Frontal and multi-frontal solvers: Dealing with singularities

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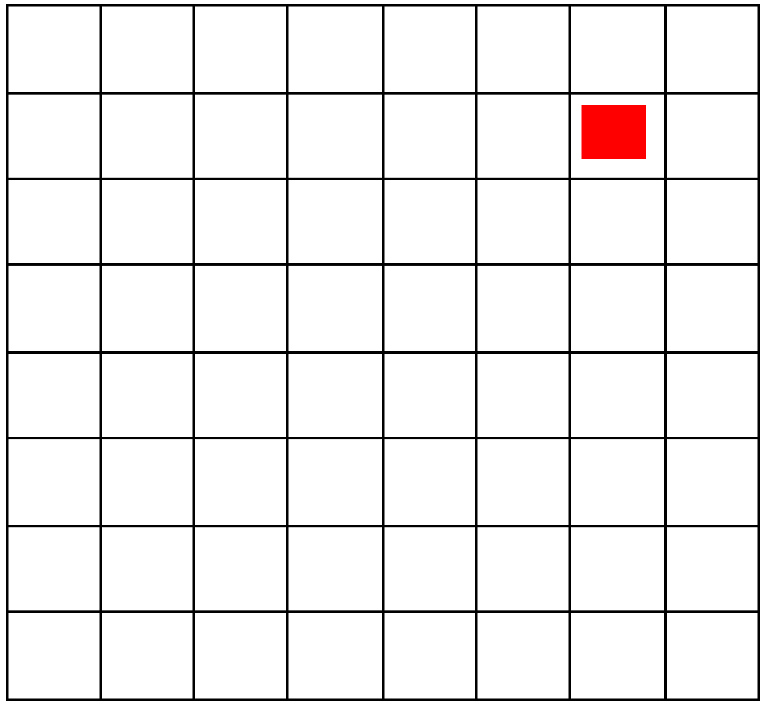
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

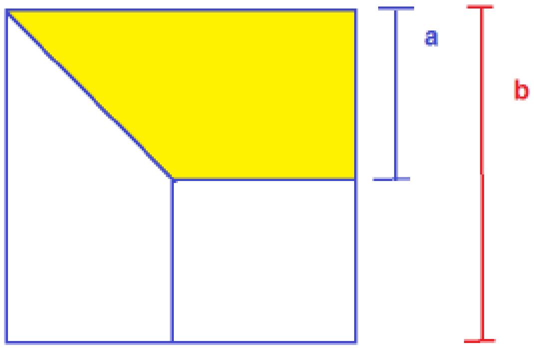


FLOPS(2D)=p^6.

FLOPS(3D)=p^9.

COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

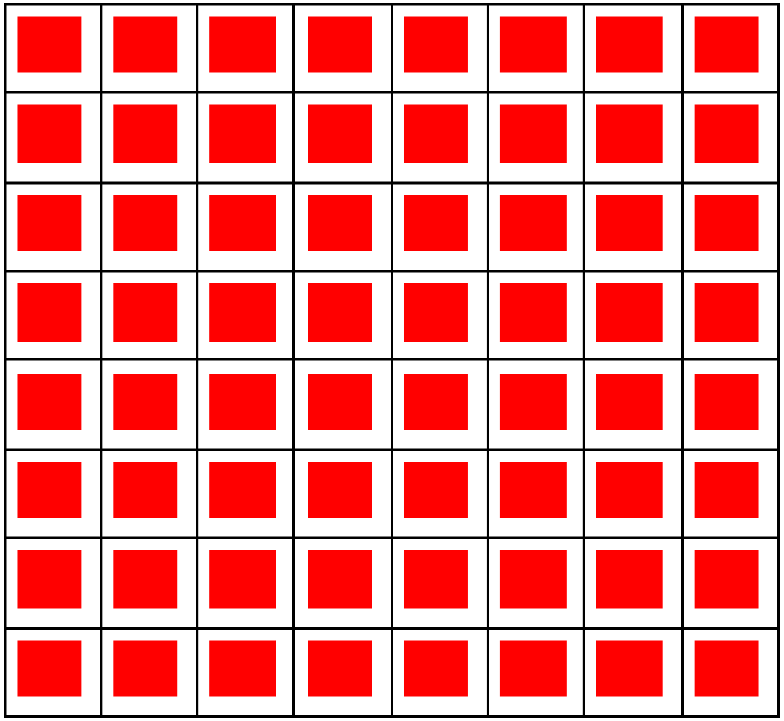
Number of operations for partial forward elimination
(Schur complement computations)



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

Computational complexity $O(ab^2)$

COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

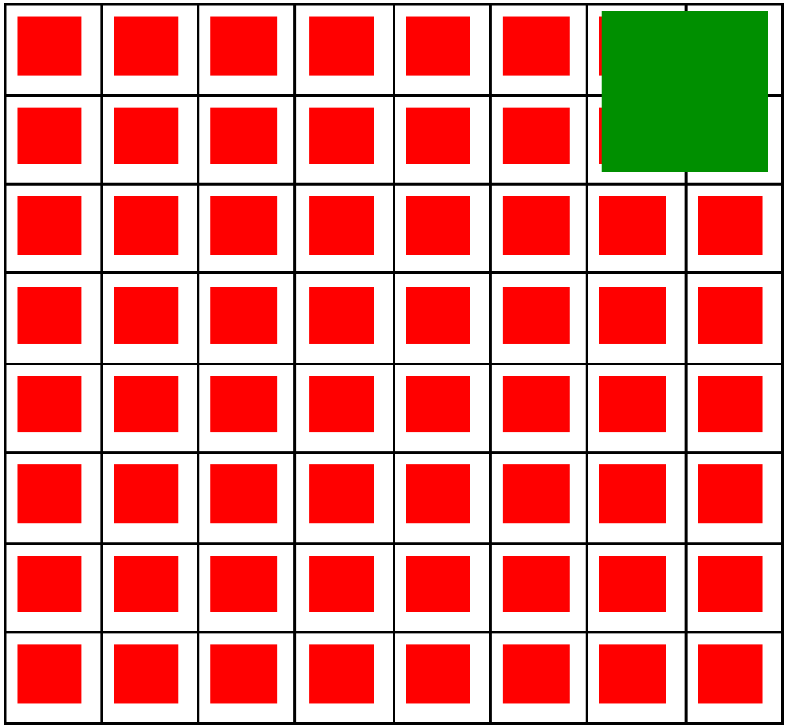


FLOPS(2D)=$2^{2s}p^6$.

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

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

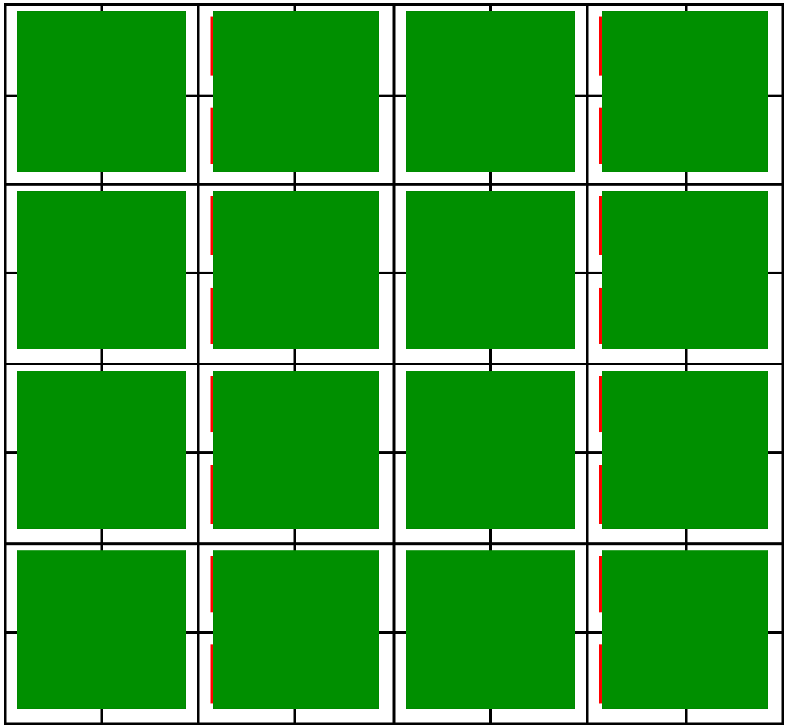
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



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

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

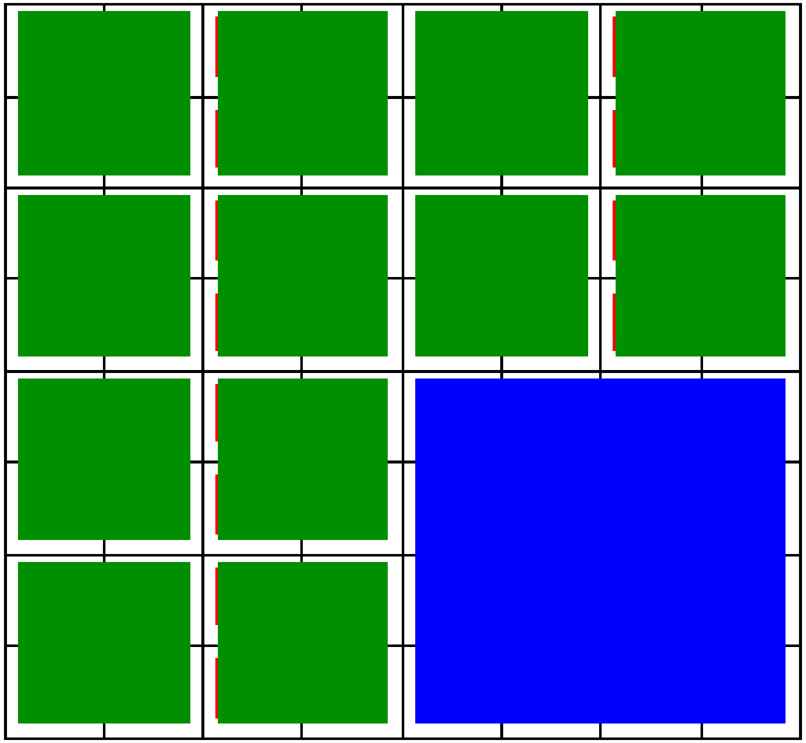
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



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

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

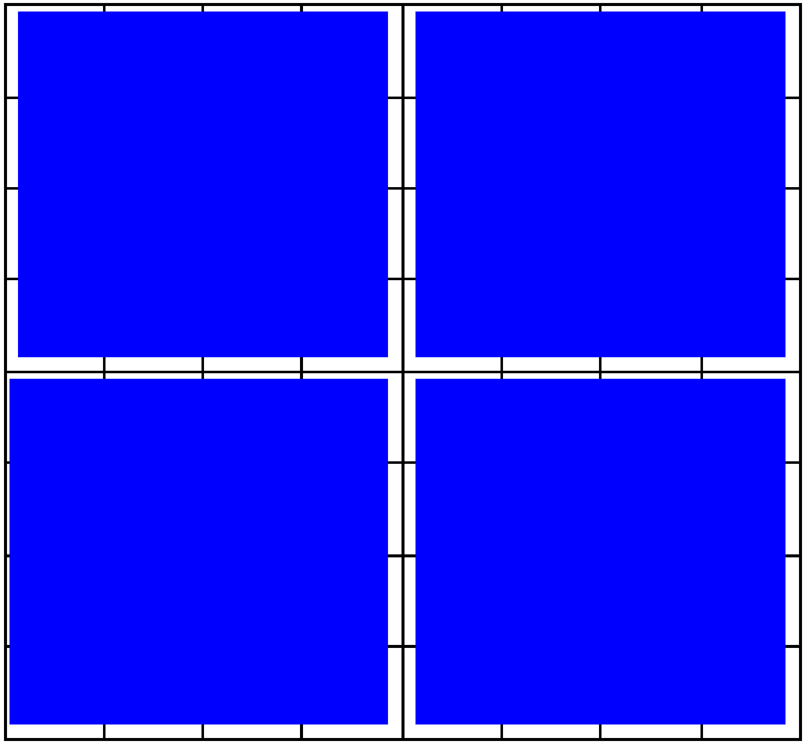
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



