Boundary Element Method for linear Partial Differential Equations

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Nuclear Science and Technology Division Seminar
10:00 AM, Research Office Building (5700), RM D307
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Abstract

This study is concerned with the development of accurate and efficient techniques for solving linear partial differential equations such as the Laplace, the diffusion and the wave equations in three-dimensional domains. The methodology is investigated in the context a Galerkin Boundary Integral Equation (BIE) approach which involves singular kernels.

It is well established that boundary-value problems with known Green's functions admit integral formulations which lead to very effective numerical schemes. The advantages of these BIE algorithms are manifold: (i) there is no need of volume discretization, only boundary mesh generation is required, (ii) the singularities in the kernels, when properly handled, lead to a discretized systems with bounded condition number, (iii) for problems in an unbounded domain, BIE systems automatically satisfy far-field conditions. A major difficulty in the numerical approximation of BIEs is the treatment of singularities in the surface integrals.

Recent developments in BIE schemes have shown that existing BIE codes can be accelerated by a matrix compression technique such as the Precorrected-FFT method to achieve a significant reduction in execution time and memory requirements. This reduction in time and computer memory scales almost linearly with the number of boundary unknowns. As a result, large-scale 3D applications (over 100,000 unknowns) with complicated geometry can be executed on a desktop computer.

In this talk, an overview of a technique for solving BIEs known as the Boundary Element Method (BEM) will be presented. Also, our strength in solving partial differential equations with the boundary element methodology will be addressed.

BOUNDARY ELEMENT METHOD
FOR
LINEAR PARTIAL DIFFERENTIAL EQUATIONS

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*Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract No. DE-AC05-00OR22725

MOTIVATION

- GENERAL PURPOSE SOLVER FOR LINEAR PDES VIA GALERKIN BEM

  3D Laplace Equation
  3D Poisson's Equation
  3D Lamé Equation
  3D Helmholtz Equation
  3D Elastodynamic Equation (Frequency Domain)
  3D Diffusion Equation
  3D Wave Equation (time Domain)
  etc...

- ACCURATE SOLUTION OF LARGE SIMULATIONS WITH COMPLEX GEOMETRY

- PROVIDE C AND FORTRAN LIBRARIES FOR SOLVING LINEAR PDES

APPLICATIONS

- ELECTROSPRAY Van Berkel G. J. et al. (1999)

  3D Laplace Equation

- CRYSTAL GROWTH Phan A-V et al. (2001)

  3D Lamé Equation + Level Set technique

- MEMS Masters N. and Ye W. (2004)

  3D Laplace + Lamé Equations

- TOKAMAK (Axisymmetric Plasma) Itagaki M. al. (2005)

