Parallelisation of $\mathcal{H}$-Matrix Computations

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Max Planck Institute for Mathematics
in the
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Winterschool on $\mathcal{H}$-Matrices
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Overview

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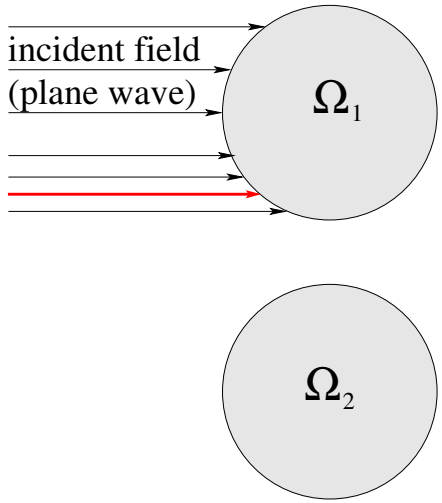
Model Problem: Acoustic Scattering

Let $\Omega_i \in \mathbb{R}^3, i = 1, \ldots, r$ be convex sets with smooth boundaries $\Gamma_i = \partial\Omega_i$.



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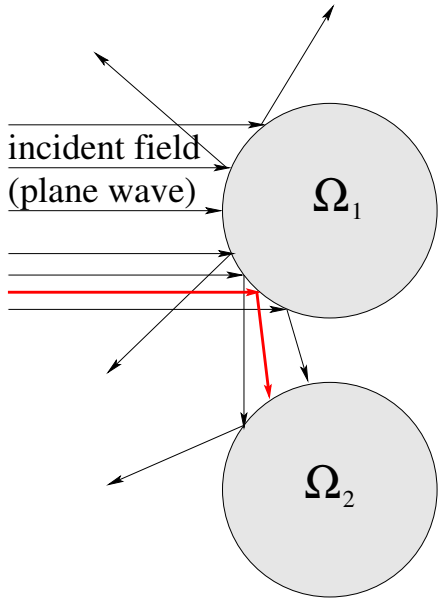

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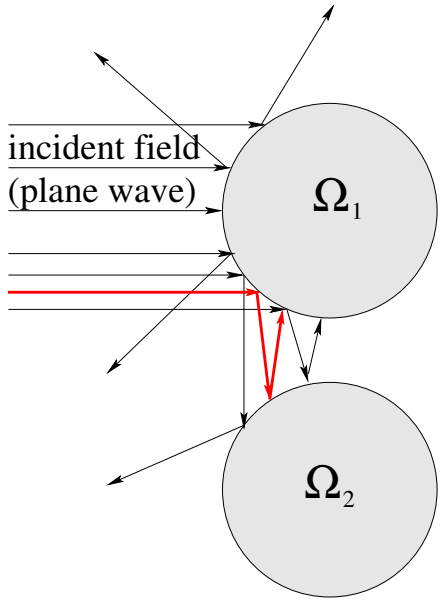

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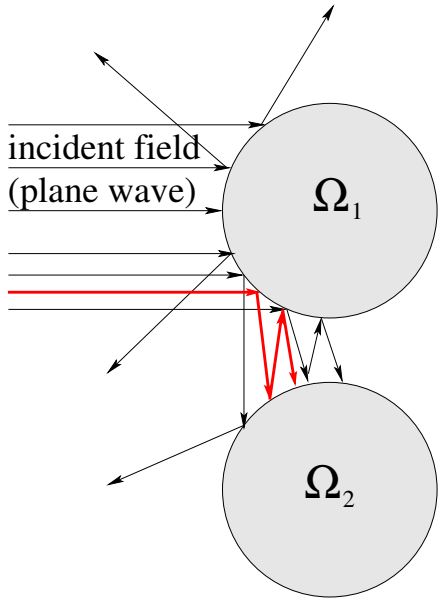

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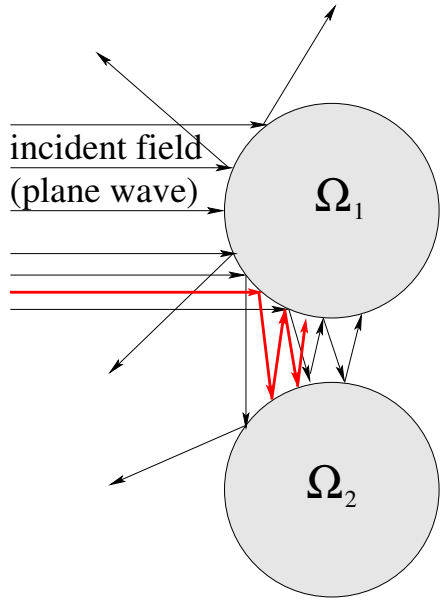

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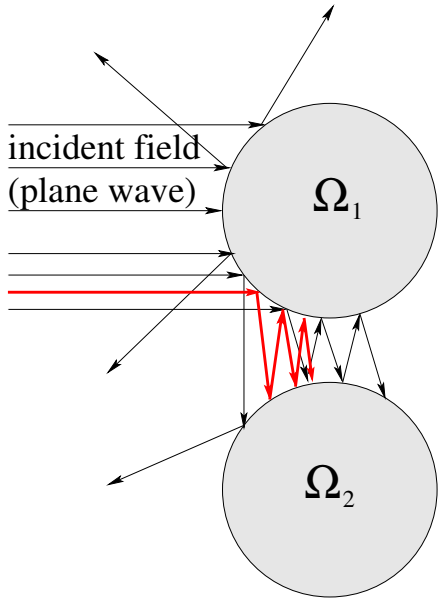

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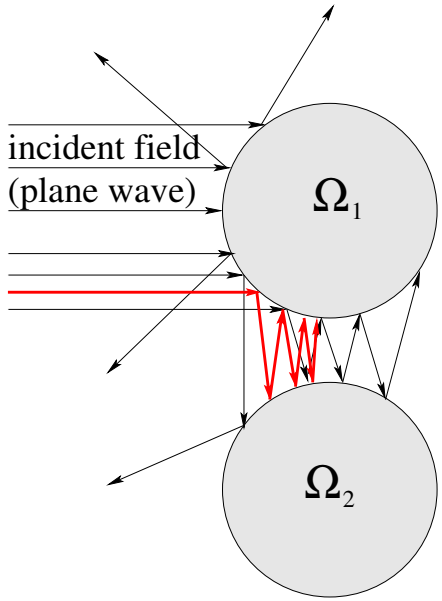

