}, \nabla \cdot \boldsymbol{v}_{1h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & = & -\left(\psi_{h,\boldsymbol{a}} \nabla u_{1h}^{k,i}, \boldsymbol{v}_{1h}\right)_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & \forall \boldsymbol{v}_{1h} \in \mathbf{V}_h^{\boldsymbol{a}}, \\ (\nabla \cdot \boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i,\boldsymbol{a}}, q_{1h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & = & (\tilde{g}_{1,h}^{k,i,\boldsymbol{a}}, q_{1h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & \forall q_{1h} \in Q_h^{\boldsymbol{a}}, \\ (\boldsymbol{\sigma}_{2h,\mathrm{disc}}^{k,i,\boldsymbol{a}}, \boldsymbol{v}_{2h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} - (\gamma_{2,h}^{k,i,\boldsymbol{a}}, \nabla \cdot \boldsymbol{v}_{2h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & = & -\left(\psi_{h,\boldsymbol{a}} \nabla u_{2h}^{k,i}, \boldsymbol{v}_{2h}\right)_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & \forall \boldsymbol{v}_{2h} \in \mathbf{V}_h^{\boldsymbol{a}}, \\ (\nabla \cdot \boldsymbol{\sigma}_{2h,\mathrm{disc}}^{k,i,\boldsymbol{a}}, q_{2h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & = & (\tilde{g}_{2,h}^{k,i,\boldsymbol{a}}, q_{2h})_{\omega_{\boldsymbol{h}}^{\boldsymbol{a}}} & \forall q_{2h} \in Q_h^{\boldsymbol{a}}. \end{cases}$$

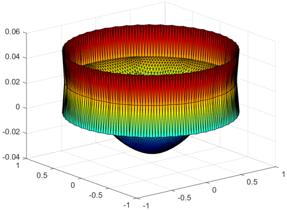
$$\boxed{\boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i} = \sum_{\boldsymbol{a} \in \mathcal{V}_{\boldsymbol{h}}} \boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i,\boldsymbol{a}} \quad \text{and} \quad \boldsymbol{\sigma}_{2,h,\mathrm{disc}}^{k,i} = \sum_{\boldsymbol{a} \in \mathcal{V}_{\boldsymbol{h}}} \boldsymbol{\sigma}_{2h,\mathrm{disc}}^{k,i,\boldsymbol{a}}}$$

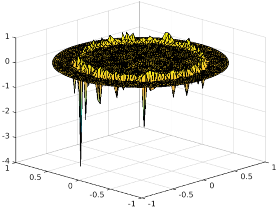
- $\boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i} \in \mathbf{H}(\mathrm{div}, \Omega)$ and $\left(\nabla \cdot \boldsymbol{\sigma}_{1,h,\mathrm{disc}}^{k,i}, 1\right)_K = \left(f_1 + \lambda_h^{k,i} - r_{1h}^{k,i}, 1\right)_K$
- $\boldsymbol{\sigma}_{2,h,\mathrm{disc}}^{k,i} \in \mathbf{H}(\mathrm{div}, \Omega)$ and $\left(\nabla \cdot \boldsymbol{\sigma}_{2,h,\mathrm{disc}}^{k,i}, 1\right)_K = \left(f_2 - \lambda_h^{k,i} - r_{2h}^{k,i}, 1\right)_K$.

- $\boldsymbol{u} = (u_1, u_2) \in \mathcal{K}_g$, $\boldsymbol{u}_h^{k,i} = (u_{1h}^{k,i}, u_{2h}^{k,i}) \in \mathbb{X}_{gh} \times \mathbb{X}_{0h}$, $\left\{\boldsymbol{\sigma}_{1h}^{k,i}, \boldsymbol{\sigma}_{2h}^{k,i}\right\} \in \mathbf{H}(\mathrm{div}, \Omega)$

Warning: $u_{1h}^{k,i}(\boldsymbol{a}) - u_{2h}^{k,i}(\boldsymbol{a})$ and $\lambda_h^{k,i}(\boldsymbol{a})$ can be negative.

Example: k=2





Motivation: Define $\boldsymbol{s}_h^{k,i} \in \mathcal{K}_{gh}$ by

$$\boldsymbol{s}_h^{k,i}(\boldsymbol{a}) = \begin{cases} \boldsymbol{u}_h^{k,i}(\boldsymbol{a}) = \left(u_{1h}^{k,i}(\boldsymbol{a}), u_{2h}^{k,i}(\boldsymbol{a})\right) & \text{if } u_{1h}^{k,i}(\boldsymbol{a}) \geq u_{2h}^{k,i}(\boldsymbol{a}), \\ \left(\dfrac{u_{1h}^{k,i}(\boldsymbol{a}) + u_{2h}^{k,i}(\boldsymbol{a})}{2}, \dfrac{u_{1h}^{k,i}(\boldsymbol{a}) + u_{2h}^{k,i}(\boldsymbol{a})}{2}\right) & \text{if } u_{1h}^{k,i}(\boldsymbol{a}) < u_{2h}^{k,i}(\boldsymbol{a}). \end{cases}$$

