Hybrid Boundary Node Method accelerated by Fast Multipole Method for 3D potential problems

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Motivation

Two main difficulties in numerical analysis of engineering problems

- Discretization of the domain into elements
- Very large computational scale

➢ To overcome the first difficulty, we developed the

Hybrid Boundary Node Method (Hybrid BNM)

➢ To overcome the second difficulty, we implemented the

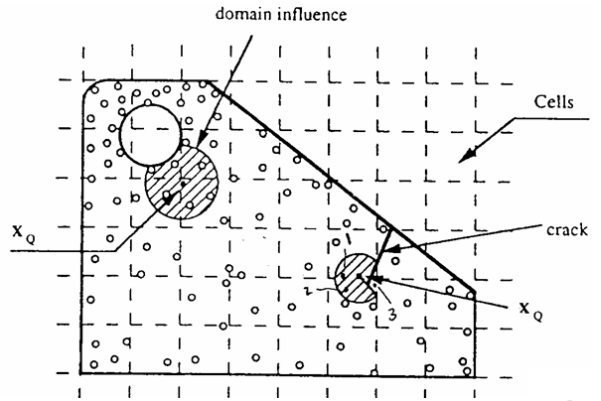
Fast Multipole Techniques (FMM)

Outline

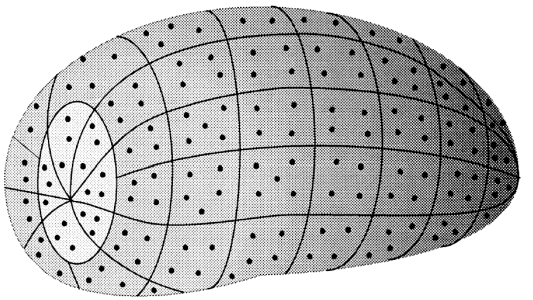
- Hybrid BNM
  - Introduction to Hybrid BNM
  - MLS approximation on an arbitrary 3D surface
  - Formulations of the Hybrid BNM for 3D potential problems
- FM-HBNM
  - Accelerate Hybrid BNM with FMM
  - Accelerate MLS with a binary tree data structure
- Numerical results
- Conclusions

Introduction to Hybrid BNM

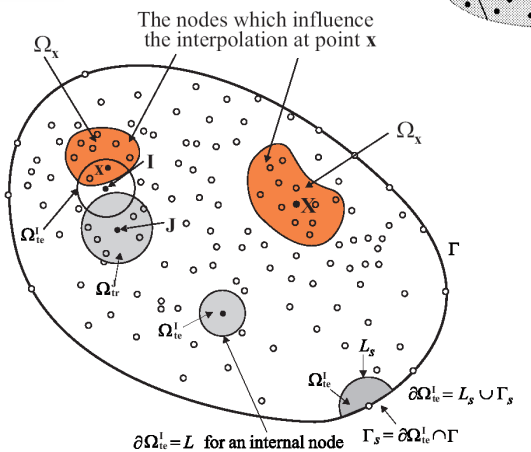
- **Element free Galerkin method (EFG)**



- **Boundary Node Method (BNM)**



- **Meshless Local Boundary Integral Equation (MLBIE)**



Introduction to Hybrid BNM (2)

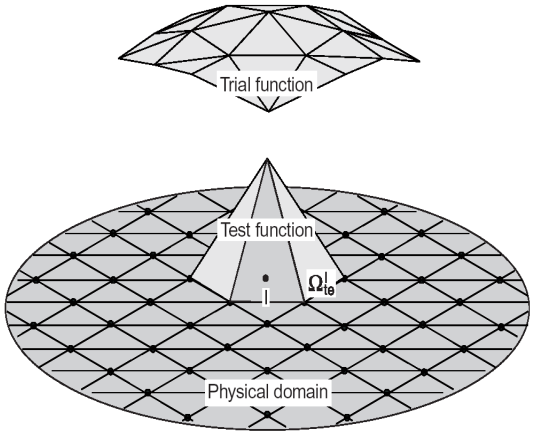
	Domain type	Boundary type
Pseudo meshless	Element free Galerkin method	Boundary node method
Truly meshless	Meshless Local Boundary Integral Equation	?

The answer is positive:

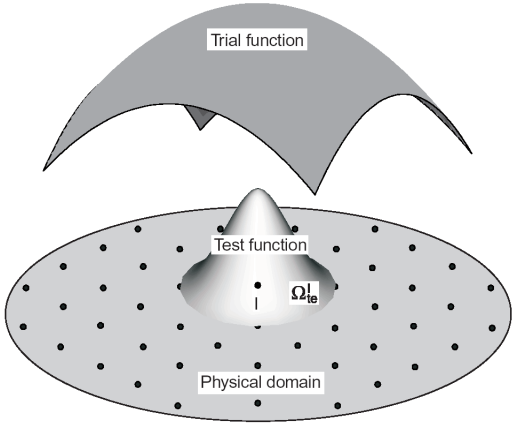
Hybrid Boundary Node Method

Combine a modified functional with the *Moving Least Squares* (MLS) approximation

MLS on arbitrary surface



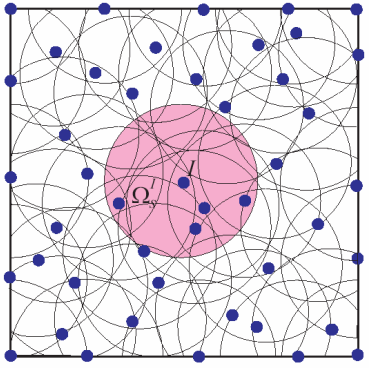
Element interpolation



MLS approximation

In Hybrid BNM, MLS is performed for boundary variables, only. To render an MLS scheme for an arbitrary surface, we construct the MLS in the parametric space of a surface.

