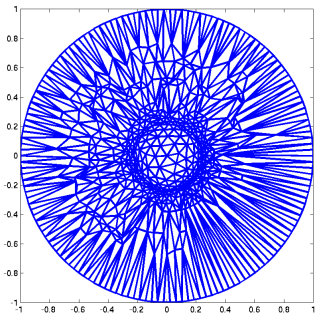
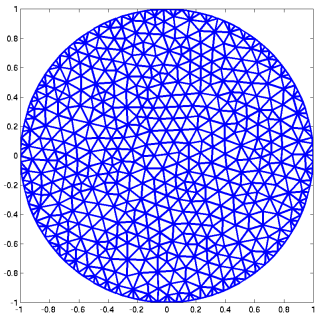
Optimizing Shape Quality





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Outline

- **Motivation**
- **Inverse Mean-Ratio Metric**
- **Optimizing the Vertex Positions**
- **Algorithm and Computational Results**
- **Conclusions**

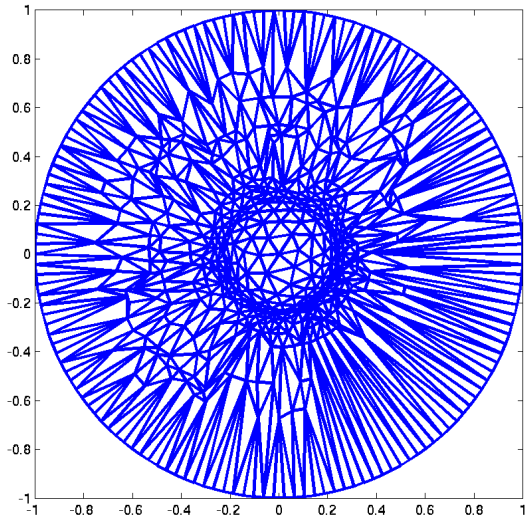
Motivation

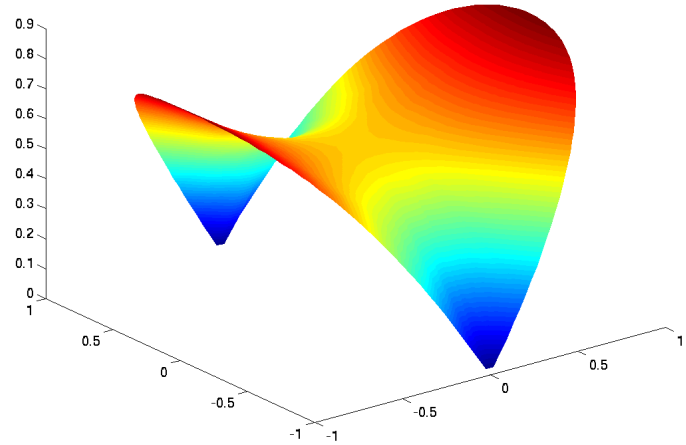
Laplace's Equation

$$
\begin{aligned}
-\Delta u &= 0 && x \in \Omega \\
u &= f(x) && x \in \partial\Omega
\end{aligned}
$$

- Approximate solution using finite-element method
  - Discretize Ω into set of elements
  - Construct matrix and right-hand side
  - Solve resulting system of equations
- Quantities to report include
  - Condition number of matrix
  - Number of conjugate gradient iterations
  - Accuracy of approximate solution

