# Nonlinear Preconditioning Methods and Applications

Xiao-Chuan Cai

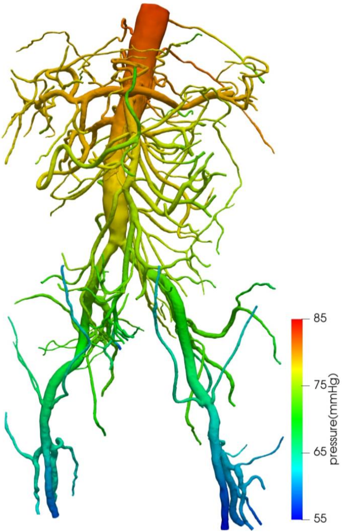
Department of Mathematics
University of Macau
&
Department of Computer Science
University of Colorado Boulder

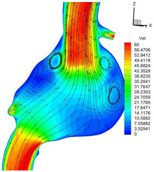
## Outline of the talk

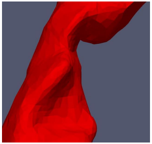
- Root Finding Problem: Find $X \in R^n$, such that $F(X) = 0$

- Motivating applications
- Nonlinearly preconditioned Newton methods
- Some nonlinearly difficult problems in fluid and solid problems in biomechanics
- Final remarks

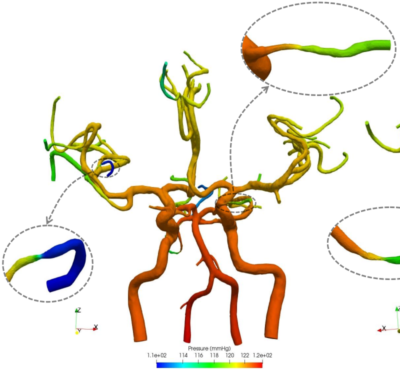
Nonlinear problems with local singularity: Blood flows in arteries with aneurysm or stenosis



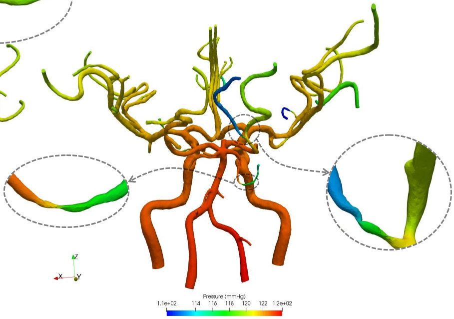



# Nonlinear problems with local singularity: Stroke

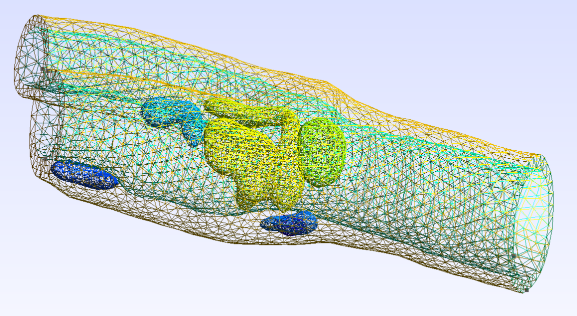



View from the front




View from the back

## Nonlinear problems with local singularity: Arterial plaques



## Motivation from linear preconditioning

- Iterative methods for solving large system of linear equations

$$Ax = b$$

  Roughly speaking, if $h$ is the mesh size and $np$ is the number of processors of a parallel machine
  - The discretization accuracy $\approx h^{\alpha}$
  - The number of iterations $\approx h^{-\beta} \cdot (np)^{\gamma}$
- Preconditioned iterative methods for solving large system of linear equations

$$M^{-1}Ax = M^{-1}b$$

- A good preconditioner reduces the impact of certain parameters on the convergence. Parameters: mesh size, number of processors, jump coefficients, ...

