# Numerical Methods for PDEs

*Integral Equation Methods, Lecture 5*
*First and Second Kind Potential Equations*

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# Outline

**Reminder about 1-D 1st and 2nd Kind Eqns**

**Three-D Laplace Problems**

- Interior Neumann Problem
- Null space issue

**First Kind Theory for 3-D Laplace**

- Informal Convergence Theory
- FEM like approach

# 1-D Reminder

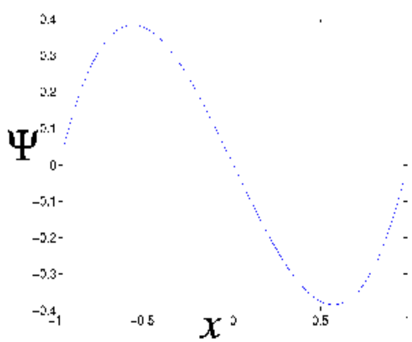
## 1st Kind Example

### First Kind Equation

$$\Psi(x) = \int_{-1}^{1} |x - x'|\sigma(x')dS' \quad x \in [-1, 1]$$

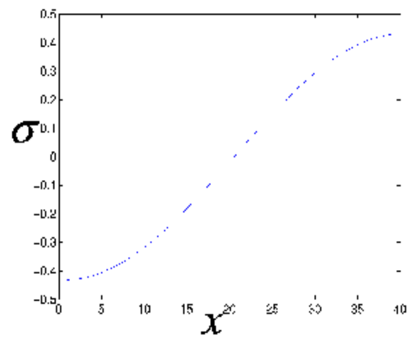
The potential is given

$$\Psi(x) = x^3 - x$$




The density must be computed

$\sigma(x)$ is unknown



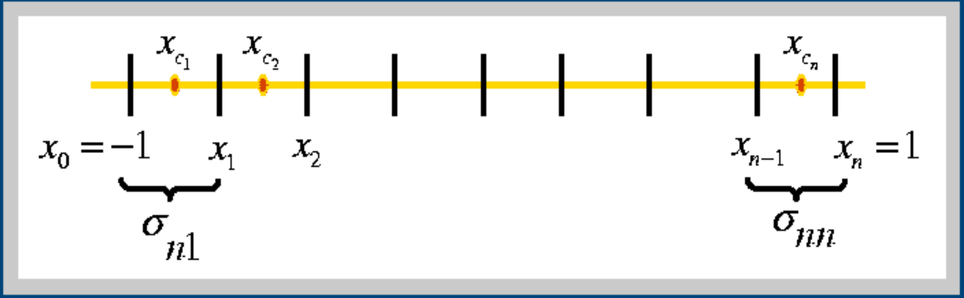
# 1-D Reminder

## 1st Kind Example

### Discretization

$$\Psi(x) = \int_{-1}^{1} |x - x'| \sigma(x') dS' \qquad x \in [-1, 1]$$

## Centroid Collocated Piecewise Constant Scheme




$$\Psi(x_{c_i}) = \sum_{j=1}^{n} \sigma_{nj} \int_{x_{j-1}}^{x_j} |x_{c_i} - x'| dS'$$

# 1-D Reminder

## 1st Kind Example

### Matrix

One column for each density value

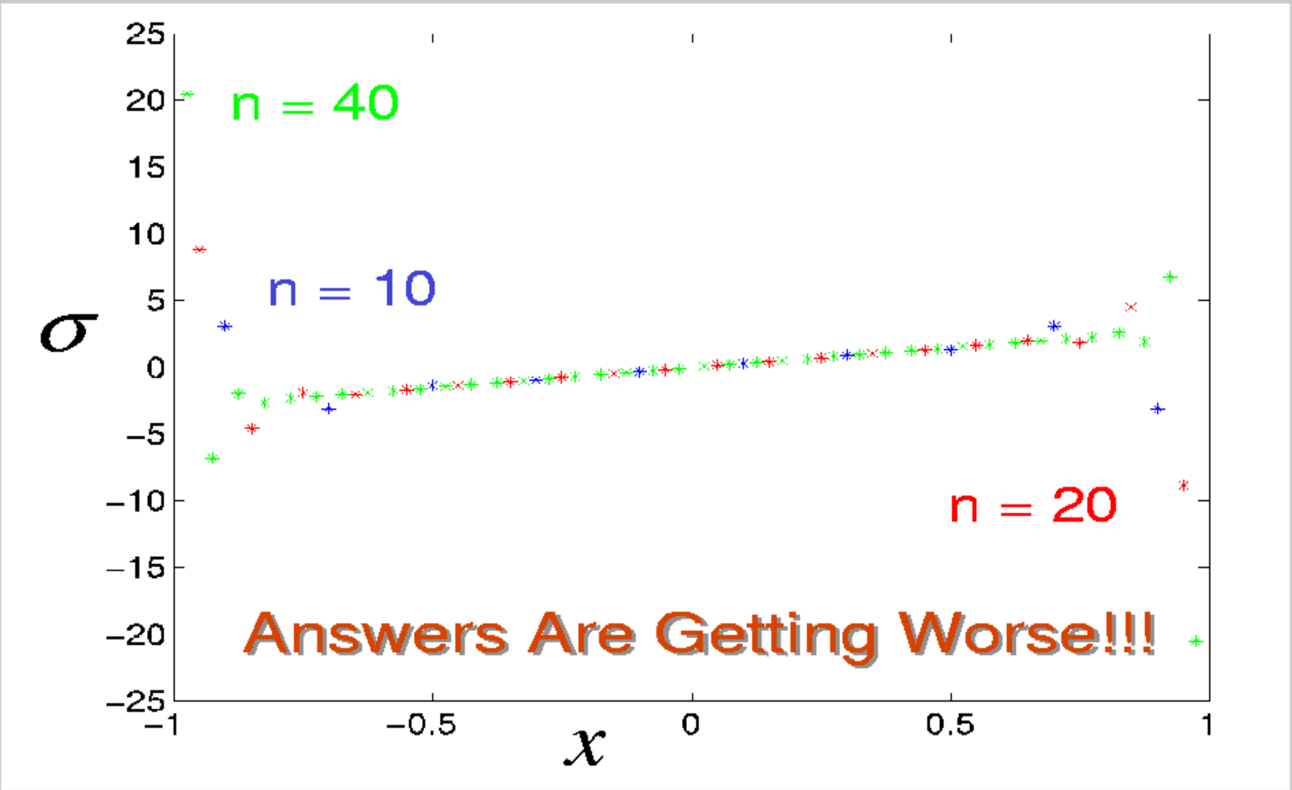
$$\begin{bmatrix} \int_{x_0}^{x_1} \left|x_{c_1} - x'\right| dS' & \cdots & \int_{x_{n-1}}^{x_n} \left|x_{c_1} - x'\right| dS' \\ \vdots & \ddots & \vdots \\ \int_{x_0}^{x_1} \left|x_{c_n} - x'\right| dS' & \cdots & \int_{x_{n-1}}^{x_n} \left|x_{c_n} - x'\right| dS' \end{bmatrix} \begin{bmatrix} \sigma_{n1} \\ \vdots \\ \sigma_{nn} \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

