MAIT 627 Fast Multipole Methods

Lecture 7

(part 2)

Outline

- Results of the MLFMM tests
  - Itemized Asymptotic Complexity of the MLFMM;
  - Optimization of the Grouping (Clustering) Parameter;
  - Regular mesh;
  - Random distributions.
- Neighborhoods and Dimensionality in MLFMM
  - Domains of Expansion Validity;
  - Domains of Translation Validity;
  - Neighborhood Increase Technique.
- Evaluation of the FMM Error

Itemized Cost of MLFMM

Regular mesh:

$$N = 2^{L_* d}, \quad s = 2^{L_s d}, \quad L = L_{\max} = L_* - L_s.$$

Assume that all translation costs are the same, *CostTranslation*(*P*)

$$CostUpward_1 = NCostExpansion(P) = O(NP).$$

$$CostUpward_2 = 2^d\left(2^{(L-1)d} + 2^{(L-2)d} + \ldots + 2^{2d}\right)CostSS(P)$$

$$< \frac{2^d}{2^d - 1}\left(2^{Ld} - 1\right)CostSS(P) \sim \frac{N}{s}CostSS(P)$$

$$CostDownward_1 \lesssim P_4(d)\left(2^{2d} + \ldots + 2^{Ld}\right)CostSR(P) \sim P_4(d)\frac{N}{s}CostSR(P),$$

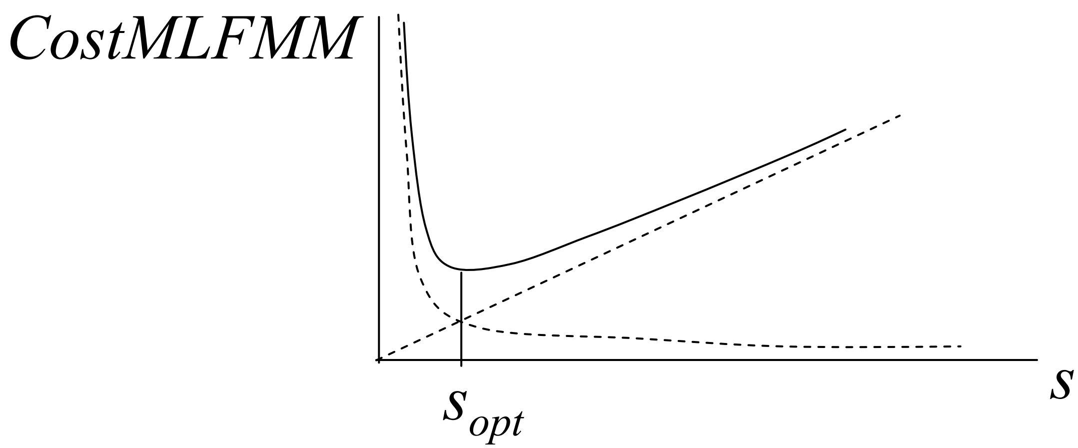
$$CostDownward_2 = 2^d\left(2^{2d} + \ldots + 2^{(L-1)d}\right)CostRR(P) \sim \frac{N}{s}CostRR(P),$$

$$CostEvaluation = M(P_2(d)sCostFunc + P).$$

Powers of E_4 and E_2 neighborhoods

$$CostMLFMM = (M+N)P + (P_4(d) + 2)\frac{N}{s}CostTranslation(P) + P_2(d)sMCostFunc$$

Optimization of the Grouping Parameter



$$CostMLFMM = (M+N)P + (P_4(d)+2)\frac{N}{s}CostTranslation(P) + P_2(d)sMCostFunc$$

$$\frac{\partial CostMLFMM}{\partial s} = -(P_4(d)+2)\frac{N}{s^2}CostTranslation(P) + P_2(d)MCostFunc = 0$$

$$s_{opt} = \left[\frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc}\right]^{1/2}.$$

$$CostMLFMM_{opt} = (M+N)P + 2[MN(P_4(d)+2)P_2(d)CostTranslation(P)CostFunc]^{1/2}.$$

Optimization of the Grouping Parameter (Example)

$$s_{opt} = \left[\frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc} \right]^{1/2}.$$

$$CostMLFMM_{opt} = (M+N)P + 2[MN(P_4(d)+2)P_2(d)CostTranslation(P)CostFunc]^{1/2}.$$

Example:

$$N = M, \quad P_4(d) = 3^d\left(2^d - 1\right), \quad P_2(d) = 3^d,$$

$$CostTranslation(P) = P^2, \quad CostFunc = 1$$

$$s_{opt} \sim 2^{d/2}P; \quad CostMLFMM_{opt} \sim 2NP\left(1 + 3^d 2^{d/2}\right)$$

$$For\ d = 2, \quad P = 10, \quad s_{opt} \sim 38, \quad CostMLFMM_{opt} \sim 38NP = 380N.$$

If non-optimized,

$$s = 1; \quad CostMLFMM \quad \sim NP\left(2 + 3^d 2^d P\right)$$

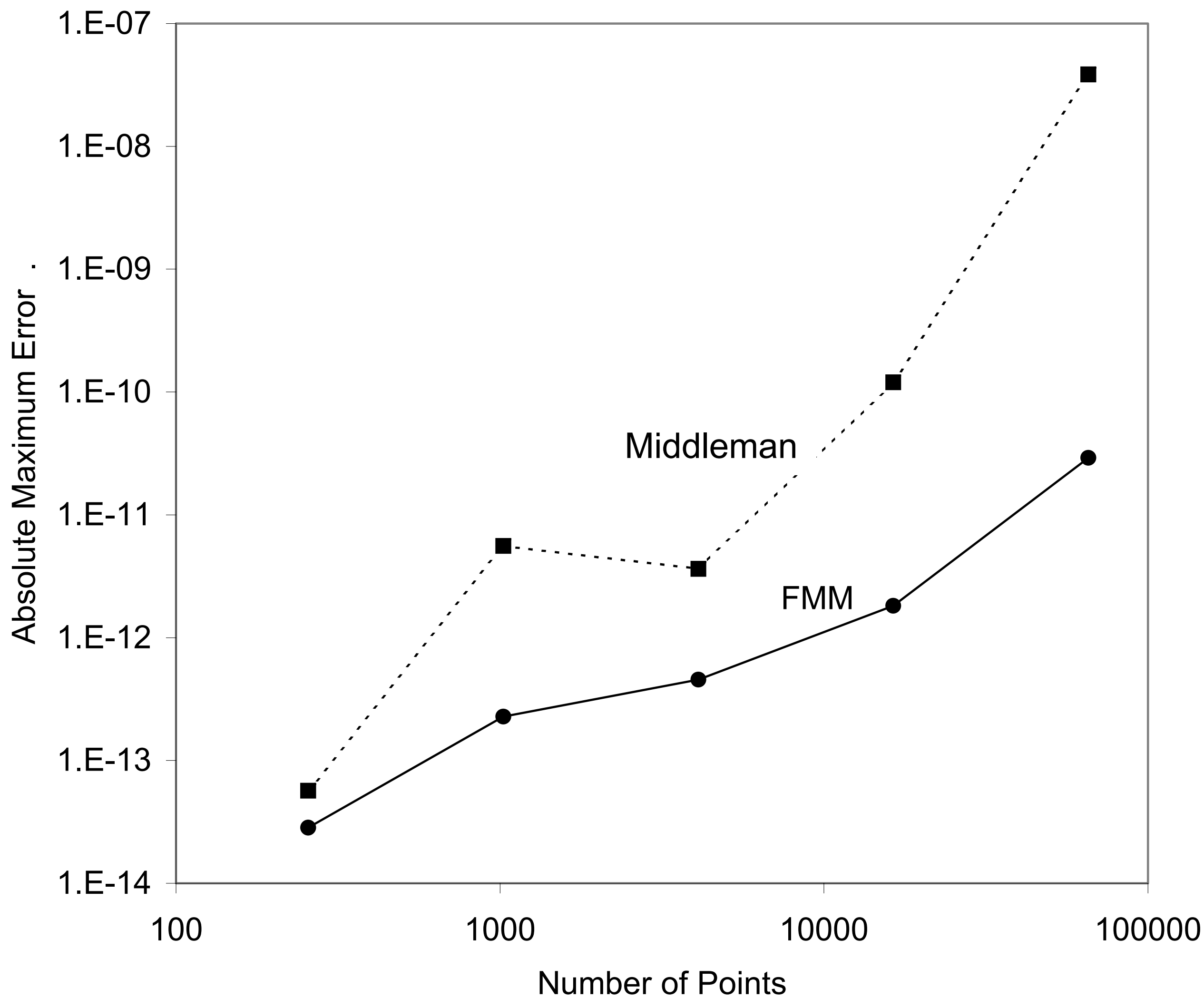
$$For\ d = 2, \quad P = 10, \quad s = 1, \quad CostMLFMM \quad \sim 360NP = 3600N.$$

In this example optimization results in about 10 times savings!