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

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

COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER



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

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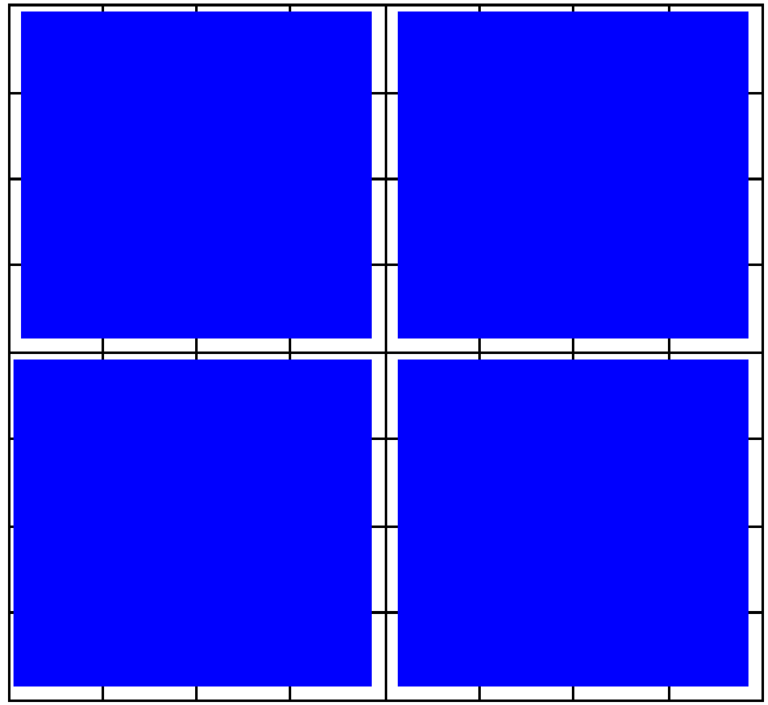
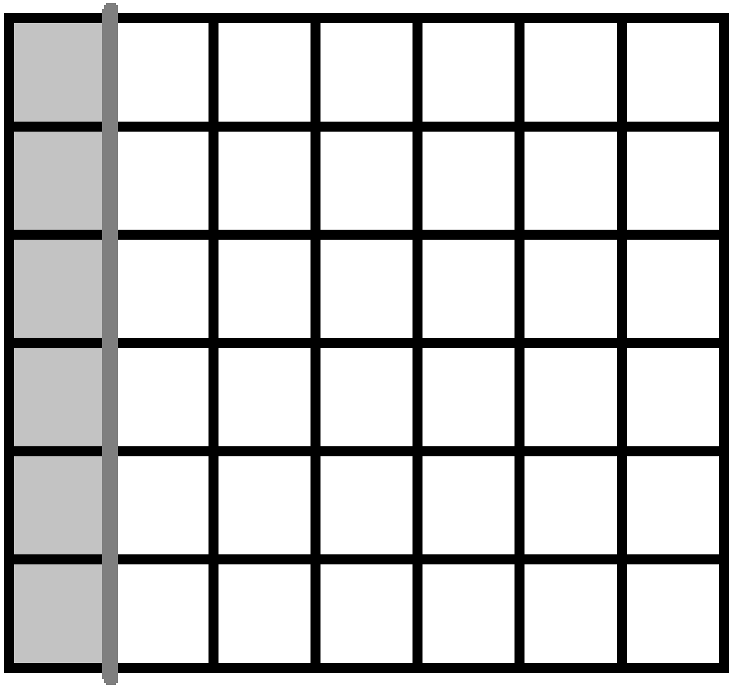
COMPUTATIONAL COST OF MULTI-FRONTAL SOLVER

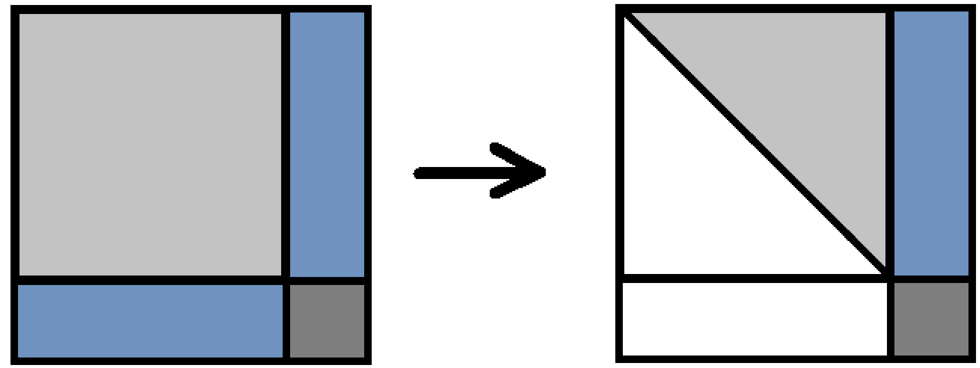


FLOPS(2D)=$2^{2s}p^6 + 2^{2(s-1)}2^4p^4 + 2^{2(s-2)}2^8p^4 + \ldots = \mathcal{O}(Np^4) + \mathcal{O}(N^{1.5})$

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

COMPUTATIONAL COST OF FRONTAL SOLVER





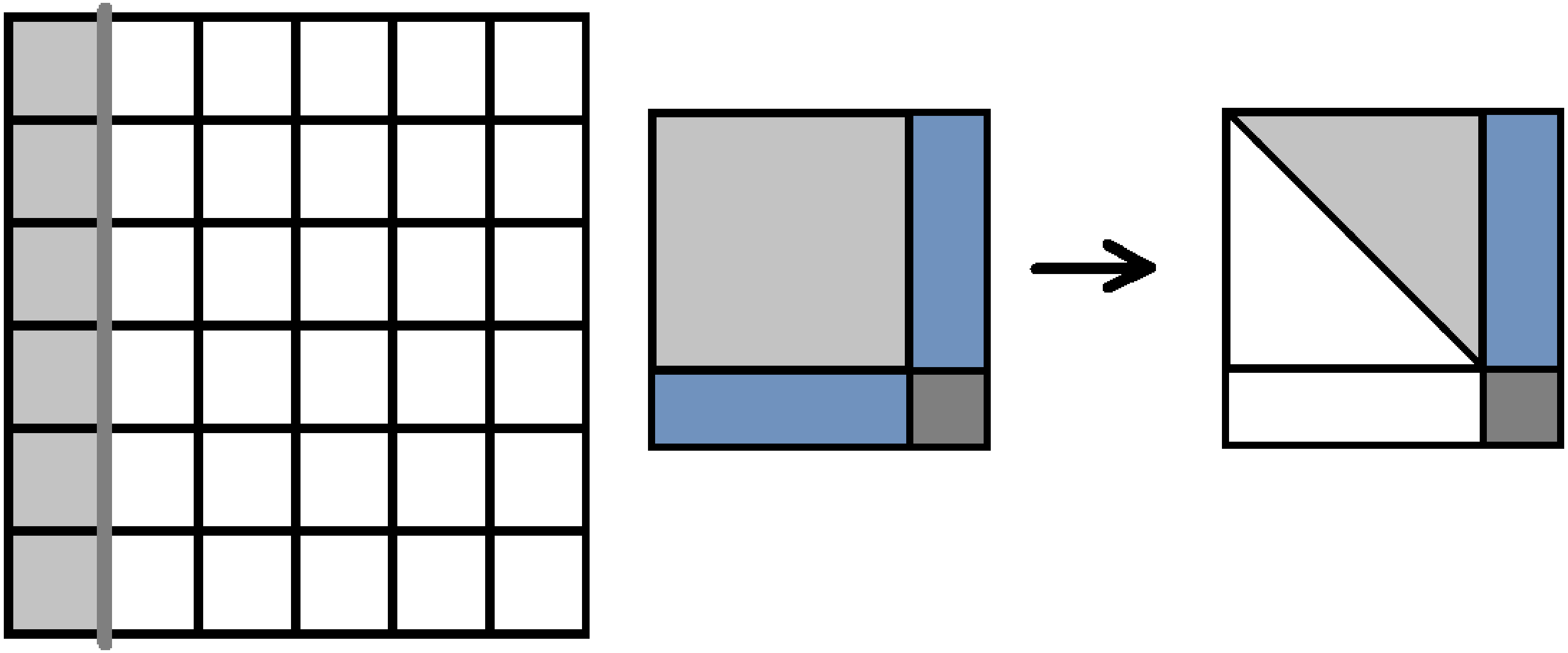
Computational cost of elimination of a single layer $O((N^{0.5})^3)=O(N^{3/2})$
Number of layers = $O(N^{0.5})$

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



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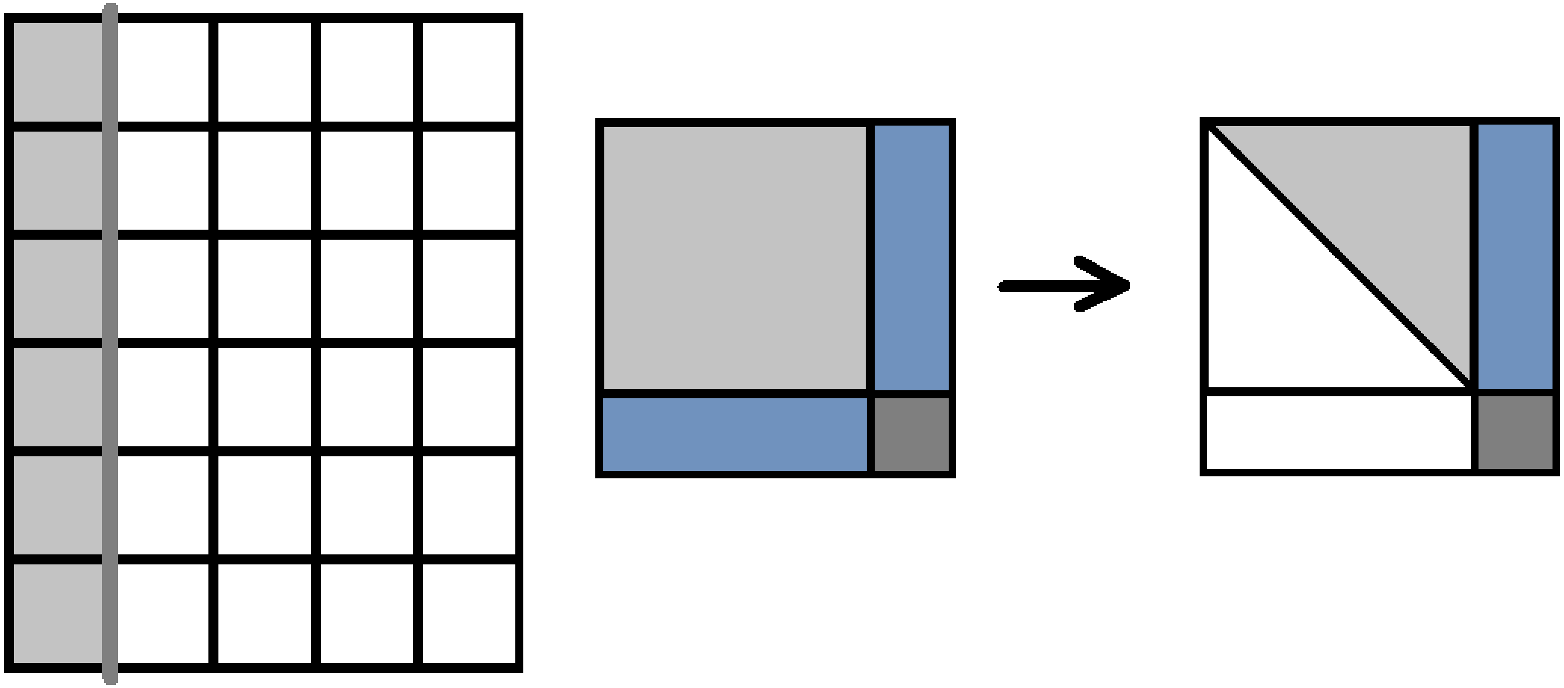

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MODEL ELIPTIC PROBLEM

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

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

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

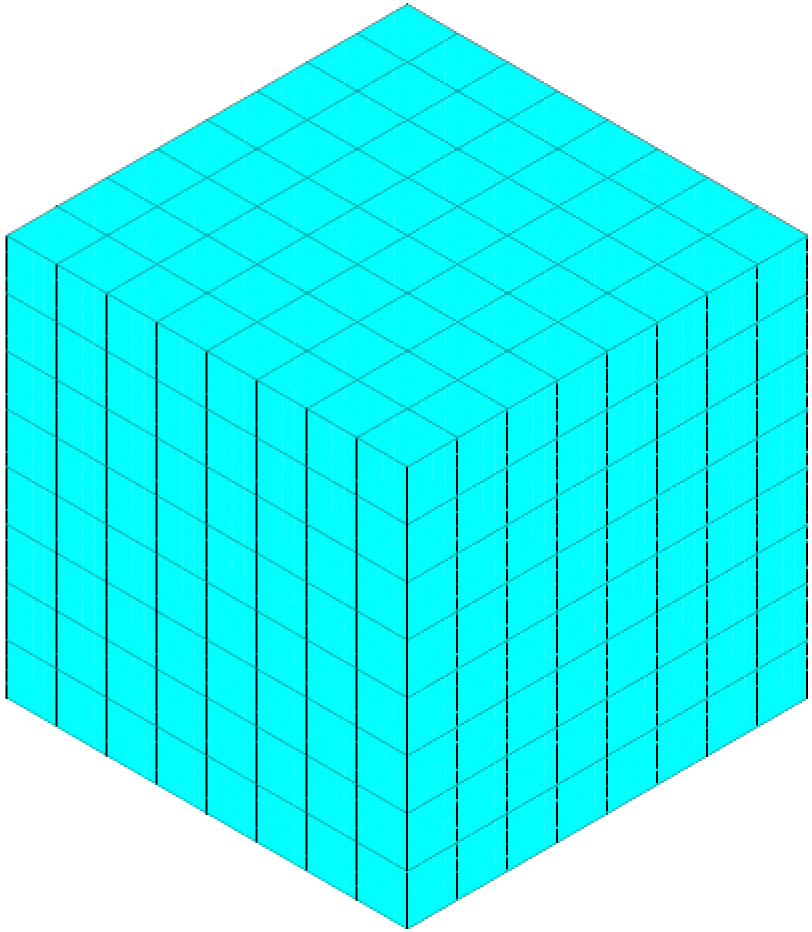
Static condensation $O(N_e*p^9)=O(N*p^6)$