One row for each collocation point

# 1-D Reminder

## 1st Kind Example

### Numerical Results



# 1-D Reminder

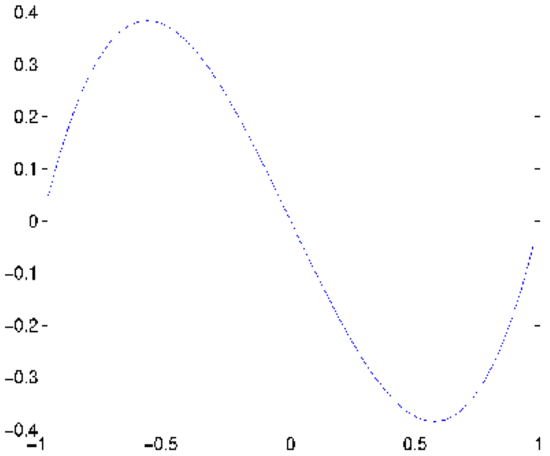
## 2nd Kind Example

### Second Kind Equation

$$\Psi(x) = \sigma(x) + \int_{-1}^{1} |x - x'| \sigma(x') dS' \quad x \in [-1, 1]$$

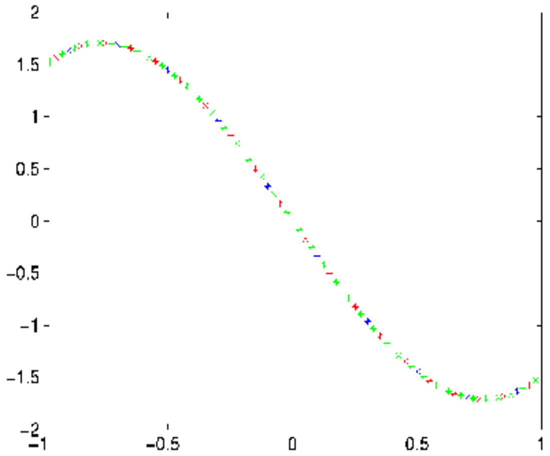
The potential is given

$$\Psi(x) = x^3 - x$$




The density must be computed

$\sigma(x)$ is unknown



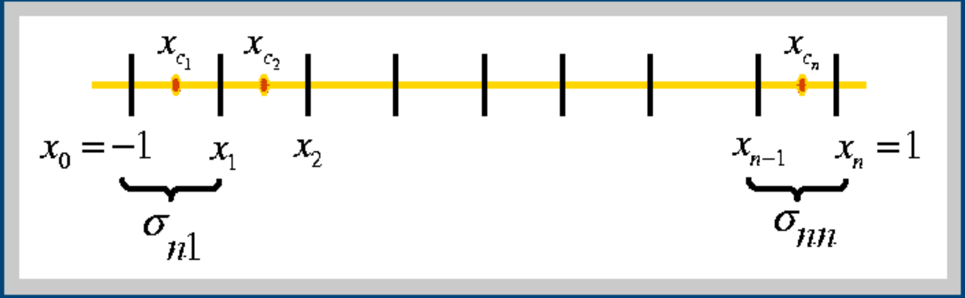
## 1-D Reminder

### 2nd Kind Example

#### Discretization

$$\Psi(x) = \sigma(x) + \int_{-1}^{1} |x - x'| \sigma(x') dS' \qquad x \in [-1, 1]$$

### Centroid Collocated Piecewise Constant Scheme




$$\Psi(x_{c_i}) = \sigma_{ni} + \sum_{j=1}^{n} \sigma_{nj} \int_{x_{j-1}}^{x_j} |x_{c_i} - x'| dS'$$

