Partitioning for applications

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CERFACS Seminar Toulouse, July 13, 2010

Mesh partitioning

- Laplacian operator
- Bulk synchronous parallel communication cost
- Diamond-shaped subdomains
- 3D partitioning

Matrix partitioning

- Parallel sparse matrix–vector multiplication (SpMV)
- Visualisation by MondriaanMovie
- Hypergraphs
- Ordering matrices for faster SpMV
- Separated Block Diagonal structure

Where meshes meet matrices

Conclusions and future work

Motivation: CFD and other applications

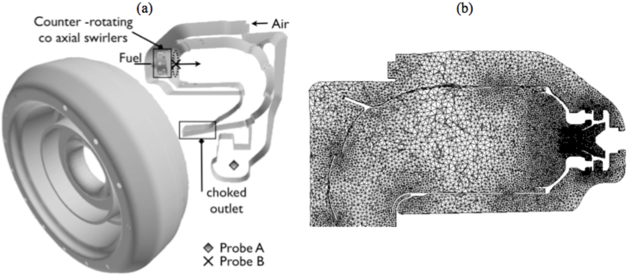
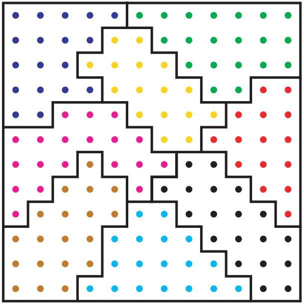


Fig. 7 Full annular aeronautical burner computed with AVBP (LES) for a thermo-acoustic analysis of the burner: (a) computational domain and (b) typical mesh resolution in the injector region.

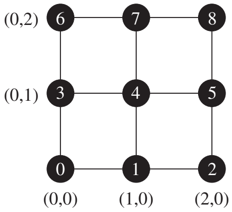
- Source: N. Gourdain et al. 'High performance Parallel Computing of Flows in Complex Geometries. Part 2: Applications' *Computational Science and Discovery* 2009.

2D rectangular mesh partitioned over 8 processors



- In many applications, a physical domain can be partitioned naturally by assigning a contiguous subdomain to every processor.
- Communication is only needed for exchanging information across the subdomain boundaries.
- Grid points interact only with a set of immediate neighbours, to the north, east, south, and west.

2D Laplacian operator for $k \times k$ grid



Compute

$$\Delta_{i,j} = x_{i-1,j} + x_{i+1,j} + x_{i,j+1} + x_{i,j-1} - 4x_{i,j}, \quad \text{for } 0 \le i,j < k,$$

where $x_{i,j}$ denotes e.g. the temperature at grid point (i,j).
By convention, $x_{i,j} = 0$ outside the grid.

- $x_{i+1,j} - x_{i,j}$ approximates the derivative of the temperature in the i-direction.
- $(x_{i+1,j} - x_{i,j}) - (x_{i,j} - x_{i-1,j}) = x_{i-1,j} + x_{i+1,j} - 2x_{i,j}$ approximates the second derivative.

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Relation operator–matrix

$$A = \begin{bmatrix} -4 & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & -4 & 1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & -4 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & -4 & 1 & \cdot & 1 & \cdot & \cdot \\ \cdot & 1 & \cdot & 1 & -4 & 1 & \cdot & 1 & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & -4 & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & -4 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 1 & -4 & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 1 & -4 \end{bmatrix}$$

$\mathbf{u} = A\mathbf{v} \Longleftrightarrow$

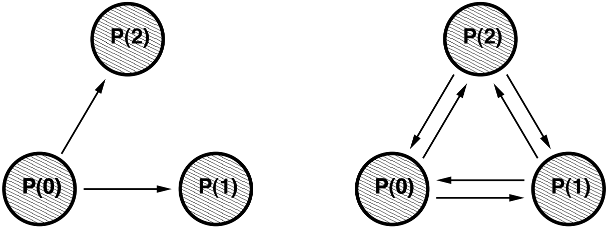
$$\Delta_{i,j} = x_{i-1,j} + x_{i+1,j} + x_{i,j+1} + x_{i,j-1} - 4x_{i,j}, \quad \text{for } 0 \leq i,j < k.$$

Finding a mesh partitioning

- We must assign each grid point to a processor.
- We assign the values $x_{i,j}$ and $\Delta_{i,j}$ to the owner of grid point (i, j).
- Each point of the grid has an amount of computation associated with it determined by the operator.
- Here, an interior point has 5 flops; a border point 4 flops; a corner point 3 flops.