  Grad-Shafranov Equation

BIEM vs Domain methods

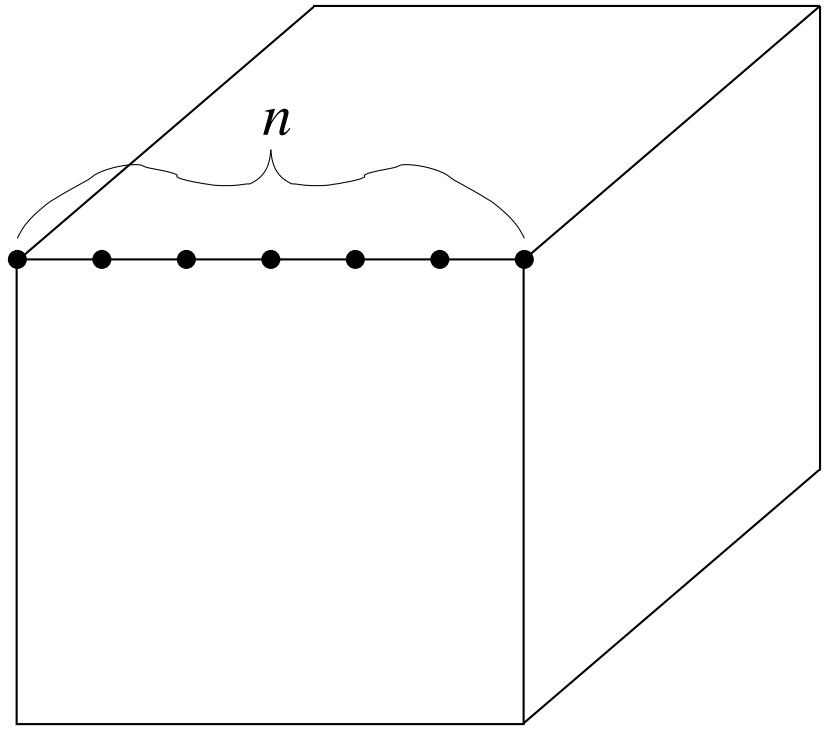
- Advantages

  Surface discretization $\Longrightarrow O(n^2)$

  Green's functions $\Longrightarrow$ High accuracy

  Diagonal Dominant matrices

  Unbounded domains



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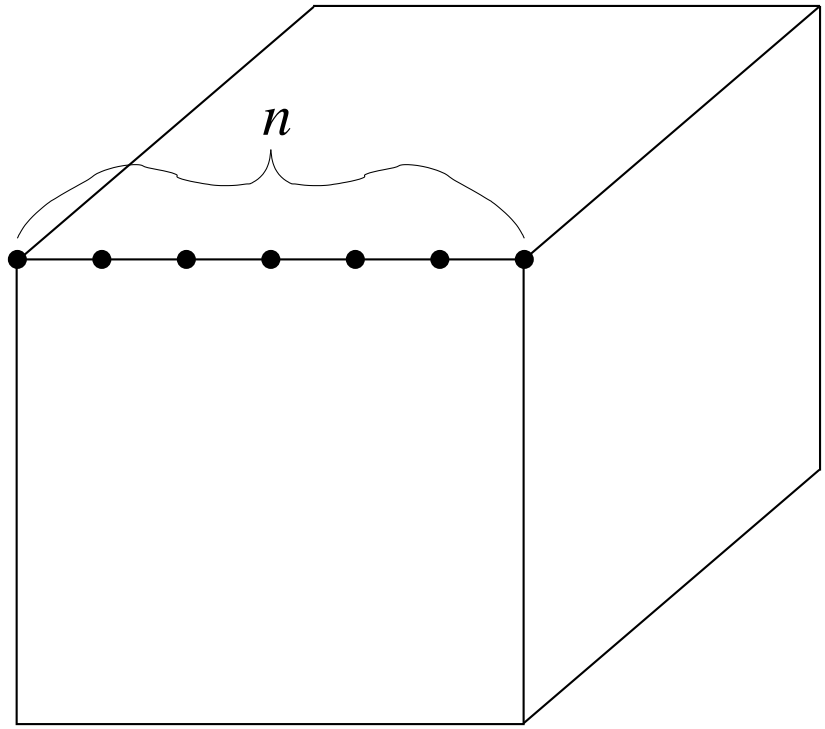

- Drawbacks

  Green's functions

  Fully-populated matrices

PROBLEM FORMULATION

- FIELD EQUATION $\nabla^2 u = 0$ in $D \subset \mathbb{R}^3$

- BOUNDARY CONDITIONS

  Dirichlet: $u = u^p$ on S

  Neumann: $t \equiv \frac{\partial u}{\partial n} = t^p$ on S

  Mixed: $u = u^p$ on S_u, $t = t^p$ on S_t, $S = S_u \cup S_t$

INTEGRAL REPRESENTATION

- GREEN'S REPRESENTATION FORMULA S is Lipschitz

$$\int_S G(\boldsymbol{x},\boldsymbol{y})\, t(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} - \int_S \boldsymbol{H}(\boldsymbol{x},\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})\, u(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} = \begin{cases} u(\boldsymbol{x}), & \boldsymbol{x}\in D \\ 0, & \boldsymbol{x}\in\mathbb{R}^3\setminus\bar{D} \end{cases}$$

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- GREEN'S FUNCTIONS

$$G(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi\|\boldsymbol{x}-\boldsymbol{y}\|}, \quad \boldsymbol{x}\neq\boldsymbol{y}, \quad \boldsymbol{x}\in\mathbb{R}^3$$

$$\boldsymbol{H}(\boldsymbol{x},\boldsymbol{y}) = \nabla_{\boldsymbol{y}} G(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi}\frac{\boldsymbol{x}-\boldsymbol{y}}{\|\boldsymbol{x}-\boldsymbol{y}\|^3}, \quad \boldsymbol{x}\neq\boldsymbol{y}, \quad \boldsymbol{x}\in\mathbb{R}^3$$

BOUNDARY INTEGRAL EQUATION

- EXTERIOR POINT $\quad \boldsymbol{x}_\varepsilon \in \mathbb{R}^3 \setminus \bar{D}, \qquad \boldsymbol{x}_\varepsilon = \boldsymbol{x} + \varepsilon \boldsymbol{n}(\boldsymbol{x}), \quad \boldsymbol{x} \in S$