Laplace's Equation



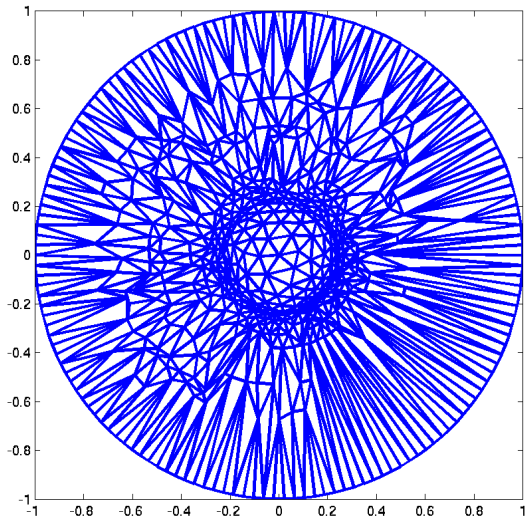


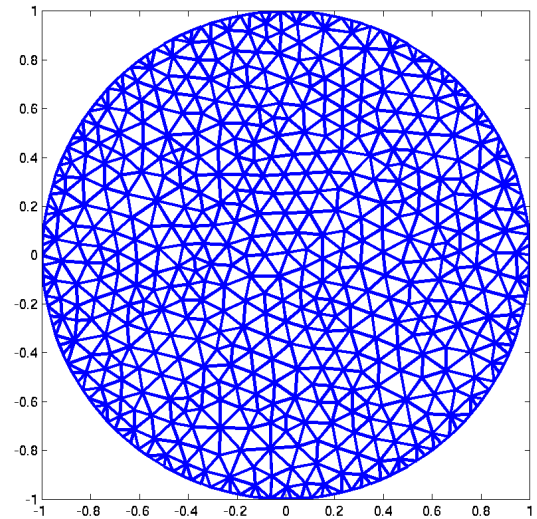
- **Objective: 1.652×10^{-1} (one digit of accuracy)**
- **Condition number: 1.164×10^{7}**
- **Conjugate gradient iterations: 423 (stalled)**

Improving the Approximate Solution

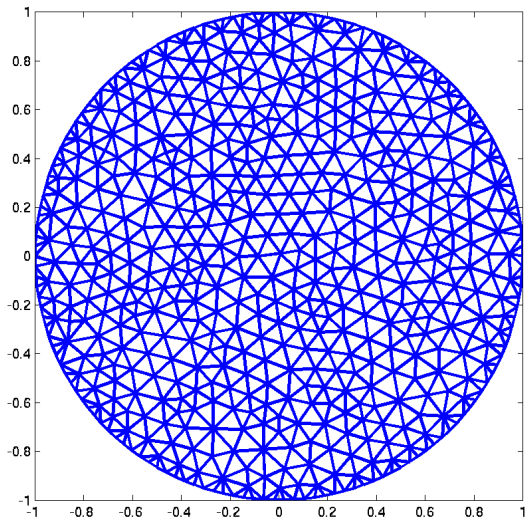
- h-refinement
  - Add elements to discretization
- p-refinement
  - Increase degree of approximation
- r-refinement
  - Improve the quality of the mesh
  - Optimize the vertex locations
  - Requires a quality metric
- Combinations of these techniques

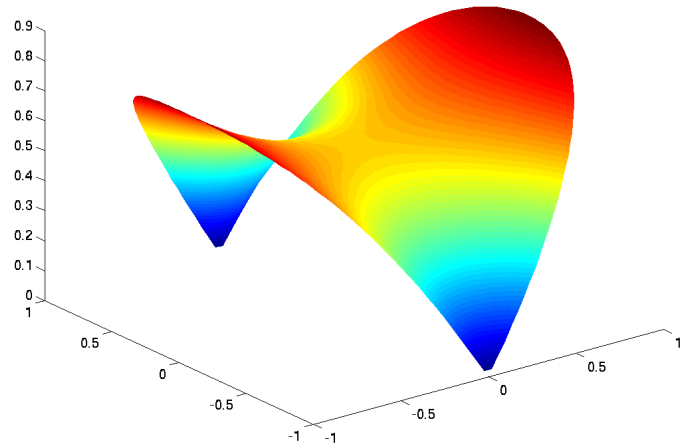
Original and Improved Mesh





Laplace's Equation





- **Objective: 1.522×10^{-1} (three digits of accuracy)**
- **Condition number: 2.997×10^{2}**
- **Conjugate gradient iterations: 85**

Inverse Mean-Ratio Metric

Incidence Function

- Given matrix of element coordinates
- Define $A : \Re^{3\times 4} \longrightarrow \Re^{3\times 3}$

$$A(x) := \begin{bmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \end{bmatrix}$$

  - Computes edge matrix for the element
  - Element volume related to $\det(A(x))$
  - Positive or negative depending on vertex ordering
- If $x \in \Re^{3\times 4}$ and $y \in \Re^{3\times 4}$ have the same shape, then

$$\begin{aligned} \|A(x)A(y)^{-1}\|_F^2 &= 3\sigma^2 \\ \det(A(x)A(y)^{-1}) &= \sigma^3 \end{aligned}$$