Our parallel cost model: BSP

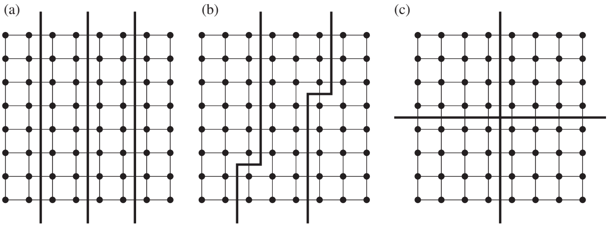
2-relations:



(a) (b)

- Bulk synchronous parallel (BSP) model by Valiant (1990): a bridging model for parallel computing
- An *h*-relation is a communication phase (superstep) in which every processor sends and receives at most h data words: $h = \max\{h_{\text{send}}, h_{\text{recv}}\}$
- $T(h) = hg + l$, where g is the time per data word and l the global synchronisation time

Partition into strips and blocks



- (a) Partition into strips: long Norwegian borders,

$$T_{\text{comm, strips}} = 2kg.$$

- (b) Boundary corrections improve load balance.
- (c) Partition into square blocks: shorter borders,

$$T_{\text{comm, squares}} = \frac{4k}{\sqrt{p}} g \qquad (\text{for } p > 4).$$

Surface-to-volume ratio

- The communication-to-computation ratio for square blocks is
$$\frac{T_{\text{comm, squares}}}{T_{\text{comp, squares}}} = \frac{4k/\sqrt{p}}{5k^2/p} g = \frac{4\sqrt{p}}{5k} g.$$
- This ratio is often called the surface-to-volume ratio, because in 3D the surface of a domain represents the communication with other processors and the volume represents the amount of computation of a processor.

What do we do at scientific workshops?

Participants of HLPP 2001, International Workshop on High-Level Parallel Programming, Orléans, France, June 2001, studying Château de Blois.

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The high-level object of our study

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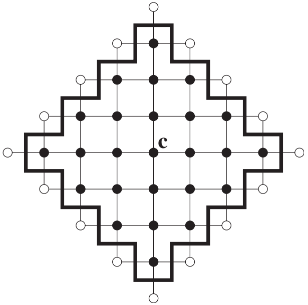
Blocks are nice, but diamonds . . .



$r = 3$

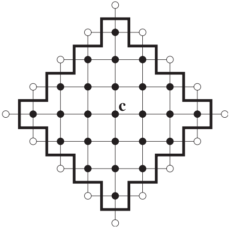
- Digital diamond, or closed l_1-sphere, defined by

$$B_r(c_0, c_1) = \{(i,j) \in \mathbf{Z}^2 : \ |i - c_0| + |j - c_1| \leq r\},$$

for integer radius $r \geq 0$ and centre $\mathbf{c} = (c_0, c_1) \in \mathbf{Z}^2$.

- $B_r(\mathbf{c})$ is the set of points with Manhattan distance $\leq r$ to the central point $\mathbf{c}$.

Points of a diamond



$r = 3$

- The number of points of $B_r(\mathbf{c})$ is

$$\begin{aligned} & 1+3+5+\cdots+(2r-1)+(2r+1)+(2r-1)+\cdots+1 \\ = \; & 2r^2+2r+1. \end{aligned}$$

- The number of neighbouring points is $4r+4$.
- This is also the number of ghost cells needed in a parallel grid computation.