MLS on arbitrary surface (3)



Parametric unit square

$$\tilde{u}(\mathbf{s}) = \sum_{I=1}^{N} \Phi_I(\mathbf{s})\hat{u}_I$$

$$\tilde{q}(\mathbf{s}) = \sum_{I=1}^{N} \Phi_I(\mathbf{s})\hat{q}_I$$

where

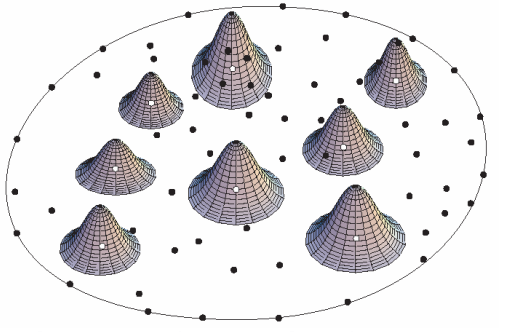
$$\Phi_I(\mathbf{s}) = \sum_{j=1}^{m} p_j(\mathbf{s})\left[A^{-1}(\mathbf{s})B(\mathbf{s})\right]_{jI}$$

$$\mathbf{p}^{\mathrm{T}}(\mathbf{s}) = [1, s_1, s_2, s_1^{\,2}, s_1 s_2, s_2^{\,2}], \qquad m = 6$$

$$A(\mathbf{s}) = \sum_{I=1}^{N} w_I(\mathbf{s})\mathbf{p}(\mathbf{s}^I)\mathbf{p}^{\mathrm{T}}(\mathbf{s}^I)$$

$$B(\mathbf{s}) = \left[w_1(\mathbf{s})\mathbf{p}(\mathbf{s}^1), w_2(\mathbf{s})\mathbf{p}(\mathbf{s}^2), \cdots, w_N(\mathbf{s})\mathbf{p}(\mathbf{s}^N)\right]$$

$$w_I(\mathbf{s}) = \begin{cases} \dfrac{\exp[-(d_I/c_I)^2] - \exp[-(\hat{d}_I/c_I)^2]}{1 - \exp[-(\hat{d}_I/c_I)^2]}, & 0 \le d_I \le \hat{d}_I \\ 0, & d_I \ge \hat{d}_I \end{cases}$$



Shape of weight function

MLS on arbitrary surface (4)

- **Remarks**
  - **Local character**

$$\Phi_I(\mathbf{s}) = \sum_{j=1}^{m} p_j(\mathbf{s}) \left[A^{-1}(\mathbf{s}) B(\mathbf{s}) \right]_{jI}$$

$$B(\mathbf{s}) = \left[w_1(\mathbf{s})\mathbf{p}(\mathbf{s}^1), w_2(\mathbf{s})\mathbf{p}(\mathbf{s}^2), \cdots, w_N(\mathbf{s})\mathbf{p}(\mathbf{s}^N) \right]$$

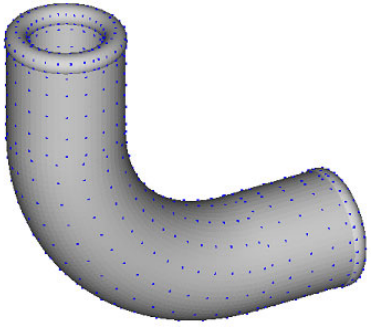
$$w_I(\mathbf{s}) = 0 \rightarrow B(\mathbf{s}) = 0 \rightarrow \Phi_I(\mathbf{s}) = 0$$

  - **No information on nodes connectivity**

Formulations of Hybrid BNM

Main features:

- Combines modified functional with the *Moving Least Squares* (MLS) approximation
- Boundary-only truly meshless method



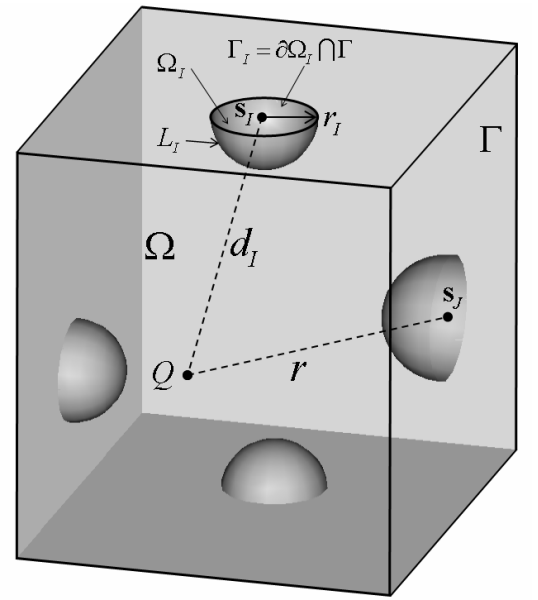
Example of meshless discretization

- Three independent variables
  - internal temperature $u = \sum_{J=1}^{N} u_J^s x_J \quad u_J^s = \frac{1}{\kappa} \frac{1}{4\pi r(Q, \mathbf{s}_J)}$
  - boundary temperature $\tilde{u}(\mathbf{s}) = \sum_{J=1}^{N} \Phi_J(\mathbf{s}) \hat{u}_J$
  - boundary normal flux $\tilde{q}(\mathbf{s}) = \sum_{J=1}^{N} \Phi_J(\mathbf{s}) \hat{q}_J$

