# FMM CMSC 878R/AMSC 698R

Lecture 13

# 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:

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

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

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

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

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

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

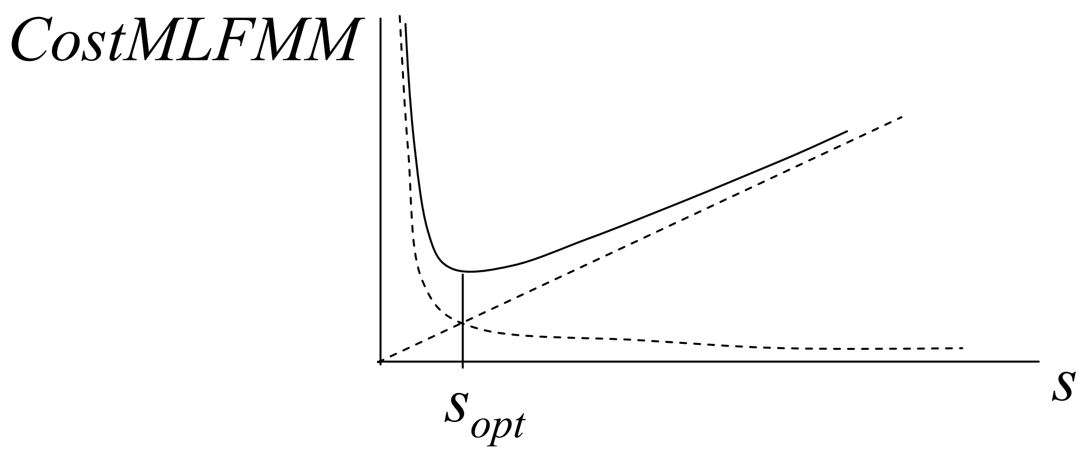
$$CostDownward_2 = 2^d\left(2^{2d} + \ldots + 2^{(L-1)d}\right)CostRR(P) \sim \frac{N}{s}CostRR(P),$$

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

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,

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

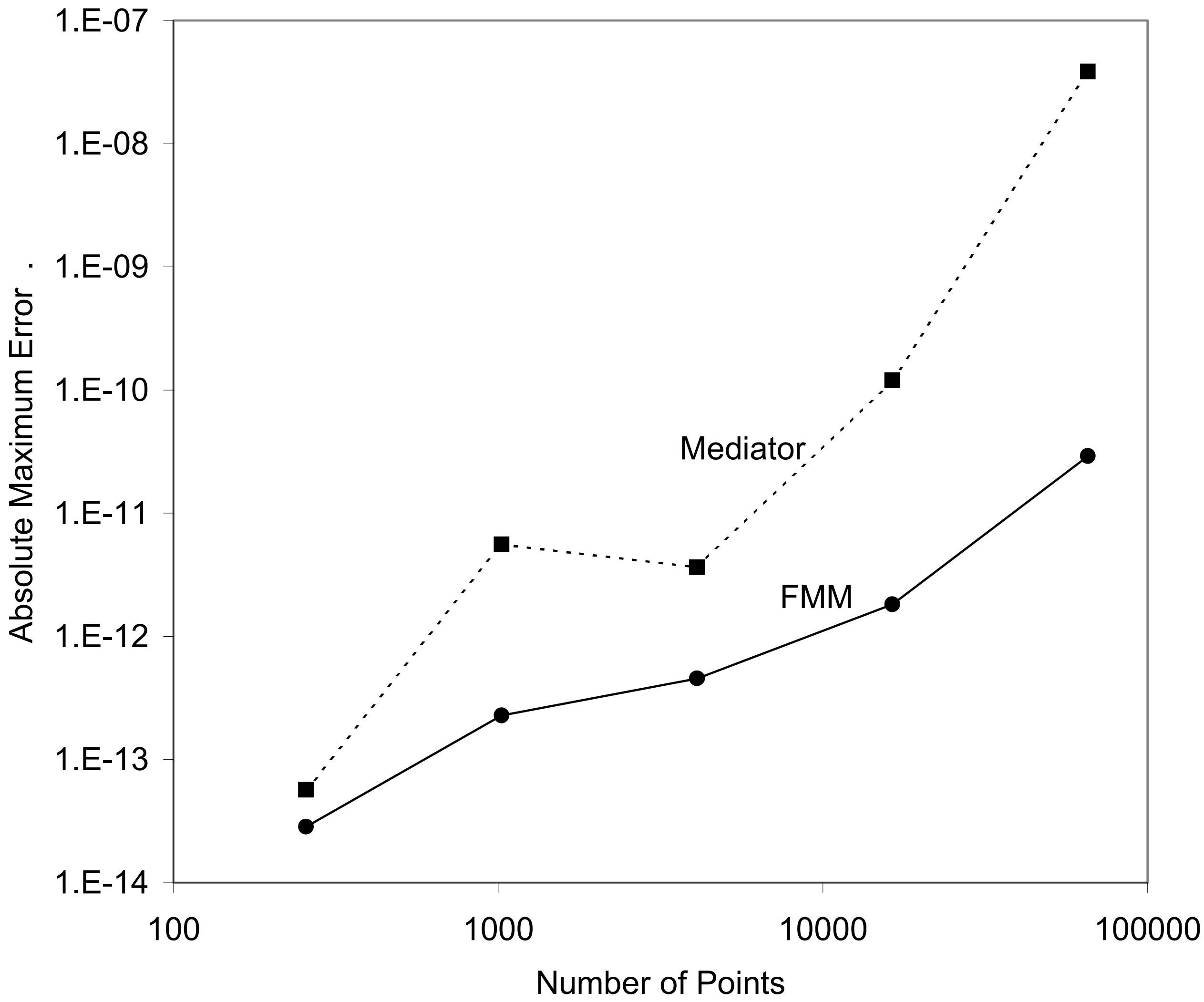
$$For\ d = 2, \quad P = 10, \quad s = 1, \quad CostMLFMM_{opt} \sim 360NP = 3600N.$$

In this example optimization results in about 10 times savings!

