

Algorithms in Scientific Computing II

Dwarf # 1 – Dense Linear Algebra

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Winter 2011/2012

The Seven Dwarfs of HPC – Dwarf # 1

- ① **dense linear algebra**
- ② sparse linear algebra
- ③ spectral methods
- ④ N-body methods
- ⑤ structured grids
- ⑥ unstructured grids
- ⑦ Monte Carlo

Part I

Matrix Multiplication



Matrix Multiplication on the PRAM

```
MatrixMult_PRAM(A:Matrix[n], B:Matrix[n], C:Matrix[n]) {  
  ! Model: CREW-PRAM with  $n*n$  processors  
  for i from 1 to n do in parallel  
    for k from 1 to n do in parallel  
      for j from 1 to n do  
         $C[i,k] = C[i,k] + A[i,j]*B[j,k]$   
      }  
}
```

Strategy:

- each processor computes one element of the result matrix
⇒ exclusive write access to $C[i,k]$
- runtime $O(n)$ on n^2 processors

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    }
```

Observation:

- synchronised execution of the for-j-loop;
→ in the first step:
- all processors $P_{i,k}$ simultaneously access $A[i,1]$
- all processors $P_{i,k}$ simultaneously access $B[1,k]$

PRAM Matrix Multiplication with Shifted Indices

```
MatrixMult_PRAM(A:Matrix[n], B:Matrix[n], C:Matrix[n]) {  
  ! Model: EREW-PRAM with n*n processors  
  for i from 1 to n do in parallel  
    for k from 1 to n do in parallel  
      for j from 1 to n do  
        C[i,k] = C[i,k]  
          + A[i,(i+j+k) mod n]*B[(i+j+k) mod n,k]  
      }  
}
```

Observation: in the first step of the j-loop

- processors $P_{i,k}$ access $A[i,(i+1+k) \bmod n]$
- processors $P_{i,k}$ access $B[(i+1+k) \bmod n,k]$
- leads to exclusive read access to A and B

Towards Cannon's Algorithm

Strategy:

- consider a 2D mesh of processors
- each processor holds one element of A, B, and C
- C element stays on a fixed processor
- during j-loop:
increase column index of A, and row index of B
⇒ A and B element have to be “transferred” to neighbouring processors

New Algorithmic Model:

Interconnection Network (2D Mesh) instead of PRAM

Matrix Multiplication on the 2D Mesh

→ “Cannon’s Algorithm”:

```
MatrMult_2Dmesh(A:Matrix[n], B:Matrix[n], C:Matrix[n]) {  
  ! Model: 2D mesh with n*n processors  
  input P[i,k]:A,B,C, range P[i,k]: 1<=i,k<=n  
  ! init : P[i,k] holds A[i,(i+k+1)mod n], B[(i+1+k) mod n,k]  
  for P[i,k]: 1<=i,k<=n do in parallel  
    for j from 1 to n do {  
      C = C + A*B;  
      P[i,k]:A <<< P[i,(k+1) mod n]:A  
      P[i,k]:B <<< P[(i+1) mod n,k]:B  
    }  
  end in parallel  
  output P[i,k]: C, range P[i,k]: 1<=i,k<=n  
}
```


Cannon's Algorithm – Time Complexity

Complexity of Cannon's Algorithm:

- n additions/multiplications on n^2 processors
- $2n$ send/receive operations (by each processor)

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Generalization:

- switch to block-oriented algorithm on p^2 processors
- $A[i,j]$, $B[j,k]$, $C[i,k]$ are matrix blocks (of size $\frac{n}{p} \times \frac{n}{p}$)
- leads to $p(n/p)^3 = n^3/p^2$ operations
- $2p$ block send/receives – total volume: $2n^2/p$ elements

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Mesh \rightarrow Torus:

- mistake in the analysis: transfer $P[i,n]:A \lll P[i,1]:A$ (similar for B) not possible in one step
- actually requires a **2D torus** network

Matrix Multiplication and Parallel External Memory

Consider: “Parallel External Memory” Model

- number of memory transfers for the PRAM program?

for i **from** 1 **to** n **do in parallel**

for k **from** 1 **to** n **do in parallel**

for j **from** 1 **to** n **do**

$$C[i,k] = C[i,k] + A[i,j]*B[j,k]$$

Matrix Multiplication and Parallel External Memory

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$$C[i,k] = C[i,k] + A[i,j]*B[j,k]$$

- each processor reads $2n$ elements
- thus $n^2 \cdot 2n/B$ transfers (each B words)
- how to use the local memory?

Block-Oriented Matrix Multiplication

Block-oriented formulation:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix}$$

→ each A_{ij} , B_{jk} , C_{ik} a square matrix block

Block operations:

- $C_{11} = A_{11}B_{11} + A_{12}B_{21} + A_{13}B_{31}$
 $C_{12} = A_{11}B_{12} + A_{12}B_{22} + A_{13}B_{32}$

...