  - Scale factor is σ

Shape-Quality Metric

- Measures distance of element from ideal shape
- Given $x \in \Re^{3\times 4}$ and $y \in \Re^{3\times 4}$ with

$$\det(A(x)) > 0$$
$$\det(A(y)) > 0$$

- Define $Q_y : \Re^{3\times 4} \rightarrow \Re$

$$Q_y(x) := \frac{\|A(x)A(y)^{-1}\|_F^2}{3\det(A(x)A(y)^{-1})^{2/3}}$$

  - Value of one when x and y have same shape
  - Greater than one otherwise
  - Invariant to scale, translation, and rotation
- Modified version used for other element types

Optimizing the Vertex Positions

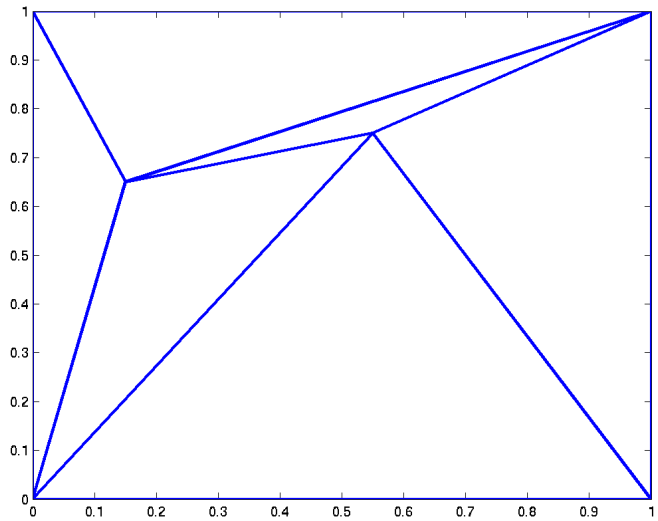
Optimization Problem

- Given $y \in \Re^{3\times 4}$ with $\det(y) > 0$
- Given initial vertex positions with $\det(A(x_e^0)) > 0 \;\; \forall e \in \mathcal{E}$
- Minimize average inverse mean-ratio metric

$$\begin{array}{lll} \min\limits_{x\in\Re^{3\times|\mathcal{V}|}} & \theta(x) := \sum\limits_{e\in\mathcal{E}} \frac{\|A(x_e)A(y)^{-1}\|_F^2}{3\det(A(x_e)A(y)^{-1})^{2/3}} & \\ \text{subject to} & \det(A(x_e)A(y)^{-1}) \geq 0 & \forall e \in \mathcal{E} \\ & x_v = \bar{x}_v & \forall v \in \mathcal{V}_B \end{array}$$

- Constraints preserve element orientation
- Area constraints not active at any local solution if
  - Mesh is edge connected
  - At least two vertices are fixed
- Metric set to infinity when $\det(A(x_e)) \leq 0$

Non-convex Optimization Problem



- **Two free vertices**
- **Hessian of objective contains**
  - **Three positive eigenvalues**
  - **One negative eigenvalue with value -70**

A Solution Strategy

- Write problem in AMPL modeling languages
  - Constrained formulation with $\det(A(x_e)A(y)^{-1}) \geq \tau$
  - Unconstrained formulation with

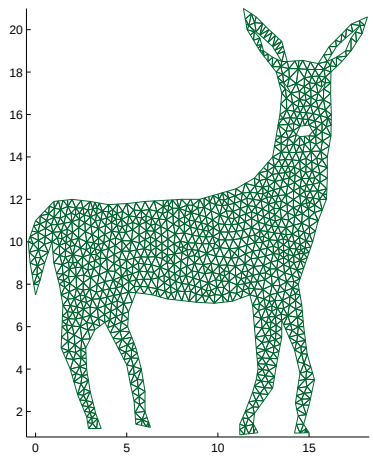
$$\tilde{Q}_y(x) := \frac{\|A(x)A(y)^{-1}\|_F^2}{3\max\{\det(A(x)A(y)^{-1}), 0\}^{2/3}}$$

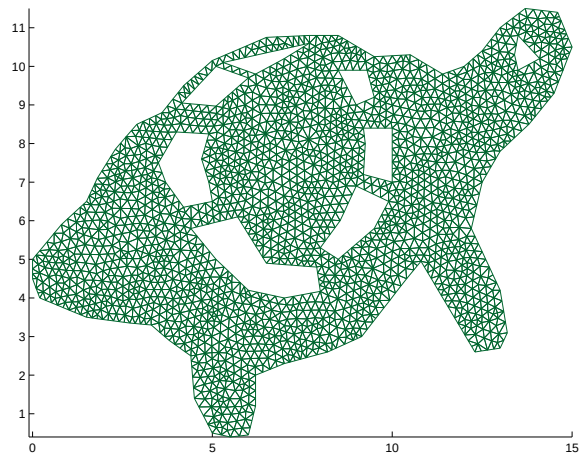
- Apply general-purpose algorithms
  - LOQO – interior-point method with line search
  - KNITRO – interior-point method with trust region
  - TRON – trust-region code for problems with bounds
- Advantage is that results can be quickly obtained

