Introduction to Simulation - Lecture 22

Integral Equation Methods

Jacob White

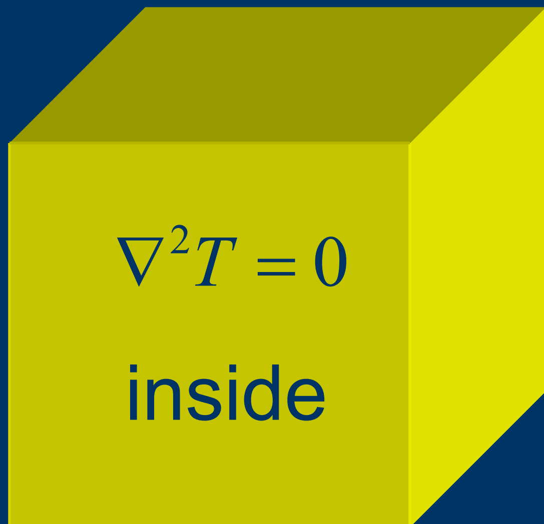
Thanks to Deepak Ramaswamy, Michal Rewienski, Xin Wang and Karen Veroy

Outline

- Integral Equation Methods
  - Exterior versus interior problems
  - Start with using point sources
- Standard Solution Methods in 2-D
  - Galerkin Method
  - Collocation Method
- Issues in 3-D
  - Panel Integration

Interior Versus Exterior Problems

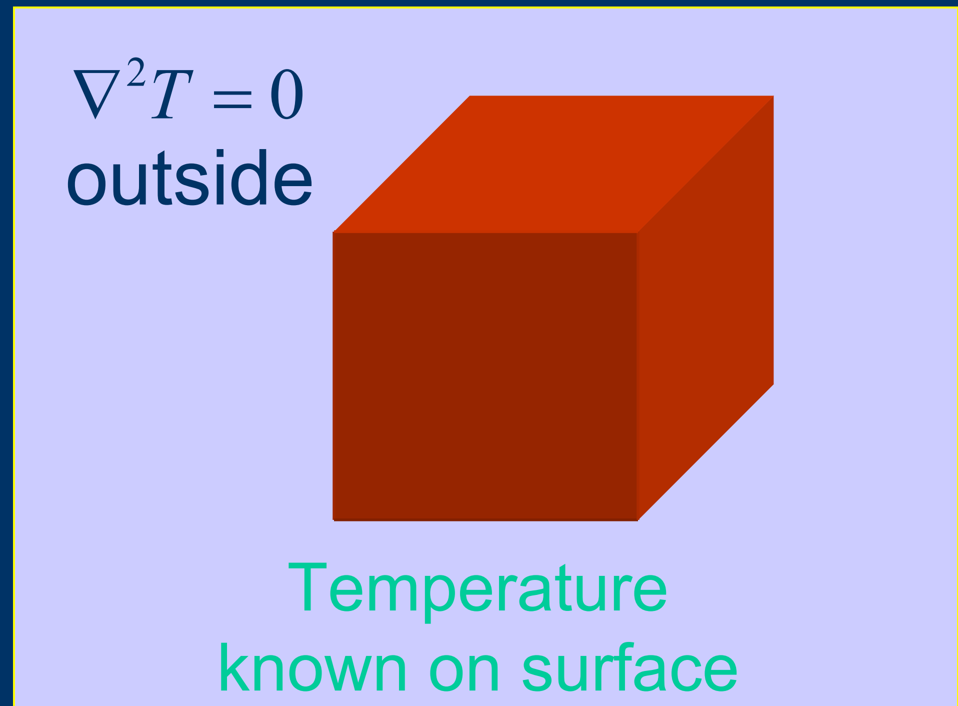
Interior



Temperature known on surface

"Temperature in a Tank"

Exterior

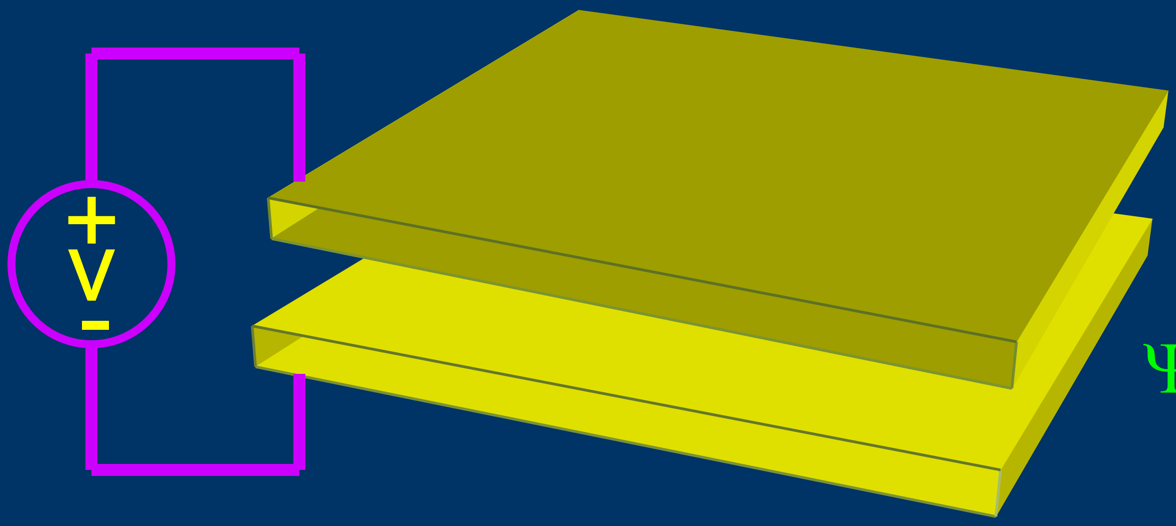


"Ice Cube in a Bath"

What is the heat flow?

$$\text{Heat Flow} = \text{Thermal conductivity} \int_{surface} \frac{\partial T}{\partial n}$$

Exterior Problem in Electrostatics



potential

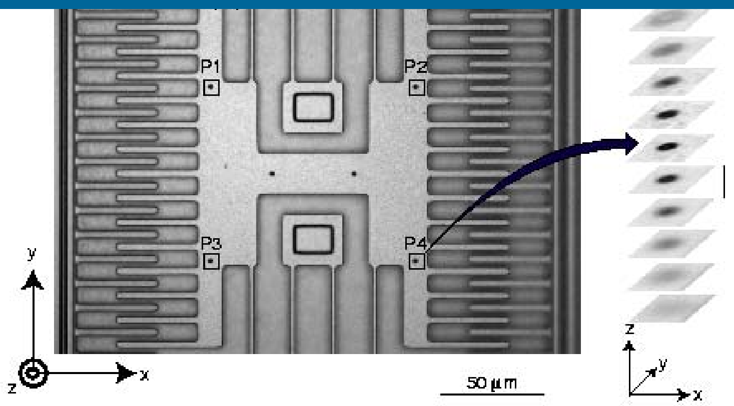
$$\nabla^2 \Psi = 0 \quad \text{Outside}$$

