Computational Methods for MEMS

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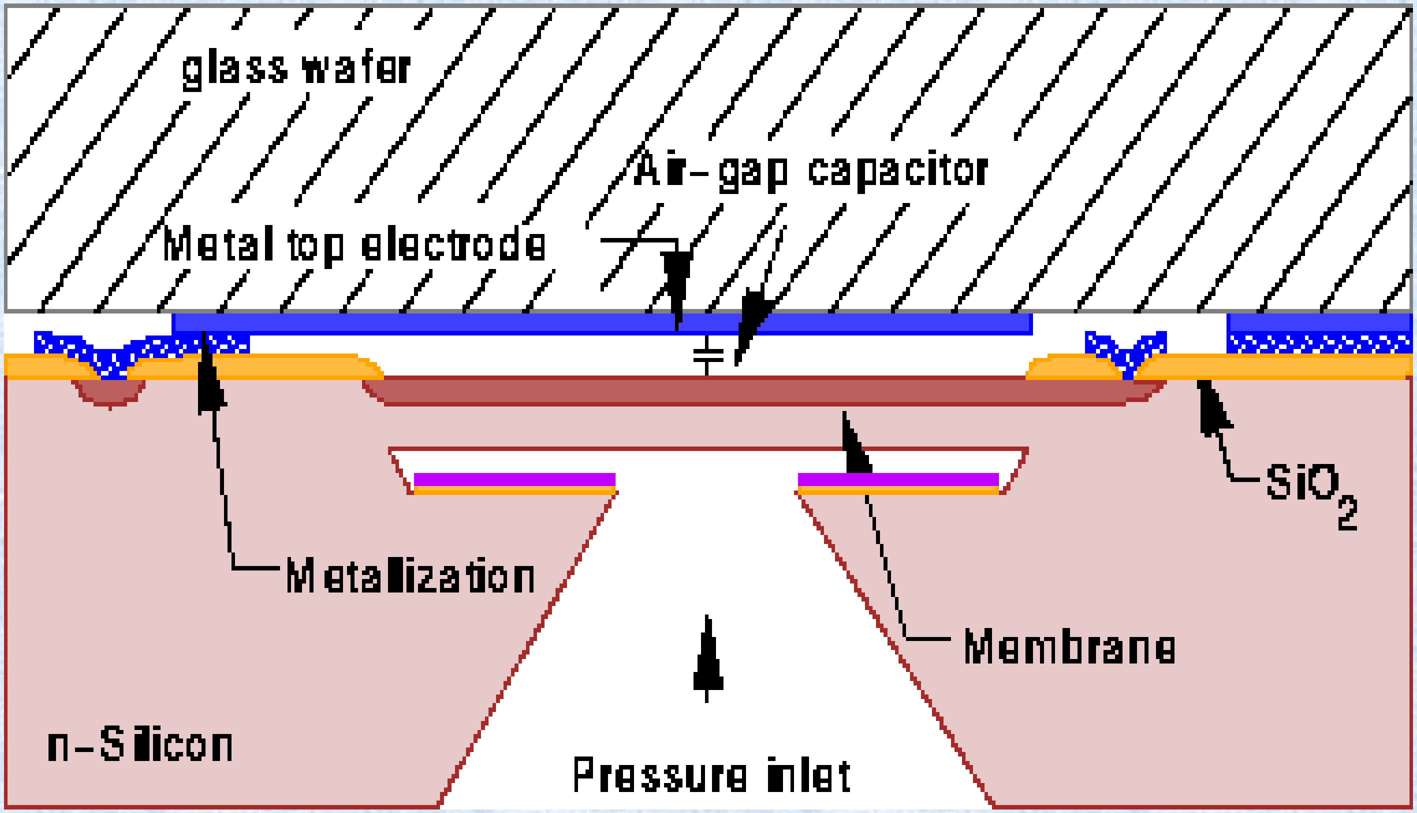
Course Objectives

- Understand how MEMS are designed
- Understand some of the computational techniques that go into the development of MEMS simulation tools
- Specific examples: electrostatic MEMS, microfluidics

Outline

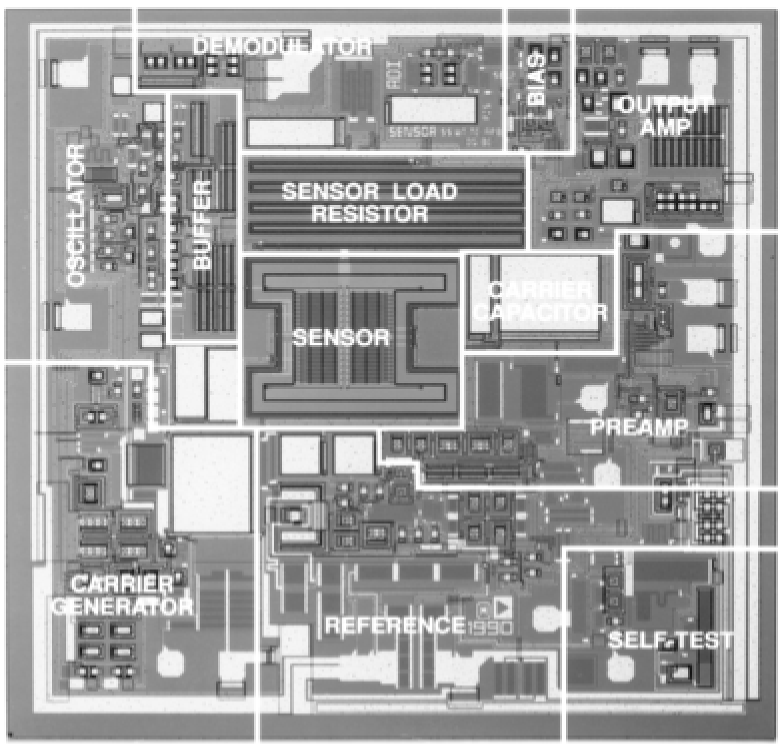
- Some MEMS Examples
- Mixed-Domain Simulation of electrostatic MEMS and microfluidics
  - Techniques for interior problems (e.g. FEM)
  - Techniques for exterior problems (e.g. BEM)
  - Algorithms

Pressure Sensor

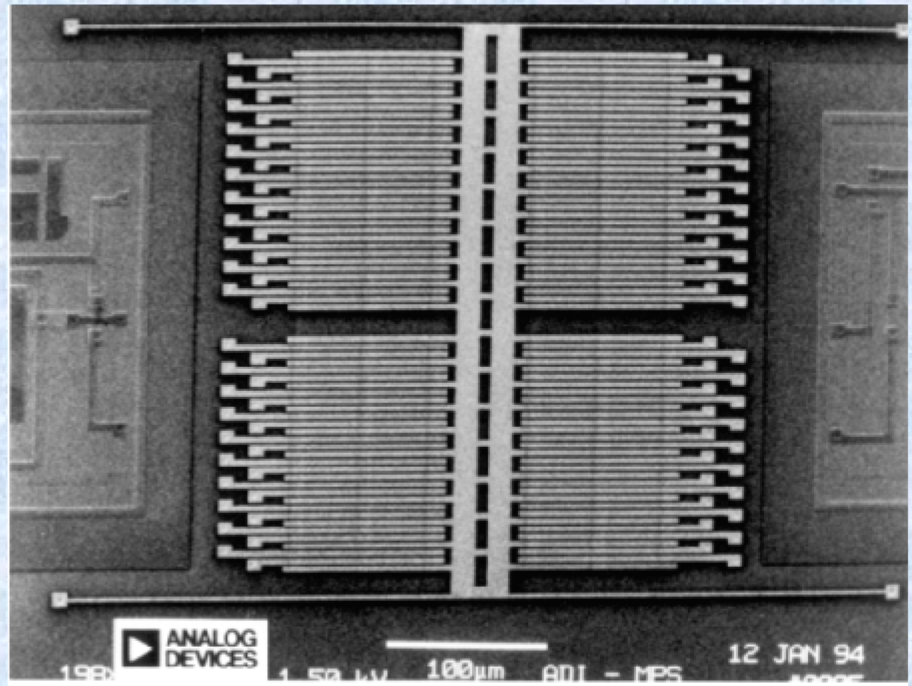


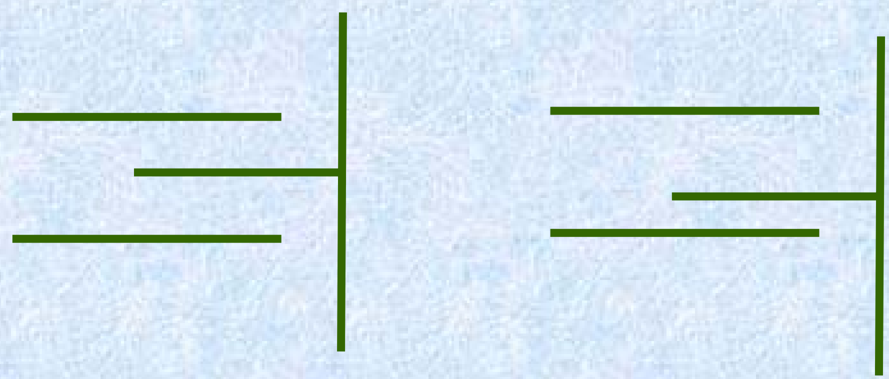
- Applications
  - Biomedical (e.g. blood pressure)

Accelerometer

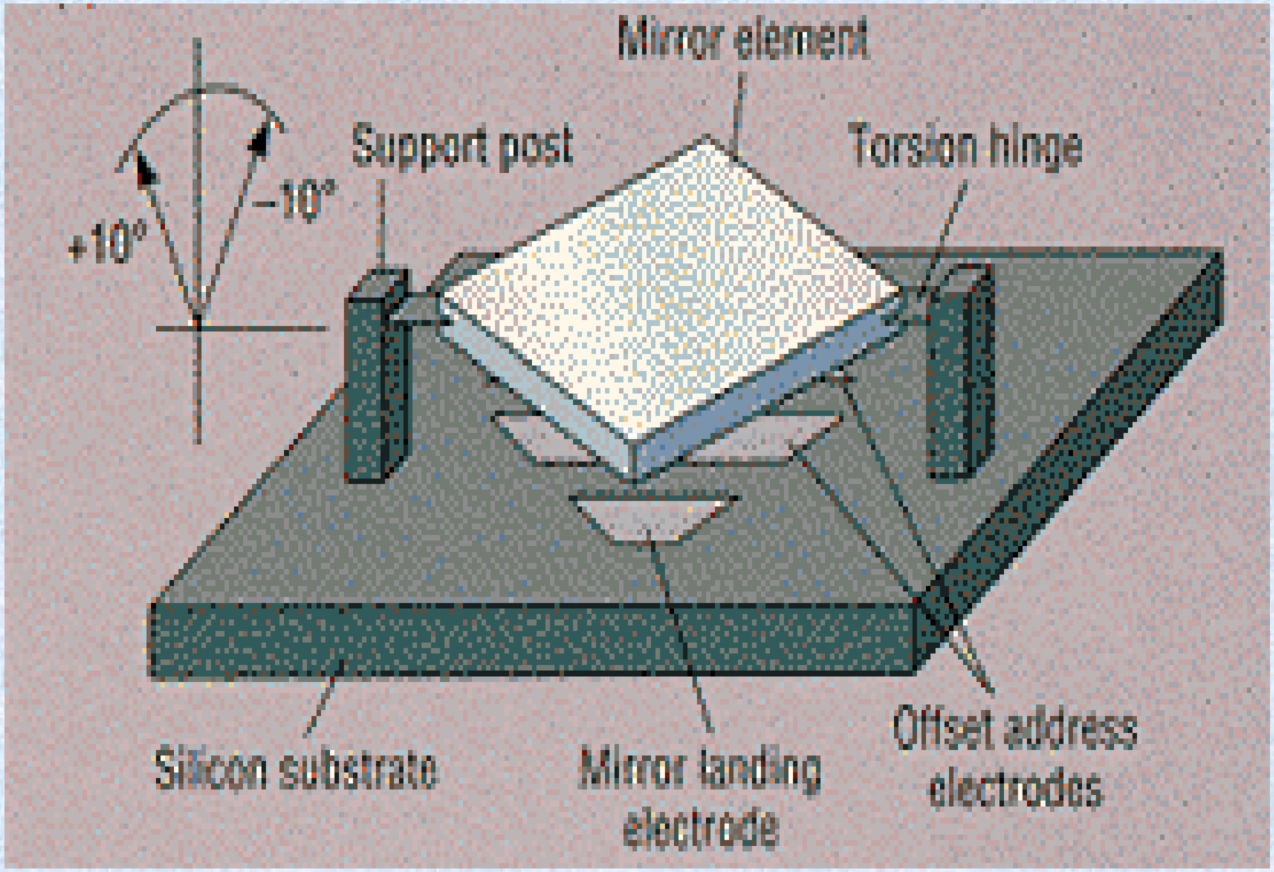


Analog Devices' ADXL-50, the industry's first surface micromachined accelerometer, includes signal conditioning on chip.





Micro Mirror



- Applications
  - High performance projection displays

Outline

- ✔ Some MEMS Examples
- ➨ Mixed-Domain Simulation of electrostatic MEMS and microfluidics
  - ➨ Techniques for interior problems (e.g. FEM)
  - ➨ Techniques for exterior problems (e.g. BEM)
  - ➨ Algorithms
- ➨ Dynamic Analysis

Is Electrostatics a good idea?

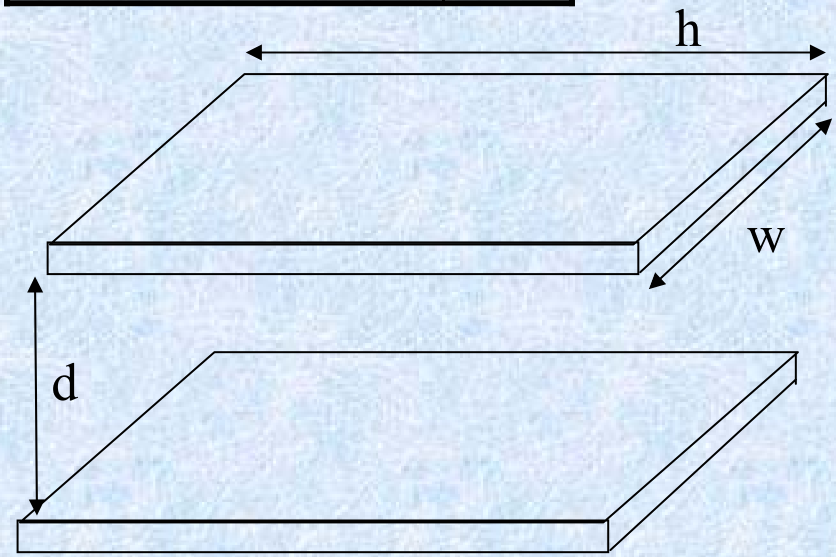
Scaling Laws

- Useful to understand where macro-theories start requiring corrections with the aim of better understanding the physical consequences of downscaling
- Develop an understanding of how systems are likely to behave when they are downsized
- Examples
  - By reducing the size of a device, the structural stiffness generally increases relative to inertially imposed loads
  - The mass or weight scales as l^3, while the surface tension scales as l as the system size becomes smaller
  - More difficult to empty liquids from a capillary compared to spilling coffee from a cup because of increased surface tension in a capillary
  - Heat loss is proportional to l^2; Heat generation is proportional to l^3; As animals get smaller, a greater percentage of their intake is required to balance heat loss; Insects are cold blooded

Scaling in Electrostatics

Distance	L
Velocity	L
Mass	L^3
Gravity	L^3
Surface Tension	L
Electrostatic force	L^2

Friction	L^2
van der Waals	$L^{1/4}$
Time	L^0
Muscle force	L^2
Power	L^3
Torque	L^3



Consider a capacitor

The electrostatic P.E. stored in a capacitor is:

$$E_{e,m} = \frac{\varepsilon_0 \varepsilon_r h w V_b^{\,2}}{2d}$$

$V_b =$ electrical breakdown voltage

Scaling in Electrostatics

Assume V_b scales linearly with d (the gap)

$$E_{e,m} = \frac{l^0 l^1 l^1 l^2}{l^1} \to l^3$$

The maximum energy stored in the capacitor scales as L^3

If L decreases by a factor of 10, the stored energy in the capacitor decreases by a factor of 1000

<u>Electrostatic Force</u>

$$F_x = -\frac{\partial}{\partial x}\left(\frac{1}{2}CV^2\right) \qquad F_y = -\frac{\partial}{\partial y}\left(\frac{1}{2}CV^2\right) \qquad F_z = -\frac{\partial}{\partial z}\left(\frac{1}{2}CV^2\right)$$

$$F_x = \frac{l^3}{l} \to l^2$$

Electrostatic force scales as L^2; This is an advantage because mass and inertial forces scale as L^3; The electrostatic force gains over inertial forces as the size of the system decreases

Scaling Laws: Vertical Bracket Notation

Different possible forces can be written as

$$F = \begin{Bmatrix} l^1 \\ l^2 \\ l^3 \\ l^4 \end{Bmatrix}$$

l^1 ← case where the force scales as L^1

l^2 ← case where the force scales as L^2

$$a = \frac{F}{m} = \left[l^F\right]\left[l^{-3}\right] = l^{F-3} \qquad t = \sqrt{\frac{2mx}{F}} = \sqrt{l^3 \cdot l \cdot l^{-F}}$$

$$\frac{P}{V_0} = \left(F\frac{x}{t}\right)\left(\frac{1}{V_0}\right) = \frac{l^F l}{\sqrt{l^{4-F}}}\frac{1}{l^3}$$

$$F = \begin{Bmatrix} l^1 \\ l^2 \\ l^3 \\ l^4 \end{Bmatrix} \rightarrow \quad a = \begin{Bmatrix} l^{-2} \\ l^{-1} \\ l^0 \\ l^1 \end{Bmatrix} \quad t = \begin{Bmatrix} l^{3/2} \\ l \\ l^{1/2} \\ 1 \end{Bmatrix} \quad \frac{P}{V_0} = \begin{Bmatrix} l^{-2.5} \\ l^{-1} \\ l^{0.5} \\ l^{2.0} \end{Bmatrix}$$