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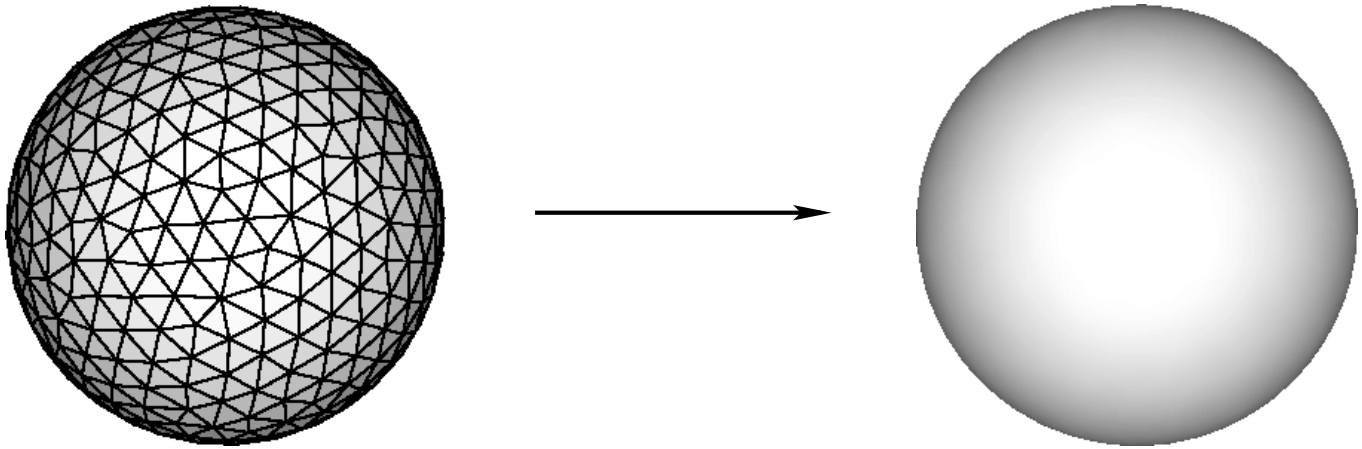
- SINGULAR BIE

$$\lim_{\boldsymbol{x}_\varepsilon \to \boldsymbol{x}} \left(\int_S G(\boldsymbol{x}_\varepsilon, \boldsymbol{y})\, t(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} - \int_S \boldsymbol{H}(\boldsymbol{x}_\varepsilon, \boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y})\, u(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} \right) = 0$$