Diamonds are forever

- For a $k \times k$ grid and p processors, we have

$$k^2 = p(2r^2 + 2r + 1) \approx 2pr^2.$$

- Just on the basis of $4r + 4$ receives from neighbour points, we have

$$\frac{T_{\text{comm, diamonds}}}{T_{\text{comp, diamonds}}} = \frac{4r+4}{5(2r^2+2r+1)} g \approx \frac{2}{5r} g \approx \frac{2\sqrt{2p}}{5k} g.$$

- Compare with value $\frac{4\sqrt{p}}{5k} g$ for square blocks: factor $\sqrt{2}$ less.
- This gain was caused by reuse of data: the value at a grid point is used twice but sent only once.
- Also $\sqrt{2}$ less memory for ghost cells.

Alhambra: tile the whole space

(2001)

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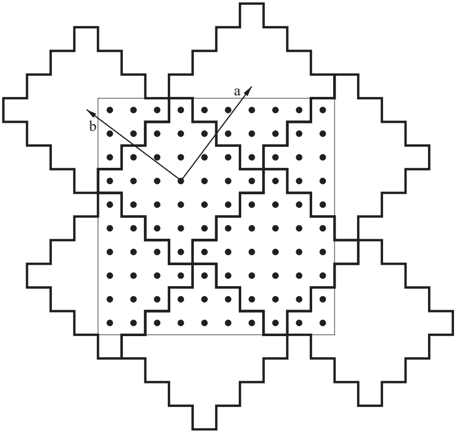
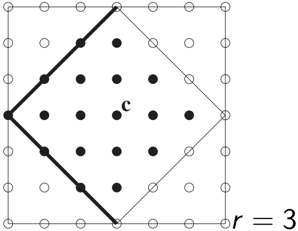
Tile the whole sky with diamonds



$r = 3$

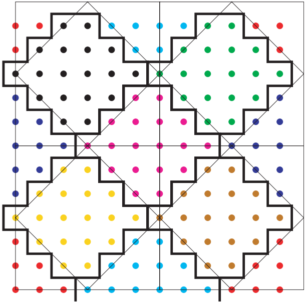
Diamond centres at $\mathbf{c} = \lambda\mathbf{a} + \mu\mathbf{b}$, $\lambda, \mu \in \mathbf{Z}$,
where $\mathbf{a} = (r, r+1)$ and $\mathbf{b} = (-r-1, r)$.
Good method for an infinite grid.

Practical method for finite grids



- Discard one layer of points from the north-eastern and south-eastern border of the diamond.
- For $r = 3$, the number of points decreases from 25 to 18.

12×12 computational grid: periodic partitioning



8 processors

- Total computation: 672 flops. Avg 84. Max 90.
- Communication: 104 values. Avg 13. Max 14.
- Total time: $90 + 14g = 90 + 14 \cdot 10 = 230$ (ignoring $2l$).
- 8 rectangular blocks of size 6×3 blocks: time is $87 + 15 \cdot 10 = 237$.

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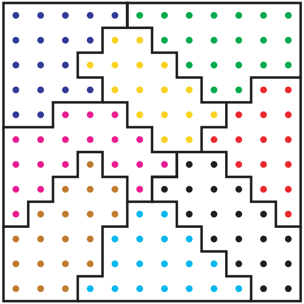
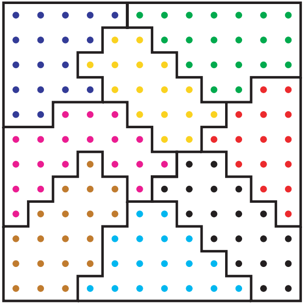
12×12 computational grid: Mondriaan partitioning



8 processors

- Partitioning obtained by translating into a sparse matrix. This treats the structured grid as unstructured.
- Total computation: 672 flops. Avg 84. Max 91. (allowed imbalance $\epsilon = 10\%$.)
- Communication: 85 values. Avg 10.525. Max 16.
- Total time: $91 + 16g = 91 + 16 \cdot 10 = 251$.

12 × 12 computational grid: challenge



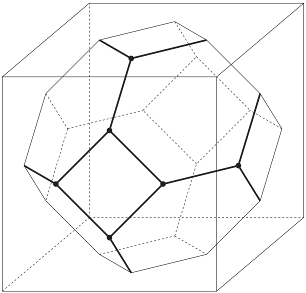
8 processors

- Find a better solution than can be obtained manually, using ideas from both solutions shown. Current best known solution is 199 (Bas den Heijer 2006).