# 1-D Reminder

## 2nd Kind Example

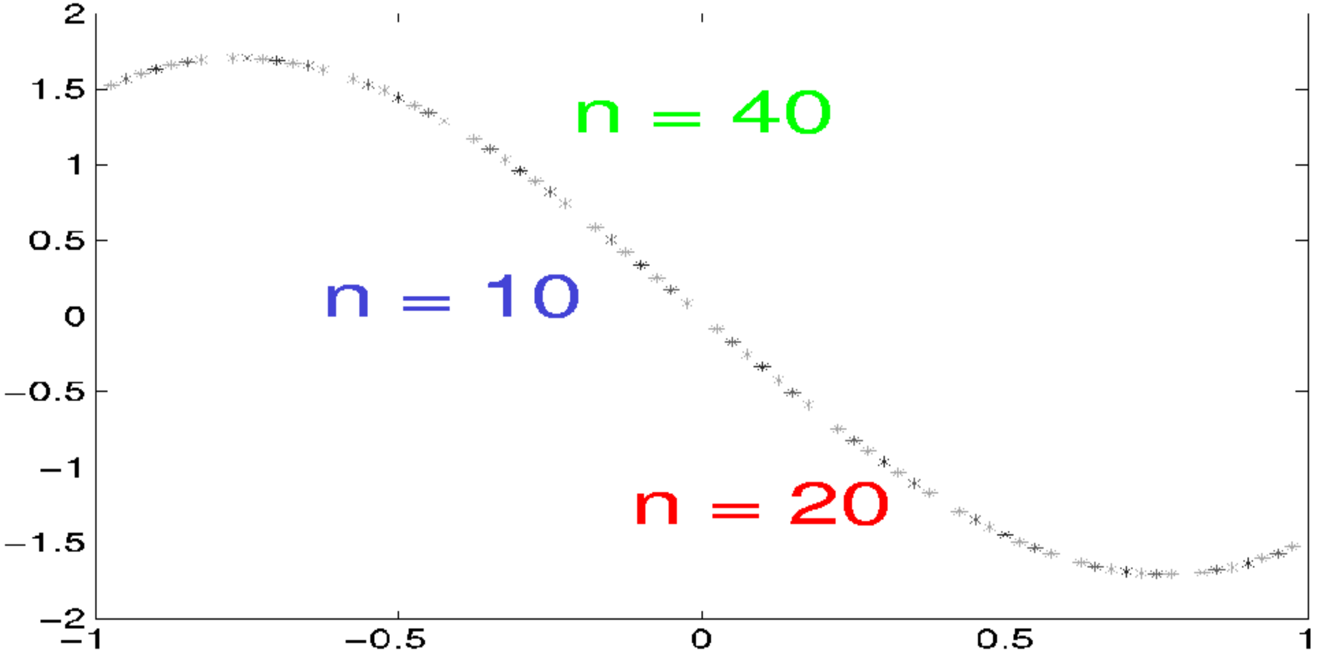
### Matrix

$$\begin{bmatrix} 1+\int_{x_0}^{x_1}\left|x_{c_1}-x'\right|dS' & \cdots & \int_{x_{n-1}}^{x_n}\left|x_{c_1}-x'\right|dS' \\ \vdots & \ddots & \vdots \\ \int_{x_0}^{x_1}\left|x_{c_n}-x'\right|dS' & \cdots & 1+\int_{x_{n-1}}^{x_n}\left|x_{c_n}-x'\right|dS' \end{bmatrix} \begin{bmatrix} \sigma_{n1} \\ \vdots \\ \sigma_{nn} \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

# 1-D Reminder

## 2nd Kind Example

### Numerical Results



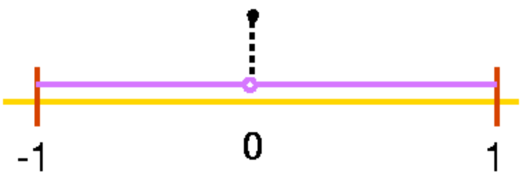

**Answers Are Improving!!!**

# 1-D Reminder

Denote the integral operator as $K$

$$K\sigma \equiv \int_{-1}^{1} |x - x'|\sigma(x')dS' \Rightarrow K\sigma = \Psi$$

The integral operator is **singular** : $K$ **has a null space**




$\sigma_0(x) = 0,\ x \neq 0,\ \sigma_0(0) = 1$

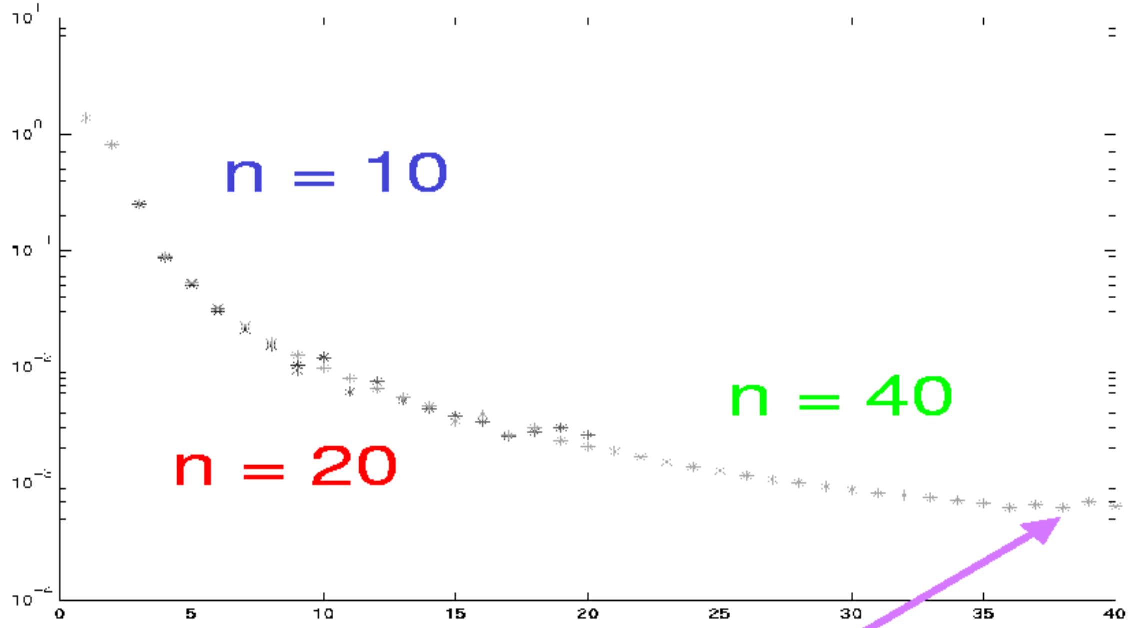
$$K\sigma_0 = \int_{-1}^{1} |x - x'|\sigma_0(x')dS' = 0$$

