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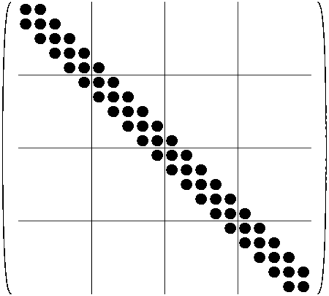
Scientific Computing

Parallele Algorithmen

Prof. Dr. Stefan Funken, Prof. Dr. Alexander Keller,
Prof. Dr. Karsten Urban | 11. Januar 2007

How to solve a tridiagonal system?



Algorithm (Tridiagonal system)

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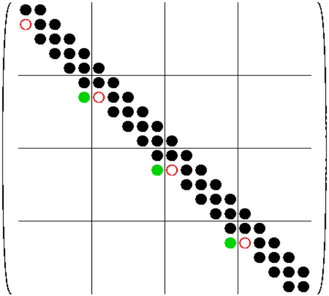

Algorithm (Tridiagonal system)

1. Eliminate in each diagonal block subdiagonal elements.

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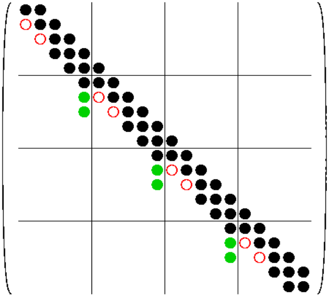

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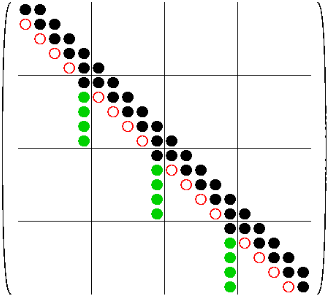

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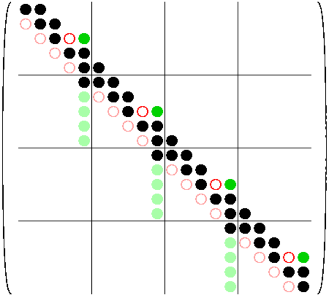

Algorithm (Tridiagonal system)

1. Eliminate in each diagonal block subdiagonal elements.
2. Eliminate in each diagonal block superdiagonal elements from third last row on.

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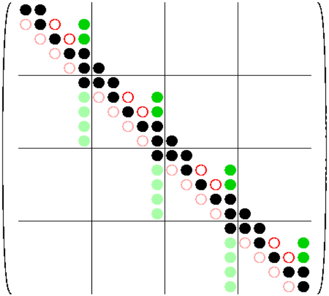

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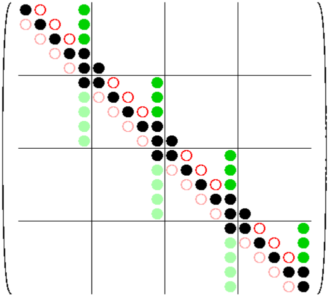

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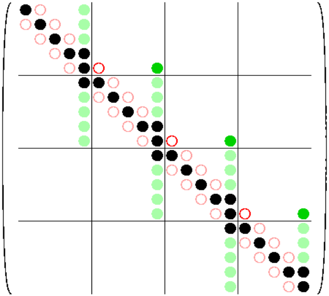

Algorithm (Tridiagonal system)

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3. Eliminate elements in superdiagonal blocks.

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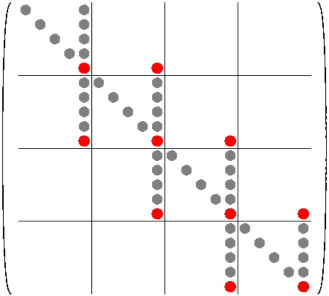

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Results in a tridiagonal subsystem with unknowns x_5, x_{10}, x_{15}, x_{20}.

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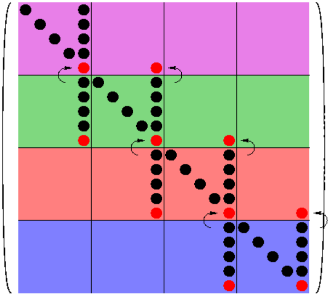

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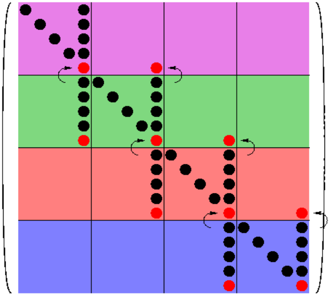

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Results in a tridiagonal subsystem with unknowns x_5, x_{10}, x_{15}, x_{20}.
If data are stored rowwise only one communication to neighbouring processor neccessary.