Ψ is given on Surface

<u>What is the capacitance?</u>

$$\text{Capacitance} = \text{Dielectric Permitivity} \int_{surface} \frac{\partial \Psi}{\partial n}$$

Drag Force in a Microresonator



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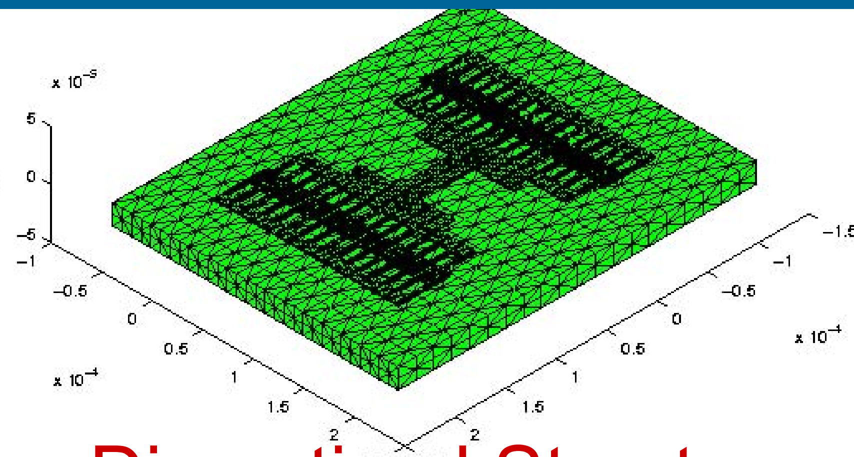
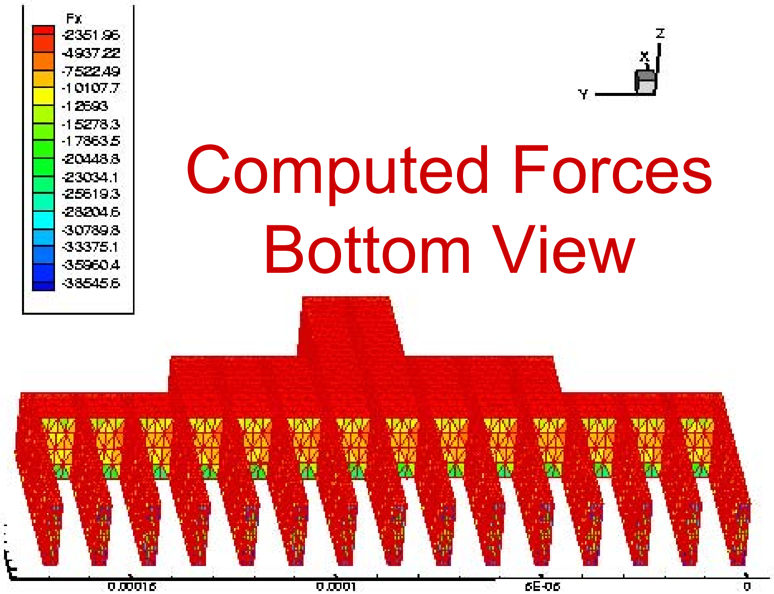
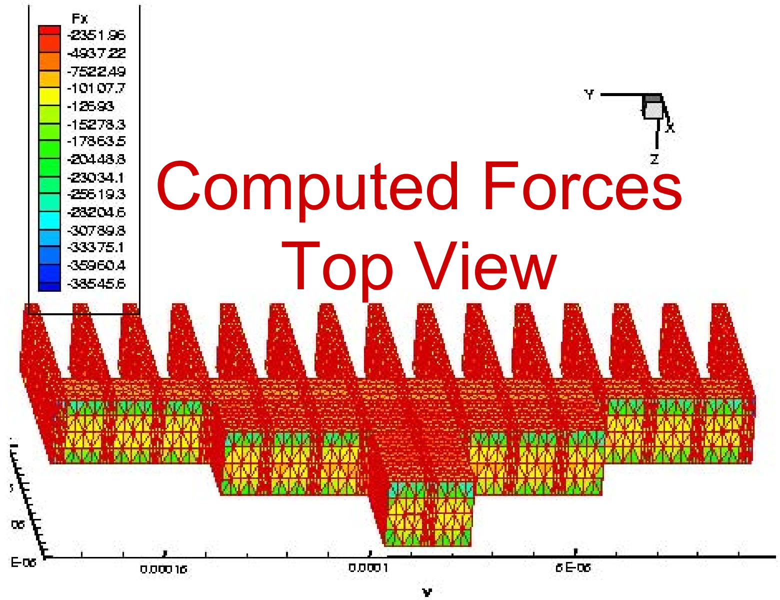
Resonator



Discretized Structure



Computed Forces Bottom View



Computed Forces Top View

What is common about these problems.

Exterior Problems

- Drag Force in MEMS device - fluid (air) creates drag.
- Coupling in a Package - Fields in exterior create coupling
- Capacitance of a Signal Line - Fields in exterior.

Quantities of Interest are on the surface

- MEMS device - Just want surface traction force
- Package - Just want coupling between conductors
- Signal Line - Just want surface charge.