If $K\sigma^a = \Psi \quad then \quad K(\sigma^a + \sigma_0) = \Psi$

# 1-D Reminder

## 1st Kind Difficulty

### Numerical Results



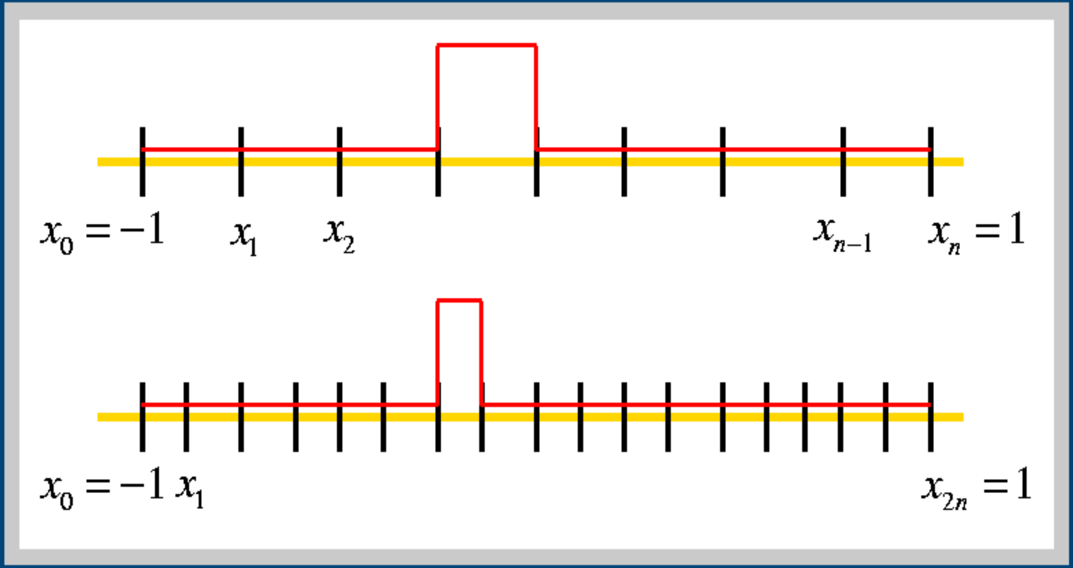

Eigenvalues accumulating at zero.

# 1-D Reminder

## 1st Kind Difficulty

### Eigenvalues

As the discretization is refined, $\sigma_0(x)$ becomes better approximated




As the discretization is refined, $K$'s null space can be more accurately represented.

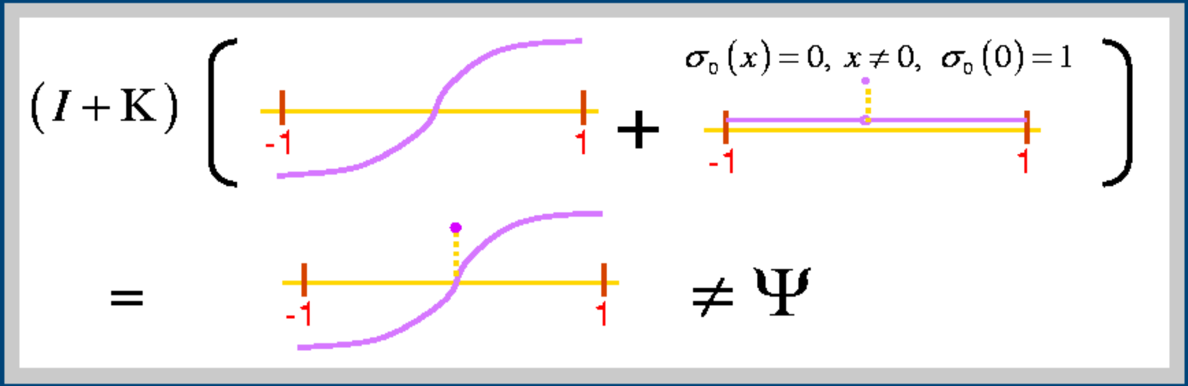
# 1-D Reminder

## 2nd Kind

Second Kind equation

$$(I+K)\sigma \equiv \sigma(x) + \int_{-1}^{1} |x-x'|\sigma(x')dS' \Rightarrow (I+K)\sigma = \Psi$$

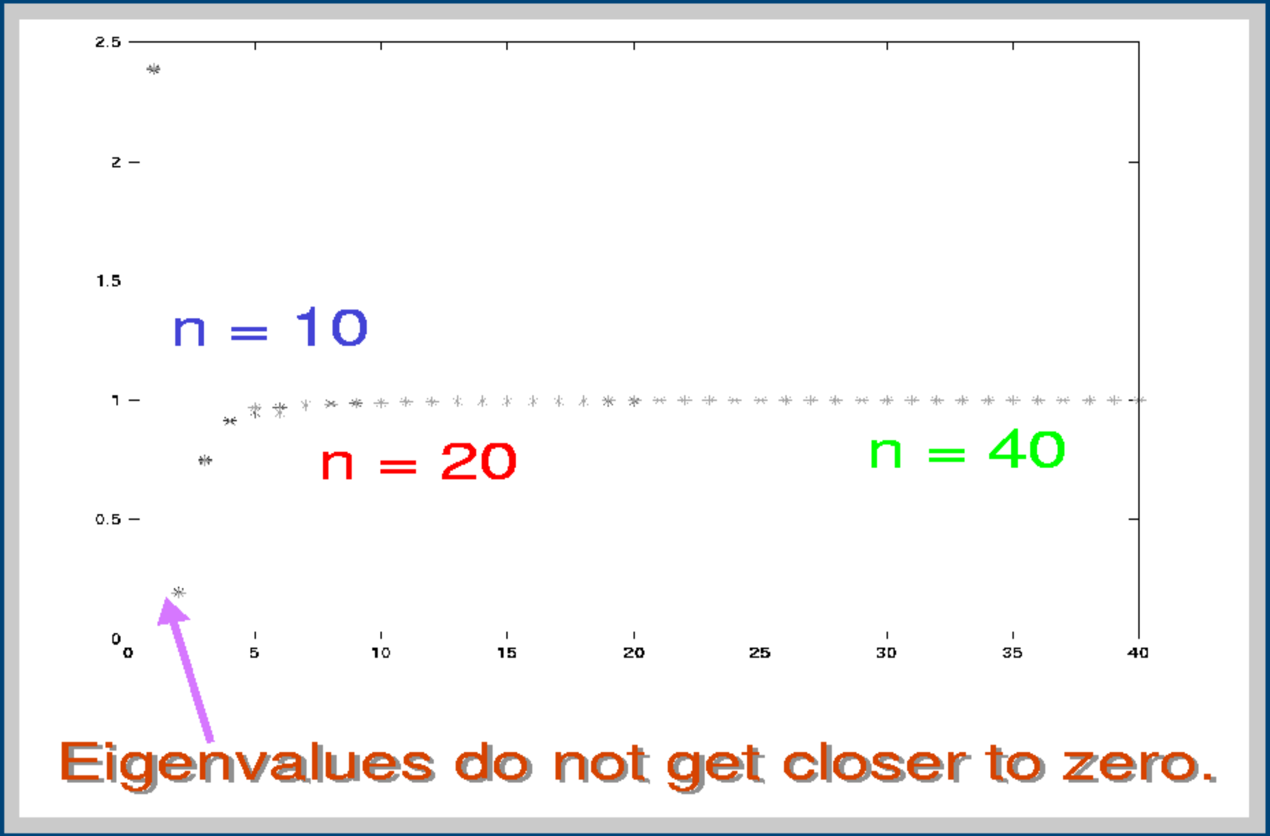
$$(I+K)(\sigma_0+\sigma) \neq (I+K)\sigma$$