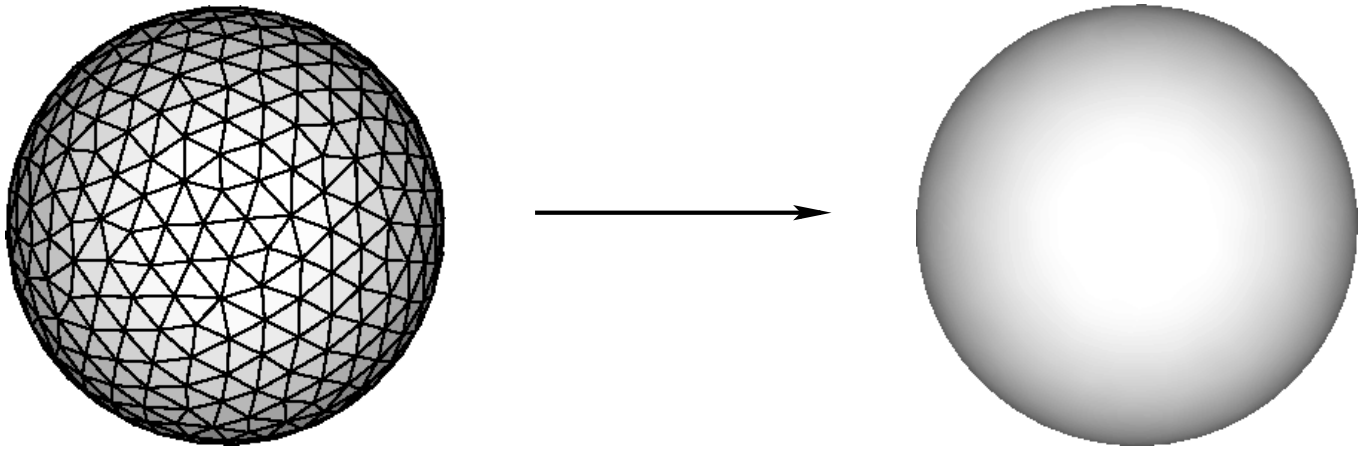
NUMERICAL APPROXIMATION



- GEOMETRIC DISCRETIZATION

$$S^h = \sum_{q=1}^{N_E} \bar{E}_q \longrightarrow S$$

NUMERICAL APPROXIMATION

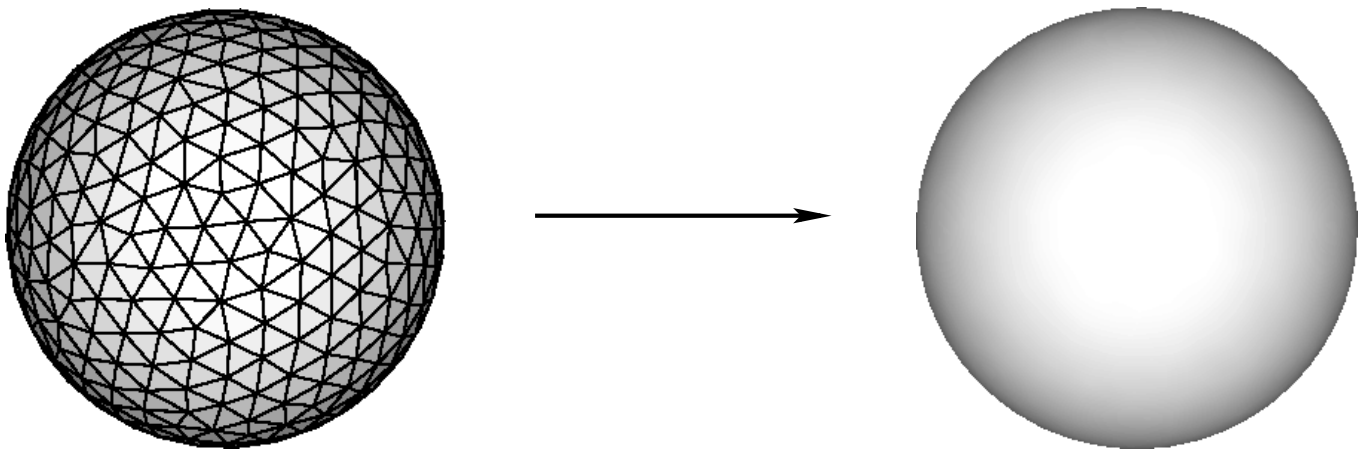


- GEOMETRIC DISCRETIZATION $$S^h = \sum_{q=1}^{N_E} \bar{E}_q \longrightarrow S$$

- DECOMPOSITION $$u(\boldsymbol{y}) = \sum_{j=1}^{N} u(\boldsymbol{y}^j)\,\psi_j(\boldsymbol{y}), \quad t(\boldsymbol{y}) = \sum_{j=1}^{N} t(\boldsymbol{y}^j)\,\psi_j(\boldsymbol{y}), \quad \boldsymbol{y} \in S^h$$

ψ_j are piecewise linear “hat” functions

NUMERICAL APPROXIMATION



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  ψ_j are piecewise linear "hat" functions

- LINEAR SYSTEM $$\mathbf{G}\{t\} = \mathbf{H}\{u\}$$

GALERKIN METHOD (WEIGHTED RESIDUAL METHOD)

- SINGULAR BIE

$$G_{ij} = \sum_{p=1}^{N_{E_i}} \sum_{q=1}^{N_{E_j}} \int_{E_p} \psi_i(\boldsymbol{x}) \left(\lim_{\boldsymbol{x}_\varepsilon \to \boldsymbol{x}} \int_{E_q} G(\boldsymbol{x}_\varepsilon, \boldsymbol{y})\, \psi_j(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} \right) \mathrm{d}s_{\boldsymbol{x}}$$

$$H_{ij} = \sum_{p=1}^{N_{E_i}} \sum_{q=1}^{N_{E_j}} \int_{E_p} \psi_i(\boldsymbol{x}) \left(\lim_{\boldsymbol{x}_\varepsilon \to \boldsymbol{x}} \int_{E_q} \boldsymbol{H}(\boldsymbol{x}_\varepsilon, \boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y})\, \psi_j(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} \right) \mathrm{d}s_{\boldsymbol{x}}$$

TRIANGULAR ELEMENTS: $E_p \in \mathrm{supp}(\psi_i)$, $E_q \in \mathrm{supp}(\psi_j)$

SURFACE POTENTIALS

- SINGLE-LAYER POTENTIAL

$$G_j^q(\boldsymbol{x}) = \int_{E_q} G(\boldsymbol{x},\boldsymbol{y})\,\psi_j(\boldsymbol{y})\,\mathrm{d}s_{\boldsymbol{y}}, \qquad \boldsymbol{x} \in \mathbb{R}^3$$

