

Frontal and multi-frontal solvers: Dealing with singularities

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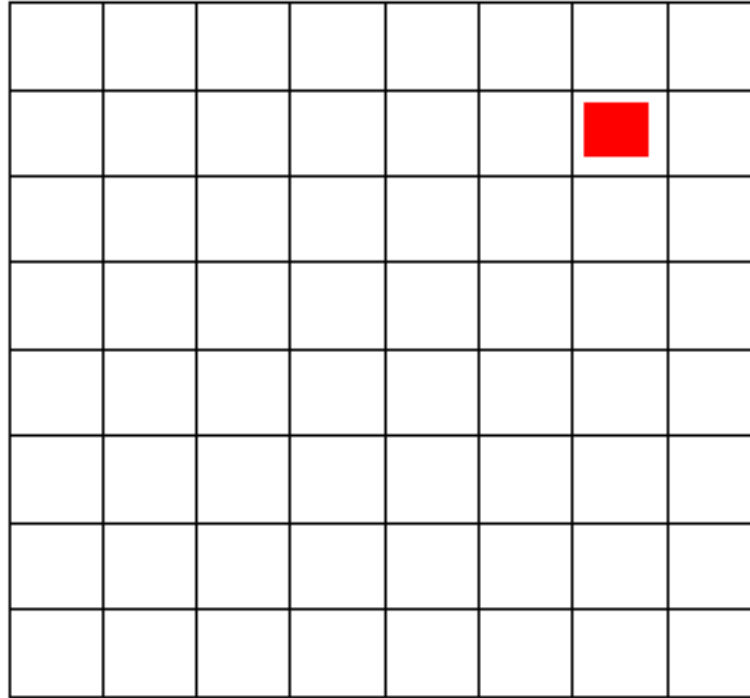
<http://www.ki.agh.edu.pl/en/research-groups/a2s>

Main collaborators

Victor Calo (KAUST)
Leszek Demkowicz (ICES, UT)
David Pardo (IKERBASQUE)



COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



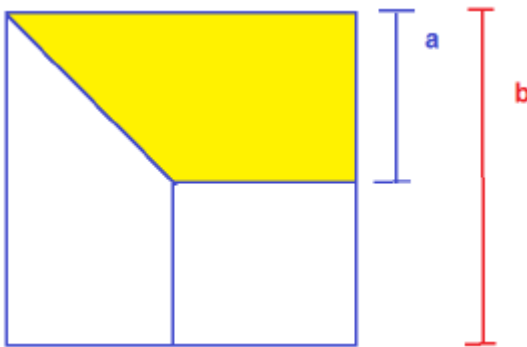
$$\text{FLOPS}(2\text{D})=p^6.$$

$$\text{FLOPS}(3\text{D})=p^9.$$



COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

Number of operations for partial forward elimination
(Schur complement computations)

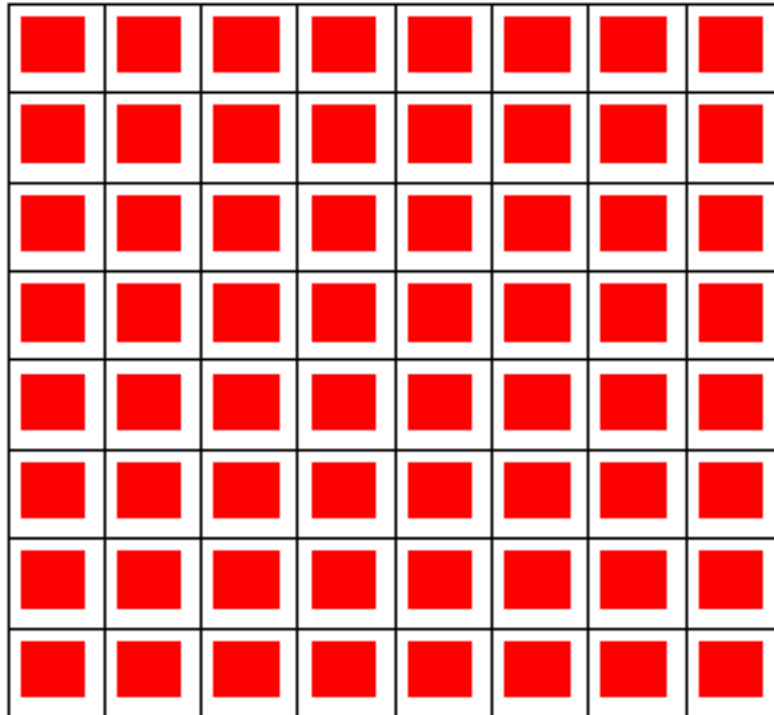


$$\sum_{m=1}^b m^2 - \sum_{m=1}^{(b-a)} m^2 = \frac{a(6b^2 - 6ab + 6b + 2a^2 - 3a + 1)}{6}$$

Computational complexity $O(ab^2)$



COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



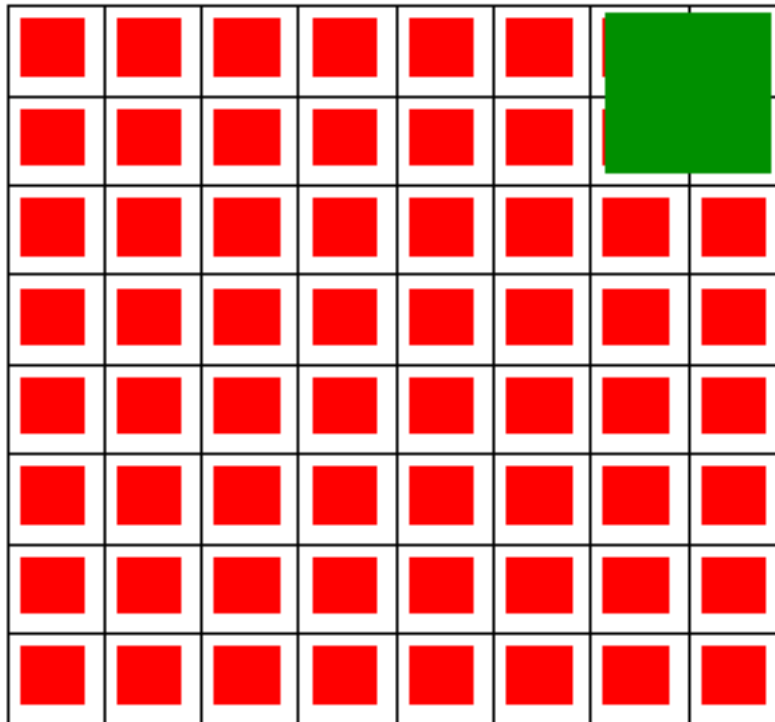
$$\text{FLOPS(2D)} = 2^{2s} p^6.$$

$$\text{FLOPS(3D)} = 2^{3s} p^9.$$

NOTE: 2^s = Number of elements in each direction ($s = 3$ here)



COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

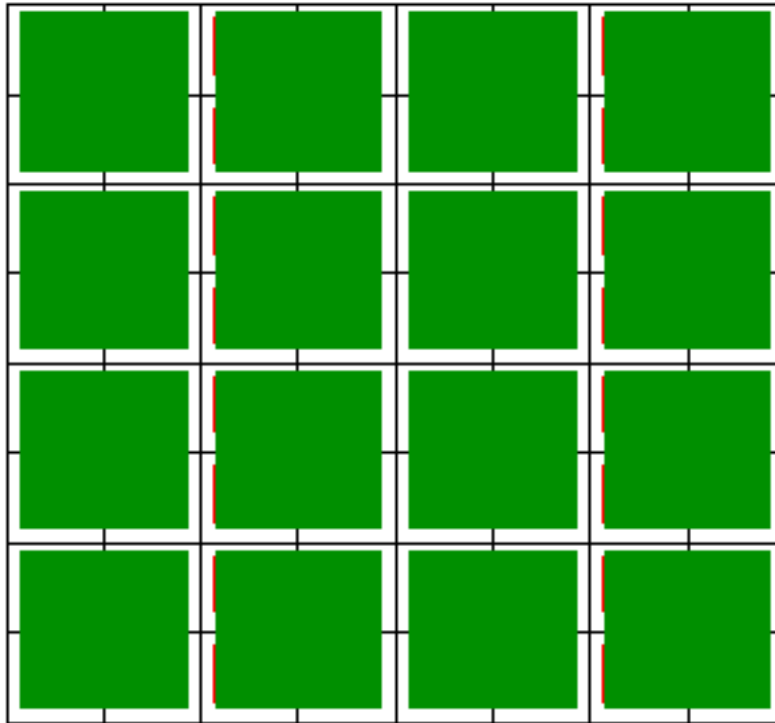


$$\text{FLOPS(2D)} = 2^{2s} p^6 + 2^4 p^3.$$

$$\text{FLOPS(3D)} = 2^{3s} p^9 + 2^6 p^6.$$



COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

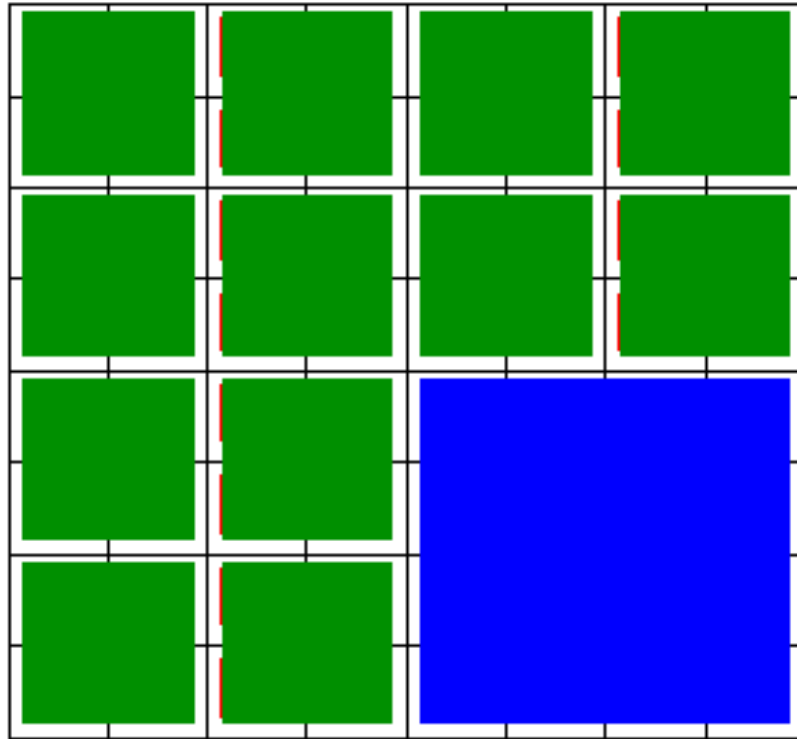


$$\text{FLOPS(2D)} = 2^{2s} p^6 + 2^{2(s-1)} 2^4 p^3.$$

$$\text{FLOPS(3D)} = 2^{3s} p^9 + 2^{3(s-1)} 2^6 p^6.$$



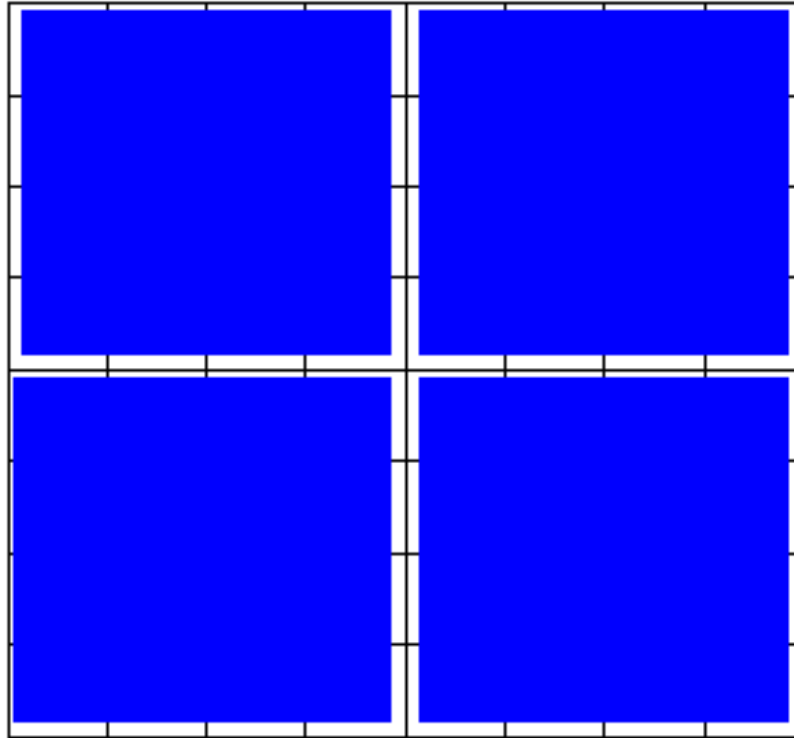
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



$$\text{FLOPS(2D)} = 2^{2s} p^6 + 2^{2(s-1)} 2^4 p^3 + 2^8 p^3$$
$$\text{FLOPS(3D)} = 2^{3s} p^9 + 2^{3(s-1)} 2^6 p^6 + 2^{12} p^6$$