# 1-D Reminder

## 2nd Kind

### Numerical Results



# 1-D Reminder

## 2nd Kind Theorem

Given $(I+K)\sigma = \Psi$ and $||(I+K)^{-1}|| < C$

(Equation uniquely solvable)

$$(I+K_n)\sigma_n = \Psi_n$$

(Discrete Equivalent )

**Consistency:**

If $lim_{n\to\infty} max_{||\sigma_{smooth}||=1} ||(K-K_n)\sigma|| \to 0$

and $lim_{n\to\infty} ||\Psi - \Psi_n|| \to 0$

**Then**

$lim_{n\to\infty} ||\sigma - \sigma_n|| \to 0$

# 1-D Reminder

## 2nd Kind Theorem

### Theorem Meaning

Final result

$$lim_{n\to\infty}||(\sigma_n - \sigma)|| \leq C\ lim_{n\to\infty}||(K - K_n)\sigma|| = 0$$

What does this mean?

The discretization convergence of a second kind integral equation solver depends on how well the integral is approximated.

## Interior Examples

# 3-D Laplace

Dirichlet Problem

$$u_\Gamma(\vec{x}) = \int_\Gamma \frac{1}{\|\vec{x} - \vec{x}'\|} \sigma(\vec{x}') d\Gamma' \quad \vec{x} \in \Gamma$$

Neumann Problem

$$\frac{\partial u_\Gamma(\vec{x})}{\partial n_{\vec{x}}} = -2\pi\sigma(\vec{x}') + \int_\Gamma^C \frac{\partial}{\partial n_{\vec{x}}} \frac{1}{\|\vec{x} - \vec{x}'\|} \sigma(\vec{x}') d\Gamma'$$

# 3-D Laplace

## Interior Examples

### Cauchy Principle Value

If $f(y)$ is singular at $y = x_0$, the Cauchy principle value integral is

$$\int_{\Gamma}^{C} f(\vec{y})d\Gamma \quad \equiv lim_{\epsilon\rightarrow 0} \int_{|y-x_0|\geq\epsilon} f(\vec{y})d\Gamma$$

when the limit exists.

If $\Gamma$ is a flat 2-D surface in 3-D

$$\int_{\Gamma}^{C} \frac{\partial}{\partial n_{\vec{x}}} \frac{1}{||\vec{x} - \vec{x}'||} d\Gamma' \quad = 0 \quad x \in \Gamma.$$

# 3-D Laplace

## Neumann Analysis

### Scaled Problem

Define

$$\Psi \equiv \frac{-1}{2\pi}\frac{\partial u_\Gamma(\vec{x})}{\partial n_{\vec{x}}}$$

$$K \equiv -\frac{1}{2\pi}\int_\Gamma^C \frac{\partial}{\partial n_{\vec{x}}}\frac{1}{\|\vec{x}-\vec{x}'\|}\sigma(\vec{x}')d\Gamma'$$

then the Neumann problem becomes

$$(I+K)\sigma = \Psi$$

# 3-D Laplace

## Neumann Analysis

### Key Property

Main assumption of second kind theory:

$$(I + K)^{-1}$$

is bounded.

Is $(I + K)^{-1}$ bounded for the Neumann Problem?

# Linear Algebra

## Inverses/Null spaces

Given $Ax = b$, $A \in \Re^{n\times n}$, $x, b \in \Re^n$

$A^{-1}$ exists and is bounded iff

$Ay = 0$ implies $y = 0$ (no null space)

If $Ay = 0$ for $y \neq 0$ then either

$Ax = b$ has an infinite # of solutions

$Ax = b$ then $A(x + \alpha y) = b$

OR

$Ax = b$ does not have a solution

$b$ is not in column space of $A$

# 3-D Laplace

## Interior Neumann

### Null Space

Consider $\tilde{\sigma}$ defined by

$$u_\Gamma(\vec{x}) = 1 = \int_\Gamma \frac{1}{\|\vec{x} - \vec{x}'\|}\tilde{\sigma}(\vec{x}')d\Gamma' \quad \vec{x} \in \Gamma$$

Then

$$\frac{\partial u_\Gamma(\vec{x})}{\partial n_{\vec{x}}} = 0 = -2\pi\tilde{\sigma}(\vec{x}') + \int_\Gamma^C \frac{\partial}{\partial n_{\vec{x}}} \frac{1}{\|\vec{x} - \vec{x}'\|}\tilde{\sigma}(\vec{x}')d\Gamma'$$

$\tilde{\sigma}$ is in the Null space of $I + K$

$(I + K)^{-1}$ is not bounded!!

# 3-D Laplace

## Interior Neumann

### Fredholm Alternative

For $I + K$ either

$(I + K)\sigma = \Psi$ has an infinite # of solutions

OR

$(I + K)\sigma = \Psi$ has no solution

For a solution to exist

$$\int_{\Gamma} \frac{\partial u_{\Gamma}(\vec{x})}{\partial n_{\vec{x}}} d\Gamma \quad = 0$$

# 3-D Laplace

## Interior Neumann

### General Theorem

The 2nd Kind Integral equation has a finite-dimensional Null Space (typically rank one).