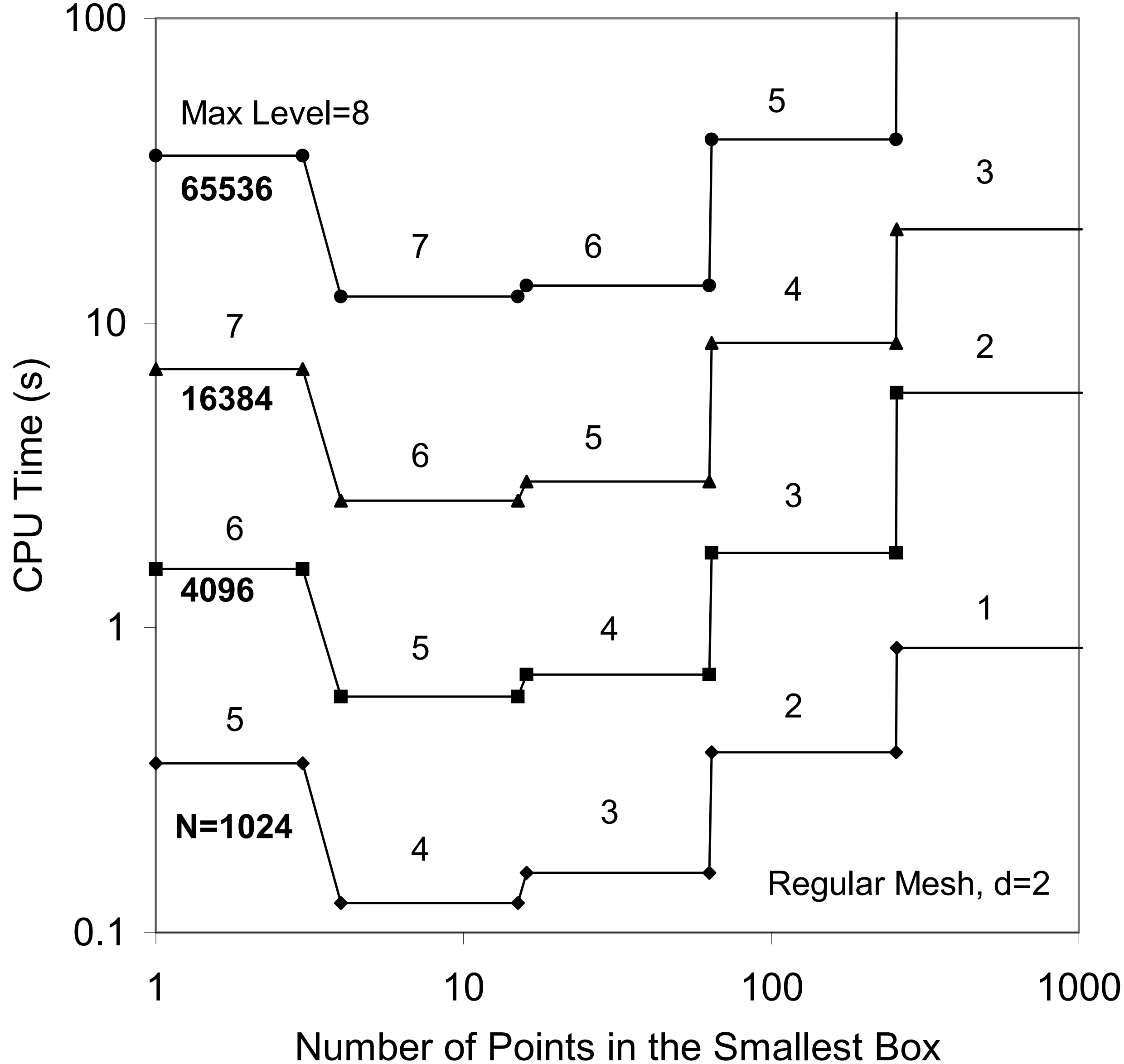
# Some Numerical Experiments with MLFMM

# Regular Mesh, $N = M$.

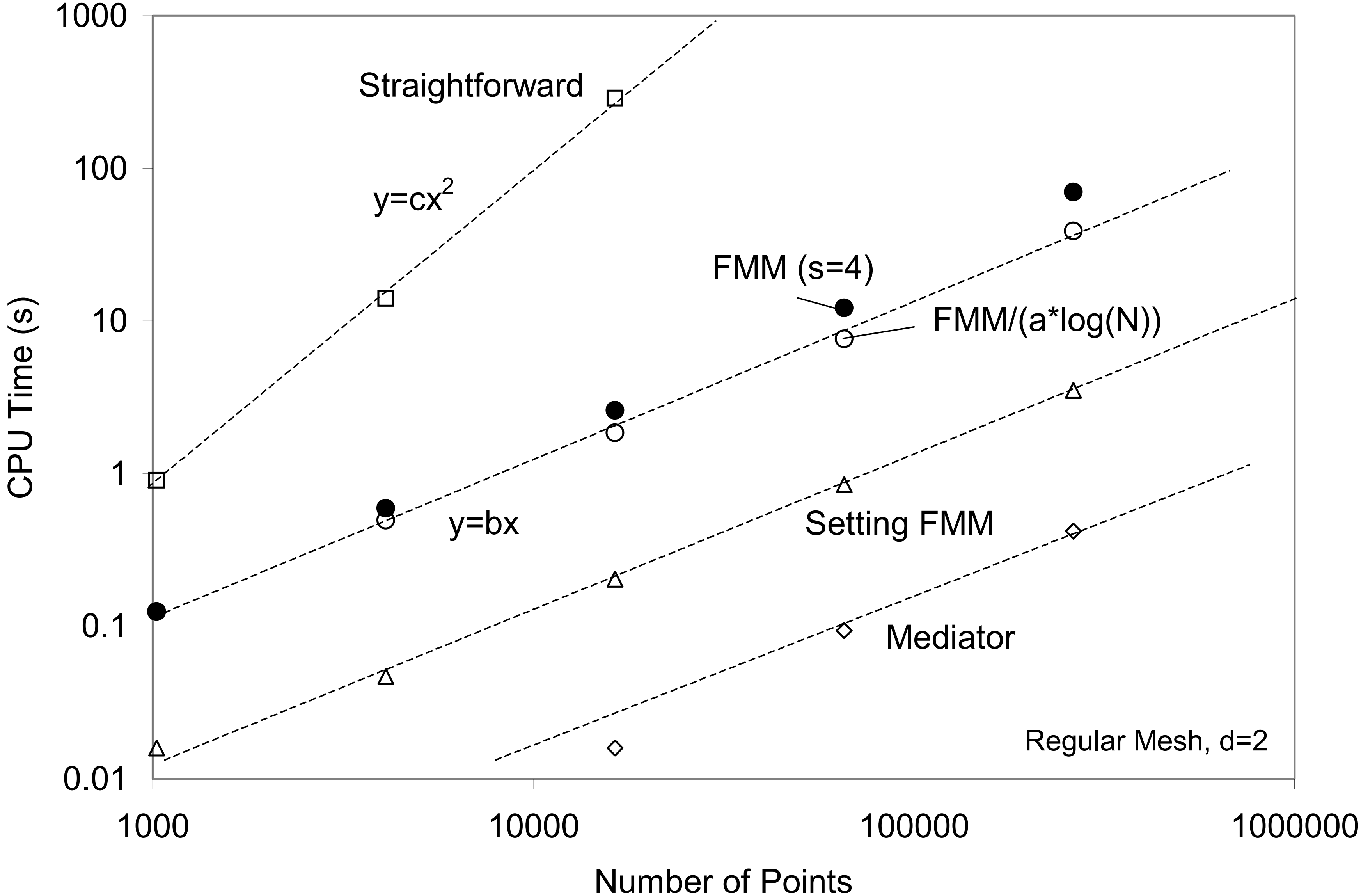
# Error Test. FMM vs Middleman.



# 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,

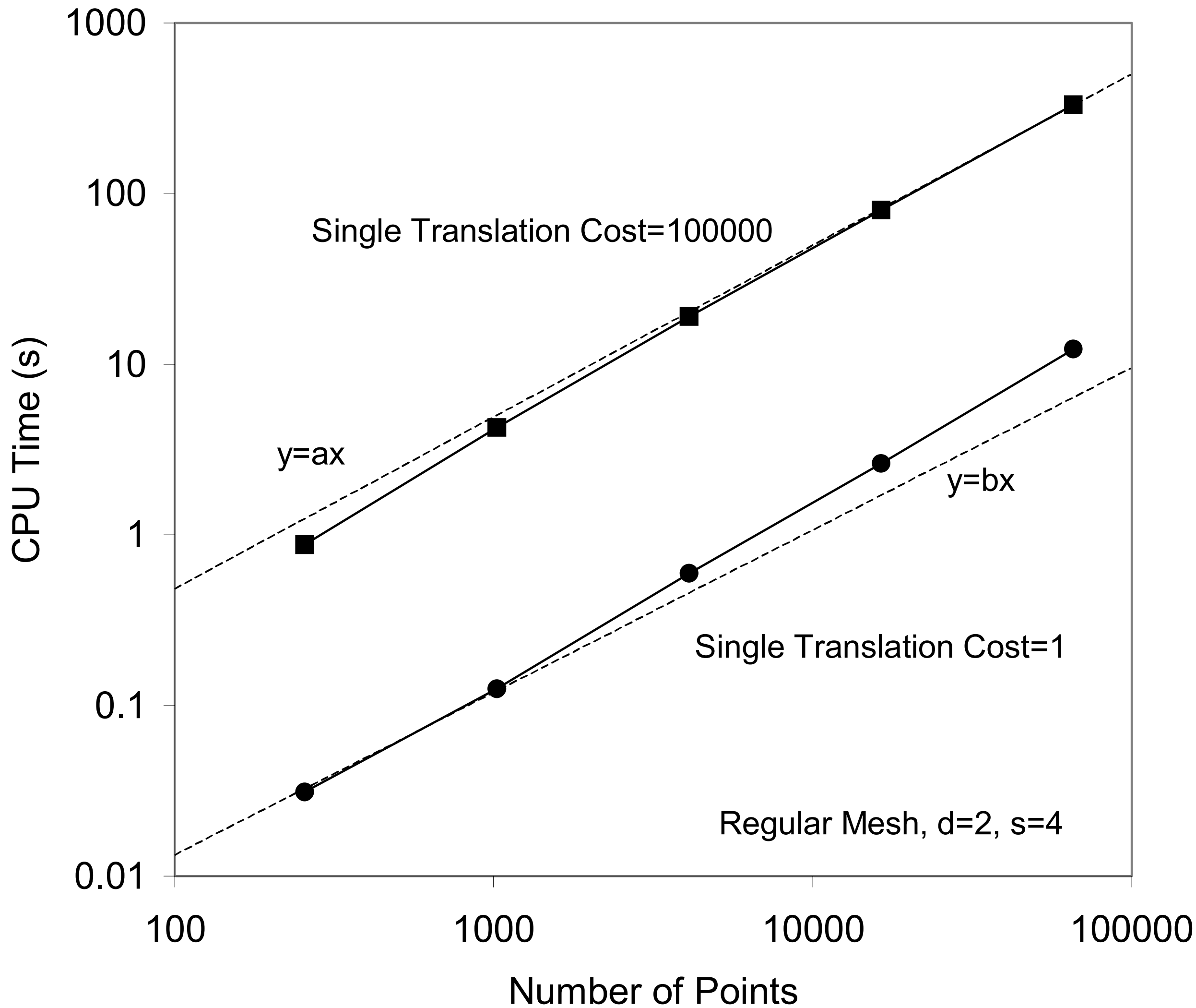
$$P = 5, \quad \beta = 1, \quad PureCostTranslation(P) = P^2 = 25, \quad \log N \sim 25, \quad N \sim 2^{25} \sim 3 \bullet 10^7,$$

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

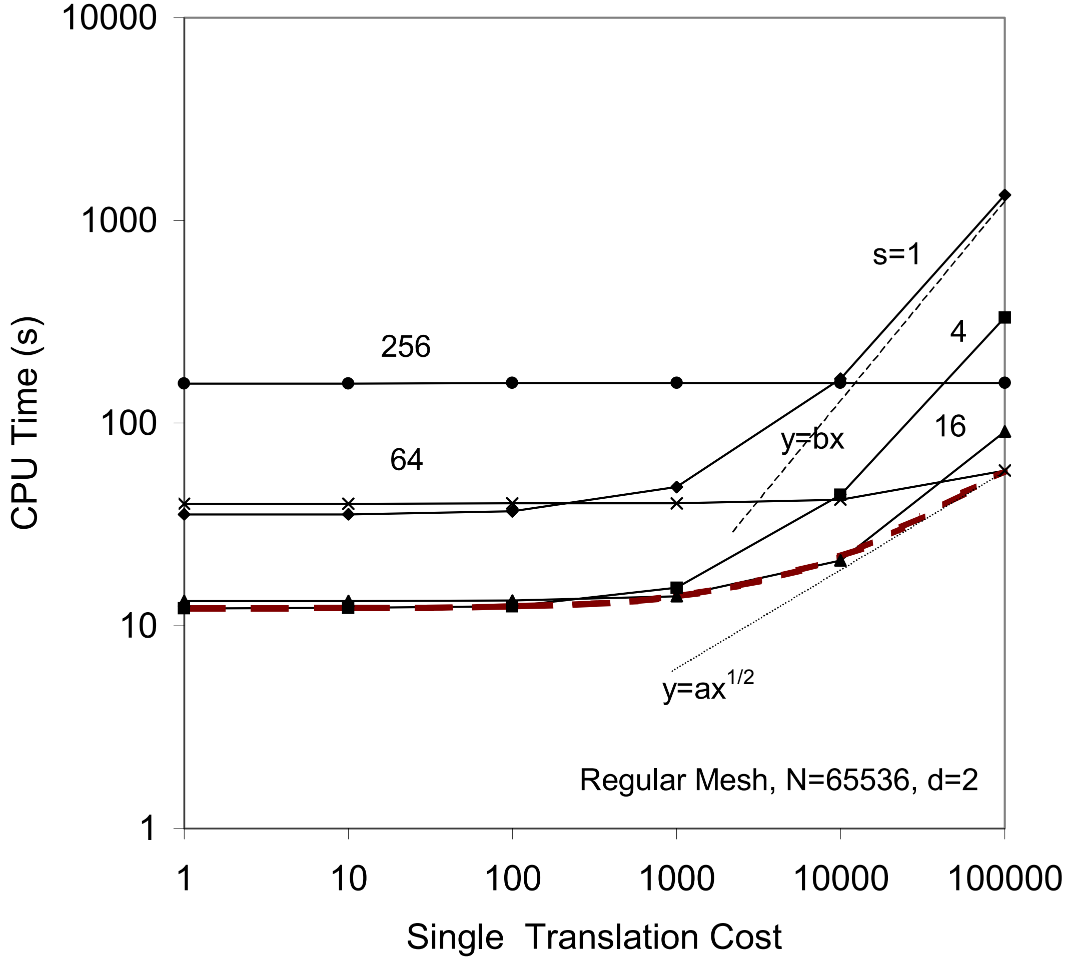
# Looks like the MLFMM complexity is $O(NlogN)$?