- three blocks need to fit in local memory!

Matrix Multiplication on Parallel External Memory

```
MatrixMult_PRAM(A:Matrix[n], B:Matrix[n], C:Matrix[n]) {  
  ! Model: CREW-PRAM with  $n*n$  processors  
  for i from 1 to  $n/b$  do in parallel  
    for k from 1 to  $n/b$  do in parallel  
      for j from 1 to  $n/b$  do {  
        ! read required blocks of A,B,C  
        for ii from 1 to b do  
          for kk from 1 to b do  
            for jj from 1 to b do  
               $C[i*b+ii, k*b+kk] = C[i*b+ii, k*b+kk]$   
                 $+ A[i*b+ii, j*b+jj]*B[j*b+jj, k*b+kk]$   
            }  
          }  
        }  
  }  
}
```

Blocked MatrixMult on PEM – Memory Transfers

Number of Memory Transfers:

- local memory can hold M words;
choose b such that $3b^2 < M$ (ideal: $3b^2 = M$)
- read/write local C block: $2b^2$ words per processor
- read all n/b A blocks and n/b B blocks:
 $2n/b \cdot b^2$ words per processor
- for all $(n/b)^2$ processors:
 $(n/b)^2 \cdot (2n/b + 2)b^2 = 2n^3/b + 2n^2$ words
- $b \in \Theta(\sqrt{M})$; move L words per transfer;
therefore: $\Theta(n^3/(L\sqrt{M}))$ memory transfers

Block-Oriented and Block-Recursive Multiplication

Block-oriented algorithms:

$$C_{ik} = \sum_j A_{ij} B_{jk}$$

Block-recursive algorithms:

$$\left(\begin{array}{cc|cc} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ \hline A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{array} \right) \left(\begin{array}{cc|cc} B_{11} & B_{12} & B_{13} & B_{14} \\ B_{21} & B_{22} & B_{23} & B_{24} \\ \hline B_{31} & B_{32} & B_{33} & B_{34} \\ B_{41} & B_{42} & B_{43} & B_{44} \end{array} \right) = \left(\begin{array}{cc|cc} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ \hline C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{array} \right)$$

→ blocking leads to better cache performance

Part II

Dense Linear Algebra



Dense Linear Algebra – Libraries

BLAS

- “Basic linear algebra subroutines for FORTRAN usage” (Lawson et al., ACM TOMS, 1979)
- BLAS level 3: dense matrix multiplication, focus on blocking to improve cache efficiency (Dongarra et al., 1990)

LAPACK

- “a portable linear algebra library for high-performance computers” (1990)
- solve systems of linear equations, least squares problems, eigenvalue problems, etc.

Dense Linear Algebra – Parallelisation

PBLAS

- parallel BLAS implementation (OpenMP, MPI)
- basis for ScaLAPACK

ScaLAPACK

- parallel library (subset of LAPACK) for distributed memory computers (v1.0: 1995; v1.8: 2007)
- basic data structure: 2D block cyclic decomposition of matrices

Multiplication of 3×3 Matrices

An optimal order of execution:

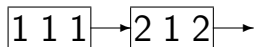
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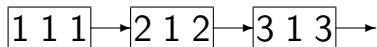
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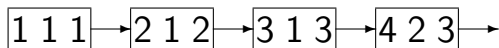
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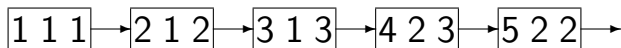