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

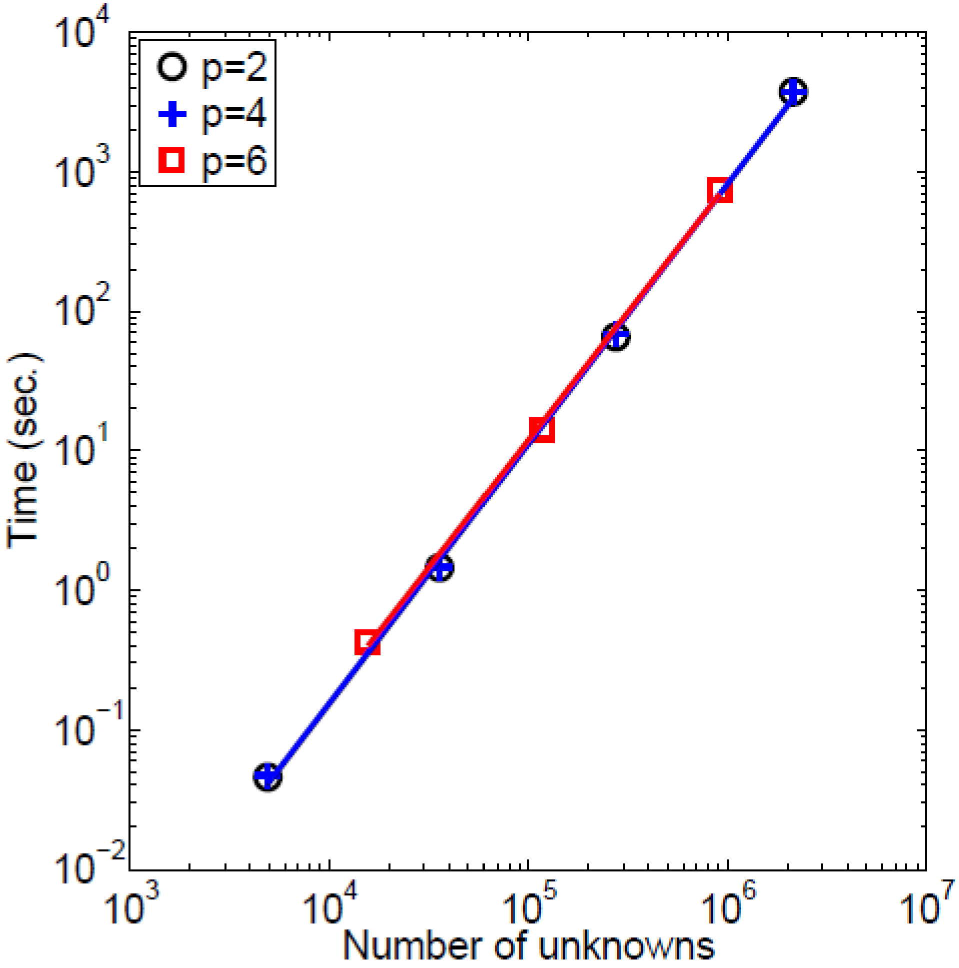
CONCLUSIONS:
For regular grid total cost is $O(N*p^6+N^2) = O(N^2)$

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

UNIFORM REFINEMENTS



Mesh



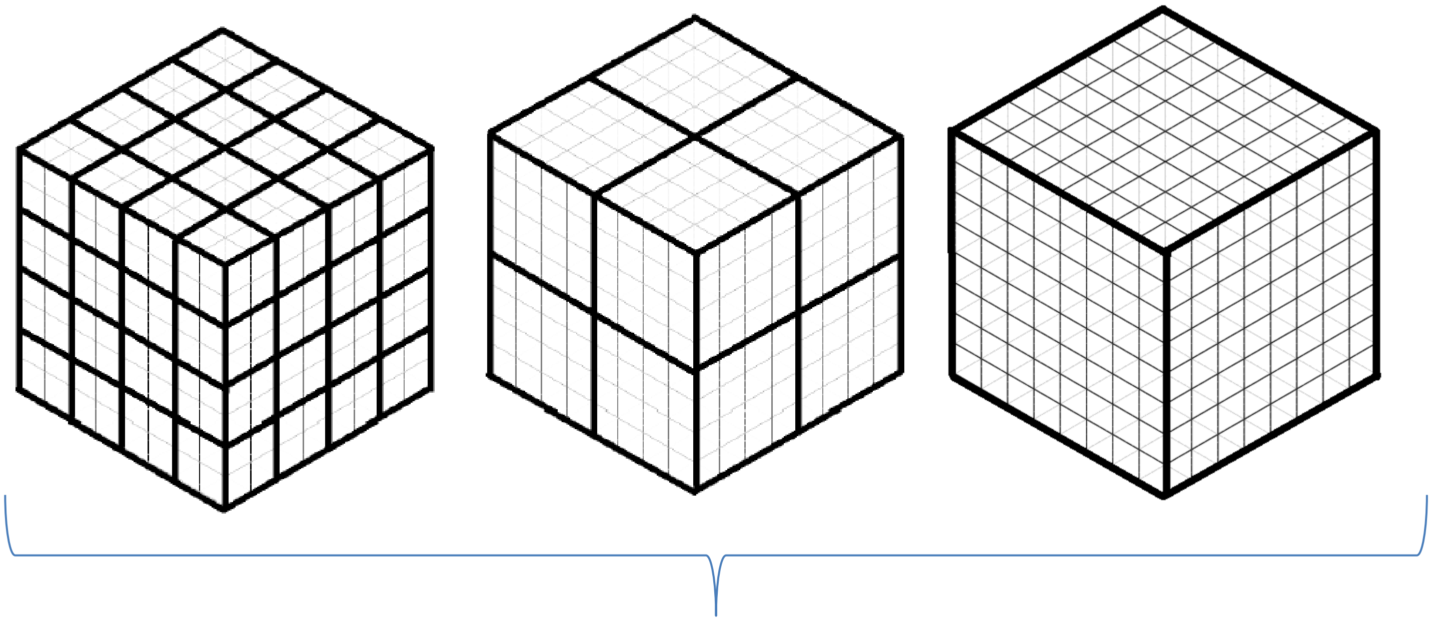
Time of LU factorization

Slope = exponent factor = 2

Location = p factor = $1=p^0$

UNIFORM REFINEMENTS
MULTI-FRONTAL SOLVER APPROACH

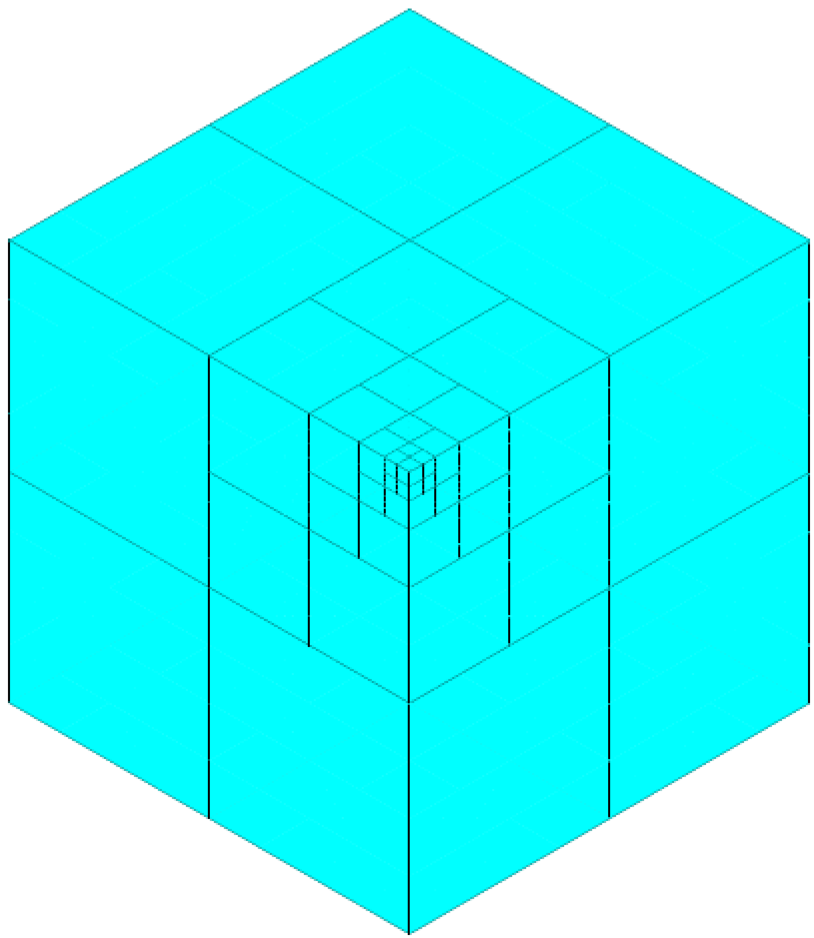
Static condensation
$O(N*p^6)$ +



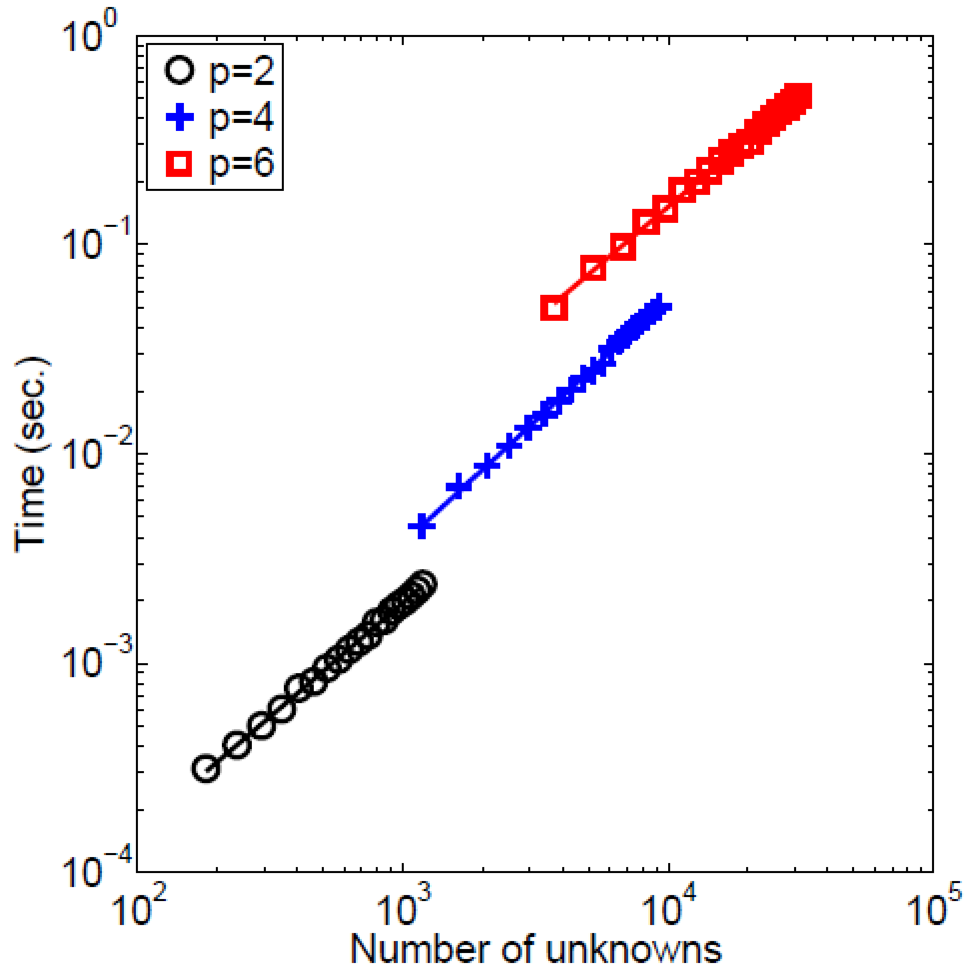
LU factorization $O(N^2)$

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

REFINEMENTS TOWARDS POINT SINGULARITY



Mesh



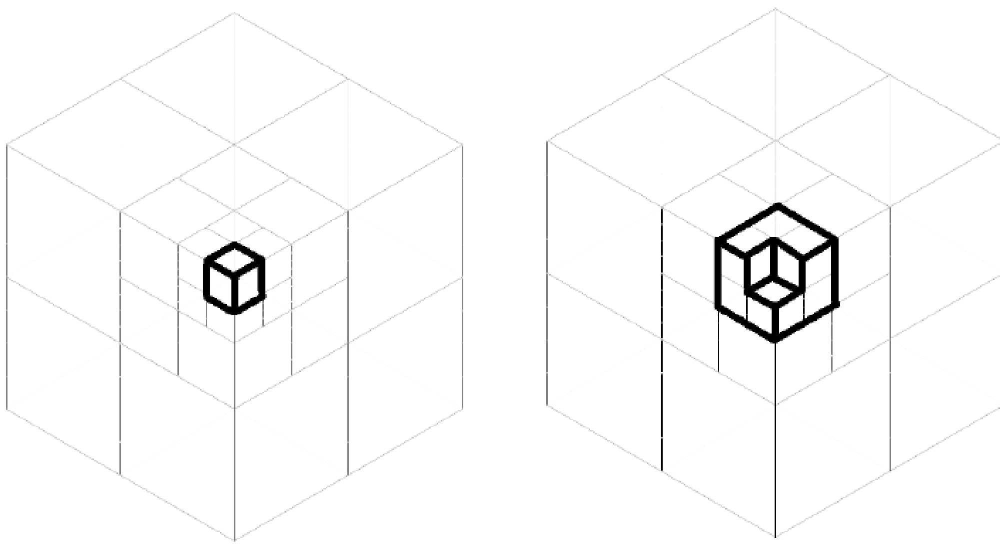
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6