Iterative Solver

Steepest Descent

The steepest descent method minimizes a differentiable function F in direction of steepest descent.
Consider $F(x) := \frac{1}{2}x^T Ax - b^T x$ where A is symmetric and positiv definite.
Hence, $\nabla F = \frac{1}{2}(A + A^T)x - b = Ax - b$

Input: Initial guess x^0

$r^0 := b - Ax^0$

Iteration: $k = 0, 1, \ldots$

$x^{k+1} := x^k + \lambda_{opt}(x^k, r^k)\, r^k$ % Update x^k

$r^{k+1} := b - Ax^{k+1}$ % Compute residual

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Using $r^{k+1} = b - Ax^{k+1}$

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Steepest Descent Method

Let $x, p \in \mathbb{R}^n$. What is the optimal $\lambda_{opt}(x, p)$ in steepest descent method:
Consider the following minimization problem:

$$f(\lambda) \stackrel{!}{=} \min \quad \text{with} \quad f(\lambda) := F(x + \lambda p)$$

Then, with $F(x) = \frac{1}{2}\langle x, Ax\rangle - \langle b, x\rangle$ we get

$$f(\lambda) = F(x + \lambda p)$$

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&= F(x) + \lambda\langle p, Ax-b\rangle + \frac{1}{2}\lambda^2\langle p, Ap\rangle
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If $p \neq 0$, $\langle p, Ap\rangle > 0$.

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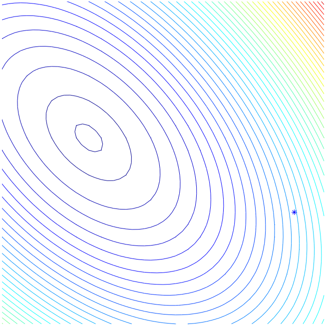
If $p \neq 0$, $\langle p, Ap\rangle > 0$.
Hence, from $0 \overset{!}{=} f'(\lambda) = \langle p, Ax - b\rangle + \lambda\langle p, Ap\rangle$ we obtain

$$\lambda_{opt}(x, p) = \frac{\langle p, b - Ax\rangle}{\langle p, Ap\rangle} \,.$$

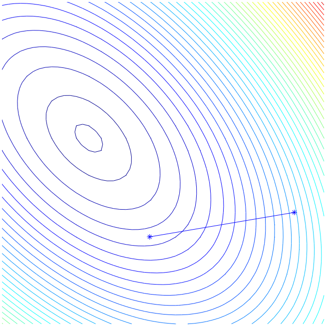
Numerical Example



2D Problem

- $A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$
- $b = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$
- $x^0 = \begin{pmatrix} 8 \\ -3 \end{pmatrix}$
- 5 iterations

Numerical Example



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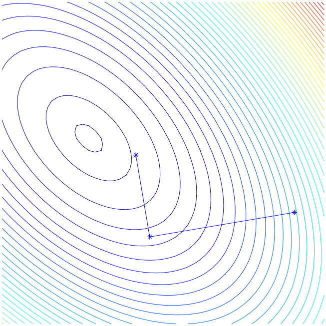

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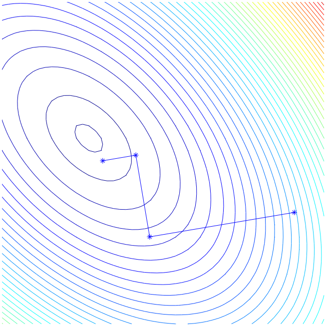

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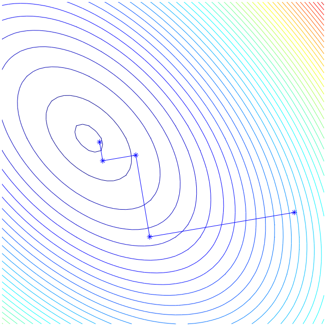

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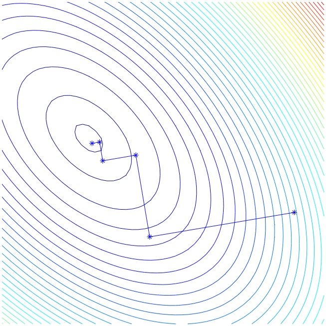

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Iteration: $k = 0, 1, \ldots$

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$x^{k+1} := x^k + \lambda_{opt}\, r^k$

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2 matrix-vector-products, 2 inner products, and 2 saxpy's per iteration

Is it possible save one matrix-vector-product?

Iterative Solver

Steepest Descent

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$a^k := Ar^k$

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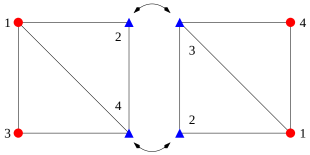
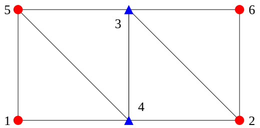


local numbering

How can vectors be given?

global numbering



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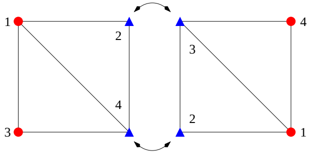

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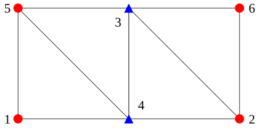

How can vectors be given?