- Discretization error estimators

$$\left.\begin{aligned}
\eta_{\mathrm{F},K,j}^{k,i} &= \left\| \mu_j^{\frac{1}{2}} \nabla u_{jh}^{k,i} + \mu_j^{-\frac{1}{2}} \boldsymbol{\sigma}_{j,h,\mathrm{disc}}^{k,i} \right\|_K \\
\eta_{\mathrm{R},K,j}^{k,i} &= \frac{h_K}{\pi} \mu_j^{-\frac{1}{2}} \left\| f_j - \nabla \cdot \boldsymbol{\sigma}_{jh}^{k,i} - (-1)^j \lambda_h^{k,i} \right\|_K \\
\eta_{\mathrm{C},K}^{k,i,\mathrm{pos}} &= 2 \left(u_{1h}^{k,i} - u_{2h}^{k,i}, \lambda_h^{k,i,\mathrm{pos}} \right)_K
\end{aligned}\right\} \Rightarrow \boldsymbol{\eta}_{\mathrm{disc}}^{k,i}$$

- Linarization error estimators

$$\left.\begin{aligned}
\eta_{\mathrm{C},K}^{k,i,\mathrm{neg}} &= 2 \left(u_{1h}^{k,i} - u_{2h}^{k,i}, -\lambda_h^{k,i,\mathrm{neg}} \right)_K \\
\eta_{\mathrm{L},K}^{k,i,\mathrm{pos}} &= \left\{ \frac{1}{\mu_1} + \frac{1}{\mu_2} \right\}^{\frac{1}{2}} \frac{h_\Omega}{\pi} \left\| \lambda_h^{k,i,\mathrm{pos}} \right\|_\Omega |||\boldsymbol{s}_h^{k,i} - \boldsymbol{u}_h^{k,i}|||_K \\
\eta_{\mathrm{L},K}^{k,i,\mathrm{neg}} &= \left\{ \frac{1}{\mu_1} + \frac{1}{\mu_2} \right\}^{\frac{1}{2}} \frac{h_\Omega}{\pi} \left\| \lambda_h^{k,i,\mathrm{neg}} \right\|_K \\
\eta_{\mathrm{P},K}^{k,i} &= |||\boldsymbol{s}_h^{k,i} - \boldsymbol{u}_h^{k,i}|||_K
\end{aligned}\right\} \Rightarrow \boldsymbol{\eta}_{\mathrm{lin}}^{k,i}$$

- Algebraic error estimators

$$\left.\eta_{\mathrm{alg},K,\mathrm{j}}^{k,i} = \left\| \mu_j^{-\frac{1}{2}} \boldsymbol{\sigma}_{j,h,\mathrm{alg}}^{k,i} \right\|_K \right\} \Rightarrow \boldsymbol{\eta}_{\mathrm{alg}}^{k,i}$$

Theorem

$$|||\boldsymbol{u} - \boldsymbol{u}_h^{k,i}||| \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{lin}}^{k,i}.$$

Adaptive inexacte semi-smooth Newton algorithm

Algorithm 1 Adaptive inexact semi-smooth Newton algorithm

Initialization: Choose an initial vector $\mathbf{X}_h^0 \in \mathcal{M}_{3N_h,1}(\mathbb{R})$, $(k=0)$

Do

$k = k+1$

Compute $\mathbb{A}^{k-1} \in \mathcal{M}_{3N_h,3N_h}(\mathbb{R})$, $\boldsymbol{B}^{k-1} \in \mathcal{M}_{3N_h,1}(\mathbb{R})$

Consider $\mathbb{A}^{k-1}\mathbf{X}_h^k = \boldsymbol{B}^{k-1}$

Initialization for the linear solver: Define $\mathbf{X}_h^{k,0} = \mathbf{X}_h^{k-1}$, $(i=0)$

Do

$i = i+1$

Compute Residual: $\boldsymbol{R}_h^{k,i} = \boldsymbol{B}^{k-1} - \mathbb{A}^{k-1}\mathbf{X}_h^{k,i}$

Compute estimators

While $\boxed{\eta_{\text{alg}}^{k,i} \geq \gamma_{\text{alg}} \max\left\{\eta_{\text{disc}}^{k,i}, \eta_{\text{lin}}^{k,i}\right\}}$

Set $\mathbf{X}_h^k = \mathbf{X}_h^{k,i} \Rightarrow$ end of linear solver

While $\boxed{\eta_{\text{lin}}^{k,i} \geq \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i}}$