Scaling Laws: Remarks

- Even in the worst case when $F = L^4$, the time required to perform a task remains constant when the system is scaled down
- Under more favorable force scaling (e.g. $F = L^2$), the time required decreases as L (a system 10 times smaller can perform an operation 10 times faster i.e. small things tend to be quick)

<u>For Electrostatics</u> $\quad l^F = l^2 \qquad a = l^{-1} \quad t = l^1 \quad \dfrac{P}{V_0} = l^{-1.0}$

- When the force scales as $F = L^2$, the power per unit volume scales as L^{-1} => When the scale decreases by a factor of 10, the power that can be generated per unit volume increases by a factor of 10

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Elastostatics

- Finite-difference methods
- Finite-element methods
- Meshless methods

Finite Element Method: Introduction

Key steps in FEM:

- Construct a weak or a variational form of the problem
- Obtain an approximate solution of the variational equations through the use of finite element functions

1-D Example: Strong and Weak Forms

- **Strong form** $u_{,xx} + f = 0 \quad 0 \le x \le 1$ (S)

  $u(1) = q$ *Dirichlet B.C.*

  $-u_{,x}(0) = h$ *Neumann B.C.*

- **Trial function** $\delta = \{ u \mid u \in H^1, u(1) = q \}$

- **Test function (or weighting functions)** $\nu = \{ w \mid w \in H^1, w(1) = 0 \}$

- **Derive *weak form*** $\int_0^1 w(u_{,xx} + f)dx = 0$

- **Integrate by parts** $wu_{,x}\Big|_0^1 - \int_0^1 w_{,x}u_{,x}dx + \int_0^1 wf\,dx = 0$

Weak form $\int_0^1 w_{,x}u_{,x}dx = \int_0^1 wf\,dx + w(0)h$ (w)

$(S) \Leftrightarrow (W)$

1-D Example: Galerkin Form

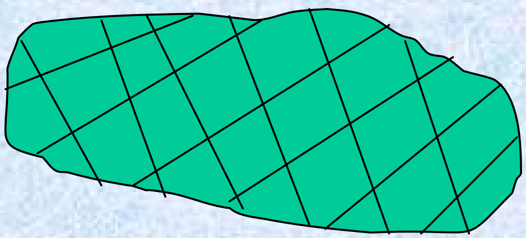
•Notations: $a(w,u) = \int_0^1 w_{,x} u_{,x} dx$ $\quad (w,f) = \int_0^1 w f \, dx$

•The weak form can be rewritten as $a(w,u) = (w,f) + w(0)h$

• Galerkin Approximation Method

$u^h \in \delta^h$

$w^h \in \nu^h$



Galerkin form	$a(w^h, u^h) = (w^h, f) + w^h(0)h$	(G)

Apply the interpolation $w^h = \sum_{A=1}^{N} N_A C_A$ $\quad u^h = \sum_{B=1}^{N} N_B d_B$

$$a\left(\sum_{A=1}^{N} N_A C_A, \sum_{B=1}^{N} N_B d_B\right) = \left(\sum_{A=1}^{N} N_A C_A, f\right) + \sum_{A=1}^{N} N_A(0) C_A h$$

1-D Example: Matrix Form

$$\sum_{A=1}^{N} C_A \left\{ \sum_{B=1}^{N} \int_\Omega N_{A,x} N_{B,x} d\Omega d_B - \int_\Omega N_A f d\Omega - N_A(0)h \right\} = 0$$

C_A's are arbitrary, so

$$\sum_{B=1}^{N} \int_\Omega N_{A,x} N_{B,x} d\Omega d_B = \int_\Omega N_A f d\Omega + N_A(0)h \qquad \text{for A=1,2, …, N}$$

where

$$\sum_{B=1}^{N} K_{AB} d_B = F_A \qquad \text{for A=1,2, …, N}$$

$$K_{AB} = \int_\Omega N_{A,x} N_{B,x} d\Omega \qquad F_A = \int_\Omega N_A f d\Omega + N_A(0)h$$

The matrix form $\quad Kd = F \quad$ (M)

1-D Example: Matrix Form

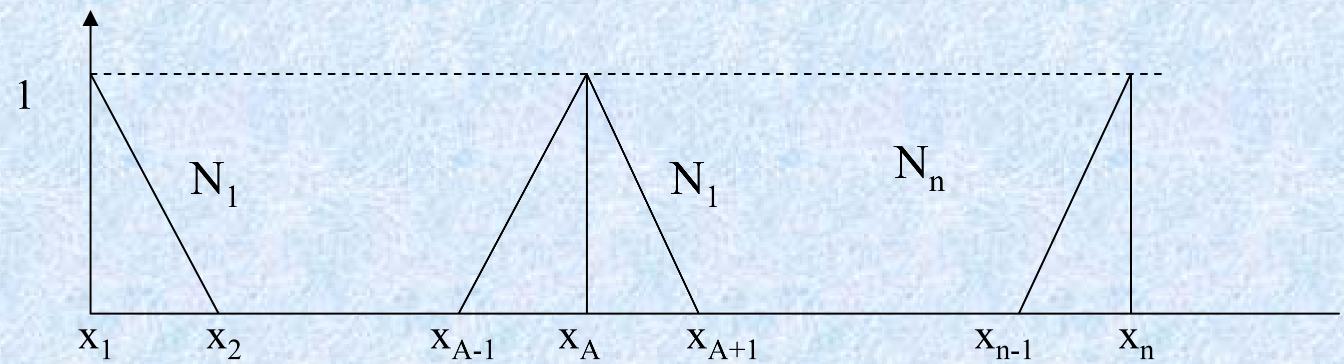
$$K = [K_{AB}] = \begin{bmatrix} K_{11} & K_{12} & \ldots\ldots & K_{1N} \\ K_{21} & K_{22} & & K_{2N} \\ \vdots & & & \\ K_{N1} & K_{N2} & & K_{NN} \end{bmatrix}$$

$$F = \{F_A\} = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_N \end{bmatrix} \qquad d = \{d_A\} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix}$$

Remarks:

- **K is symmetric;**
- **For any given problem,** $(S) \Leftrightarrow (W) \approx (G) \Leftrightarrow (M)$

Shape Functions



Shape functions

$$N_A(x)=\begin{cases} \dfrac{x-x_{A-1}}{h_{A-1}}, & x_{A-1}\le x\le x_A \\ \dfrac{x_{A+1}-x}{h_A}, & x_A\le x\le x_{A+1} \\ 0, & otherwize \end{cases}$$

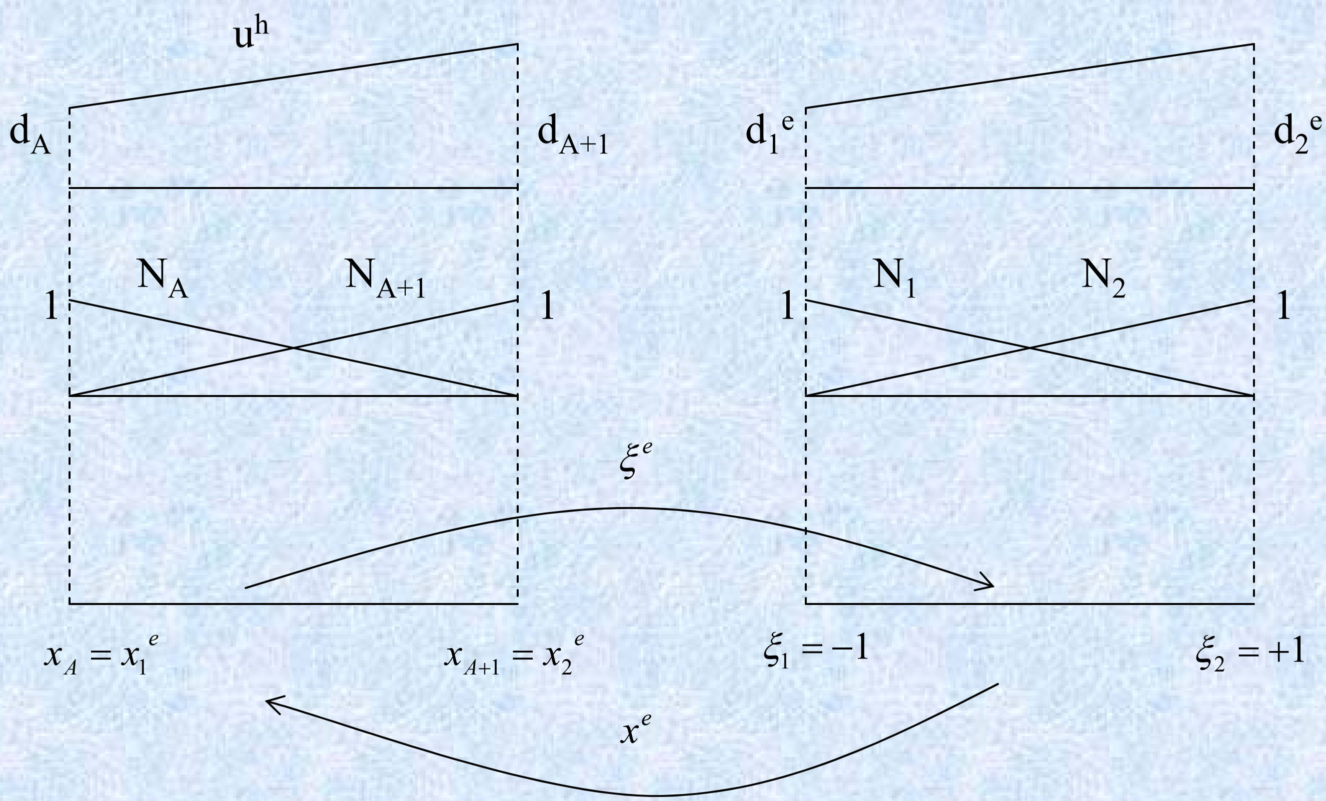
$$N_1(x)=\frac{x_2-x}{h_1},\quad x_1\le x\le x_2 \qquad N_N(x)=\frac{x-x_{N-1}}{h_{N-1}},\quad x_{n-1}\le x\le x_n$$

Local/Element Point of View

For a linear finite element

	global	local
Domain	$\left[x_A, x_{A+1}\right]$	$\left[\xi_1, \xi_2\right]$
Nodes	$\left\{x_A, x_{A+1}\right\}$	$\left\{\xi_1, \xi_2\right\}$
Degree of freedom	$\left\{d_A, d_{A+1}\right\}$	$\left\{d_1, d_2\right\}$
Shape functions	$\left\{N_A, N_{A+1}\right\}$	$\left\{N_1, N_2\right\}$
Interpolation function	$u^h(x) = N_A(x) d_A + N_{A+1}(x) d_{A+1}$	$u^h(\xi) = N_1(\xi) d_1 + N_2(\xi) d_2$

Mapping



u^h
d_A
d_{A+1}
d_1^e
d_2^e
N_A
N_{A+1}
N_1
N_2
1
1
1
1
ξ^e
$x_A = x_1^e$
$x_{A+1} = x_2^e$
$\xi_1 = -1$
$\xi_2 = +1$
x^e

Mapping

- **Local Shape function** $$N_a(\xi) = \frac{1}{2}(1 + \xi_a \xi)$$

$$N_1 = \frac{1}{2}(1 - \xi) \qquad N_2 = \frac{1}{2}(1 + \xi)$$

where $$\xi(x) = \frac{2x - x_A - x_{A-1}}{h_A}$$

$$x_{,\xi}{}^{e} = \frac{h^e}{2} = \frac{x_2{}^e - x_1{}^e}{2} \qquad \xi_{,x}{}^{e} = \left(x_{,\xi}{}^{e}\right)^{-1} = \frac{2}{h^e}$$

$$x^e(\xi) = \sum_{a=1}^{2} N_a(\xi) x_a{}^e = N_1(\xi) x_1{}^e + N_2(\xi) x_2{}^e$$

- **Derivative of the Shape function**

$$N_{a,\xi} = \frac{\xi_a}{2} = \frac{(-1)^a}{2}$$

Matrix Assembly

- **Global stiffness** $$K = \sum_{e=1}^{nel} K^e \qquad K^e = \left[K^e{}_{AB}\right]$$
- **Force vector** $$F = \sum_{e=1}^{nel} F^e \qquad F^e = \left[F^e{}_A\right]$$

where $$K^e{}_{AB} = a\left(N_A, N_B\right)^e = \int_{\Omega^e} N_{A,x} N_{B,x} dx$$

$$F^e{}_A = \left(N_A, f\right)^e + N_A(0)h$$

where $\Omega^e = \left[x^e{}_1, x^e{}_2\right]$ is the domain of the e-th element

$$K^e{}_{ab} = \int_{\Omega^e} N_{a,x}(x) N_{b,x}(x) dx$$

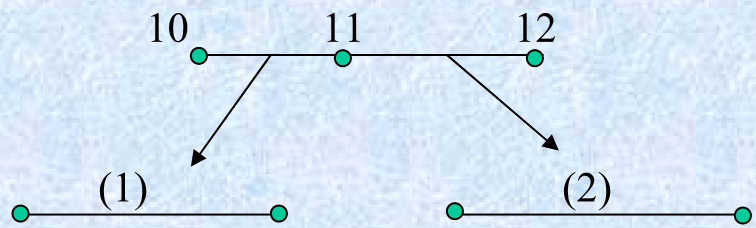
$$= \int_{-1}^{+1} N_{a,x}(x(\xi)) N_{b,x}(x(\xi)) x_{,\xi} d\xi = \int_{-1}^{+1} N_{a,\xi} N_{b,\xi} \left(x_{,\xi}\right)^{-1} d\xi$$

local stiffness

$$K^e = \frac{1}{h^e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

Assembly Process

example



local stiffness

$$K^{(1)} = \frac{1}{h^{(1)}}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad K^{(2)} = \frac{1}{h^{(2)}}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

Global stiffness

$$K = \begin{array}{cc} \begin{bmatrix} & & \vdots & \vdots & \vdots & & \\ & & \vdots & \vdots & \vdots & & \\ \cdots & \cdots & X & -X & & \cdots & \cdots \\ \cdots & \cdots & -X & X+Y & -Y & \cdots & \cdots \\ \cdots & \cdots & & -Y & Y & \cdots & \cdots \\ & & \vdots & \vdots & \vdots & & \\ & & \vdots & \vdots & \vdots & & \end{bmatrix} & \begin{array}{c} \\ \\ 10 \\ 11 \\ 12 \\ \\ \\ \end{array} \\ \begin{array}{ccccccc} & & 10 & 11 & 12 & & \end{array} & \end{array}$$

FEM: Multidimensional Problems

Divergence theorem $\int_{\Omega} f_{,i} d\Omega = \oint_{\Gamma} f n_i d\Gamma$

Integration by parts $\int_{\Omega} f_{,i} g d\Omega = \oint_{\Gamma} g f n_i d\Gamma - \int_{\Omega} f g_{,i} d\Omega$

Heat Conduction

Strong form: given $f : \Omega \rightarrow \Re, \quad g : \Gamma_g \rightarrow \Re, \quad h : \Gamma_h \rightarrow \Re$

find $u : \Omega \rightarrow \Re$ such that

$$q_{i,i} = f \quad in\, \Omega$$
$$u = g \quad on\, \Gamma_g$$
$$-q_i n_i = h \quad on\, \Gamma_h$$

where $q_i = -K_{ij} u_{,j}$ K_{ij} are the conductivities

Weak Form: Heat Conduction Problem

$$\int_\Omega w\left(q_{i,i} - f\right) d\Omega = 0$$

$$\int_\Gamma w q_i n_i d\Gamma - \int_\Omega w_{,i} q_i d\Omega - \int_\Omega w f d\Omega = 0$$

Apply the property of the weighting function $w = 0 \quad on\, \Gamma_g$

$$-\int_\Omega w_{,i} q_i d\Omega = \int_\Omega w f d\Omega + \int_{\Gamma_h} w h d\Gamma$$

Notation: $a(w,u) = \int_\Omega w_{,i} K_{ij} u_{,j} d\Omega$

$$(w,f) = \int_\Omega w f d\Omega \qquad (w,h)_\Gamma = \int_{\Gamma_h} w h d\Gamma$$

- **Weak form** $a(w,u) = (w,f) + (w,h)_{\Gamma_h}$
- **Galerkin form** $a(w^h,u^h) = (w^h,f) + (w^h,h)_{\Gamma_h}$

Heat Conduction Problem: Matrix Form

Substitute the interpolation $w^h = \sum_{A=1}^{N} N_A C_A$ $\quad u^h = \sum_{B=1}^{N} N_B d_B$

$$a\left(\sum_{A=1}^{N} N_A C_A, \sum_{B=1}^{N} N_B d_B\right) = \left(\sum_{A=1}^{N} N_A C_A, f\right) + \left(\sum_{A=1}^{N} N_A C_A, h\right)_\Gamma$$

$$\sum_{B=1}^{N} a(N_A, N_B) d_B = (N_A, f) + (N_A, h)_\Gamma$$

- Matrix form

$$K d = F$$

where

$$K_{AB} = a(N_A, N_B)$$

$$F_A = (N_A, f) + (N_A, h)_\Gamma$$

FEM for Elastostatics

Strong form: given f_i, g_i and h_i, find u_i such that

$$\sigma_{ij,j} + f_i = 0 \quad in\, \Omega$$
$$u_i = g_i \qquad on\, \Gamma_{gi}$$
$$\sigma_{ij} n_j = h_i \quad on\, \Gamma_h$$