Formulations of Hybrid BNM(2)

➢Local weak form

$$\int_\Gamma (q-\tilde{q})\delta u d\Gamma - \int_\Omega u_{,ii}\delta u d\Omega + \int_{\Gamma_q} (\tilde{q}-\overline{q})\delta\tilde{u} d\Gamma - \int_\Gamma (u-\tilde{u})\delta\tilde{q} d\Gamma = 0$$



$$\sum_{J=1}^{N}\int_{\Gamma_I} u_J^s v_I(Q)x_J d\Gamma = \sum_{J=1}^{n}\int_{\Gamma_I} \Phi_J(\mathbf{s})v_I(Q)\hat{u}_J d\Gamma$$

$$\sum_{J=1}^{N}\int_{\Gamma_I} \frac{\partial u_J^s}{\partial n} v_I(Q)x_J d\Gamma = \sum_{J=1}^{n}\int_{\Gamma_I} \Phi_J(\mathbf{s})v_I(Q)\hat{q}_J d\Gamma$$

Formulations of Hybrid BNM(3)

➢System of equations – final form

$$\mathbf{Ux} = \mathbf{H\hat{u}}$$

$$\mathbf{Qx} = \mathbf{H\hat{q}}$$

where

$$U_{IJ} = \int_{\Gamma_I} u_J^s v_I(Q) d\Gamma$$

$$Q_{IJ} = \int_{\Gamma_I} \frac{\partial u_J^s}{\partial n} v_I(Q) d\Gamma$$

$$H_{IJ} = \int_{\Gamma_I} \Phi_J(\mathbf{s}) v_I(Q) d\Gamma$$

➢Solution procedure

$$\left.\begin{array}{l}\mathbf{Ux} = \mathbf{H\hat{u}} \\ \mathbf{Qx} = \mathbf{H\hat{q}}\end{array}\right\} \rightarrow \mathbf{Ax} = \mathbf{d} \rightarrow \mathbf{x} = \mathbf{A}^{-1}\mathbf{d}$$

$$\mathbf{Ux} = \mathbf{H\hat{u}} \rightarrow \hat{\mathbf{u}} = \mathbf{H}^{-1}\mathbf{Ux}$$

$$\mathbf{Qx} = \mathbf{H\hat{q}} \rightarrow \hat{\mathbf{q}} = \mathbf{H}^{-1}\mathbf{Qx}$$

For a direct solver

Memory requirement: $O(N^2)$

Computational time: $O(N^3)$

Accelerate Hybrid BNM with FMM

➢ Iterative equation solver – GMRES

The most time-consuming part of an iterative method is the calculation of matrix-vector product, **Ux** or **Qx**, at each iteration step.

$$\text{The } I\text{ - th row of } \mathbf{Ux} = \sum_{J=1}^{N} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma$$

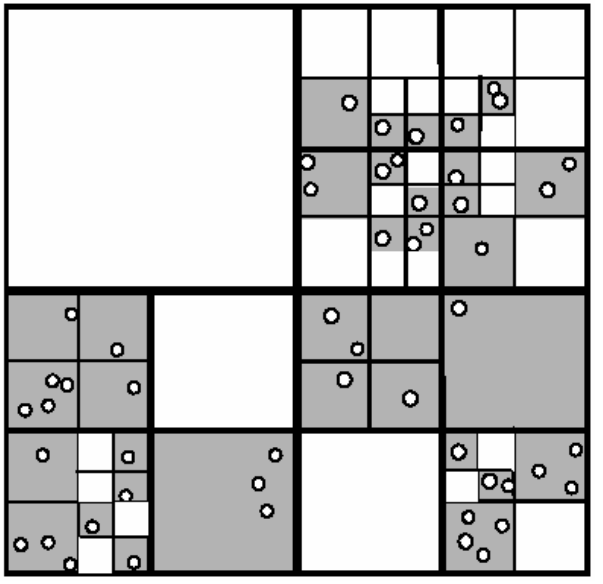
$$\text{The } I\text{ - th row of } \mathbf{Qx} = \sum_{J=1}^{N} \int_{\Gamma_I} \frac{\partial u_J^s}{\partial n} v_I(Q) x_J d\Gamma$$

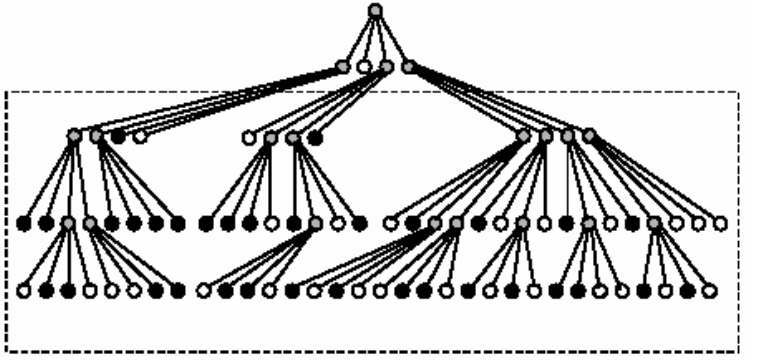
For an iterative solver
Memory requirement: $O(N^2)$
Computational time: $O(N^3)$

We use FMM to speed up these summations.