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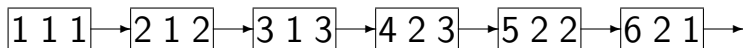
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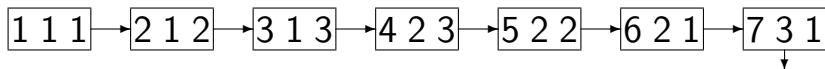
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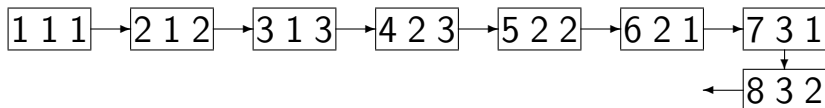
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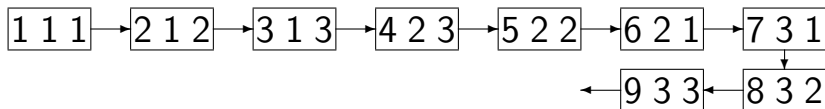
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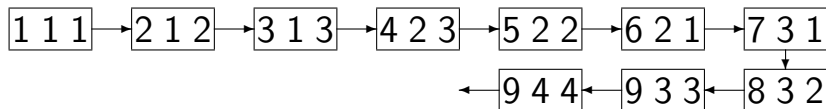
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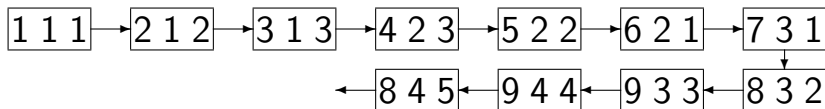
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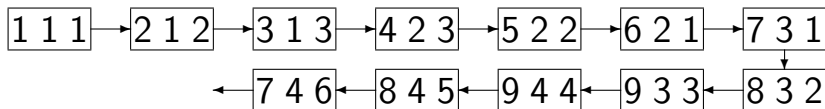
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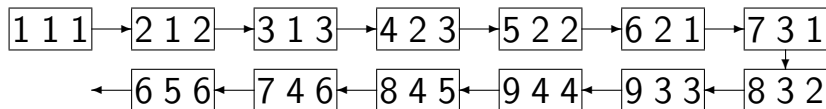
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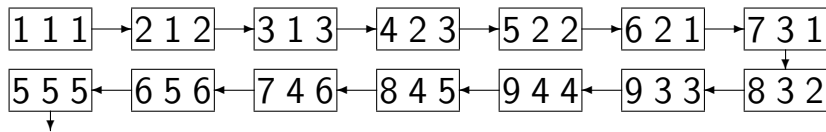
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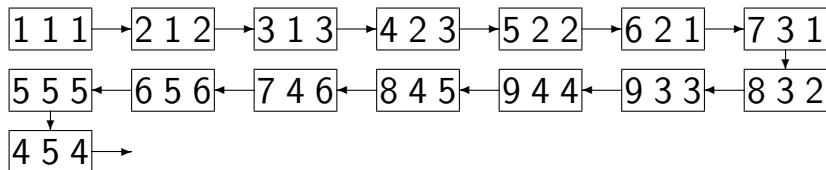
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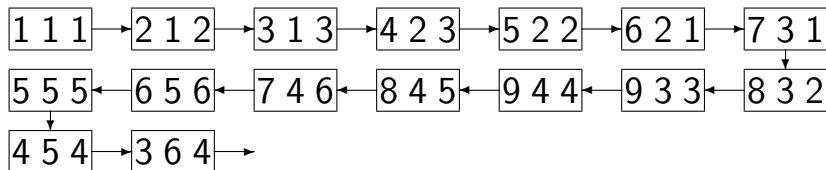
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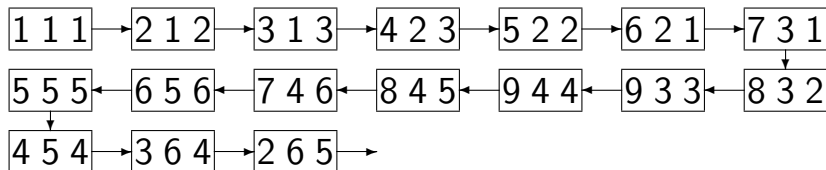
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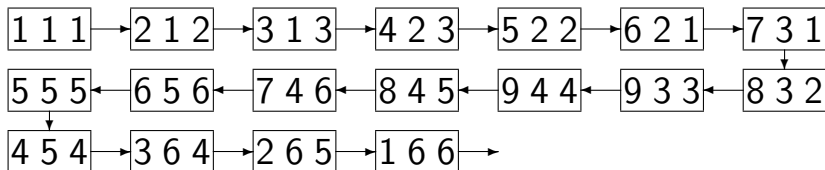
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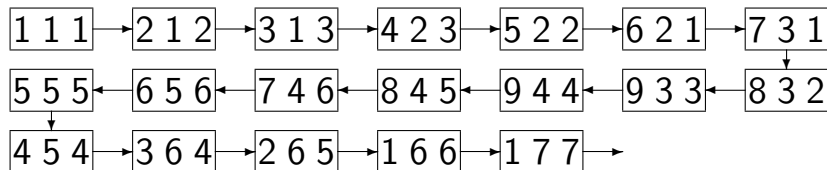
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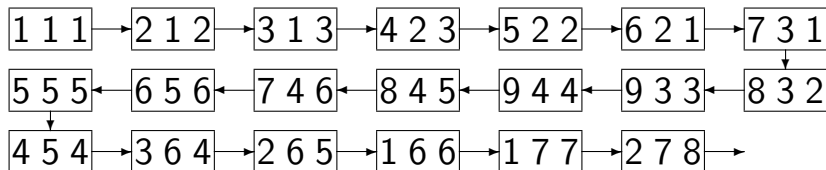
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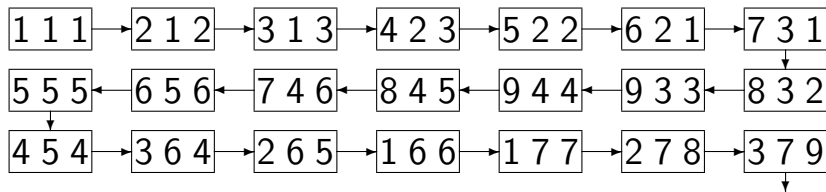