REFINEMENTS TOWARDS POINT SINGULARITY
FRONTAL SOLVER APPROACH

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



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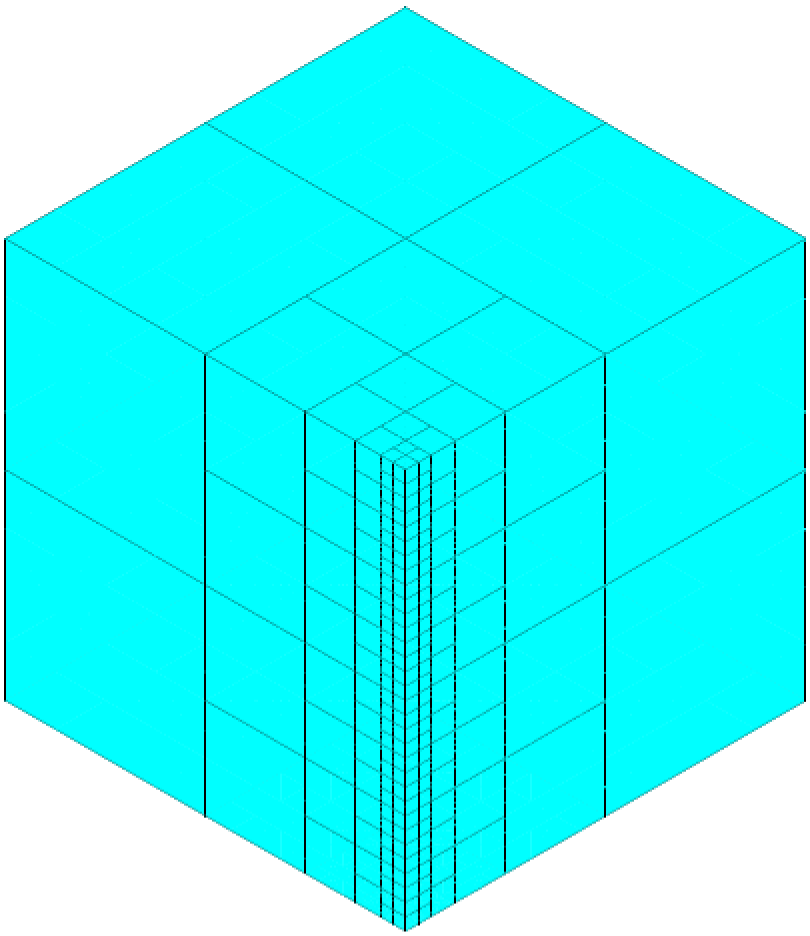
Schur complent of a single layer $O(p^6)$
Number of layers $k=O(N_e)=O(N/p^3)$

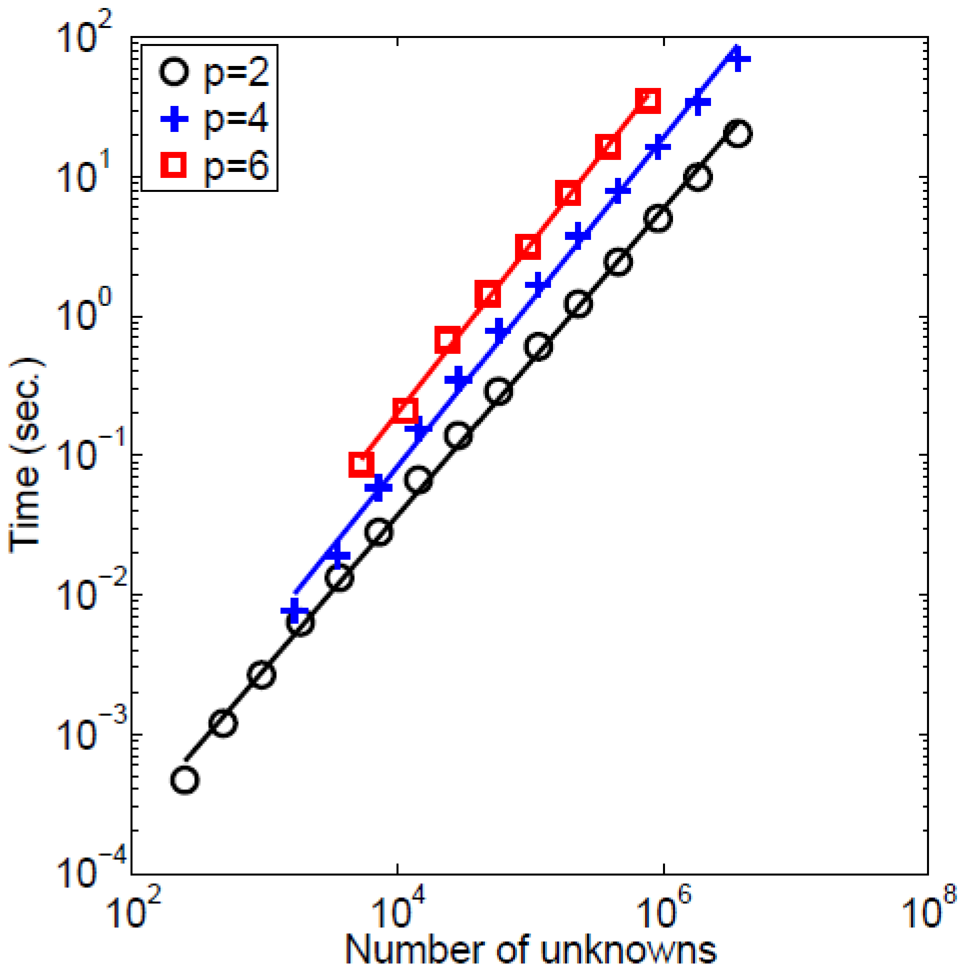
Total cost of LU factorization $O(p^6*k)=O(p^6*N/p^3)= O(N*p^3)$

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

ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY



Mesh



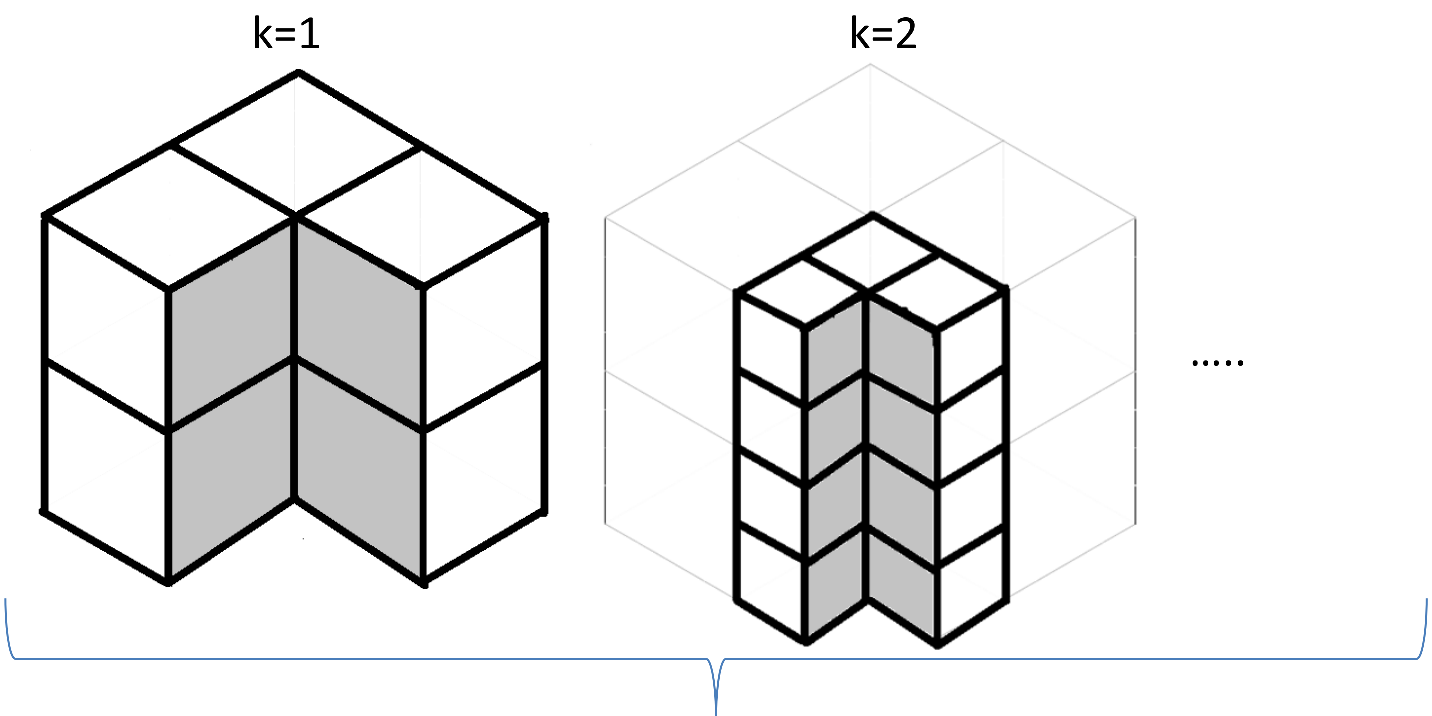
Time of LU factorization

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

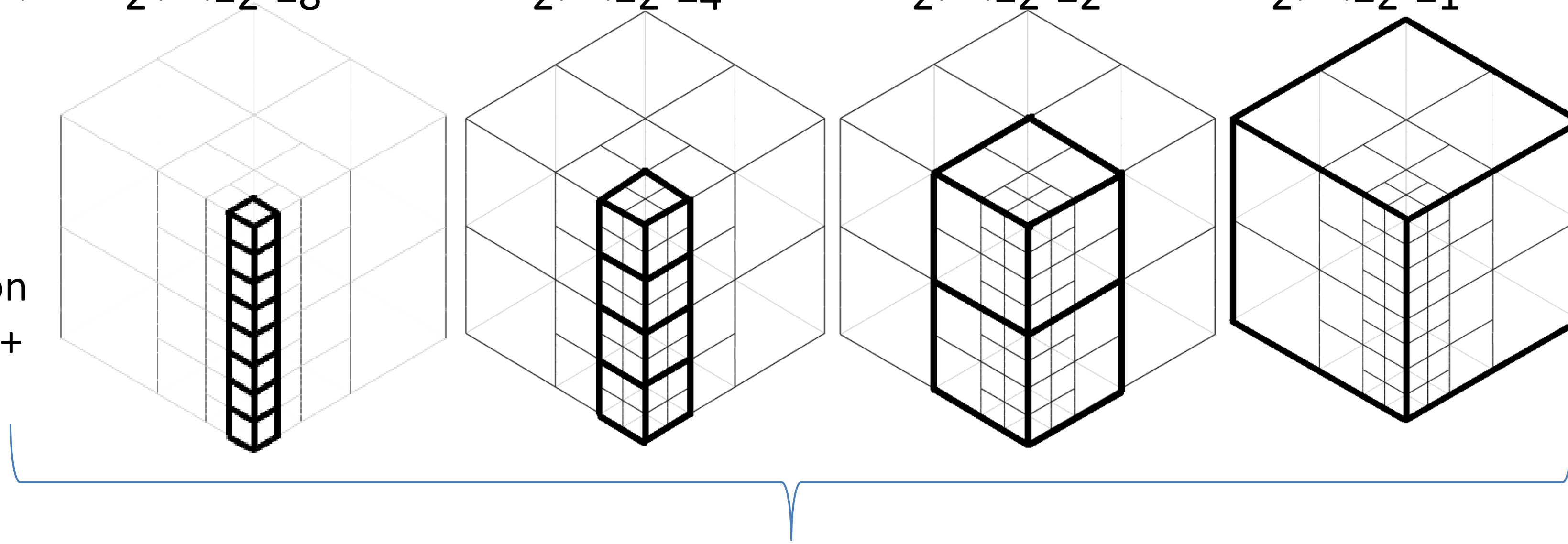
Cost of LU factorization $O\left(\sum_{k=1}^{s} 2^{3k} p^6\right) = O(p^6 2^{3s}) = O(N^3/p^3)$

DO NOT USE FRONTAL SOLVER APPROACH

ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY MULTI-FRONTAL SOLVER APPROACH

	k=1	k=2	k=3	k=4
$2^{(s-k)}$	$2^{(4-1)}=2^3=8$	$2^{(4-2)}=2^2=4$	$2^{(4-3)}=2^1=2$	$2^{(4-4)}=2^0=1$