- Preconditioned iterative methods for solving large system of nonlinear equations

$$F(X) = 0 \iff G(F(X)) = 0 \iff F(G(X)) = 0$$

- A good nonlinear preconditioner can sometimes drastically improve the robustness of the nonlinear convergence by reducing the impact of certain parameters on the nonlinear convergence
- Parameters: Reynolds number, Mach number, Grashof number, ..., plus mesh size, number of processors, ...
- Note: Linear preconditioning doesn't help much with the "nonlinear parameters"

# A little history of nonlinear preconditioning

- X.-C. Cai, W. D. Gropp, D. E. Keyes, R. G. Melvin, and D. P. Young, Parallel Newton-Krylov-Schwarz algorithms for the transonic full potential equation, SIAM J. Sci. Comput., 19 (1998), pp. 246-265.
(a shock wave problem)
- X.-C. Cai, D. E. Keyes, and D. P. Young, A nonlinear additive Schwarz preconditioned inexact Newton method for shocked duct flow, Proceedings of the 13th International Conference on Domain Decomposition Methods, Oct. 9-12, 2000, France.
(a shock wave problem solved using nonlinear preconditioning)
- X.-C. Cai and D. E. Keyes, Nonlinearly preconditioned inexact Newton algorithms, SIAM J. Sci. Comput., 24 (2002), pp. 183-200.
(left nonlinear preconditioning)
- X.-C. Cai and X. Li, Inexact Newton methods with restricted additive Schwarz based nonlinear elimination for problems with high local nonlinearity, SIAM J. Sci. Comput., 33 (2011), pp. 746-762.
(right nonlinear preconditioning)

In general, we can use the classical Newton's method for

$$F(X) = 0,$$

where $X = (x_1, x_2, \ldots, x_n)^T$ and $F = (f_1, f_2, \ldots, f_n)^T$

$$X^{k+1} = X^k - F'(X^k)^{-1} F(X^k)$$

or, equivalently,

$$X^{k+1} = X^k + H^k$$

$$F'(X^k) H^k = -F(X^k),$$

which requires the solving of a large linear system of equations at every iteration

Inexact Newton's method: $H^k$ is chosen such that

$$\|F'(X^k) H^k + F(X^k)\| \le \eta^k \|F(X^k)\|,$$

for a given $\eta^k > 0$ (which may or may not depend on $k$)

## Globally convergent Newton's methods

- Linesearch: Changing the steplength by a factor of $\lambda^k \in (0, 1]$
$$X^{k+1} = X^k - \lambda^k H^k$$
In other words, $H^k$ is a good search direction if a non-zero $\lambda^k$ can be found such that
$$\frac{1}{2}\|F(X^{k+1})\|^2 \leq \frac{1}{2}\|F(X^k)\|^2 - \alpha\lambda^k (H^k)^T JF(X^k)$$
where $\alpha$ is small positive parameter
- Trust region: Changing the search direction $H^k$

## What happens when inexact Newton is applied to a large system with unbalanced nonlinearities?

- The convergence, or fast convergence, happens only if a good initial guess is available
- Generally it is very difficult to obtain such an initial guess especially for nonlinear equations that have unbalanced nonlinearities
- The step length $\lambda^k$ is often determined by the components with the strongest nonlinearities, and this may lead to an extended period of stagnation in the nonlinear residual curve
- We say that the nonlinearities are "unbalanced" when $\lambda^k$ is, in effect, determined by a subset of the overall degrees of freedom

We consider a one-dimensional compressible flow problem described by the full potential equation in a variable-area duct. The problem is to determine the solution potential $u(x)$ satisfying

$$(A\rho u_x)_x = 0,$$

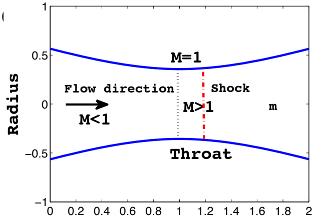
for $0 < x < 2$ and $u(0) = 0$ and $u(2) = u_R$ given. The duct area

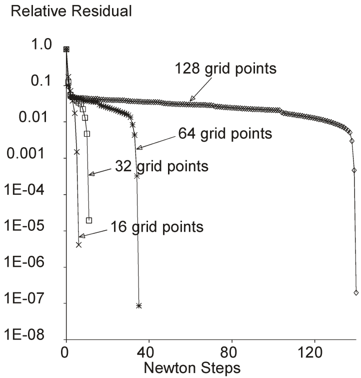
$$A = A(x) = 0.4 + 0.6(x-1)^2,$$

and the density $\rho$ is given by

$$\rho = \rho(v) = (c^2)^{1/(\gamma-1)} = \left(1 + \frac{\gamma-1}{2}(1-v^2)\right)^{1/(\gamma-1)}.$$