Accelerate Hybrid BNM with FMM (2)

- **First, construct a hierarchy of boxes which refine the computational domain into small regions**



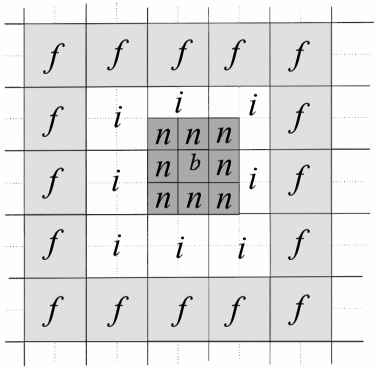


Quad-tree in 2D
Oct-tree in 3D

For simplicity, taking 2D case as an example.

Accelerate Hybrid BNM with FMM (3)

- **Using the hierarchical decomposition, we divide the sum into two parts**



f: far field

i: interaction list

n: neighbor

Near nodes $\sim n+b$

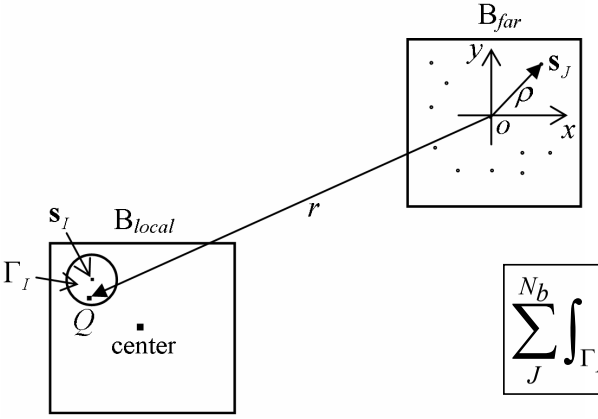
Far nodes $\sim i+f$

$$\sum_{J=1}^{N} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma = \overset{Near\ nodes}{\sum_{J}} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma + \overset{Far\ nodes}{\sum_{J}} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma$$

We compute the sum over near nodes directly, while use multipole expansions to speed up the summation over far nodes.

Accelerate Hybrid BNM with FMM (4)

- Consider two leaves B_{local} and B_{far}. B_{far} is on the interaction list of B_{local}. B_{local} contains node s_I, while B_{far} contains N_b nodes



$$u_J^s = \frac{1}{4\pi}\frac{1}{r(Q,\mathbf{s}_J)} = \frac{1}{4\pi}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\rho^n Y_n^{-m}(\alpha,\beta)\frac{Y_n^m(\theta,\phi)}{r^{n+1}}$$

$$\sum_J^{N_b}\int_{\Gamma_I} u_J^s v_I(Q)x_J d\Gamma = \frac{1}{4\pi}\sum_{n=0}^{\infty}\sum_{m=-n}^{n} M_n^m \int_{\Gamma_I}\frac{Y_n^m(\theta,\phi)}{r^{n+1}} v_I(Q)d\Gamma$$

Condition: $r > \rho$

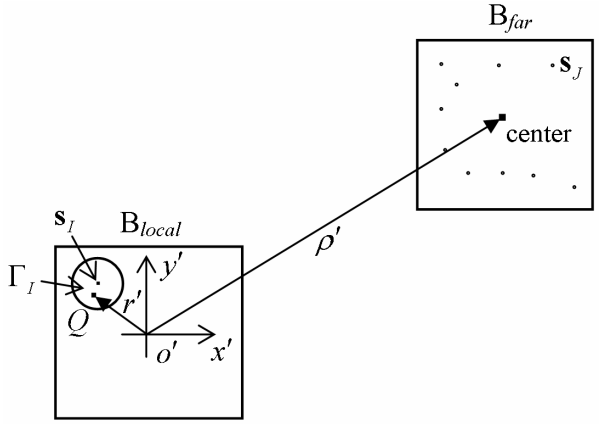
$$M_n^m = \sum_J^{N_b}\rho_J^n Y_n^{-m}(\alpha_J,\beta_J)x_J$$

In above expanded expression, the pair of points Q and $\mathbf{s}_J$ is separated.

Accelerate Hybrid BNM with FMM (5)

- **Move origin of spherical coordinate system to B_{local}'s center**

$$\frac{Y_n^m(\theta,\phi)}{r^{n+1}} = \sum_{j=0}^{\infty}\sum_{k=-j}^{j} \frac{i^{|k-m|-|k|-|m|} A_n^m A_j^k Y_{n+j}^{m-k}(\alpha',\beta')}{(-1)^n A_{n+j}^{m-k} \rho'^{j+n+1}} Y_j^k(\theta',\phi') r'^j$$



$$\sum_{J}^{N_b} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma = \sum_{j=0}^{\infty}\sum_{k=-j}^{j} L_j^k S_j^k$$

$$L_j^k = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} M_n^m \frac{i^{|k-m|-|k|-|m|} A_n^m A_j^k Y_{n+j}^{m-k}(\alpha',\beta')}{(-1)^n A_{n+j}^{m-k} \rho'^{j+n+1}}$$