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



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 $O(kp^2)$

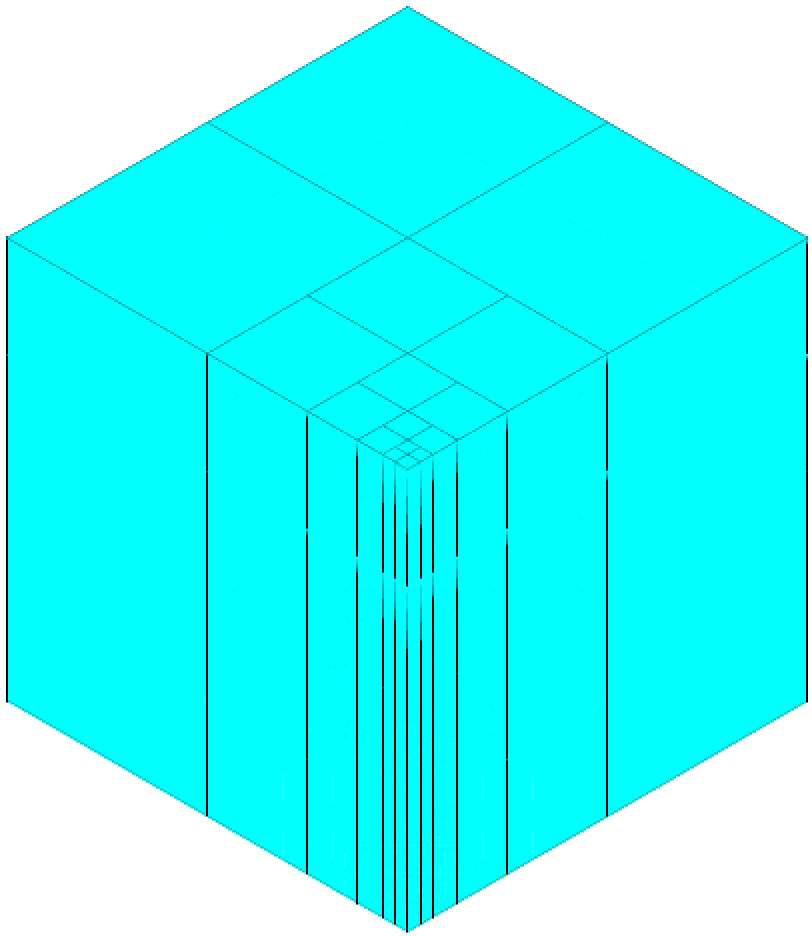
Cost of Schur complement of a single layer $O(2^{s-k}k^3p^6)$

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

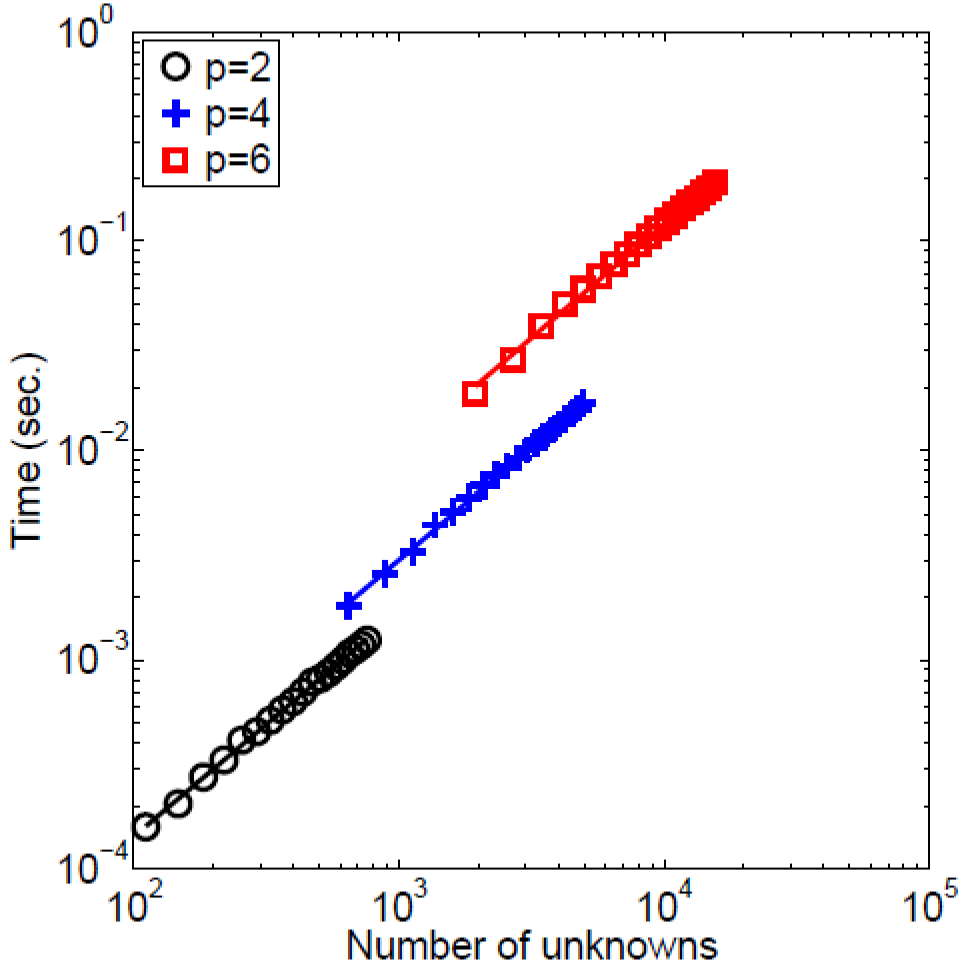
Cost of LU factorization $O\left(\sum_{k=1}^{s} 2^{s-k} k^3 p^6\right) < O(s^3 p^6 2^s) = O(Np^3 (\log_2{}^3 N_e))$

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

ANISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY



Mesh



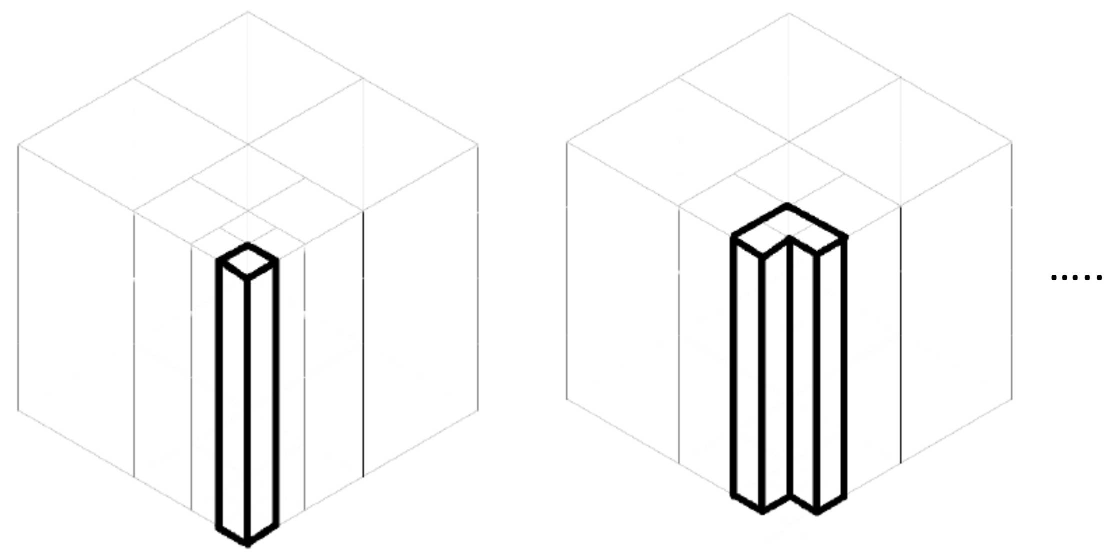
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6

ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY FRONTAL SOLVER APPROACH

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

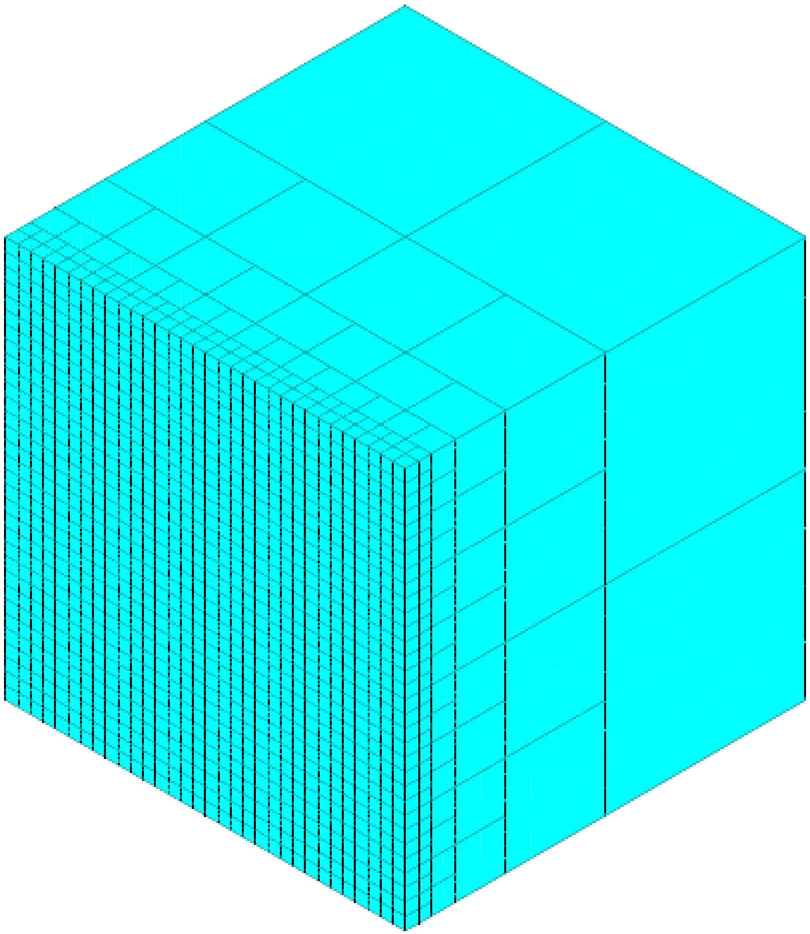


Number of dofs in a layer $O(p^2)$
Number of interfaces dofs in a layer $O(p^2)$
Number of layers $k=O(N_e)=O(N/p^3)$

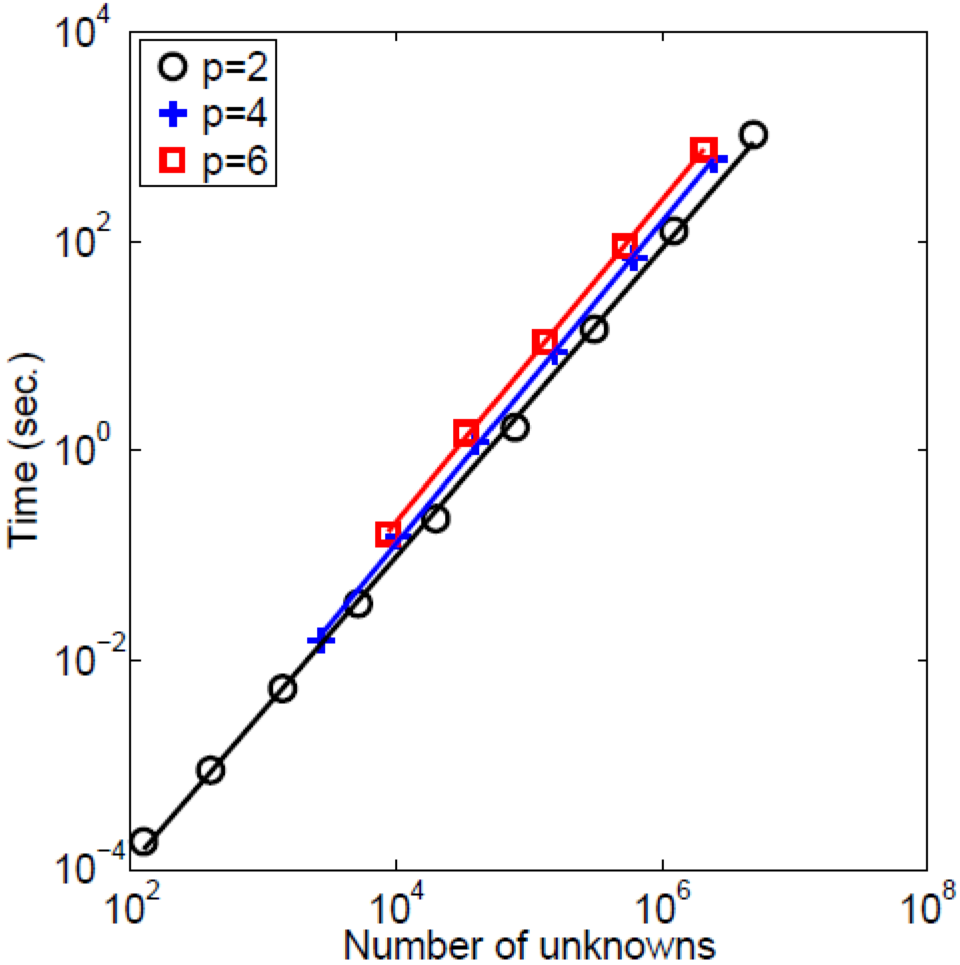
Total cost of LU factorization $O(p^6*k)=O(p^6*N/p^3)= O(N*p^3)$