- Full value at each node, e.g. given

$$u_\ell = (1,1,1,1)^T \quad u_r = (1,1,1,1)^T\,.$$

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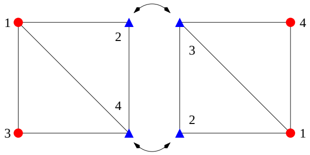

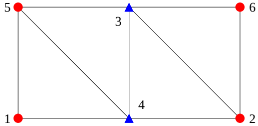

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$$u_\ell = (1,1,1,1)^T \quad u_r = (1,1,1,1)^T\,.$$

Using incidence matrices C_ℓ and C_r.

$$C_\ell = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad C_r = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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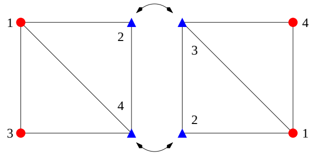

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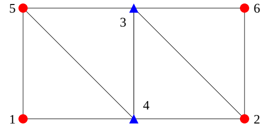

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Note

$$u_\ell : \quad \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

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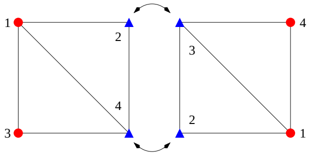
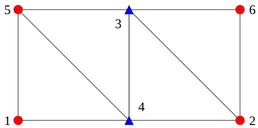




How can vectors be given?

- Full value at each node, e.g. given

$$u_\ell = (1,1,1,1)^T \quad u_r = (1,1,1,1)^T \,.$$

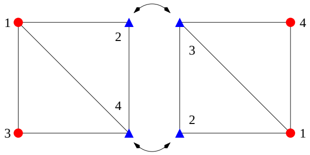
Hence

$$\begin{aligned} u &= C_\ell(1,1,1,1)^T + C_r(1,1,1,1)^T \\ &= (1,0,1,1,1,0)^T + (0,1,1,1,0,1)^T \\ &= (1,1,2,2,1,1)^T \neq (1,1,1,1,1,1)^T \end{aligned}$$

resp.

$$u = C_\ell u_\ell + C_r u_r$$

Numbering



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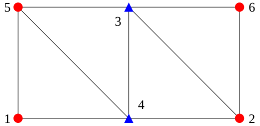


How can vectors be given?

- Full value at each node be given.
- Value is given after assembling all data, e.g. given

$$u_\ell = (1, \frac{1}{2}, 1, \frac{1}{2})^T \quad u_r = (1, \frac{1}{2}, \frac{1}{2}, 1)^T$$

results in

$$\begin{aligned} u &= C_\ell u_\ell + C_r u_r \\ &= (1, 0, \frac{1}{2}, \frac{1}{2}, 1, 0)^T + (0, 1, \frac{1}{2}, \frac{1}{2}, 0, 1)^T \\ &= (1, 1, 1, 1, 1, 1)^T \end{aligned}$$

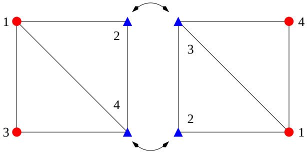
Types of Vectors

Two types of vectors, depending on the storage type:

type I: $\overline{u}$ is stored on P_k as restriction $\overline{u}_k = C_k \overline{u}$.
'Complete' value accessable on P_k.

type II: $\underline{r}$ is stored on P_k as $\underline{r}_k$, s.t.
$\underline{r} = \sum_{k=1}^{p} C_k^T \underline{r}_k$.
Nodes on the interface have only a part of the full value.

Numbering

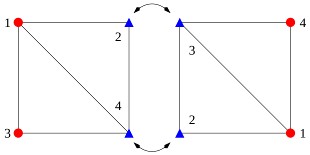


local numbering

Let matrices on both subdomains be given, for example:

$$A_\ell = \begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix} \quad A_r = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 1 & 3 & -7 & 2 \\ -2 & -9 & 4 & 0 \\ 3 & 7 & 1 & 5 \end{pmatrix}$$

Numbering



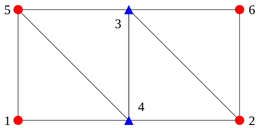
local numbering

Let matrices on both subdomains be given, for example:

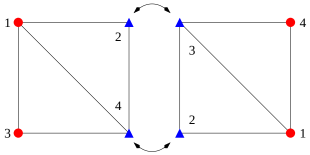
$$A_\ell = \begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix} \quad A_r = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 1 & 3 & -7 & 2 \\ -2 & -9 & 4 & 0 \\ 3 & 7 & 1 & 5 \end{pmatrix}$$

How to construct matrix A w.r.t global numbering from A_ℓ and A_r?

global numbering



Numbering



local numbering

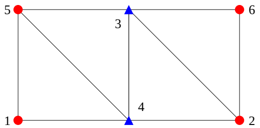
Let matrices on both subdomains be given, for example:

$$A_\ell = \begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix} \quad A_r = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 1 & 3 & -7 & 2 \\ -2 & -9 & 4 & 0 \\ 3 & 7 & 1 & 5 \end{pmatrix}$$

How to construct matrix A w.r.t global numbering from A_ℓ and A_r?

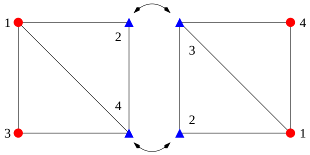
Use incidence matrices C_ℓ and C_r.

global numbering



$$C_\ell = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad C_r = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Numbering



local numbering

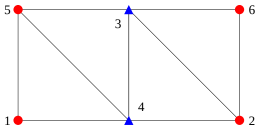
Let matrices on both subdomains be given, for example:

$$A_\ell = \begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix} \quad A_r = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 1 & 3 & -7 & 2 \\ -2 & -9 & 4 & 0 \\ 3 & 7 & 1 & 5 \end{pmatrix}$$

How to construct matrix A w.r.t global numbering from A_ℓ and A_r?