Exterior Problem is linear and space-invariant

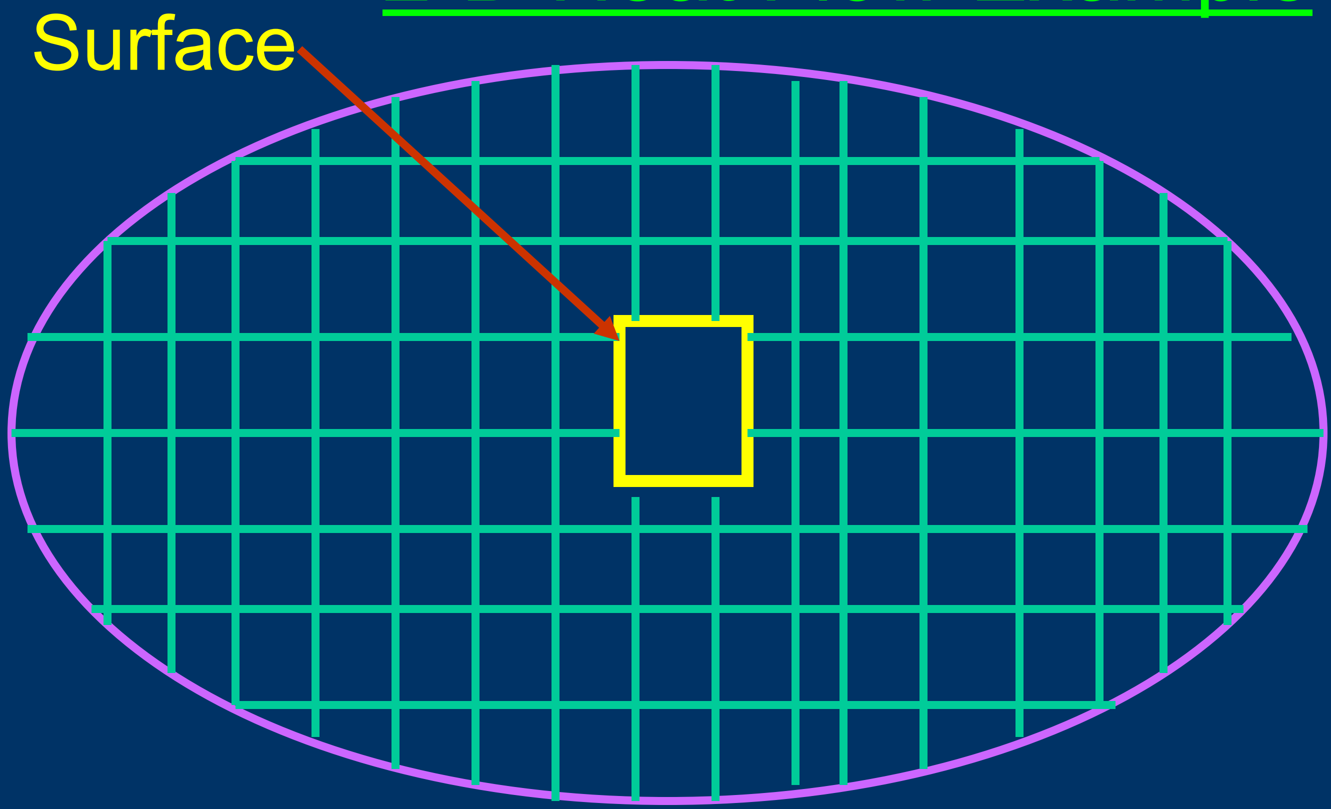
- MEMS - Exterior Stokes Flow equation (linear).
- Package - Maxwell's equations in free space (linear).
- Signal Line - Laplace's equation in free space (linear).

But problems are geometrically very complex!

Exterior Problems

Why not use Finite-Difference or FEM methods

2-D Heat Flow Example



$T = 0 \text{ at } \infty$

But, must truncate the mesh

Only need $\frac{\partial T}{\partial n}$ on the surface, but T is computed everywhere

Must truncate the mesh, $\Rightarrow T(\infty) = 0$ becomes $T(R) = 0$

Laplace's Equation

In 2-D

$$\text{If } u = \log\left(\sqrt{(x - x_0)^2 + (y - y_0)^2}\right)$$

$$\text{then } \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{for all } (x, y) \neq (x_0, y_0)$$

In 3-D

$$\text{If } u = \frac{1}{\sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2}}$$

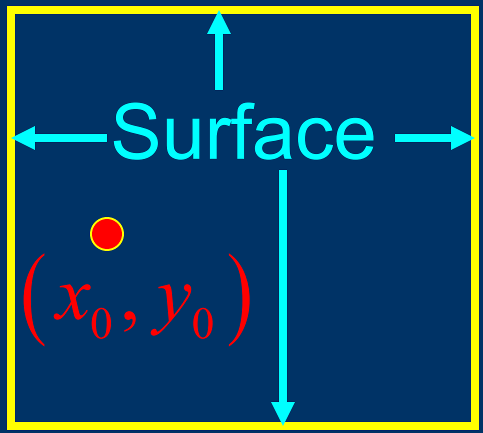
$$\text{then } \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0 \quad \text{for all } (x, y, z) \neq (x_0, y_0, z_0)$$

Proof: Just differentiate and see!

Laplace's Equation in 2-D

Simple Idea

u is given on surface



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{outside}$$

Let $u = \log\left(\sqrt{(x - x_0)^2 + (y - y_0)^2}\right)$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{outside}$$

~~Problem Solved~~

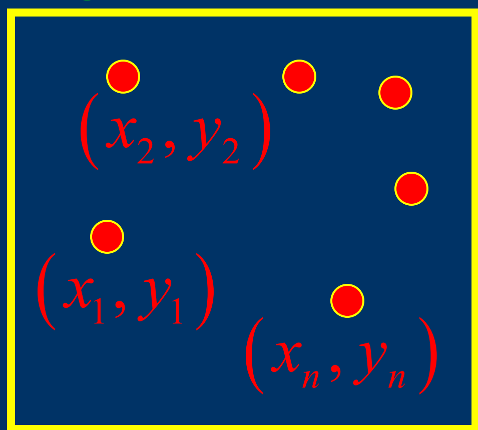
Does not match boundary conditions!

Laplace's Equation in 2-D

Simple Idea

"More Points"

u is given on surface



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{outside}$$

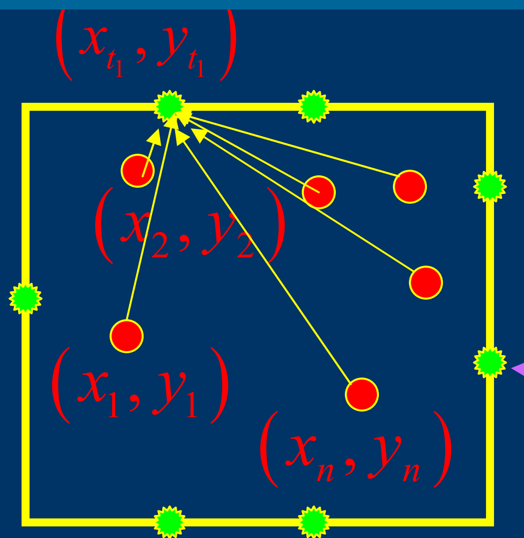
$$\text{Let } u = \sum_{i=1}^{n} \omega_i \log\left(\sqrt{(x - x_i)^2 + (y - y_i)^2}\right) = \sum_{i=1}^{n} \omega_i G(x - x_i, y - y_i)$$

Pick the ω_i's to match the boundary conditions!