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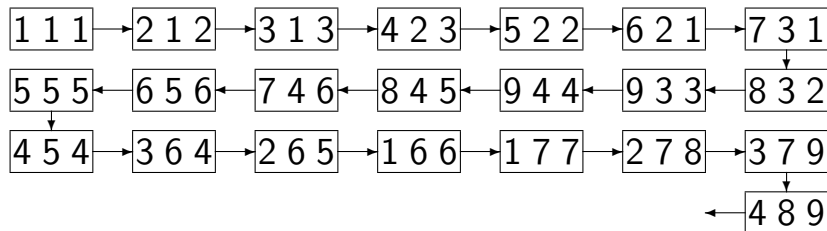
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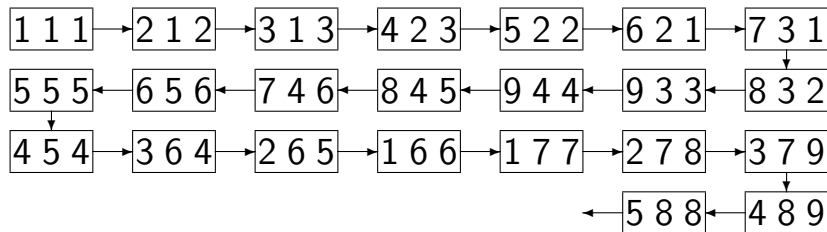
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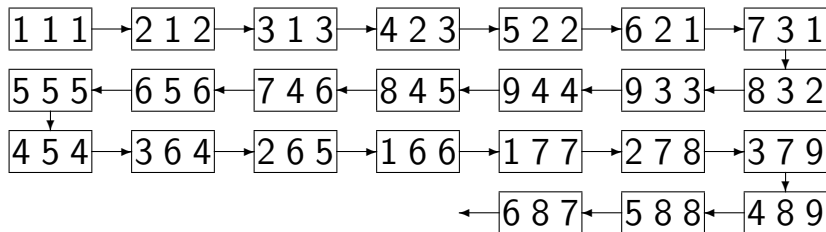
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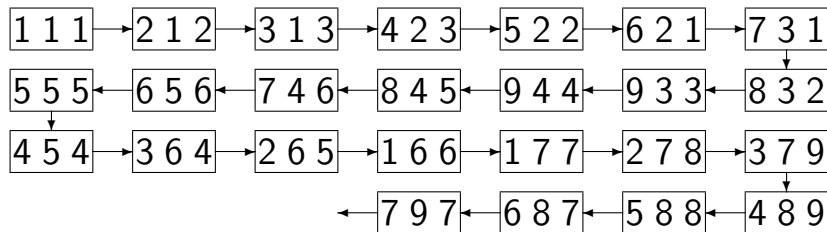
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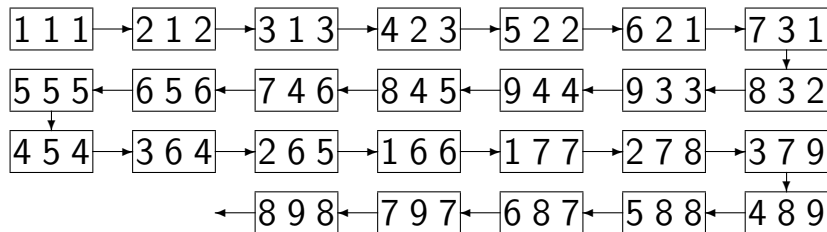
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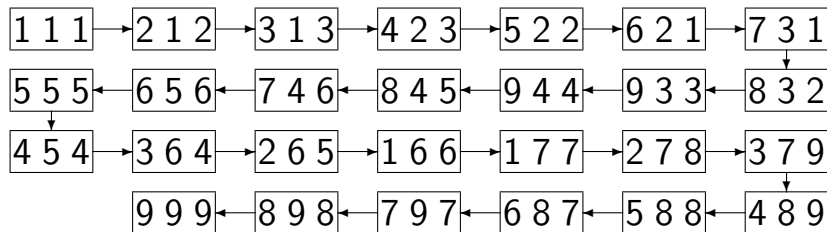
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Multiplication of 3×3 Matrices

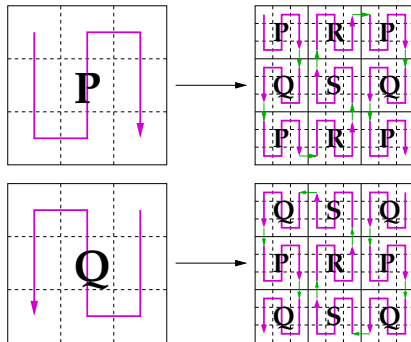
An optimal order of execution:

$$\begin{pmatrix} 1 & 6 & 7 \\ 2 & 5 & 8 \\ 3 & 4 & 9 \end{pmatrix} \begin{pmatrix} 1 & 6 & 7 \\ 2 & 5 & 8 \\ 3 & 4 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 6 & 7 \\ 2 & 5 & 8 \\ 3 & 4 & 9 \end{pmatrix}$$



Block-recursive Peano Element Order

- indexing according to iteration of a Peano curve



- in practice: stopped on *L1 blocks*
(size tuned to L1 cache \rightarrow 2 matrix blocks should fit)
- use column-major layout within L1-blocks

Block-recursive Multiplication

- multiplication of block matrices (cmp. 3×3 -scheme):

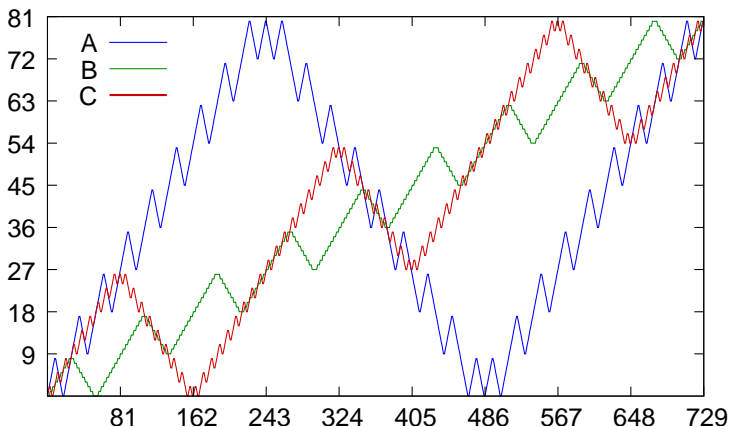
$$\begin{pmatrix} P_{A0} & R_{A5} & P_{A6} \\ Q_{A1} & S_{A4} & Q_{A7} \\ P_{A2} & R_{A3} & P_{A8} \end{pmatrix} \begin{pmatrix} P_{B0} & R_{B5} & P_{B6} \\ Q_{B1} & S_{B4} & Q_{B7} \\ P_{B2} & R_{B3} & P_{B8} \end{pmatrix} = \begin{pmatrix} P_{C0} & R_{C5} & P_{C6} \\ Q_{C1} & S_{C4} & Q_{C7} \\ P_{C2} & R_{C3} & P_{C8} \end{pmatrix}$$