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

ISOTROPIC REFINEMENTS TOWARDS FACE SINGULARITY



Mesh



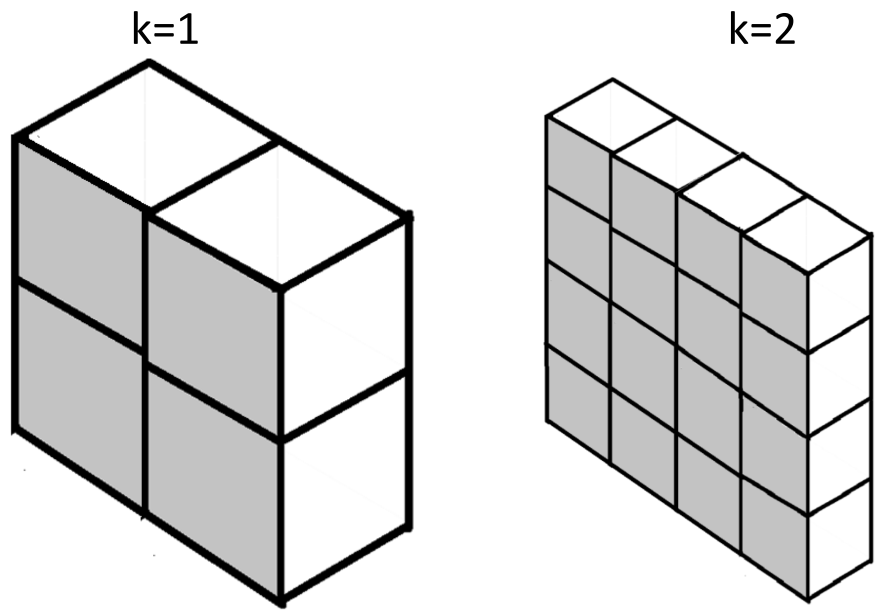
Time of LU factorization

Slope = exponent factor = 1.5

Location = p factor = $p^{1.5}$

ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY
FRONTAL SOLVER APPROACH

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



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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

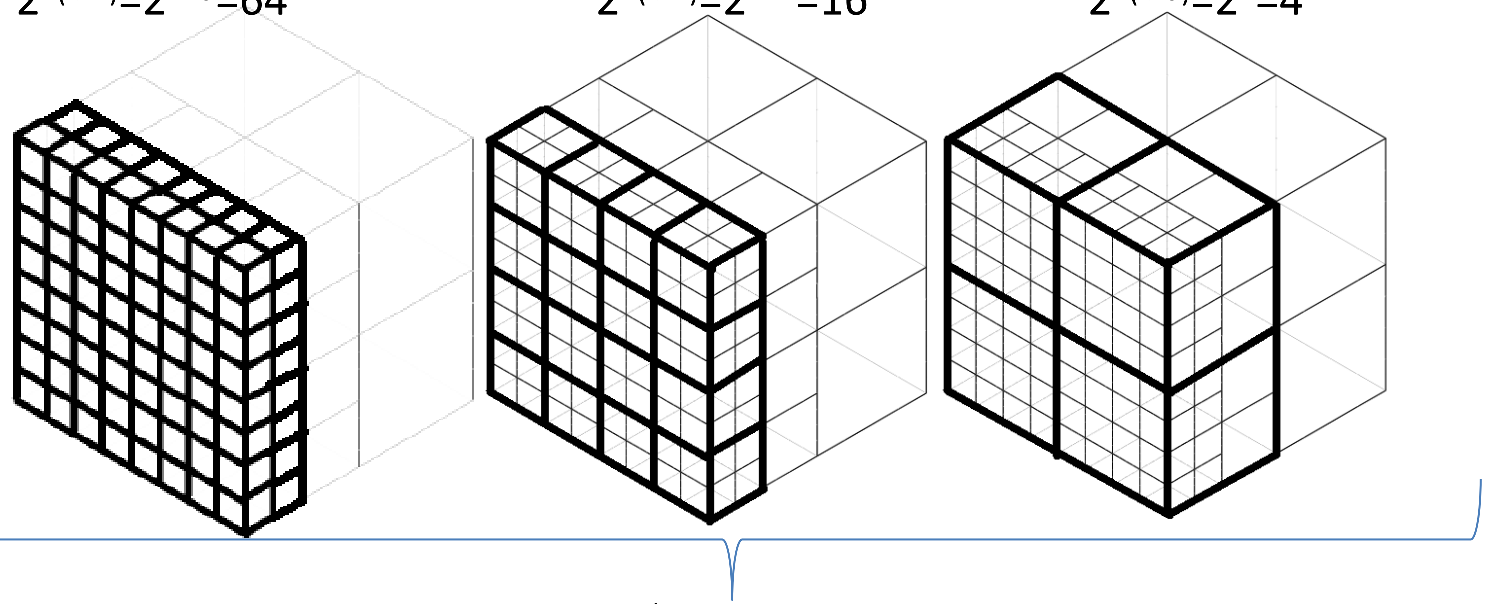
$2^{2(s-k)}$

k=1 $2^{2(4-1)}=2^{2*3}=64$

k=2 $2^{2(4-2)}=2^{2*2}=16$

k=3 $2^{2(4-3)}=2^{2}=4$

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



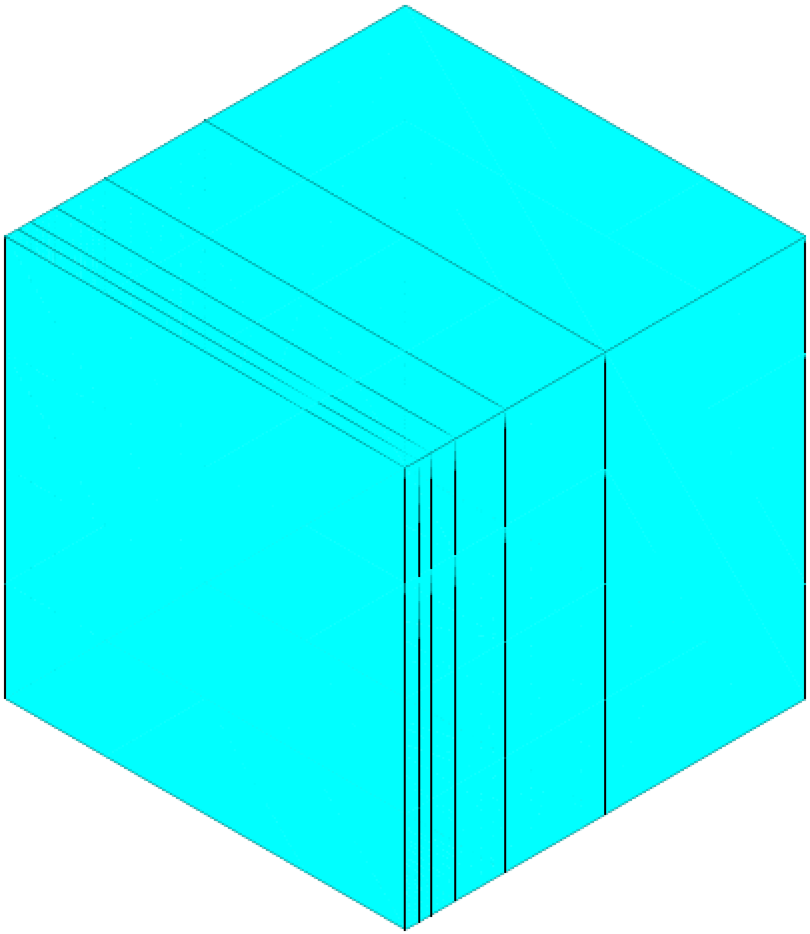
Number of dofs in a patch $O(2^k p^2)$
Numbers of patches in a layer $O(2^{2(s-k)})$
Number of interfaces dofs in a patch $O(2^k p^2)$
Cost of Schur complement of a single layer $O(2^{2(s-k)} 2^{3k} p^6)$

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

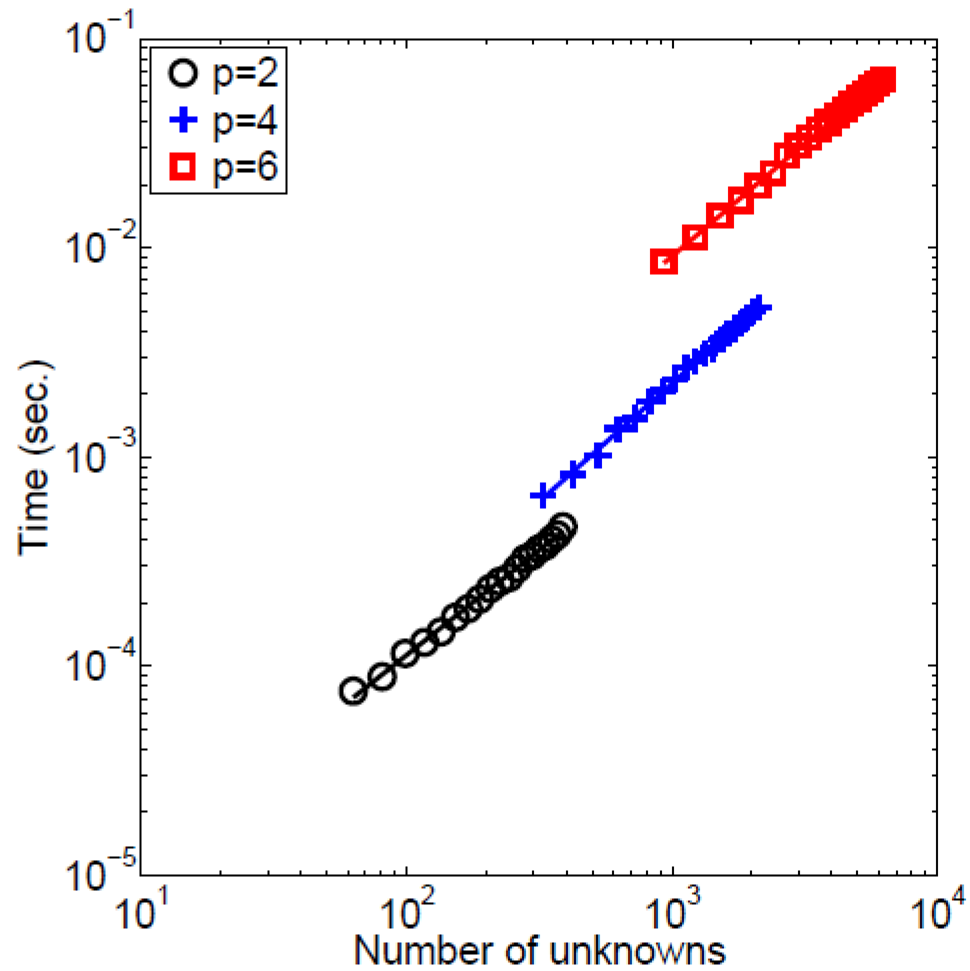
Cost of LU factorization $O\left(\sum_{k=1}^{s} 2^{2(s-k)} 2^{3k} p^6\right) = O(p^6 2^{3s}) = O(N^{1.5} * p^{1.5})$

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

ANISOTROPIC REFINEMENTS TOWARDS FACE SINGULARITY



Mesh



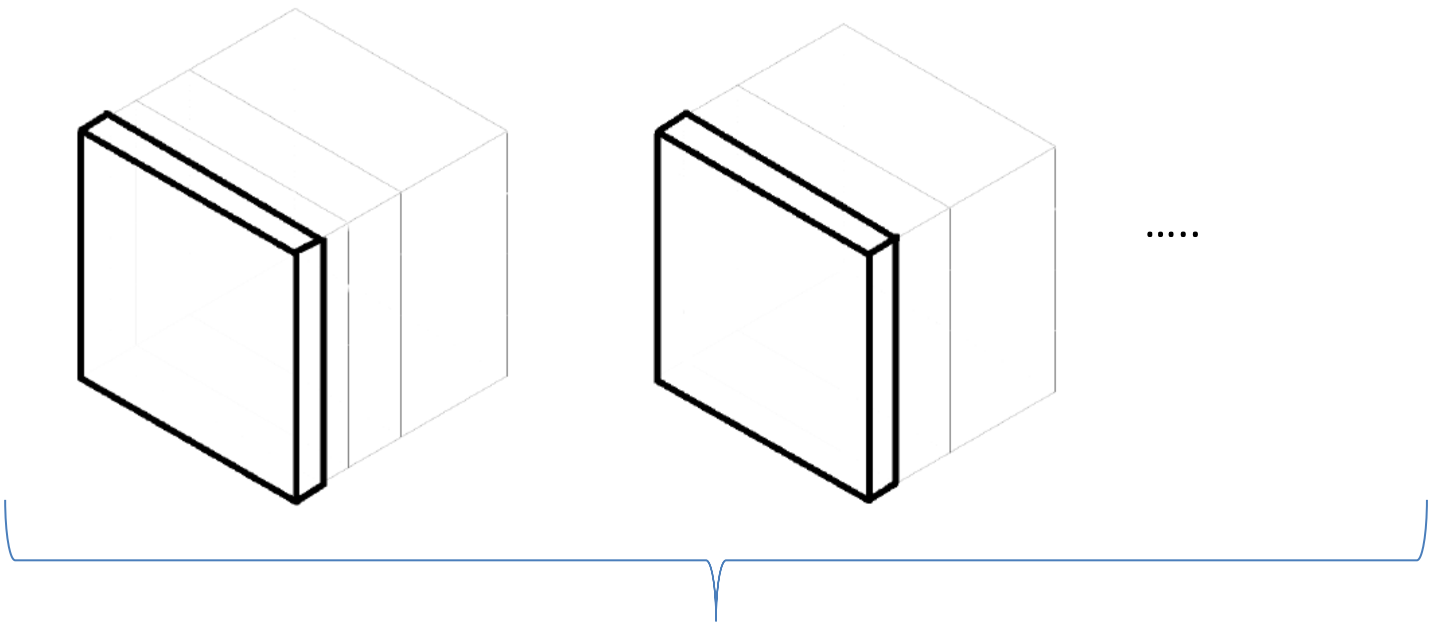
Time of LU factorization

Slope = exponent factor = 1

Location = p factor = p^6

ISOTROPIC REFINEMENTS TOWARDS EDGE SINGULARITY
FRONTAL SOLVER APPROACH

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

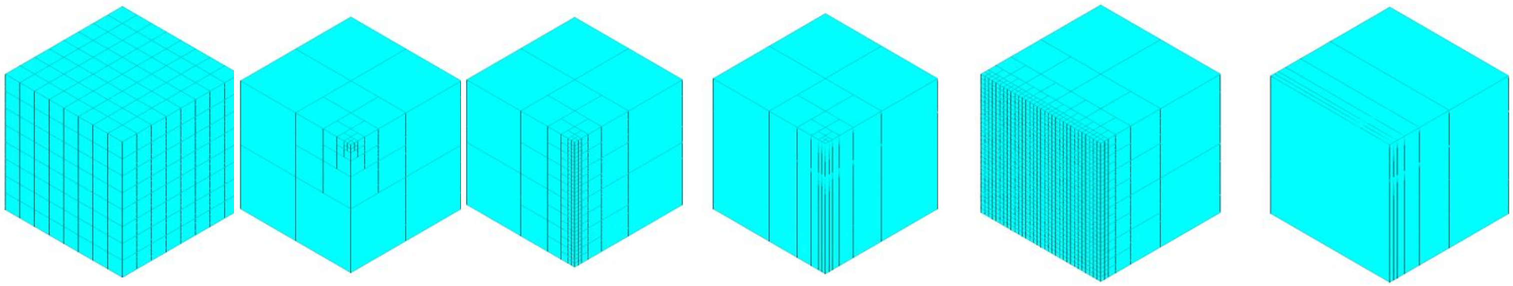


Number of dofs in a layer $O(p^2)$
Number of interfaces dofs in a layer $O(p^2)$
Number of layers $k=O(N_e)=O(N/p^3)$