Use incidence matrices C_ℓ and C_r.

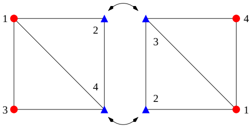
global numbering



$$C_\ell = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad C_r = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Now we get $A = C_\ell A_\ell C_\ell^T + C_r A_r C_r^T$.

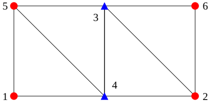
Numbering



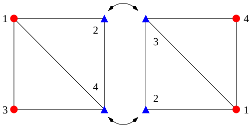
local numbering

$$A = C_\ell A_\ell C_\ell^T + C_r A_r C_r^T$$

global numbering



Numbering

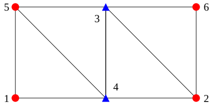


local numbering

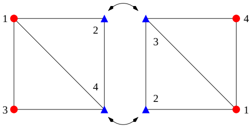
$$A = C_\ell A_\ell C_\ell^T + C_r A_r C_r^T$$

$$= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} + \dots$$

global numbering



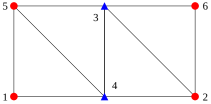
Numbering



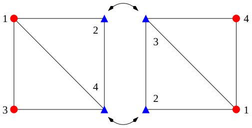
local numbering

$$
\begin{aligned}
A &= C_\ell A_\ell C_\ell^T + C_r A_r C_r^T \\
&= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix}
\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} + \ldots \\
&= \begin{pmatrix} 6 & 0 & 3 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -7 & 0 & 4 & 3 & -3 & 0 \\ 1 & 0 & -2 & 2 & 5 & 0 \\ 3 & 0 & 1 & -2 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}
+ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & -2 & 4 & -9 & 0 & 0 \\ 0 & 1 & -7 & 3 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 7 & 0 & 5 \end{pmatrix}
\end{aligned}
$$

global numbering



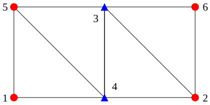
Numbering



local numbering

$$
\begin{aligned}
A &= C_\ell A_\ell C_\ell^T + C_r A_r C_r^T \\
&= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\begin{pmatrix} 2 & 1 & 3 & -2 \\ -3 & 4 & -7 & 3 \\ 4 & 3 & 6 & 0 \\ 5 & -2 & 1 & 2 \end{pmatrix}
\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} + \ldots \\
&= \begin{pmatrix} 6 & 0 & 3 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -7 & 0 & 4 & 3 & -3 & 0 \\ 1 & 0 & -2 & 2 & 5 & 0 \\ 3 & 0 & 1 & -2 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} +
\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & -2 & 4 & -9 & 0 & 0 \\ 0 & 1 & -7 & 3 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 7 & 0 & 5 \end{pmatrix} \\
&= \begin{pmatrix} 6 & 0 & 3 & 0 & 4 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ -7 & -2 & 4+4 & -9+3 & -3 & 0 \\ 1 & 1 & -7-2 & 3+2 & 5 & 2 \\ 3 & 0 & 1 & -2 & 2 & 0 \\ 0 & 3 & 1 & 7 & 0 & 5 \end{pmatrix}
\end{aligned}
$$

global numbering



Types of Matrices

There are two types of matrices:

type I: 'Complete' (but not all) entries are accessable on P_k.

type II: The matrix is stored in a distrubuted manner similiar to type II.

$$A = \sum_{k=1}^{p} C_k A_k C_k^T$$

where A_k belongs to processor P_k, resp. to the subdomain Ω_i.

Converting Type

Obviously, addition, subtraction (and similiar operations) of vectors can be done without communication, if they are of the same type.

- Converting from type I to type II needs communication.
  Mapping is not unique, e.g.

$$\underline{u}_i = C_i \left(\sum_{k=1}^{p} C_k C_k^T \right)^{-1} C_k^T \overline{u}_k$$

- Converting from type II to type I needs communication.

$$\overline{r}_i = C_i \sum_{k=1}^{p} C_k^T \underline{r}_k$$

Inner Product

The inner product of two vectors $\overline{u}$, $\underline{r}$ of different type needs only one reduce-communication.

$$\langle \overline{u}, \underline{r} \rangle$$

Inner Product

The inner product of two vectors $\overline{u}$, $\underline{r}$ of different type needs only one reduce-communication.

$$\begin{aligned} & \langle \overline{u}, \underline{r} \rangle \\ = \; & \overline{u}^T \sum_{k=1}^{p} C_k^T \underline{r}_k \end{aligned}$$

Inner Product

The inner product of two vectors $\overline{u}$, $\underline{r}$ of different type needs only one reduce-communication.

$$
\begin{aligned}
&\langle \overline{u}, \underline{r} \rangle \\
= \quad & \overline{u}^T \sum_{k=1}^{p} C_k^T \underline{r}_k \\
= \quad & \sum_{k=1}^{p} \overline{u}^T C_k^T \underline{r}_k
\end{aligned}
$$

Inner Product

The inner product of two vectors $\overline{u}$, $\underline{r}$ of different type needs only one reduce-communication.