Test Problem Statistics

Mesh	Type	Vertices	Elements	Variables
deer	triangular	1,122	1,896	1,520
turtle	triangular	2,222	4,025	3,578
rand1000	triangular	1,152	2,170	2,048
rand10000	triangular	10,400	20,394	20,000
foam	tetrahedral	1,337	4,847	867
gear	tetrahedral	866	3,116	780
hook	tetrahedral	1,190	4,675	1,200
duct20	tetrahedral	1,067	4,104	1,146
duct15	tetrahedral	2,139	9,000	2,868
duct12	tetrahedral	4,199	19,222	6,906

Sample Meshes





Preliminary Computational Results

	Constrained		Unconstrained		
Mesh	LOQO	KNITRO	LOQO	KNITRO	TRON
deer	†	1.25	1.31	0.59	0.76
turtle	33.59	4.33	2.43	1.76	2.11
rand1000	12.79	‡	2.95	*	*
rand10000	80.95	‡	49.21	*	*
foam5	6.53	4.70	4.51	2.87	2.79
gear	3.75	4.28	2.59	‡	2.60
hook	8.86	7.25	8.71	3.30	3.82
duct20	11.63	6.12	16.15	3.50	4.02
duct15	41.65	16.59	40.42	9.27	10.74
duct12	112.00	61.20	127.93	*	29.20

Algorithm and Computational Results

Inexact Newton Method with a Line Search

1. Given x^0 and set $k = 0$
2. Stop if $\|\nabla\theta(x^k)\| < \epsilon$
3. Calculate direction by approximately solving

$$\nabla^2\theta(x^k)d^k = -\nabla\theta(x^k)$$

   - Apply conjugate gradient method
   - Block diagonal preconditioner

4. Find β such that $\theta(x^k + \beta d^k) < \theta(x^k)$
5. Let $x^{k+1} = x^k + \beta d^k$, set $k = k + 1$, and repeat

Preconditioner Properties

- Hessian matrix may be indefinite
- Need positive definite block diagonal submatrix
- Some useful properties of inverse mean-ratio metric
  - $\det(A(x_1, x_2, x_3, x_4)A(y)^{-1})$ is linear in x_1
  - $\det(A(x_1, x_2, x_3, x_4)A(y)^{-1})^{\frac{2}{3}}$ is concave in x_1
  - $\|A(x_1, x_2, x_3, x_4)A(y)^{-1}\|_F^2$ is strongly convex in x_1
- $Q_y(x_1, x_2, x_3, x_4)$ is a pseudoconvex function of x_1
- Prove $Q_y(x_1, x_2, x_3, x_4)$ is a strictly convex function of x_1
  - Implies $Q_y(x_1, x_2, x_3, x_4)$ is strictly convex function of x_i

$$Q_{[y_1,y_2,y_3,y_4]}(x_1, x_2, x_3, x_4) = Q_{[y_2,y_1,y_4,y_3]}(x_2, x_1, x_4, x_2)$$

  - Moreover $\sum_{e \in E} \nabla^2_{x_i,x_i} Q_y(x_e)$ is positive definite
  - Block diagonal preconditioner is positive definite

Convexity of Fractional Functions

Proposition 1 *Let $f : \Re^n \to \Re$ and $g : \Re^n \to \Re$, and let $\Omega \subseteq \Re^n$ be a convex set. Assume the following properties are satisfied:*

1. *g is a positive, concave function on Ω.*
2. *f is a nonnegative, uniformly convex function with constant κ on Ω.*
3. *For all $(x, y) \in \Theta := \left\{(x, y) \in \Omega \times \Omega \mid \frac{f(y)}{g(y)} \geq \frac{f(x)}{g(x)} \text{ and } g(y) \geq g(x)\right\}$,*