- DOUBLE-LAYER POTENTIAL

$$H_j^q(\boldsymbol{x}) = \int_{E_q} \boldsymbol{H}(\boldsymbol{x},\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})\,\psi_j(\boldsymbol{y})\,\mathrm{d}s_{\boldsymbol{y}}, \qquad \boldsymbol{x} \in \mathbb{R}^3$$

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Feature: $\forall \boldsymbol{x} \in \mathbb{R}^3, \quad G_j^q(\boldsymbol{x})$ and $H_j^q(\boldsymbol{x})$ are integrated exactly

EXAMPLES: INTERIOR DIRICHLET PROBLEM

STANDARD CUBE

- $D = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < x_1, x_2, x_3 < 1\}, \qquad u|_S = x_1^2 + x_2^2 - 2x_3^2$

	GBEM:SBIE			GBEM:HBIE		
N	T	L_2-$error$	n_{it}	T	L_2-$error$	n_{it}
54	0.05	4.659×10^{-1}	43	0.05	4.331×10^{-1}	25
150	0.27	1.730×10^{-1}	74	0.33	1.690×10^{-1}	33
384	1.81	7.969×10^{-2}	104	2.19	7.873×10^{-2}	33
1014	14	3.729×10^{-2}	152	16	3.681×10^{-2}	34
2646	99	1.769×10^{-2}	170	116	1.760×10^{-2}	41
4374	285	1.204×10^{-2}	177	328	1.200×10^{-2}	33
6534	625	9.080×10^{-3}	188	731	8.842×10^{-3}	33
8664	1167	7.406×10^{-3}	212	1351	7.168×10^{-3}	33
10086	1573	6.434×10^{-3}	182	1865	6.376×10^{-3}	33

$T = T_{\text{MAT}} + T_{\text{BiCGSTAB(4)}} + T_{\text{RHS}}$ $\qquad$ $T =$ Total time in seconds

$n_{it} =$ Number of iterations by BiCGSTAB(4)

Dell Latitude D820 Laptop 2.0GHz/4MB L2 cache/ 2GB RAM

EXAMPLES: INTERIOR DIRICHLET PROBLEM

RHOMBUS

- $D =$ Rhombus, $\quad u|_S = x_1^2 + x_2^2 - 2x_3^2$

	GBEM:SBIE			GBEM:HBIE		
N	T	L_2-$error$	n_{it}	T	L_2-$error$	n_{it}
864	9.70	3.414×10^{-2}	145	12	3.496×10^{-2}	41
1734	42	1.970×10^{-2}	157	49	2.033×10^{-2}	49
2904	123	1.311×10^{-2}	175	143	1.379×10^{-2}	41
6144	592	7.217×10^{-3}	193	685	7.758×10^{-3}	41
8214	1053	5.719×10^{-3}	205	1217	6.305×10^{-3}	41
10086	1577	4.897×10^{-3}	199	1846	5.396×10^{-3}	41

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PRECORRECTED-FFT(PFFT)

- COMPUTATIONAL COST

$$\mathbf{G}, \ \mathbf{H} \Longrightarrow \text{Dense Matrices} \Longrightarrow O(N^2)$$

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- ACCELERATION TECHNIQUES

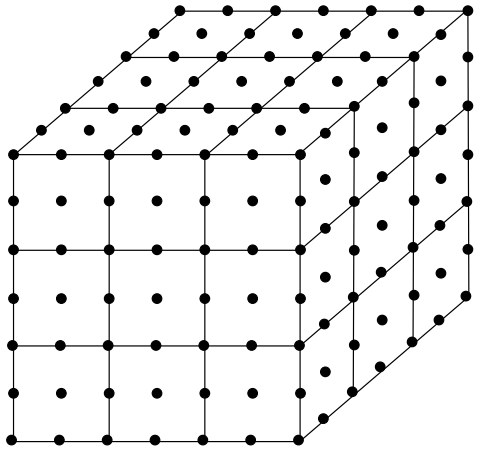
Greengard L. and Rokhlin V. (1987) $\Longrightarrow$ FMM