Laplace's Equation in 2-D

Simple Idea

"More Points Equations"

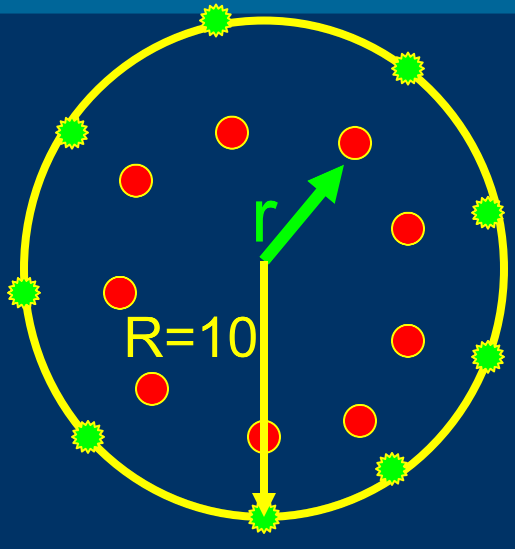


Source Strengths selected to give correct potential at test points.

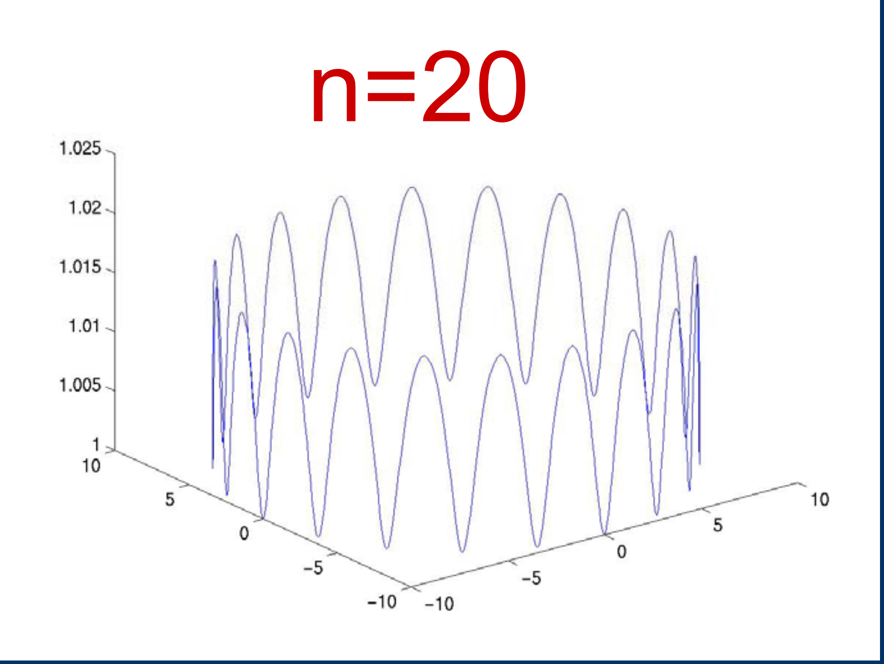
$$
\begin{bmatrix}
G\left(x_{t_1}-x_1, y_{t_1}-y_1\right) & \cdots & \cdots & G\left(x_{t_1}-x_n, y_{t_1}-y_n\right) \\
\vdots & \ddots & & \vdots \\
\vdots & & \ddots & \vdots \\
G\left(x_{t_n}-x_1, y_{t_n}-y_1\right) & \cdots & \cdots & G\left(x_{t_n}-x_n, y_{t_n}-y_n\right)
\end{bmatrix}
\begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix}
=
\begin{bmatrix} \Psi\left(x_{t_1}, y_{t_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{t_n}, y_{t_n}\right) \end{bmatrix}
$$

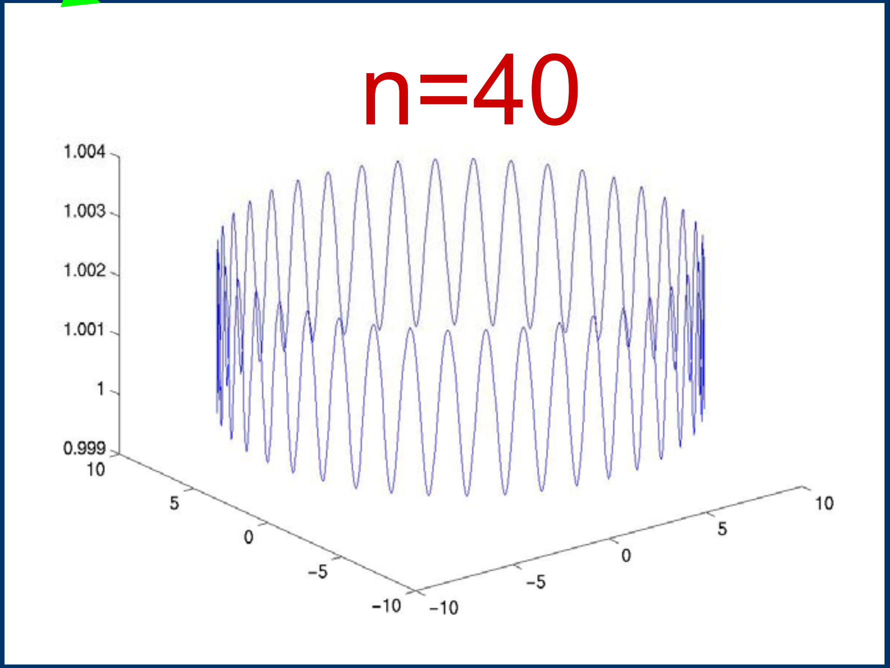
Computational results using points approach

Circle with Charges r=9.5

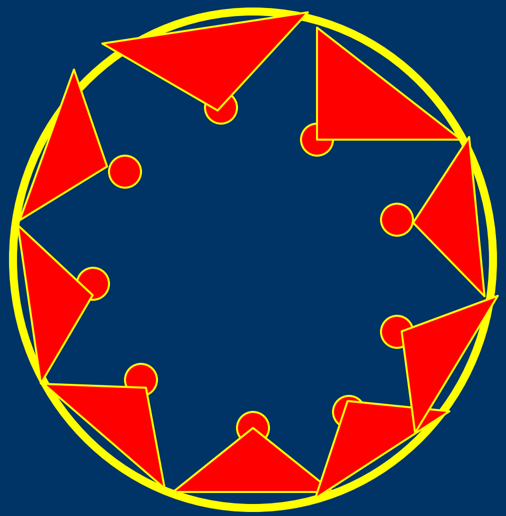


Potentials on the Circle





Want to smear point charges onto surface



Results in an Integral Equation

$$\Psi(x) = \int_{surface} G(x, x')\sigma(x')dS'$$

How do we solve the integral equation?