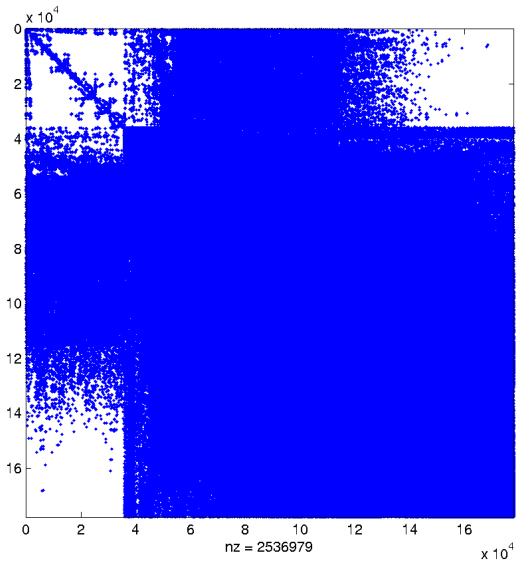
$$\left(\frac{f(y)}{g(y)} - \frac{f(x)}{g(x)}\right)(g(y) - g(x)) \leq \kappa \|y - x\|_2^2.$$

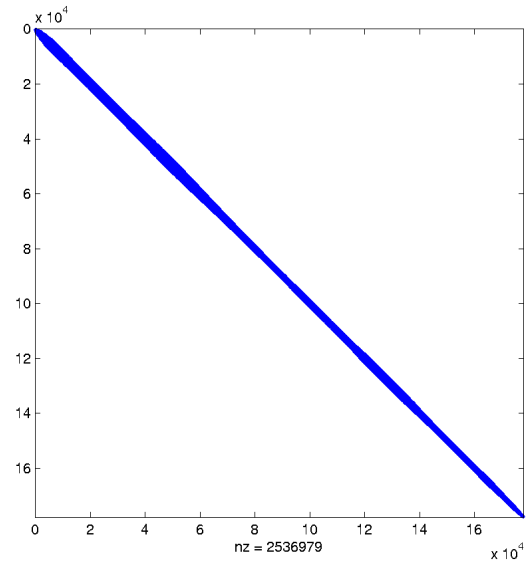
Then, $\frac{f}{g}$ is a nonnegative, convex function on Ω.

Algorithm Implementation

- Analytic gradient and Hessian evaluations
- Upper triangular part of Hessian stored
- Newton direction found by conjugate gradients
  - Block diagonal preconditioner (positive definite)
  - Blocked matrix-vector product
  - Terminates based on
    - Relative tolerance
    - Direction of negative curvature
- Monotone Armijo linesearch
- Reverse breadth-first search ordering

Ordering Effects





Computational Results

	Best Time			
Mesh	**LOQO**	**KNITRO**	**TRON**	**Newton Code**
deer	**1.21**	**0.55**	**0.60**	**0.04**
turtle	**2.20**	**1.61**	**1.73**	**0.12**
rand1000	**2.44**	†	†	**0.16**
rand10000	**42.78**	†	†	**4.43**
foam5	**4.45**	**2.87**	**2.72**	**0.12**
gear	**2.48**	**4.00**	**2.31**	**0.07**
hook	**7.27**	**3.23**	**3.73**	**0.11**
duct20	**10.42**	**3.20**	**3.37**	**0.07**
duct15	**28.01**	**8.39**	**9.78**	**0.21**
duct12	**79.80**	**51.94**	**24.20**	**0.48**

Analysis

- AMPL and general-purpose solvers
  - Fail on some examples
  - Take 9.5–50 times longer to compute solutions
  - Consume 100 times the memory
  - Easy to model and solve test problems
- Special-purpose code
  - Solves all example problems
  - Achieves 20–25% of peak performance in kernels
  - Time consuming to code and validate
- Challenge is to narrow the gap

Conclusions

- r-refinement is useful
  - Improved solution accuracy
  - Reduced condition number
- Fast algorithms are required
  - Modeling languages great for prototyping
  - May be insufficient as final solution strategy
- Special-purpose code is very efficient
  - Analytic derivatives necessary
  - Positive definite preconditioner required
  - Reordering significantly improves performance

Availability

http://www.mcs.anl.gov/~tmunson/codes/feasnewt12.zip

- **Algorithms**
  - **Gauss-Seidel method**
  - **Newton line-search method**
  - **Newton trust-region method**
- **Inverse mean-ratio and distance-from-target metrics**
  - **Triangular and quadrilateral elements**
  - **Tetrahedral and hexahedral elements**
- **All test problems included**
- **Mesh validity checker**

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