Here $v = u_x$ is the velocity, $\gamma = 1.4$ is the ratio of specific heat and $c$ is the speed of soun




Relative Residual
1.0
0.1
0.01
0.001
1E-04
1E-05
1E-06
1E-07
1E-08
0
40
80
120
Newton Steps
128 grid points
64 grid points
32 grid points
16 grid points
Step Length
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
40
80
120
Newton Steps
128 grid points
64 grid points
32 grid points

## Some observations

- To advance from $X^k$ to $X^{k+1}$, all $n$ variables and equations need to be updated even though in many situations $n$ can be very large, but only a small number of components of $X^k$ receive significant updates
- If a small number of components of the initial guess $X^0$ are not acceptable, the entire $X^0$ is declared bad
- There are two global control variables $\eta^k$ and $\lambda^k$. Any slight change of $F(\cdot)$ may result in the change of $\eta^k$ or $\lambda^k$, and any slight change of $\eta^k$ or $\lambda^k$ may result in some global function evaluations and/or the solving of global Jacobian systems

## Can we remove those bad components, just like Gaussian elimination?

For example

$$\begin{cases} F_1(x_1, x_2) = 0 \\ F_2(x_1, x_2) = 0 \end{cases}$$

Eliminate (implicit function theorem) the bad component $x_2$

$$x_2 = G(x_1)$$

The leftover is a slightly smaller and easier to solve nonlinear system

$$F_1(x_1, G(x_1)) = 0$$

## A simple example with one bad component

- Consider a $2 \times 2$ system

$$F(x_1, x_2) \equiv \begin{bmatrix} F_1(x_1, x_2) \\ F_2(x_1, x_2) \end{bmatrix} = \begin{bmatrix} (x_1 - x_2^3 + 1)^m - x_2^m \\ x_1 + 2x_2 - 3 \end{bmatrix} = 0$$

where $m = 1, 3, 5$. $x^* = [1, 1]^T$ is the root

| | IN | | | PIN | | |
|---|---|---|---|---|---|---|
| $x^{(0)}$ | $m$=1 | $m$=3 | $m$=5 | $m$=1 | $m$=3 | $m$=5 |
| $(0, 0)^T$ | 5 | 8 | 10 | 5 | 6 | 6 |
| $(0, 2)^T$ | 5 | 11 | 12 | 5 | 6 | 6 |
| $(2, 0)^T$ | 5 | 1 | 7 | 5 | 1 | 5 |
| $(2, 2)^T$ | 5 | 12 | 13 | 5 | 5 | 6 |

- As $m$ increases, one of the equations is more nonlinear than the other; the number of iterations increases and is also more sensitive to the choice of the initial guess

## Nonlinear elimination – peak removing

Consider a nonlinear problem $F(x) = 0$ defined on $\Omega$ with the current approximate solution $x_c$.

- Identify the worst region. A peak of $F$ is a region $\omega \in \Omega$ such that $\|F(x_c)\|_{2(\omega)}$ is large
- Solve a local nonlinear problem

$$F|_\omega(x_\omega) = 0, \text{ with boundary condition } x_\omega|_{\partial\omega} = x_c|_{\partial\omega}$$

- Locally correct the solution

$$x_{new} = \begin{cases} x_\omega & \text{in } \omega \\ x_c & \text{in } \Omega \setminus \omega \end{cases}$$

## Linear and nonlinear Schwarz preconditioners

- $R_i^\delta$, $R_i^0$ restriction with and without overlap. $\delta$ is the overlapping size
- Additive Schwarz

$$\text{Linear}: \sum_{i=1}^{N} (R_i^\delta)^T A_i^{-1} R_i^\delta \qquad \text{Nonlinear}: \sum_{i=1}^{N} (R_i^\delta)^T F_i^{-1} (R_i^\delta x)$$