# 3-D Laplace

## Interior Neumann

### Fixes

**Add a point constraint**

Fix $u$ at some point

**Force $\sigma$ orthogonal to null space**

Need the null space

May need to solve 1st kind equation

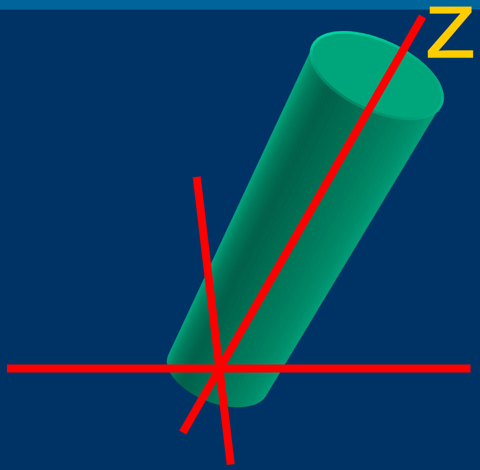
**Use SVD to solve singular system**

Can be computationally expensive

# 3-D Laplace's Equation

## First Kind Issues

### The singular Kernel Saves the day




Spike Function=1 on a disk

$$\sigma_0 = 0 \qquad \sqrt{x^2+y^2} > R$$

$$\sigma_0 = 1 \qquad \sqrt{x^2+y^2} \leq R$$

Singular Kernel Case
$$\int_{disk} \frac{1}{\left\| x_{c_i} - x' \right\|} \sigma_0(x') dS' = \int_0^R \int_0^{2\pi} \frac{1}{r} r dr d\theta = 2\pi R$$

Smooth Kernel Case
$$\int_{disk} 1 \, \sigma_0(x') dS' = \pi R^2$$

Smooth kernel $\rightarrow$ 0 faster as $R \rightarrow 0$, more singular

# 3-D Laplace's Equation



Partial Differential Equation form

$$\nabla^2 u = f \quad in \quad \Omega \qquad \Omega \text{ is the volume domain}$$

$$u = 0 \quad on \quad \Gamma \qquad \Gamma \text{ is the problem surface}$$

"Nearly" Equivalent weak form

$$\underbrace{\int_\Omega \nabla u \nabla v \, dx}_{a(u,v)} = \underbrace{\int_\Omega f \, v \, dx}_{l(v)} \quad \text{for all } v \in H^1(\Omega)$$

Introduced an abstract notation for the equation u must satisfy

$$a(u,v) = l(v) \quad \text{for all } v \in H^1(\Omega)$$

Introduce an approximate solution $u^n = \sum_{i=1}^{n} \alpha_i \varphi_i$

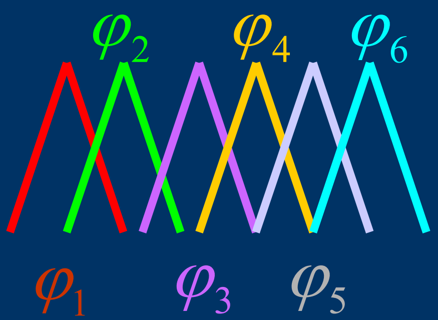
$\Rightarrow$ $u^n$ is a weighted sum of basis functions

The basis functions define a space

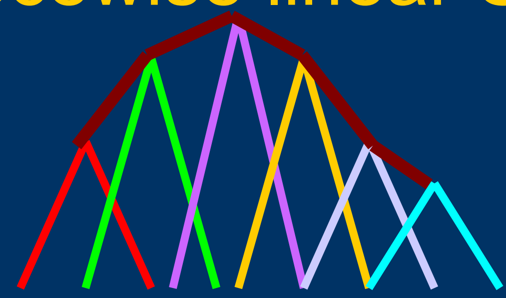
$$X_n = \left\{ v \in X_n \mid v = \sum_{i=1}^{n} \beta_i \varphi_i \text{ for some } \beta_i\text{'s} \right\}$$

## Example

"Hat" basis functions




Piecewise linear Space



## Key Idea

$a(u,u)$ defines a norm on $H_0^1(\Omega)$ $\quad a(u,u) \equiv \|u\|$

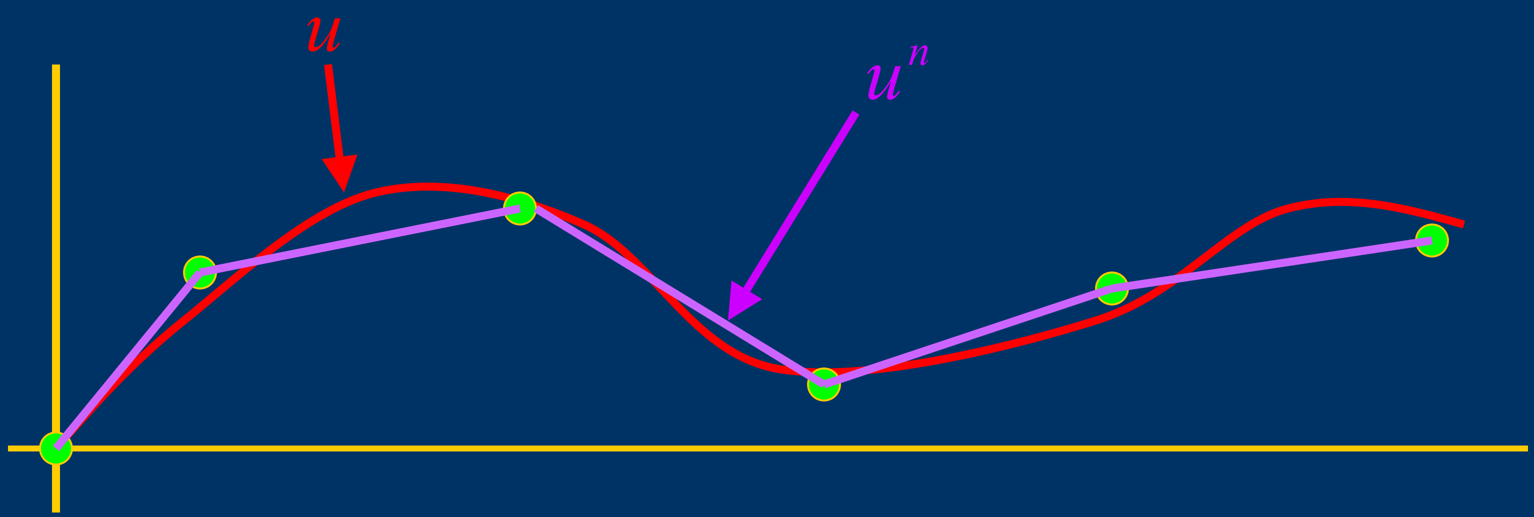
U is restricted to be 0 at 0 and1!!