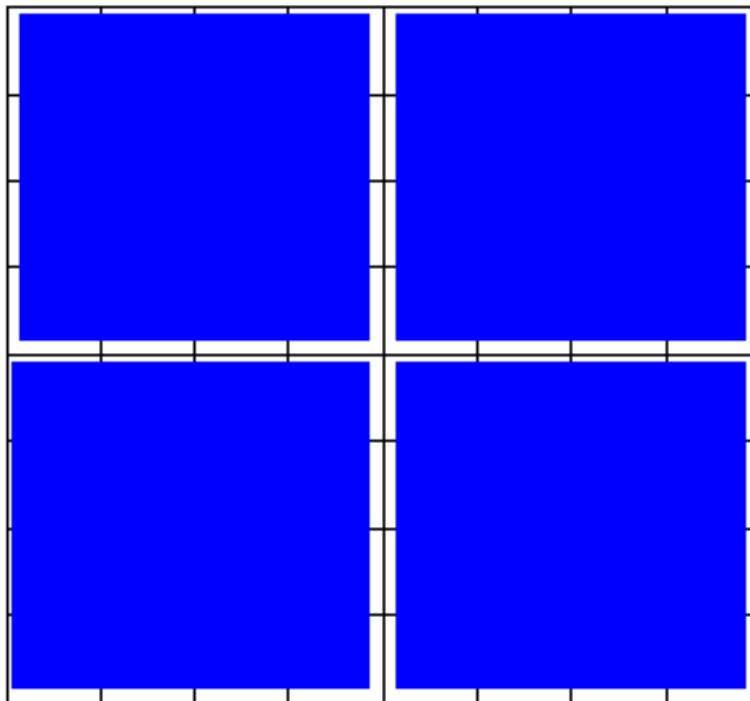
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



$$\text{FLOPS(2D)} = 2^{2s}p^6 + 2^{2(s-1)}2^4p^3 + 2^{2(s-2)}2^8p^3$$
$$\text{FLOPS(3D)} = 2^{3s}p^9 + 2^{3(s-1)}2^6p^6 + 2^{3(s-2)}2^{12}p^6$$



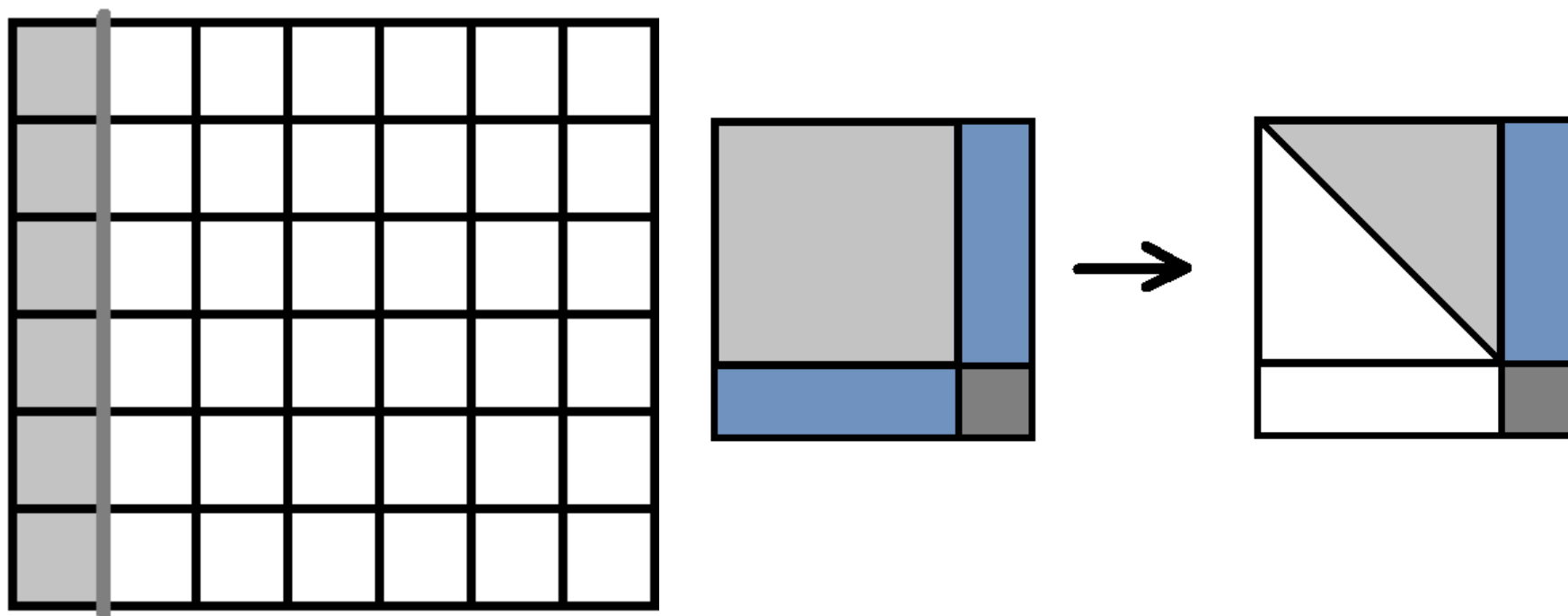
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



$$\text{FLOPS(2D)} = 2^{2s}p^6 + 2^{2(s-1)}2^4p^4 + 2^{2(s-2)}2^8p^4 + \dots = \mathcal{O}(Np^4) + \mathcal{O}(N^{1.5})$$
$$\text{FLOPS(3D)} = 2^{3s}p^9 + 2^{3(s-1)}2^6p^6 + 2^{3(s-2)}2^{12}p^6 + \dots = \mathcal{O}(Np^6) + \mathcal{O}(N^2)$$



COMPUTATIONAL COST OF FRONTAL SOLVER



Computational cost of elimination of a single layer $O((N^{0.5})^3) = O(N^{3/2})$
Number of layers = $O(N^{0.5})$

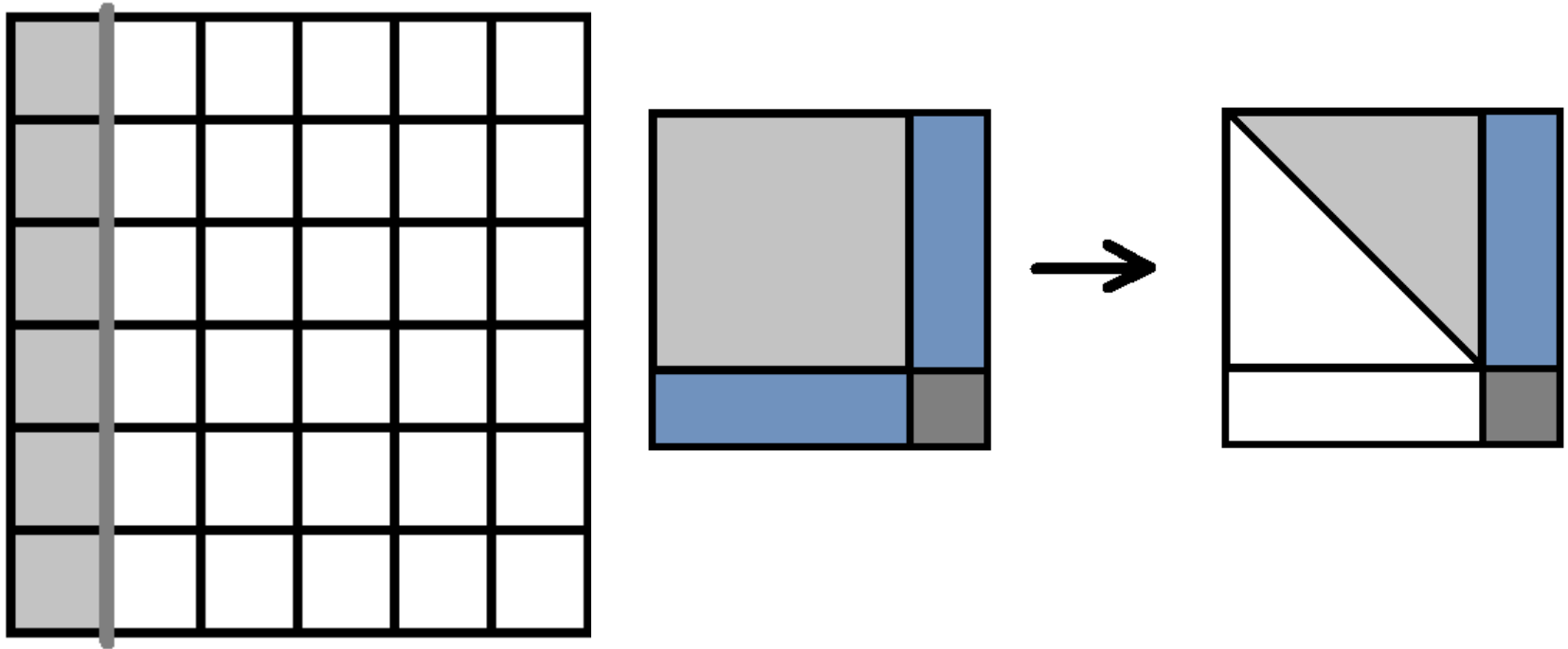
Computational cost of elimination of entire mesh
= computational cost of elimination of a single layer * number of layers

$O(N^{0.5}N^{3/2}) = O(N^2)$ in 2D

$O(N^{1/3}N^{6/3}) = O(N^{7/3})$ in 3D



COMPUTATIONAL COST OF FRONTAL SOLVER



Computational cost of elimination of a single layer $O((N^{0.5})^3) = O(N^{3/2})$
Number of layers = $O(N^{0.5})$

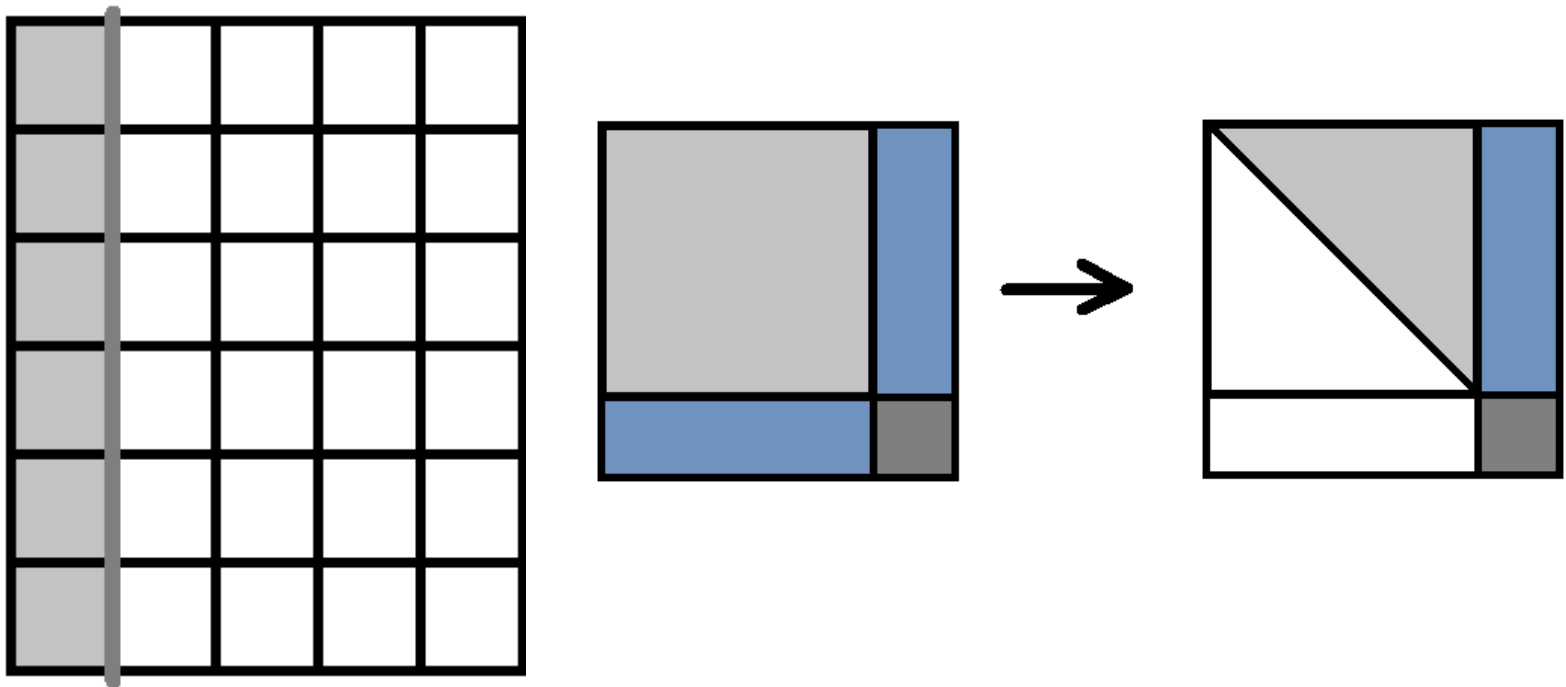
Computational cost of elimination of entire mesh
= computational cost of elimination of a single layer * number of layers

$O(N^{0.5}N^{3/2}) = O(N^2)$ in 2D

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COMPUTATIONAL COST OF FRONTAL SOLVER



Computational cost of elimination of a single layer $O((N^{0.5})^3) = O(N^{3/2})$
Number of layers = $O(N^{0.5})$

Computational cost of elimination of entire mesh
= computational cost of elimination of a single layer * number of layers

$$O(N^{0.5}N^{3/2}) = O(N^2) \text{ in 2D}$$

$$O(N^{1/3}N^{6/3}) = O(N^{7/3}) \text{ in 3D}$$



MODEL ELIPTIC PROBLEM

Find $u = u(x, y, z) \in H^1(\Omega)$ such that $\Delta u = 0$

where $\Omega = (0, 1)^3$, with boundary conditions

$$u(:, :, 0) = 0$$

$$u(:, :, 1) = 1$$

$$\frac{\partial u}{\partial x}(0, :, :) = \frac{\partial u}{\partial x}(1, :, :) = \frac{\partial u}{\partial y}(:, 0, :) = \frac{\partial u}{\partial y}(:, 1, :) = 0$$

Find $u \in V = \{u \in H^1(\Omega) : u(:, :, 0) = u(:, :, 1) = 0\}$

such that $b(u, v) = l(v), \forall v \in V$

$$b(u, v) = \int_{\Omega} \nabla u \cdot \nabla v dV \quad l(v) = - \int_{\Omega} \frac{\partial v}{\partial z} dV$$