The stress is related to the strain by Hooke's law

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

Strain tensor $\varepsilon_{ij} = \dfrac{u_{i,j} + u_{j,i}}{2} = u(i,j)$

$$\int_\Omega w_i(\sigma_{ij,j} + f_i)d\Omega = -\int_\Omega w_{i,j}\sigma_{ij}d\Omega + \int_\Gamma w_i\sigma_{ij}n_j d\Gamma + \int_\Omega w_i f_i d\Omega = 0$$

- **Weak form**

$$\int_\Omega w(i,j)\sigma_{ij}d\Omega = \int_\Omega w_i f_i d\Omega + \sum_{i=1}^{nsd}\left(\int_\Gamma w_i h_i d\Gamma\right)$$

FEM for Elastostatics

Why $\boldsymbol{w_{i,j}\sigma_{ij} = w(i,j)\sigma_{ij}}$

rewrite $w_{i,j} = w(i,j) + w[i,j]$

where $w(i,j) = \dfrac{w_{i,j} + w_{j,i}}{2}$ (symmetric)

$w[i,j] = \dfrac{w_{i,j} - w_{j,i}}{2}$ (skew symmetric)

since
$$w_{i,j}\sigma_{ij} = (w(i,j) + w[i,j])\sigma_{ij}$$
$$= w(i,j)\sigma_{ij} + w[i,j]\sigma_{ij}$$

and $w[i,j]\sigma_{ij} = -w[j,i]\sigma_{ij} = -w[j,i]\sigma_{ji} = -w[i,j]\sigma_{ij}$

$$w[i,j]\sigma_{ij} = 0$$

So
$$\boldsymbol{w_{i,j}\sigma_{ij} = w(i,j)\sigma_{ij}}$$

FEM for Elastostatics

Notation:

$$a(w,u) = \int_\Omega w(i,j) c_{ijkl} u(k,l) d\Omega$$

$$(w,f) = \int_\Omega w_i f_i d\Omega \qquad (w,h)_\Gamma = \sum_{i=1}^{nsd} \left(\int_{\Gamma_{hi}} w_i h_i d\Gamma \right)$$

- Weak form

$$a(w,u) = (w,f) + (w,h)_\Gamma \quad \text{for all } w \in v$$

- Galerkin form

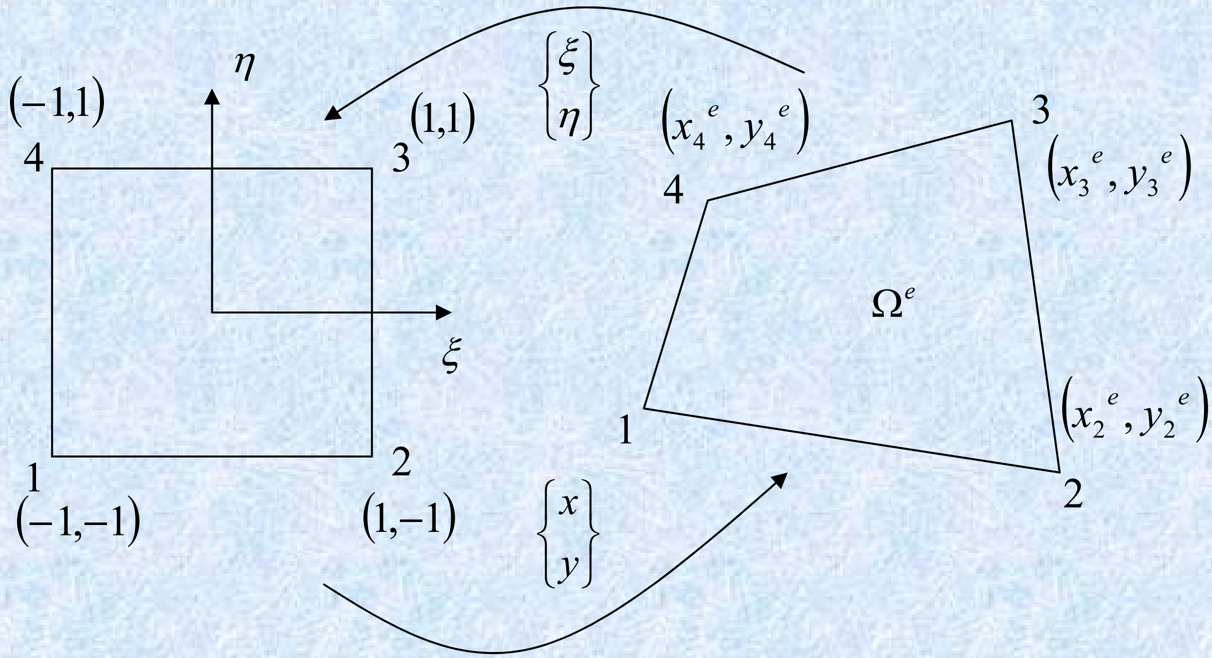
$$a(w^h,u^h) = (w^h,f) + (w^h,h)_\Gamma$$

$$u_i^h = \sum_{A=1}^{n} N_A d_{iA} \quad i = 1,2,3 \ (\ 3\ dof's)$$

- Matrix form

$$Kd = F$$

Bilinear Quadrilateral Element



$$x(\xi,\eta) = \sum_{a=1}^{4} N_a(\xi,\eta) x_a^{\ e}$$

$$y(\xi,\eta) = \sum_{a=1}^{4} N_a(\xi,\eta) y_a^{\ e}$$

Shape Functions

- **Shape functions**

$$N_1(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta)$$

$$N_2(\xi,\eta)=\frac{1}{4}(1+\xi)(1-\eta)$$

$$N_3(\xi,\eta)=\frac{1}{4}(1+\xi)(1+\eta)$$

$$N_4(\xi,\eta)=\frac{1}{4}(1-\xi)(1+\eta)$$

Property of the shape function

$$\sum_{a=1}^{nen} N_a(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta)+\frac{1}{4}(1+\xi)(1-\eta)+\frac{1}{4}(1+\xi)(1+\eta)+\frac{1}{4}(1-\xi)(1+\eta)$$
$$=1$$

Numerical Integration

Numerical integration

$$\int_{-1}^{+1} g(\xi)d\xi = \sum_{l}^{n_{\text{int}}} g(\xi_l)w_l + R \cong \sum_{l}^{n_{\text{int}}} g(\xi_l)w_l$$

- **Trapezoidal rule**

$$n_{\text{int}} = 2 \qquad w_l = 1 \qquad l = 1,2$$
$$\bar{\xi}_1 = -1$$
$$\bar{\xi}_2 = +1$$
$$R = -\frac{2}{3} g_{,\xi\xi}(\bar{\xi})$$

- **Simpson's rule**

$$n_{\text{int}} = 3 \qquad w_1 = w_3 = \frac{1}{3}$$
$$\bar{\xi}_1 = -1$$
$$\bar{\xi}_2 = 0 \qquad w_2 = \frac{4}{3}$$
$$\bar{\xi}_3 = 1$$
$$R = -\frac{1}{90} g^{(4)}(\bar{\xi})$$

Gaussian Quadrature Rules

$n_{\text{int}} = 1$

$$\bar{\xi}_1 = 0 \qquad w_1 = 2$$

$$R = \frac{g_{,\xi\xi}\left(\bar{\xi}\right)}{3}$$

$n_{\text{int}} = 2$

$$\bar{\xi}_1 = -\frac{1}{\sqrt{3}} \qquad \bar{\xi}_2 = \frac{1}{\sqrt{3}}$$

$$w_1 = w_2 = 1$$

$$R = \frac{g^{(4)}\left(\bar{\xi}\right)}{135}$$

$n_{\text{int}} = 3$

$$\bar{\xi}_1 = -\sqrt{\frac{3}{5}} \qquad \bar{\xi}_2 = 0 \qquad \bar{\xi}_3 = \sqrt{\frac{3}{5}}$$

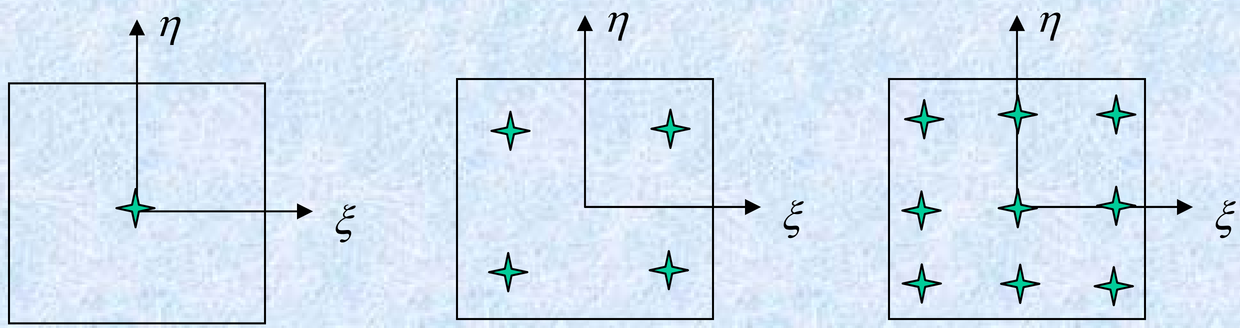
$$w_1 = w_3 = \frac{5}{9} \qquad w_2 = \frac{8}{9}$$

$$R = \frac{g^{(6)}\left(\bar{\xi}\right)}{15750}$$

Gaussian Quadrature Rules in 2-D

$$\int_{-1}^{+1}\int_{-1}^{+1} g(\xi,\eta)\,d\xi\,d\eta \cong \int_{-1}^{+1}\left\{\sum_{l^{(1)}=1}^{n_{int}^{(1)}} g\left(\bar{\xi}_{l^{(1)}}^{(1)},\eta\right) w_{l^{(1)}}^{(1)}\right\} d\eta$$

$$\cong \sum_{l^{(1)}=1}^{n_{int}^{(1)}} \sum g\left(\bar{\xi}^{(1)}_{l^{(1)}}, \bar{\eta}^{(2)}_{l^{(2)}}\right) w^{(1)}_{l^{(1)}} w^{(2)}_{l^{(2)}}$$

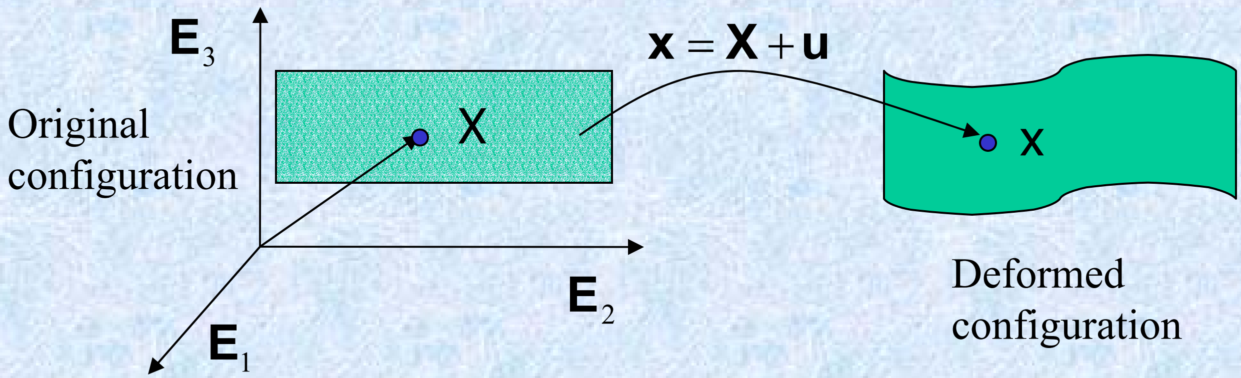


examples

$$\int_{-1}^{+1}\int_{-1}^{+1} g(\xi,\eta)\,d\xi\,d\eta = 4\,g(0,0)$$

$$\int_{-1}^{+1}\int_{-1}^{+1} g(\xi,\eta)\,d\xi\,d\eta = g\left(-\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right) + g\left(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right)$$

Finite Deformation Elastodynamics



Transformation function $\mathbf{x} = \varphi(\mathbf{X})$ $d\mathbf{x} = \mathbf{F}d\mathbf{X}$

Deformation gradient

$$\mathbf{F} = D\varphi(\mathbf{X}) = \begin{bmatrix} \frac{\partial \varphi_1}{\partial X_1} & \frac{\partial \varphi_1}{\partial X_2} & \frac{\partial \varphi_1}{\partial X_3} \\ \frac{\partial \varphi_2}{\partial X_1} & \frac{\partial \varphi_2}{\partial X_2} & \frac{\partial \varphi_2}{\partial X_3} \\ \frac{\partial \varphi_3}{\partial X_1} & \frac{\partial \varphi_3}{\partial X_2} & \frac{\partial \varphi_3}{\partial X_3} \end{bmatrix}$$

$$J(\varphi) = \det[\mathbf{F}]$$

Volume transformation $dv = JdV$

Area transformation $(d\mathbf{s})\mathbf{n} = J(d\mathbf{S})(\mathbf{F}^T)^{-1}\mathbf{N}$

Density transformation $\rho = \frac{1}{J}\rho_0$

Velocity $\mathbf{V} = \frac{\partial \varphi}{\partial t}$

Cauchy stress $\sigma = \frac{1}{J}\mathbf{P}\mathbf{F}^T$

Elastodynamics: Governing Equations

Strong form:

$$\rho_0 \frac{\partial^2 \varphi}{\partial t^2} = Div[\mathbf{P}] + \rho_0 \mathbf{B}$$

where $\mathbf{P} = \mathbf{F}\,\mathbf{S}$

$$\mathbf{S} = \mathbf{c}\,\mathbf{E} \qquad \mathbf{c} = \mathbf{F}^T\mathbf{F} \qquad \mathbf{E} = \frac{1}{2}[\mathbf{c} - \mathbf{I}]$$

- **Boundary conditions:**

$$\varphi = \mathbf{g} \quad \text{on } \Gamma_g \quad \text{at } [0,T]$$

$$P_{iA} n_A = h_i \quad \text{on } \Gamma_{h_i} \quad \text{at } [0,T]$$

- **Initial conditions:**

$$\varphi\big|_{t=0} = \varphi^0 \quad \text{in } \Omega$$

$$\mathbf{V}\big|_{t=0} = \mathbf{V}^{(0)} \quad \text{in } \Omega$$

FEM for Elastodynamics

- **Weak form**:

$$G(\varphi,\eta)=\int_\Omega Grad[\eta]:[D\varphi\,\mathbf{S}(\mathbf{E}(\varphi))]dV-\int_\Omega \rho_0\mathbf{B}\cdot\eta\, dV-\int_{\Gamma_h}\eta\cdot\mathbf{h}\,d\Gamma=0$$

- **Galerkin form:**

$$G(\varphi^h,\eta^h)=\int_\Omega Grad[\eta^h]:[D\varphi^h\,\mathbf{S}^h]dV-\int_\Omega \rho_0\mathbf{B}\cdot\eta^h dV-\int_{\Gamma_h}\eta^h\cdot\mathbf{h}\,d\Gamma=0$$

$$\Downarrow$$

Nonlinear equations: $\mathcal{F}^{\text{int}}(\mathbf{d})-\mathcal{F}^{ext}=0$

Where

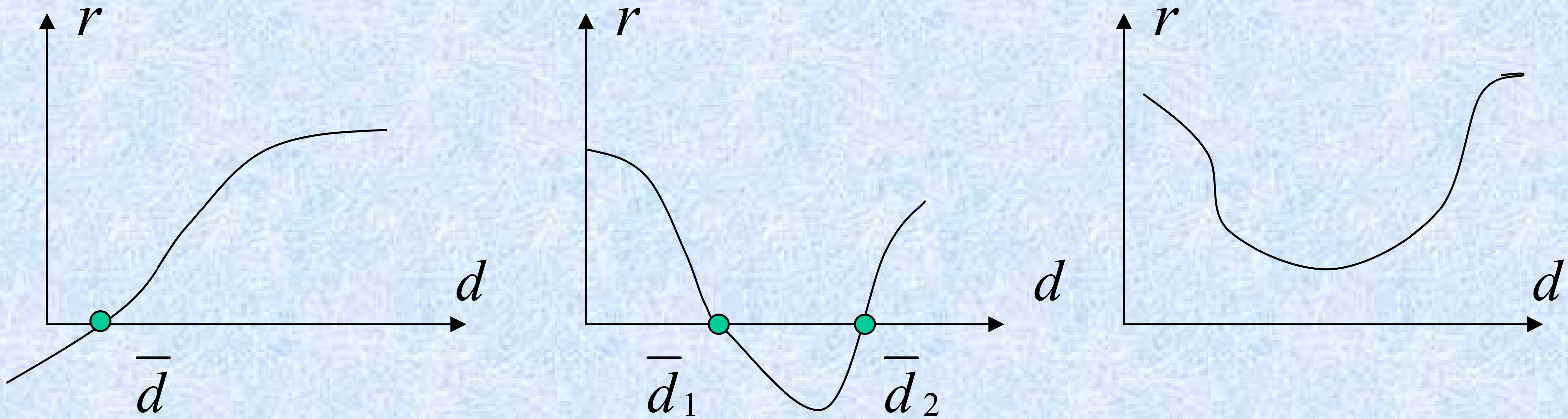
$$\mathcal{F}^{\text{int}}(\mathbf{d})=\int_\Omega \mathcal{B}^T\hat{\mathbf{S}}\,dV \qquad \mathcal{F}^{ext}=\int_\Omega \rho_0\mathbf{B}\cdot\mathbf{N}\,dV+\int_{\Gamma_h}\mathbf{h}\cdot\mathbf{N}\,d\Gamma$$