- Restricted additive Schwarz

$$\text{Linear}: \sum_{i=1}^{N} (R_i^0)^T A_i^{-1} R_i^\delta \qquad \text{Nonlinear}: \sum_{i=1}^{N} (R_i^0)^T F_i^{-1} (R_i^\delta x)$$

# A general scalable nonlinear equation solver: RAS-NKS

- **Step 1 (The Nonlinearity Checking Step):** Check stopping conditions.
  - If the global condition is satisfied, **stop**.
  - If the local nonlinearities are not balanced, go to **Step 2**.
  - If the local conditions indicate the nonlinearities are balanced, set $\tilde{u}^{(k)} = u^{(k)}$, go to **Step 3**.
- **Step 2 (The RAS Step):** Solve local nonlinear problems on the overlapping subdomains to obtain the subdomain correction $v_i^\delta$

  $$R_i^\delta F(u^{(k)} + v_i^\delta) = 0, \ \text{for} \ \ i = 1, \cdots, N$$

  Drop the solution in the overlapping part of the subdomain and compute the global function $G(u^{(k)})$

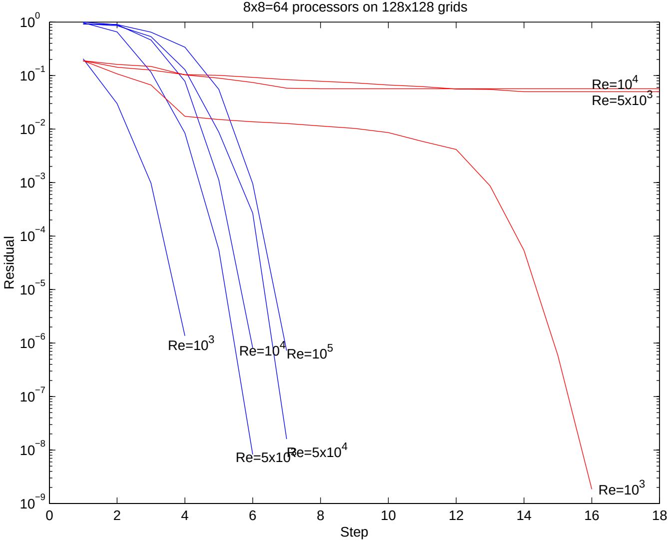
  $$G(u^{(k)}) = \sum_{i=1}^{N} R_i^0 (u^{(k)} + v_i^\delta), \quad \text{and set} \ \ \tilde{u}^{(k)} = G(u^{(k)}).$$

- **Step 3 (The NKS Step):** Compute the next approximate solution $u^{(k+1)}$ by solving the following equation

  $$F(u) = 0$$

  with one step of NKS iteration using $\tilde{u}^{(k)}$ as the initial guess.
  Go to **Step 1**

# Comparing NKS and RAS-NKS

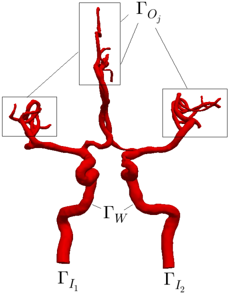


## Blood flow in the cerebral artery of a stroke patient

Time-dependent incompressible Navier-Stokes equations

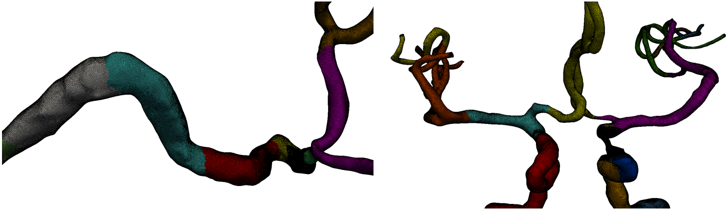
$$\begin{cases} \rho\left(\dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) - \nabla\cdot\boldsymbol{\sigma} = \mathbf{0}, \\ \nabla\cdot\mathbf{u} = 0 \end{cases}$$

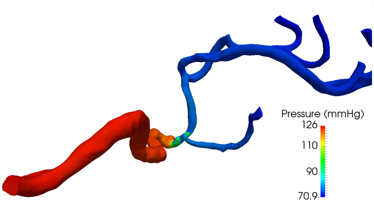
Here $\rho$ is the blood density, $\mu$ is the viscosity, and $\boldsymbol{\sigma} = -p\mathbf{I} + \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)$ is the Cauchy stress tensor, $\mathbf{u}$ is the velocity, $p$ is the pressure.