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

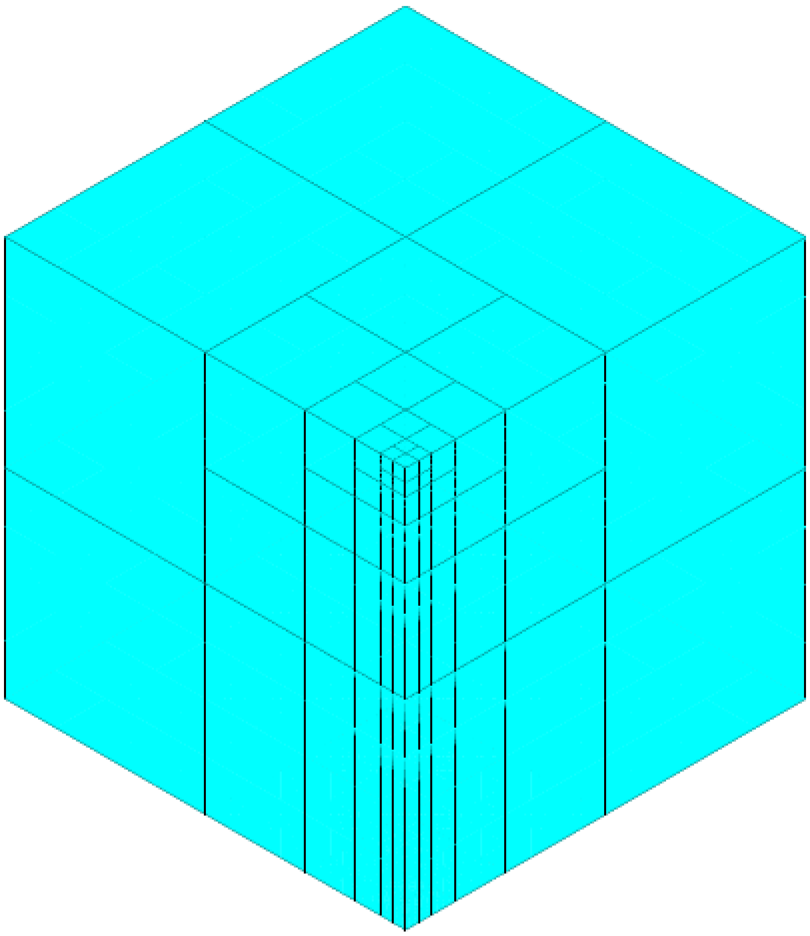
Total cost is $O(N*p^6+N*p^3) = O(Np^6)$

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

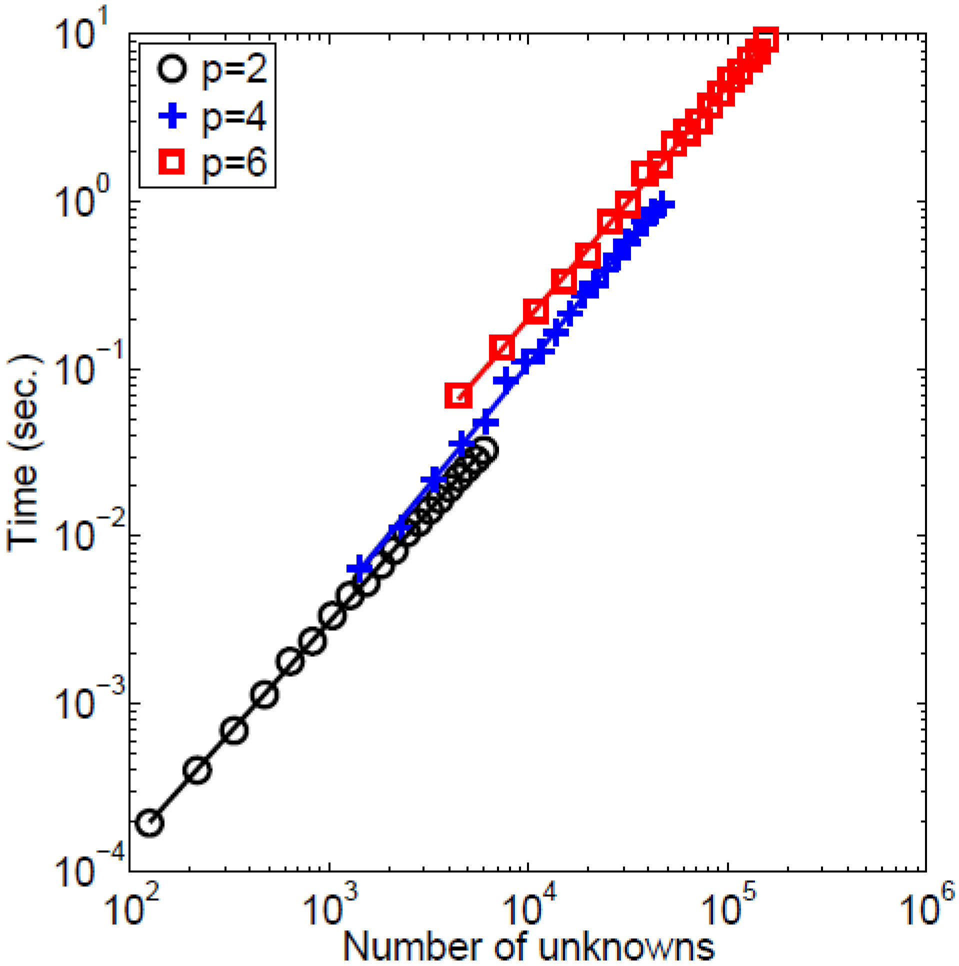


	Uniform	Point	Edge Isotropic	Edge Anisotropic	Face Isotropic	Face Anisotropic
$p = 2$	1.86	1.09	1.10	1.07	1.47	1.01
$p = 4$	1.86	1.17	1.18	1.07	1.47	1.12
$p = 6$	1.83	1.08	1.21	1.09	1.54	1.08
Theoretical	2	1	1	1	1.5	1