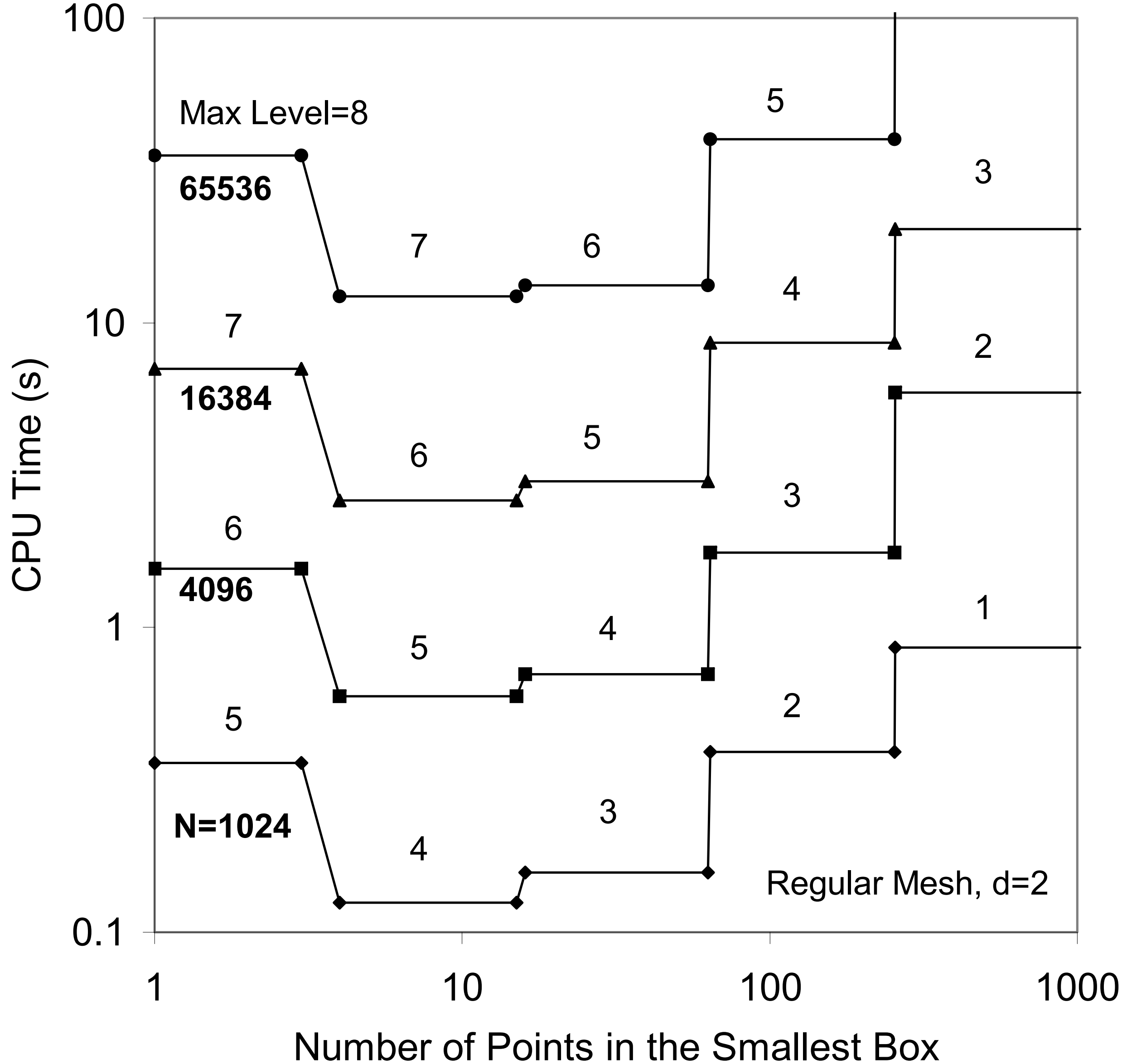
Some Numerical Experiments with MLFMM

Regular Mesh, $N = M$.

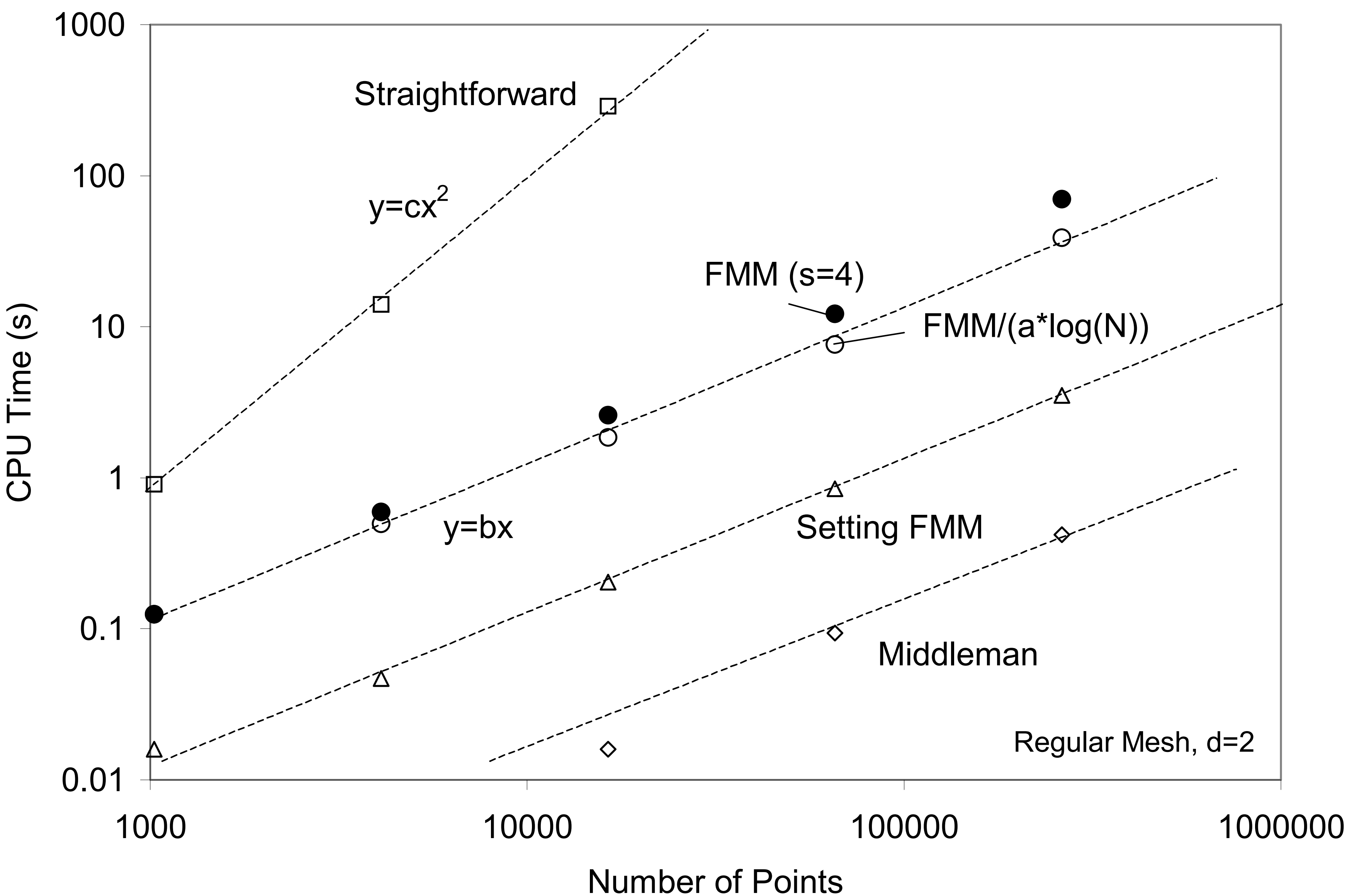
Error Test. FMM vs Middleman.



Test with Varying Grouping Parameter.



Test with Varying N.