Three dimensions

- If a processor has a cubic block of $N = k^3/p$ points, about $\frac{6k^2}{p^{2/3}} = 6N^{2/3}$ are boundary points. In 2D, only $4N^{1/2}$.
- If a processor has a $10 \times 10 \times 10$ block, 488 points are on the boundary. About half!
- Thus, communication is important in 3D.
- Based on the surface-to-volume ratio of a 3D digital diamond, we can aim for a reduction by a factor $\sqrt{3} \approx 1.73$ in communication cost.
- The prime application of diamond-shaped distributions will most likely be in 3D.

Basic cell for 3D



- Basic cell: grid points in a truncated octahedron.
- For load balancing, take care with the boundaries.
- What You See, Is What You Get (WYSIWYG):
  4 hexagons and 3 squares visible at the front are included.
  Also 12 edges, 6 vertices.
- Gain factor of 1.68 achieved for $p = 2q^3$.

Comparing partitioning methods in 2D and 3D

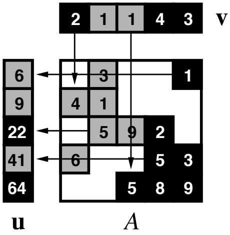
Grid	p	Rectangular	Mondriaan	Diamond
1024×1024	2	1024	1024	2046
	4	1024	1240	2048
	8	1280	1378	1026
	16	1024	1044	1024
	32	768	766	514
	64	512	548	512
	128	384	395	258
$64 \times 64 \times 64$	16	4096	2836	2402
	128	1024	829	626

Communication cost (in g) for a Laplacian operation on a grid.
Mondriaan with $\epsilon = 10\%$.

Parallel sparse matrix–vector multiplication $\mathbf{u} := A\mathbf{v}$

A sparse $m \times n$ matrix, $\mathbf{u}$ dense m-vector, $\mathbf{v}$ dense n-vector

$$u_i := \sum_{j=0}^{n-1} a_{ij} v_j$$

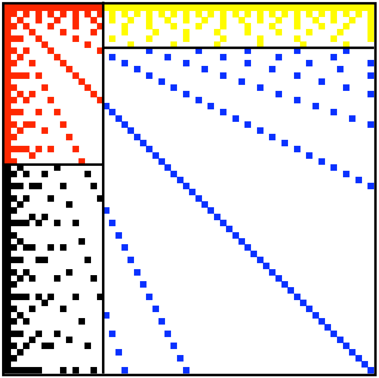


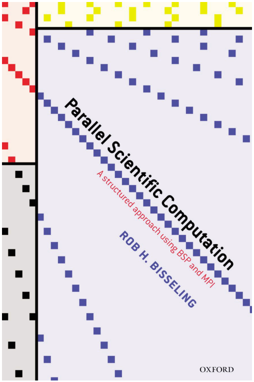
$p = 2$

4 supersteps: communicate, compute, communicate, compute

Divide evenly over 4 processors

Matrix prime60





- Mondriaan block partitioning of 60×60 matrix `prime60` with 462 nonzeros, for $p = 4$
- $a_{ij} \neq 0 \iff i|j \text{ or } j|i \qquad (1 \leq i, j \leq 60)$

Avoid communication completely, if you can

All nonzeros in a row or column have the same colour.

Permute the matrix rows/columns

First the green rows/columns, then the blue ones.