POINT + ANISOTROPIC EDGE SINGULARITY

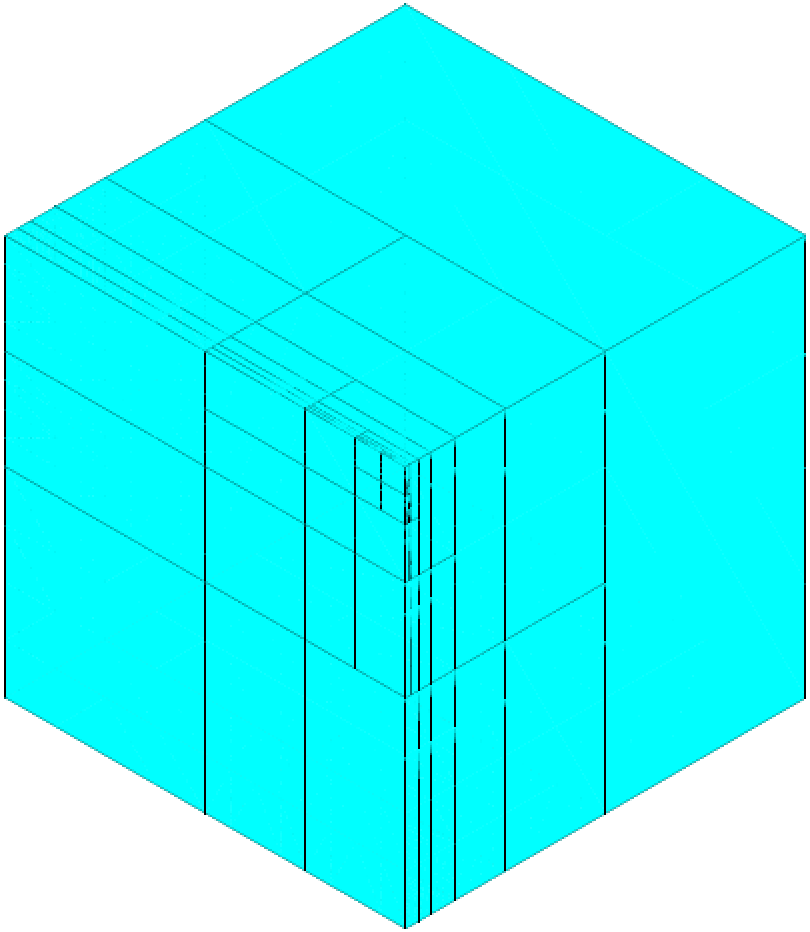


Mesh

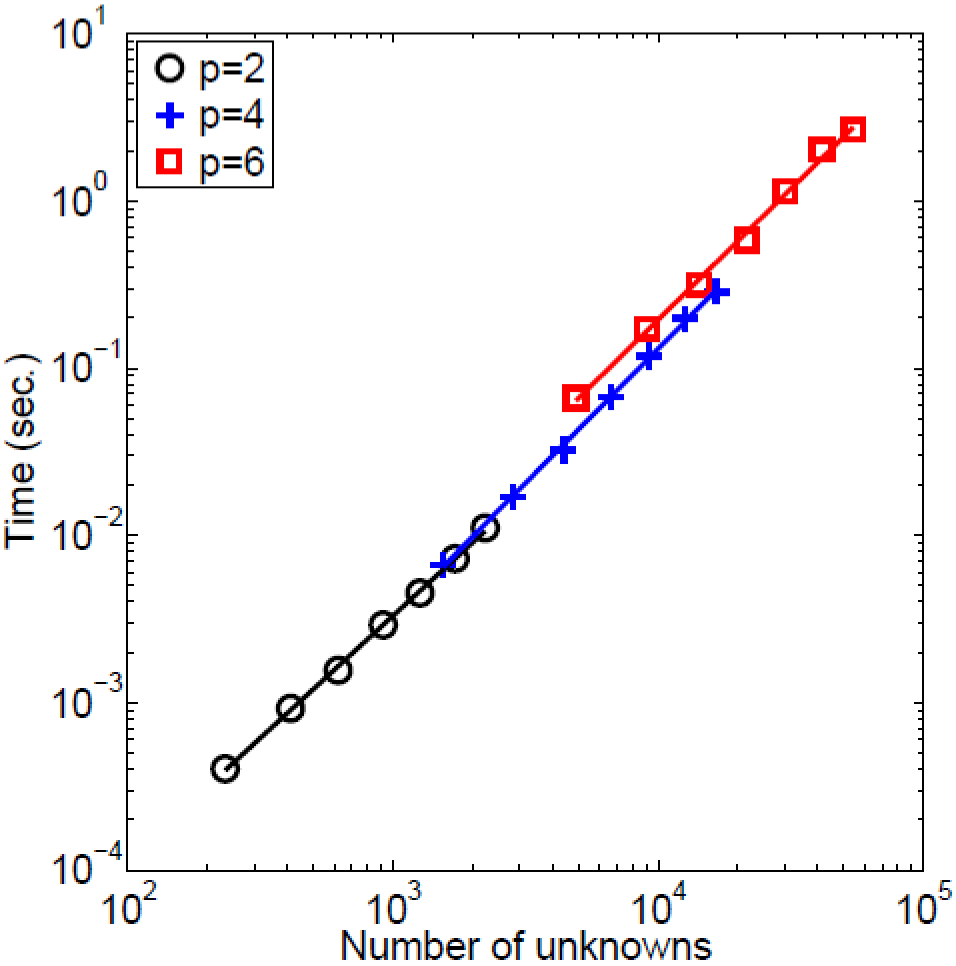


Time of LU factorization

POINT + ANISOTROPIC FACE SINGULARITY

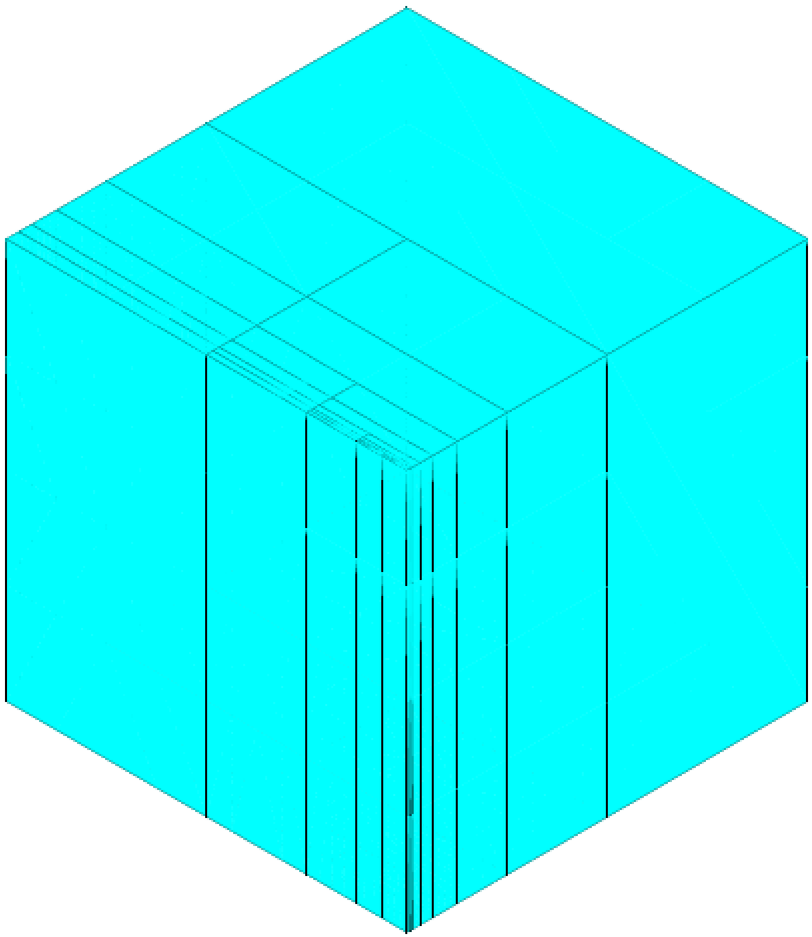


Mesh

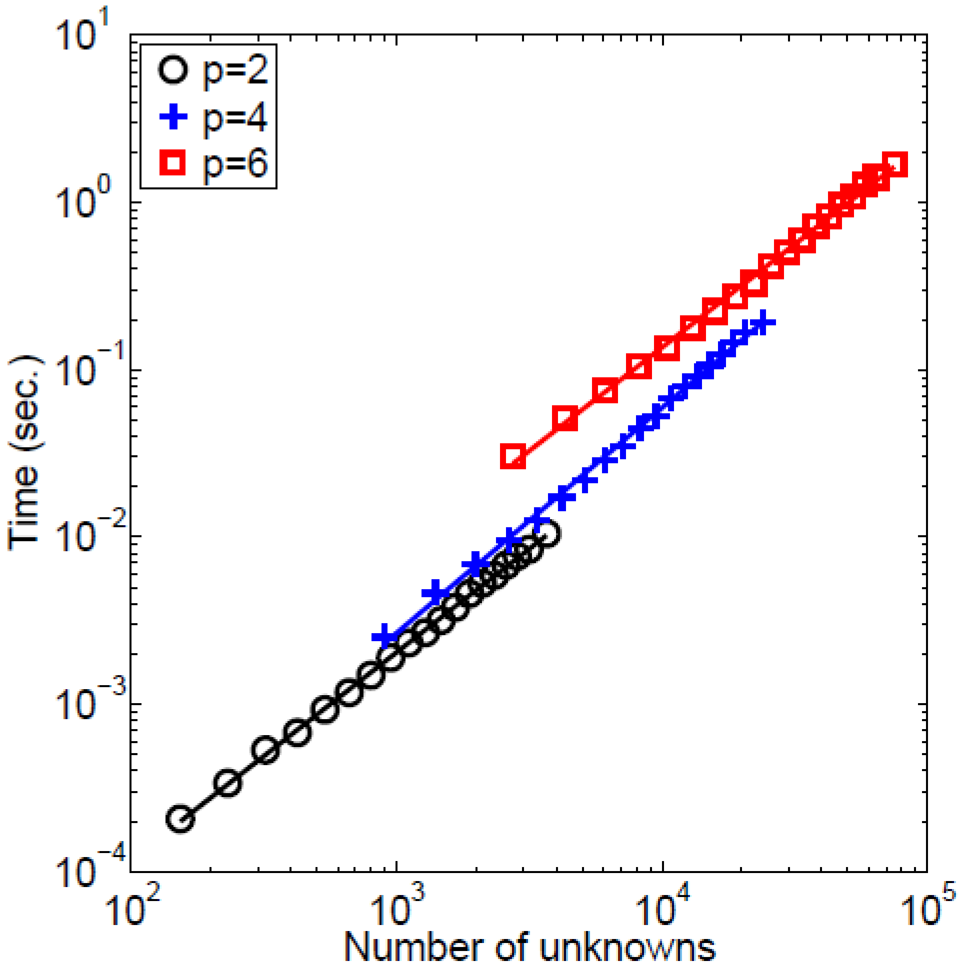


Time of LU factorization

ANISOTROPIC EDGE + ANISOTROPIC FACE SINGULARITY

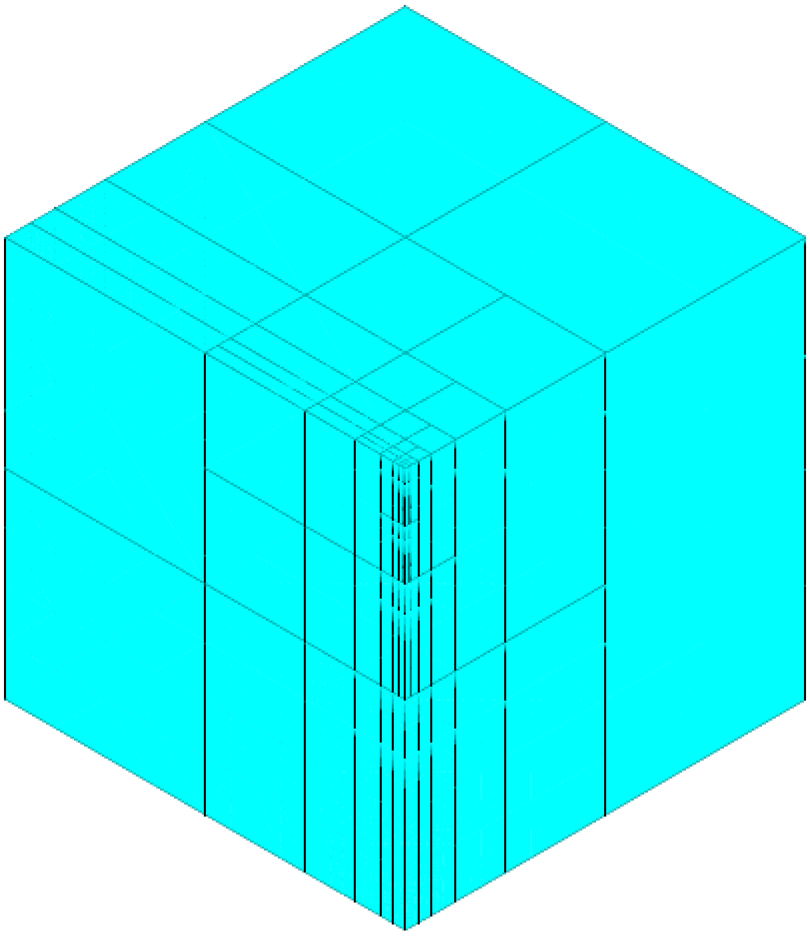


Mesh

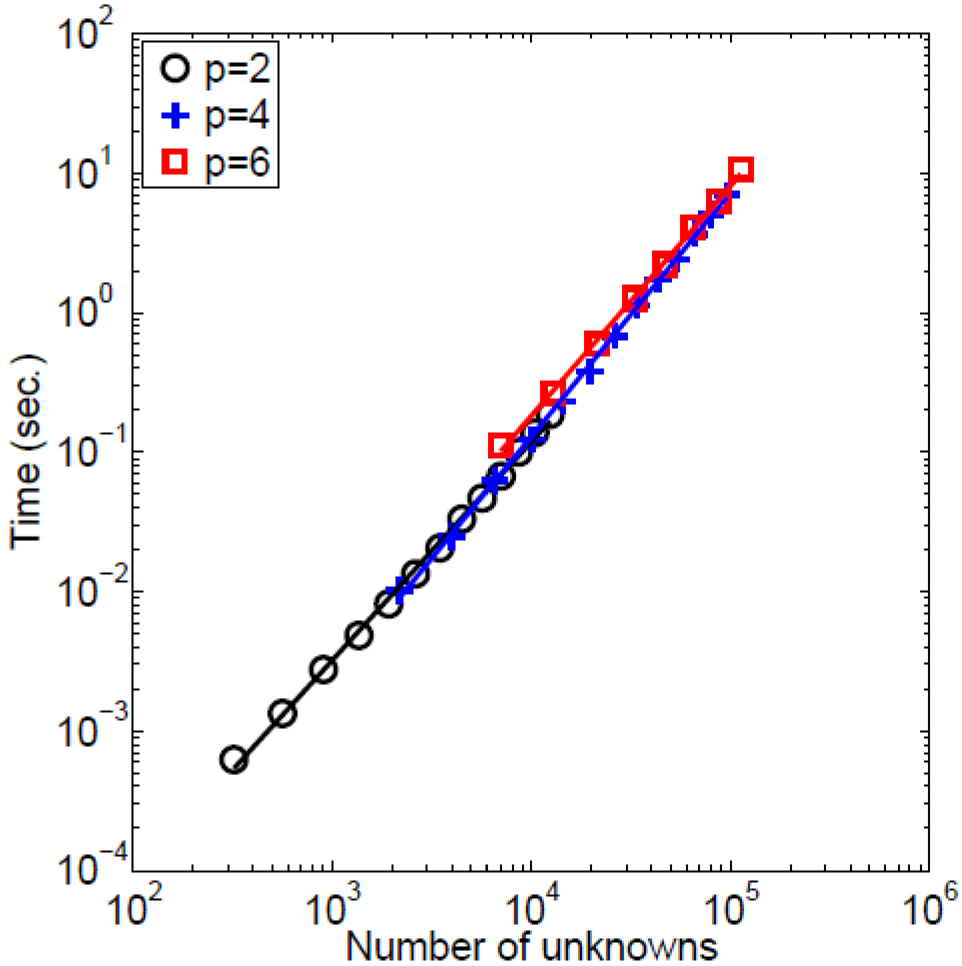


Time of LU factorization

POINT + ANISOTROPIC EDGE + ANISOTROPIC FACE SINGULARITY

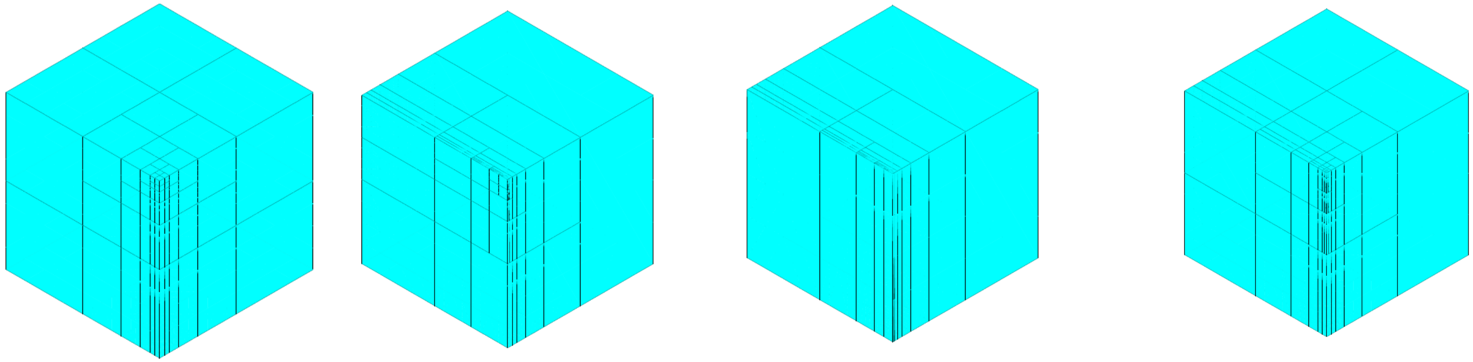


Mesh



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, Victor Calo
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submitted to ***Computers and Mathematics with Applications***, 2014

Damian Goik, Konrad Jopek, Maciej Paszynski, Andrew Lenharth, Donald Nguyen, Keshav Pingali
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Procedia Computer Science, 29 (2014) 960-969

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COMPUTATIONAL COST ESTIMATES FOR PARALLEL SHARED MEMORY ISOGEOMETRIC MULTI-FRONTAL SOLVERS,
Computers and Mathematics with Applications, 67(10) (2014) 1864-1883.

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Computer Methods in Applied Mechanics and Engineering, 284 (2015) 971-987.