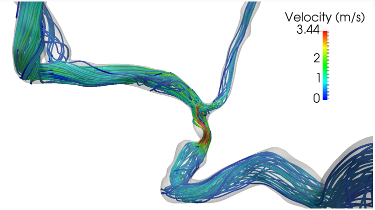
# Two cases of patient-specific arteries

| Case | Mean Reynolds | # of inlets | # of outlets | # of nodes | # of elements |
|---|---|---|---|---|---|
| One-inlet | 443.2 | 1 | 6 | 437,538 | 2,190,164 |
| Two-inlet | 262.6 | 2 | 15 | 1,069,767 | 5,225,949 |

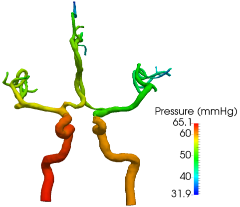




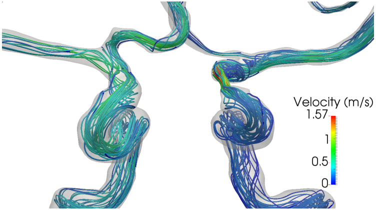

(a) Pressure




(b) Streamlines




(c) Pressure



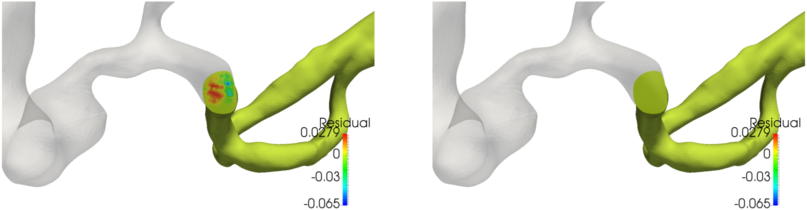

(d) Streamlines

Figure: Numerical solutions at $t = 0.7$s.

We form the following nonlinear system in the region with large residuals

$$\mathcal{G}(\mathbf{x}) \equiv \mathcal{R}_b^k\left(\mathcal{F}\left(\mathbf{x}\right)\right) + \mathcal{R}_g^k\left(\mathbf{x} - \mathbf{x}_k^n\right) = \mathbf{0}.$$

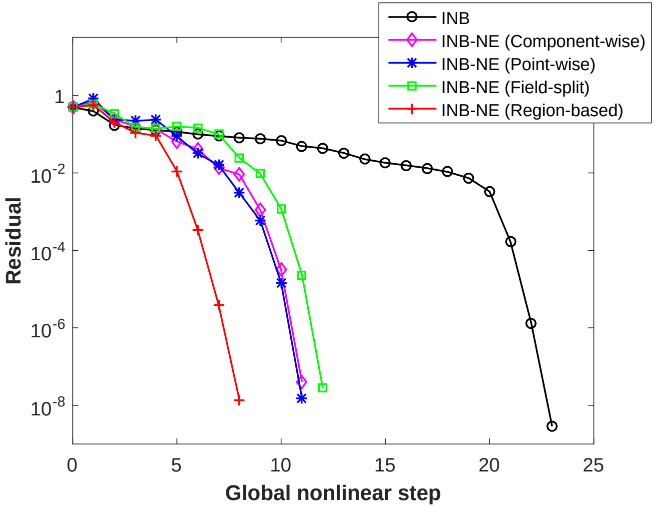
$\mathbf{x}_k^*$ is accepted as the approximate solution if the stopping condition $\|\mathcal{G}(\mathbf{x}_k^*)\| \leq \gamma_r^{NE}\|\mathcal{G}(\mathbf{x}_k^n)\|$ is satisfied.




(a) Before the subspace correction (b) After the subspace correction

Figure: The one-inlet case: residual contours for the $u$ component at the second nonlinear step during the second time step.