$$
\begin{aligned}
& \langle \overline{u}, \underline{r} \rangle \\
= \ & \overline{u}^T \sum_{k=1}^{p} C_k^T \underline{r}_k \\
= \ & \sum_{k=1}^{p} \overline{u}^T C_k^T \underline{r}_k \\
= \ & \sum_{k=1}^{p} \langle C_k \overline{u}, \underline{r}_k \rangle
\end{aligned}
$$

Inner Product

The inner product of two vectors $\overline{u}$, $\underline{r}$ of different type needs only one reduce-communication.

$$
\begin{aligned}
& \langle \overline{u}, \underline{r} \rangle \\
= \; & \overline{u}^T \sum_{k=1}^{p} C_k^T \underline{r}_k \\
= \; & \sum_{k=1}^{p} \overline{u}^T C_k^T \underline{r}_k \\
= \; & \sum_{k=1}^{p} \langle C_k \overline{u}, \underline{r}_k \rangle \\
= \; & \sum_{k=1}^{p} \langle \overline{u}_k, \underline{r}_k \rangle
\end{aligned}
$$

Matrix-Vector Multiplications

- type II - matrix $\times$ type I - vector
  result is a type II vector, no communication!!!
  Consider $A = \sum_{k=1}^{p} C_k A_k C_k^T$.

$$A\overline{u}$$

Matrix-Vector Multiplications

- type II - matrix $\times$ type I - vector
  result is a type II vector, no communication!!!
  Consider $A = \sum_{k=1}^{p} C_k A_k C_k^T$.

$$A\overline{u} = \sum_{k=1}^{p} C_k A_k C_k^T \overline{u}$$

Matrix-Vector Multiplications

- type II - matrix $\times$ type I - vector
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  Consider $A = \sum_{k=1}^{p} C_k A_k C_k^T$.

$$A\overline{u} = \sum_{k=1}^{p} C_k A_k C_k^T \overline{u} = \sum_{k=1}^{p} C_k \underbrace{A_k \overline{u}_k}_{\underline{r}_k}$$

Matrix-Vector Multiplications

- type II - matrix × type I - vector
  result is a type II vector, no communication!!!
  Consider $A = \sum_{k=1}^{p} C_k A_k C_k^T$.

$$A\overline{u} = \sum_{k=1}^{p} C_k A_k C_k^T \overline{u} = \sum_{k=1}^{p} C_k \underbrace{A_k \overline{u}_k}_{\underline{r}_k} = \underline{r}$$

- type II - matrix × type II - vector
  type conversion neccessary, needs communication

Steepest Descent

Parallel Version

Input: Initial guess $\overline{x}^0$

$\underline{r}^0 := \underline{b} - A\overline{x}^0$

$\overline{w}^0 := \sum_{\ell=1}^{p} C_\ell^T \underline{r}^0$

Iteration: $k = 0, 1, \ldots$

$\underline{a}^k := A\overline{w}^k$

$\lambda := \frac{\langle \overline{w}^k, \underline{r}^k \rangle}{\langle \overline{w}^k, \underline{a}^k \rangle}$

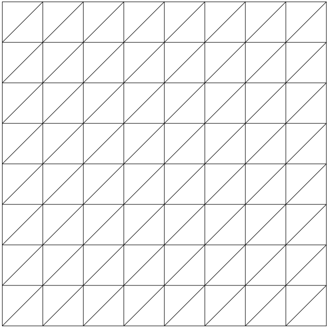
$\overline{x}^{k+1} := \overline{x}^k + \lambda\, \overline{w}^k$

$\underline{r}^{k+1} := \underline{r}^k - \lambda\, \underline{a}^k$

$\overline{w}^k := \sum_{\ell=1}^{p} C_\ell^T \underline{r}^k$

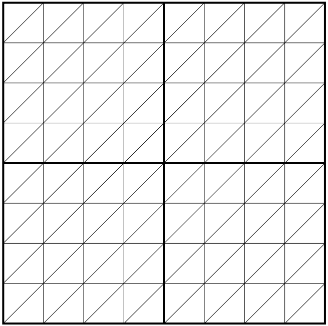
Only two allreduce-communications and one vector accumulation per iteration necessary!

Non-overlapping Subdomains



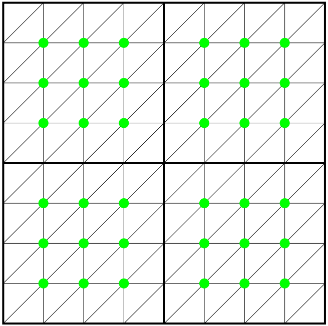
Different Indizes

Non-overlapping Subdomains



Different Indizes

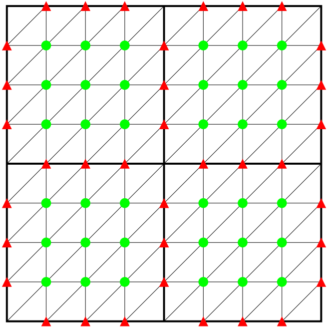
Non-overlapping Subdomains



Different Indizes

1. **I** nodes in interior of subdomains $[N_I = \sum_{j=1}^{p} N_{I,j}]$.