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



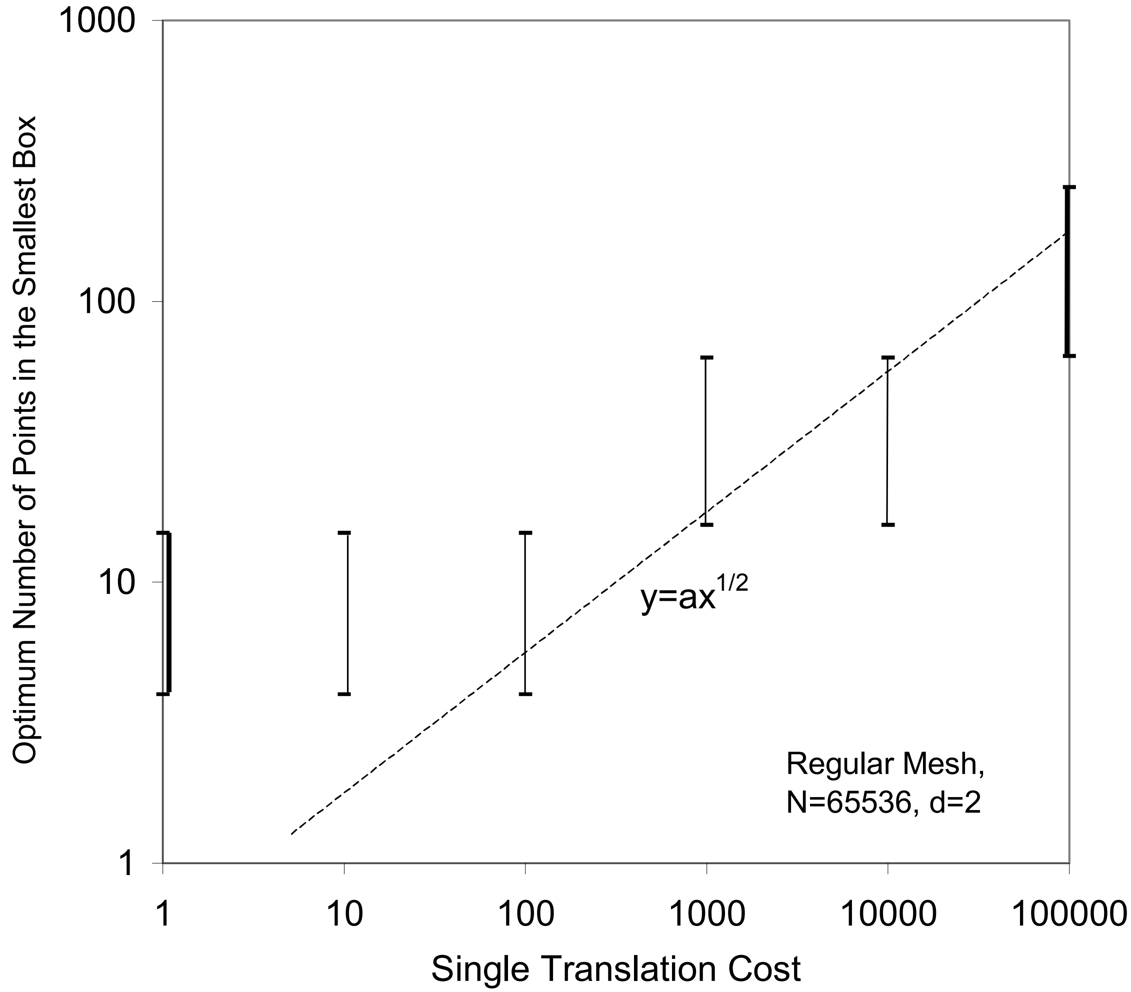
# Test with Varying *TranslationCost*(*P*)




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

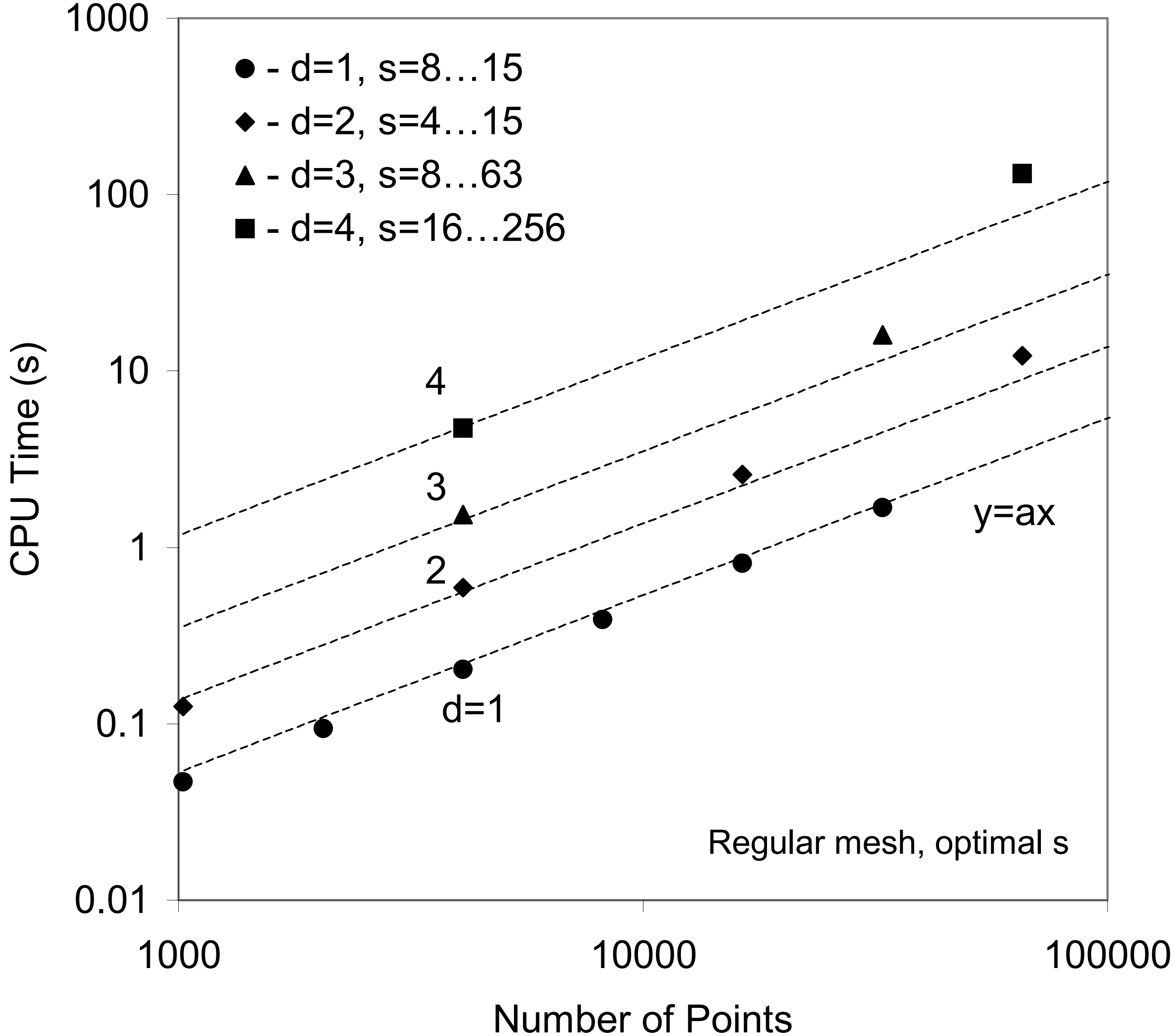
$$CostMLFMM_{opt} = (M+N)P + 2[MN(P_4(d)+2)P_2(d)CostTranslation(P)CostFunc]^{1/2}.$$

# Test with Varying *TranslationCost*(*P*)

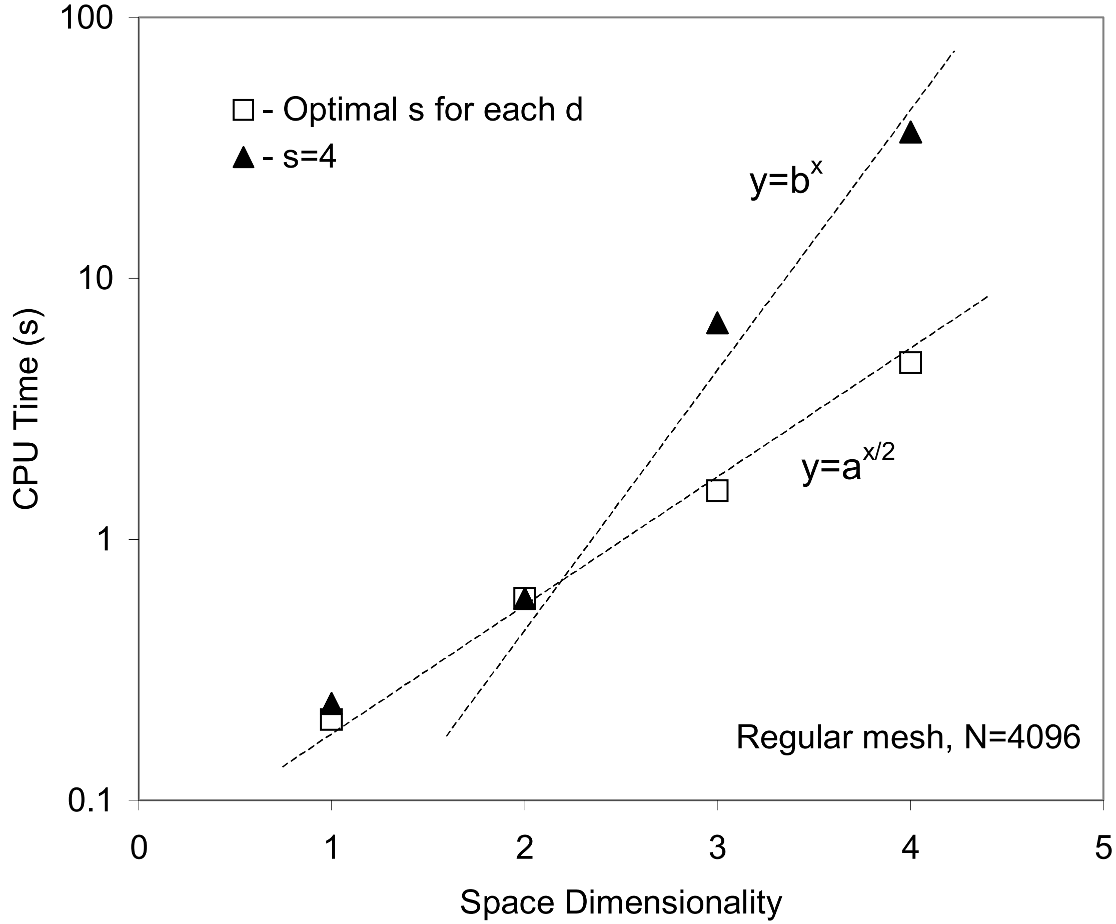



$$s_{opt} = \left[ \frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc} \right]^{1/2}.$$