- leads to **eight** different combinations (w.r.t. block numbering):

$$\begin{array}{cccc} PP \rightarrow P & QR \rightarrow S & RS \rightarrow R & SQ \rightarrow Q \\ PR \rightarrow R & QP \rightarrow Q & RQ \rightarrow P & SS \rightarrow S \end{array}$$

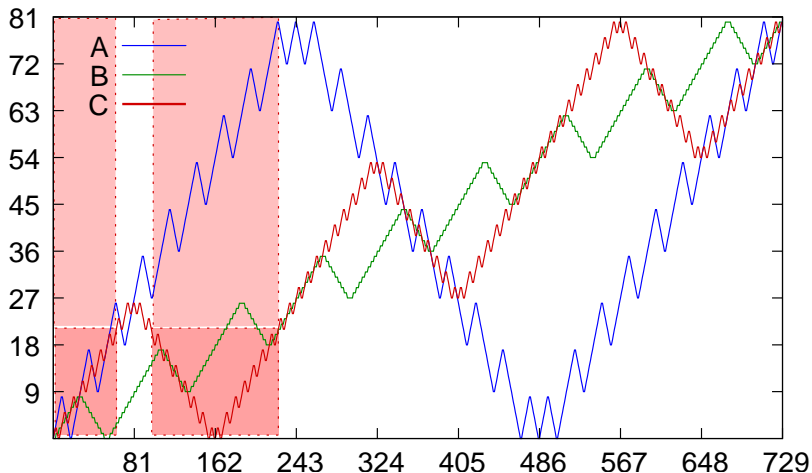
- all schemes similar to $PP \rightarrow P$ (but revers order)

Access Pattern to the Matrix Blocks



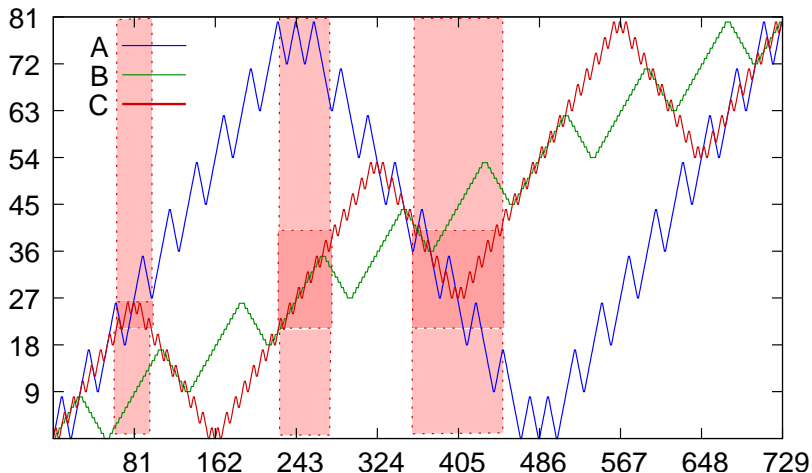
- Increment/Decrement access to elements
- $\mathcal{O}(k^3)$ operations on any block of k^2 elements

Parallelisation: *Owner-Computes-Partitioning*



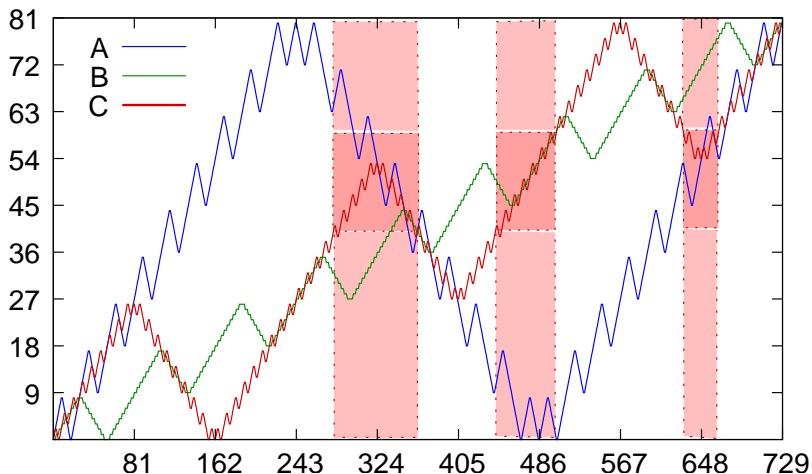
Partition matrix C according to Peano order \rightarrow defines thread

Parallelisation: *Owner-Computes-Partitioning*



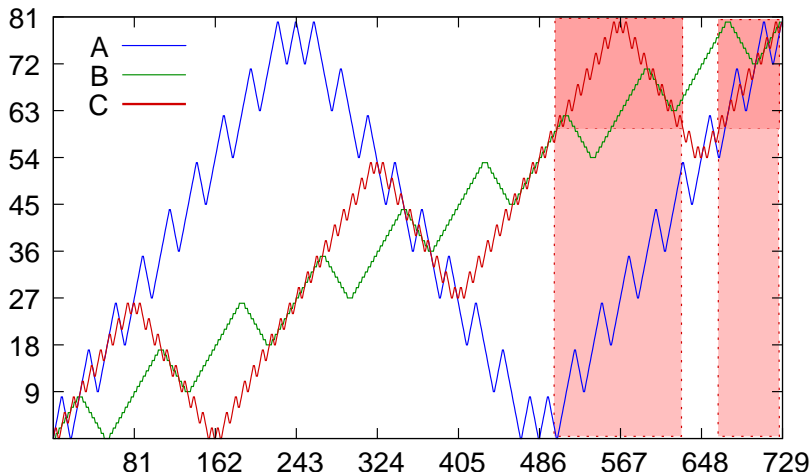
Partition matrix C according to Peano order \rightarrow defines thread

Parallelisation: *Owner-Computes-Partitioning*



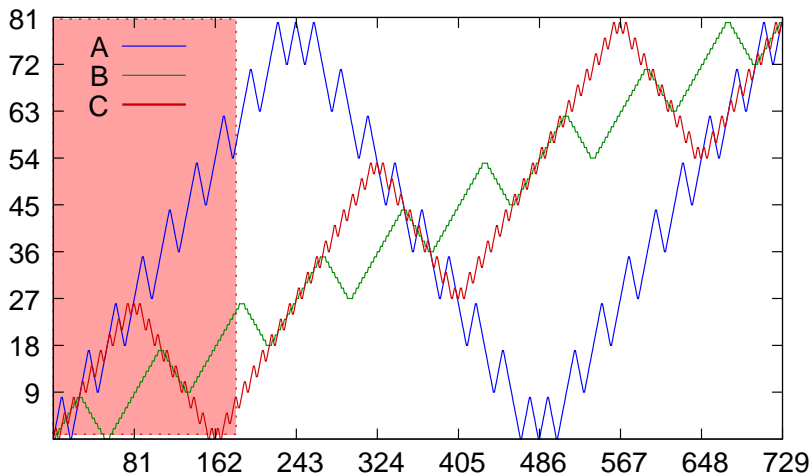
Partition matrix C according to Peano order \rightarrow defines thread

Parallelisation: *Owner-Computes-Partitioning*



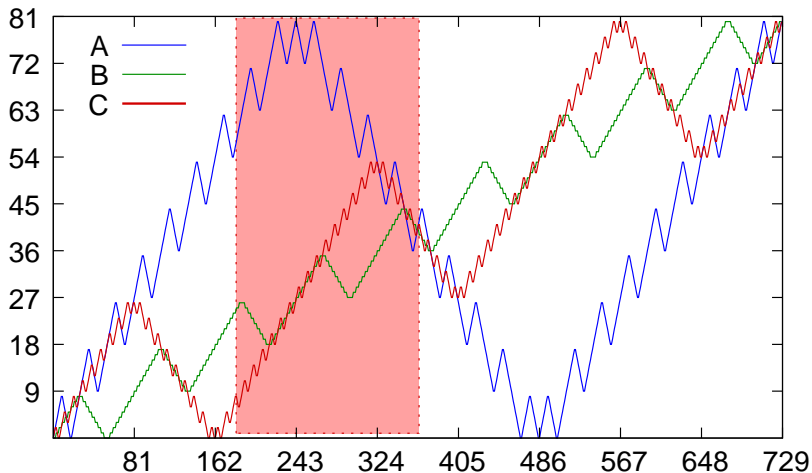
Partition matrix C according to Peano order \rightarrow defines thread

Parallelisation: *Work-Oriented-Partitioning*



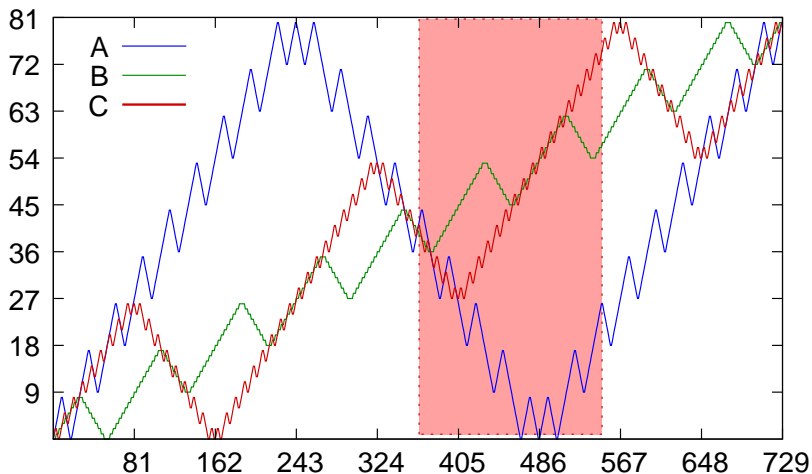
Partition element operations according to 3D Peano order
→ defines thread