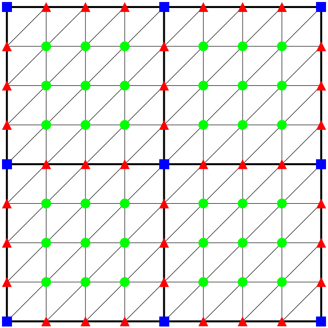
Non-overlapping Subdomains



Different Indizes

1. **I** nodes in interior of subdomains $[N_I = \sum_{j=1}^{p} N_{I,j}]$.
2. **E** nodes in interior of subdomains-edges $[N_E = \sum_{j=1}^{n_e} N_{E,j}]$. ($n_e$ number of subdomain-edges)

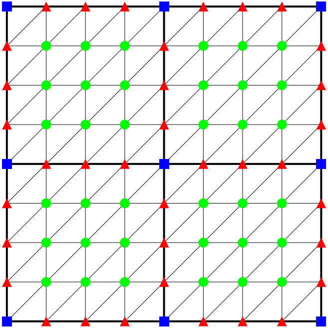
Non-overlapping Subdomains



Different Indizes

1. **I** nodes in interior of subdomains $[N_I = \sum_{j=1}^{p} N_{I,j}]$.
2. **E** nodes in interior of subdomains-edges $[N_E = \sum_{j=1}^{n_e} N_{E,j}]$. ($n_e$ number of subdomain-edges)
3. **V** crosspoints, i.e. endpoints of subdomain-edges $[N_V]$

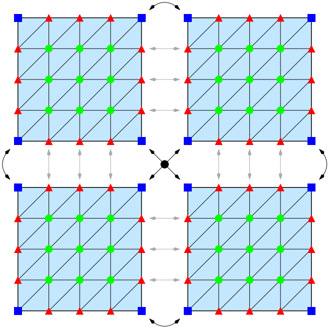
Non-overlapping Subdomains



Different Indizes

1. **I** nodes in interior of subdomains $[N_I = \sum_{j=1}^{p} N_{I,j}]$.
2. **E** nodes in interior of subdomains-edges $[N_E = \sum_{j=1}^{n_e} N_{E,j}]$. ($n_e$ number of subdomain-edges)
3. **V** crosspoints, i.e. endpoints of subdomain-edges $[N_V]$
4. **E** and **V** are often denoted as coupling nodes with index **C** $[N_C = N_E + N_V]$

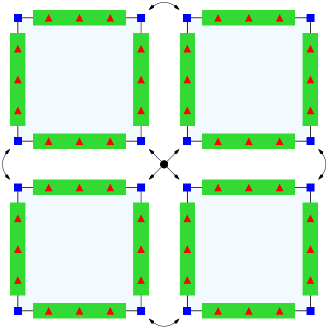
Non-overlapping Subdomains



Communication

1. Communication only neccessary for nodes on the coupling boundaries.

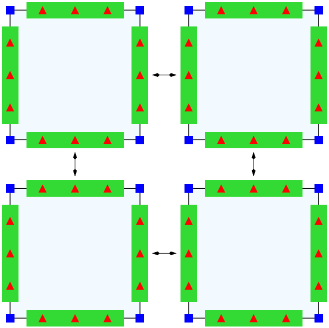
Non-overlapping Subdomains



Communication

1. Communication only neccessary for nodes on the coupling boundaries.
2. Global communication for crosspoints.

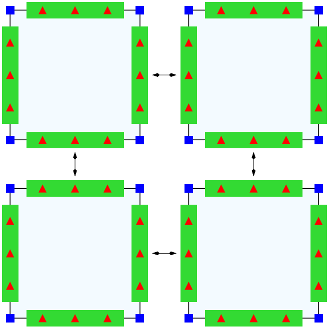
Non-overlapping Subdomains



Communication

1. Communication only neccessary for nodes on the coupling boundaries.
2. Global communication for crosspoints.
3. Only communication to the neighbouring subdomain for edge-nodes.

Non-overlapping Subdomains

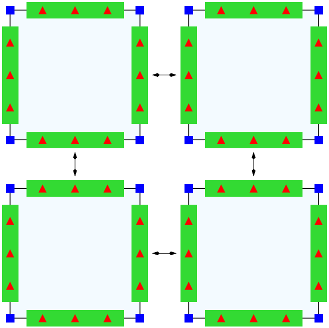


Communication

1. Communication only neccessary for nodes on the coupling boundaries.
2. Global communication for crosspoints.
3. Only communication to the neighbouring subdomain for edge-nodes.
4. Not all nodes have to be 'touched' for a vector accumulation

$$\overline{w} := \sum_{\ell=1}^{p} C_\ell^T \underline{r}$$

Non-overlapping Subdomains



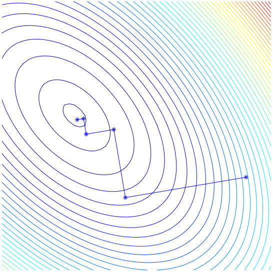
Communication

1. Communication only neccessary for nodes on the coupling boundaries.
2. Global communication for crosspoints.
3. Only communication to the neighbouring subdomain for edge-nodes.
4. Not all nodes have to be 'touched' for a vector accumulation

$$\overline{w} := \sum_{\ell=1}^{p} C_\ell^T \underline{r}$$

5. Split into communication between neighbouring subdomains and one global communication for all crosspoints.

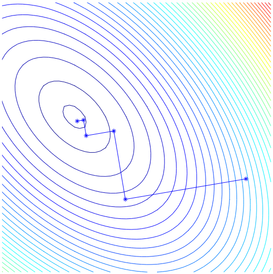
Numerical Example



Notice the following properties of the algorithm

$$r^m \perp r^{m+1} = r^m - \lambda_{opt}(x^m, r^m)\, Ar^m = r^m - \frac{\langle r^m, b - Ax^m \rangle}{\langle r^m, Ar^m \rangle} Ar^m$$