# Comparisons for different dimensionalities



# Test at different dimensionalities



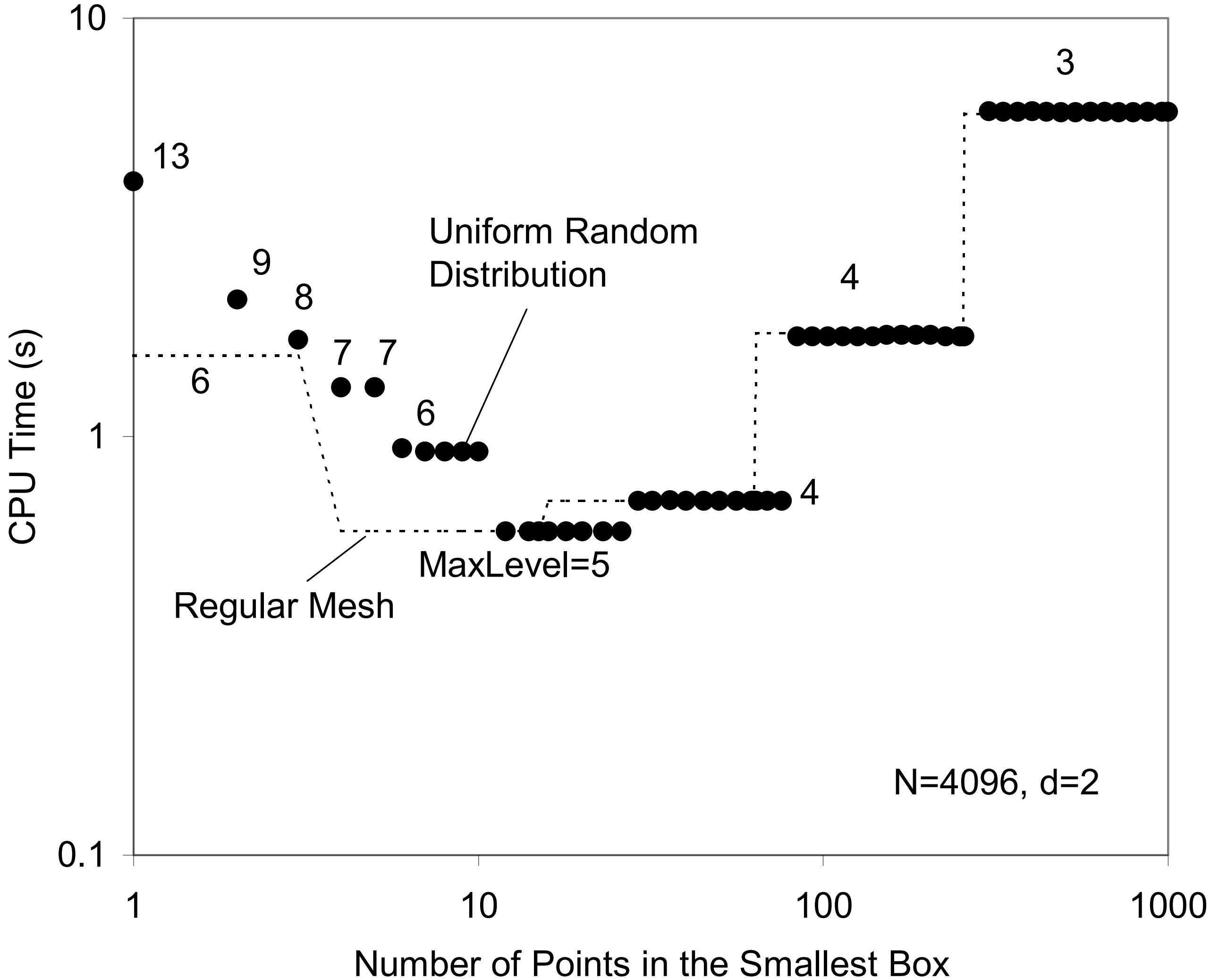

$$P_4(d) \sim c_4^d, \quad P_2(d) \sim c_2^d$$

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

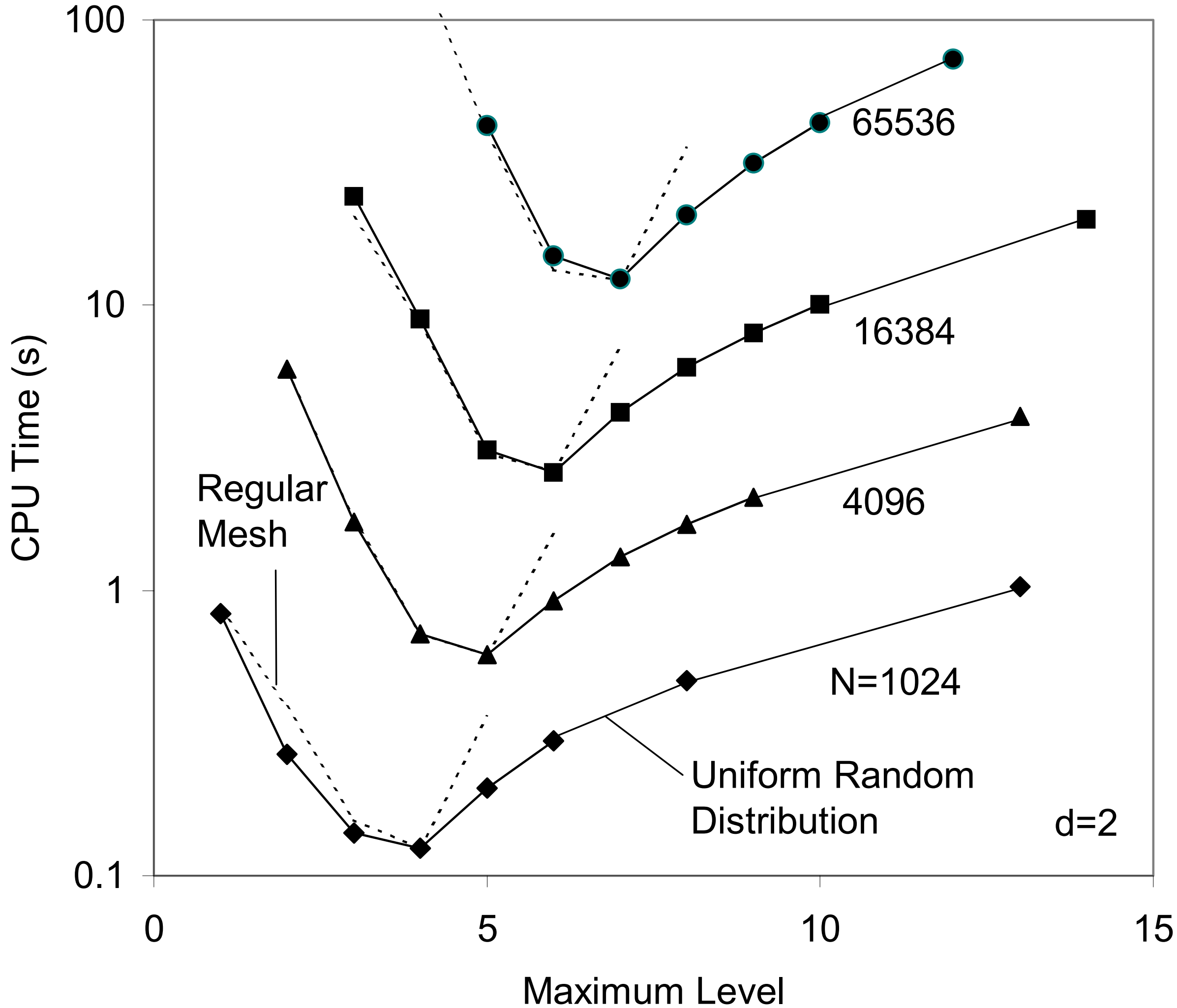
$$CostMLFMM_{opt} = (M+N)P + 2[MN(P_4(d)+2)P_2(d)CostTranslation(P)CostFunc]^{1/2}.$$

# Random Distributions

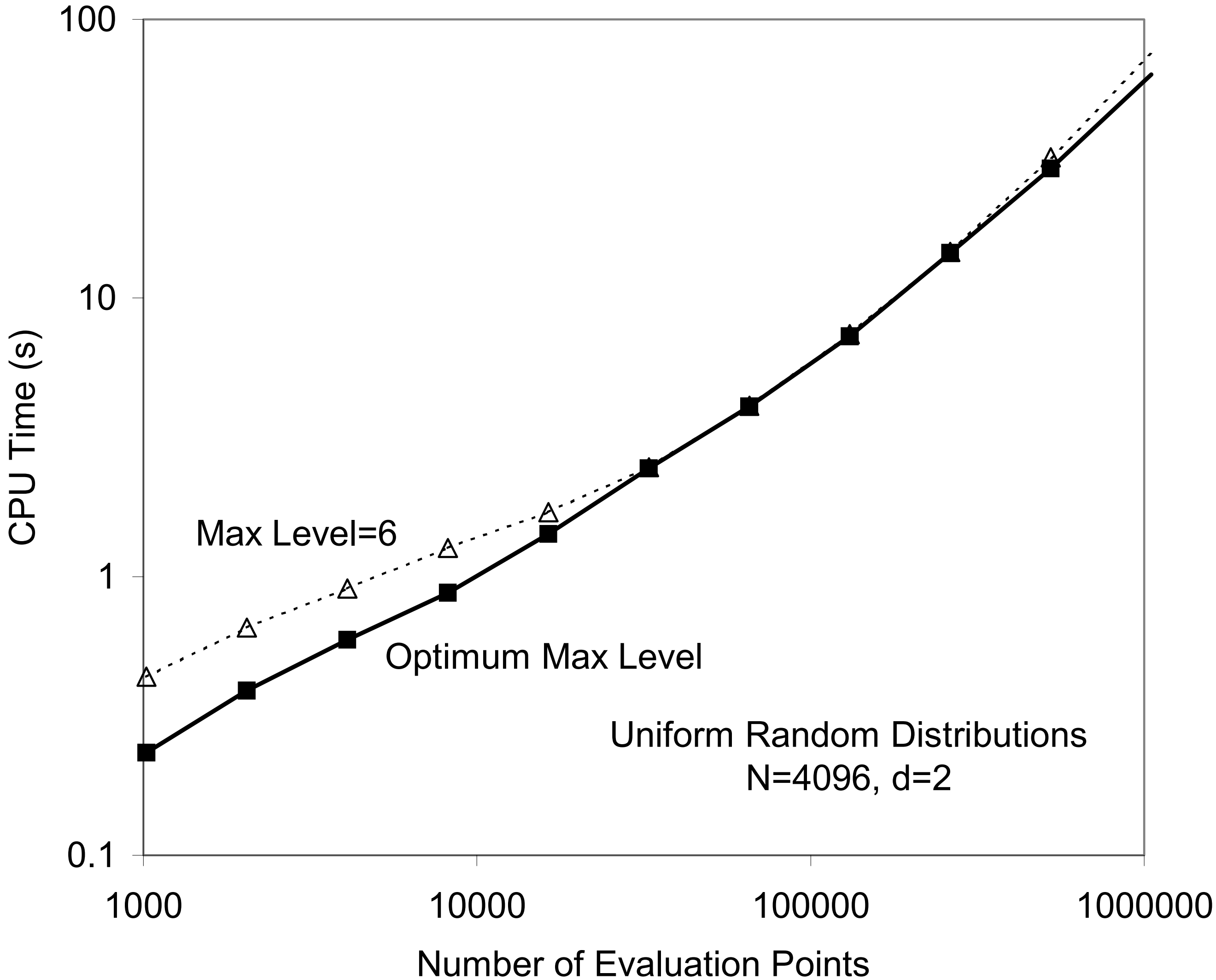
# Dependence of CPU Time on the Grouping Parameter, s