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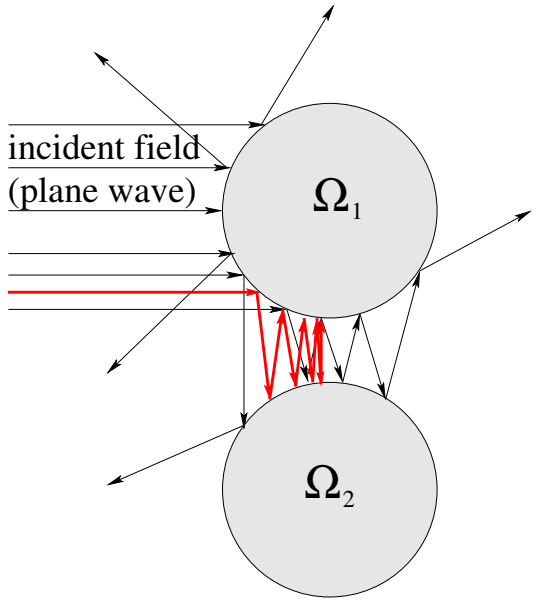

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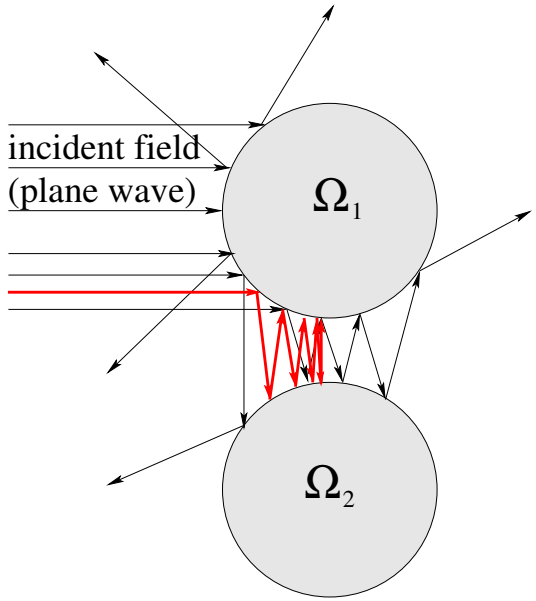
Let $\Omega_i \in \mathbb{R}^3, i = 1, \ldots, r$ be convex sets with smooth boundaries $\Gamma_i = \partial\Omega_i$.

Let $\nu = \nu_1, \nu_2, \ldots$ with $1 \leq \nu_i \leq r$ be a sequence, such that $\nu_i \neq \nu_{i+1}$ for all i.

To compute: densities η_{ν_i} on Γ_{ν_i} defined by



$$\eta_{\nu_i} - \mathcal{K}_{\nu_i}\eta_{\nu_i} = g_{\nu_i},$$

with

$$(\mathcal{K}_{\nu_i}\eta_{\nu_i})(x) := \int_{\Gamma_{\nu_i}} \frac{\partial G(x,y)}{\partial n(x)} \eta_{\nu_i}(y) dy, \quad x \in \Gamma_{\nu_i}$$

with $G(x,y) = -\frac{1}{2\pi}\frac{e^{ik|x-y|}}{|x-y|}$, $k > 0$

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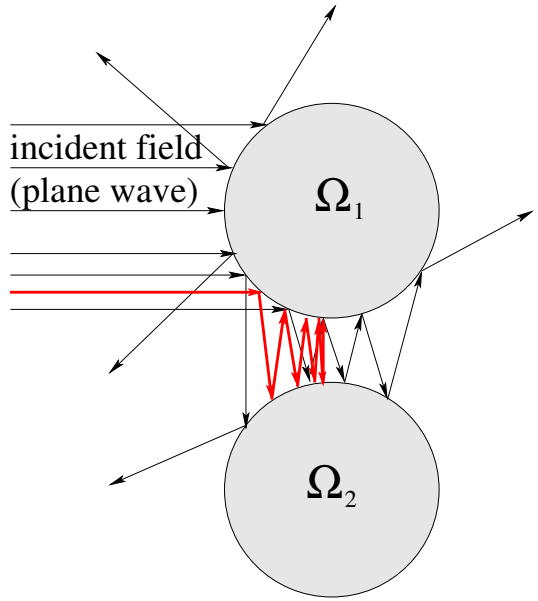

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with $G(x,y) = -\frac{1}{2\pi}\frac{e^{ik|x-y|}}{|x-y|}$, $k > 0$, and with $d \in \mathbb{R}^3$, $|d| = 1$,

$$g_{\nu_i}(x) := \begin{cases} 2\frac{\partial e^{ik\langle d,x\rangle}}{\partial n(x)}, & i = 1 \\ (\mathcal{K}_{\nu_{i-1}}\eta_{\nu_{i-1}})(x), \ x \in \Gamma_{\nu_i} & i > 1 \end{cases}$$

Model Problem: Acoustic Scattering

Discrete System

With a standard Galerkin discretisation using constant ansatz functions, one gets the following matrices

$$K_{ij}^{\nu_i,\nu_i} := \frac{1}{2\pi} \int_{\Gamma_{\nu_i}} \int_{\Gamma_{\nu_i}} e^{ik|x-y|} \frac{1 - ik|x-y|}{|x-y|^3} \langle x - y, n(x) \rangle dy dx$$

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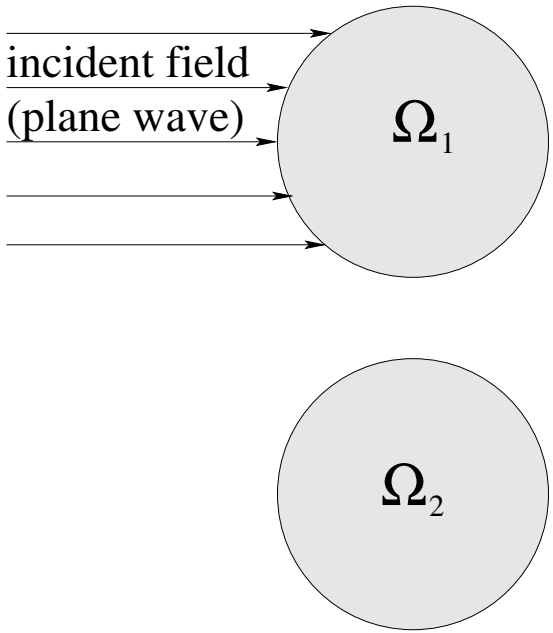
Properties

- expensive integrals to compute,
- complex valued arithmetic even more costly

Model Problem: Acoustic Scattering

Algorithm for two Objects ($\nu = 1, 2, 1, 2, 1, 2, \ldots$)

build $K^{1,1}, K^{2,2}, K^{2,1}$ and $K^{1,2}$;
build initial right hand side $b_{1,1} := g_1$;
for $i = 1, \cdots$ **do**
  solve $(I - K^{1,1})\eta_{i,1} = b_{i,1}$;
  if $\eta_{i,1}/\eta_{i-1,1}$ converged **then stop**
  $b_{i,2} := K^{2,1}\eta_{i,1}$;
  solve $(I - K^{2,2})\eta_{i,2} = b_{i,2}$;
  $b_{i,1} := K^{1,2}\eta_{i,2}$;
endfor