Solution of Nonlinear Systems: Newton Methods

The scalar problem: $\boldsymbol{r}(\boldsymbol{d})$ is a scalar nonlinear function of $\boldsymbol{d}$. Find $\bar{d}$ such that

$$\boldsymbol{r}\left(\bar{\boldsymbol{d}}\right) = \mathbf{0}$$

Possibilities:



one unique solution

several solutions

no solutions

Newton's Method

- **Solution strategy:**

Guess a "good" d_0 close to the solution;

$$r(\bar{d}) = r(d_0) + \frac{d}{d\varepsilon} r(d_0 + \varepsilon \Delta d)\Big|_{\varepsilon=0} + \frac{1}{2!}\frac{d^2}{d\varepsilon^2} r(d_0 + \varepsilon \Delta d)\Big|_{\varepsilon=0} + \ldots\ldots$$

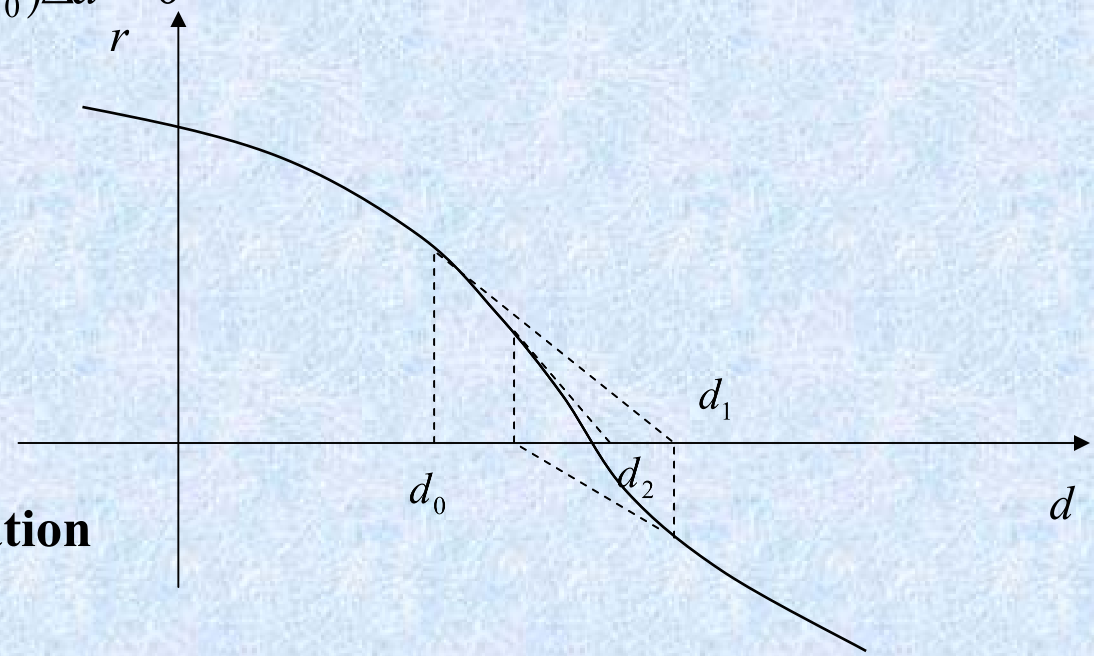
$$r(\bar{d}) \cong r(d_0) + \frac{d}{d\varepsilon} r(d_0 + \varepsilon \Delta d)\Big|_{\varepsilon=0}$$

$$= r(d_0) + K(d_0)\Delta d = 0$$

$$\Delta d = -\frac{r(d_0)}{K(d_0)}$$

$$d_1 = d_0 + \Delta d$$

- **Geometric interpretation**



Algorithm: Newton's Method

$$
\begin{aligned}
& i = 0 \\
& d_i = d_0 \\
& \text{for } i = 1,2,\ldots\ldots \text{ until convergence} \\
& \quad \text{if } |r(d_i)| < tol \\
& \qquad \bar{d} = d_i \\
& \quad \text{else} \\
& \qquad \Delta d = -\frac{r(d_i)}{r'(d_i)} \\
& \qquad d_{i+1} = d_i + \Delta d \\
& \quad \text{end if} \\
& \text{end for}
\end{aligned}
$$

The error at the i-th iteration is given by $e^{(i)} = d_i - \bar{d}$

if $\left|e^{(i+1)}\right| \leq C\left|e^{(i)}\right|^k$ then we say the algorithm converges with order k.

Newton's method has quadratic convergence, i.e. k=2

Modified Newton's Method

Advantages of Newton's method

- Optimal (quadratic) convergence close to solution

Disadvantages of Newton's method

- Poor or no convergence far away from the solution;
- Computation of K(d_i) is very expensive in the general multidimensional case (K (d_i) is a matrix).

Algorithm: modified Newton's method

$$
\begin{aligned}
& i = 0 \\
& d_i = d_0 \\
& \text{for } \; i = 1,2,\ldots\ldots \text{ until convergence} \\
& \quad \text{if } \left| r(d_i) \right| < tol \\
& \qquad \bar{d} = d_i \\
& \quad \text{else} \\
& \qquad \Delta d = -\frac{r(d_i)}{r'(d_0)} \\
& \qquad d_{i+1} = d_i + \Delta d \\
& \quad \text{end if} \\
& \text{end}
\end{aligned}
$$

Newton Method: Multidimensional Case

Let $\underline{R}(\underline{d})$ be a n-dimensional vector valued nonlinear function of the n-dimensional vector $\underline{d}$

$$R_1 = \hat{R}_1(d_1, d_2, \ldots\ldots, d_n)$$
$$R_2 = \hat{R}_2(d_1, d_2, \ldots\ldots, d_n)$$
$$\vdots \qquad \vdots$$
$$R_n = \hat{R}_n(d_1, d_2, \ldots\ldots, d_n)$$

• **Directional or Frechet derivative**

$$\frac{d}{d\varepsilon}\underline{R}(\underline{d}+\varepsilon\underline{u})\Big|_{\varepsilon=0} = \nabla\underline{R}\underline{u}$$

$$= \begin{bmatrix} \frac{\partial R_1}{\partial d_1} & \frac{\partial R_1}{\partial d_2} & \cdots & \frac{\partial R_1}{\partial d_n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial R_n}{\partial d_1} & \frac{\partial R_n}{\partial d_n} & \cdots & \frac{\partial R_n}{\partial d_n} \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{Bmatrix}$$

Similar to the scalar case

$$\underline{R}(\overline{\underline{d}}) = \underline{R}(\underline{d_0}) + \frac{d}{d\varepsilon}\underline{R}(\underline{d_0}+\varepsilon\Delta\underline{d})\Big|_{\varepsilon=0} + \frac{1}{2!}\frac{d^2}{d\varepsilon^2}\underline{R}(\underline{d_0}+\varepsilon\Delta\underline{d})\Big|_{\varepsilon=0} + \ldots\ldots$$
$$\cong \underline{R}(d_0) + \frac{d}{d\varepsilon}\underline{R}(\underline{d_0}+\varepsilon\Delta\underline{d})\Big|_{\varepsilon=0}$$
$$= \underline{R}(d_0) + \underline{K}_T(\underline{d_0})\Delta\underline{d} = 0$$

$\underline{K}_T(\underline{d_0})$ is called the tangent stiffness matrix

Newton-Raphson Method: Algorithm

$n = 0$

step loop (load stepping e.g)

$i = 0$

$\underline{d}^{(i)} = \underline{d}_n$

do (iteration loop)

$$\underline{\mathrm{K}}_T\left(\underline{d}^{(i)}\right)\Delta\underline{d}^{(i)} = -\underline{R}^{(i)}$$

$$:= \underline{F}_{n+1}^{ext} - \underline{F}_{n+1}^{\mathrm{int}}\left(\underline{d}^{(i)}\right)$$

$$\underline{d}^{(i+1)} = \underline{d}^{(i)} + \Delta\underline{d}^{(i)}$$

$$i = i + 1$$

until $\left\|\underline{R}^{(i+1)}\right\| < \varepsilon\left\|\underline{R}^{(i)}\right\|$

$\underline{d}_{n+1} = \underline{d}^{(i)}$

$n \leftarrow n + 1$

Remarks:

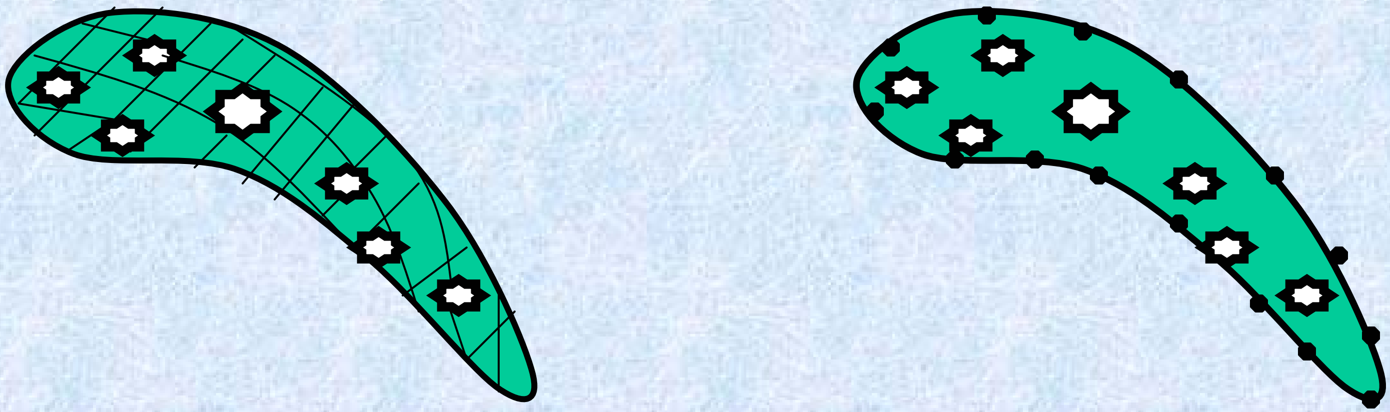
- The load step is needed since the method might not converge if the entire load is applied at once. Instead the load is applied incrementally. Each increment is converged before the next step is applied.
- Likewise one might have to apply the "g" b.c.'s incrementally. This method is called "displacement control".
- In practice, the terminology "Newton-Raphson method"is often used to denote algorithms in which a new left hand size matrix is formed for each iteration. If KT is not updated in each iteration, but kept frozen for a couple of iterations, the term "modified Newton" method is used.

Outline

- ✔ Some MEMS Examples
- ➡ Mixed-Domain Simulation of electrostatic MEMS and microfluidics
  - ✔ Techniques for interior problems (e.g. FEM)
  - ☞ Techniques for exterior problems (e.g. BEM)
  - ➡ Algorithms

BEM - Introduction

- What is Boundary Element Method ?
  - Boundary discretization only
  - Integral based method



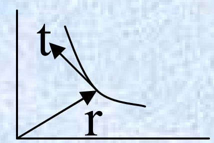
Analysis of a turbine blade using FEM and BEM

- Approaches available for solving boundary integral equations
  - BEM based on Collocation
  - BEM based on Galerkin

Comparison of FEM and BEM

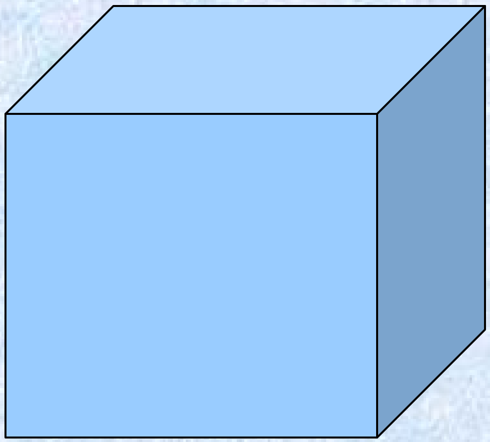
FEM	BEM
Local approach	Global approach, Integral based
Domain mesh (2D/3D)	Boundary mesh (1D/2D)
Symmetric, sparse and large matrices	Unsymmetric, dense and smaller matrices
Lot of commercial packages available	Fewer packages available

Table 1

Problems ($\nabla^2\phi = 0$)	**Scalar function** (ϕ)	**Dirichlet b.c.** ($\phi = \bar{\phi}$)	**Neumann b.c.** ($K\frac{\partial\phi}{\partial n} = \bar{q}$)	**Constant** (K)
Heat Transfer	Temperature ($T \equiv Deg.$)	($T = \bar{T}$)	Heat flow ($-\lambda\frac{\partial T}{\partial n} = \bar{q}$)	Thermal conductivity(λ)
Elastic torsion	Warping function (ψ)		($r\cos(r,t) = \bar{q}$)	
Ideal fluid flow	Stream function ($\phi \equiv m^2 s^{-1}$)	($\phi = \bar{\phi}$)	($\frac{\partial\phi}{\partial n} = \bar{q}$)	
Electrostatic	Field potential ($V \equiv volt$)	($V = \bar{V}$)	Electric flow ($-\varepsilon\frac{\partial V}{\partial n} = \bar{q}$)	Permittivity (ε)
Electric conduction	Electro-potential ($E \equiv volt$)	($E = \bar{E}$)	Electric current ($\frac{1}{k}\frac{\partial E}{\partial n} = \bar{q}$)	Resistivity (k)

Boundary Integral Formulation

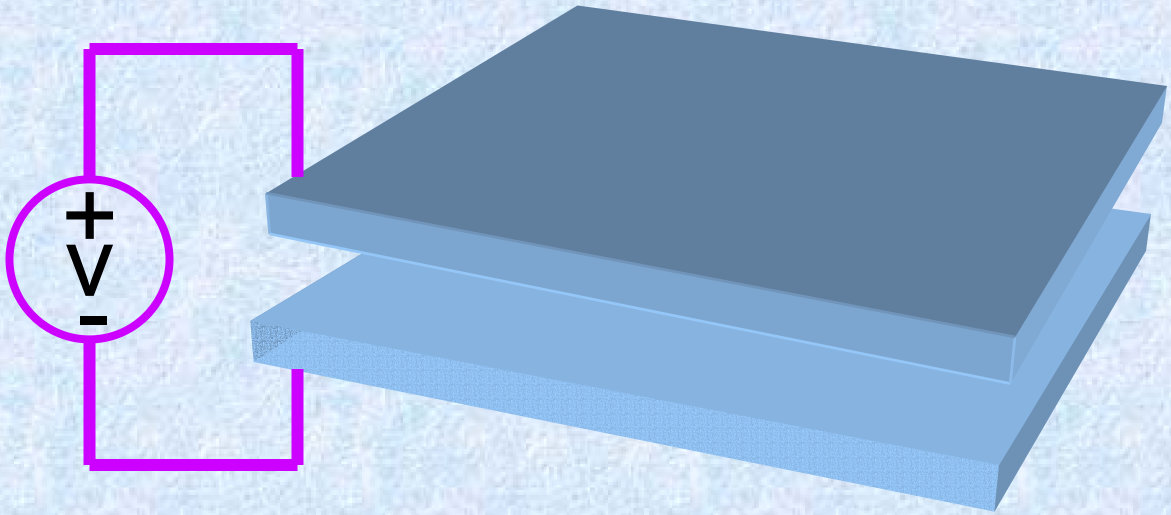
- Laplace equation represents many problems in engineering (Table 1)



$\nabla^2 T = 0$ inside

Temperature 'T' known on the surface

Interior problem



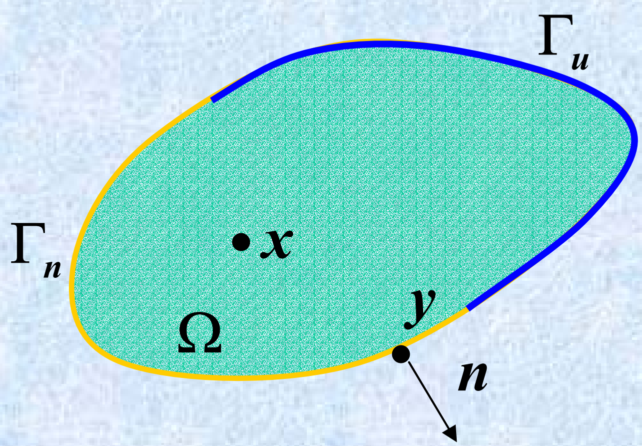
$\nabla^2 \phi = 0$ outside

Potential ϕ known on the surface

Exterior problem

Boundary Integral Formulation

- **BEM is based on the Second Theorem of Green**
- **Problem definition**



Definition of the problem

- **Governing equation:**

$$\nabla^2 \phi = p(x) \qquad x \in \Omega$$

$$p(x) \begin{cases} = 0\,;\ Laplace \\ \neq 0\,;\ Poisson \end{cases}$$

- **Dirichlet boundary condition (b.c):**

$$\phi(y) = \overline{\phi}(y) \qquad y \in \Gamma_u$$

- **Neumann boundary condition (b.c):**

$$\left.\frac{\partial \phi(x)}{\partial n}\right|_{x=y} = \overline{q}(y) \qquad y \in \Gamma_n$$

Boundary Integral Formulation

Derivation of BIE:

Multiplying $(\nabla^2\phi - p)$ **with** ϕ^* **and integrating over** Ω

$$\int_\Omega \left(\nabla^2\phi - p\right)\phi^* d\Omega = 0 \qquad \ldots \; (1)$$

Integrating by parts we get (2D case),

$$\int_\Gamma \phi^* \nabla\phi \cdot \boldsymbol{n} d\Gamma - \int_\Omega \left(\nabla\phi \cdot \nabla\phi^* + p\phi^*\right) d\Omega + = 0$$