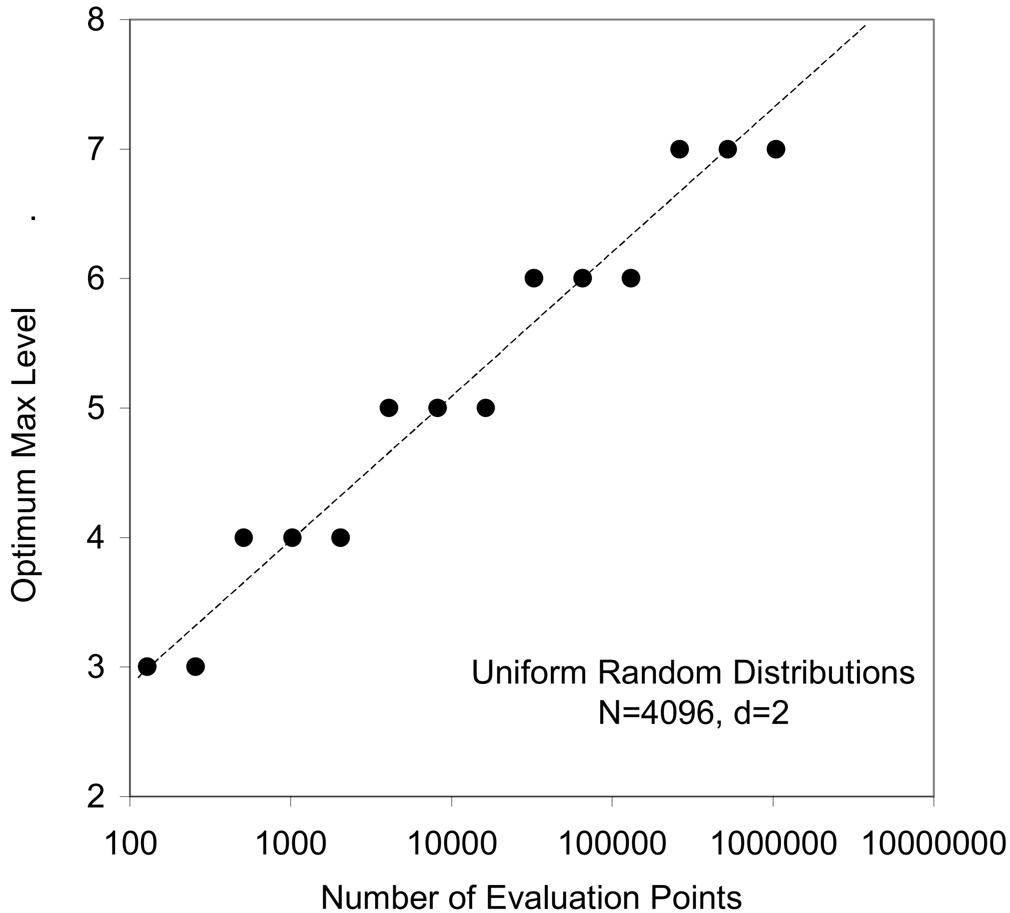
# Dependence of CPU Time on the Maximum Space Subdivision Level



# Dependence of CPU Time on *M*



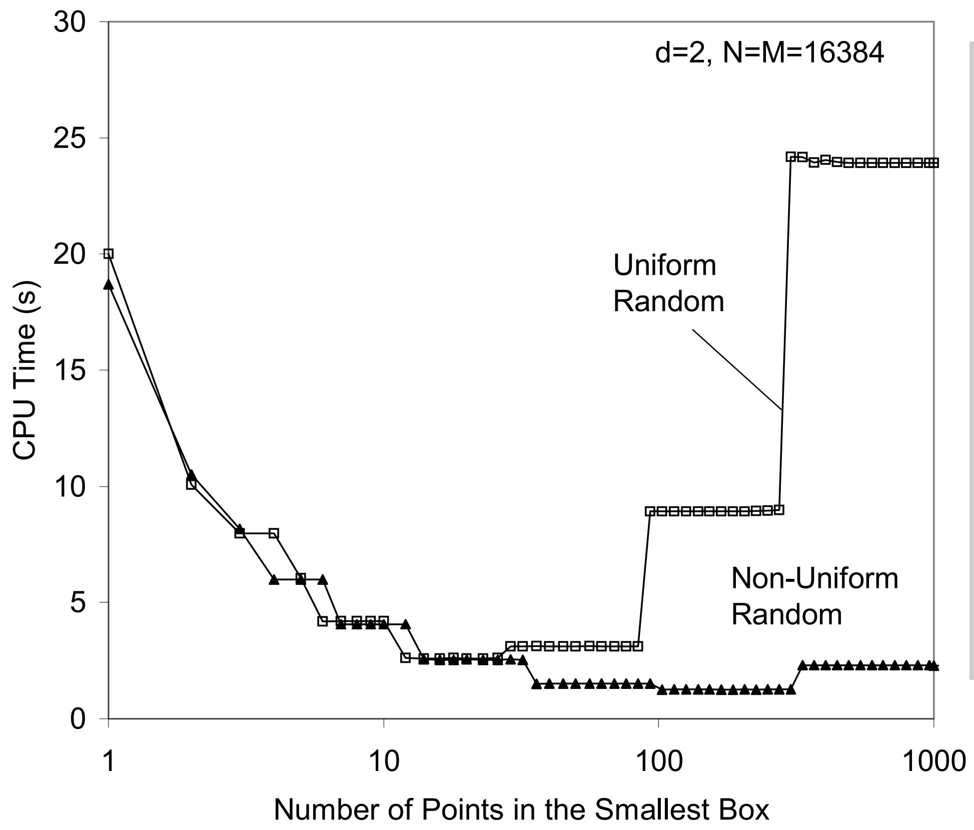
# Dependence of Optimum Max Level on $M$

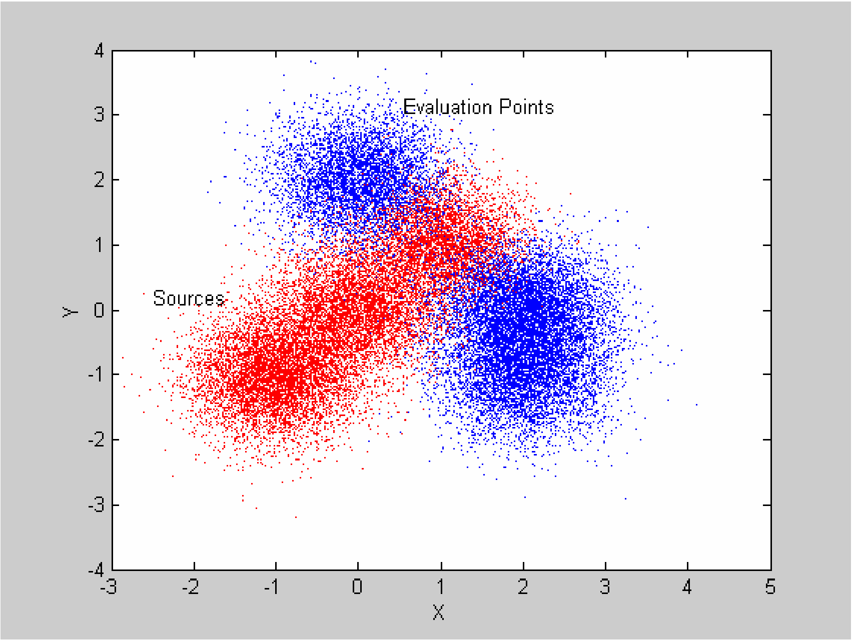



$$s_{opt} = \left[ \frac{N(P_4(d)+2)CostTranslation(P)}{MP_2(d)CostFunc} \right]^{1/2} \sim M^{-1/2},$$

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

# Example of A Non-Uniform Random Distribution



# Domains of Expansion Validity (1)

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

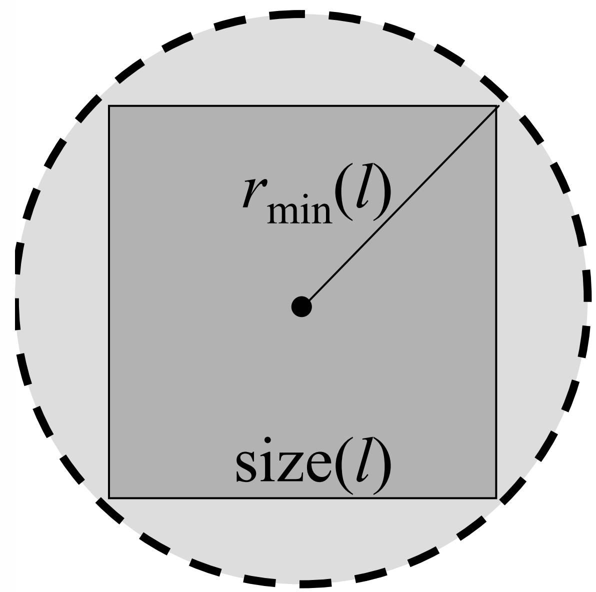
$$size(l) = 2^{-l}.$$

Half of diagonal of box at level $l$ :

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

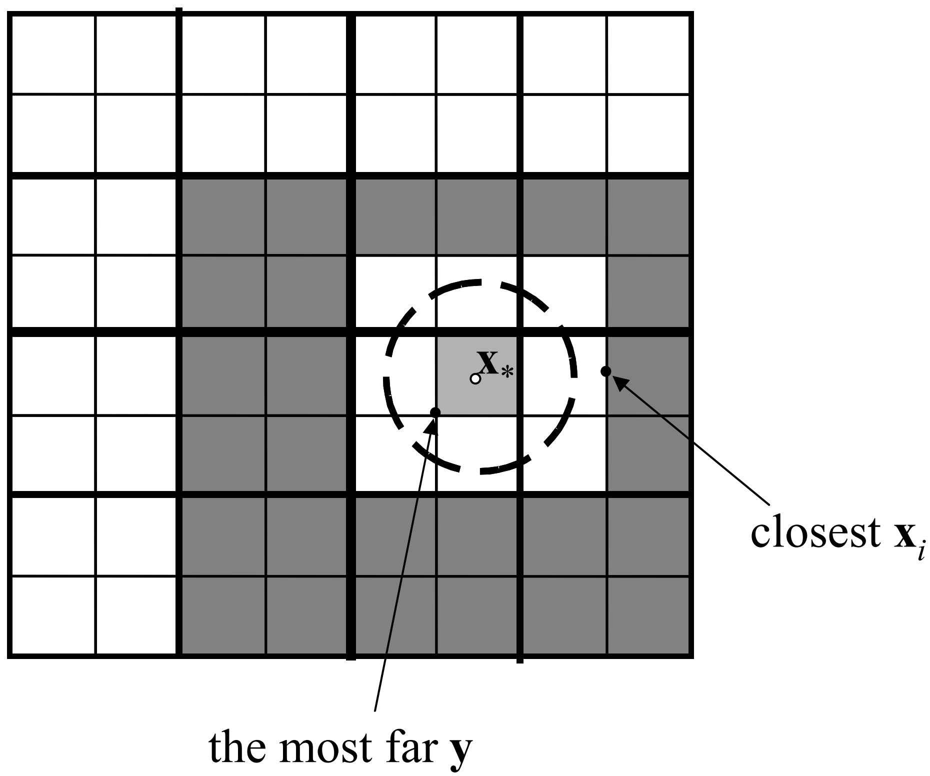
Minimum sphere radius containing the box