COMPUTATIONAL COST OF 3D DIRECT SOLVER

Notation:

N = number of degrees of freedom

N_e = number of elements

p = polynomial order of approximation

$$O(N) = O(N_e * p^3)$$

**Computational cost of direct solvers =
cost of static condensation + cost of LU factorization**

$$\text{Static condensation } O(N_e * p^9) = O(N * p^6)$$

Cost of LU factorization over regular grid $O(N^2)$

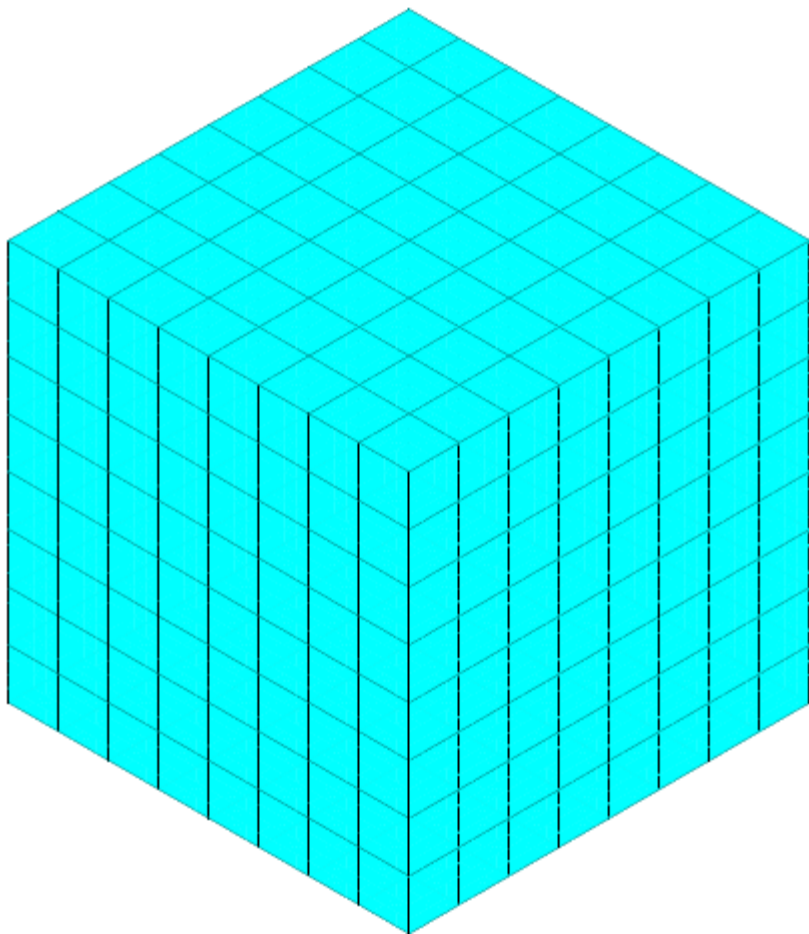
CONCLUSIONS:

For regular grid total cost is $O(N * p^6 + N^2) = O(N^2)$

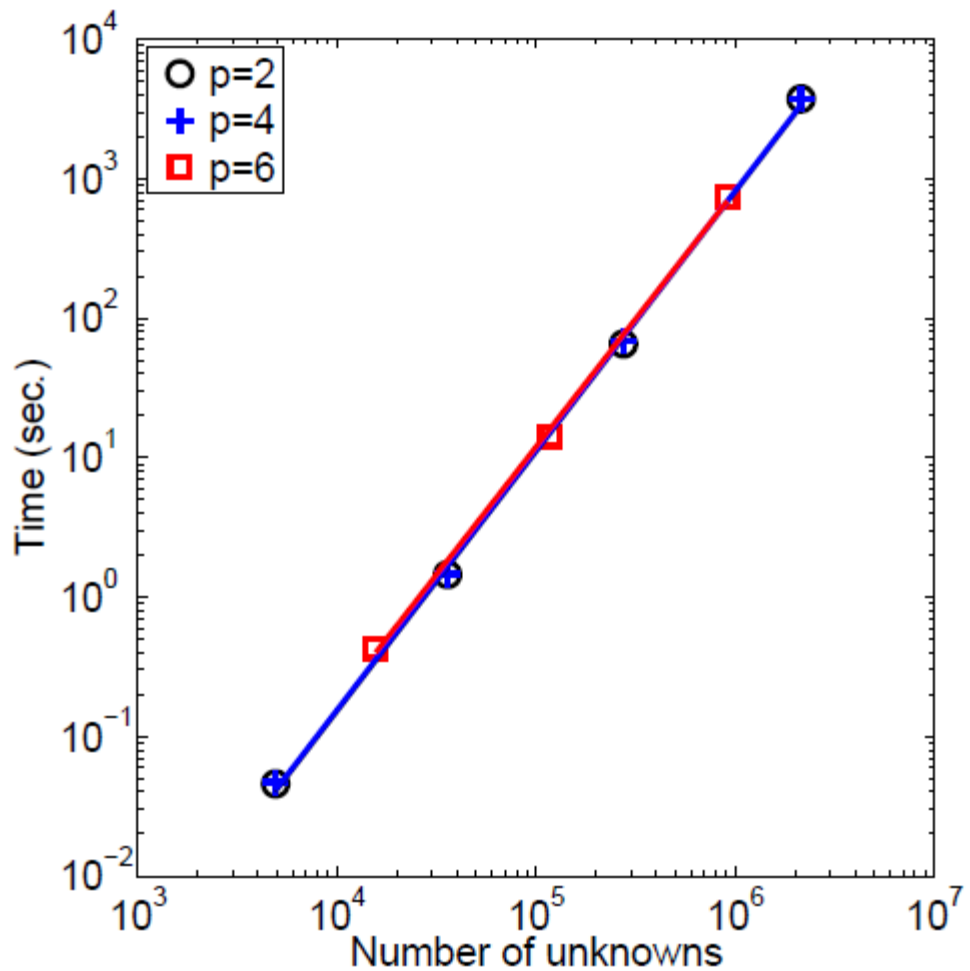
For other grids it is not always the case (static condensation may dominate)



UNIFORM REFINEMENTS



Mesh

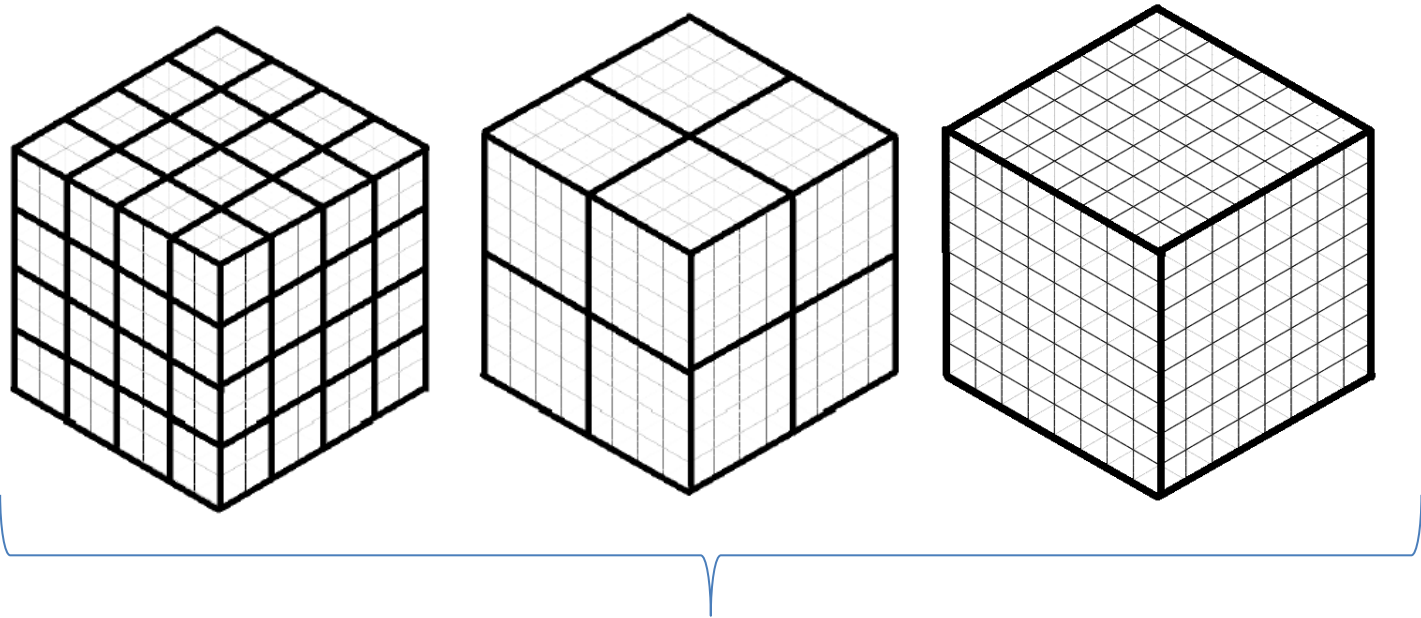


Time of LU factorization
Slope = exponent factor = 2
Location = p factor = $1=p^0$



UNIFORM REFINEMENTS MULTI-FRONTAL SOLVER APPROACH

Static condensation
 $O(N * p^6)$ +

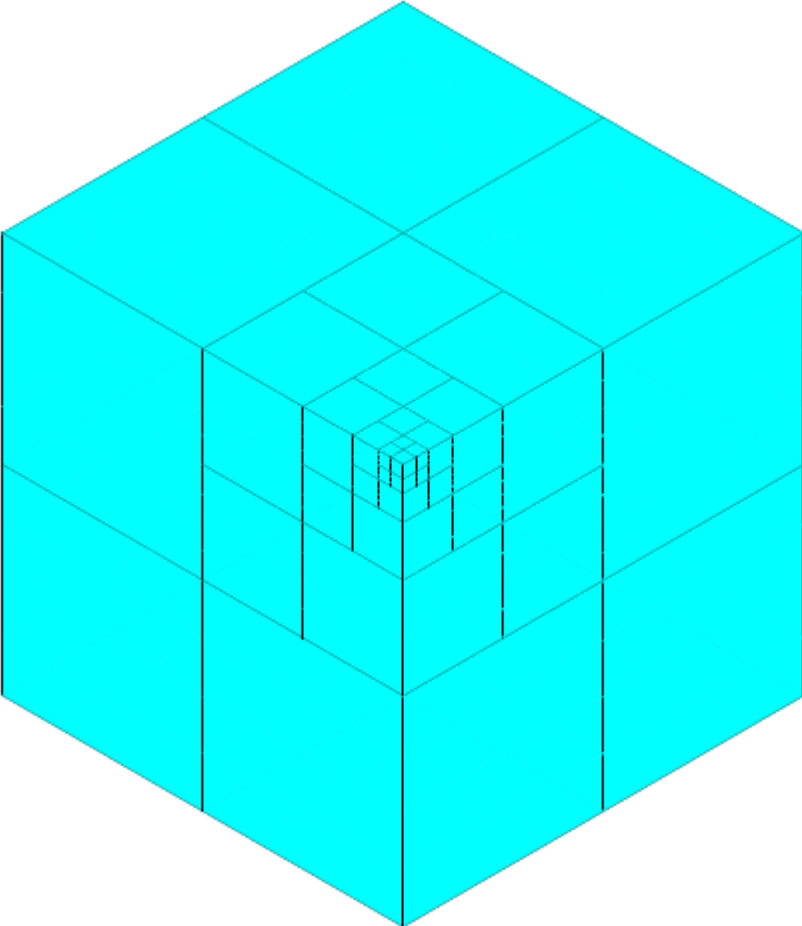


LU factorization $O(N^2)$

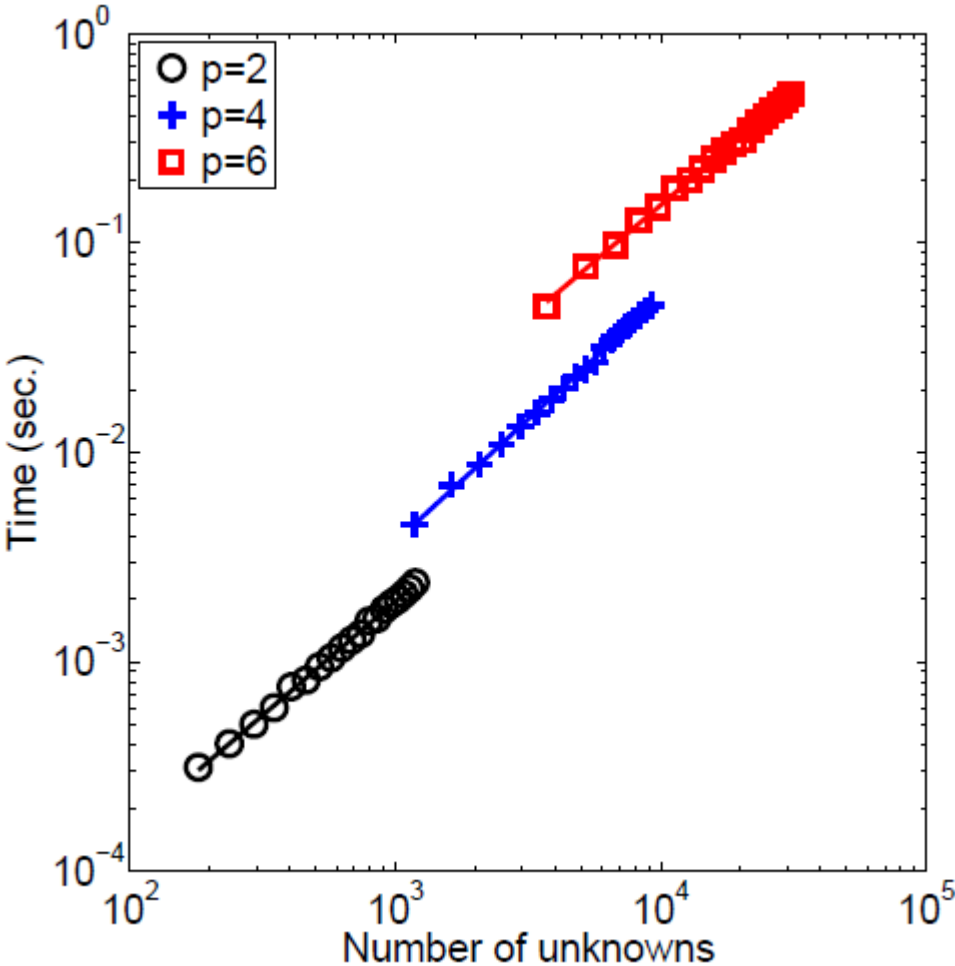
Total cost is $O(N * p^6 + N^2) = O(N^2)$