Looks like the MLFMM complexity is $O(NlogN)$?

$$CostMLFMM = (M+N)P + (P_4(d)+2)\frac{N}{s}CostTranslation(P) + P_2(d)sMCostFunc,$$

$$CostTranslation(P) = PureCostTranslation(P) + \beta \log N.$$

$$s_{opt} = \left[\frac{N(P_4(d)+2)(PureCostTranslation(P) + \beta \log N)}{MP_2(d)CostFunc}\right]^{1/2}$$

$$CostMLFMM_{opt} \sim (M+N)P + [MN(C+\log N)]^{1/2}$$

Asymptotic Complexity of the optimized $MLFMM$ at $M \sim N$ is

$$CostMLFMM_{opt} = O(N \log^{1/2} N)$$

Asymptotic Complexity of non-optimized $MLFMM$ at $M \sim N$ is

$$CostMLFMM_{opt} = O(N \log N)$$

To have this asymptotics realized one may need incredibly large N. For example,

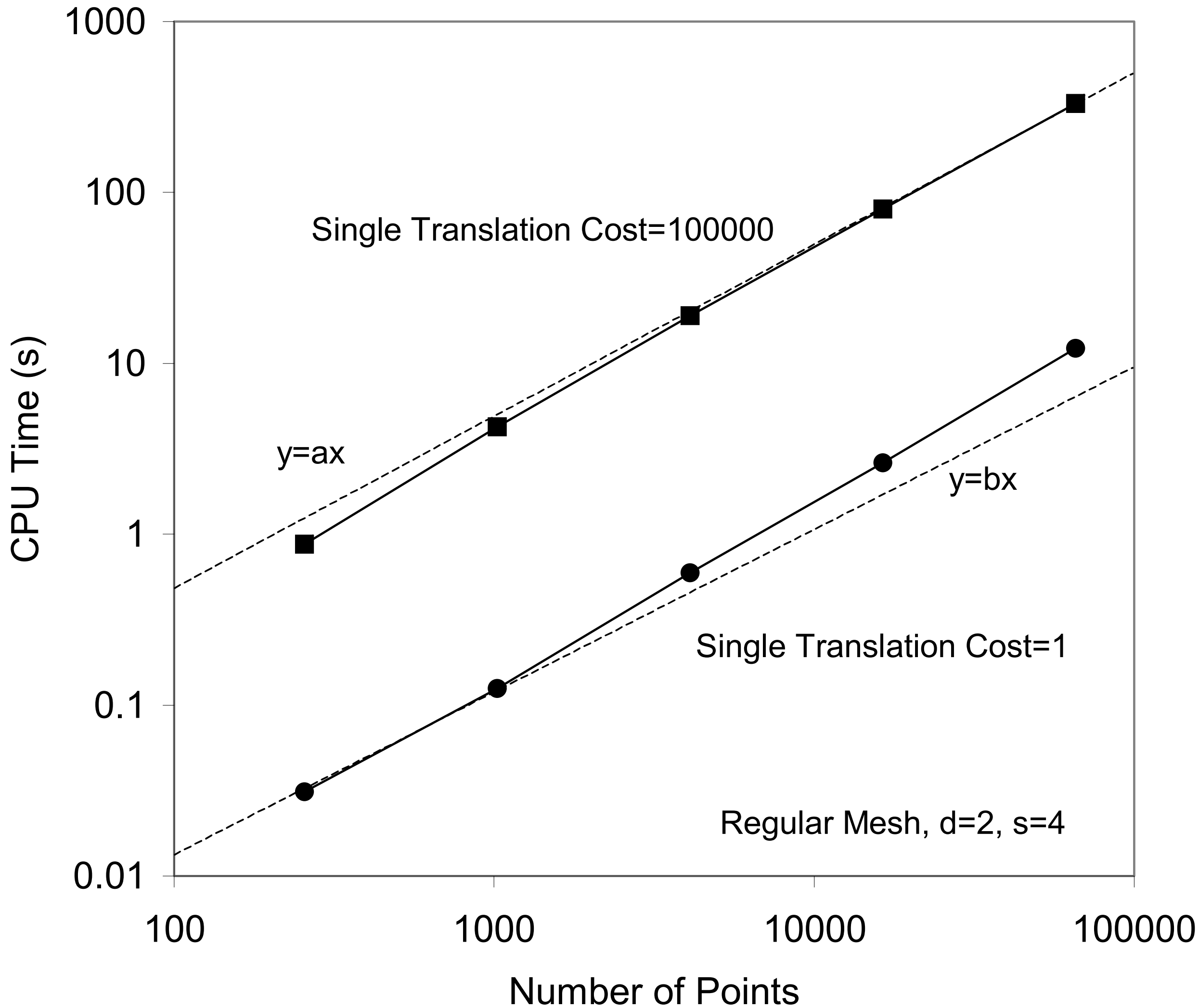
$$P = 5, \quad \beta = 1, \quad PureCostTranslation(P) = P^2 = 25, \quad \log N \sim 25, \quad N \sim 2^{25} \sim 3 \bullet 10^7,$$

$$P = 10, \quad \beta = 1, \quad PureCostTranslation(P) = P^2 = 100, \quad \log N \sim 100, \quad N \sim 2^{100} \sim 10^{60}.$$

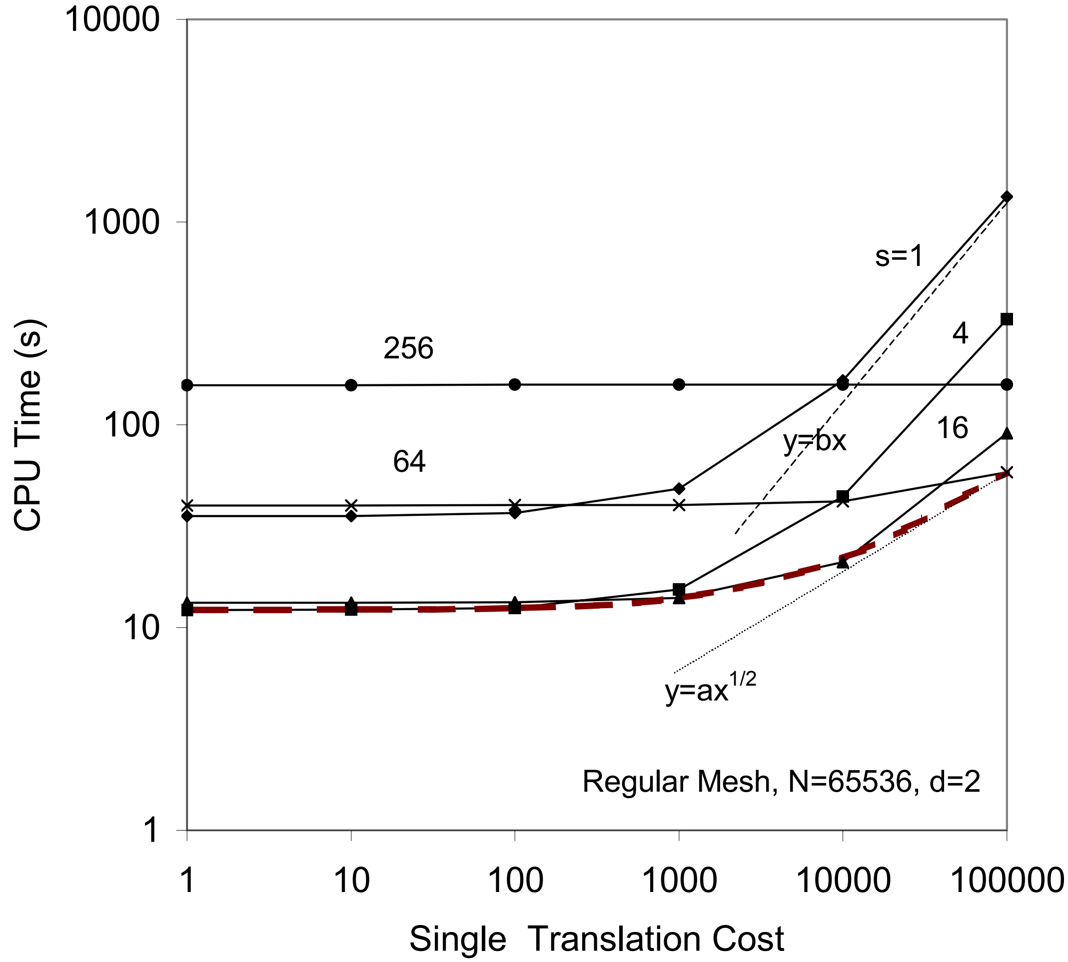
Looks like the MLFMM complexity is $O(NlogN)$?

Explanation of log behavior in the numerical example: Translation was very cheap, PureCostTranslation ~ 5, while β was also small (say 0.2-0.5), so some influence of log dependence was observable.