## Nonlinear residual history

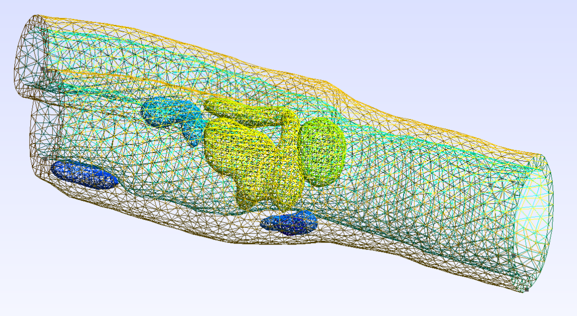


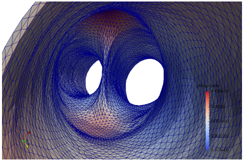
## Parallel scalability of INB-NE

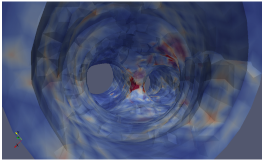
Table: Scalability test for the two-inlet case obtained using the INB-NE method with different fill-in levels of the ILU subsolve. A fixed mesh with 5,225,949 elements and 1,069,767 nodes is used. The overlap size of RAS preconditioner is $\delta = 1$. The time step size is 0.0025s.

| *np* | Subsolve | $NI_{global}$ | $LI_{global}$ | $NI_{ne}$ | $LI_{ne}$ | $Time_{ne}$(s) | $Time_{total}$(s) |
|---|---|---|---|---|---|---|---|
| 240 | ILU(0) | 3.83 | 1068.52 | 1.33 | 6.75 | 11.04 | 243.79 |
| | ILU(1) | 3.67 | 668.59 | 1.20 | 3.66 | 10.42 | 171.54 |
| | ILU(2) | 3.83 | 525.70 | 1.20 | 3.33 | 10.82 | 171.83 |
| | ILU(3) | 3.50 | 488.47 | 1.20 | 3.00 | 11.54 | 179.63 |
| 480 | ILU(0) | 3.83 | 1115.04 | 1.33 | 6.50 | 6.19 | 133.81 |
| | ILU(1) | 3.50 | 683.47 | 1.20 | 4.00 | 5.83 | 87.84 |
| | ILU(2) | 3.67 | 532.91 | 1.20 | 3.67 | 6.05 | 88.66 |
| | ILU(3) | 3.50 | 491.91 | 1.20 | 3.50 | 6.47 | 96.40 |
| 960 | ILU(0) | 3.83 | 1179.70 | 1.33 | 6.63 | 3.72 | 77.45 |
| | ILU(1) | 3.50 | 743.81 | 1.20 | 4.00 | 3.69 | 52.88 |
| | ILU(2) | 3.50 | 541.76 | 1.20 | 3.67 | 3.76 | 48.08 |
| | ILU(3) | 3.67 | 505.50 | 1.20 | 3.50 | 4.02 | 56.74 |
| 1920 | ILU(0) | 3.83 | 1436.56 | 1.20 | 5.00 | 2.27 | 53.17 |
| | ILU(1) | 3.67 | 900.36 | 1.20 | 4.16 | 2.30 | 38.33 |
| | ILU(2) | 3.67 | 653.05 | 1.20 | 3.67 | 2.34 | 33.31 |
| | ILU(3) | 3.67 | 630.18 | 1.20 | 3.83 | 2.43 | 38.58 |

# A carotid artery with plaques







# Hyperelastic model for arterial wall

- Energy functional

$$\psi = \psi^{iso}(C) + \psi^{vol}(C) + \psi^{ti}(C, M^{(i)}),$$

where $C$ is Cauthy-Green tensor, $M^{(i)}$ are the structural tensors

- Momentum equation

$$\mathrm{div} P = -f$$

where $P = FS, S = \frac{\partial \psi}{\partial C}$

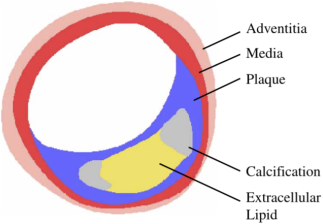



Figure: Cross-section of artery [Klawonn et al., 2008]