REFINEMENTS TOWARDS POINT SINGULARITY



Mesh



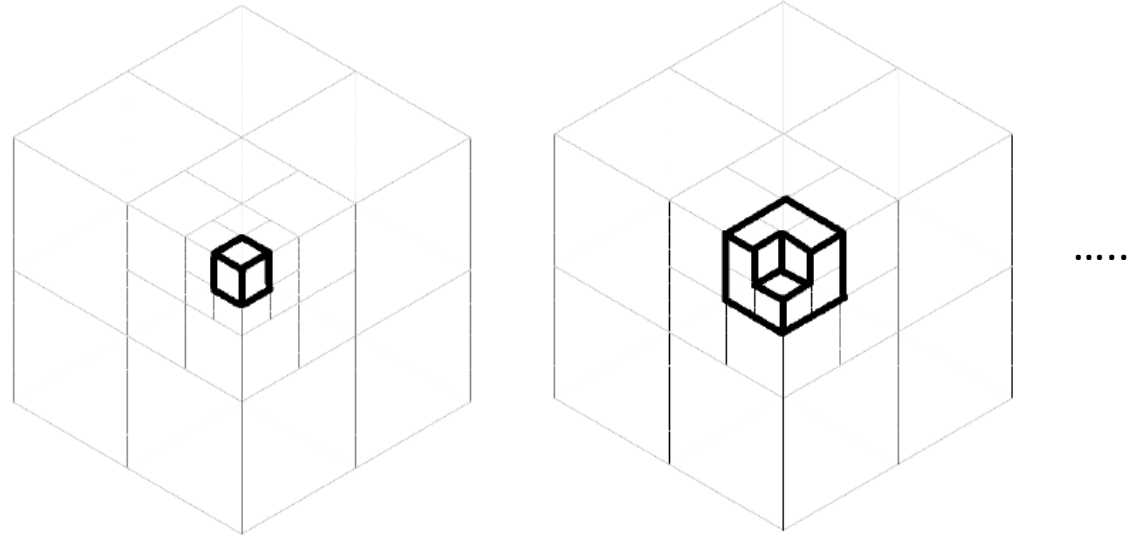
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6



REFINEMENTS TOWARDS POINT SINGULARITY FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

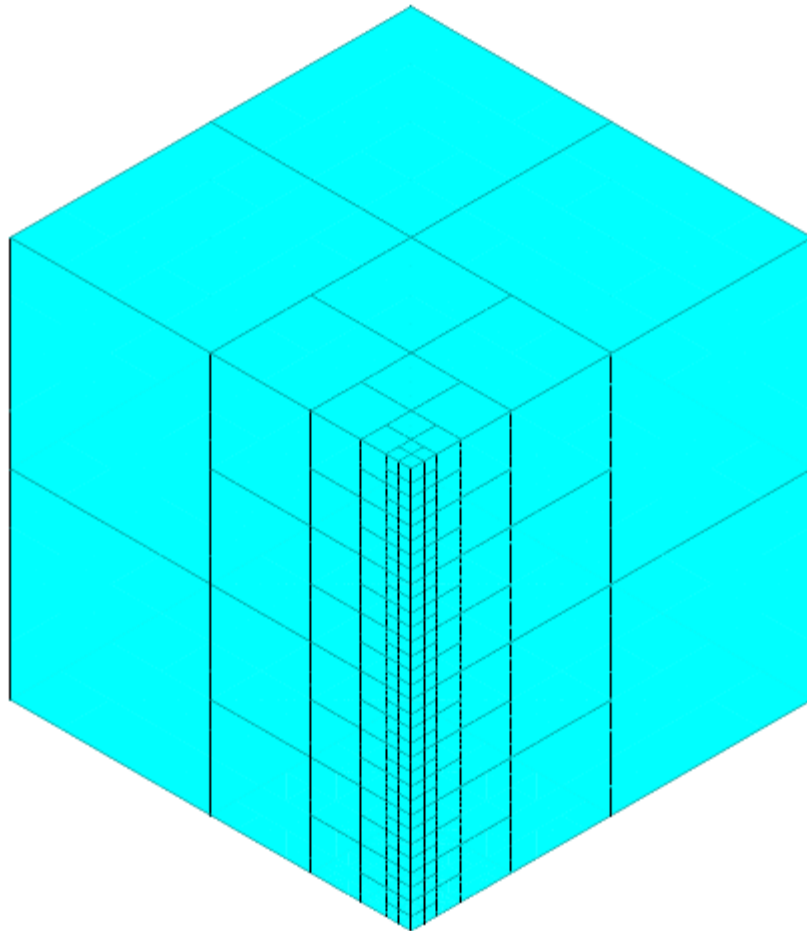
Schur complement of a single layer $O(p^6)$
Number of layers $k = O(N_e) = O(N/p^3)$

Total cost of LU factorization $O(p^6 * k) = O(p^6 * N/p^3) = O(N * p^3)$

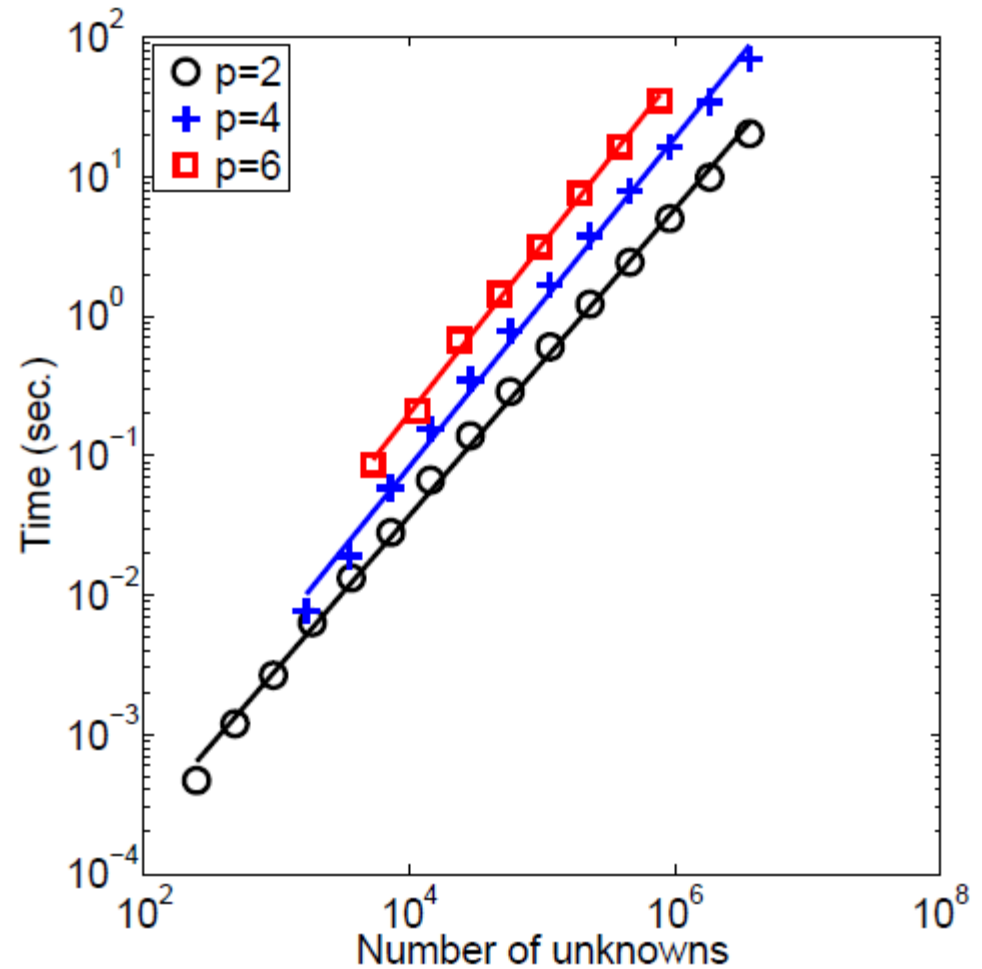
Total cost is $O(N * p^6 + N * p^3) = O(N * p^6)$



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY



Mesh



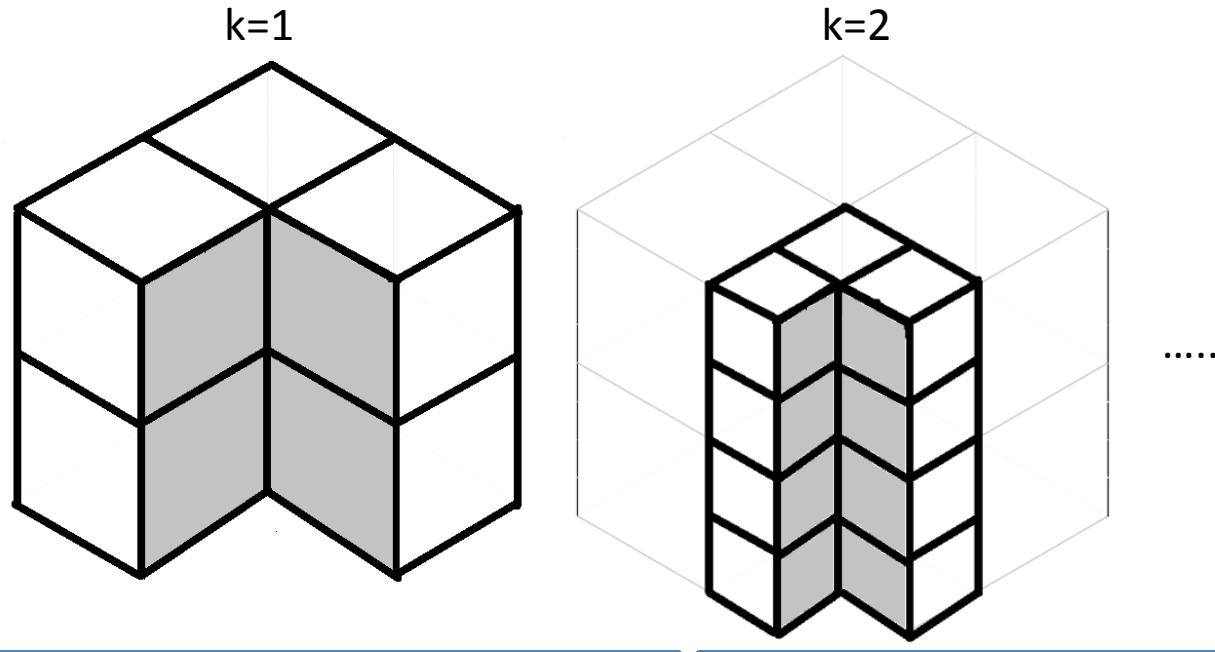
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

Number of dofs in a layer $3 * 2^k p^2 = O(2^k p^2)$

Number of interfaces dofs in a layer $2 * 2^k p^2 = O(2^k p^2)$

Cost of Schur complement of a single layer $O(2^{3k} p^6)$

$s = \text{number of layers, } N = O\left(\sum_{k=1}^s 3 * 2^k p^3\right) = O\left(\sum_{k=1}^s 2^k p^3\right) = O(p^3 2^s)$

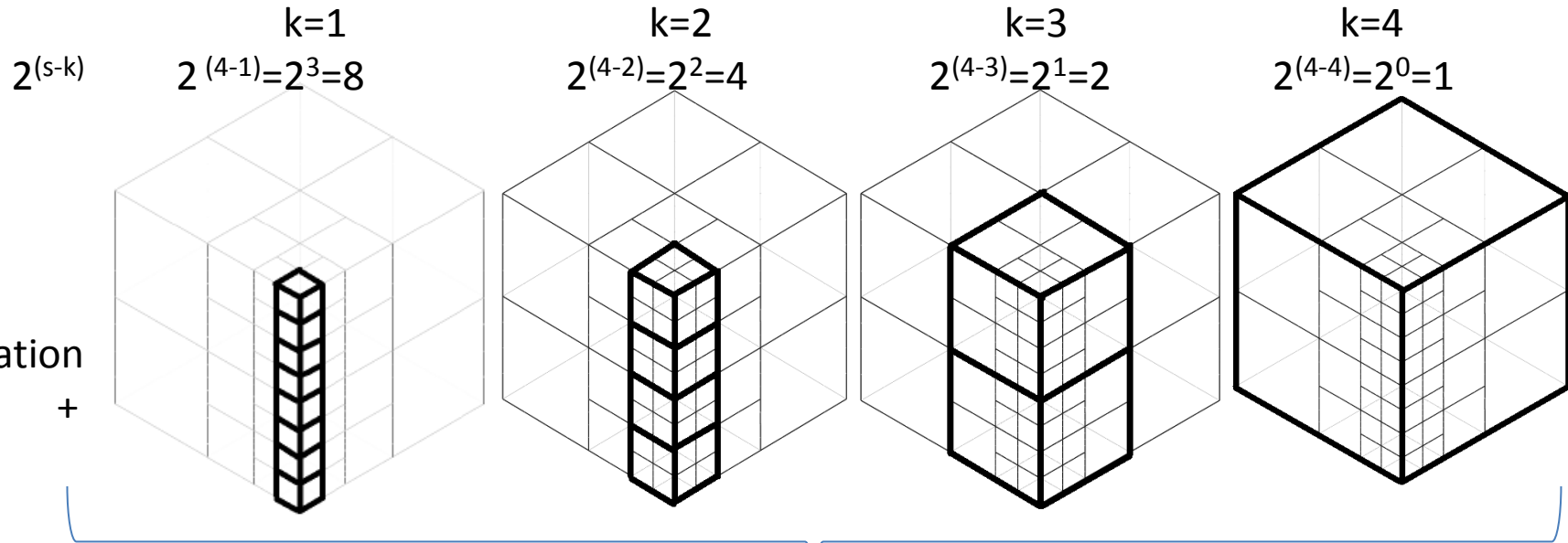
Cost of LU factorization $O\left(\sum_{k=1}^s 2^{3k} p^6\right) = O(p^6 2^{3s}) = O(N^3 / p^3)$