Test at different translation costs



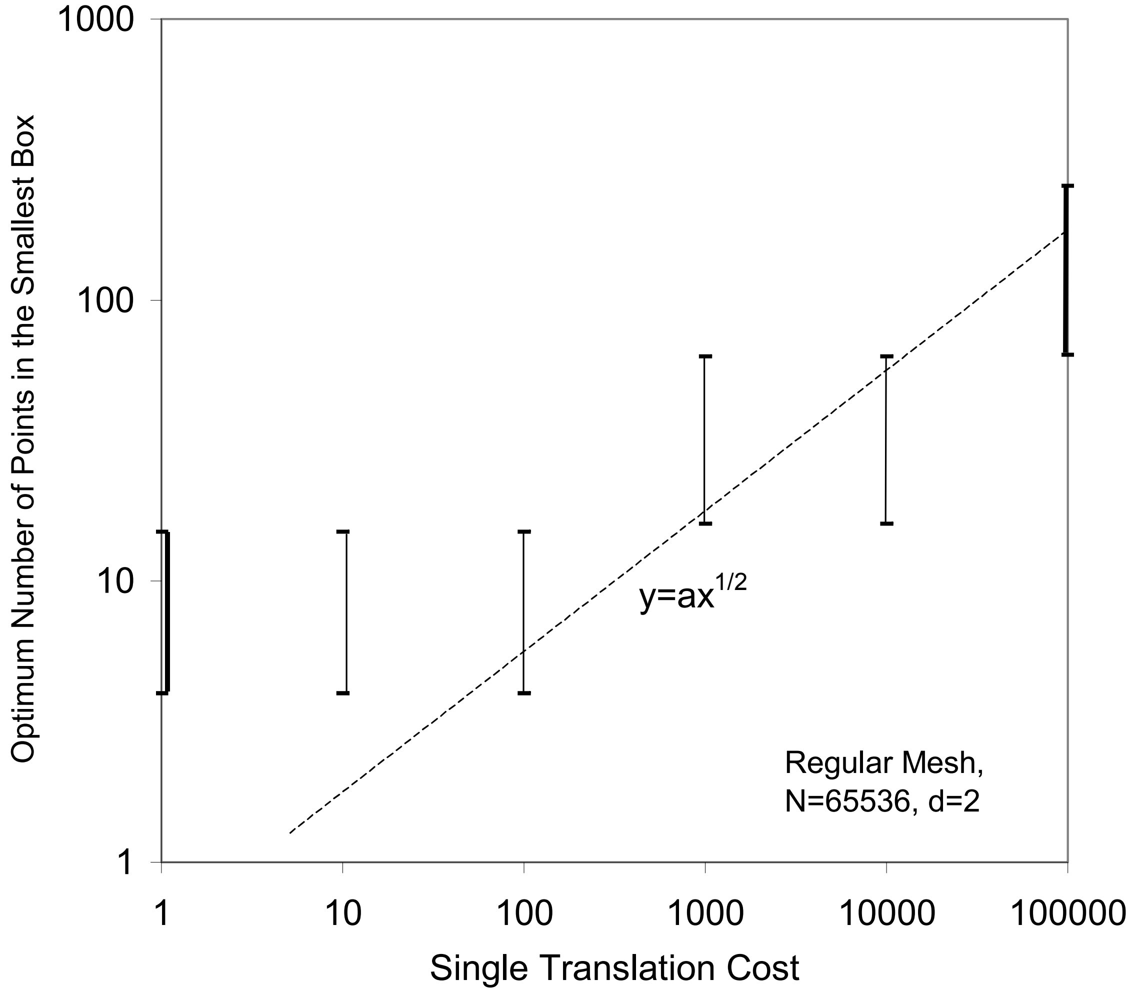
Test with Varying *TranslationCost*(*P*)



$$CostMLFMM = (M+N)P + (P_4(d)+2)\frac{N}{s}CostTranslation(P) + P_2(d)sMCostFunc,$$

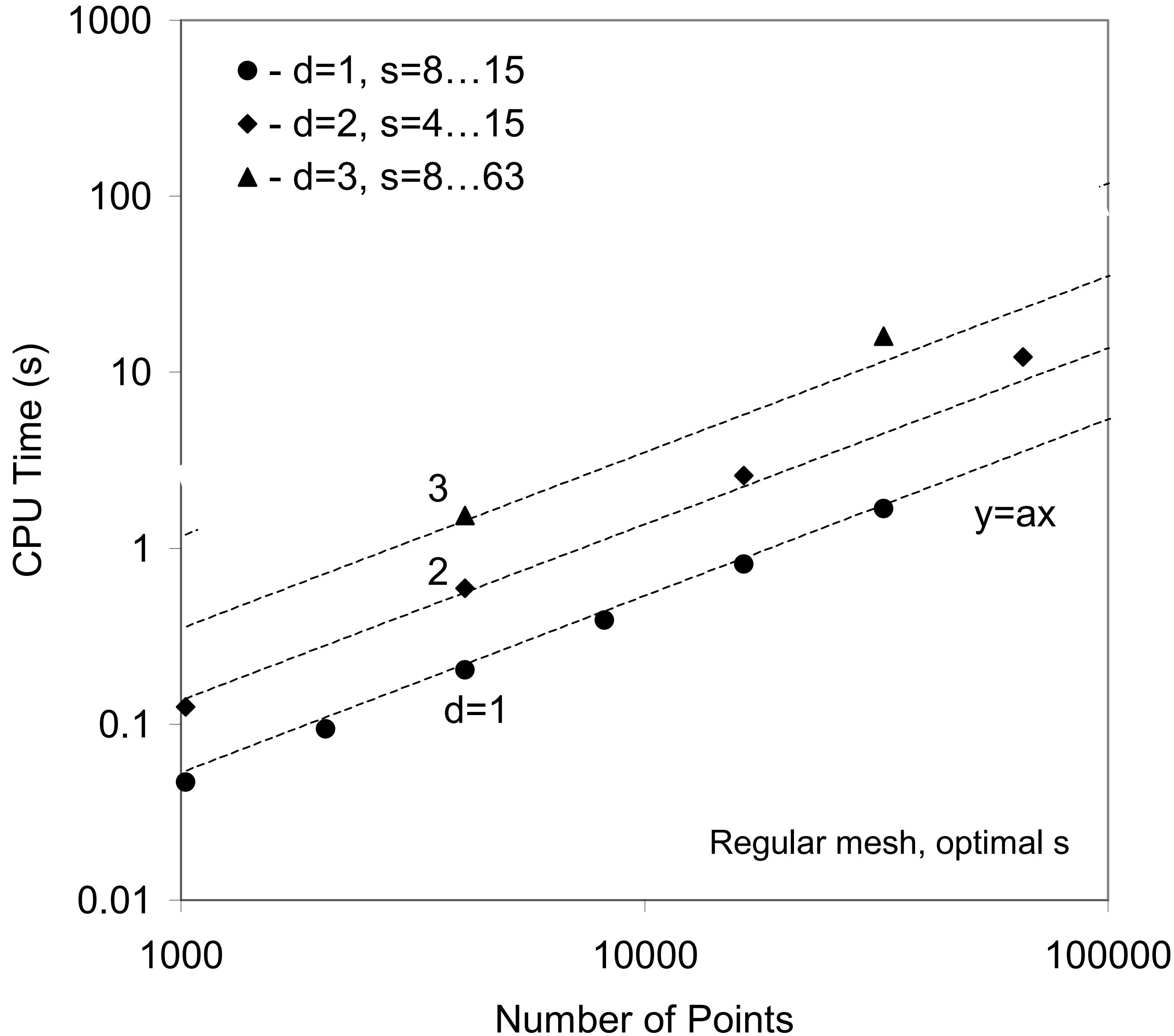
$$CostMLFMM_{opt} = (M+N)P + 2[MN(P_4(d)+2)P_2(d)CostTranslation(P)CostFunc]^{1/2}.$$

Test with Varying *TranslationCost*(*P*)