Parallelisation: *Work-Oriented-Partitioning*



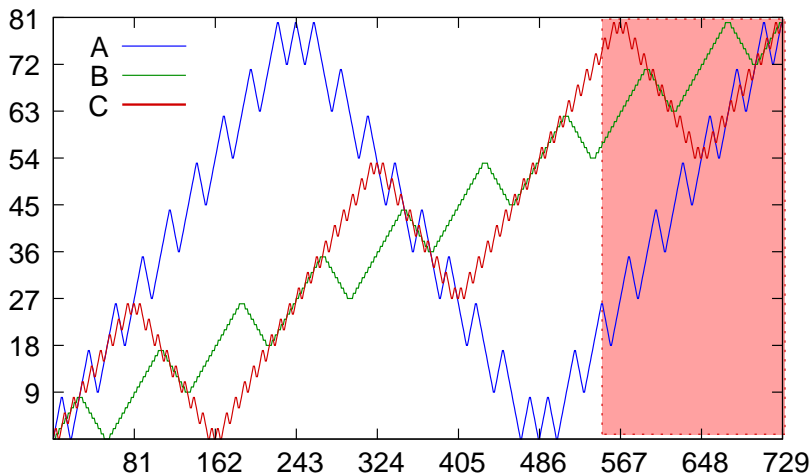
Partition element operations according to 3D Peano order
→ defines thread

Parallelisation: *Work-Oriented-Partitioning*



Partition element operations according to 3D Peano order
→ defines thread

Parallelisation: *Work-Oriented-Partitioning*



Partition element operations according to 3D Peano order
→ defines thread

“Peano” Multiplication – Properties

- access to matrix elements entirely local:
use increment and decrement operators only
- optimal re-use of data:
 $\mathcal{O}(k^3)$ operations on any block of k^2 contiguous elements
- number of cache misses on an *ideal cache* (M lines of length L):

$$\mathcal{O}\left(\frac{N^3}{L\sqrt{M}}\right)$$

shown to be asymptotically optimal

- results can be extended to Parallel External Memory model

Example: LU Decomposition

Block-oriented formulation:

$$\begin{pmatrix} \hat{L}_{11} & 0 & 0 \\ L_{21} & \hat{L}_{22} & 0 \\ L_{31} & L_{32} & \hat{L}_{33} \end{pmatrix} \begin{pmatrix} \tilde{U}_{11} & U_{12} & U_{13} \\ 0 & \tilde{U}_{22} & U_{23} \\ 0 & 0 & \tilde{U}_{33} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix},$$

Block operations:

- 1 LU decomposition: $\hat{L}_{11} \tilde{U}_{11} = A_{11}$
- 2 “find left”: $L_{21} \tilde{U}_{11} = A_{21}$, $L_{31} \tilde{U}_{11} = A_{31}$
- 3 “find right”: $\hat{L}_{11} U_{12} = A_{12}$, $\hat{L}_{11} U_{13} = A_{13}$
- 4 block updates: $A_{22} = A_{22} - L_{21} U_{12}$

etc.