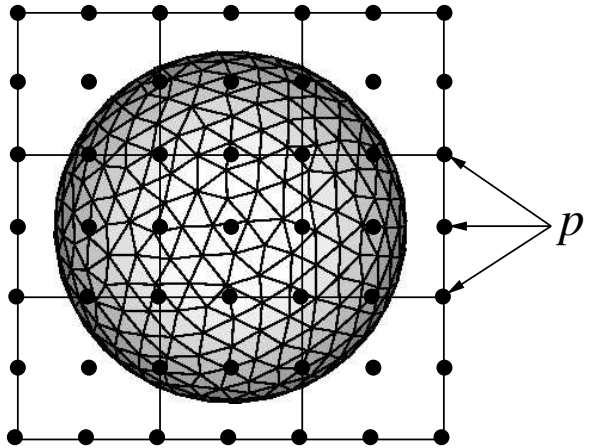
Hackbusch W. (1999) $\Longrightarrow$ H-matrices $\qquad O(N^{1+\alpha}\log^{\beta} N),\ 0 \leq \alpha < 1,\ \beta \geq 0$

Fann G. et al. (2004) $\Longrightarrow$ Multiwavelet method

Nintcheu Fata S. (2008) $\Longrightarrow$ Precorrected-FFT

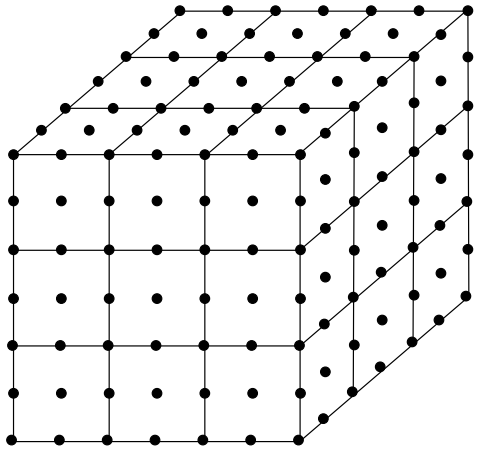
REGULAR GRID APPROXIMATION

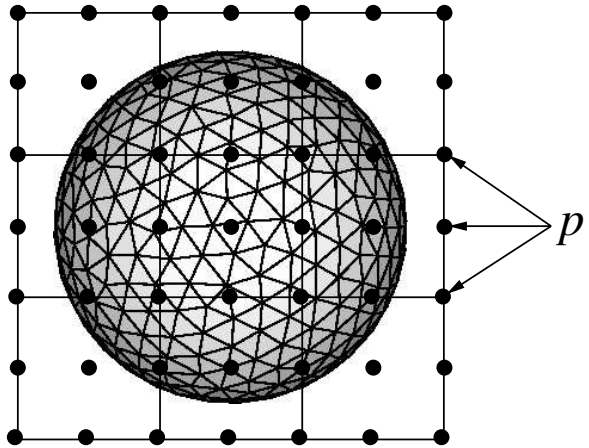




- GALERKIN INTEGRAL $$\mathsf{H}_{ij}^{kl} = \sum_{s=1}^{N_{E_k}} \sum_{t=1}^{N_{E_l}} \int_{E_s} \int_{E_t} \psi_i(\boldsymbol{x})\, \boldsymbol{H}(\boldsymbol{x},\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y})\, \psi_j(\boldsymbol{y})\, \mathrm{d}s_{\boldsymbol{y}} \mathrm{d}s_{\boldsymbol{x}}$$

REGULAR GRID APPROXIMATION





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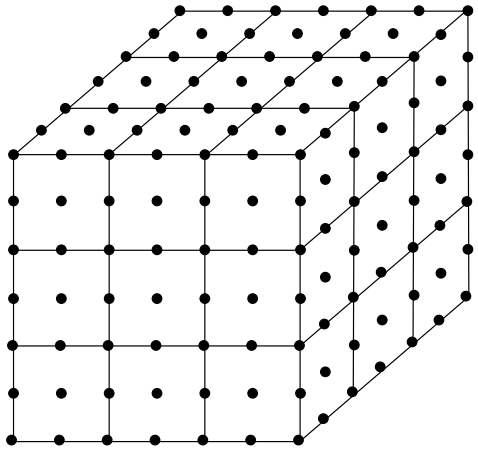
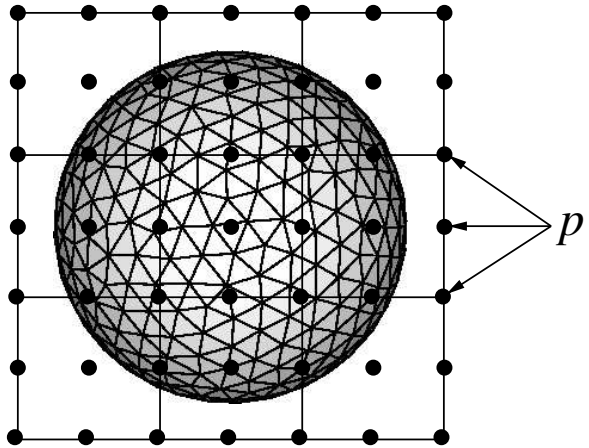
- QUADRATURE ESTIMATE $$\mathsf{H}_{ij}^{kl(s,t)} = \sum_{\beta=1}^{N_G} \sum_{\alpha=1}^{N_G} C_i^{s\beta} C_j^{t\alpha}\, n_f^{t\alpha} H_f(\boldsymbol{x}^{s\beta}, \boldsymbol{y}^{t\alpha})$$