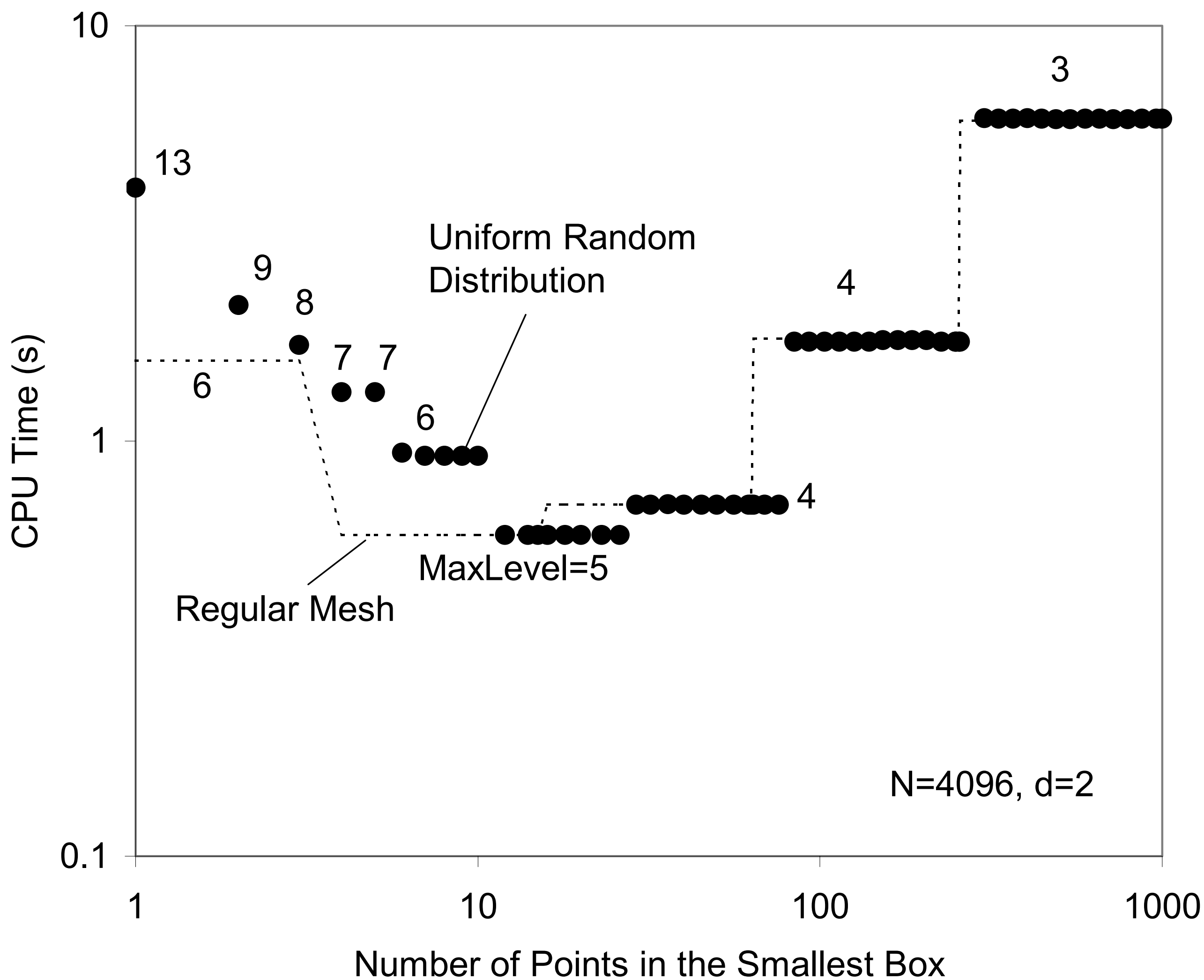
$$s_{opt} = \left[\frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc} \right]^{1/2}.$$

Comparisons for different dimensionalities

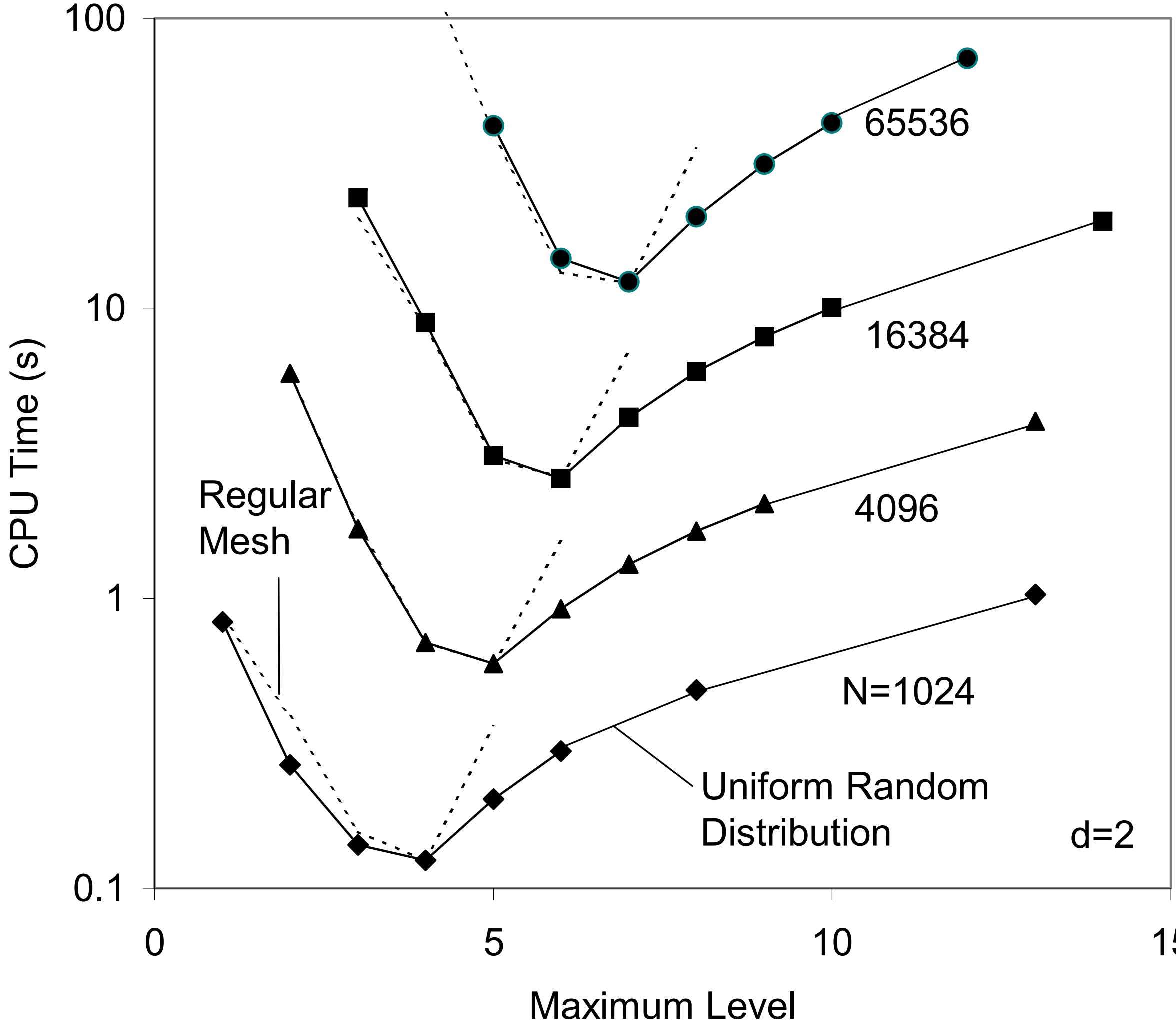


Random Distributions

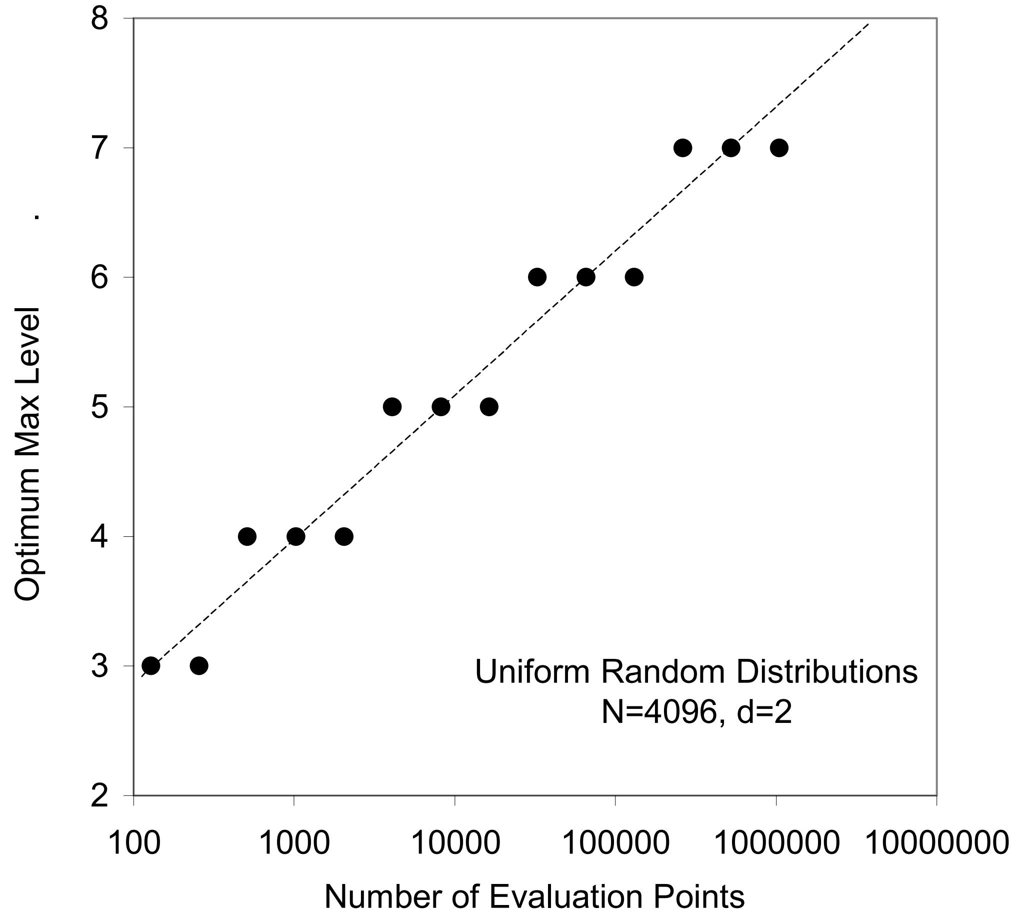
Dependence of CPU Time on the Grouping Parameter, s