Integrating by parts the second integral we get,

$$\int_\Gamma \phi^* \nabla\phi \cdot \boldsymbol{n} d\Gamma - \int_\Gamma \phi\nabla\phi^* \cdot \boldsymbol{n} d\Gamma + \int_\Omega \left(\phi\nabla^2\phi^* - p\phi^*\right) d\Omega = 0$$

where *n* is the outward normal to the boundary Γ

Boundary Integral Formulation

Therefore, Equation (*1*) can be written as,

$$\int_{\Omega}\left(\nabla^{2}\phi - p\right)\phi^{*}\,d\Omega = \int_{\Omega}\left(\phi\nabla^{2}\phi^{*} - p\phi^{*}\right)d\Omega + \int_{\Gamma}\phi^{*}\frac{\partial\phi}{\partial n}\,d\Gamma - \int_{\Gamma}\phi\frac{\partial\phi^{*}}{\partial n}\,d\Gamma = 0$$

$$\boxed{\Rightarrow \int_{\Omega}\left[\left(\nabla^{2}\phi\right)\phi^{*} - \left(\nabla^{2}\phi^{*}\right)\phi\right]d\Omega = \int_{\Gamma}\left(\phi^{*}\frac{\partial\phi}{\partial n} - \phi\frac{\partial\phi^{*}}{\partial n}\right)d\Gamma} \qquad \ldots\ (2)$$

ϕ^{*} **is the** ***Fundamental Solution of Laplace equation.***

Boundary Integral Formulation

Fundamental Solution ϕ^* for Laplace equation :

- satisfies Laplace equation
- represents field generated by a concentrated unit charge acting at a point '*i*'
- effect of this charge is propagated from '*i*' to infinity

$$\nabla^2\phi^* + \delta(i,j) = 0 \qquad \delta(i,j) = \text{Dirac Delta function}$$

Multiplying with ϕ and integrating we get,

$$\int_\Omega \phi(\nabla^2\phi^*)\,d\Omega = \int_\Omega \phi(-\delta(i,j))\,d\Omega = -\phi^i$$

Therefore,

$$\boxed{\phi^i + \int_\Gamma \phi\left(\frac{\partial\phi^*}{\partial n}\right)d\Gamma = \int_\Gamma \left(\frac{\partial\phi}{\partial n}\right)\phi^*\,d\Gamma} \qquad \ldots(3)$$

Boundary Integral Formulation

Fundamental Solutions : One Dimensional Equations

	Equation	Fundamental Solution
Laplace	$\nabla^2\phi^* + \delta_0 = 0$	$\phi^* = \frac{r}{2}, r = \lvert x \rvert$
Helmholtz	$\nabla^2\phi^* + \lambda^2\phi^* + \delta_0 = 0$	$\phi^* = -\frac{1}{2\lambda}\sin(\lambda r)$
Wave Equation	$c^2\nabla^2\phi^* - \frac{\partial^2\phi^*}{\partial t^2} + \delta_0\delta(t) = 0$	$\phi^* = \frac{1}{2c}H(ct - r)$ H=Heaviside function
Diffusion Equation	$\nabla^2\phi^* - \frac{1}{k}\frac{\partial\phi^*}{\partial t^2} + \delta_0\delta(t) = 0$	$\phi^* = \frac{-H(t)}{\sqrt{4\pi kt}}\exp\left(\frac{-r^2}{4kt}\right)$
Convection/decay Equation	$\frac{\partial\phi^*}{\partial t} + \bar{\phi}\frac{\partial\phi^*}{\partial x} + \beta\phi^* + \delta_0\delta(t) = 0$	$\phi^* = -e^{-\beta\frac{r}{\bar{\phi}}}\delta\left(t - \frac{r}{\bar{\phi}}\right)$

Boundary Integral Formulation

Fundamental Solutions : Two Dimensional Equations

	Equation	Fundamental Solution
Laplace	$\nabla^2\phi^* + \delta_0 = 0$	$\phi^* = \frac{1}{2\pi} ln\left(\frac{1}{r}\right), r = \sqrt{x_1^2 + x_2^2}$
Helmholtz	$\nabla^2\phi^* + \lambda^2\phi^* + \delta_0 = 0$	$\phi^* = \frac{1}{4i} H_0^{(2)}(\lambda r)$ H_0 = Hankel function
D'Arcy (orthotropic case)	$k_1 \frac{d^2\phi^*}{dx_1^2} + k_2 \frac{d^2\phi^*}{dx_2^2} + \delta_0 = 0$	$\phi^* = -\frac{1}{\sqrt{k_1 k_2}} \frac{1}{2\pi} ln\left[\left(\frac{x_1^2}{k_1} + \frac{x_2^2}{k_2}\right)^{\frac{1}{2}}\right]$
Wave Equation	$c^2\nabla^2\phi^* - \frac{\partial^2\phi^*}{\partial t^2} + \delta_0\delta(t) = 0$	$\phi^* = -\frac{H(ct - r)}{2\pi c\left(c^2t^2 - r^2\right)}$
Plate Equation	$\left(\frac{\partial^2}{\partial t^2} - \mu^2\nabla^4\right)\phi^* + \delta_0\delta(t) = 0$	$\phi^* = +\frac{H(t)}{4\pi\mu} S_i\left(\frac{r}{4\pi t}\right)$ S_i = Integral sine function
Navier's Equation	$\frac{\partial\sigma_{jk}^*}{\partial x_j} + \delta_l = 0$	$\phi_k^* = U_{lk}^* e_l$

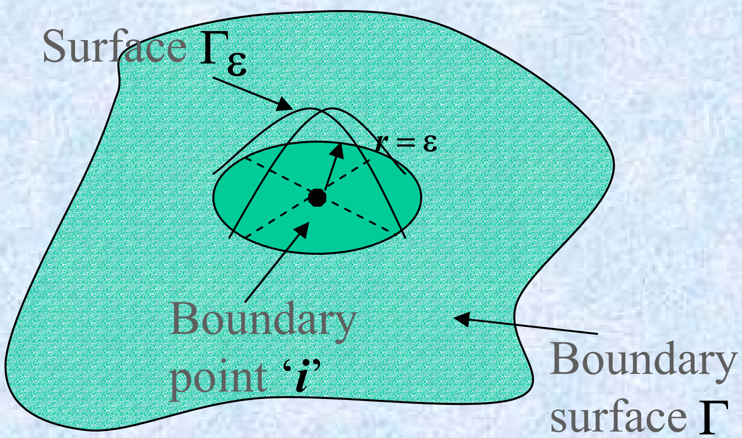
Boundary Integral Formulation

Fundamental Solutions : Three Dimensional Equations

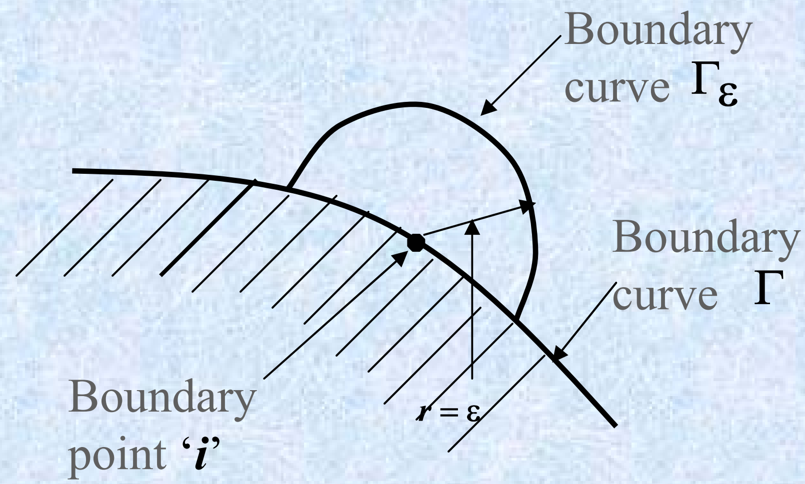
	Equation	Fundamental Solution
Laplace	$\nabla^2\phi^* + \delta_0 = 0$	$\phi^* = \frac{1}{4\pi r}, r = \sqrt{x_1^2 + x_2^2 + x_3^2}$
Helmholtz	$\nabla^2\phi^* + \lambda^2\phi^* + \delta_0 = 0$	$\phi^* = \frac{1}{4\pi r} e^{-i\lambda r}$
D'Arcy	$k_1 \frac{d^2\phi^*}{dx_1^2} + k_2 \frac{d^2\phi^*}{dx_2^2} + k_3 \frac{d^2\phi^*}{dx_3^2} + \delta_0 = 0$	$\phi^* = -\frac{1}{\sqrt{k_1 k_2 k_3}} \frac{1}{4\pi} \left(\frac{x_1^2}{k_1} + \frac{x_2^2}{k_2} + \frac{x_3^2}{k_3} \right)^{\frac{-1}{2}}$
Wave Equation	$c^2\nabla^2\phi^* - \frac{\partial^2\phi^*}{\partial t^2} + \delta_0\delta(t) = 0$	$\phi^* = \frac{\delta\left(t - \frac{r}{c}\right)}{4\pi r}$
Navier's Equation (Isotropic homogenous)	$\frac{\partial \sigma_{jk}^*}{\partial x_j} + \delta_l = 0$	$\phi_k^* = U_{lk}^* e_l$

Boundary Integral Formulation

What happens when point '*i*' is on Γ ?



3D case - Hemisphere around point '*i*'



2D case - Semicircle around point '*i*'

Augment the boundary with

- **Hemisphere of radius ε in 3D**
- **Semicircle of radius ε in 2D**

Boundary Integral Formulation

Consider equation (*3*) before any boundary conditions have been applied,

$$\phi^i + \int_\Gamma \phi \left(\frac{\partial \phi^*}{\partial n} \right) d\Gamma = \int_\Gamma \phi^* \left(\frac{\partial \phi}{\partial n} \right) d\Gamma$$

- **RHS integral** easy to deal (lower order singularity),

$$\lim_{\varepsilon \to 0} \left\{ \int_{\Gamma_\varepsilon} \frac{\partial \phi}{\partial n} \phi^* d\Gamma \right\} = \lim_{\varepsilon \to 0} \left\{ \int_{\Gamma_\varepsilon} \frac{\partial \phi}{\partial n} \frac{1}{4\pi\varepsilon} d\Gamma \right\} = \lim_{\varepsilon \to 0} \left\{ \frac{\partial \phi}{\partial n} \frac{2\pi\varepsilon^2}{4\pi\varepsilon} \right\} \equiv 0$$

- **LHS integral** behaves as,

$$\lim_{\varepsilon \to 0} \left\{ \int_{\Gamma_\varepsilon} \phi \frac{\partial \phi^*}{\partial n} d\Gamma \right\} = \lim_{\varepsilon \to 0} \left\{ - \int_{\Gamma_\varepsilon} \phi \frac{1}{4\pi\varepsilon^2} d\Gamma \right\} = \lim_{\varepsilon \to 0} \left\{ - \phi \frac{2\pi\varepsilon^2}{4\pi\varepsilon^2} \right\} = -\frac{1}{2} \phi^i$$

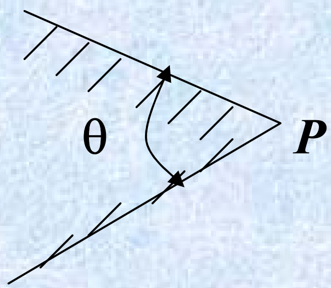
Boundary Integral Formulation

Therefore,

$$c\,\phi^{i} + \int_{\Gamma} \phi \left(\frac{\partial \phi^{*}}{\partial n} \right) d\Gamma = \int_{\Gamma} \phi^{*} \left(\frac{\partial \phi}{\partial n} \right) d\Gamma \qquad \cdots \; (4)$$

$$c = \frac{1}{2}, \quad \text{for smooth boundaries}$$

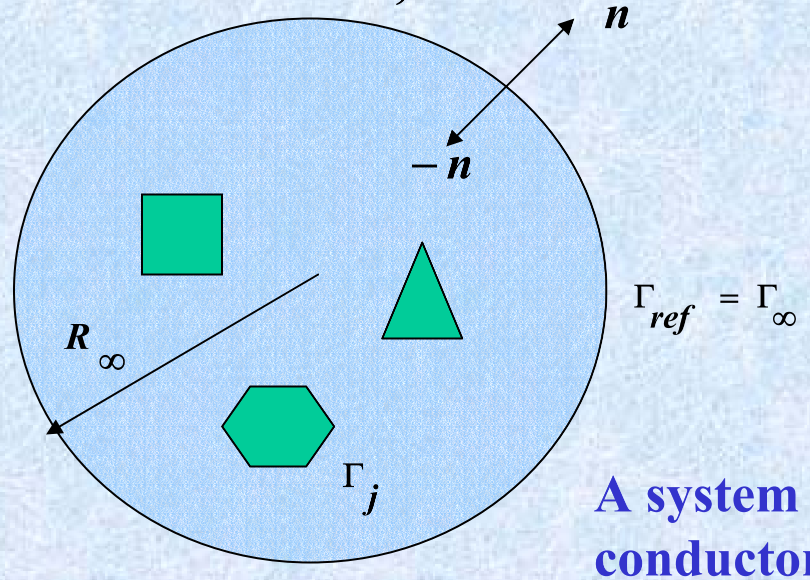
$$c = \frac{\theta}{2\pi} \quad \text{for corner points}$$



Boundary with corner point

Boundary Integral Formulation (contd.)

Exterior Problem - Electrostatics,



A system of 'N_c', ideal conductors

$\nabla^2\phi = 0$ outside

Potential ϕ known on the surface of each conductor

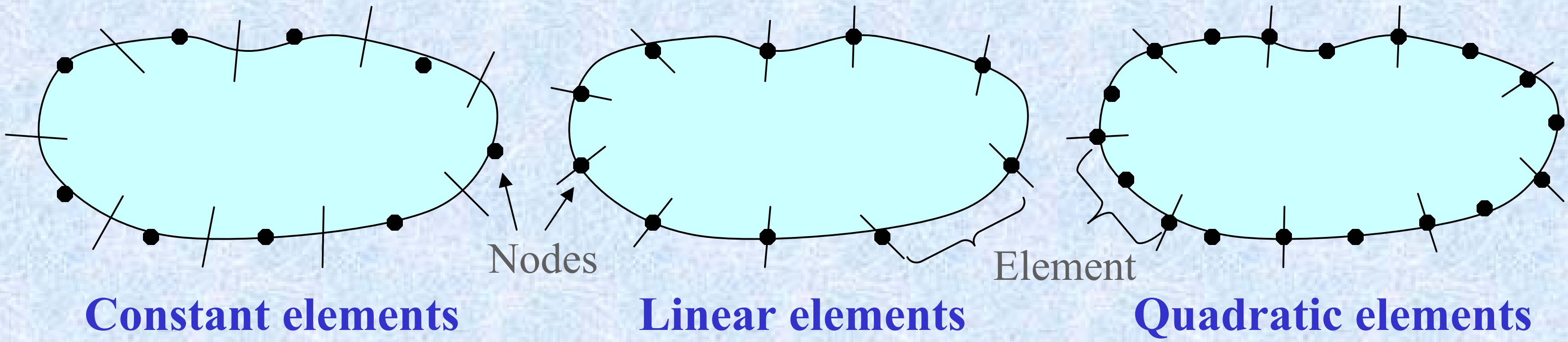
For 3D Electrostatic problem the boundary integral equation is,

$$\phi^i = \sum_{j=1}^{N_c} \int_{\Gamma_j} \frac{\partial \phi}{\partial n} \phi^* d\Gamma$$

Boundary Element Method

Equation (*4*) is discretized to find system of equations

Boundary is divided into *N* elements



Discretized form of equation (*3*) at point '*i*' is given as,

$$c\phi^{i} + \sum_{j=1}^{N} \int_{\Gamma_j} \phi \frac{\partial \phi^{*}}{\partial n} d\Gamma = \sum_{j=1}^{N} \int_{\Gamma_j} \frac{\partial \phi}{\partial n} \phi^{*} d\Gamma$$

Boundary Element Method

In matrix form,

$$[H]\{\Phi\} = [G]\left\{\frac{\partial \Phi}{\partial n}\right\}$$

where H^{ij} and G^{ij} are the influence coefficients given as,

'i' is the source point (where fundamental solution is acting)
'j' is the field point (any other nodes on the boundary)

Boundary Element Method

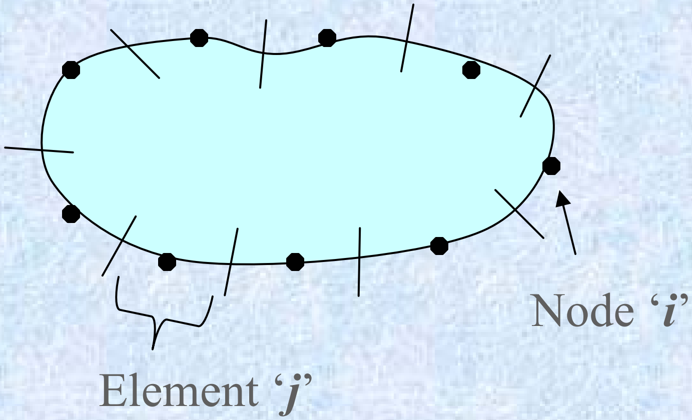
Constant Elements:

- ϕ and ϕ^* are assumed to be constant over each element
- The value of ϕ and ϕ^* is assumed equal to that at mid-element node

The influence coefficients, H^{ij} and G^{ij} are given as,

$$H^{ij} = \frac{1}{2}\delta(i,j) + \int_{\Gamma_j} \frac{\partial \phi^*}{\partial n} d\Gamma$$

$$G^{ij} = \int_{\Gamma_j} \phi^* d\Gamma$$

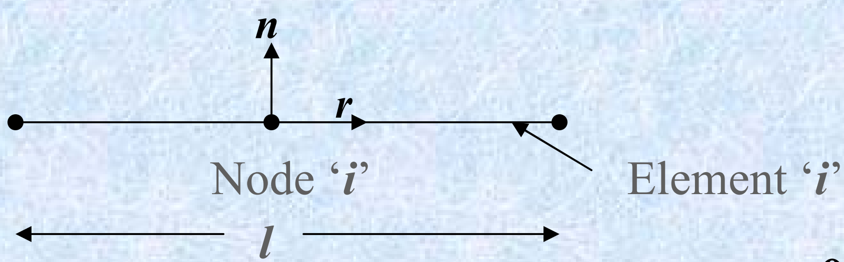


'i' is the source point (where fundamental solution is acting)
'j' is the field point (any other nodes on the boundary)