DO NOT USE FRONTAL SOLVER APPROACH



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY

MULTI-FRONTAL SOLVER APPROACH



Number of dofs in a patch $O(kp^2)$

Number of patches in a single layer $O(2^{s-k})$

Number of interfaces dofs in a patch $O(kp^2)$

Cost of Schur complement of a single layer $O(2^{s-k} k^3 p^6)$

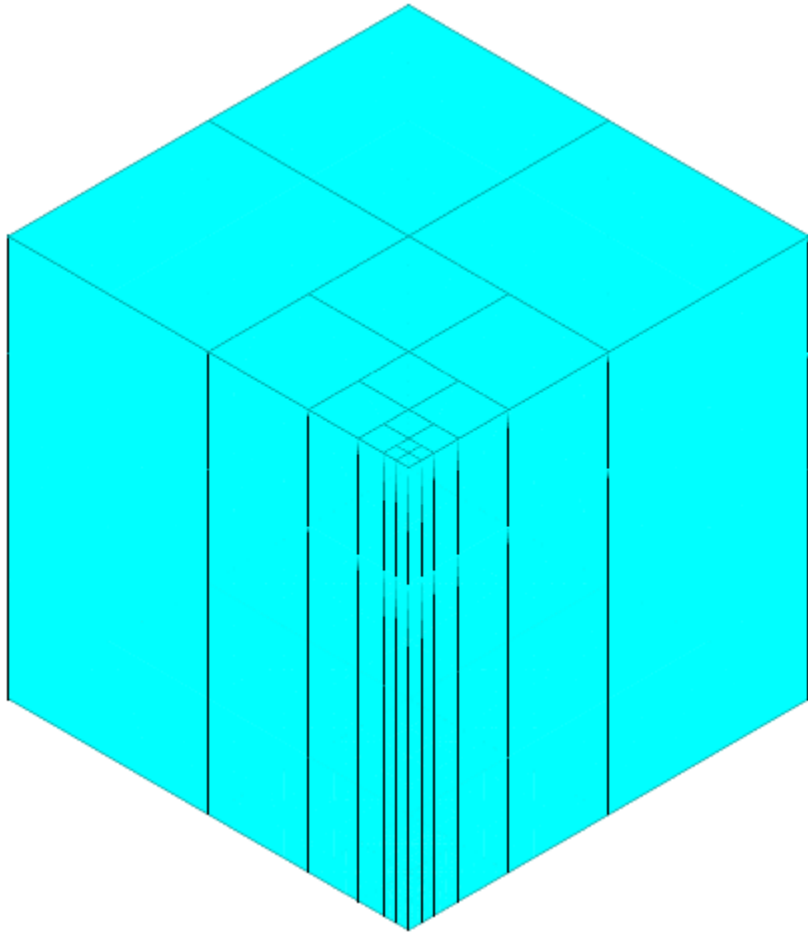
$s = \text{number of layers, } N = O\left(\sum_{k=1}^s 3 * 2^k p^3\right) O\left(\sum_{k=1}^s 2^k p^3\right) O(p^3 2^s)$

Cost of LU factorization $O\left(\sum_{k=1}^s 2^{s-k} k^3 p^6\right) O(s^3 p^6 2^s) = O(N p^3 (\log_2^3 N_e))$

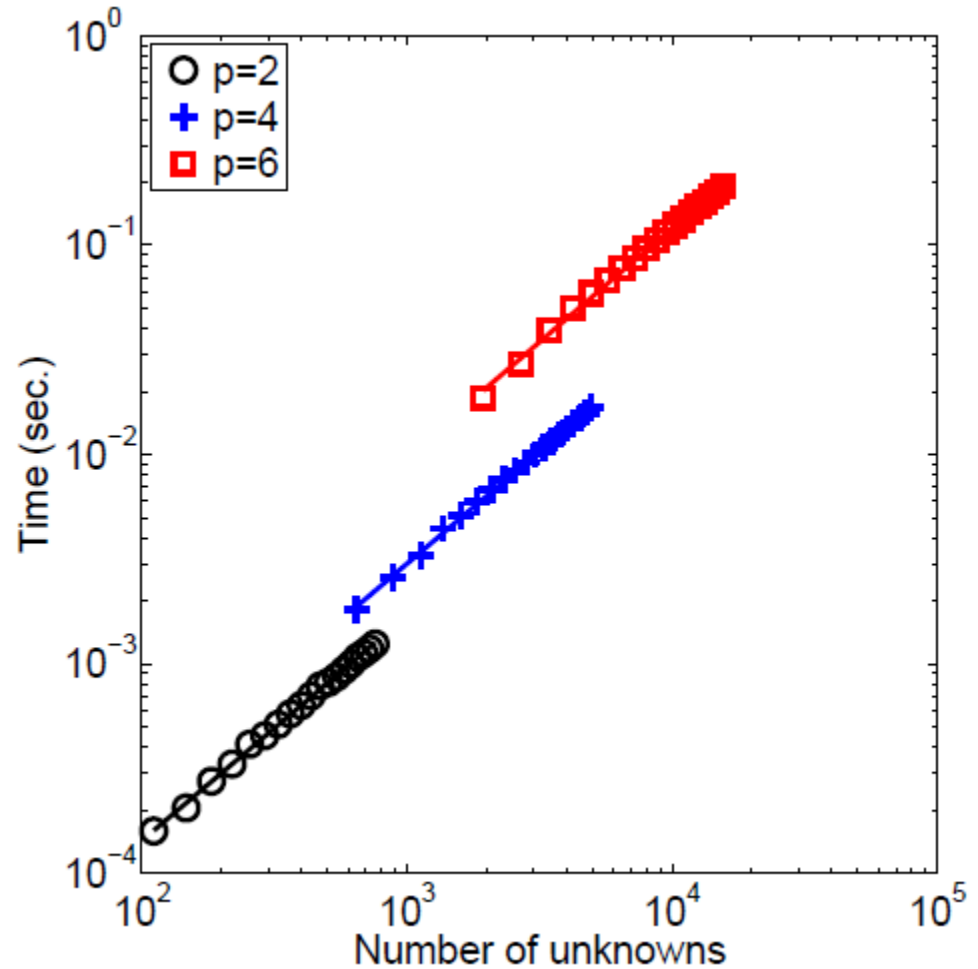
Total cost is $< O(N * p^6 + N p^3 (\log_2^3 N_e))$



ANISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY



Mesh



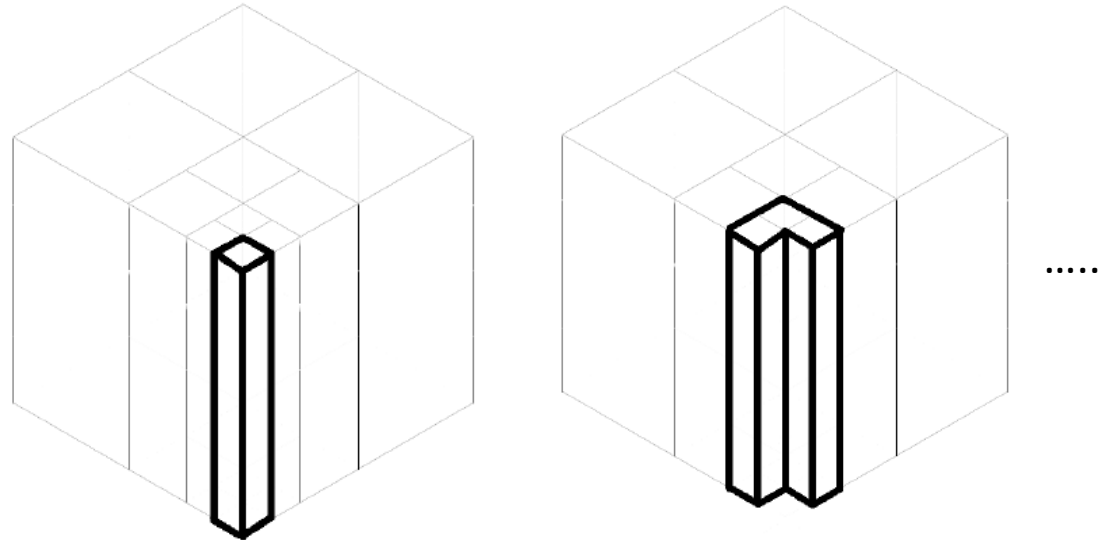
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

Number of dofs in a layer $O(p^2)$

Number of interfaces dofs in a layer $O(p^2)$

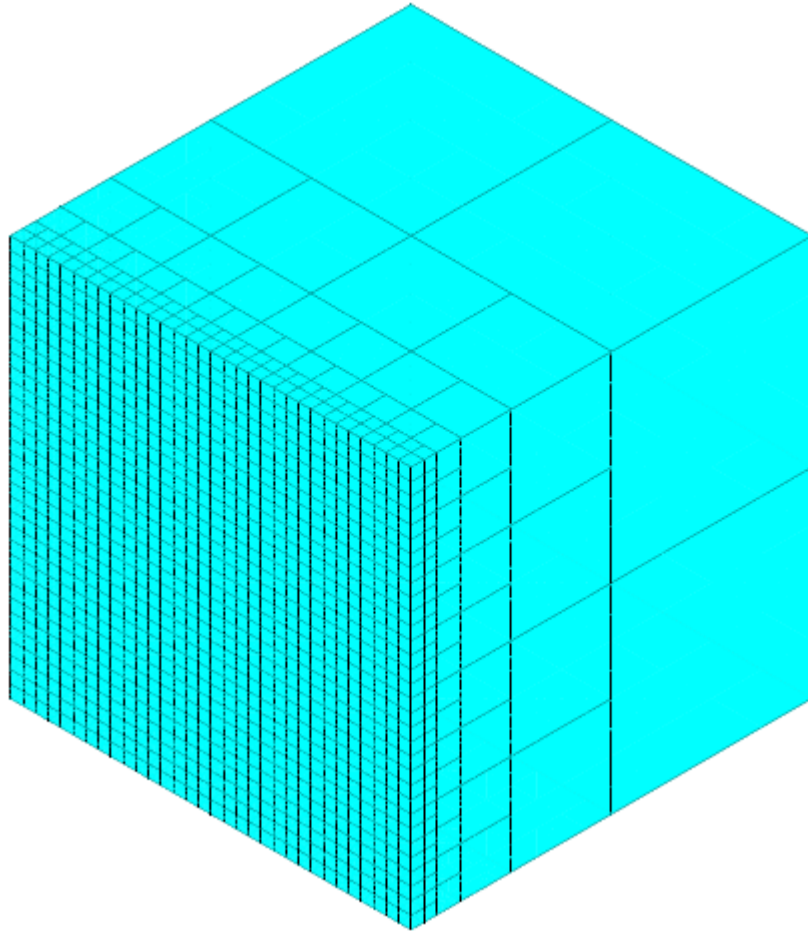
Number of layers $k = O(N_e) = O(N/p^3)$

Total cost of LU factorization $O(p^6 * k) = O(p^6 * N/p^3) = O(N * p^3)$

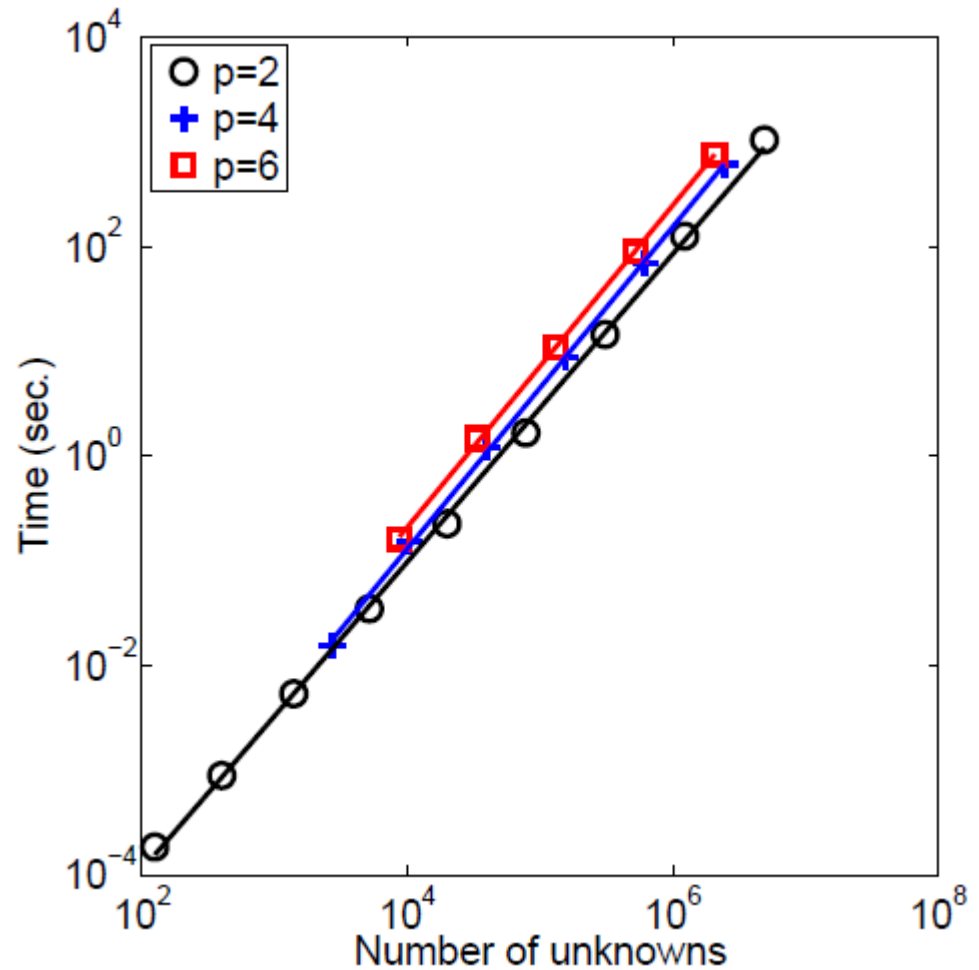
Total cost is $O(N * p^6 + N * p^3) = O(Np^6)$