Basis Function Approach

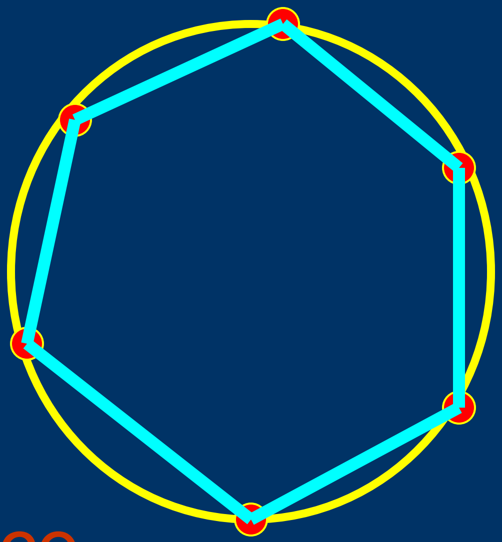
Basic Idea

Represent $\sigma(x) = \sum_{i=1}^{n} \omega_i \underbrace{\varphi_i(x)}_{\text{Basis Functions}}$

Example Basis

Represent circle with straight lines

Assume σ is constant along each line



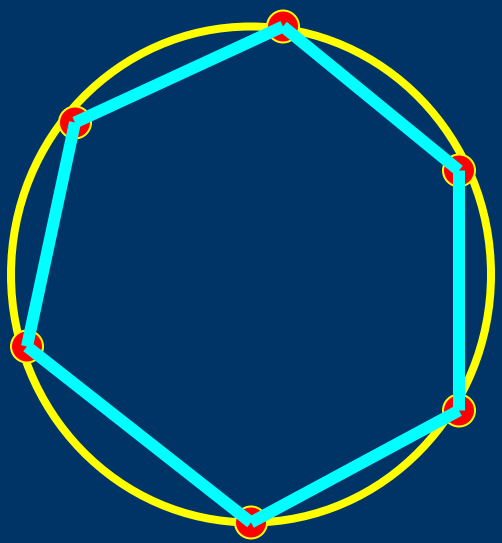
The basis functions are "on" the surface

Can be used to approximate the density

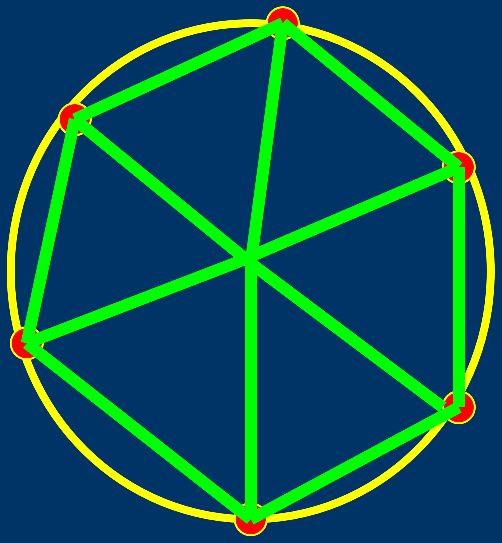
May also approximate the geometry

Laplace's Equation in 2-D

Geometric Approximation is not new.



Piecewise Straight surface basis Functions approximate the circle



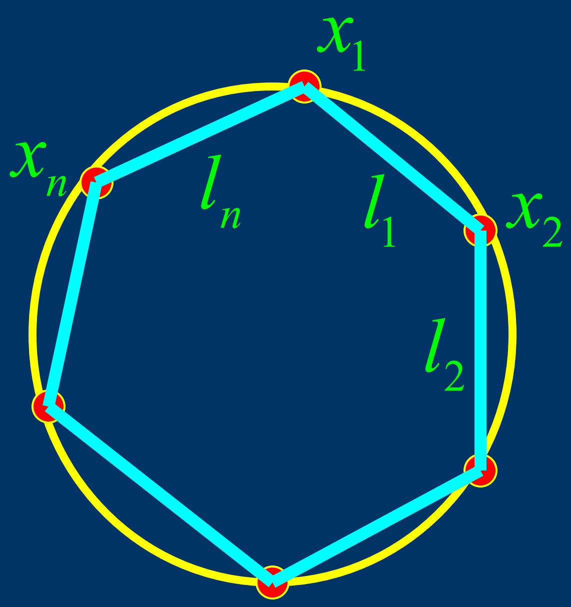
Triangles for 2-D FEM approximate the circle too!

$$\Psi(x) = \int_{\substack{approx\\surface}} G(x, x') \sum_{i=1}^{n} \omega_i \varphi_i(x') dS'$$

Laplace's Equation in 2-D

Basis Function Approach

Piecewise Constant Straight Sections Example.



1) Pick a set of n Points on the surface

2) Define a new surface by connecting points with n lines.

3) Define $\varphi_i(x) = 1$ if x is on line l_i otherwise, $\varphi_i(x) = 0$

$$\Psi(x) = \int_{\substack{approx \\ surface}} G(x,x') \sum_{i=1}^{n} \omega_i \varphi_i(x') \, dS' = \sum_{i=1}^{n} \omega_i \int_{line\ l_i} G(x,x') \, dS'$$

How do we determine the ω_i's?

Laplace's Equation in 2-D

Basis Function Approach

Residual Definition and minimization

$$R(x) \equiv \Psi(x) - \int_{\substack{approx\\surface}} G(x,x') \sum_{i=1}^{n} \omega_i \varphi_i(x') dS'$$

We will pick the ω_i's to make $R(x)$ small.

General Approach: Pick a set of test functions $\phi_1, \ldots, \phi_n$, and force $R(x)$ to be orthogonal to the set

$$\int \phi_i(x) R(x) dS = 0 \quad \text{for all } i.$$

Laplace's Equation in 2-D

Basis Function Approach

Residual minimization using test functions

$$\int \phi_i(x)\, R(x)\, dS = \int \phi_i(x)\, \Psi(x)\, dS - \int \int_{\substack{approx\\surface}} \phi_i(x)\, G(x,x') \sum_{j=1}^{n} \omega_j \varphi_j(x')\, dS' dS = 0$$

We will generate different methods by chosing the $\phi_1, \ldots, \phi_n$,

Collocation: $\phi_i(x) = \delta\left(x - x_{t_i}\right)$ (point-matching)

Galerkin Method: $\phi_i(x) = \varphi_i(x)$ (basis = test)

Laplace's Equation in 2-D

Basis Function Approach

Collocation

Collocation: $\phi_i(x) = \delta(x_i)$ (point-matching)

$$\int \delta\left(x - x_{t_i}\right) R(x)\, dS = R\left(x_{t_i}\right) = \Psi\left(x_{t_i}\right) - \int_{\substack{approx\\surface}} G\left(x_{t_i}, x'\right) \sum_{j=1}^{n} \omega_j \varphi_j(x')\, dS' = 0$$