Barrier/Tile-Oriented Parallelisation

$$L_{11}U_{11} = A_{11}$$

$$L_{21}U_{11} = A_{21}$$

$$L_{31}U_{11} = A_{31}$$

$$L_{11}U_{12} = A_{12}$$

$$L_{11}U_{13} = A_{13}$$

$$A_{23} = L_{21}U_{13}$$

$$A_{22} = L_{21}U_{12}$$

$$A_{32} = L_{31}U_{12}$$

$$A_{33} = L_{31}U_{13}$$

$$L_{22}U_{22} = A_{22}$$

$$L_{32}U_{22} = A_{32}$$

$$L_{22}U_{23} = A_{23}$$

$$A_{33} = L_{32}U_{23}$$

$$L_{33}U_{33} = A_{33}$$

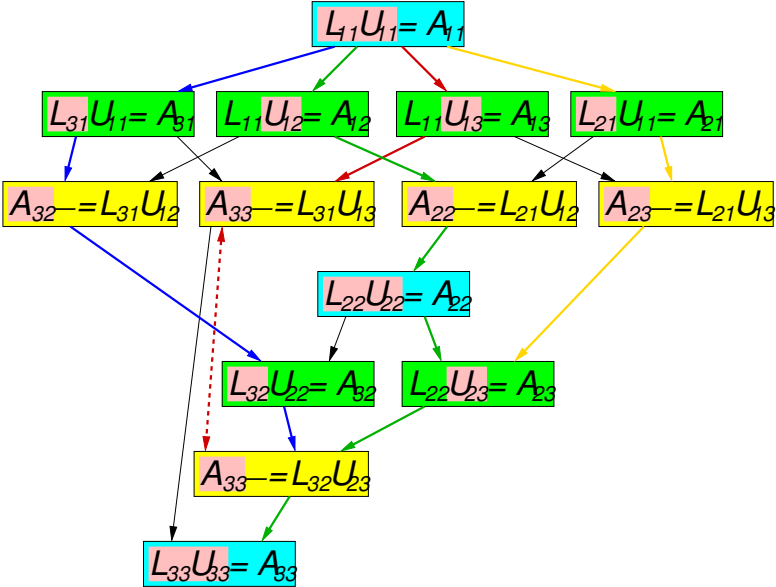
2D Block Cyclic Decomposition

A_{11}	A_{12}	A_{13}	A_{14}	A_{15}	A_{16}	A_{17}	A_{18}
A_{21}	A_{22}	A_{23}	A_{24}	A_{25}	A_{26}	A_{27}	A_{28}
A_{31}	A_{32}	A_{33}	A_{34}	A_{35}	A_{36}	A_{37}	A_{38}
A_{41}	A_{42}	A_{43}	A_{44}	A_{45}	A_{46}	A_{47}	A_{48}
A_{51}	A_{52}	A_{53}	A_{54}	A_{55}	A_{56}	A_{57}	A_{58}
A_{61}	A_{62}	A_{63}	A_{64}	A_{65}	A_{66}	A_{67}	A_{68}
A_{71}	A_{72}	A_{73}	A_{74}	A_{75}	A_{76}	A_{77}	A_{78}
A_{81}	A_{82}	A_{83}	A_{84}	A_{85}	A_{86}	A_{87}	A_{88}

	0	1	2					
	A_{11}	A_{14}	A_{17}	A_{12}	A_{15}	A_{18}	A_{13}	A_{16}
0	A_{31}	A_{34}	A_{37}	A_{32}	A_{35}	A_{38}	A_{33}	A_{36}
	A_{51}	A_{54}	A_{57}	A_{52}	A_{55}	A_{58}	A_{53}	A_{56}
	A_{71}	A_{74}	A_{77}	A_{72}	A_{75}	A_{78}	A_{73}	A_{76}
	A_{21}	A_{24}	A_{27}	A_{22}	A_{25}	A_{28}	A_{23}	A_{26}
1	A_{41}	A_{44}	A_{47}	A_{42}	A_{45}	A_{48}	A_{43}	A_{46}
	A_{61}	A_{64}	A_{67}	A_{62}	A_{65}	A_{68}	A_{63}	A_{66}
	A_{81}	A_{84}	A_{87}	A_{82}	A_{85}	A_{88}	A_{83}	A_{86}

(source: ScaLAPACK)

Graph-Oriented Parallelisation



Current Library Projects

PLASMA (<http://www.netlib.org/plasma/>):

- new library project to replace ScaLAPACK
- block-oriented algorithms for dense linear algebra
- DAG-based scheduling of operations
- MAGMA: version for GPUs

FLAME (<http://z.cs.utexas.edu/wiki/flame.wiki/>):

- “formal linear algebra methods environment”
- block-oriented algorithms for dense linear algebra
- based on block-oriented notation of algorithms; concept to transfer notation into program code

Current Library Projects (2)

SMP superscalar

(http://www.bsc.es/plantillaG.php?cat_id=385):

- pragma-based programming model (similar to OpenMP)
- input/output qualifiers to declare data dependencies
- scheduling of operations according to DAG