REGULAR GRID APPROXIMATION





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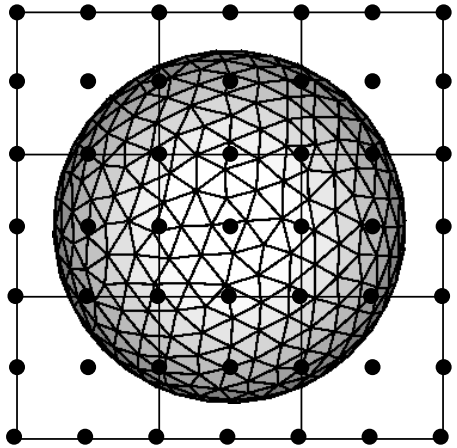
- LOCAL INTERPOLATION $$H_f(\boldsymbol{x}^{s\beta}, \boldsymbol{y}^{t\alpha}) = \sum_{r=1}^{p^3} \sum_{q=1}^{p^3} d_r^{s\beta}\, d_q^{t\alpha}\, H_f(\widehat{\boldsymbol{x}}^r, \widehat{\boldsymbol{y}}^q)$$

PRECORRECTION

SINGULAR BIE

SINGLE-LAYER KERNEL

- CELL-NEIGHBOR $\mathbf{P}^{kl} = \mathbf{G}^{kl} - \mathbf{W}^{k^\top} \widehat{\mathbf{G}}^{kl} \mathbf{W}^{l}$
- DECOMPOSITION $\mathbf{G} = \mathbf{P} + \mathbf{W}^\top \widehat{\mathbf{G}} \mathbf{W}$



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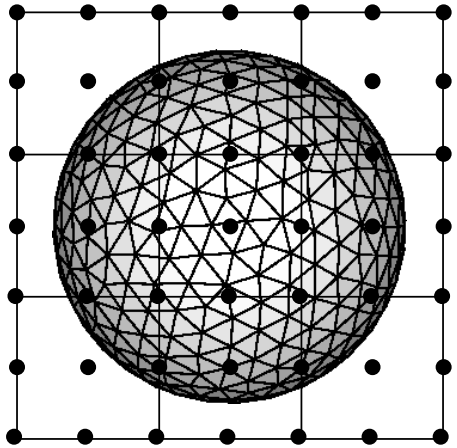

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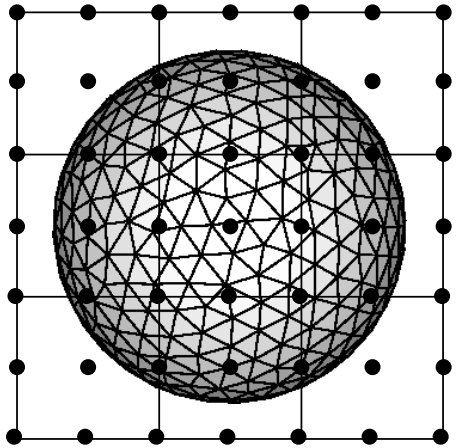
DOUBLE-LAYER KERNEL

- CELL-NEIGHBOR $\mathbf{P}^{kl} = \mathbf{H}^{kl} - \sum_{i=1}^{3} \mathbf{W}^{k^\top} \widehat{\mathbf{H}}_i^{kl} \mathbf{V}^{l,i}$
- DECOMPOSITION $\mathbf{H} = \mathbf{P} + \sum_{i=1}^{3} \mathbf{W}^\top \widehat{\mathbf{H}}_i \mathbf{V}^{i}$

Feature: $\mathbf{P}, \quad \mathbf{W}, \quad \mathbf{V}^i \Longrightarrow$ Sparse $\Longrightarrow O(N)$

PRECORRECTION

SINGULAR BIE



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Feature: $\mathbf{P}, \quad \mathbf{W}, \quad \mathbf{V}^i \Longrightarrow$ Sparse $\Longrightarrow O(N)$