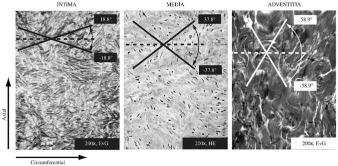


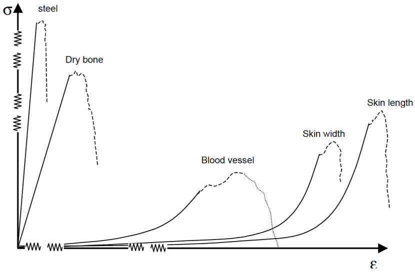

Figure: Collagen fibre reinforced [Holzapfel et al.,

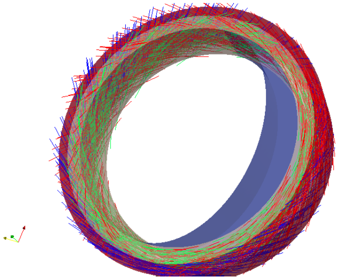
# Computational difficulties

Standard NKS doesn't work well under the following 3 conditions, and the issue is not the linear solver

- Large deformation
- Nearly incompressible
- Highly anisotropic

| Material | Poisson's Ratio |
|---|---|
| rubber | 0.4999 |
| soft tissue | 0.45 - 0.49 |
| gold | 0.42 - 0.44 |
| clay | 0.3 - 0.45 |
| stainless steel | 0.3 - 0.31 |
| glass | 0.18 - 0.3 |
| concrete | 0.1 - 0.2 |



# 3 situations

## From Klawonn, Rheinbach et al 2008

$$\begin{array}{lcccccc} \psi_A & = & \psi^{isochoric} & + & \psi^{volumetric} & + & \psi^{ti} \\ & := & c_1\left(\frac{I_1}{I_3^{1/3}} - 3\right) & + & \epsilon_1\left(I_3^{\epsilon_2} + \frac{1}{I_3^{\epsilon_2}} - 2\right) & + & \sum_{i=1}^{2} \alpha_1 \langle I_1 J_4^{(i)} - J_5^{(i)} - 2\rangle^{\alpha_2} \end{array}$$

| Set | Layer | $c_1$ | $\epsilon_1$ | $\epsilon_2$(-) | $\alpha_1$ | $\alpha_2$ | Purpose |
|---|---|---|---|---|---|---|---|
| D1 | – | 1.e3 | 1.e3 | 1.0 | 0.0 | 0.0 | Deformations by different forces |
| C1 | – | 1.e3 | 1.e3 | 1.0 | 0.0 | 0.0 | Different compressibility |
| C2 | – | 1.e3 | 1.e4 | 1.0 | 0.0 | 0.0 | |
| C3 | – | 1.e3 | 1.e5 | 1.0 | 0.0 | 0.0 | |
| A1 | Adv. | 7.5 | 100.0 | 20.0 | 1.5e10 | 20.0 | Highly anisotropic arterial walls[1] |
| | Med. | 17.5 | 100.0 | 50.0 | 5.0e5 | 7.0 | |
| A2 | Adv. | 6.6 | 23.9 | 10 | 1503.0 | 6.3 | |
| | Med. | 17.5 | 499.8 | 2.4 | 30001.9 | 5.1 | |
| A3 | Adv. | 7.8 | 70.0 | 8.5 | 1503.0 | 6.3 | |
| | Med. | 9.2 | 360.0 | 9.0 | 30001.9 | 5.1 | |

Table: Model parameter sets of $\psi_A$

[1] kPa for $c_1, \epsilon_1, \alpha_1$.

# Test for large deformation

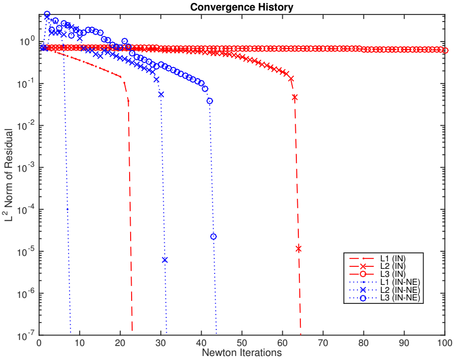



Figure: Convergence history of IN and IN-NE.