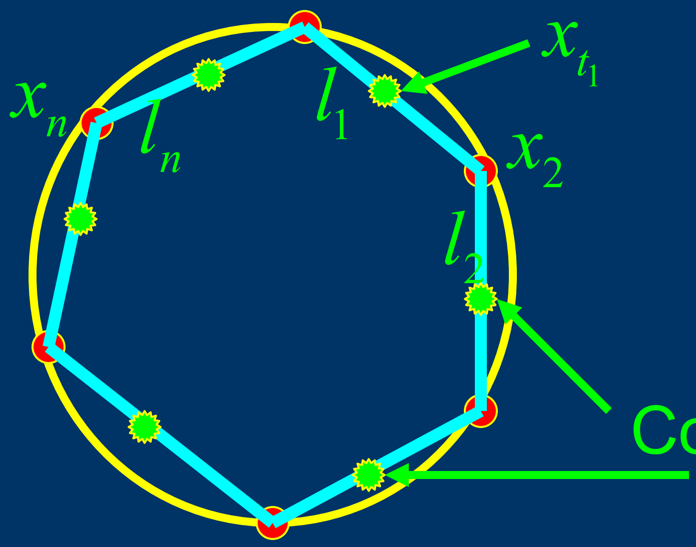
$$\Rightarrow \Psi\left(x_{t_i}\right) = \sum_{j=1}^{n} \omega_j \underbrace{\int_{\substack{approx\\surface}} G\left(x_{t_i}, x'\right) \varphi_j(x')\, dS'}_{A_{i,j}}$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{t_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{t_n}\right) \end{bmatrix}$$

Laplace's Equation in 2-D

Basis Function Approach

Centroid Collocation for Piecewise Constant Bases



$$\Psi\left(x_{t_i}\right) = \sum_{j=1}^{n} \omega_j \int_{\substack{approx \\ surface}} G\left(x_{t_i}, x'\right) \varphi_j\left(x'\right) dS'$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{t_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{t_n}\right) \end{bmatrix}$$

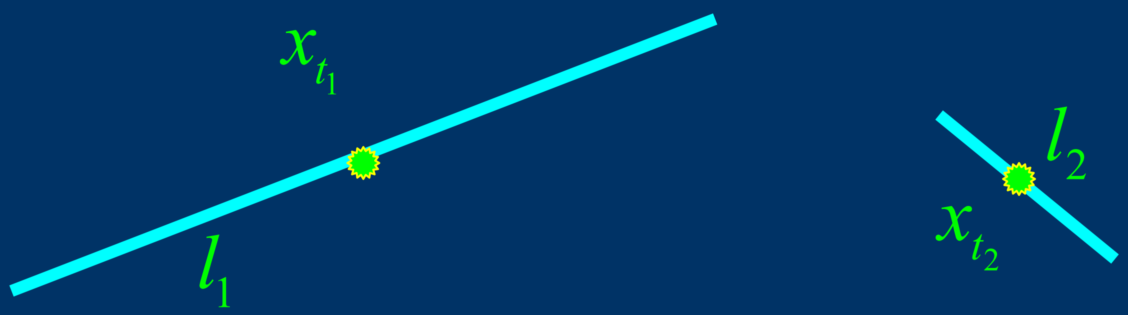
$$\Psi\left(x_{t_i}\right) = \sum_{j=1}^{n} \omega_j \underbrace{\int_{line\ j} G\left(x_{t_i}, x'\right) dS'}_{A_{i,j}}$$

Laplace's Equation in 2-D

Basis Function Approach

Centroid Collocation Generates a nonsymmetric A

$$\Psi\left(x_{t_i}\right) = \sum_{j=1}^{n} \omega_j \underbrace{\int_{line\ j} G\left(x_{t_i}, x'\right) dS'}_{A_{i,j}}$$



$$A_{1,2} = \int_{line\,2} G\left(x_{t_1}, x'\right) dS' \neq \int_{line\,1} G\left(x_{t_2}, x'\right) dS' = A_{2,1}$$

Laplace's Equation in 2-D

Basis Function Approach

Galerkin

Galerkin: $\phi_i(x) = \varphi_i(x)$ (test=basis)

$$\int \varphi_i(x)\, R(x)\, dS = \int \varphi_i(x)\, \Psi(x)\, dS - \int \int_{\substack{approx\\surface}} \varphi_i(x)\, G(x,x') \sum_{j=1}^{n} \omega_j \varphi_j(x')\, dS' dS = 0$$

$$\underbrace{\int_{\substack{approx\\surface}} \varphi_i(x)\Psi(x)\, dS}_{b_i} = \sum_{j=1}^{n} \omega_j \underbrace{\int_{\substack{approx\\surface}} \int_{\substack{approx\\surface}} G(x,x')\varphi_i(x)\varphi_j(x')\, dS' dS}_{A_{i,j}}$$

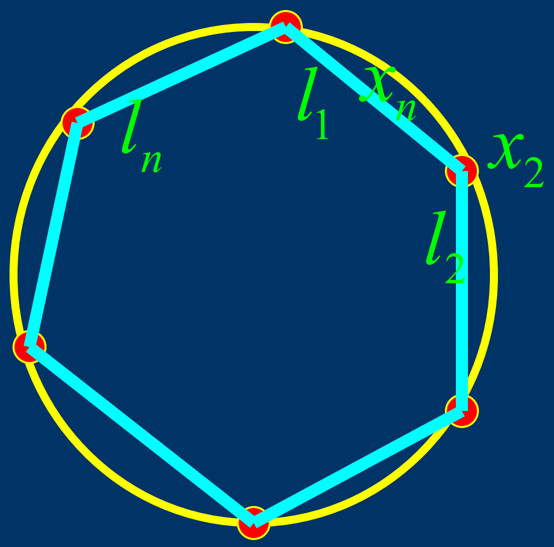
$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_n \end{bmatrix}$$

If $G(x,x') = G(x',x)$ then $A_{i,j} = A_{j,i}$ A is symmetric

Laplace's Equation in 2-D

Basis Function Approach

Galerkin for Piecewise Constant Bases



$$\underbrace{\int_{line_i} \Psi(x)\, dS}_{b_i} = \sum_{j=1}^{n} \omega_j \underbrace{\int_{line_i} \int_{line_j} G(x, x')\, dS' dS}_{A_{i,j}}$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_n \end{bmatrix}$$