Boundary Element Method

Evaluation of integrals:

- H^{ij} and G^{ij} can be calculated numerically, for the case $i \neq j$
- For the case $i = j$, H^{ij} and G^{ij} are evaluated analytically



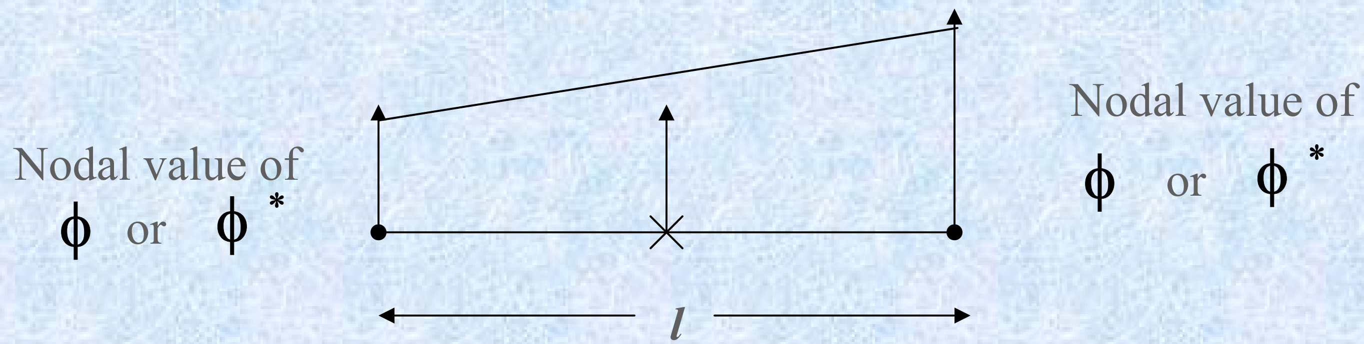
$$H^{ii} = \frac{1}{2} + \int_{\Gamma_j} \frac{\partial \phi^*}{\partial n} d\Gamma = \frac{1}{2} + \int_{\Gamma} \left(\frac{\partial \phi^*}{\partial r} \cancelto{0}{\frac{\partial r}{\partial n}} \right) d\Gamma = \frac{1}{2}$$

$$G^{ii} = \int_{\Gamma_i} \phi^* d\Gamma = \frac{1}{2\pi} \int_{\Gamma_i} ln\left(\frac{1}{r}\right) d\Gamma = \frac{1}{\pi}\left(\frac{l}{2}\right)\left[ln\left(\frac{1}{l/2}\right) + 1 \right]$$

Boundary Element Method

Linear Elements:

- ϕ and ϕ^* are assumed to vary linearly over each element

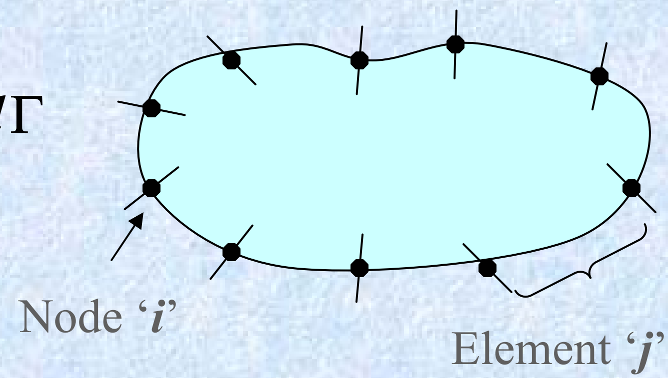


$$\phi = \begin{bmatrix} N_1 & N_2 \end{bmatrix} \begin{Bmatrix} \phi^1 \\ \phi^2 \end{Bmatrix} \qquad \frac{\partial \phi}{\partial n} = \begin{bmatrix} N_1 & N_2 \end{bmatrix} \begin{Bmatrix} \partial \phi^1 / \partial n \\ \partial \phi^2 / \partial n \end{Bmatrix}$$

Therefore,

$$H^{ij} = \frac{1}{2}\delta(i,j) + \int_{\Gamma_j} \begin{bmatrix} N_1 & N_2 \end{bmatrix} \frac{\partial \phi^*}{\partial n} d\Gamma$$

$$G^{ij} = \int_{\Gamma_j} \begin{bmatrix} N_1 & N_2 \end{bmatrix} \phi^* d\Gamma$$

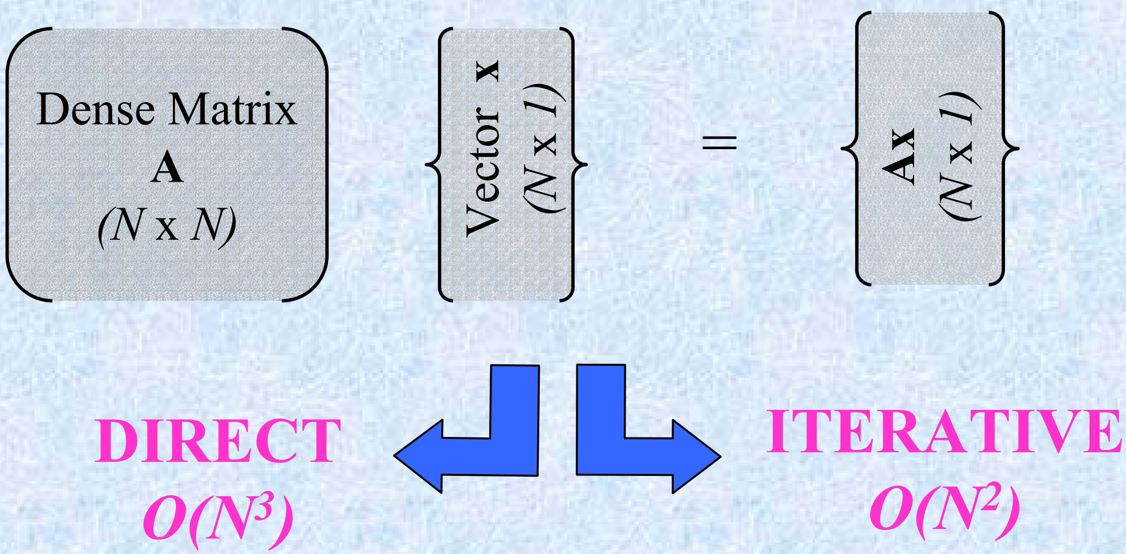


Boundary Element Method

Putting all the unknowns on LHS we get,

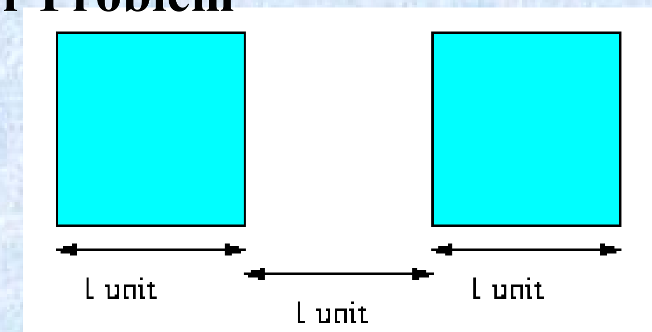
$$[A]\{x\} = \{F\}$$

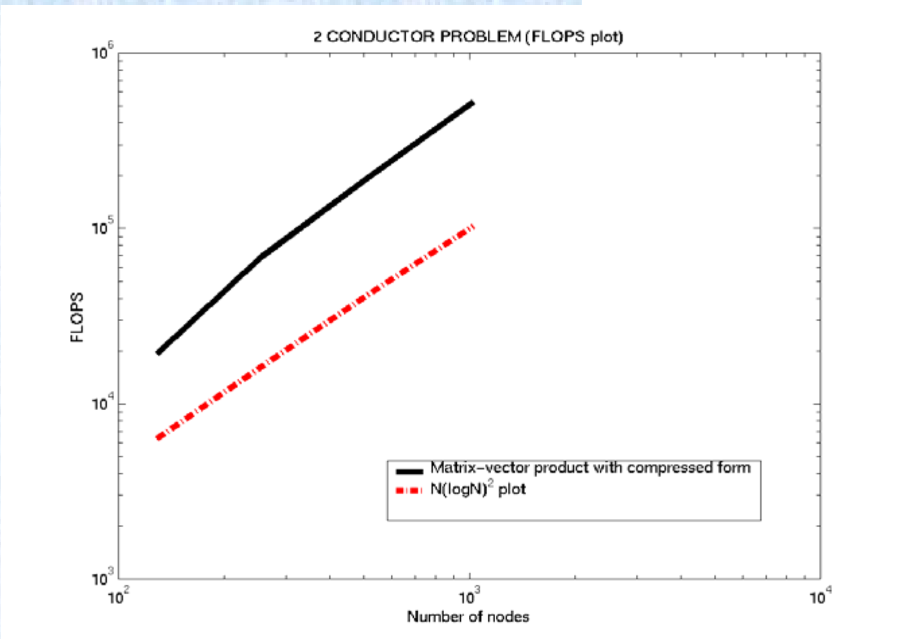
Note: *A* is a dense matrix

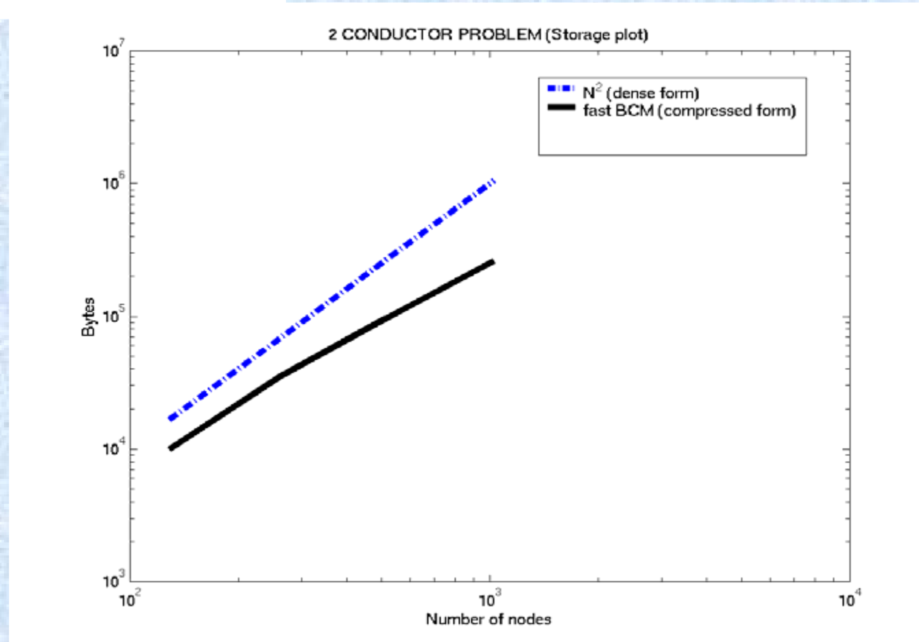


Fast Integral Equation Solver

Results : 2-Conductor Problem





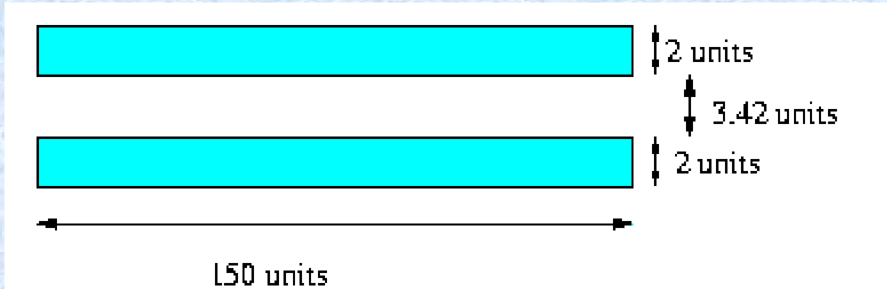


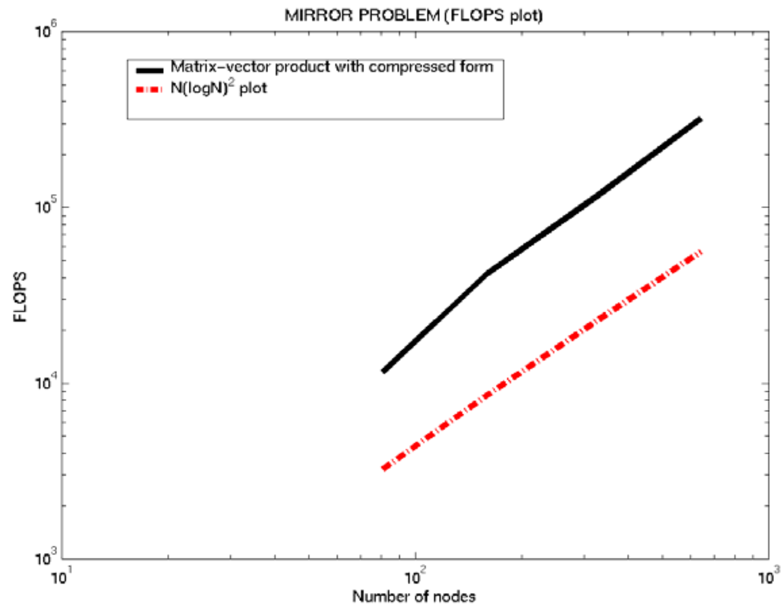
Matrix-Vector multiplication: ***$O(N(\log N)^2)$***

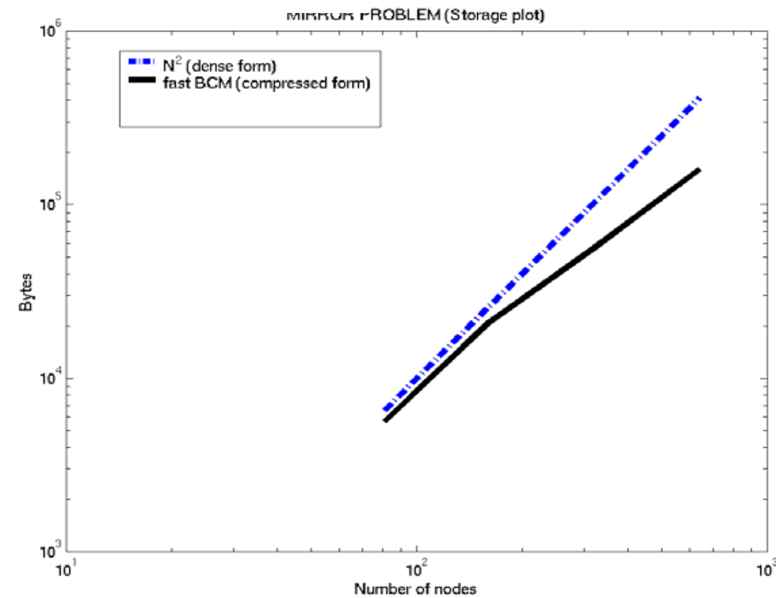
Storage: ***$O(N(\log N)^2)$***

Fast Integral Equation Solver

Results : Mirror Problem





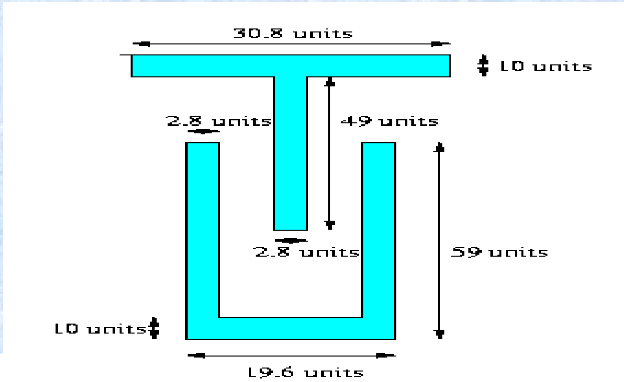


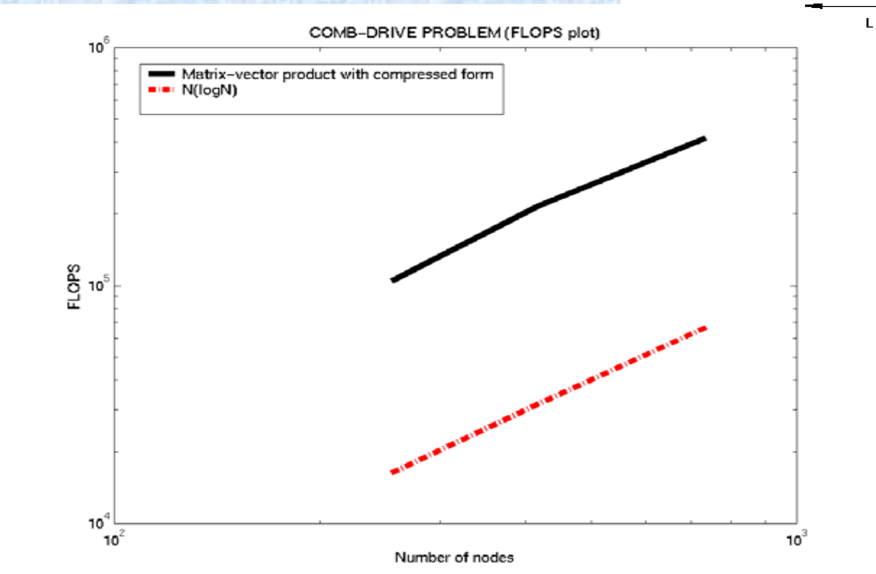
Matrix-Vector multiplication: ***$O(N(\log N)^2)$***