Using the norm properties, it is possible to show

*If* $a(u^n, \varphi_i) = l(\varphi_i)$ for all $\varphi_i \in \{\varphi_1, \varphi_2, \ldots, \varphi_n\}$

*Then* $\underbrace{\left\| u - u^n \right\|}_{\text{Solution Error}} = \min_{w_n \in X_n} \underbrace{\left\| u - w^n \right\|}_{\text{Projection Error}}$

# The question is only




How well can you fit u with a member of $X_n$

But you must measure the error in the ||| ||| norm

For piecewise linear:
$$\underbrace{\left|\left|\left| u - u^n \right|\right|\right|}_{error} \leq \left|\left|\left| u - \Pi_n^a u \right|\right|\right| = O\left(\frac{1}{n}\right)$$

# 3-D Laplace's Equation

"Weak" Form for the integral equation

$$\underbrace{\iint_{\Gamma} v(x)\frac{1}{\|x-x'\|}\sigma(x')\,dS'dS}_{a(\sigma,v)} = \underbrace{\int_{\Gamma} v(x)\Psi(x)\,dS}_{l(v)} \quad \text{for all } v \in \bar{H}(\Gamma)$$

The difficulty is defining $\bar{H}(\Gamma)$ with right properties

Must exclude $\sigma(x)$'s where $\int \frac{1}{\|x-x'\|}\sigma(x')\,dS' = 0$

$\bar{H}(\Gamma)$ is a fractional Sobolev Space

We won't say more about this

# 3-D Laplace's Equation

## Convergence Analysis

### Applying FEM approach to first kind integral equations

## Use FEM key Idea

$a(\sigma,\sigma)$ defines a norm on $\bar{H}(\Gamma)$ $\quad a(\sigma,\sigma) = \|\sigma\|$

$$\sigma^n = \sum_{i=1}^{n} \alpha_i \underbrace{\varphi_i(x)}_{\text{Basis Functions}} \qquad X_n = \left\{ v \in X_n \mid v = \sum_{i=1}^{n} \beta_i \varphi_i \text{ for some } \beta_i\text{'s} \right\}$$

Using the norm properties, it is possible to show

*If* $a(\sigma^n, \varphi_i) = l(\varphi_i)$ for all $\varphi_i \in \{\varphi_1, \varphi_2, \ldots, \varphi_n\}$

*Then* $$\underbrace{\|\sigma - \sigma^n\|}_{\textit{Solution Error}} = \min_{w_n \in X_n} \underbrace{\|\sigma - w^n\|}_{\textit{Projection Error}}$$

# MEMS Performance Depends on Air Damping of Complicated 3-D Structures

Bosch angular rate sensor

ADXL76 accelerometer

TI 3x3 mirror array

Resonator

Lucent micromirror

# Drag In MEMS is Incompressible Stokes

Velocity integral equation for Stokes flow

$$u_j(\vec{x}_o) = -\frac{1}{8\pi\mu}\int_s f_i(\vec{x}) G_{ij}(\vec{x} - \vec{x}_o) ds$$

where

$$G_{ij} = \frac{\delta_{ij}}{R} + \frac{\hat{x}_i \hat{x}_j}{R^3};$$

$$R = \left| \vec{x}_o - \vec{x} \right|; \qquad \hat{x}_i = x_{oi} - x_i$$

# Null Space of the Stokes Equation

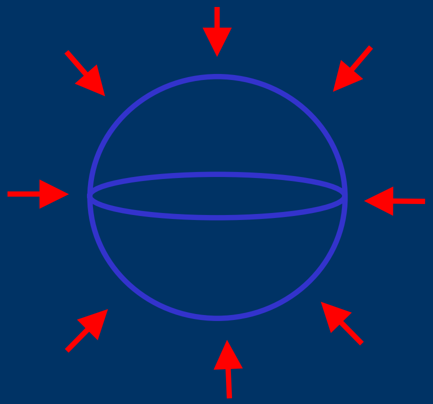
Constant pressure a singular mode, generates zero velocity.

Differential Form of Stokes, independent of absolute pressure

$$\begin{cases} 0 = -\nabla P + \mu \nabla^2 \vec{u} \\ \nabla \bullet \vec{u} = 0 \end{cases}$$

Integral Form of Stokes, constant pressure must not change velocity

$$u_j(\vec{x}_o) = -\frac{1}{8\pi\mu} \int_s f_i(\vec{x}) G_{ij}(\vec{x} - \vec{x}_o) ds$$



If $P = \text{constant}, \quad u_i = 0; f_i = -P n_i$

$$\Rightarrow \int_s G_{ij}(\vec{x} - \vec{x}_o) n_i(\vec{x}) ds = 0$$

# Null Space of the Singular BEM Operators

- Stokes Integral Operator has a null space
  - The solution is not uniquely defined.
  - A pressure boundary condition is needed.
- Null space must be removed
  - so as to avoid numerical error.

$$F = F^{\text{correct solution}} + XN + \varepsilon$$

- Two-step method:
  1. Modify GMRES to calculate a null-space-free solution.
  2. Use pressure condition to adjust solution

# Krylov Subspace Iterative methods

## Linear System

Start with $Ax = b$

## Determine the Krylov Subspace $r^0 = b - Ax^0$

Krylov Subspace $\equiv span\{r^0, Ar^0, \ldots, A^k r^0\}$

## Select Solution from the Krylov Subspace

$$x^{k+1} = x^0 + y^k, \quad y^k \in span\{r^0, Ar^0, \ldots, A^k r^0\}$$

GMRES picks a residual-minimizing $y^k$.