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

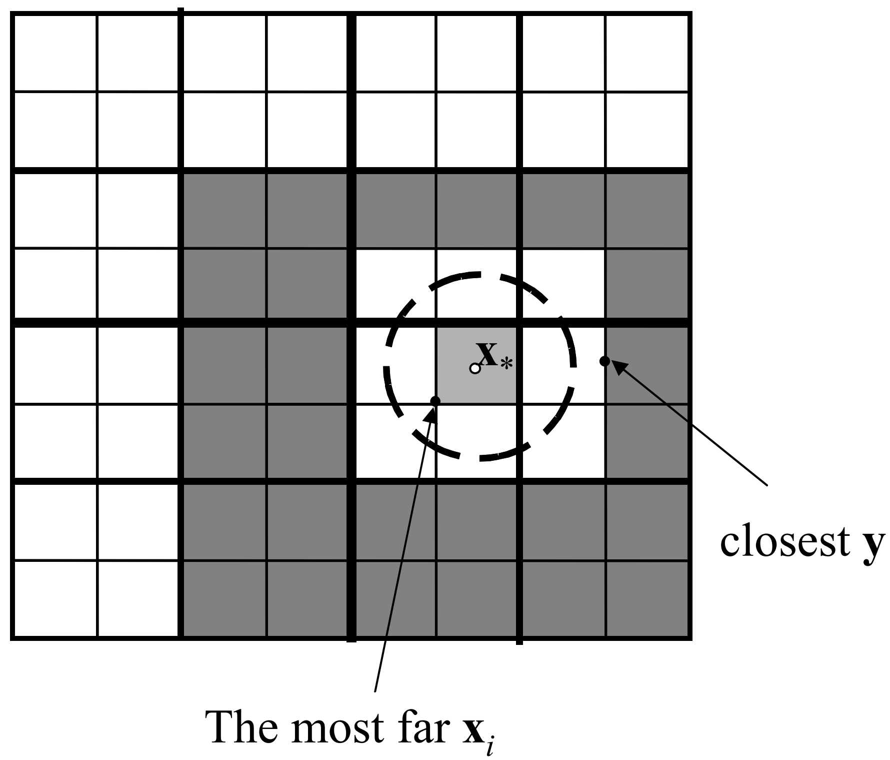


# Domains of Expansion Validity (2)

R-expansion




S-expansion



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

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

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

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

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

Strict unequality:

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

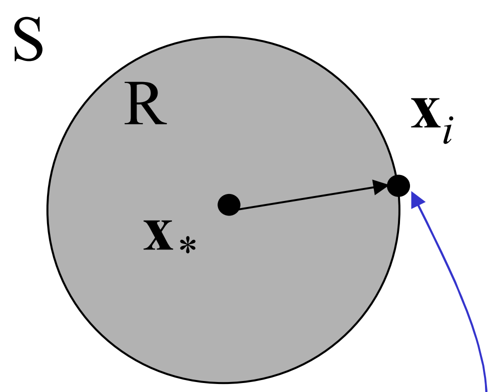
$$2^{-l-1}\sqrt{d} < \frac{3}{2}2^{-l}, \quad d < 9.$$

For $d = 9$ this condition also holds, if the requirements are weaker:

$$\Phi(\mathbf{x}_i,\mathbf{y}) = \mathrm{A}(\mathbf{x}_i,\mathbf{x}_*) \circ \mathrm{R}(\mathbf{y}-\mathbf{x}_*), \quad |\mathbf{y}-\mathbf{x}_*| \leqslant |\mathbf{x}_i - \mathbf{x}_*|, \quad \mathbf{y} \neq \mathbf{x}_i \quad i = 1,...,N$$

# Domains of Expansion Validity (4)

Picture from Lecture 4




What frequently happens, is that that both S and R expansions converge even on the sphere of radius $|\mathbf{x}_* - \mathbf{x}_i|$, except of point $\mathbf{y} = \mathbf{x}_i$.

If this is the case, $d = 9$ is OK for R-expansion with the $E_3$ neighborhood.

Singular Point is located at the Boundary of regions for the R- and S-expansions!

# Domains of Expansion Validity (5). S-expansion.

strict

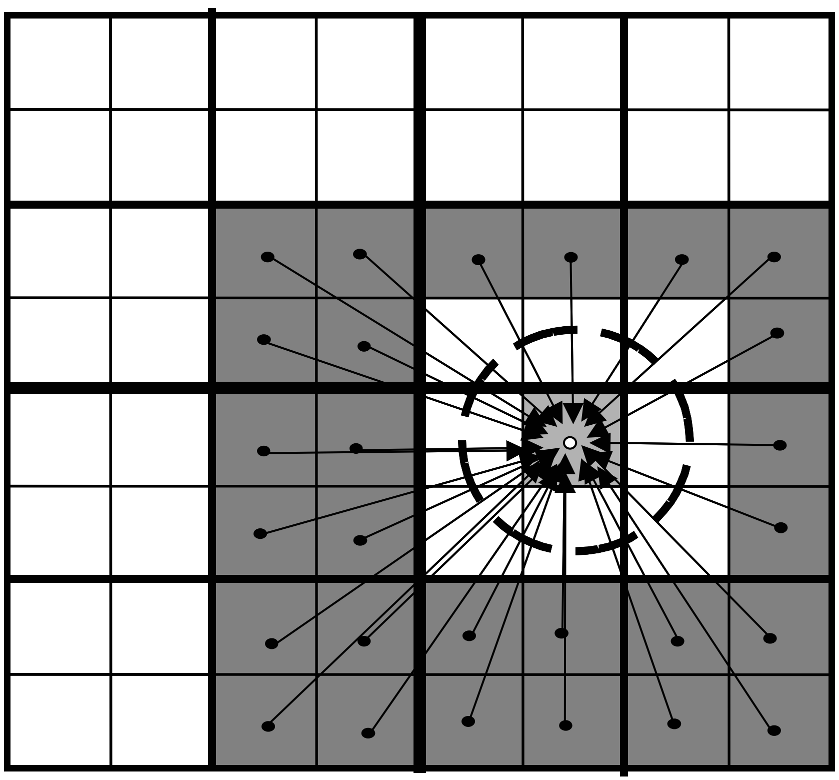
Potentials (functions) can be factorized as (far field expansion):

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

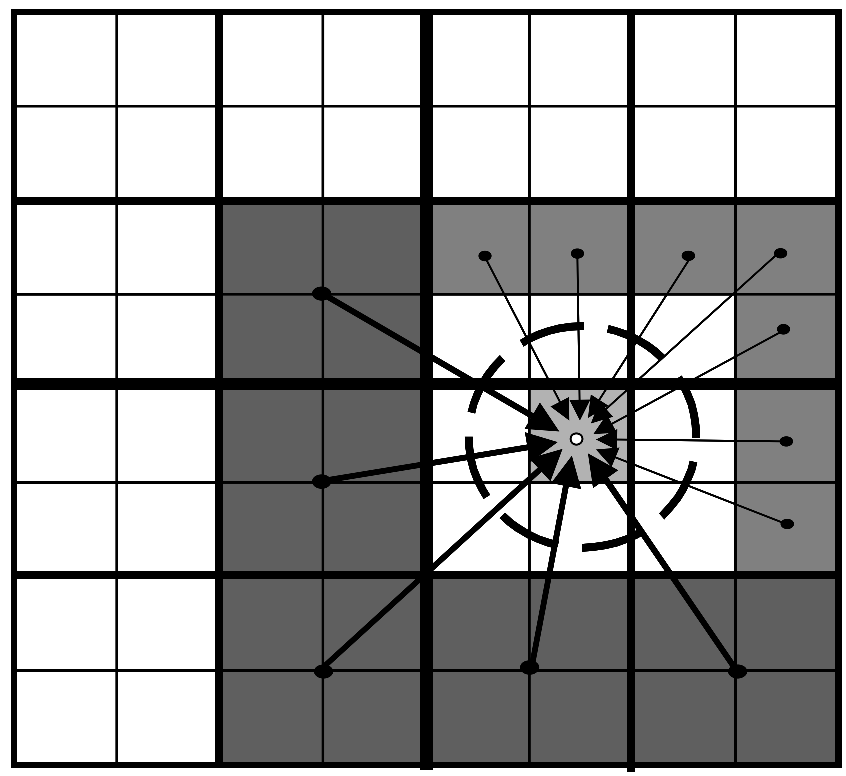
$$\Phi(\mathbf{x}_i,\mathbf{y}) = \mathbf{B}(\mathbf{x}_i,\mathbf{x}_*) \circ \mathbf{S}(\mathbf{y}-\mathbf{x}_*), \quad |\mathbf{y}-\mathbf{x}_*| \geqslant |\mathbf{x}_i-\mathbf{x}_*|, \quad \mathbf{y} \neq \mathbf{x}_i,\ i = 1,\dots,N$$

weak

Original



Reduced



# Domains of Expansion Validity (6). S-expansion.

In case of original FMM scheme the limitation for dimensionality coming from S-expansion validity is the same as for R-expansion validity:

$d < 9$ – strict,
$d \leq 9$ – weak.