Dependence of CPU Time on the Maximum Space Subdivision Level



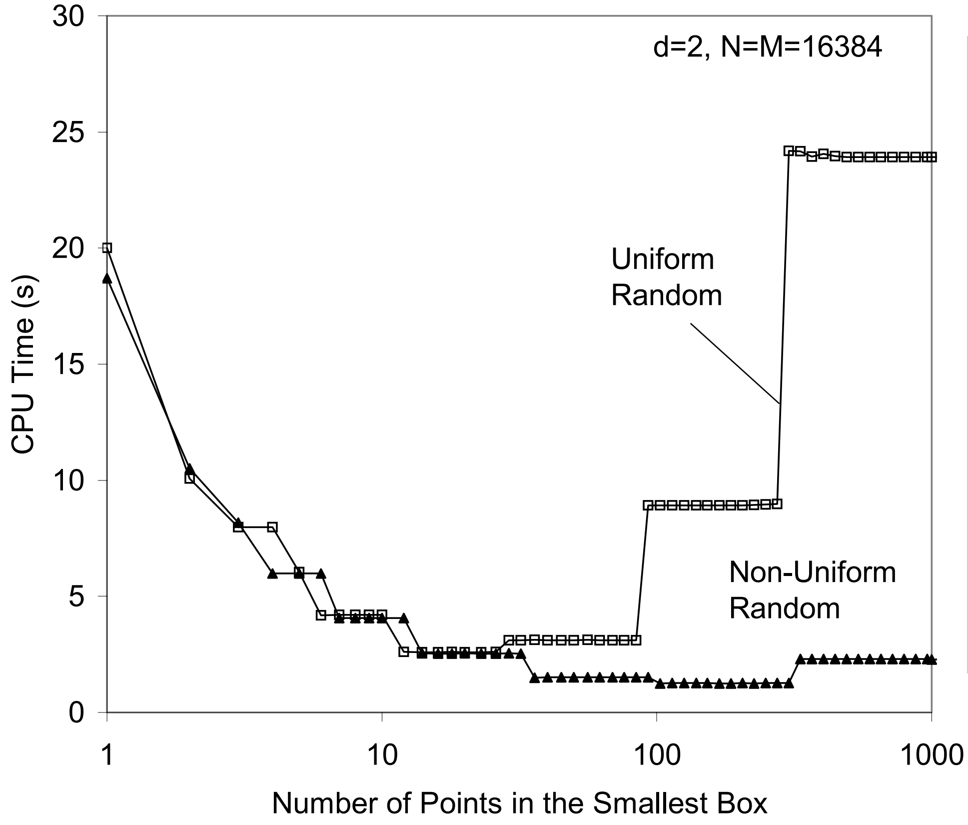
Dependence of Optimum Max Level on *M*

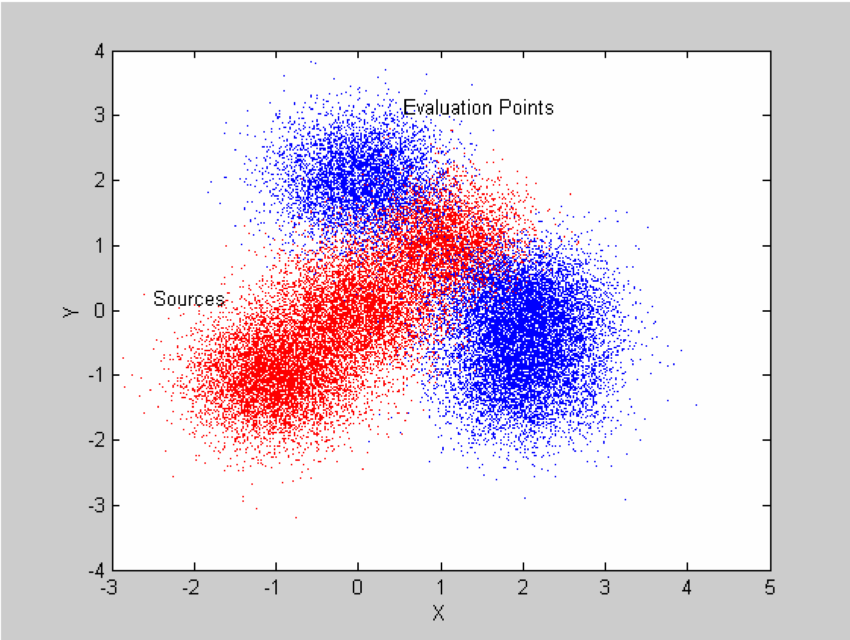


$$s_{opt} = \left[\frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc} \right]^{1/2} \sim M^{-1/2},$$

$$L_{opt} \sim L_* - \left[\frac{1}{d} \log_2 s_{opt} \right] \sim L_* + \left[\frac{1}{2d} \log_2 M \right]$$

Example of A Non-Uniform Random Distribution





Domains of Expansion Validity (1)

Consider d –dimensional space.
Size of box at level l :

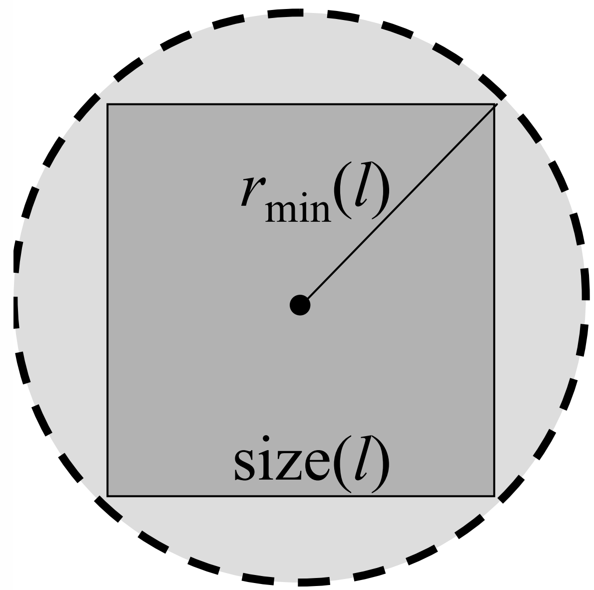
$$size(l) = 2^{-l}.$$

Half of diagonal of box at level l :

$$diag(l) = 2^{-l}\frac{1}{2}\,\square\sqrt{d} = 2^{-l-1}\sqrt{d}.$$

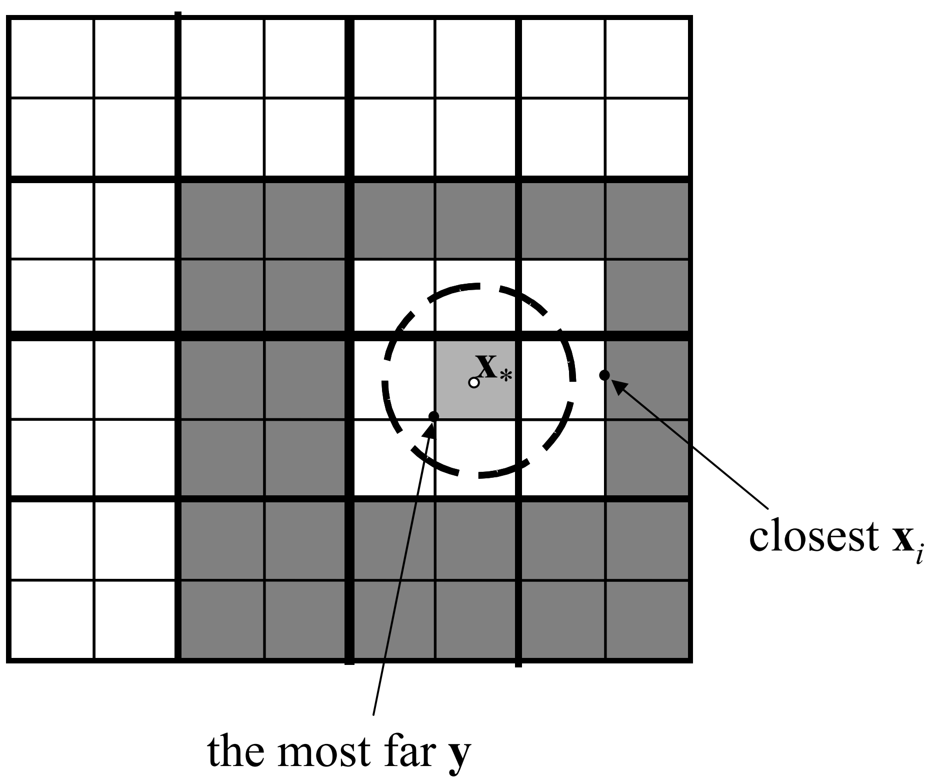
Minimum sphere radius containing the box