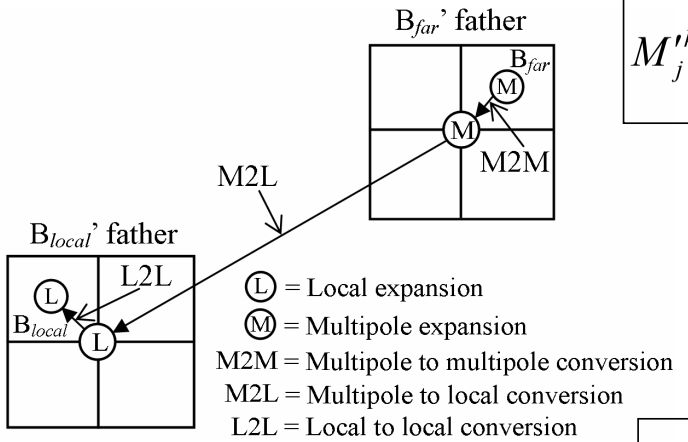
multipole to local conversion

Condition: $\rho' > 2r'$

$$S_j^k = \frac{1}{4\pi} \int_{\Gamma_I} Y_j^k(\theta',\phi') r'^j v_I(Q) d\Gamma$$

Accelerate Hybrid BNM with FMM (6)

- **When B_{far}'s parent belongs to the interaction list of B_{local}'s parent**



$$M'^{k}_{j} = \sum_{n=0}^{j} \sum_{m=-n}^{n} M^{k-m}_{j-n} \frac{i^{|k|-|m|-|k-m|} A^{m}_{n} A^{k-m}_{j-n} \rho^{n} Y^{-m}_{n}(\alpha,\beta)}{A^{k}_{j}}$$

multipole to multipole conversion

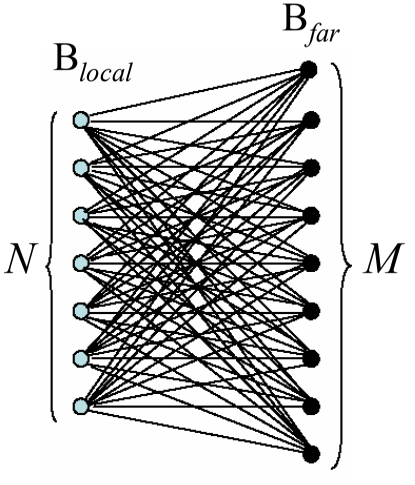
$$L^{k}_{j} = \sum_{n=j}^{\infty} \sum_{m=-n}^{n} L'^{m}_{n} \frac{i^{|m|-|m-k|-|k|} A^{m-k}_{n-j} A^{k}_{j} Y^{m-k}_{n-j}(\alpha,\beta) \rho^{n-j}}{(-1)^{n+j} A^{m}_{n}}$$

local to local conversion

Accelerate Hybrid BNM with FMM (7)

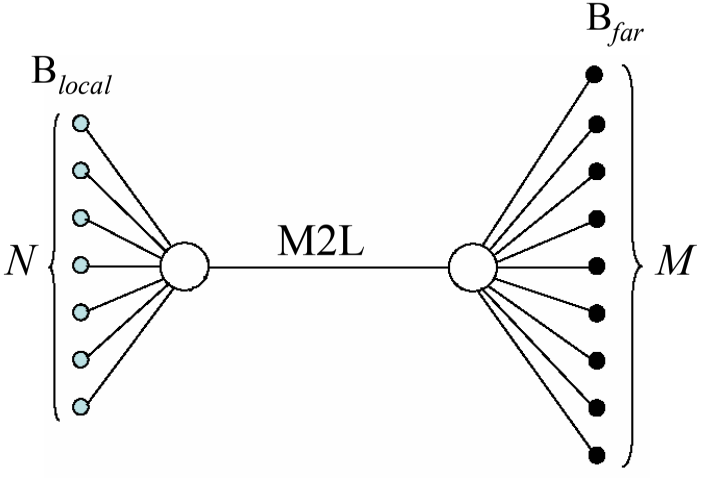
- **Comparison of the standard and multipole algorithms**

Standard algorithm



Total number of operations O(*NM*)

Multipole expansion algorithm

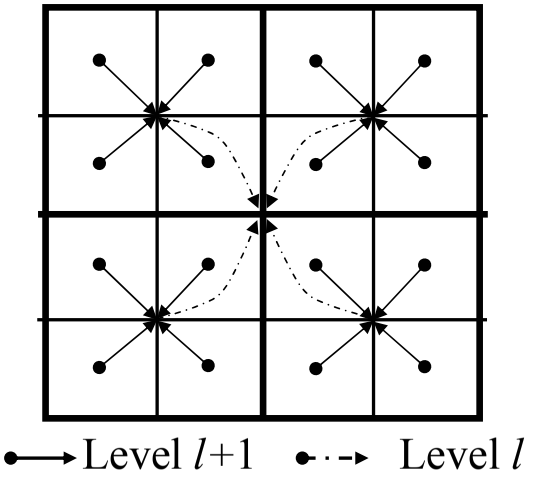


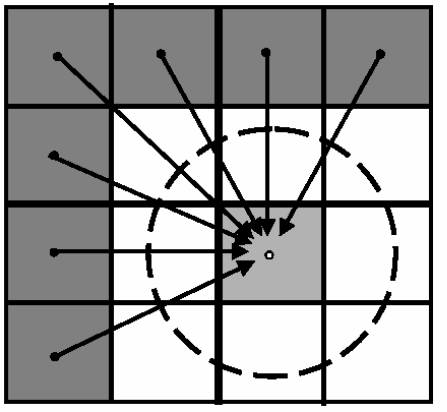
Total number of operations O(*N*+*M*)

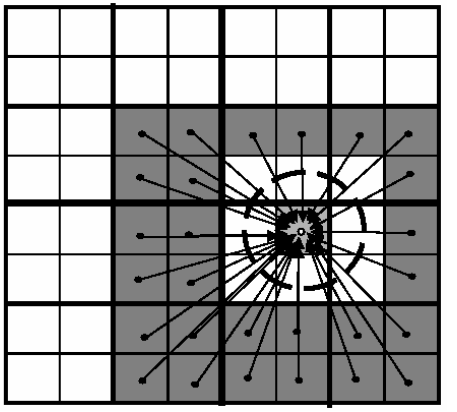
Accelerate Hybrid BNM with FMM (8)

➢ Upward pass and Downward pass

In FMM, the multipole and local moments are orchestrated in the hierarchy of boxes.