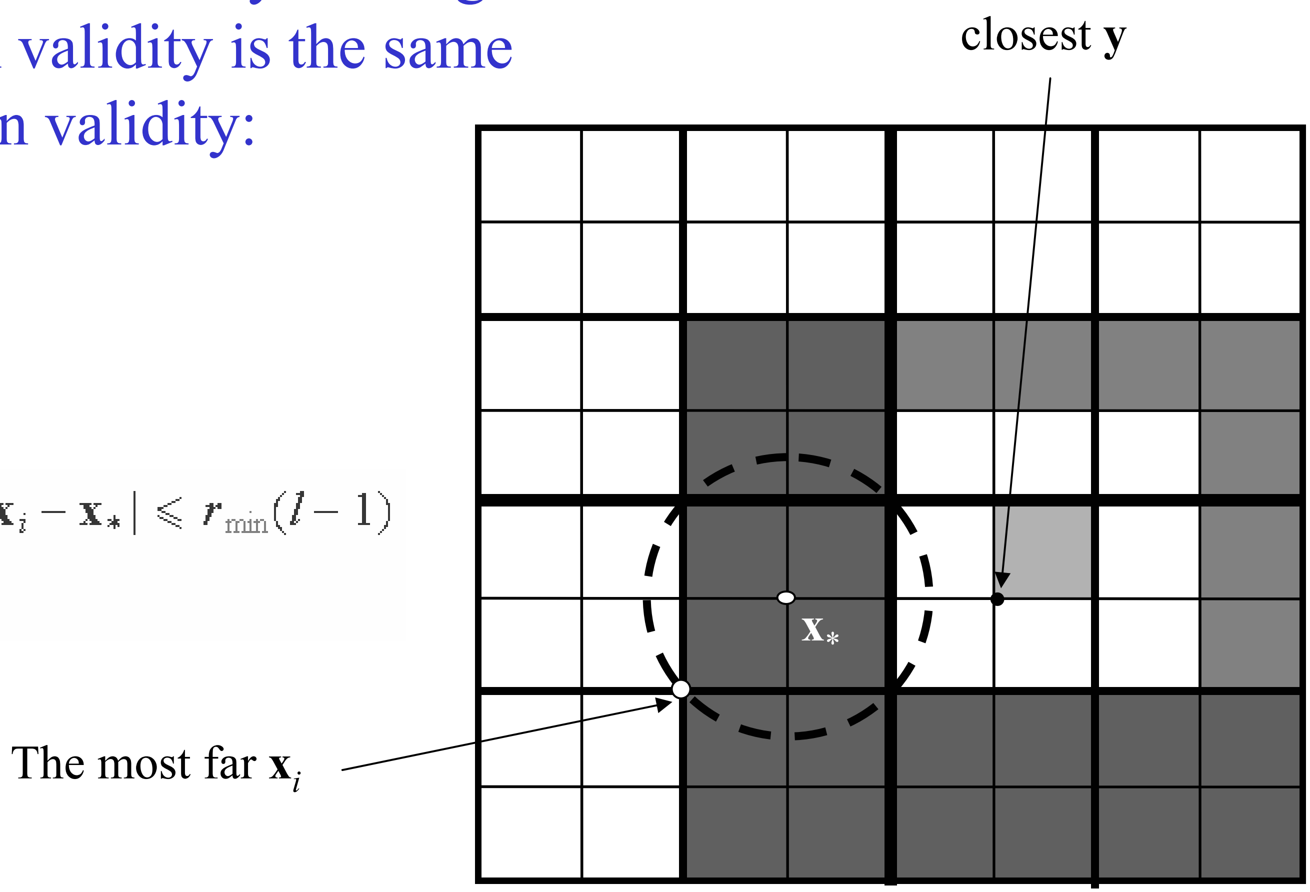
# Domains of Expansion Validity (7). S-expansion.

In case of reduced FMM scheme the limitation for dimensionality coming from S-expansion validity is the same as for R-expansion validity:

$d < 4$ – strict,
$d \leq 4$ – weak.

$$|\mathbf{y} - \mathbf{x}_*| \geqslant size(l-1), \quad |\mathbf{x}_i - \mathbf{x}_*| \leqslant r_{\min}(l-1)$$

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



# Domains of Expansion Validity (8). R|R and S|S-translations.

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

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

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

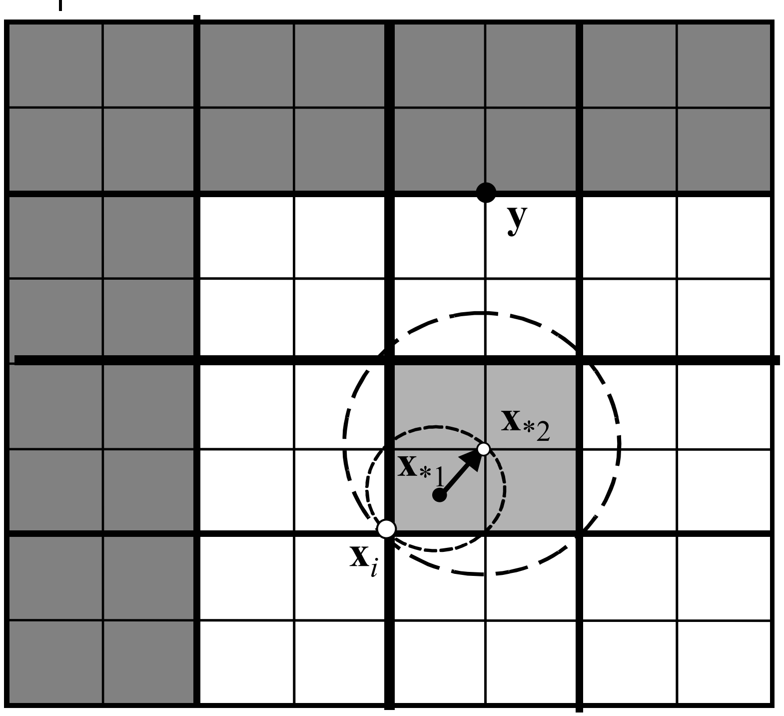
- $S$-expansion coefficients can be $S|S$-translated:

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

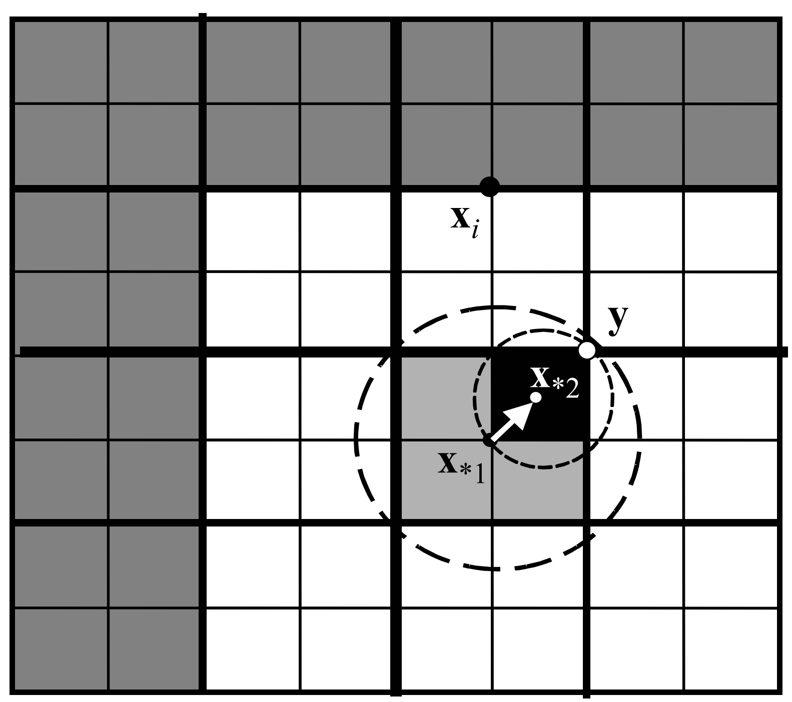
$$\mathbf{B}(\mathbf{x}_i,\mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{S})(\mathbf{x}_{*2}-\mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i,\mathbf{x}_{*1})$$

No additional constraints

S|S




R|R



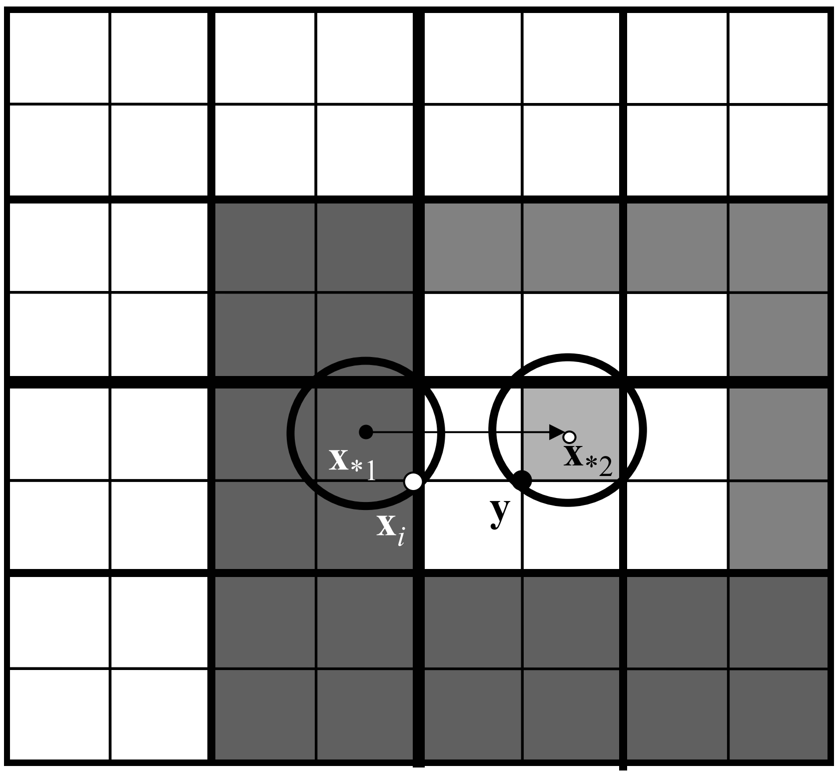
# Domains of Expansion Validity (9). S|R-translation.

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

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

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

Original




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

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

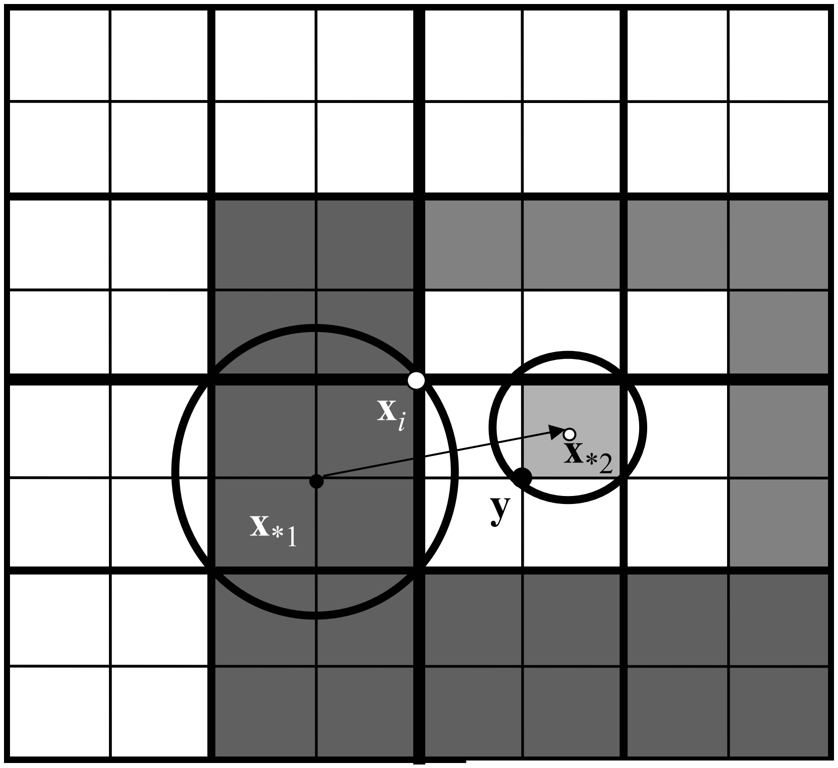
$$2^{-l-1}\sqrt{d} + 2^{-l-1}\sqrt{d} \leqslant 2^{-l+1}, \quad d \leqslant 4.$$

$d < 4$ – strict,

$d \leq 4$ – weak.