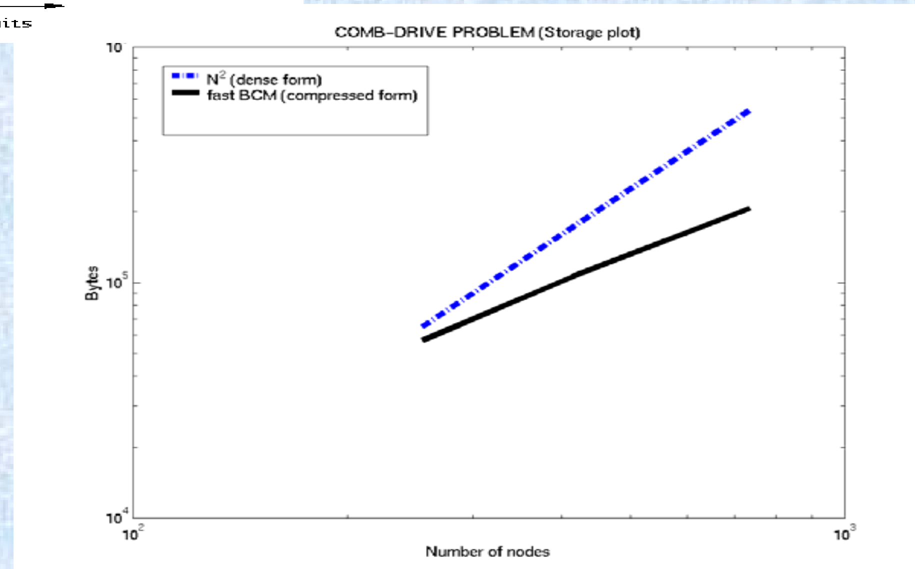
Storage: ***$O(N(\log N)^2)$***

Fast Integral Equation Solver

Results : Comb-Drive Problem







Matrix-Vector multiplication: ***O(NlogN)***
Storage: ***O(NlogN)***

References

- **P.K. Banerjee, *The Boundary Element Method in Engineering*, Mc-Graw Hill, 1994**
- **G. Beer, *Programming the Boundary Element Method*, Wiley, 2001**
- **C.A. Brebbia and J. Dominguez *Boundary Elements An Introductory Course*, Mc-Graw Hill, 1996**
- **J.H. Kane, *Boundary Element Analysis in Engineering Continuum Mechanics*, Prentice Hall, 1994**

Outline

- ✔ Some MEMS Examples
- ➨ Mixed-Domain Simulation of electrostatic MEMS and microfluidics
  - ✔ Techniques for interior problems (e.g. FEM)
  - ✔ Techniques for exterior problems (e.g. BEM)
  - ☞ Algorithms

Coupled Electromechanical Analysis

- We need to self-consistently solve the coupled electrical and mechanical equations to compute the equilibrium displacements and forces. Three approaches –
  - Relaxation technique
  - Full-Newton method
  - Multi-level Newton method
- Solution of elastostatic equations is represented by

$$u = R_M(P(q))$$

- Solution of electrostatic equations is represented by

$$q = R_E(u, V)$$

Relaxation Technique

- Simplest black-box approach
- Data is passed back and forth between black-box electrostatic and elastostatic analysis programs until a converged solution is obtained

$$\boldsymbol{k} = \mathbf{1}; \boldsymbol{u}^k = \mathbf{0}$$

Repeat

Compute $\boldsymbol{q}^k = \boldsymbol{R}_E(\boldsymbol{u}^k)$

Compute $\boldsymbol{u}^{(k+1)} = \boldsymbol{R}_M(\boldsymbol{P}(\boldsymbol{q}^k))$

$$\boldsymbol{k} = \boldsymbol{k} + \mathbf{1}$$

Until $\left\| \boldsymbol{u}^k - \boldsymbol{u}^{k+1} \right\| \le \varepsilon \qquad \left\| \boldsymbol{q}^k - \boldsymbol{q}^{k+1} \right\| \le \varepsilon$

Relaxation Technique

- Advantages
  - Very quick implementation based on black-boxes
  - Existing mechanical and electrical solvers can be used

- Disadvantages
  - Fails to converge for strong coupling between electrical and mechanical domains

Multi-Level Newton Algorithm

- Matrix-free approaches: Matrix-vector product involving a Jacobian and a vector can be computed as

$$\frac{\partial R}{\partial u}\Delta u = \frac{R(u+\varepsilon\Delta u)-R(u)}{\varepsilon}$$

- Define a new residual

$$R(u,q) = \begin{Bmatrix} q - R_E(u) \\ u - R_M(q) \end{Bmatrix}$$

- The Jacobian of the residual is given by

$$J(u,q) = \begin{bmatrix} \frac{\partial R_1}{\partial q} & \frac{\partial R_1}{\partial u} \\ \frac{\partial R_2}{\partial q} & \frac{\partial R_2}{\partial u} \end{bmatrix} = \begin{bmatrix} I & -\frac{\partial R_E}{\partial u} \\ -\frac{\partial R_M}{\partial q} & I \end{bmatrix}$$

Multi-Level Newton Algorithm

$$k = 1; u^k = 0; q^k = 0$$

use an iterative solver

Repeat

solve $\boxed{J(u^k, q^k)\begin{Bmatrix}\delta q \\ \delta u\end{Bmatrix} = -R(u^k, q^k)}$

set $u^{k+1} = u^k + \delta u$

set $q^{k+1} = q^k + \delta q$

$k = k + 1$

until $\left\| u^k - u^{k+1} \right\| \le \varepsilon \qquad \left\| q^k - q^{k+1} \right\| \le \varepsilon$

Iterative Solution of Linear Systems

- Lets say we need to solve $Pq = \bar{p}$
- Key steps in GMRES algorithm

make an initial guess to the solution, q_0
set k = 0
do {
compute the residual, $r^k = \bar{p} - Pq^k$
if $\|r^k\| \le tol,$ return q^k as the solution
else {
choose $\alpha's$ and β in

$$q^{k+1} = \sum_{j=0}^{k} \alpha_j q^j + \beta r^k$$

to minimize $\|r^{k+1}\|$
set $k = k + 1$
}
}

Multi-Level Newton Algorithm

$$\frac{\partial R}{\partial u} * r = \frac{R(u + \theta * r) - R(u)}{\theta}$$

$$\theta = sign(u * r) * a \frac{\|u\|}{\|r\|}$$

$$a \in (0.01, 0.5)$$

$$J(u,q)\begin{Bmatrix} \delta q \\ \delta u \end{Bmatrix} = \begin{bmatrix} I & -\frac{\partial R_E}{\partial u} \\ -\frac{\partial R_M}{\partial q} & I \end{bmatrix} \begin{Bmatrix} \delta q \\ \delta u \end{Bmatrix} = \begin{Bmatrix} \delta q - \frac{1}{\theta}\left[R_E(u + \theta \delta u) - R_E(u)\right] \\ \delta u - \frac{1}{\theta}\left[R_M(q + \theta \delta q) - R_M(q)\right] \end{Bmatrix}$$

Multi-Level Newton Algorithm

- Advantages
  - Black box based approach
  - Superior global convergence

- Disadvantages
  - Can be sensitive to the choice of the matrix-free parameter

Full-Newton Technique

- Represent the mechanical and electrical equations as

$$R_M(u,q) = f^{\text{int}}(u) - f^{ext}(q) = 0$$

$$R_E(u,q) = P(u)q - V = 0$$

- Let $\bar{u}$ and $\bar{q}$ be self-consistent solutions

$$R_M(\bar{u},\bar{q}) = 0$$

$$R_E(\bar{u},\bar{q}) = 0$$

- Let u_0 and q_0 be some initial guess

$$R_M(\bar{u},\bar{q}) = R_M(u_0,q_0) + \frac{\partial R_M}{\partial u}\Delta u + \frac{\partial R_M}{\partial q}\Delta q + h.o.t = 0$$

$$R_E(\bar{u},\bar{q}) = R_E(u_0,q_0) + \frac{\partial R_E}{\partial u}\Delta u + \frac{\partial R_E}{\partial q}\Delta q + h.o.t = 0$$

Full-Newton Technique

- **Neglecting h.o.t**

$$\frac{\partial R_M}{\partial u}\Delta u+\frac{\partial R_M}{\partial q}\Delta q=-R_M(u_0,q_0)$$

$$\frac{\partial R_E}{\partial u}\Delta u+\frac{\partial R_E}{\partial q}\Delta q=-R_E(u_0,q_0)$$

- **In matrix form**

$$\begin{bmatrix}\frac{\partial R_M}{\partial u} & \frac{\partial R_M}{\partial q}\\ \frac{\partial R_E}{\partial u} & \frac{\partial R_E}{\partial q}\end{bmatrix}\begin{Bmatrix}\Delta u\\ \Delta q\end{Bmatrix}=-\begin{Bmatrix}R_M(u_0,q_0)\\ R_E(u_0,q_0)\end{Bmatrix}$$

Full Newton Algorithm

$$i = 0; u^{(i)} = 0; q^{(i)} = 0$$

Repeat

solve $$\begin{bmatrix} \dfrac{\partial R_M}{\partial u} & \dfrac{\partial R_M}{\partial q} \\ \dfrac{\partial R_E}{\partial u} & \dfrac{\partial R_E}{\partial q} \end{bmatrix} \begin{Bmatrix} \Delta u^{(i)} \\ \Delta q^{(i)} \end{Bmatrix} = -\begin{Bmatrix} R_M(u^{(i-1)}, q^{(i-1)}) \\ R_E(u^{(i-1)}, q^{(i-1)}) \end{Bmatrix}$$

set $u^{(i)} = u^{(i-1)} + \Delta u^{(i)}$

set $q^{(i)} = q^{(i-1)} + \Delta q^{(i)}$

$$i = i + 1$$

until $\left|\Delta u^{(i)}\right| \le \varepsilon$ $\left|\Delta q^{(i)}\right| \le \varepsilon$

Full Newton Algorithm

$$\frac{\partial \boldsymbol{R}_M}{\partial \boldsymbol{u}} \rightarrow \frac{\partial \boldsymbol{f}^{\text{int}}(\boldsymbol{u})}{\partial \boldsymbol{u}} \rightarrow$$ entirely elastostatic part

$$\frac{\partial \boldsymbol{R}_E}{\partial \boldsymbol{q}} \rightarrow \frac{\partial (\boldsymbol{P}\boldsymbol{q} - \boldsymbol{V})}{\partial \boldsymbol{q}} = \boldsymbol{P} \rightarrow$$ entirely electrostatic part

$$\frac{\partial \boldsymbol{R}_M}{\partial \boldsymbol{q}} \rightarrow \frac{\partial \boldsymbol{f}^{ext}(\boldsymbol{q})}{\partial \boldsymbol{q}} \rightarrow$$ electrical to mechanical coupling term

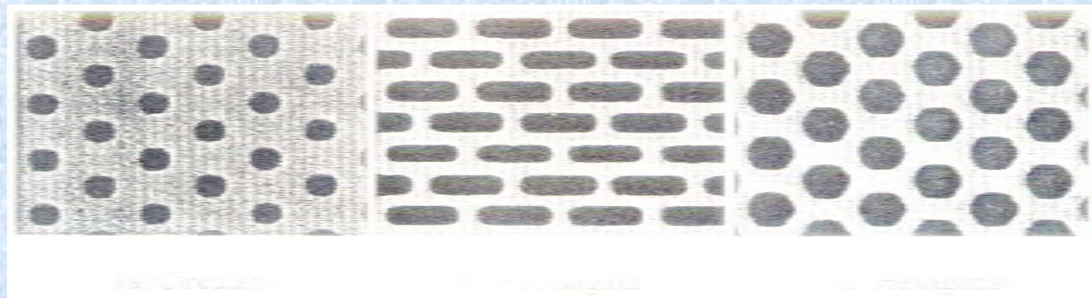
$$\frac{\partial \boldsymbol{R}_E}{\partial \boldsymbol{u}} \rightarrow \frac{\partial (\boldsymbol{P}\boldsymbol{q} - \boldsymbol{V})}{\partial \boldsymbol{u}} = \frac{\partial \boldsymbol{P}(\boldsymbol{u})}{\partial \boldsymbol{u}} \boldsymbol{q} \rightarrow$$ mechanical to electrical coupling term

Microfluidics: Gas Flows

Introduction to Microfilters

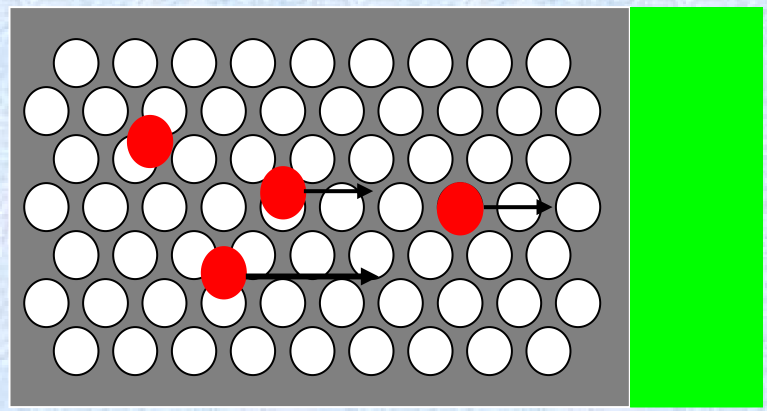
Microfilter properties:

- Openings of various shapes
- Thickness between 1 and 5μm
- Opening size as small as 2nm
- High burst pressure achieved



Design issues:

- Flow profiles
- Estimation of flow rate
- Dependence of flow rate on:
  - geometry
  - surface properties
  - pressure difference



Rarefaction effects observed due to small dimensions

Characteristics of Flows in Micro-Channels

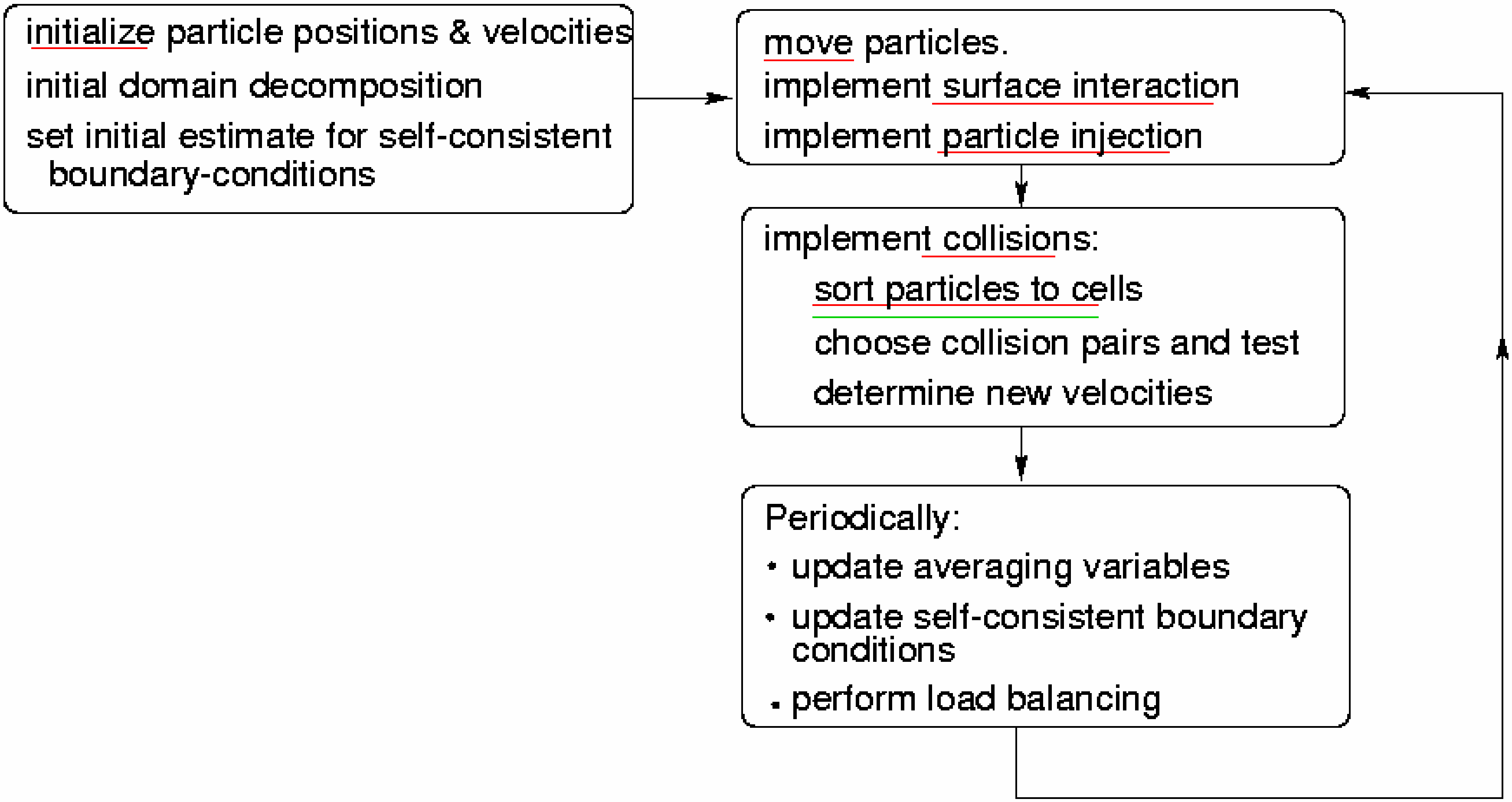
Typical Characteristics:

- Compressible
- High Kn #
- Small Re #
- Small Ma #
- Wide range of Kn #
- Reacting

Effects of high Knudsen Number:

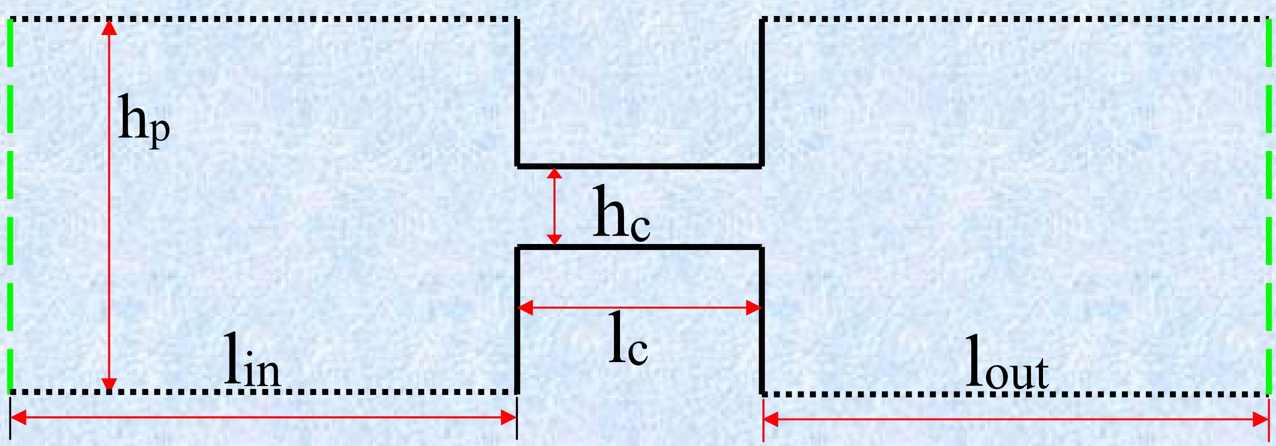
- Slip velocity
- Thermal jump
- Strong interaction with walls

DSMC Flow Chart

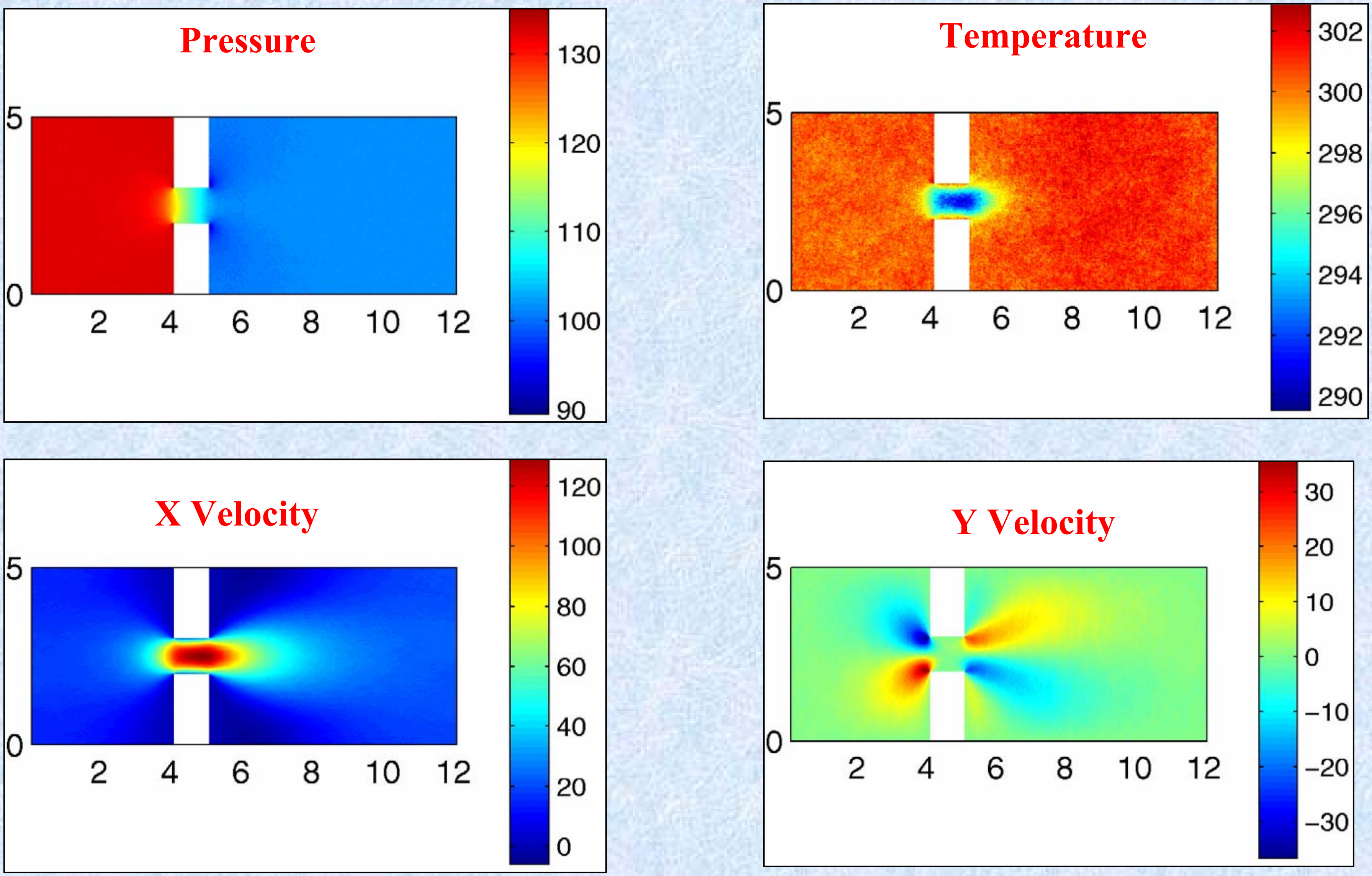


Micro-Filter Elements

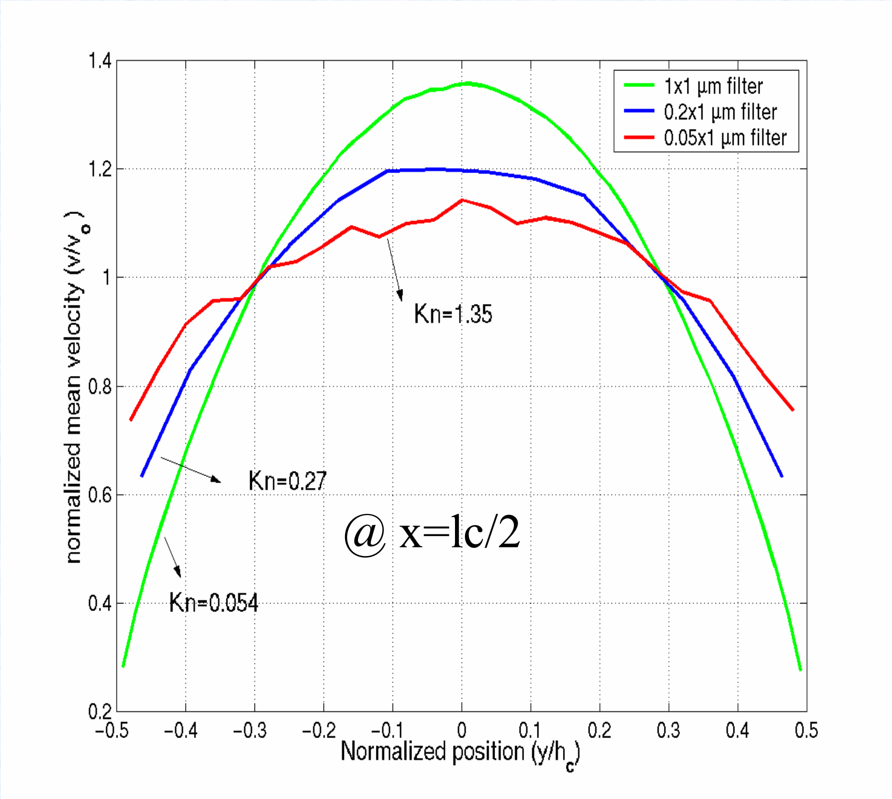
	1x1	1x5	0.2x1	1x10	0.05x1	0.2x2
h_c (μm)	1	1	0.2	1	0.05	0.2
l_c (μm)	1	5	1	10	1	2
h_p (μm)	5	5	1	5	1	1
l_{in} (μm)	4	6	4	4	4	4
l_{out} (μm)	7	7	5	7	7	5
Kn	0.054	0.054	0.27	0.054	1.1	0.27

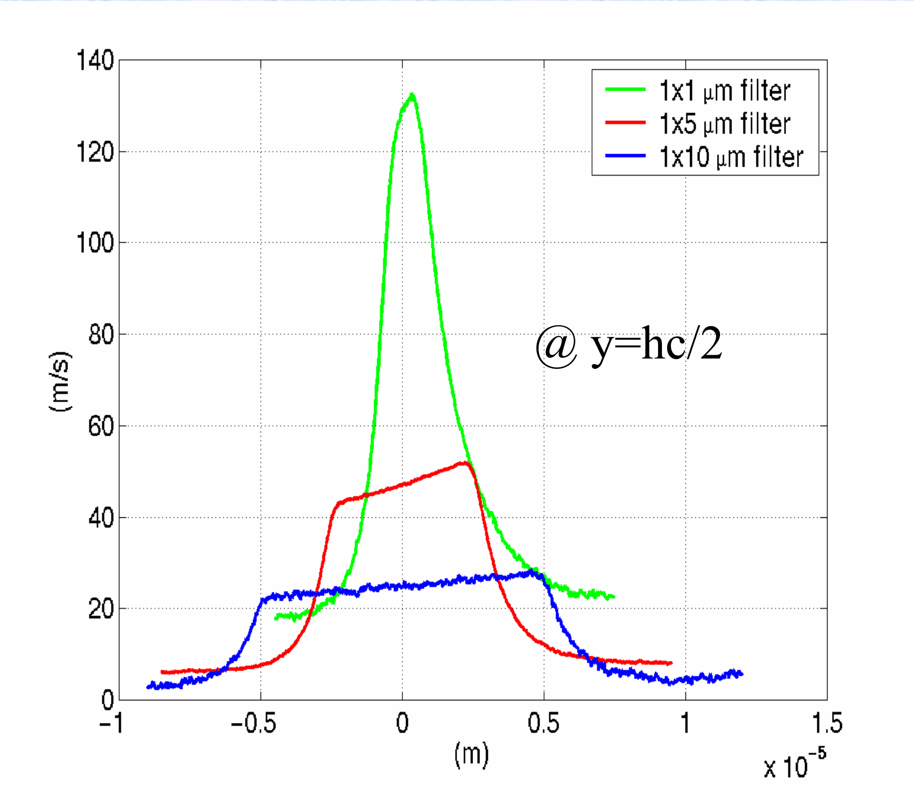


1μmX1μm Filter Element



Knudsen Number and Length Effects





Effect of Kn:

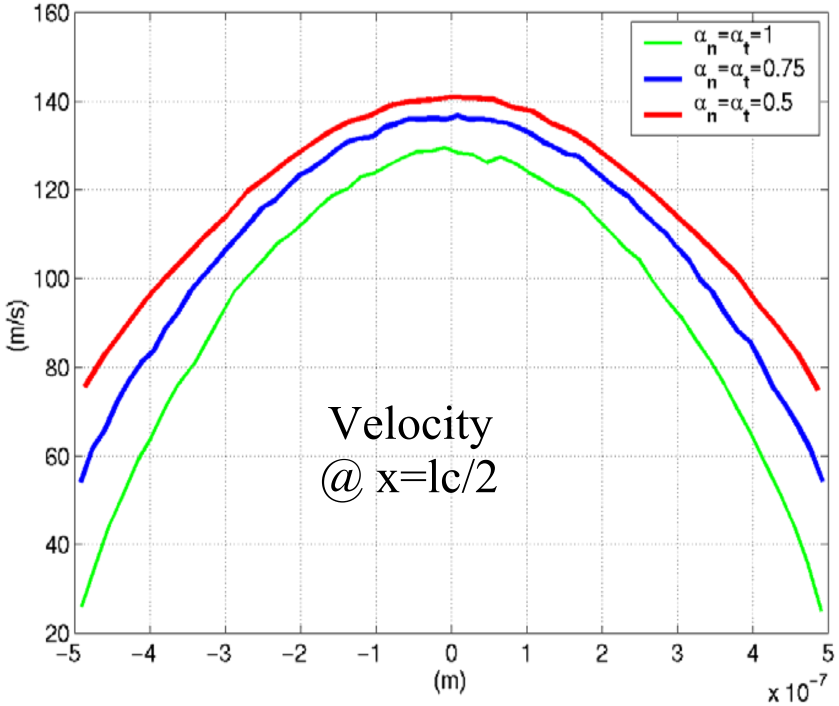
- Slip velocity increases with Kn

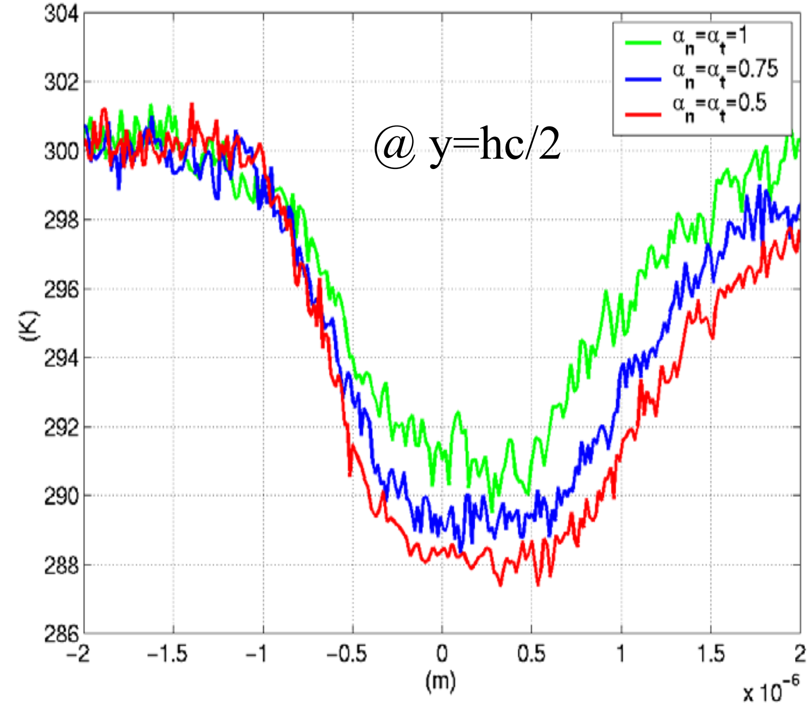
Effect of Length:

- As lc/hc increases, 2D channel approximation holds good for smaller Kn

Effect of Surface Accommodation

1x1 μm filter

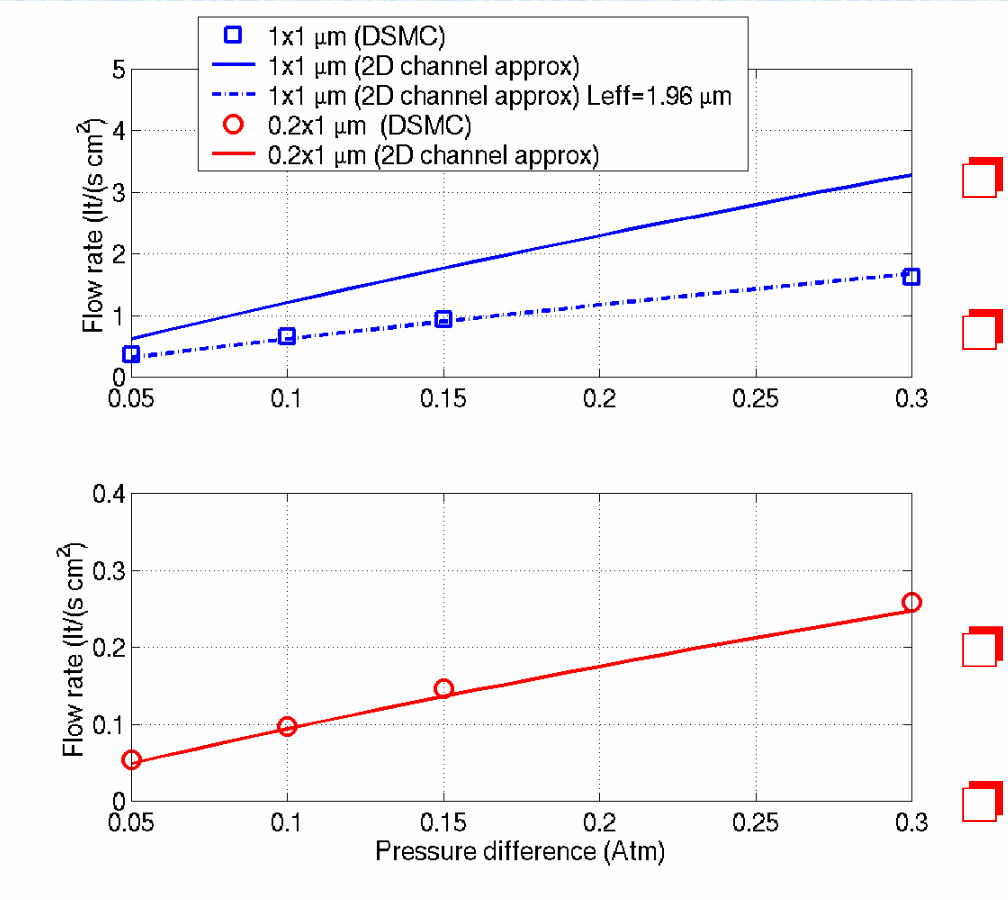




Smaller accomodation coefficients:

- **Strong increase in slip velocity**
- **Temperature drop increases**

Flow Rate vs. Pressure Difference



- Dependence of flow rate on pressure is linear
- Qualitative behavior is captured by 2D channel formula + 1st order slip BC (Arkilic & Breuer, 1997)
- Good agreement for large lc/hc
- Effective length can be used for smaller lc/hc

Conclusions

- MEMS design is still an art
- Critical issues
  - Mixed-domain simulation tools
  - Multiscale approaches
  - System level modeling tools
- Need fast and radically simpler techniques for MEMS modeling