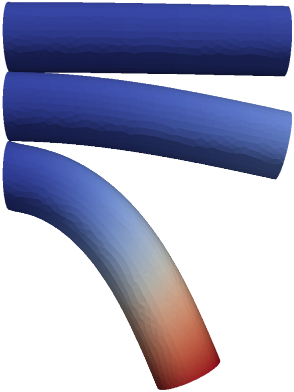


Figure: Deformations by different pulls.

# Test for compressibility

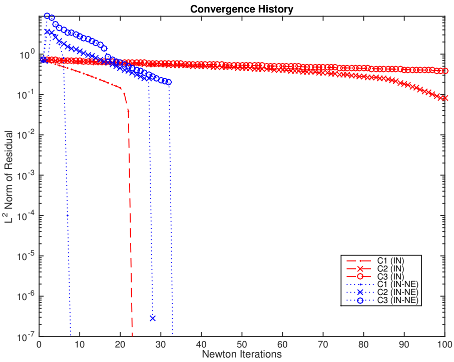



Figure: Convergence history of IN and IN-NE.

For consistency with linear elasticity,

$$C_1 = \frac{\mu}{2}, \epsilon_1 = \frac{\kappa}{2},$$

where $\mu, \kappa$ and the shear and bulk modulus. The Poisson ratio can be computed by

$$\nu = \frac{3K - 2G}{2(3K + G)}$$

| Set | Poisson's Ratio |
|---|---|
| C1 | 0.125 |
| C2 | 0.452 |
| C3 | 0.495 |

# Test for anisotropic arterial wall

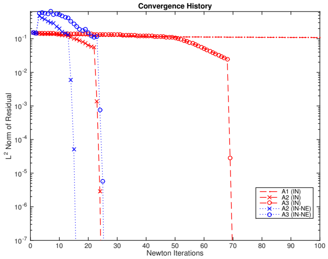



Figure: Convergence history of IN and IN-NE.

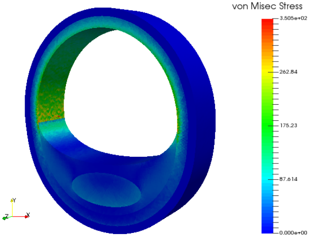



Figure: von Mises stress

## Some final remarks

- For problems with uniform global nonlinearity, NKS is a good general purpose parallel solver. Multilevel maybe necessary if the number of processors is large
- For problems with unbalanced global and local nonlinearities, a combination of full space Newton and subspace Newton, in the form of a nonlinear elimination preconditioned Newton, offers a good strategy
- It may not be easy to identify the local 'bad' region
- For problems with only local nonlinearities, subspace Newton is often sufficient
- It is often difficult to tell what types of nonlinearities a problem may have
- The norm of the residual function, $\|F(x)\|_2$, is often not a good monitor, unfortunately all existing nonlinear theories and algorithms are based on $\|F(x)\|_2$
- Many parameters (stopping conditions)

## Some recent publications


- L. Luo, X.-C. Cai, and D. Keyes, Nonlinear preconditioning strategies for two-phase flows in porous media discretizated by a fully implicit discondinuous Galerkin method, SIAM J. Sci. Comput., (2021, to appear)
- L. Luo, X.-C. Cai, Z. Yan, L. Xu, and D. Keyes, A multi-layer nonlinear elimination preconditioned inexact Newton method for steady-state incompressible flow problems in 3D, SIAM J. Sci. Comput., 42 (2020), pp. B1404-1428
- L. Luo, W.-S. Shiu, R. Chen, and X.-C. Cai, A nonlinear elimination preconditioned inexact Newton method for blood flow problems in human artery with stenosis, J. Comp. Phys., 399 (2019), 108926
- S. Gong and X.-C. Cai, A nonlinear elimination preconditioned Newton method for heterogeneous hyperelasticity, SIAM J. Sci. Comput., 41 (2019), pp. S390-S408