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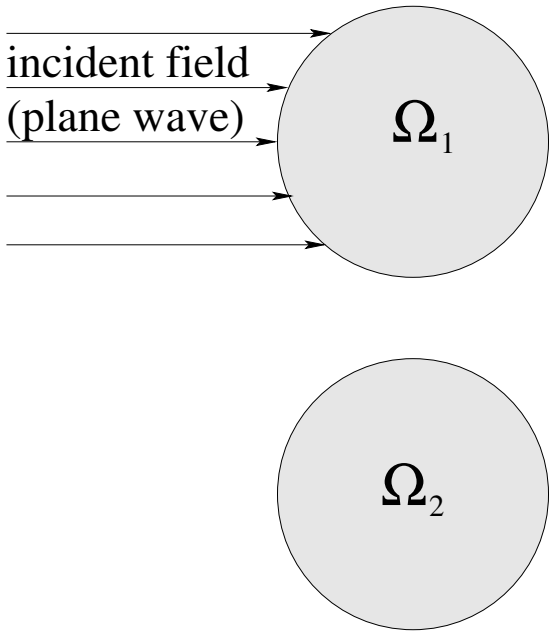
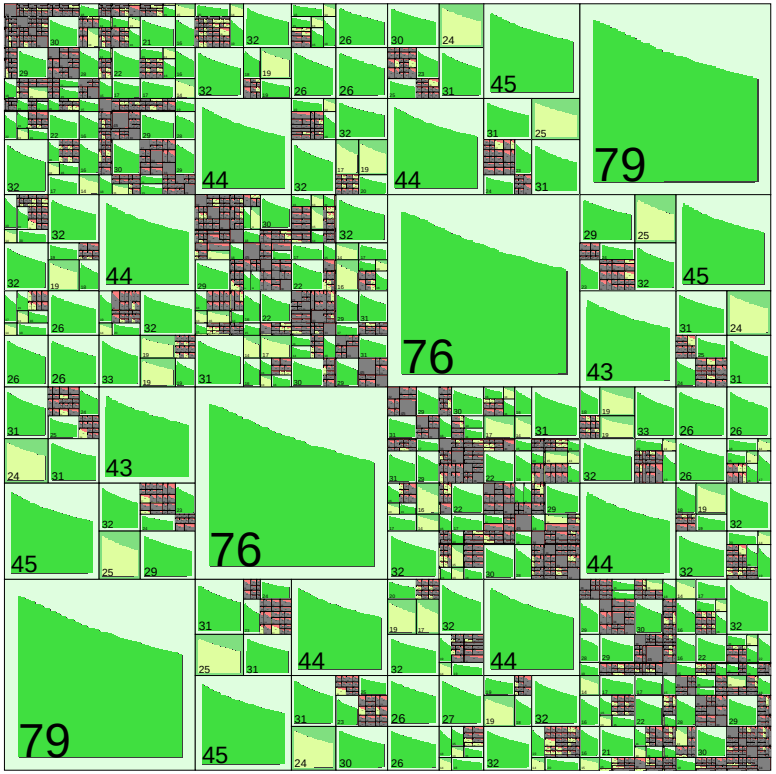


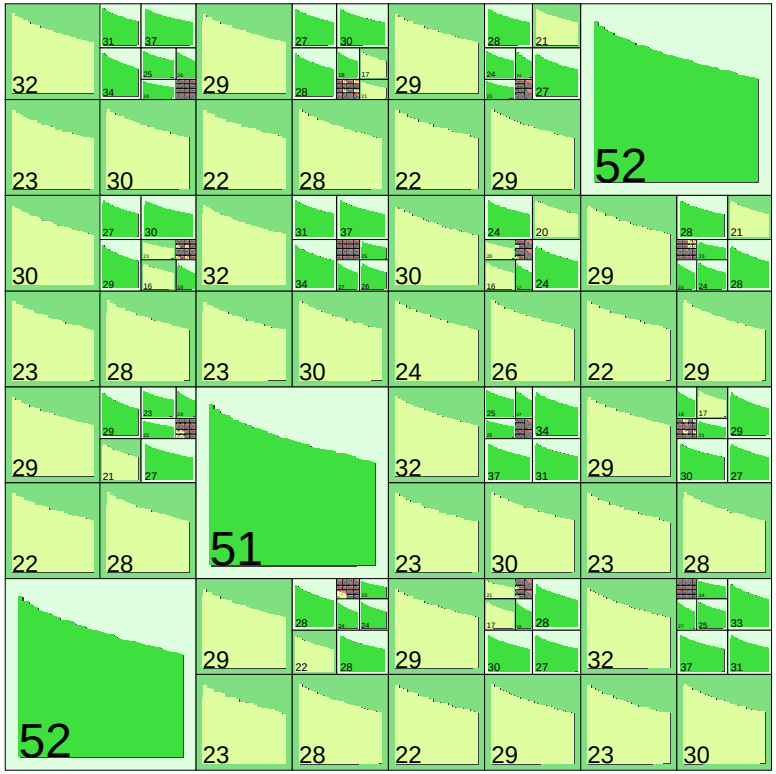
Involved $\mathcal{H}$-Arithmetics

- Matrix-Construction,
- solving linear equation systems with $\mathcal{H}$-Preconditioner and
- Matrix-Vector Multiplication

Model Problem: Acoustic Scattering

Example





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Problem

- Matrix-Construction is very expensive, especially for large k
- $\mathcal{H}$-Preconditioner via $\mathcal{H}$-Inversion or $\mathcal{H}$-LU-Factorisation can be expensive

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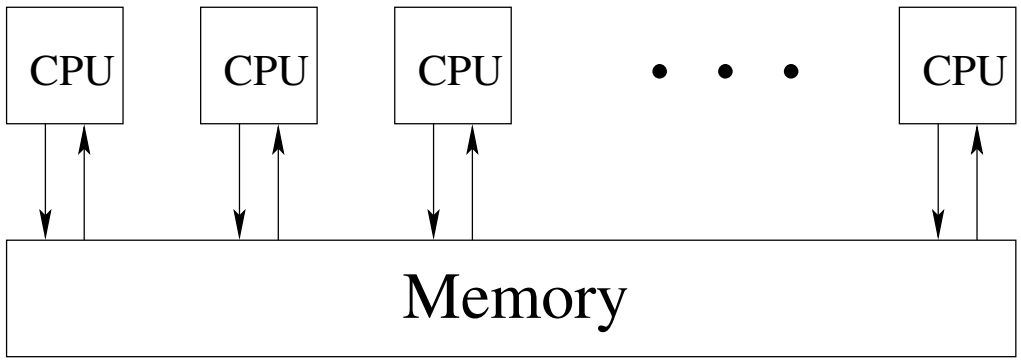
Goal

Use parallel algorithms for involved $\mathcal{H}$-Arithmetic with small programming effort but high efficiency on workstations or small compute servers.