PRODUCTS $\widehat{\mathbf{G}}\{\hat{z}\}, \quad \widehat{\mathbf{H}}_i\{\hat{z}\} \Longrightarrow$ FFT $\Longrightarrow O(N \log N)$

EXAMPLES: INTERIOR DIRICHLET PROBLEM

STANDARD CUBE GBEM:HBIE

- $D = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < x_1, x_2, x_3 < 1\}, \qquad u|_S = x_1^2 + x_2^2 - 2x_3^2$

	CA			PFFT$(m, 4, 3.5, 3, 100)$			
N	T_{CA}	L_2-$error$	Mem	T_{PFFT}	L_2-$error$	Mem	m
384	2	7.873×10^{-2}	3.5	2	7.873×10^{-2}	6.9	1
1014	16	3.681×10^{-2}	17	9	3.681×10^{-2}	21	4
2646	116	1.760×10^{-2}	110	24	1.760×10^{-2}	59	8
4374	328	1.200×10^{-2}	297	45	1.199×10^{-2}	88	8
6534	731	8.842×10^{-3}	659	82	8.838×10^{-3}	156	8
8664	1351	7.168×10^{-3}	1126	110	7.159×10^{-3}	382	20
10086	1865	6.376×10^{-3}	1536	125	6.369×10^{-3}	402	20
20886	8225	3.654×10^{-3}	6491	285	3.654×10^{-3}	593	20
41334	32694	$--$	25276	849	2.253×10^{-3}	1126	20
61206	72037	$--$	55317	1744	1.706×10^{-3}	1434	20

$T_{\mathsf{CA}} = T_{\mathsf{MAT}} + T_{\mathsf{BiCGSTAB(4)}} + T_{\mathsf{RHS}} \qquad T_{\mathsf{PFFT}} = T_{\mathsf{P}} + T_{\mathsf{BiCGSTAB(4)}} + T_{\mathsf{RHS}}$

$T_{\mathsf{CA}}, T_{\mathsf{PFFT}} =$ Total time in seconds

Dell Latitude D820 Laptop 2.0GHz/4MB L2 cache/ 2GB RAM

FUTURE DIRECTIONS

- GALERKIN BEM FOR LAPLACE EQUATION (Testing)
- FAST SPECTRAL (PFFT) METHOD FOR LAPLACE EQUATION (to complete)
- PRECONDITIONER FOR FAST SPECTRAL METHOD (to complete)
- ANALYTIC INTEGRATION FOR LAMÉ EQUATION

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- PRECONDITIONER FOR FAST SPECTRAL METHOD (to complete)
- ANALYTIC INTEGRATION FOR LAMÉ EQUATION
- FAST VOLUME INTEGRATION $\Longrightarrow$ Poisson's equation and Non-linear effect

$$B(\boldsymbol{x}) = \int_D G(\boldsymbol{x}, \boldsymbol{y})\, b(\boldsymbol{y})\, \mathrm{d}V_{\boldsymbol{y}}, \qquad \boldsymbol{x} \in \mathbb{R}^3$$

$$B_i = \int_S \int_D \psi_i(\boldsymbol{x})\, G(\boldsymbol{x}, \boldsymbol{y})\, b(\boldsymbol{y})\, \mathrm{d}V_{\boldsymbol{y}}\, \mathrm{d}s_{\boldsymbol{x}}$$

FUTURE DIRECTIONS

- GALERKIN BEM FOR LAPLACE EQUATION (Testing)
- FAST SPECTRAL (PFFT) METHOD FOR LAPLACE EQUATION (to complete)
- PRECONDITIONER FOR FAST SPECTRAL METHOD (to complete)
- ANALYTIC INTEGRATION FOR LAMÉ EQUATION
- FAST VOLUME INTEGRATION $\Longrightarrow$ Poisson's equation and Non-linear effect

$$B(\boldsymbol{x}) = \int_D G(\boldsymbol{x}, \boldsymbol{y})\, b(\boldsymbol{y})\, \mathrm{d}V_{\boldsymbol{y}}, \qquad \boldsymbol{x} \in \mathbb{R}^3$$

$$B_i = \int_S \int_D \psi_i(\boldsymbol{x})\, G(\boldsymbol{x}, \boldsymbol{y})\, b(\boldsymbol{y})\, \mathrm{d}V_{\boldsymbol{y}}\, \mathrm{d}s_{\boldsymbol{x}}$$

- GALERKIN BEM FOR AXISYMMETRIC PLASMA $\Longrightarrow$ GRAD-SHAFRANOV EQUATION
- GALERKIN BEM FOR DIFFUSION EQUATION
- GALERKIN BEM FOR WAVE EQUATION