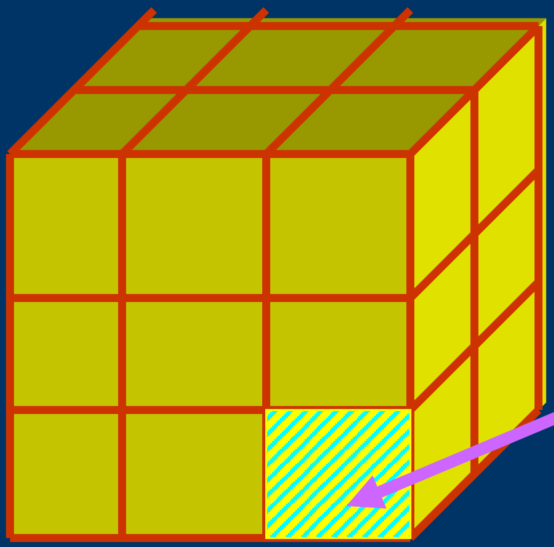
3-D Laplace's Equation

Basis Function Approach

Piecewise Constant Basis

Integral Equation: $\Psi(x) = \int_{surface} \frac{1}{\|x - x'\|} \sigma(x') \, dS'$

Discretize Surface into Panels



Panel j

Represent $\sigma(x) \approx \sum_{i=1}^{n} \omega_i \underbrace{\varphi_i(x)}_{\text{Basis Functions}}$

$\varphi_j(x) = 1$ if x is on panel j

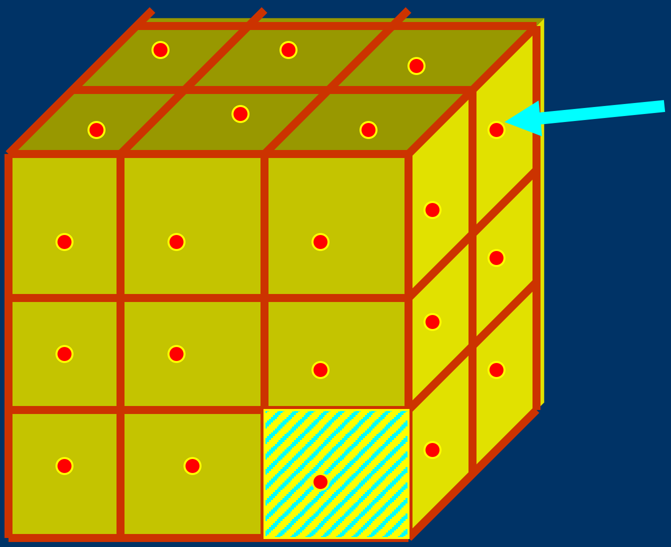
$\varphi_j(x) = 0$ otherwise

3-D Laplace's Equation

Basis Function Approach

Centroid Collocation

Put collocation points at panel centroids



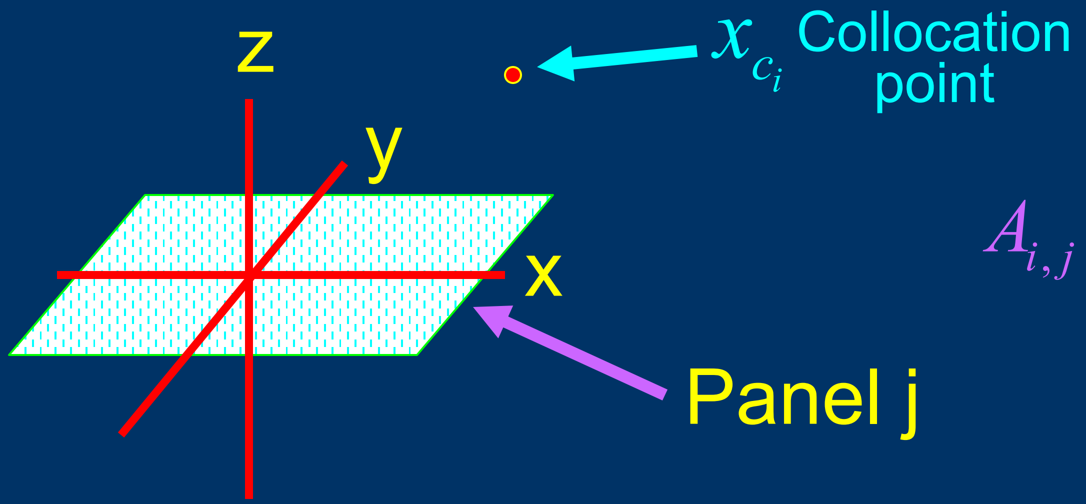
x_{c_i} Collocation point

$$\Psi\left(x_{c_i}\right) = \sum_{j=1}^{n} \omega_j \underbrace{\int_{panel\ j} G\left(x_{c_i}, x'\right) dS'}_{A_{i,j}}$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

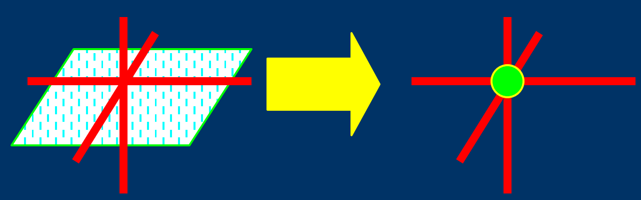
3-D Laplace's Equation

Calculating Matrix Elements



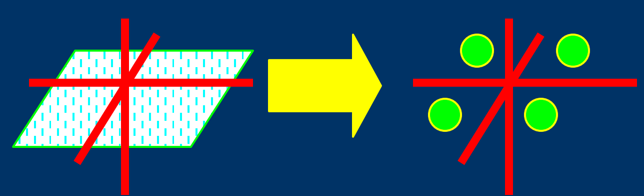
$$A_{i,j} = \int_{panel\ j} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

One point quadrature Approximation



$$A_{i,j} \approx \frac{Panel\ \ Area}{\left\| x_{c_i} - x_{centroid_j} \right\|}$$