$$r_{\min}(l) = diag(l).$$

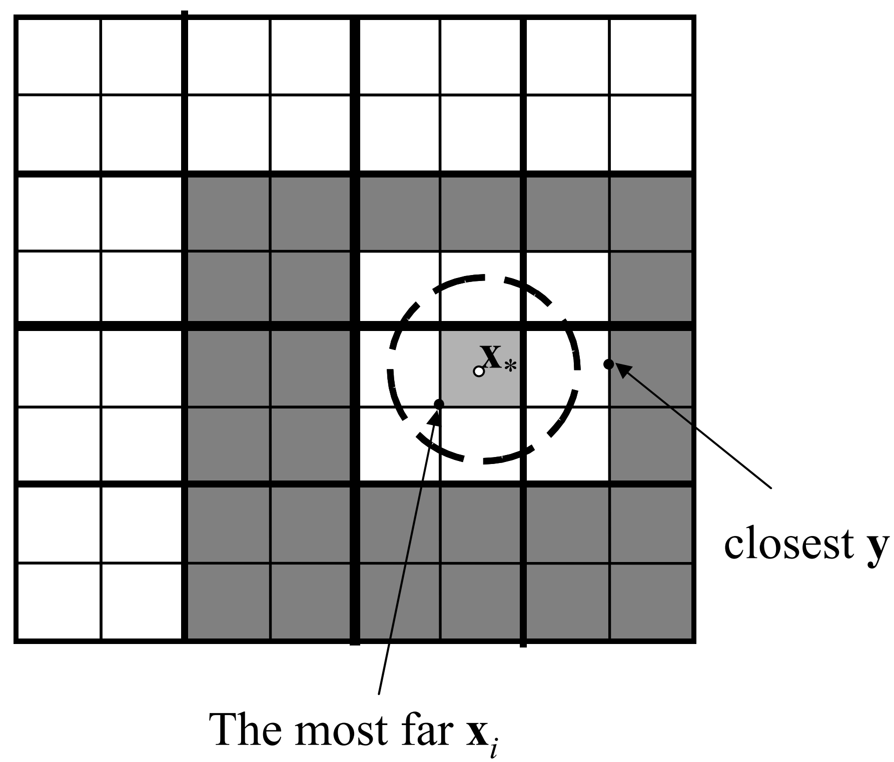


Domains of Expansion Validity (2)

R-expansion



S-expansion



Domains of Expansion Validity (3). R-expansion.

- Potentials (functions) can be factorized as (local expansion):

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{A}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| < r < |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, \ldots, N$$

$$|\mathbf{y} - \mathbf{x}_*| \leqslant r_{\min}(l),$$

$$|\mathbf{x}_i - \mathbf{x}_*| \geqslant \frac{3}{2} size(l).$$

Strict inequality

i

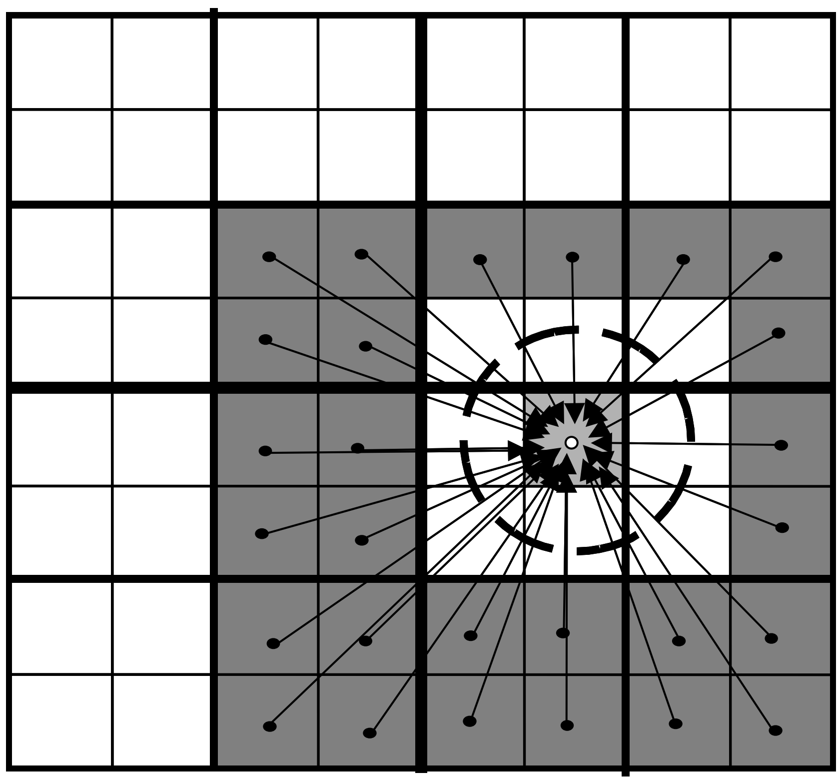
$$r_{\min}(l) < \frac{3}{2} size(l)$$

$$2^{-l-1}\sqrt{d} < \frac{3}{2} 2^{-l}, \quad d < 9.$$

Domains of Expansion Validity (4). S-expansion.

Potentials (functions) can be factorized as (far field expansion):

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{B}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| > R > |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, \ldots, N$$



Domains of Expansion Validity (5). R|R and S|S-translations.

- R-expansion coefficients can be $R|R$-translated:

$$|\mathbf{y}-\mathbf{x}_{*2}| < |\mathbf{x}_i-\mathbf{x}_{*1}| - |\mathbf{x}_{*1}-\mathbf{x}_{*2}| :$$

$$\mathbf{A}(\mathbf{x}_i,\mathbf{x}_{*2}) = (\mathbf{R}|\mathbf{R})(\mathbf{x}_{*2}-\mathbf{x}_{*1})\mathbf{A}(\mathbf{x}_i,\mathbf{x}_{*1})$$

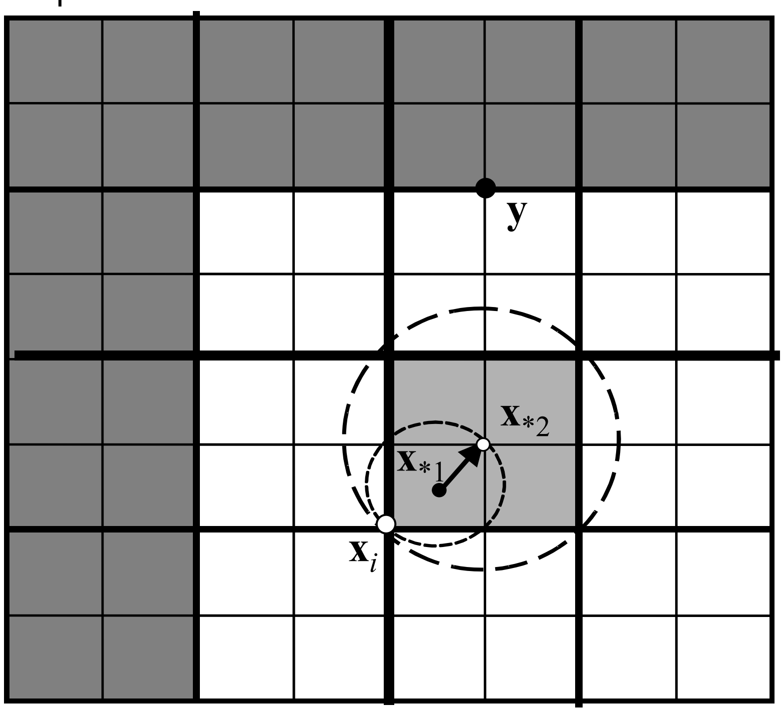
- S-expansion coefficients can be $S|S$-translated:

$$|\mathbf{y}-\mathbf{x}_{*2}| > |\mathbf{x}_{*1}-\mathbf{x}_{*2}| + |\mathbf{x}_i-\mathbf{x}_{*1}|,$$