ISOTROPIC REFINEMENTS TOWARDS FACE SINGULARITY



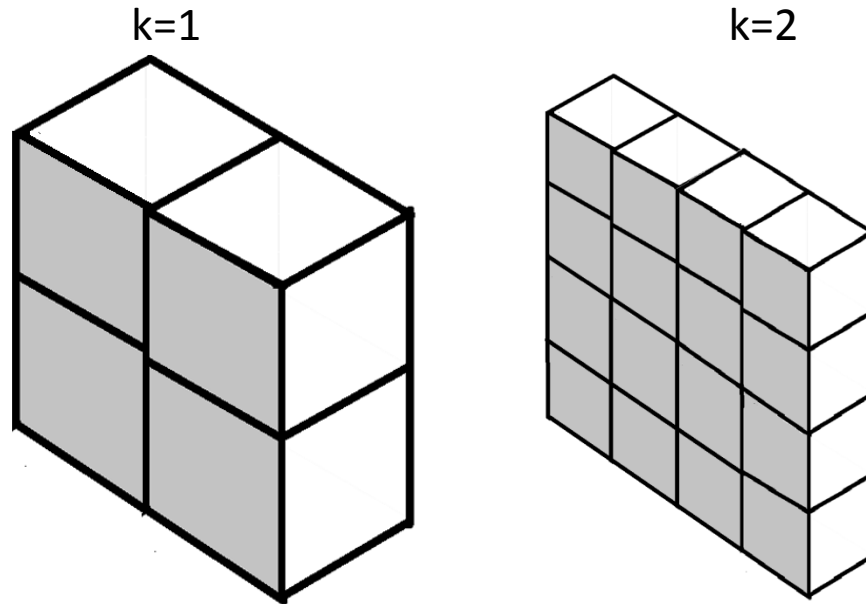
Mesh



Time of LU factorization
Slope = exponent factor = 1.5
Location = p factor = $p^{1.5}$



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

Number of dofs in a layer $2^{2k}p^2 = O(2^{2k}p^2)$
 Number of interfaces dofs in a layer $2^{2k}p^2 = O(2^{2k}p^2)$
 Cost of Schur complement of a single layer $O(2^{6k}p^6)$

s =number of layers, $N = O\left(\sum_{k=1}^s 2^{2k}p^3\right) = O(p^3 2^{2s})$

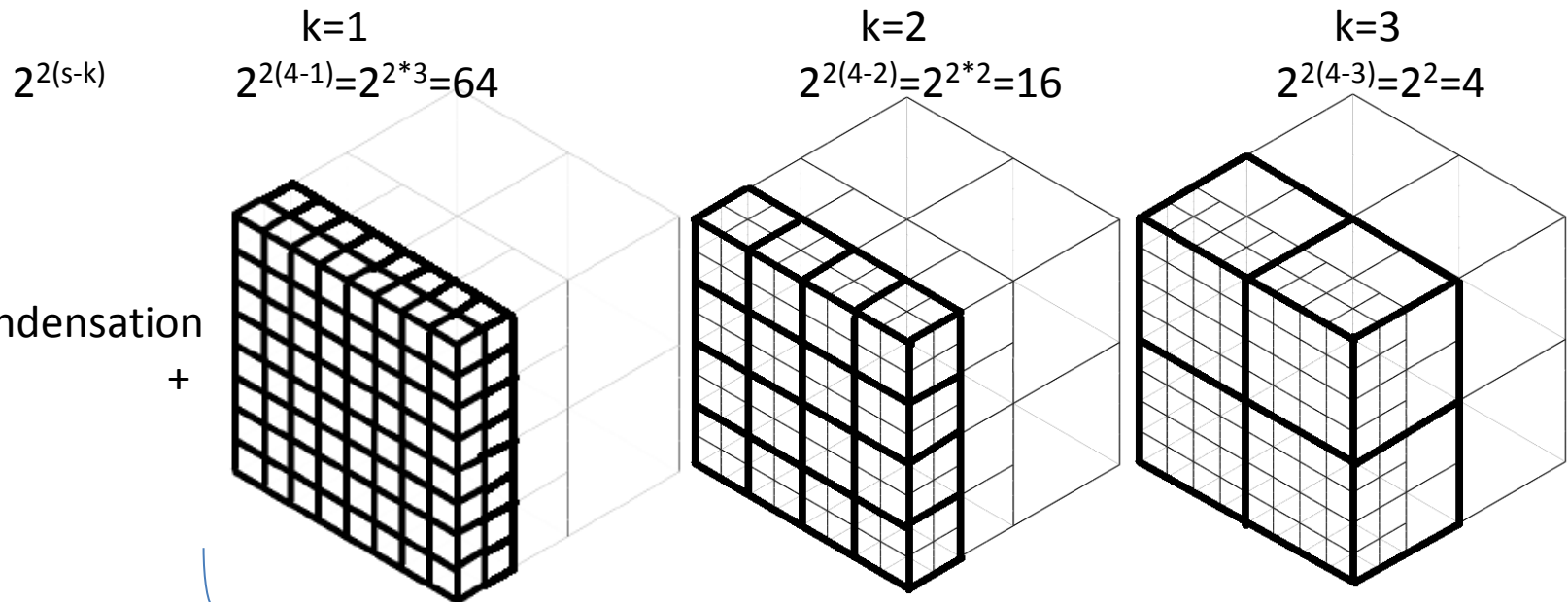
Cost of LU factorization $O\left(\sum_{k=1}^s 2^{6k}p^3\right) = O(p^6 2^{6s}) = O(N^3/p^3)$

DO NOT USE FRONTAL SOLVER APPROACH



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY

MULTI-FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

- Number of dofs in a patch $O(2^k p^2)$
- Numbers of patches in a layer $O(2^{2(s-k)})$
- Number of interfaces dofs in a patch $O(2^k p^2)$
- Cost of Schur complement of a single layer $O(2^{2(s-k)} 2^{3k} p^6)$

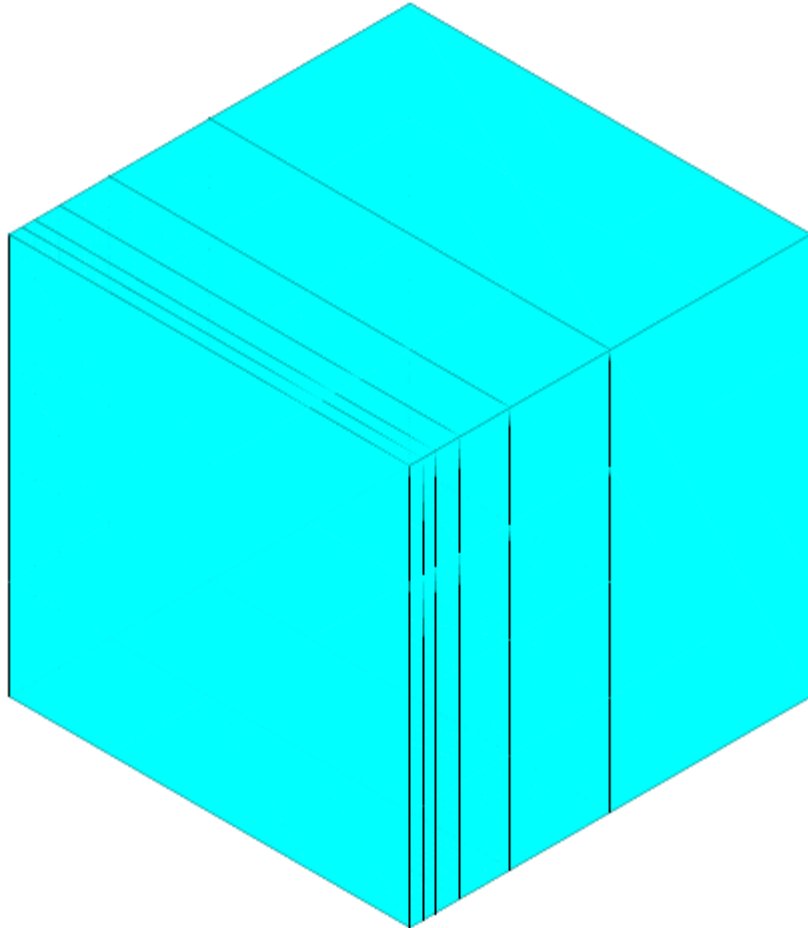
s =number of layers, $N = O\left(\sum_{k=1}^s 2^{2k} p^3\right) = O(p^3 2^{2s})$

Cost of LU factorization $O\left(\sum_{k=1}^s 2^{2(s-k)} 2^{3k} p^6\right) = O(p^6 2^{3s}) = O(N^{1.5} * p^{1.5})$

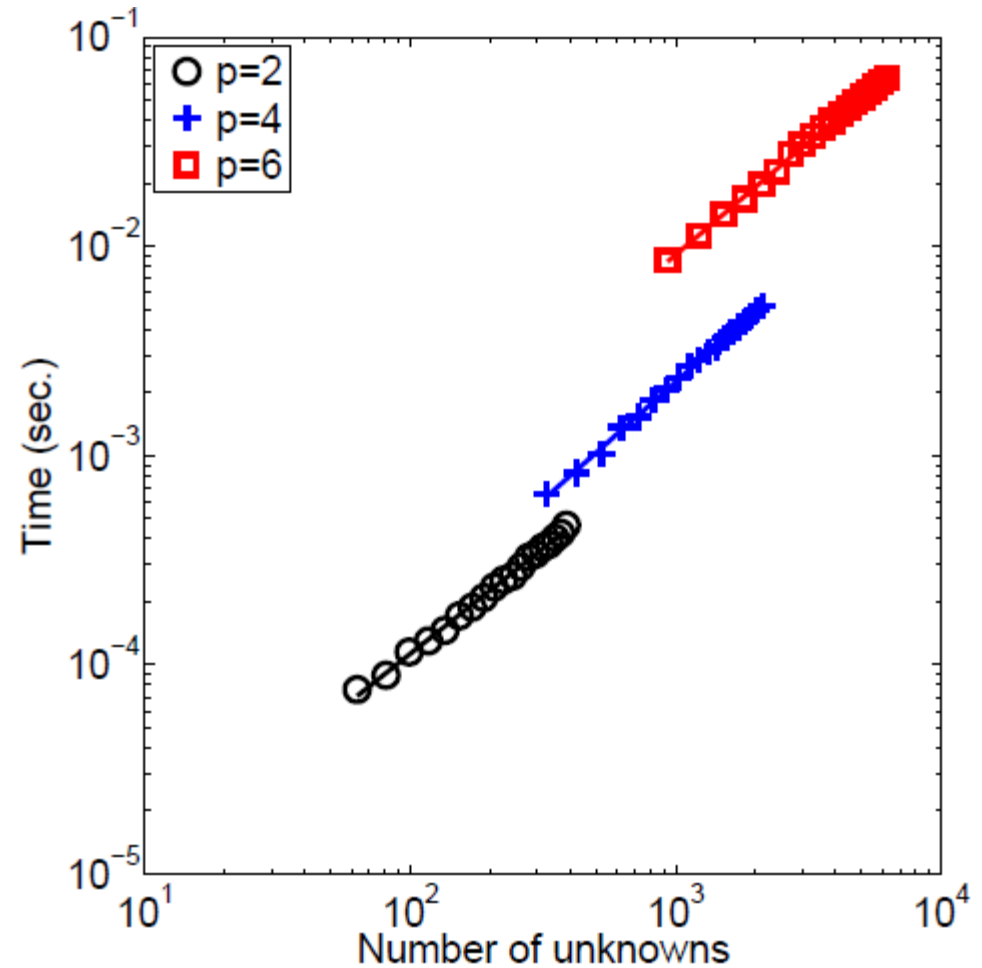
Total cost is $O(N * p^6 + N^{1.5} * p^{1.5})$



ANISOTROPIC REFINEMENTS TOWARDS FACE SINGULARITY



Mesh



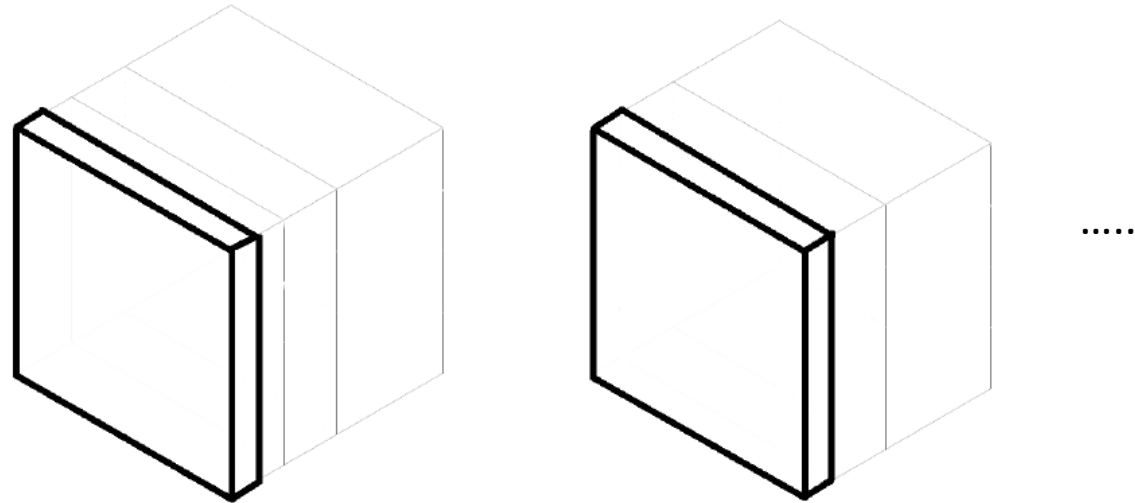
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6



ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY FRONTAL SOLVER APPROACH



Static condensation
 $O(N * p^6)$ +

Number of dofs in a layer $O(p^2)$

Number of interfaces dofs in a layer $O(p^2)$

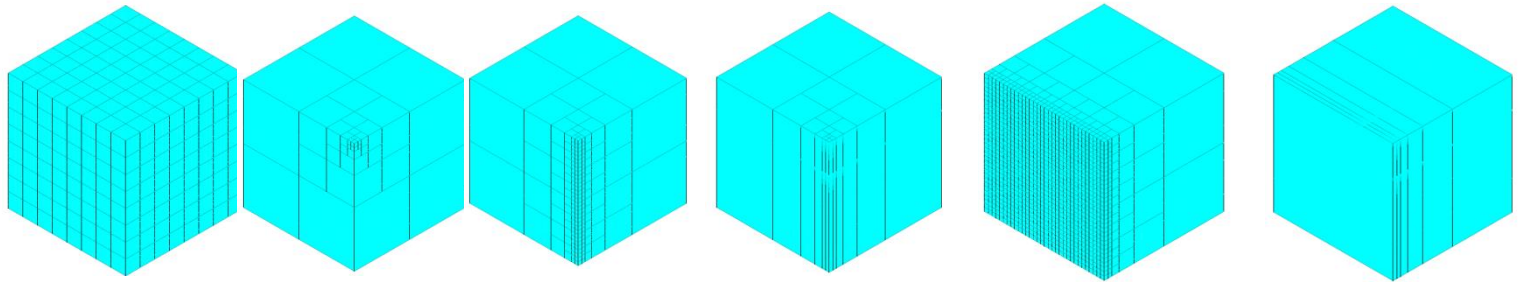
Number of layers $k = O(N_e) = O(N/p^3)$

Total cost of LU factorization $O(p^6 * k) = O(p^6 * N/p^3) = O(N * p^3)$

Total cost is $O(N * p^6 + N * p^3) = O(Np^6)$



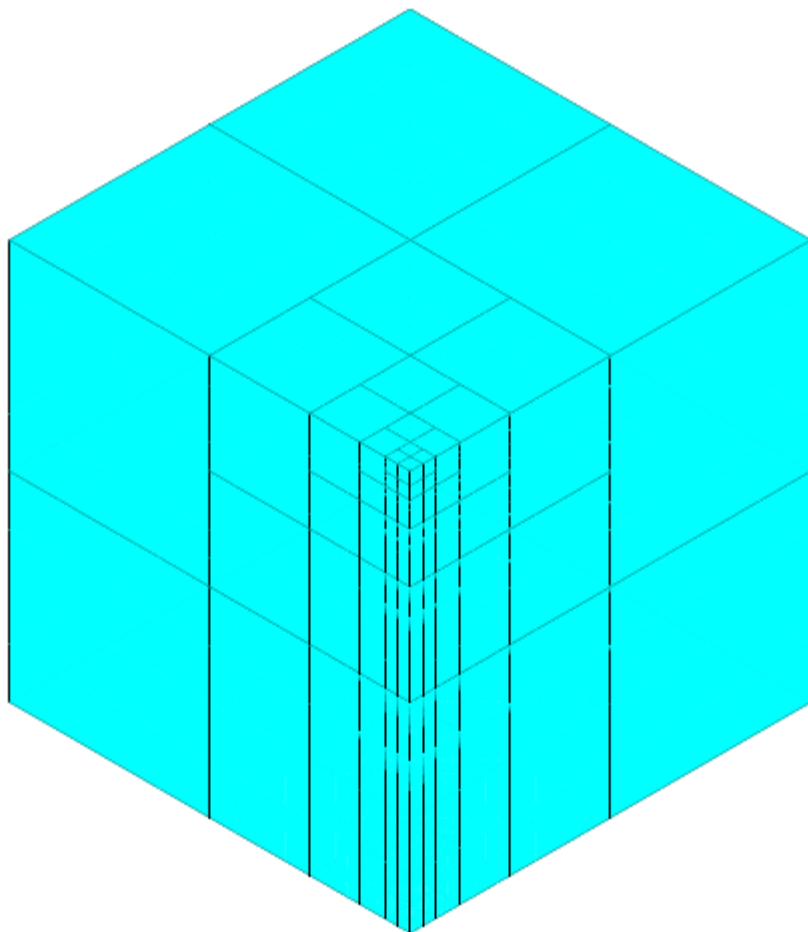
COMPARISON OF NUMERICAL AND THEORETICAL SCALABILITY EXPONENT FACTORS FOR REFINEMENTS TOWARDS A SINGLE ENTITY



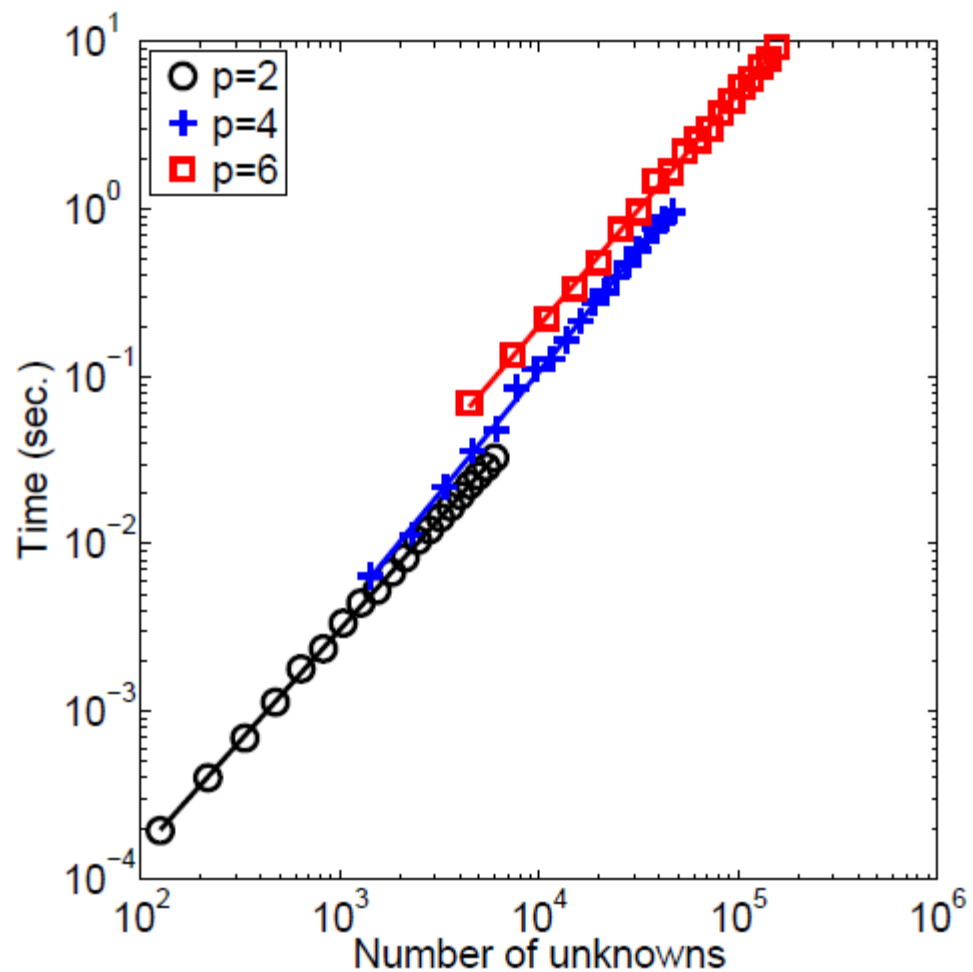
	Uniform	Point	Edge Isotropic	Edge Anisotropic	Face Isotropic	Face Anisotropic
$p = 2$	1.86	1.09	1.10	1.07	1.47	1.01
$p = 4$	1.86	1.17	1.18	1.07	1.47	1.12
$p = 6$	1.83	1.08	1.21	1.09	1.54	1.08
Theoretical	2	1	1	1	1.5	1