Overview

System Architecture

Workstations and small compute servers are usually systems with a shared memory, e.g. all processors have direct access to the same memory:



Technical Prerequisites

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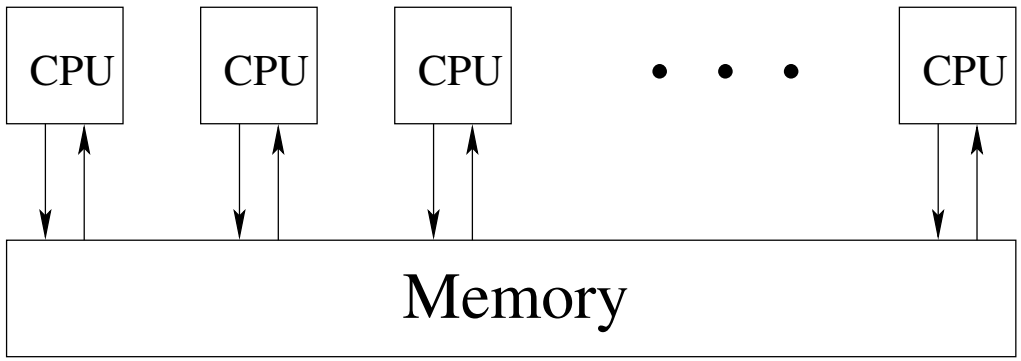

Consequences

- simplified programming because no communications involved,
- but protection of critical resources necessary, e.g. simultaneous access to the same memory position

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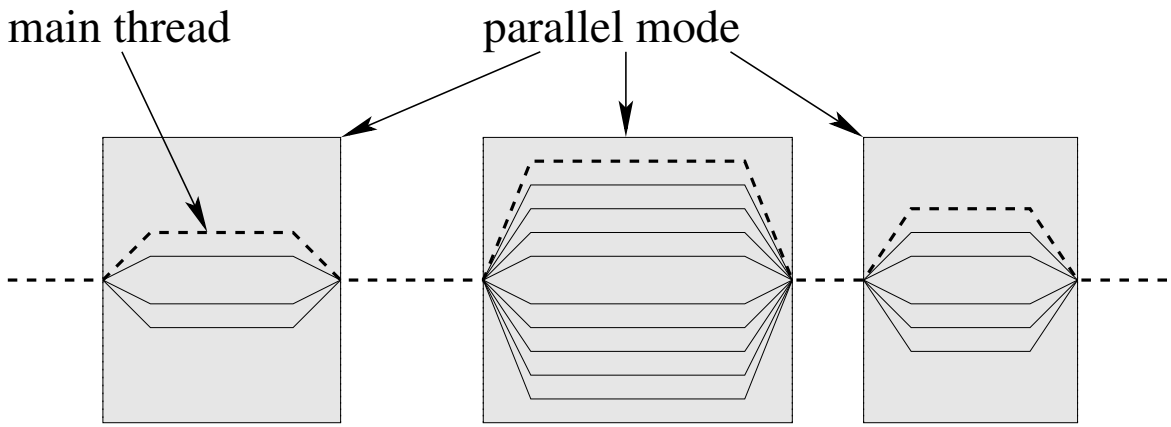

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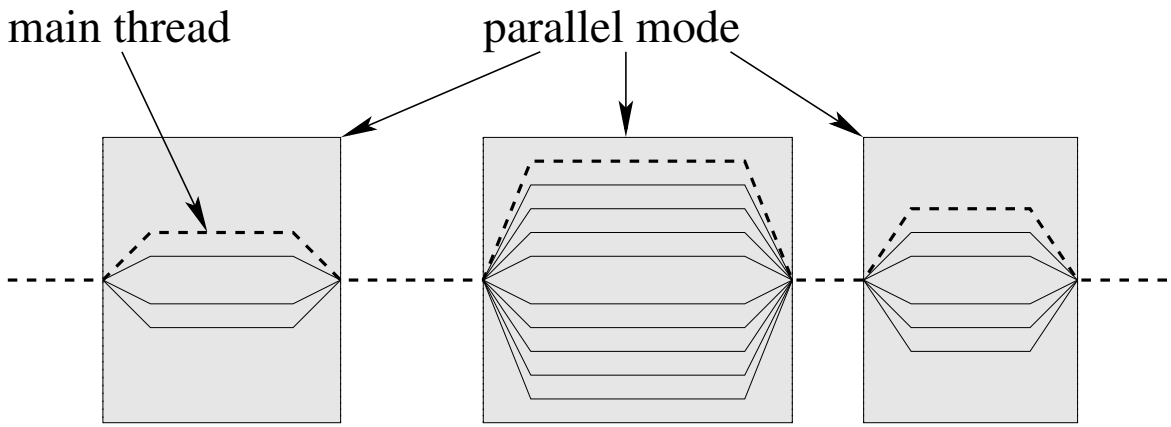

Functions for threads:

- `t = tcreate( f )`: create thread `t` and start function `f`,
- `tsync( t )`: synchronise with thread `t`, e.g. wait until `t` has finished.

Mutices

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Example: compute $A := A + \sum_{i=1}^{4} A_i$, with matrices A and $A_i, i = 1, \ldots, 4$

On thread 1:

$$T_1 := A_1 + A_2;$$

$$A := A + T_1;$$

On thread 2:

$$T_2 := A_3 + A_4;$$

$$A := A + T_2;$$

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On thread 1:

$T_1 := A_1 + A_2;$
LOCK(m);
$A := A + T_1;$
UNLOCK(m);

On thread 2:

$T_2 := A_3 + A_4;$
LOCK(m);
$A := A + T_2;$
UNLOCK(m);

with common mutex m

Overview

Matrix Construction

Let I be an index set with $|I| = n$, $T(I)$ a cluster tree over I and $T(I \times I)$ a block cluster tree over $I \times I$.
Let $p > 0$ be the number of processors.

Sequential Algorithm without Hierarchy

Build matrix blocks only for leaves in block cluster tree:

for $(t, s) \in \mathcal{L}(T(I \times I))$ **do**
    if (t, s) is admissible **then** build low rank matrix;
    else build dense matrix;
endfor;

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Properties

- $\mathcal{L}(T(I \times I)) \gg p$, e.g. enough to do for each processor,
- all matrix blocks can be built independently.