# Domains of Expansion Validity (9). S|R-translation.

Reduced




$d < 3$ – strict,

$d \leq 3$ – weak.

$$|\mathbf{y} - \mathbf{x}_*| \leqslant r_{\min}(l), \quad |\mathbf{x}_i - \mathbf{x}_*| \leqslant r_{\min}(l-1) = 2r_{\min}(l),$$

$$\min|\mathbf{x}_{*1} - \mathbf{x}_{*2}| = \sqrt{\left[\frac{5}{2}size(l)\right]^2 + \left[\frac{1}{2}size(l)\sqrt{d-1}\right]^2},$$

$$\left[\frac{5}{2}size(l)\right]^2 + \left[\frac{1}{2}size(l)\sqrt{d-1}\right]^2 \geqslant [r_{\min}(l) + 2r_{\min}(l)]^2 = 9r_{\min}^2(l)$$

$$\frac{25}{4} + \frac{d-1}{4} \geqslant \frac{9d}{4},$$

$$d \leqslant 3.$$

What to do in larger dimensions?

# Neighborhood Increase Technique

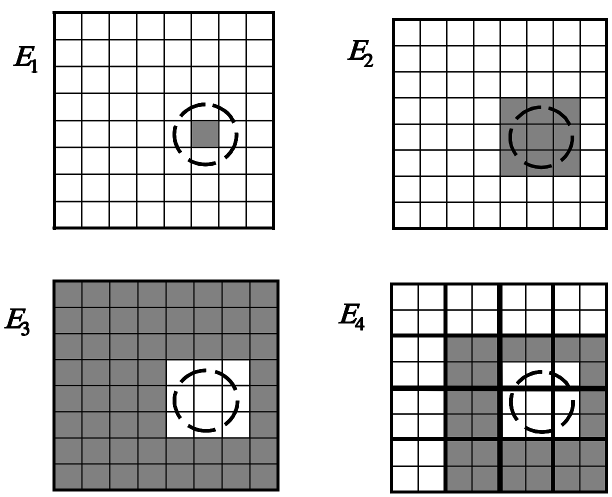
# Neighborhood Increase Technique

Recipe: Build a fractal structure with larger neighborhood

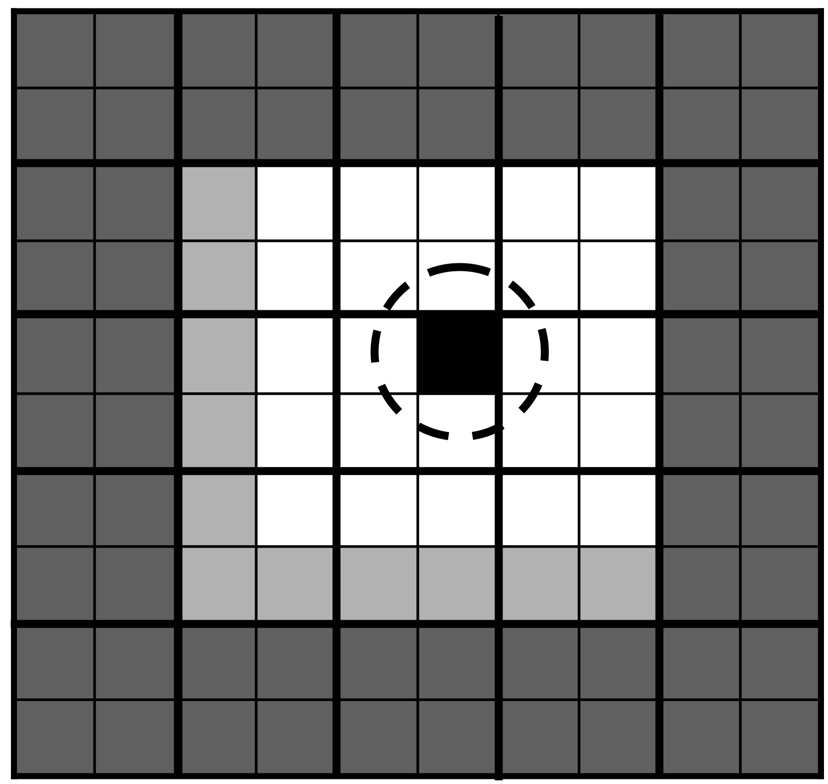
Everything works by the same way, but $E_2$ and $E_4$ are larger

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

5-neighborhood

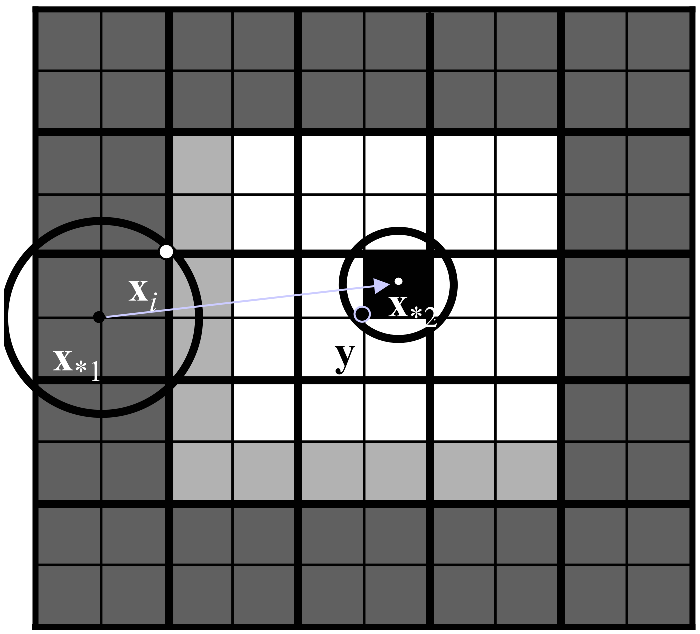



3-neighborhood



# Neighborhood Increase Technique

5-neighborhood, Translation Reduction Trick




$$|\mathbf{y}-\mathbf{x}_*| \leqslant r_{\min}(l), \quad |\mathbf{x}_i-\mathbf{x}_*| \leqslant r_{\min}(l-1) = 2r_{\min}(l),$$

$$\min|\mathbf{x}_{*1}-\mathbf{x}_{*2}| = \sqrt{\left[\frac{7}{2}size(l)\right]^2 + \left[\frac{1}{2}size(l)\sqrt{d-1}\right]^2},$$

$$\left[\frac{7}{2}size(l)\right]^2 + \left[\frac{1}{2}size(l)\sqrt{d-1}\right]^2 \geqslant [r_{\min}(l) + 2r_{\min}(l)]^2 = 9r_{\min}^2(l)$$

$$\frac{49}{4} + \frac{d-1}{4} \geqslant \frac{9d}{4},$$

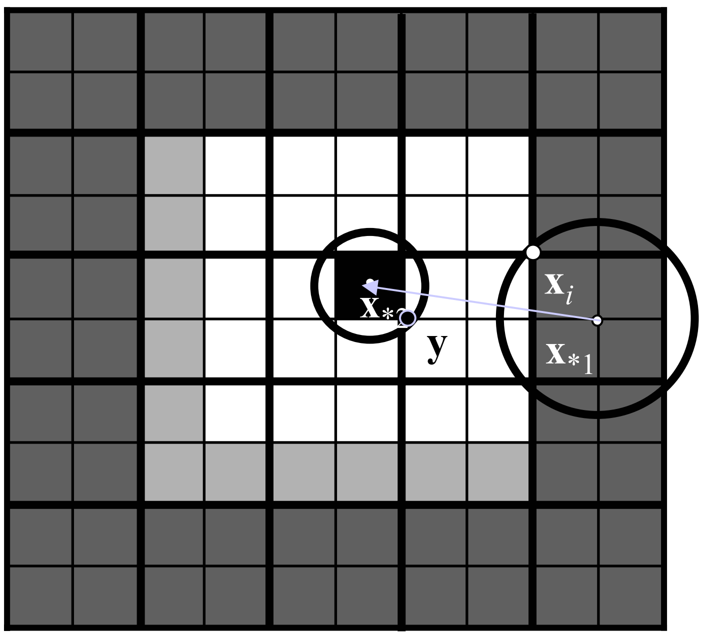
$$d \leqslant 6.$$

$d < 6$ – strict,

$d \leq 6$ – weak.

# Neighborhood Increase Technique

5-neighborhood




The same as for non-reduced scheme with 3-neighborhoods!

Number of Translations:

$$P_4^{(reduced)} = PowerOfE_4Neighborhood = 5^d - 3^d + 2^d 3^d - 5^d = 3^d\left(2^d - 1\right).$$

# Neighborhood Increase Technique

Advantages:

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

Unfortunately, cannot Increase Indefinitely…

# Evaluation of the Error of FMM

- Each Translation introduces an error;
- This includes error of expansion/evaluation;

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

Error:

$$ErrorMLFMM = (P_4(d)+2)\frac{N}{s}ErrorTranslation(P).$$

or

$$ErrorMLFMM_{opt} = \left[MN(P_4(d)+2)P_2(d)\frac{CostFunc}{CostTranslation(P)}\right]^{1/2} ErrorTranslation(P).$$

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

Translation error depends on the size of neighborhood.

# Example

Example (see Homework 4), $\Phi = \frac{1}{y - x_i}$,

$$ErrorTranslation(p) \leqslant \frac{2}{l_{\min} \cdot 3^p}, \quad x_i \in \left[-\frac{l_{\min}}{2}, \frac{l_{\min}}{2}\right], \quad y \in \left[\frac{3l_{\min}}{2}, \frac{5l_{\min}}{2}\right],$$

$$ErrorTranslation(p) \leqslant \frac{2}{l_{\min} \cdot 5^p}, \quad x_i \in \left[-\frac{l_{\min}}{2}, \frac{l_{\min}}{2}\right], \quad y \in \left[\frac{5l_{\min}}{2}, \frac{7l_{\min}}{2}\right].$$

$M = N, CostTranslation(P) = 10, CostFunc = 1.$

3-neighborhood:

$$P_4(1) = 3, \quad P_2(d) = 3, \quad s_{opt} \sim 4, \quad \epsilon = ErrorMLFMM_{opt}^{(3)} = \frac{5N}{4} \frac{2}{l_{\min} \cdot 3^p},$$

$$p^{(3)} = \frac{1}{\log 3} \log\left(\frac{5N}{2l_{\min}\epsilon}\right)$$

For p=10, about 100 times higher accuracy!

5-neighborhood:

$$P_4(1) = 5, \quad P_2(d) = 5, \quad s_{opt} \sim 4, \quad ErrorMLFMM_{opt}^{(5)} = \frac{7N}{4} \frac{2}{l_{\min} \cdot 5^p},$$

$$p^{(5)} = \frac{1}{\log 5} \log\left(\frac{7N}{2l_{\min}\epsilon}\right).$$

For the same error, about 1.5 times smaller *p*

# Problem:

Let the error is specified. What method is faster
Smaller neighborhood with larger p or
Larger neighborhood with smaller p?