# Modify Krylov-Subspace Method to Calculate Null-Space-Free Solution

- The discretized Stokes equation $GF = U$
- The Krylov subspace is

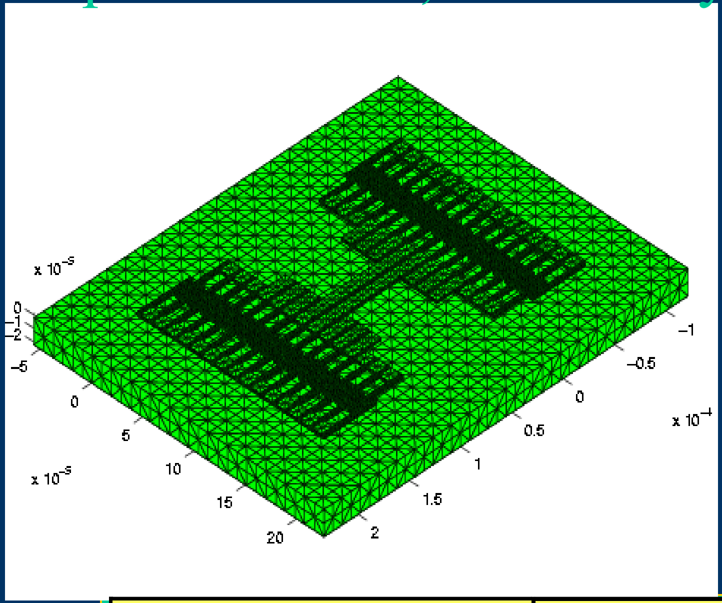
$$\mathcal{K} = span\left\{U, GU, G^2U, G^3U, G^4U, \cdots\cdots\right\}$$

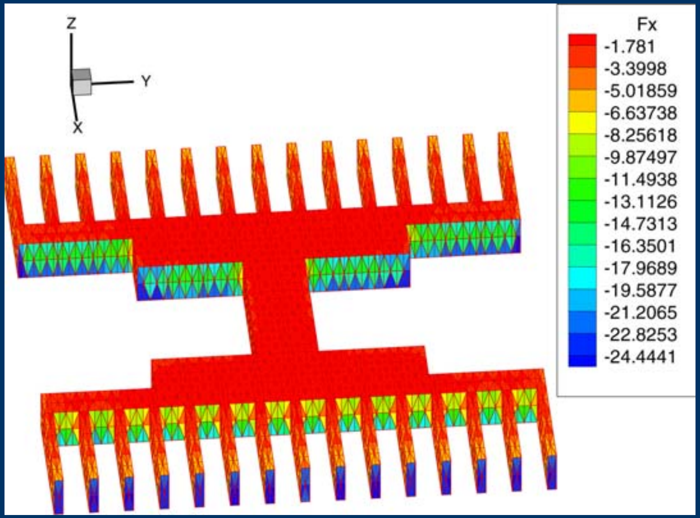
- If $\mathcal{K} \perp Null(G)$ then $F = F^{\perp} \perp Null(G)$

Remove *Null(G)* from every Krylov subspace vector

# FastStokes Simulation Result

## In-plane motion, 3-D steady incompressible Stokes, 16k panels

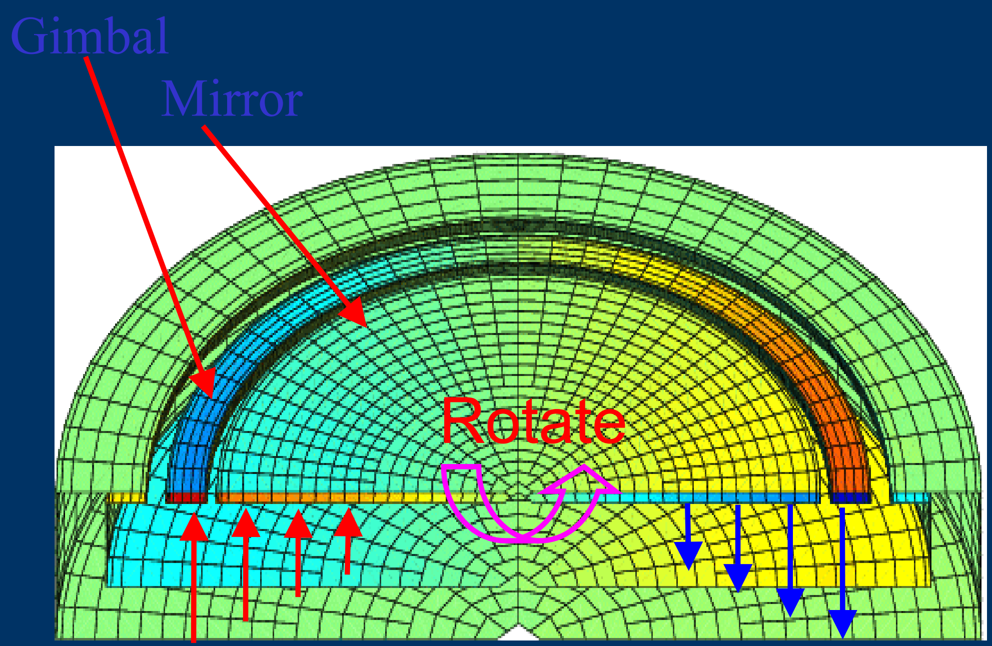





| | Drag Force (nN) | | | | | Q |
|---|---|---|---|---|---|---|
| | Total | Bottom | Top | Inter-finger | End and others | |
| Couette Model | 123.7 | 108.9 | | 14.8 | | 50.1 |
| 1-D Stokes | 137.1 | 108.9 | 13.5 | 14.8 | | 45.20 |
| FastStokes | 223.7 | 123.0 (55%) | 26.8 (12%) | 73.8 (33%) | | 27.7 |
| Measurement | | | | | | 27 |

Computation finished in 10 minutes

# Micromirror Q-factor




| | Mode | Q | | Error (%) |
|---|---|---|---|---|
| | | Simulated | Measured | |
| Mirror 1 | Mirror+Gimbal | 2.36 | 2.31 | 2.16 |
| | Mirror | 3.14 | 3.45 | 8.99 |
| Mirrror 2 | Mirror+Gimbal | 4.69 | 4.27 | 9.84 |
| | Mirror | 10.16 | 10.63 | 4.42 |

# Summary

- Reminder about $2^{nd}$ Kind theory
  - Convergence Theory
- Fredholm Alternative for $2^{nd}$ Kind
  - Finite Dimensional Null Space
- First Kind Convergence Theory, sort of
  - Connection to the FEM results
- MEMS Drag Example