POINT + ANISOTROPIC EDGE SINGULARITY



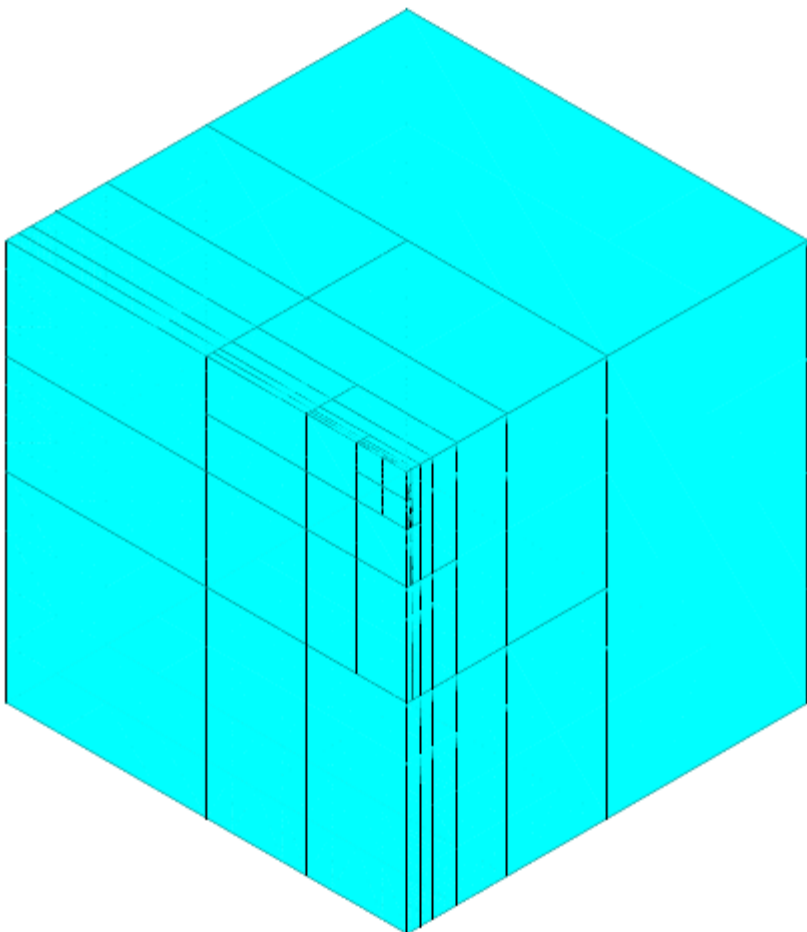
Mesh



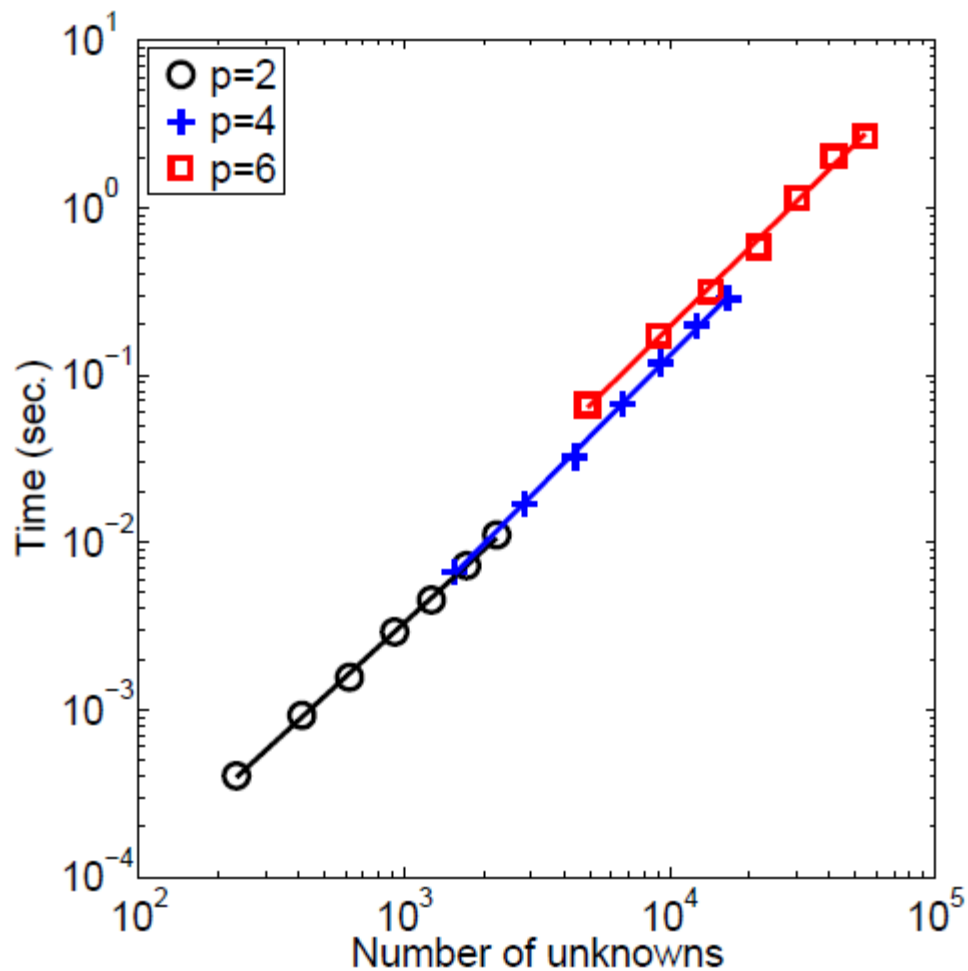
Time of LU factorization



POINT + ANISOTROPIC FACE SINGULARITY



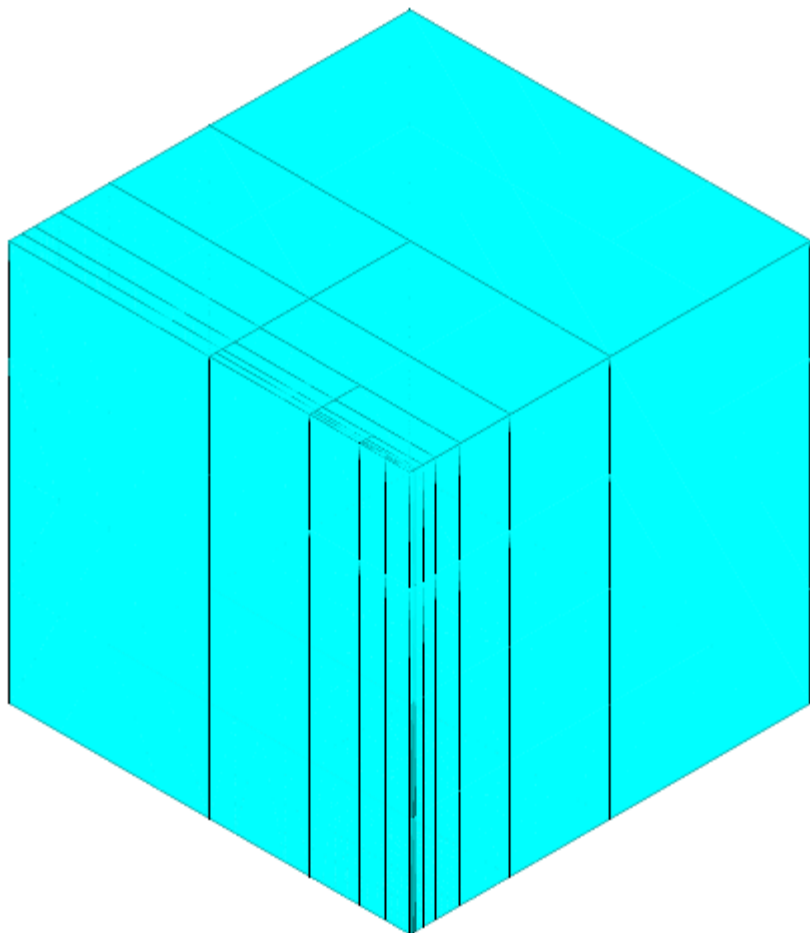
Mesh



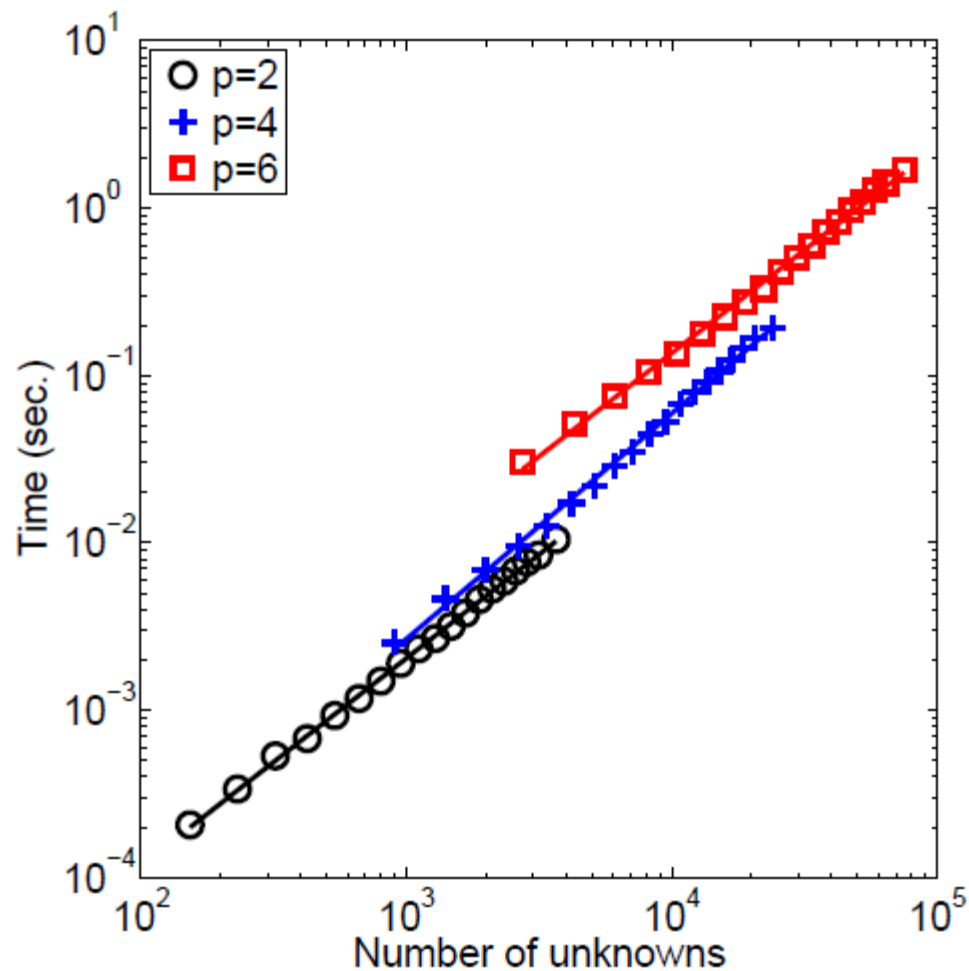
Time of LU factorization



ANISOTROPIC EDGE + ANISOTROPIC FACE SINGULARITY



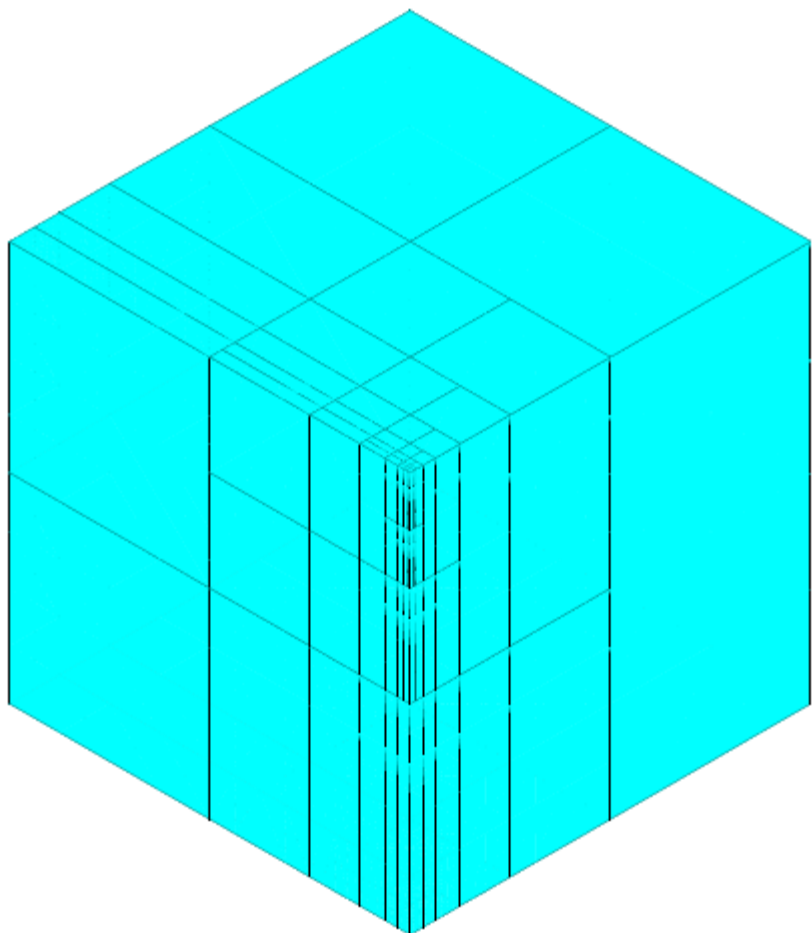
Mesh



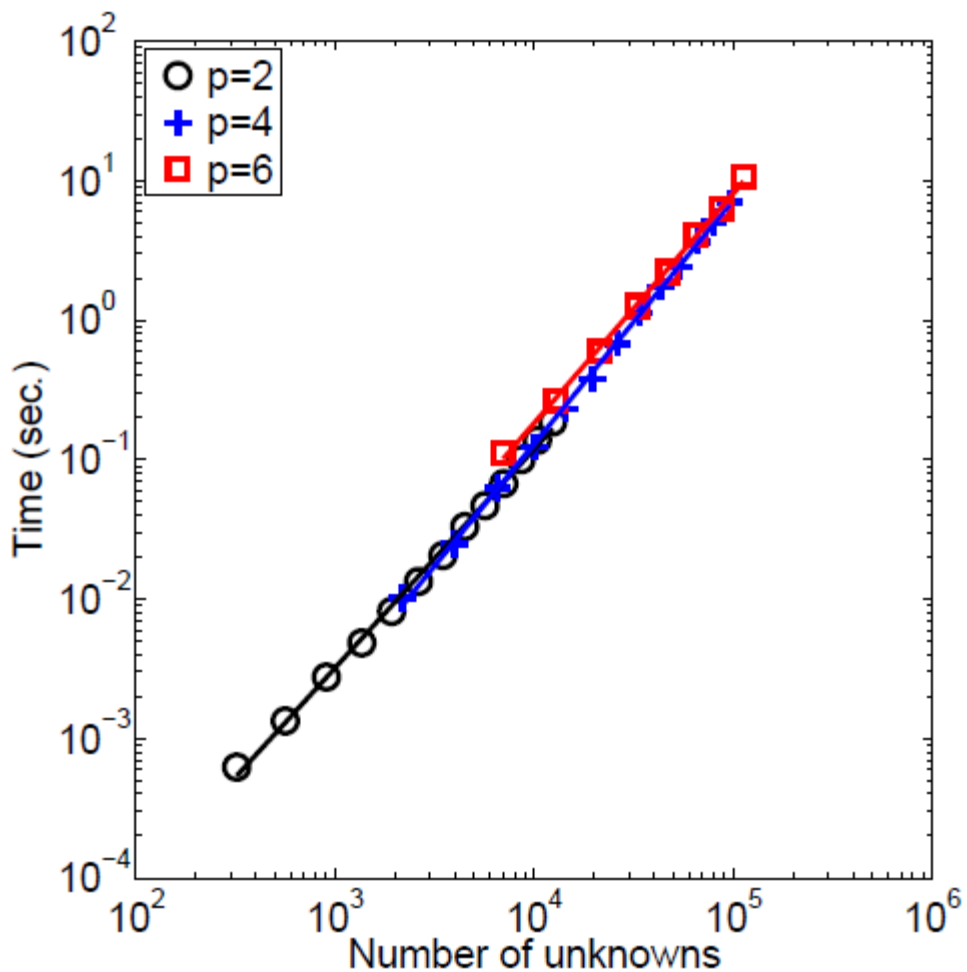
Time of LU factorization



POINT + ANISOTROPIC EDGE + ANISOTROPIC FACE SINGULARITY



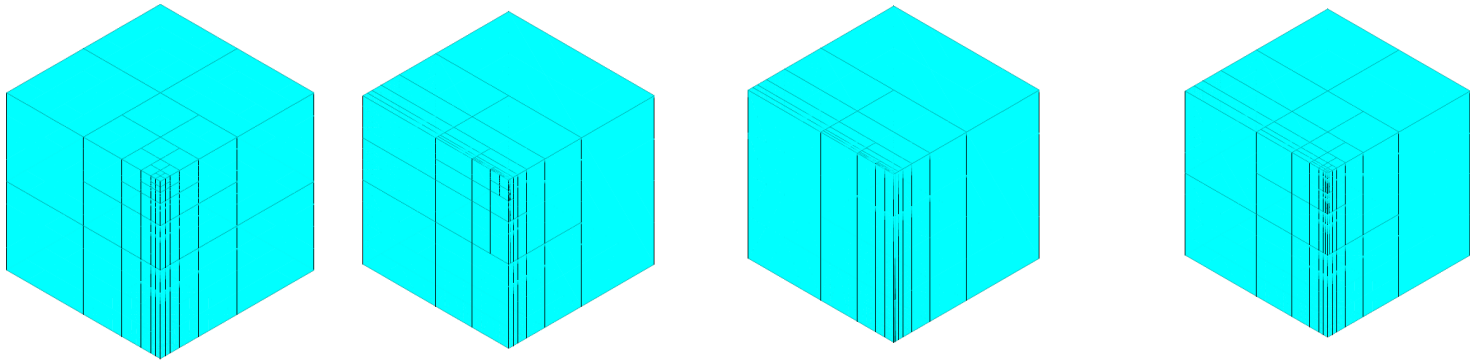
Mesh



Time of LU factorization



NUMERICAL SCALABILITY EXPONENT FACTORS FOR REFINEMENTS TOWARDS MULTIPLE SINGULARITIES



	Point + Edge	Point + Face	Edge + Face	Point + Edge + Face
$p = 2$	1.33	1.46	1.24	1.57
$p = 4$	1.45	1.60	1.35	1.75
$p = 6$	1.39	1.56	1.23	1.65



PAPERS

Maciej Paszyński, David Pardo, Damian Goik

PERFORMANCE OF DIRECT SOLVERS ON H-ADAPTED GRIDS

submitted to *SIAM Journal of Numerical Analysis*, 2013