Matrix Construction

Parallel Algorithm without Hierarchy

Compute each matrix block in own thread.

procedure build ((t, s))
    if (t, s) is admissible **then** build low rank matrix;
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for $(t, s) \in \mathcal{L}(T(I \times I))$ **do**
    $\mathcal{T} := \mathcal{T} \cup \{$ `tcreate`(build((t, s)) $\}$;
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Complexity

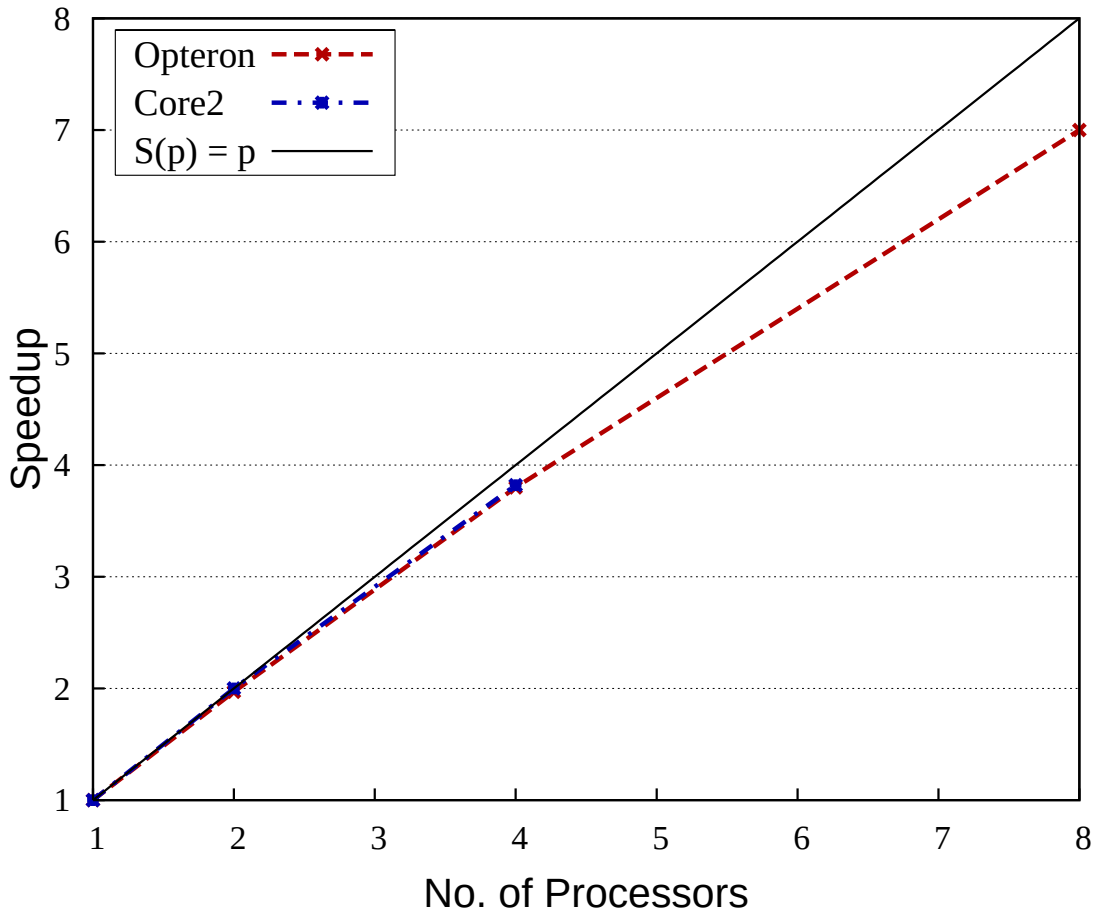
Simple, automatic load balancing by thread implementation leads to optimal parallel complexity:

$$\mathcal{W}_{\text{Con}}(n, p) = \mathcal{O}\left(\frac{n \log n}{p}\right)$$

Matrix Construction

Numerical Experiments ($K^{1,1}, n = 8192, k = 8$)

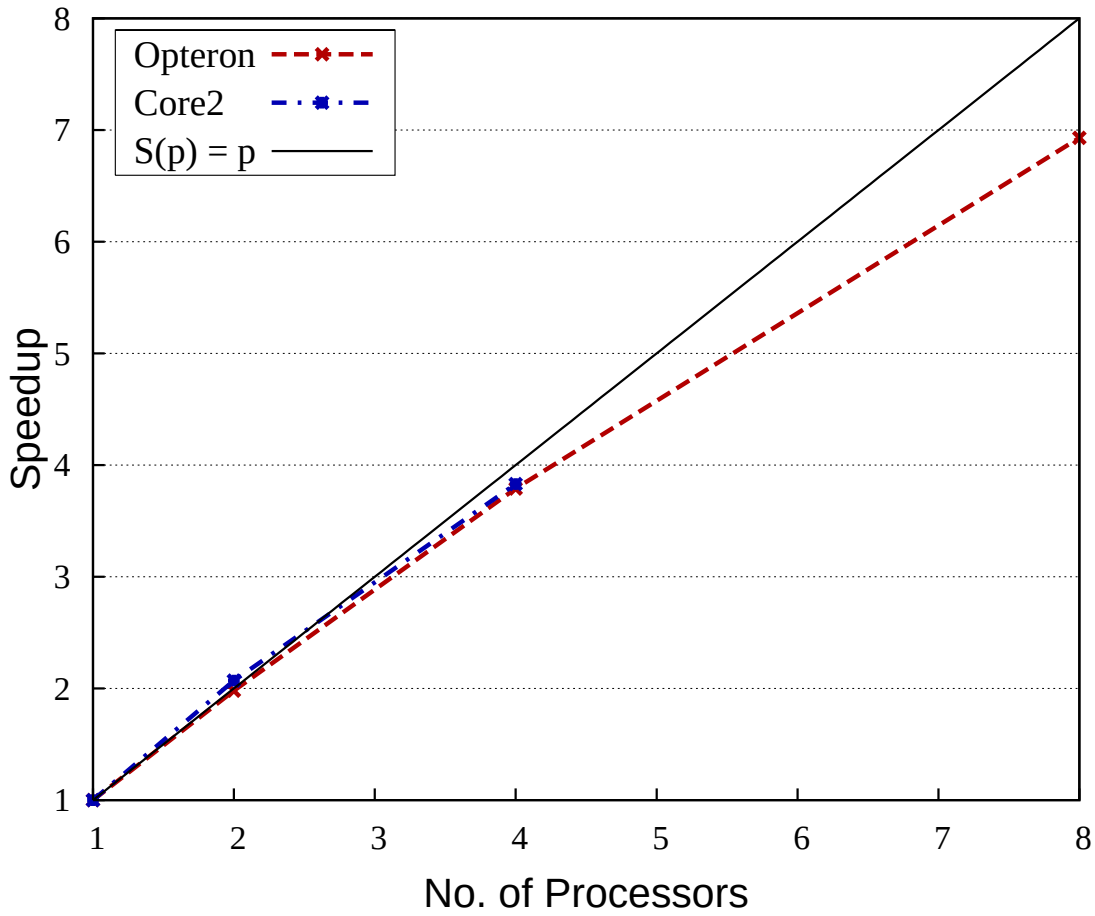
p	Opteron	Core2
1	899.1 s	895.8 s
2	455.5 s	448.0 s
4	236.3 s	234.0 s
8	128.4 s	