Multipole moments are accumulated from leaves of the tree to the root (***Upward pass***); and local moments are distributed from the root to the leaves (***Downward pass***). This is accomplished in order of N operations.

Accelerate Hybrid BNM with FMM (9)

- **Product** $\mathbf{Qx} \sim \sum_{I=1}^{N} \int_{\Gamma_J} \frac{\partial u_I^s}{\partial n} v_J(Q) x_I d\Gamma$

$$\mathbf{Qx} \sim \sum_{J}^{N_b} \int_{\Gamma_I} \frac{\partial u_J^s}{\partial n} v_I(Q) x_J d\Gamma = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k \frac{\partial S_j^k}{\partial n}$$

$$\frac{\partial S_j^k}{\partial n} = \frac{1}{4\pi} \int_{\Gamma_I} \frac{\partial Y_j^k(\theta', \phi') r'^j}{\partial n} v_I(Q) d\Gamma$$

$$L_j^k = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_n^m \frac{i^{|k-m|-|k|-|m|} A_n^m A_j^k Y_{n+j}^{m-k}(\alpha', \beta')}{(-1)^n A_{n+j}^{m-k} \rho'^{j+n+1}}$$

$$\mathbf{Ux} \sim \sum_{J=1}^{N_b} \int_{\Gamma_I} u_J^s v_I(Q) x_J d\Gamma = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} L_j^k S_j^k$$

$$S_j^k = \frac{1}{4\pi} \int_{\Gamma_I} Y_j^k(\theta', \phi') r'^j v_I(Q) d\Gamma$$

$$L_j^k = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_n^m \frac{i^{|k-m|-|k|-|m|} A_n^m A_j^k Y_{n+j}^{m-k}(\alpha', \beta')}{(-1)^n A_{n+j}^{m-k} \rho'^{j+n+1}}$$

Coefficients of local expansion L_j^k are the same for **Qx** and **Ux.**

Accelerate MLS with binary tree

- **Computation of matrix H**

Solution procedure

$$\left.\begin{array}{l}\mathbf{Qx}=\mathbf{H}\hat{\mathbf{q}}\\ \mathbf{Ux}=\mathbf{H}\hat{\mathbf{u}}\end{array}\right\} \rightarrow \mathbf{Ax}=\mathbf{d} \rightarrow \mathbf{x}=\mathbf{A}^{-1}\mathbf{d}$$

$$\mathbf{Qx}=\mathbf{H}\hat{\mathbf{q}} \rightarrow \hat{\mathbf{q}}=\mathbf{H}^{-1}\mathbf{Qx}$$

$$\mathbf{Ux}=\mathbf{H}\hat{\mathbf{u}} \rightarrow \hat{\mathbf{u}}=\mathbf{H}^{-1}\mathbf{Ux}$$

$$H_{IJ}=\int_{\Gamma_s^J}\Phi_I(\mathbf{s})v_J(Q)d\Gamma$$

FMM deals with only matrices **U** and **V**, while leaves matrix **H** intact.

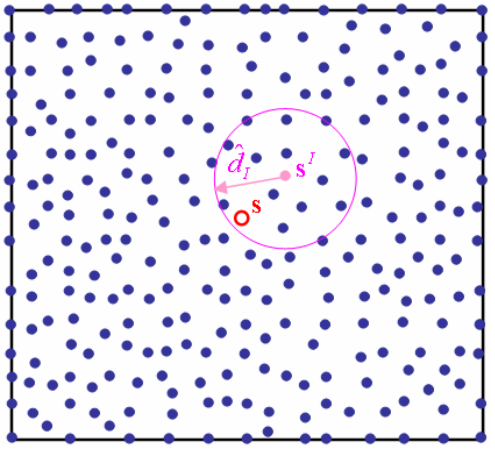
Accelerate MLS with binary tree (2)

Original MLS algorithm

$$A(\mathbf{s}) = \sum_{I=1}^{n} w_I(\mathbf{s})\mathbf{p}(\mathbf{s}^I)\mathbf{p}^{\mathrm{T}}(\mathbf{s}^I)$$

$$B(\mathbf{s}) = \left[w_1(\mathbf{s})\mathbf{p}(\mathbf{s}^1), w_2(\mathbf{s})\mathbf{p}(\mathbf{s}^2), \cdots, w_N(\mathbf{s})\mathbf{p}(\mathbf{s}^N) \right]$$

$$\Phi_I(\mathbf{s}) = \sum_{j=1}^{m} p_j(\mathbf{s}) \left[A^{-1}(\mathbf{s})B(\mathbf{s}) \right]_{jI}$$