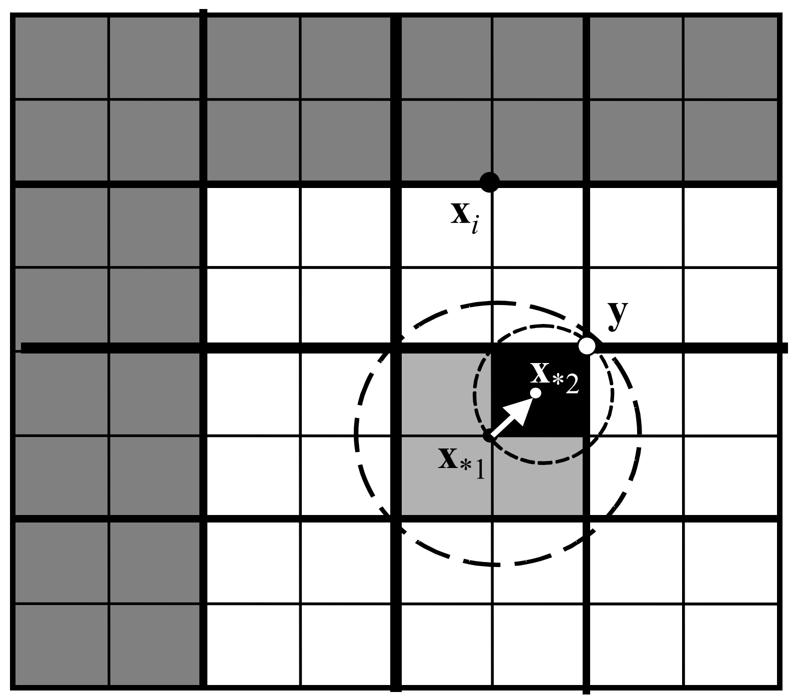
$$\mathbf{B}(\mathbf{x}_i,\mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{S})(\mathbf{x}_{*2}-\mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i,\mathbf{x}_{*1})$$

No additional constraints

S|S



R|R

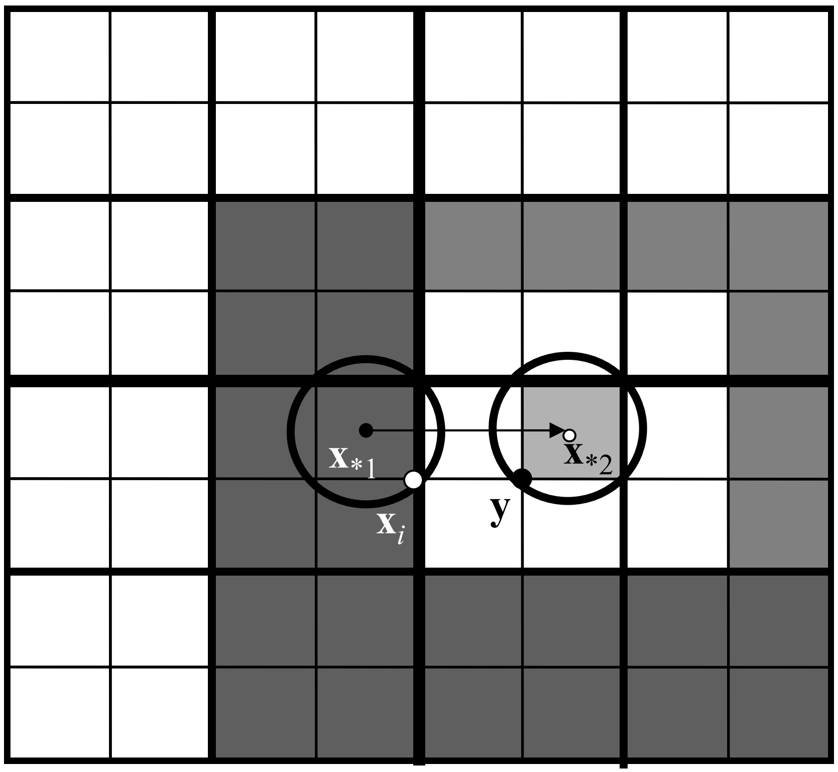


Domains of Expansion Validity (6). S|R-translation.

- S-expansion coefficients can be $S|R$-translated (converted to R-expansion coefficients)

$$|\mathbf{y}-\mathbf{x}_{*2}| < |\mathbf{x}_{*1}-\mathbf{x}_{*2}| - |\mathbf{x}_i-\mathbf{x}_{*1}|,$$

$$\mathrm{A}(\mathbf{x}_i,\mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{R})(\mathbf{x}_{*2}-\mathbf{x}_{*1})\mathrm{B}(\mathbf{x}_i,\mathbf{x}_{*1})$$



$$|\mathbf{y}-\mathbf{x}_*| < r_{\min}(l), \quad |\mathbf{x}_i-\mathbf{x}_*| < r_{\min}(l),$$

$$\min|\mathbf{x}_{*1}-\mathbf{x}_{*2}| = 2size(l).$$

$$2^{-l-1}\sqrt{d} + 2^{-l-1}\sqrt{d} < 2^{-l+1}, \quad d < 4.$$

$$d < 4$$

What to do in larger dimensions?

Neighborhood Increase Technique

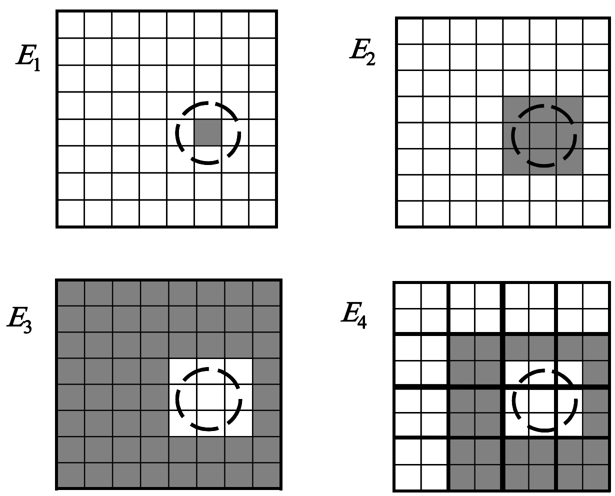
Neighborhood Increase Technique

Recipe: Build a fractal structure with larger neighborhood

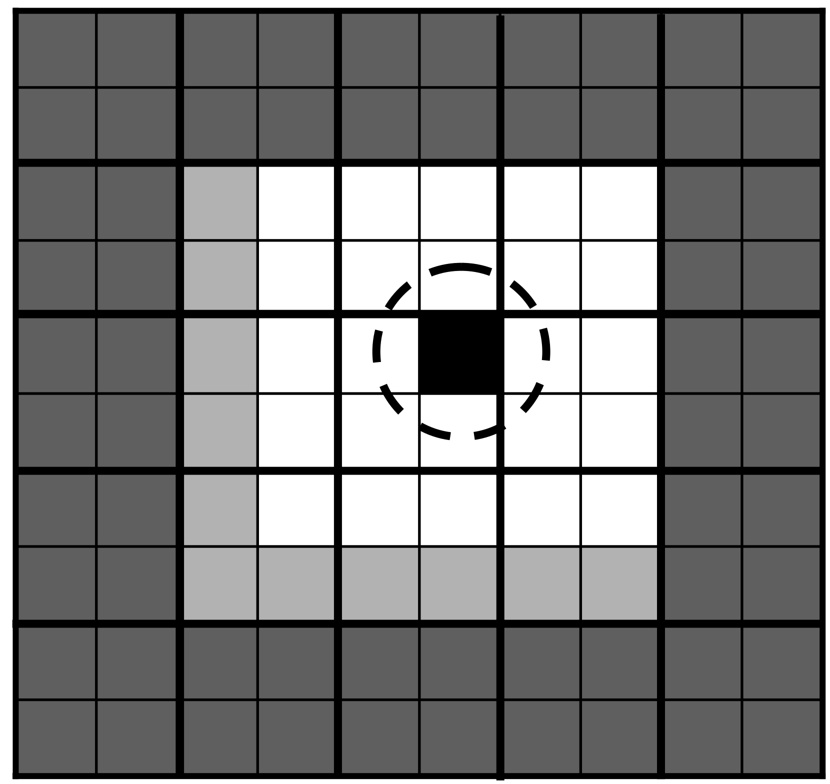
Everything works by the same way, but E_2 and E_4 are larger

We need only: $E_3 = \overline{E}_2$, $E_3(Parent(n),l\text{-}1) \cup E_4(n,l) = E_3(n,l)$.

2-neighborhoods



1-neighborhood



Neighborhood Increase Technique

Advantages:

1) Enables larger dimensionality of the problem;
2) Smaller error (or smaller truncation number).

(Error of the MLFMM will be considered in a separate lecture).

Unfortunately, cannot Increase Indefinitely…

Disadvantages:

1) Usually larger number of operations;
2) Costly search of nonempty boxes in the neighborhood.

Recommended Reading:

N.A. Gumerov, R. Duraiswami & E.A. Borovikov

Data Structures, Optimal Choice of Parameters, and Complexity Results for Generalized Multilevel Fast Multipole Methods in *d* Dimensions.

UMIACS TR 2003-28,
Also issued as *Computer Science Technical Report CS-TR-# 4458*.
University of Maryland, College Park, 2003.

Available online via
http://www.umiacs.umd.edu/~ramani/pubs/umiacs-tr-2003-28.pdf