Matrix Construction

Numerical Experiments ($K^{1,2}, n = 8192, k = 8$)

p	**Opteron**	**Core2**
1	349.8 s	346.0 s
2	176.9 s	167.5 s
4	92.2 s	88.2 s
8	50.5 s	



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Matrix Inversion

Let $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$ be an $\mathcal{H}$-Matrix. The inverse of A can be computed as

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} + A_{11}^{-1} A_{12} S^{-1} A_{21} A_{11}^{-1} & -A_{11}^{-1} A_{12} S^{-1} \\ -S^{-1} A_{21} A_{11}^{-1} & S^{-1} \end{pmatrix},$$

with the *Schur-complement*

$$S = A_{22} - A_{21} A_{11}^{-1} A_{12}.$$

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Sequential Algorithm

procedure invert (A, C)
    invert(A_{00}, C_{00});
    $T_{12} := C_{11} \cdot A_{12}$; $T_{21} := A_{21} \cdot C_{11}$;
    $A_{22} := A_{22} - A_{21} \cdot T_{12}$;
    invert(A_{22}, C_{22});
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Assumption: complexity of parallel matrix multiplication on p processors is

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Then, by using the parallel matrix multiplication for all products in the inversion algorithm, for the complexity of the $\mathcal{H}$-matrix inversion one gets

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$$\mathcal{W}_{\text{Inv}}(n, p) = \mathcal{O}\left(n + \frac{n \log^2 n}{p}\right)$$

Remark: sequential part due to diagonal decreases for larger n.

Parallel Matrix Multiplication

To compute:

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Sequential Algorithm for a $m \times m$ block matrix:

```
procedure mul( α, A, B, β, C )
    if A, B and C are block matrices then
        for i := 1, ..., m do
            for j := 1, ..., m do
                for l := 1, ..., m do
                    mul( α, A_il, B_lj, β, C_ij );
    else
8:      C := αAB + βC;
end;
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Matrix Inversion

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Sequential Algorithm for a $m \times m$ block matrix:

```
    procedure mul( α, A, B, β, C )
        if A, B and C are block matrices then
            for i := 1, ..., m do
                for j := 1, ..., m do
                    for l := 1, ..., m do
                        mul( α, A_il, B_lj, β, C_ij );
        else
8:          tcreate( C := αAB + βC );
    end;
```

First parallelisation ansatz: execute line 8 in a thread

Matrix Inversion

Parallel Matrix Multiplication

Consider

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} := \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} + \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

The parallel execution of

$$C_{11} = C_{11} + A_{11}B_{11} \quad \text{and} \quad C_{11} = C_{11} + A_{12}B_{21}.$$

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leads to a collision and has to be guarded by a mutex:

LOCK(m); $C_{11} := C_{11} + A_{11}B_{11}$; UNLOCK(m);	LOCK(m); $C_{11} := C_{11} + A_{12}B_{21}$; UNLOCK(m);

This blocks one of the threads and therefore enforces sequential execution.

Matrix Multiplication (2nd Try)

Simulate matrix multiplication to collect all products $A \cdot B$ for a destination block C and execute list of products for each C in a different thread.

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procedure $\mathrm{sim\_mul}(\ A, B, C\ )$
  if A, B and C are block matrices **then**
    for $i, j, l := 1, \ldots, m$ **do**
      sim_mul(A_{il}, B_{lj}, C_{ij});
  else
    $\mathcal{P}(C) := \mathcal{P}(C) \cup \{(A, B)\}$; $\mathcal{L}_{\mathrm{MM}} := \mathcal{L}_{\mathrm{MM}} \cup \{C\}$;
end;

Matrix Multiplication (2nd Try)

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procedure sim_mul(A, B, C)
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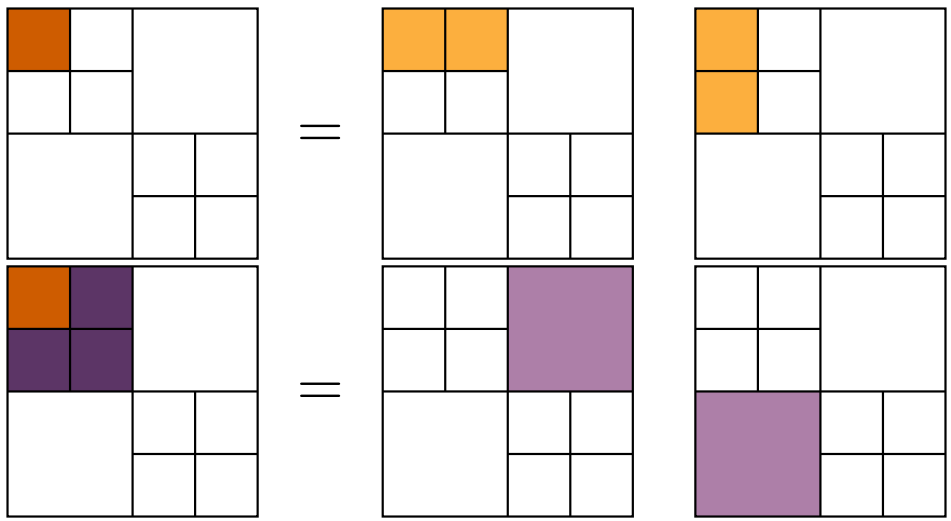
  else
    $\mathcal{P}(C) := \mathcal{P}(C) \cup \{(A, B)\}$; $\mathcal{L}_{\text{MM}} := \mathcal{L}_{\text{MM}} \cup \{C\}$;
end;

procedure mul_block(C)
  for all $(A, B) \in \mathcal{P}(C)$ **do** $C := C + \alpha AB$;

procedure mul($\alpha, \beta, \mathcal{L}_{\text{MM}}$)
  for all $C \in \mathcal{L}_{\text{MM}}$ **do** $\mathcal{T} := \mathcal{T} \cup \{$ `tcreate`(mul_block(C)) $\}$;
  for $\texttt{t} \in \mathcal{T}$ **do** tsync(t);

Matrix Multiplication (2nd Try)

Even in the second algorithm collisions can occur, e.g.



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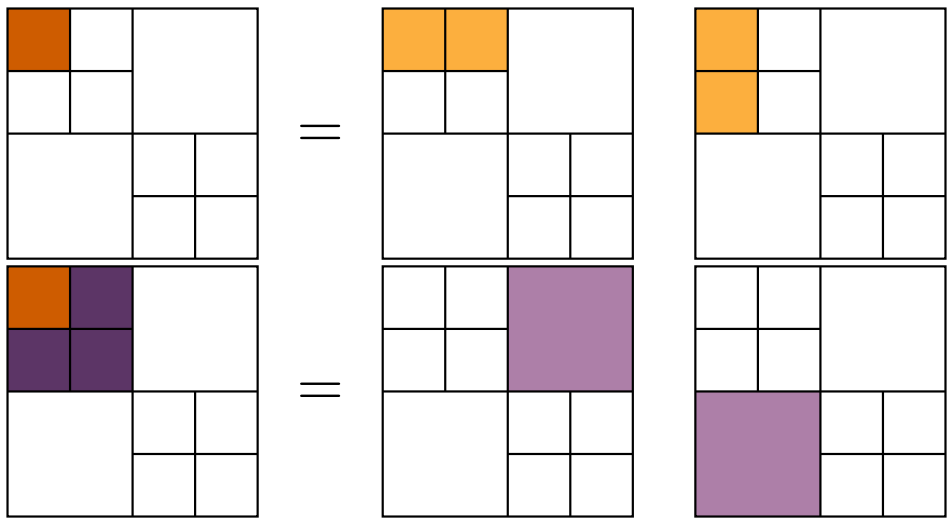

Therefore, all matrix blocks have to guarded by a mutex, e.g.

procedure mul_block(C)
  for all $(A, B) \in \mathcal{P}(C)$ **do**
    LOCK(m(C)); $C := C + \alpha AB$; UNLOCK(m(C));
end;

Matrix Multiplication

For moderate p, collisions are very seldom or non-existent at all, hence:

$$\mathcal{W}_{\text{Mul}}(n, p) = \mathcal{O}\left(\frac{n \log^2 n}{p}\right)$$

Matrix Inversion

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Complexity of Matrix Inversion

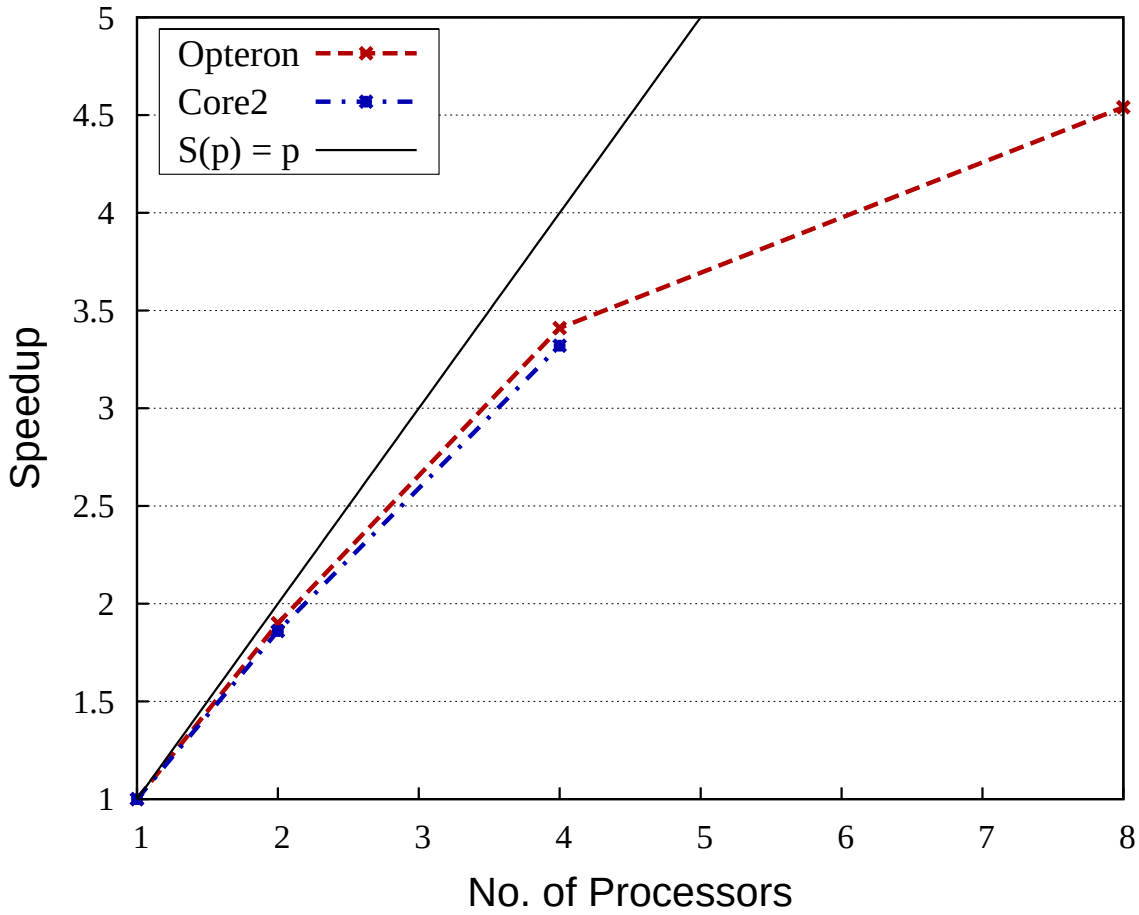
Since previous assumption about complexity of matrix multiplication was justified, the complexity of matrix inversion is truly

$$\mathcal{W}_{\text{Inv}}(n, p) = \mathcal{O}\left(n + \frac{n \log^2 n}{p}\right)$$

Matrix Inversion

Numerical Experiments ($K^{1,1}, n = 8192, k = 8$)

p	**Opteron**	**Core2**
1	221.2 s	217.1 s
2	116.6 s	116.9 s
4	64.8 s	65.4 s
8	48.7 s	



Remark about LU Factorisation

The same technique can be applied for the LU factorisation of an $\mathcal{H}$-Matrix, but in contrast to inversion, the recursion also takes place in the off-diagonal blocks (solving L and U). This increases the sequential part of the algorithm and one gets:

$$\mathcal{W}_{\mathrm{LU}}(n,p) = \mathcal{O}\left(n\log^2 n + \frac{n\log^2 n}{p}\right)$$

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But for small p, the parallel speedup of the algorithm is nevertheless acceptable:

System	$p=1$	$p=2$	$p=4$	$p=8$
Opteron	84.9 sec	45.5 sec	37.2 sec	34.6 sec
Core2	85.6 sec	49.2 sec	38.0 sec	

Overview

Matrix-Vector Multiplication

For $\mathcal{H}$-Matrix A and vectors x and y compute

$$y := Ax$$

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Sequential Algorithm

Compute matrix-vector product for matrix blocks corresponding to leaves in block cluster tree:

for $(t, s) \in \mathcal{L}(T(I \times I))$ **do**
    $y|_t := y|_t + A|_{(t,s)} \cdot x|_s$;
endfor;

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    $y|_t := y|_t + A|_{(t,s)} \cdot x|_s$;
endfor;

Parallelisation

Use same idea as in matrix construction: execute local matrix-vector multiplication in own thread.

procedure mulvec($A, x, y, (t, s)$)
    $y|_t := y|_t + A|_{(t,s)} \cdot x|_s$;

for $(t, s) \in \mathcal{L}(T(I \times I))$ **do** $\mathcal{T} := \mathcal{T} \cup \{$`tcreate`($A, x, y, (t, s)$)$\}$;
for `t` $\in \mathcal{T}$ **do** `tsync( t )`;

Matrix-Vector Multiplication

Collisions

If two threads update y, the access to y has to be guarded:

procedure $\mathrm{mulvec}(\ A, x, y, (t, s)\ )$
    LOCK(m); $y|_t := y|_t + A|_{(t,s)} \cdot x|_s$; UNLOCK(m);
end;

which prohibits parallel execution.

Matrix-Vector Multiplication

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If two threads update y, the access to y has to be guarded:

procedure $\mathrm{mulvec}(\ A, x, y, (t, s)\ )$
    LOCK(m); $y|_t := y|_t + A|_{(t,s)} \cdot x|_s$; UNLOCK(m);
end;

which prohibits parallel execution.

Parallelisation (2nd Try)

Use local result vectors y^i per processor $1 \leq i \leq p$:

procedure $\mathrm{mulvec}(\ A, x, y, (t, s)\ )$
    Let i be index of local processor;
    $y^i|_t := y^i|_t + A|_{(t,s)} \cdot x|_s$;
end;

for $(t, s) \in \mathcal{L}(T(I \times I))$ **do** $\mathcal{T} := \mathcal{T} \cup \{$`tcreate(` $A, x, y, (t, s)$ `)`$\}$;
for `t` $\in \mathcal{T}$ **do** `tsync( t )`;
$y := y + \sum_{i=1}^{p} y_i$;

Matrix-Vector Multiplication

Complexity

Again, automatic load balancing due to threads gives optimal parallel speedup. Together with sequential summation of p vectors one gets:

$$\mathcal{W}_{\text{Vec}}(n, p) = \mathcal{O}\left(\frac{n \log n}{p} + pn\right)$$

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$$\mathcal{W}_{\text{Vec}}(n,p) = \mathcal{O}\left(\frac{n \log n}{p} + n\right)$$

Remark

With better load balancing based on space-filling curves one can achieve

$$\mathcal{W}_{\text{Vec}}(n,p) = \mathcal{O}\left(\frac{n \log n}{p} + \frac{n}{\sqrt{p}}\right)$$

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With better load balancing based on space-filling curves one can achieve

$$\mathcal{W}_{\text{Vec}}(n,p) = \mathcal{O}\left(\frac{n \log n}{p} + \frac{n}{\sqrt{p}}\right)$$

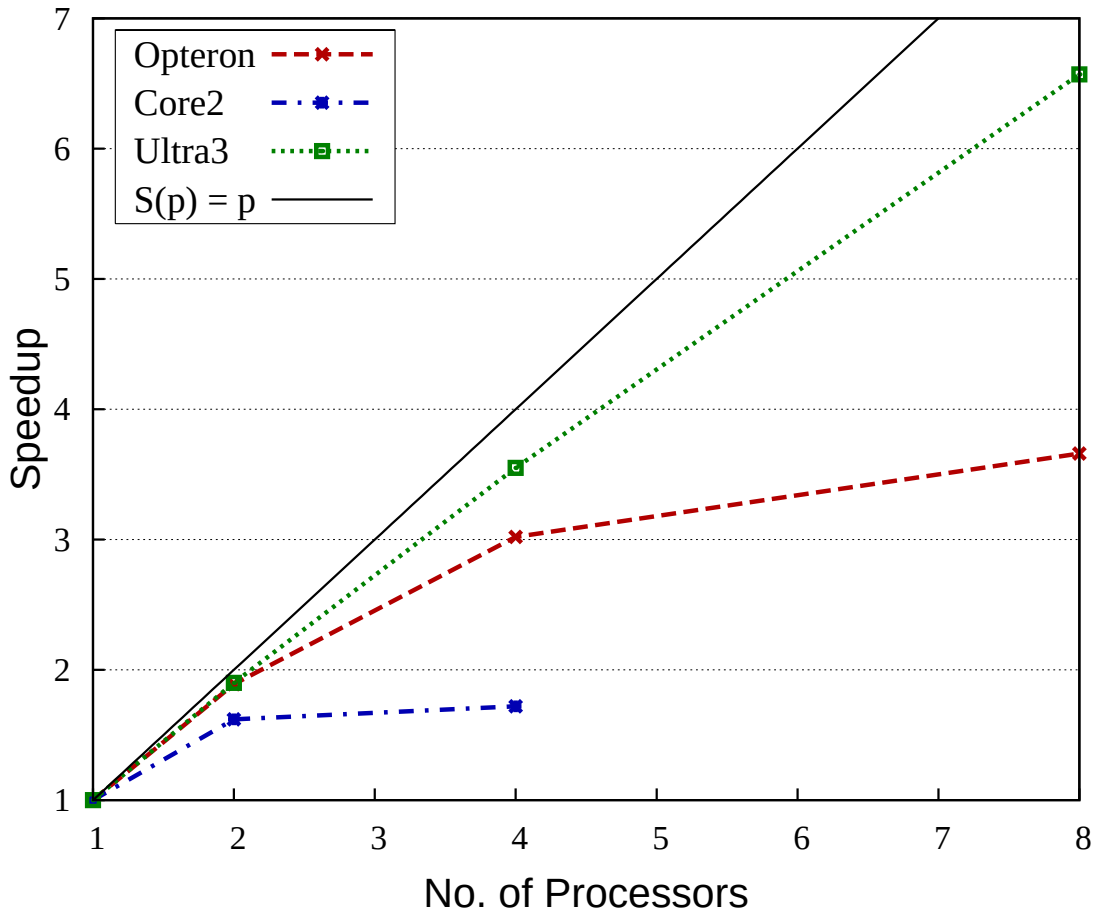
and with alternative data distribution

$$\mathcal{W}_{\text{Vec}}(n,p) = \mathcal{O}\left(\frac{n \log n}{p}\right)$$

Matrix-Vector Multiplication

Numerical Experiments ($n = 131072$)

p	Opteron	Core2
1	1.13 s	0.45 s
2	0.60 s	0.28 s
4	0.48 s	0.26 s
8	0.31 s	



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