Set $\mathbf{X}_h^k = \mathbf{X}_h \Rightarrow$ end of non linear solver

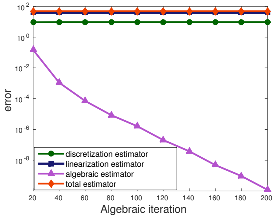
End

Numerical experiments

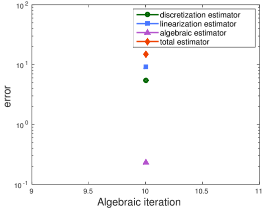
- Ω = unit disk, $J = 3$, $\mu_1 = \mu_2 = 1$, $g = 0.05$, $\gamma_{\mathrm{lin}} = 0.1$ $\gamma_{\mathrm{alg}} = 0.01$

Non linear solver: **Newton-min** iterative linear solver: **GMRES**.

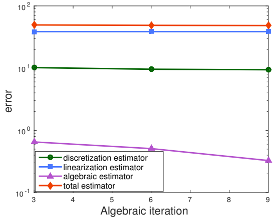
Exact Newton



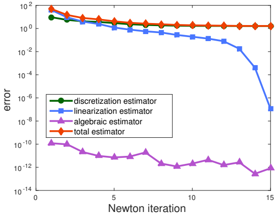
Inexact Newton



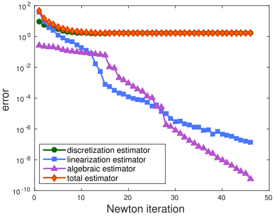
Adaptive inexact Newton



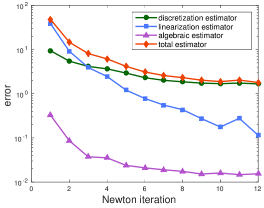
Exact Newton



Inexact Newton

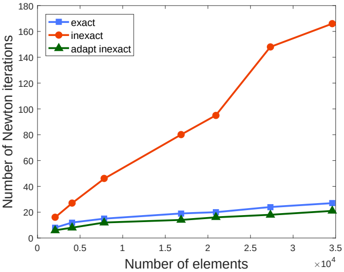


Adaptive Inexact Newton

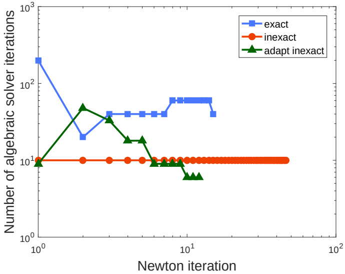


Overall performance of the three approaches:

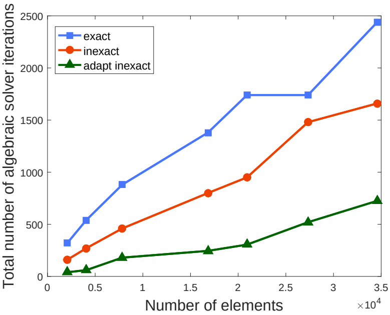
Newton



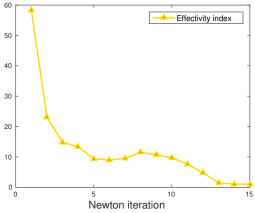
GMRES



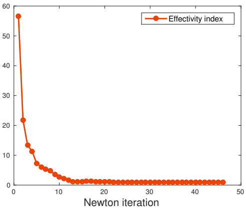
Total iter



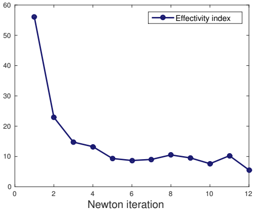
Exact Newton



Inexact Newton

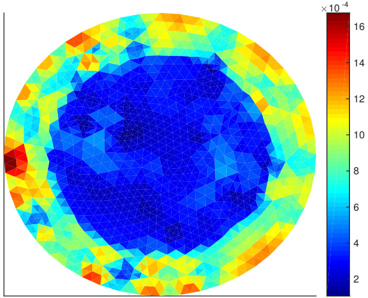


Adaptive inexact Newton

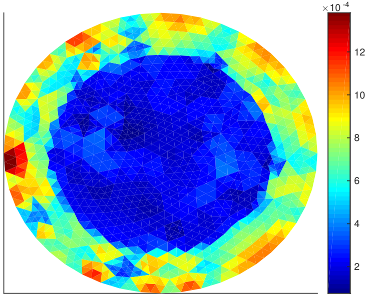


Distribution of the error:

Actual error



Estimated error



Conclusion

- We devised an a posteriori error estimate between $\boldsymbol{u}$ and $\boldsymbol{u}_h^{k,i}$ for a wide class of semi-smooth Newton methods.
- The adaptive inexact semi-smooth Newton method requires less non linear and linear steps.
- Extension of this work to multiphase flow problem with exchange between phases (non linear complementarity conditions) in porous media.

Thank you for your attention!