Four point quadrature Approximation

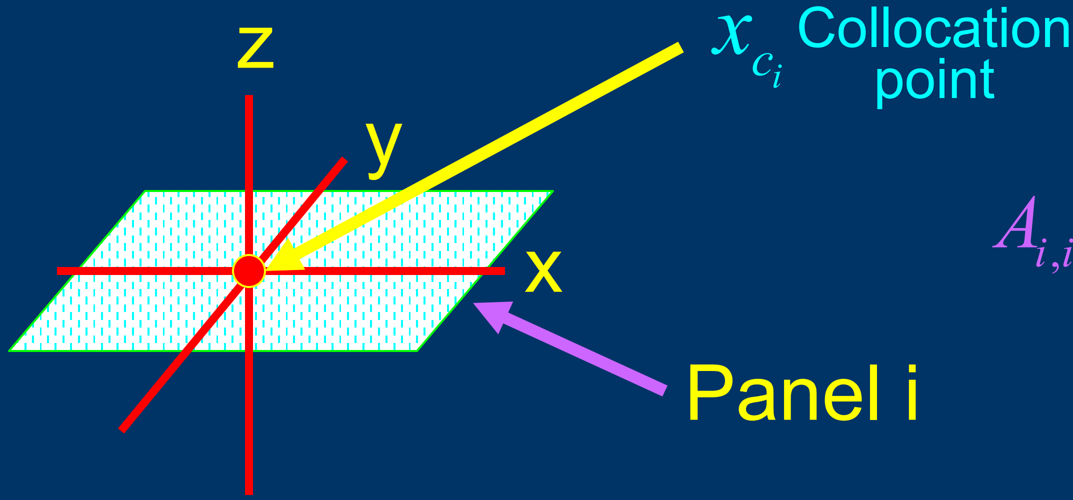


$$A_{i,j} \approx \sum_{j=1}^{4} \frac{0.25 * Area}{\left\| x_{c_i} - x_{point_j} \right\|}$$

3-D Laplace's Equation

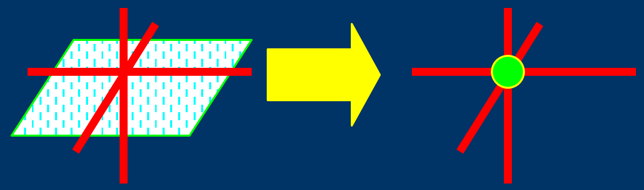
Basis Function Approach

Calculating "Self-Term"



$$A_{i,i} = \int_{panel\ i} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

One point quadrature Approximation



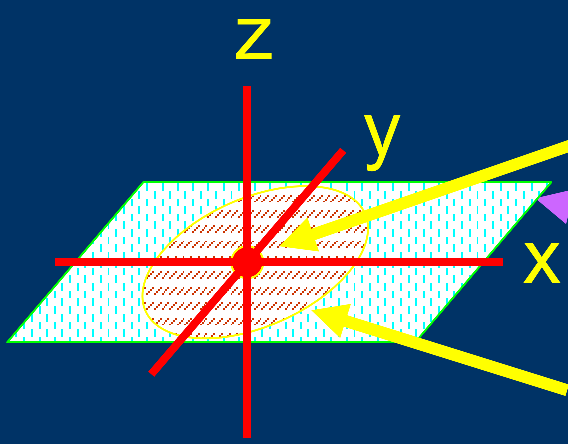
$$A_{i,i} \approx \frac{Panel\ \ Area}{\underbrace{\left\| x_{c_i} - x_{c_i} \right\|}_{0}}$$

$$A_{i,i} = \int_{panel\ i} \frac{1}{\left\| x_{c_i} - x' \right\|} dS' \quad \text{is an integrable singularity}$$

3-D Laplace's Equation

Basis Function Approach

Calculating "Self-Term" Tricks of the trade



$$A_{i,i} = \int_{panel\ i} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

Integrate in two pieces

$$A_{i,i} = \int_{disk} \frac{1}{\left\| x_{c_i} - x' \right\|} dS' + \int_{rest\ of\ panel} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

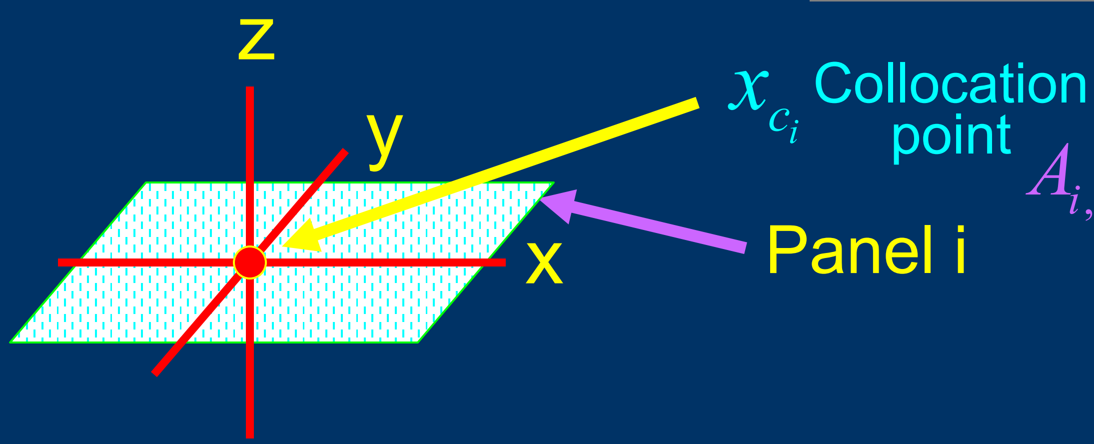
Disk Integral has singularity but has analytic formula

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

3-D Laplace's Equation

Basis Function Approach

Calculating "Self-Term"
Other Tricks of the trade



$$A_{i,i} = \int_{panel\ i} \underbrace{\frac{1}{\left\| x_{c_i} - x' \right\|}}_{\text{Integrand is singular}} dS'$$

1) If panel is a flat polygon, analytical formulas exist

2) Curve panels can be handled with projection

3-D Laplace's Equation

Basis Function Approach

Galerkin (test=basis)

$$\underbrace{\int \varphi_i(x)\Psi(x)\,dS}_{b_i} = \sum_{j=1}^{n} \omega_j \underbrace{\int\int \varphi_i(x) G(x,x') \varphi_j(x')\,dS'dS}_{A_{i,j}}$$

<u>For piecewise constant Basis</u>

$$\underbrace{\int \Psi(x)\,dS'}_{b_i} = \sum_{j=1}^{n} \omega_j \underbrace{\int_{panel\ i}\int_{panel\ j} \frac{1}{\|x-x'\|}\,dS'dS}_{A_{i,j}}$$

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_n \end{bmatrix}$$

3-D Laplace's Equation

Basis Function Approach

Problem with dense matrix

Integral Equation Method Generate Huge Dense Matrices

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \omega_1 \\ \vdots \\ \vdots \\ \omega_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

Gaussian Elimination Much Too Slow!

Summary

Integral Equation Methods
- Exterior versus interior problems
- Start with using point sources

Standard Solution Methods
- Collocation Method
- Galerkin Method

Next Time → "Fast" Solvers
- Use a Krylov-Subspace Iterative Method
- Compute MV products Approximately