Numerical Example



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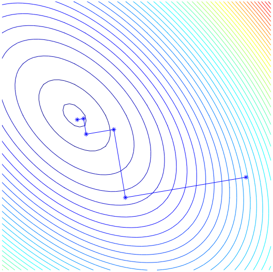
resp.

$$\langle r^m, r^{m+1} \rangle$$

Numerical Example



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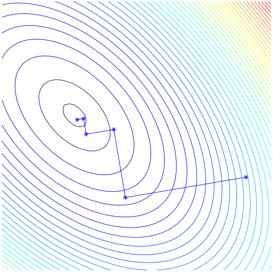
resp.

$$\langle r^m, r^{m+1} \rangle = \langle r^m, r^m \rangle - \frac{\langle r^m, b - Ax^m \rangle}{\langle r^m, Ar^m \rangle} \langle r^m, Ar^m \rangle = 0$$

Numerical Example



Notice the following properties of the algorithm

$$r^m \perp r^{m+1} = r^m - \lambda_{opt}(x^m, r^m)\, Ar^m = r^m - \frac{\langle r^m, b - Ax^m\rangle}{\langle r^m, Ar^m\rangle} Ar^m$$

resp.

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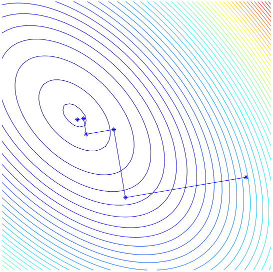
but not $r^m \perp r^{m+2}$.

Numerical Example



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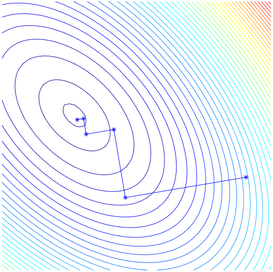

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There exists a better algorithm for symmetric and positive definite matrices, as they arise in the finite element method!!! The CG-algorithm.

Preconditioned Conjugate Gradient Method

Solve $Ax = b$ (A, W sym, + def), W^{-1} 'easy' to compute, s.t. $W^{-1}A \approx I$ (e.g. $W^{-1} = I$, $W^{-1} = k$-iterations of Jacobi/Gauss-Seidel)

Input: Initial guess x^0

$r^0 := b - Ax^0$

$p^0 := W^{-1} r^0$

$\sigma_0 := \langle p^0, r^0 \rangle$

Iteration: $k = 0, 1, \ldots$ (as long as $k < n$, $r^k \neq 0$)

$a^k := Ap^k$

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Parallel Preconditioned Conjugate Gradient Method

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How should we choose W^{-1} ???

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- prefix each message with the process rank, sort by rank!

  messages received from different processes do not necessarily arrive in chronological order

Debugging MPI Programs

Practical debugging strategies

- run parallel program on single process,

  tests most of functionality, such as I/O
- run parallel program with two processes,

  or more, such that all functionality can be exercised
- run with smallest problem size that exercises all functionality

  solving a 4×4-system is the same as 1024×1024
- use 'printf'-debugger
- put `fflush(stdout);` after every `printf`
- for point-to-point communication, print data being sent and received
- prefix each message with the process rank, sort by rank!

  messages received from different processes do not necessarily arrive in chronological order
- make sure that all the data structures have been set up correctly

Most frequent sources of trouble

Sequential programming

1. interface problems (types, storage of pointers to data)

Parallel programming

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2. pointer and dynamical memory management

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1. communication

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Parallel programming

1. communication
2. races

Most frequent sources of trouble

Sequential programming

1. interface problems (types, storage of pointers to data)
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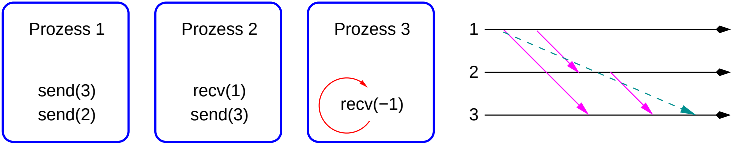
Parallel programming

1. communication
2. races
3. deadlocks

Races

Definition: A race produces an unpredictable program state and behavior due to un-synchronized concurrent executions.
Most often data races occur, which are caused by unordered concurrent accesses of the same memory location from multiple processes.

Example: 'triangle inequality'



Effect: non-deterministic, non-reproducable program running

Communication with MPI

Deadlock I

Time	Process A	Process B
1	`MPI_Send` to B, tag $= 0$	local work
2	`MPI_Send` to B, tag $= 1$	local work
3	local work	`MPI_Recv` from A, tag $= 1$
4	local work	`MPI_Recv` from A, tag $= 0$

Communication with MPI

Deadlock I

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- The program will deadlock, if system provides no buffer.