n nodes on a panel

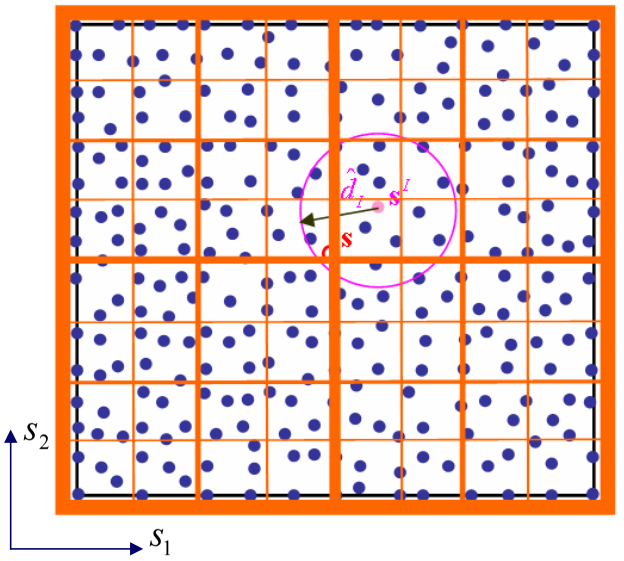
1. Loop over all nodes located on the panel
   - determine the nodes $\mathbf{s}^I$ that $w_I(\mathbf{s}) > 0$;
   - calculate $w_I(\mathbf{s})\mathbf{p}(\mathbf{s}^I)\mathbf{p}^{\mathrm{T}}(\mathbf{s}^I)$;
2. Solve the inversion of A(s).
3. Loop over all nodes located on the panel. Calculate $\Phi_I(\mathbf{s})$.

Remarks:

1. Loop has to be over all the nodes on the panel.
2. Size of matrix H ($H_{IJ} = \int_{\Gamma_s^J} \Phi_I(\mathbf{s}) v_J(Q) d\Gamma$) is $n \times n$.

Accelerate MLS with binary tree (3)

- Panel partitioning with cells

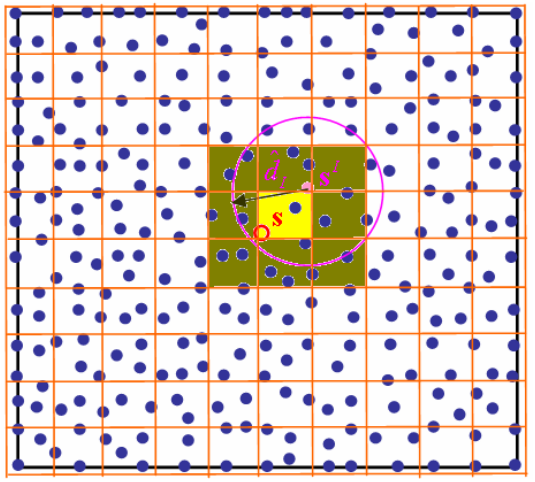


Build the binary tree

1. Let the root cell contains the entire panel.
2. Recursively repeat:
   if *H.s1* > *Dmax.s1*, subdivide a cell into two equal cells in s_1 direction;
   if *H.s2* > *Dmax.s2*, subdivide a cell into two equal cells in s_2 direction.
3. Refer the cells at the finest level as *leaves*. Create a *neighbor list* for each leaf.
4. Associate each leaf a $j \times k$ sub-matrix h_{jk}.
   j denotes the number of nodes included in the leaf, and k the number of nodes in the neighborhood.

Accelerate MLS with binary tree (4)

- **Algorithm with a binary tree**



1. Find the leaf that includes the evaluation point.
2. Loop over the nodes included in the neighborhood
   - determine the nodes s^I that $w_I(s) > 0$;
   - calculate $w_I(s)p(s^I)p^T(s^I)$;
3. Solve the inversion of A(s).
4. Loop over the nodes included in the neighborhood. calculate $\Phi_I(s)$.

Near nodes

$$A(s) = \sum_I w_I(s)p(s^I)p^T(s^I)$$

$$B(s) = \left[w_1(s)p(s^1), w_2(s)p(s^2), \cdots \right]$$

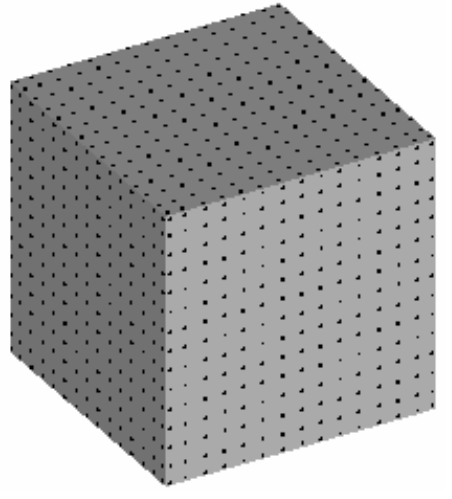
$$\Phi_I(s) = \sum_{j=1}^{m} p_j(s)\left[A^{-1}(s)B(s) \right]_{jI}$$

Remarks:

1. Loop is restricted to the neighboring nodes.
2. Matrix H is replaced by a number of sub-matrices h_{jk}.

Numerical results

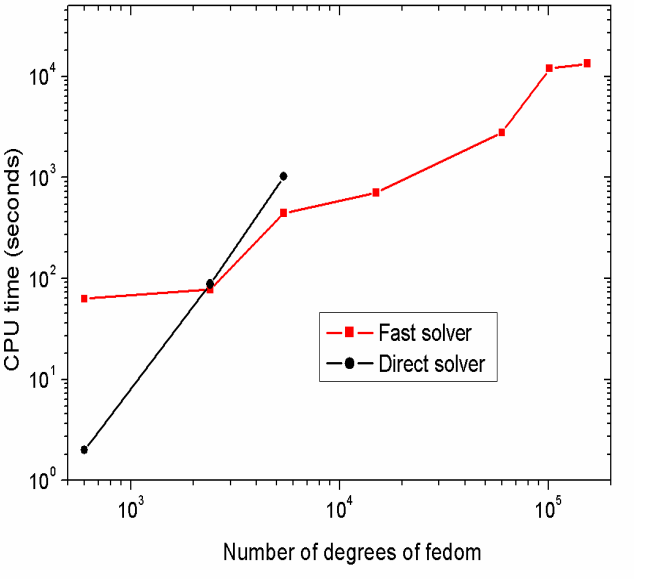
- **Results of a cube**



Max number of unknowns

Direct computation: 5400

FMM computation: 153600

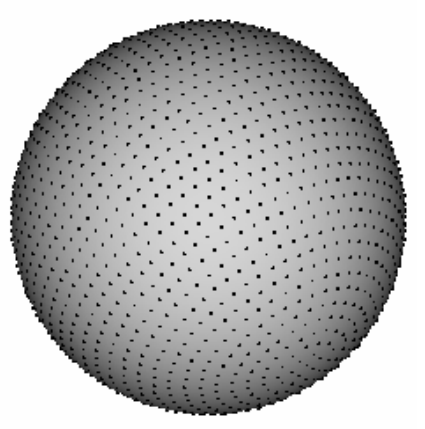


CPU time vs number of unknowns

Performed on a desktop computer with an Intel(R) Pentium(R) 4 CPU (1.99GHz)

Numerical results (2)

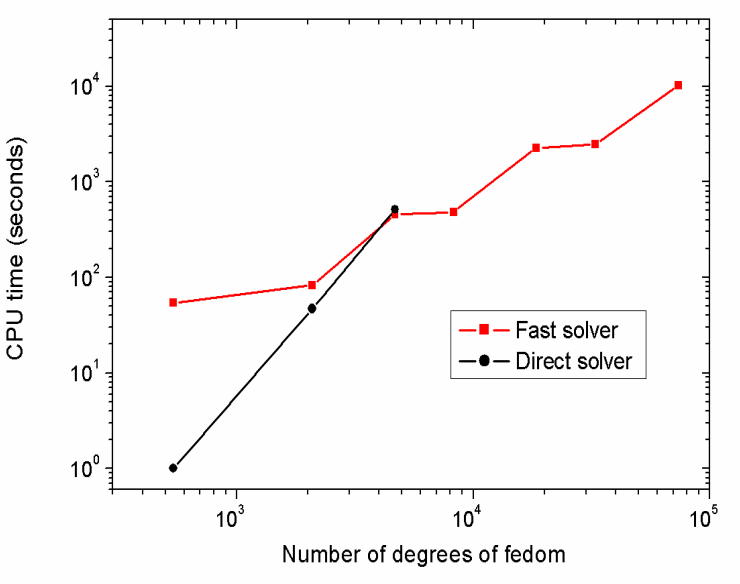
- **Results of a sphere**



Max number of unknowns

Direct computation: 4664

FMM computation: 73664

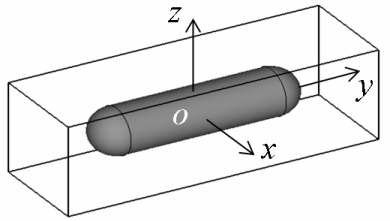


CPU time vs number of unknowns

Performed on a desktop computer with an Intel(R) Pentium(R) 4 CPU (1.99GHz)

Numerical results (3)

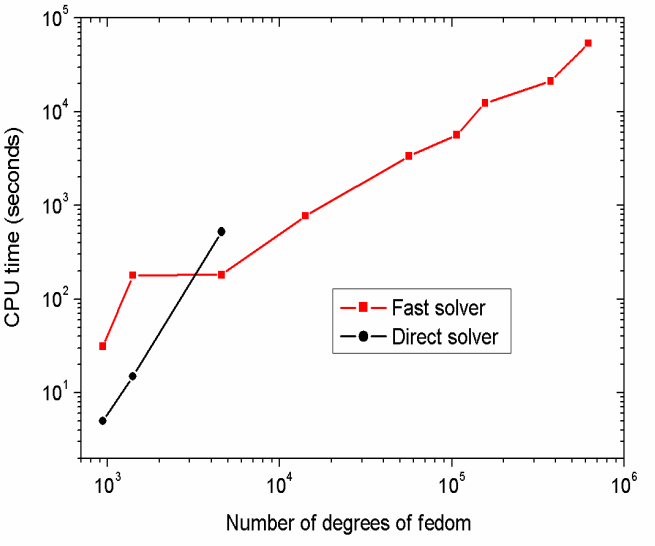
- **Results of a cuboid**



Max number of unknowns

Direct computation: 4598

FMM computation: 620708



CPU time vs number of unknowns

Performed on a desktop computer with an Intel(R) Pentium(R) 4 CPU (1.99GHz)

Conclusions

- The FMM has been incorporated into the Hybrid BNM. Numerical results clearly demonstrate that FM-HBNM is more efficient than the original Hybrid BNM when the number of unknowns is more than about 2000.

- The FM-HBNM retains the advantages of both the meshless method and the fast solver. It not only results in considerable savings in computing time and memory, but also substantially simplifies the discretization tasks for problems with complicated geometries. Therefore, the proposed method is especially applicable for large-scale simulations of bodies with intricate geometries.