Communication with MPI

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1	`MPI_Send` to B, tag $= 0$	local work
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- The program will deadlock, if system provides no buffer.
- Process A is not able to send message with tag=0.

Communication with MPI

Deadlock I

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1	`MPI_Send` to B, tag $= 0$	local work
2	`MPI_Send` to B, tag $= 1$	local work
3	local work	`MPI_Recv` from A, tag $= 1$
4	local work	`MPI_Recv` from A, tag $= 0$

- The program will deadlock, if system provides no buffer.
- Process A is not able to send message with tag=0.
- Process B is not able to receive message with tag=1.

Communication with MPI

Deadlock II

Time	Process A	Process B
1	MPI_Send to B	MPI_Send to A
2	MPI_Recv from B B	MPI_Recv from A

Communication with MPI

Deadlock II

Time	Process A	Process B
1	MPI_Send to B	MPI_Send to A
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Communication with MPI

Deadlock II

Time	Process A	Process B
1	MPI_Send to B	MPI_Send to A
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- The program will deadlock, if system provides no buffer.
- Process A and Process B are not able to send messages.

Communication with MPI

Deadlock II

Time	Process A	Process B
1	`MPI_Send` to B	`MPI_Send` to A
2	`MPI_Recv` from B B	`MPI_Recv` from A

- The program will deadlock, if system provides no buffer.
- Process A and Process B are not able to send messages.
- Order communications in the right way!

Communication with MPI

Example: Exchange of messages

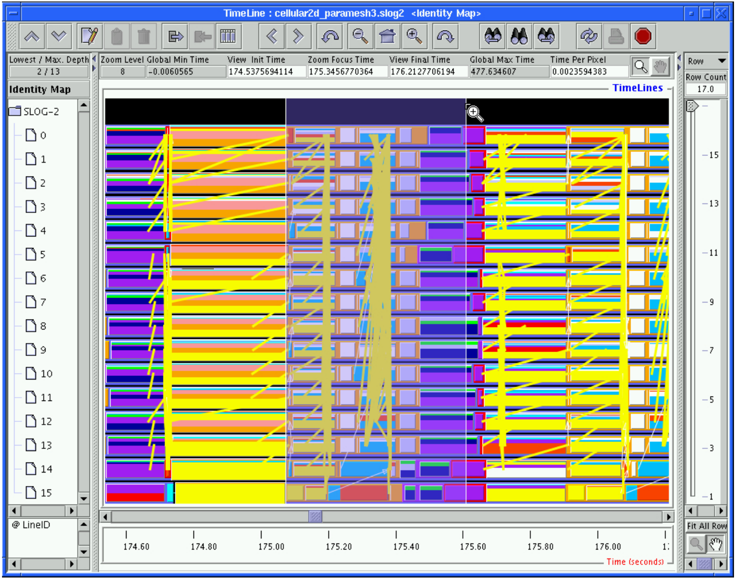
```
if (myrank == 0) {
    MPI_Send( sendbuf, 20, MPI_INT, 1, tag, communicator);
    MPI_Recv( recvbuf, 20, MPI_INT, 1, tag, communicator, &status);
}
else if (myrank == 1) {
    MPI_Recv( recvbuf, 20, MPI_INT, 0, tag, communicator, &status);
    MPI_Send( sendbuf, 20, MPI_INT, 0, tag, communicator);
}
```

- This code succeeds even with no buffer space at all !!!
- **Important note: Code which relies on buffering is considered unsafe !!!**

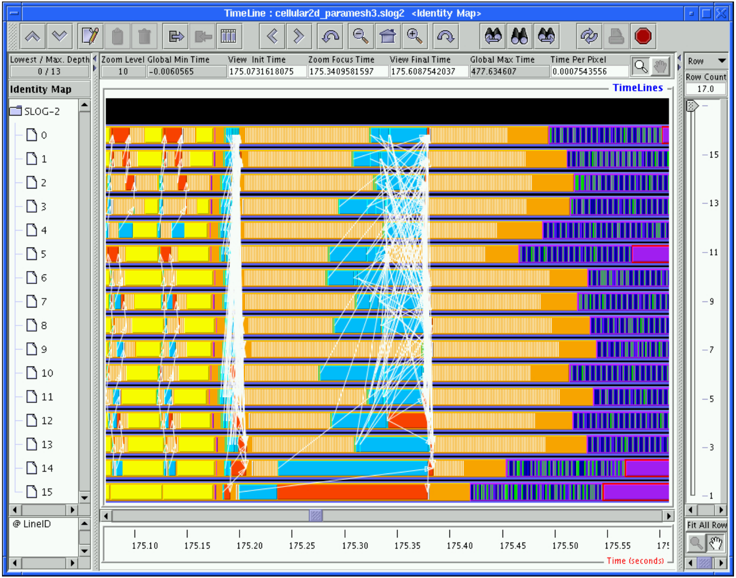
Performance Visualization for Parallel Programs

- MPE is a software package for MPI programmers.
- useful tools for MPI programs, mainly performance visualization
- latest version is called MPE2
- current tools are:
  1. profiling libraries to create logfiles
  2. postmortem visualization of logfiles when program is executed
  3. shared-display parallel X graphics library
  4. . . .

Performance Visualization for Parallel Programs



Performance Visualization for Parallel Programs



Performance Visualization for Parallel Programs