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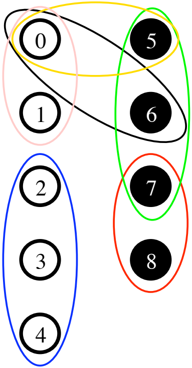
Combinatorial problem: sparse matrix partitioning

Problem: Split the set of nonzeros A of the matrix into p subsets, $A_0, A_1, \ldots, A_{p-1}$, minimising the communication volume $V(A_0, A_1, \ldots, A_{p-1})$ under the load imbalance constraint

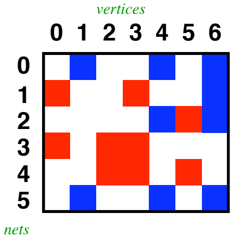
$$nz(A_i) \leq \frac{nz(A)}{p}(1+\epsilon), \quad 0 \leq i < p.$$

The hypergraph connection



Hypergraph with 9 vertices and 6 hyperedges (nets), partitioned over 2 processors, black and white

1D matrix partitioning using hypergraphs



- Hypergraph $\mathcal{H} = (\mathcal{V}, \mathcal{N}) \Rightarrow$ exact communication volume in sparse matrix–vector multiplication.
- Columns $\equiv$ Vertices: $0, 1, 2, 3, 4, 5, 6$.
  Rows $\equiv$ Hyperedges (nets, subsets of $\mathcal{V}$):

$$n_0 = \{1,4,6\}, \quad n_1 = \{0,3,6\}, \quad n_2 = \{4,5,6\},$$
$$n_3 = \{0,2,3\}, \quad n_4 = \{2,3,5\}, \quad n_5 = \{1,4,6\}.$$

$(\lambda - 1)$-metric for hypergraph partitioning

- 138×138 symmetric matrix `bcsstk22`, $nz = 696$, $p = 8$
- Reordered to Bordered Block Diagonal (BBD) form
- Split of row i over λ_i processors causes a communication volume of $\lambda_i - 1$ data words

Cut-net metric for hypergraph partitioning

- Row split has unit cost, irrespective of λ_i

Mondriaan 2D matrix partitioning

- $p = 4$, $\epsilon = 0.2$, global non-permuted view

Fine-grain 2D matrix partitioning

- Each individual nonzero is a vertex in the hypergraph
Çatalyürek and Aykanat, 2001.

Mondriaan 2.0, Released July 14, 2008

- New algorithms for vector partitioning.
- Much faster, by a factor of 10 compared to version 1.0.
- 10% better quality of the matrix partitioning.
- Inclusion of fine-grain partitioning method
- Inclusion of hybrid between original Mondriaan and fine-grain methods.
- Can also handle $p \neq 2^q$.

Matrix lns3937 (Navier–Stokes, fluid flow)

Splitting the 3937×3937 sparse matrix lns3937 into 5 parts.

Recursive, adaptive bipartitioning algorithm

$\textsf{MatrixPartition}(A, p, \epsilon)$

input: p = number of processors, $p = 2^q$

ϵ = allowed load imbalance, $\epsilon > 0$.

output: p-way partitioning of A with imbalance $\le \epsilon$.

if $p > 1$ **then**

$q := \log_2 p$;

$(A_0^{\rm r}, A_1^{\rm r}) := h(A, {\rm row}, \epsilon/q)$; hypergraph splitting

$(A_0^{\rm c}, A_1^{\rm c}) := h(A, {\rm col}, \epsilon/q)$;

$(A_0^{\rm f}, A_1^{\rm f}) := h(A, {\rm fine}, \epsilon/q)$;

$(A_0, A_1) :=$ best of $(A_0^{\rm r}, A_1^{\rm r})$, $(A_0^{\rm c}, A_1^{\rm c})$, $(A_0^{\rm f}, A_1^{\rm f})$;

$maxnz := \frac{nz(A)}{p}(1+\epsilon)$;

$\epsilon_0 := \frac{maxnz}{nz(A_0)} \cdot \frac{p}{2} - 1$; $\textsf{MatrixPartition}(A_0, p/2, \epsilon_0)$;

$\epsilon_1 := \frac{maxnz}{nz(A_1)} \cdot \frac{p}{2} - 1$; $\textsf{MatrixPartition}(A_1, p/2, \epsilon_1)$;

else output A;

Mondriaan version 1 vs. 3 (Preliminary)

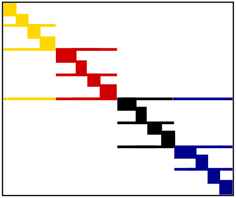
Name	p	v1.0	v3.0
`dfl001`	4	1484	1404
	16	3713	3631
	64	6224	6071
`cre_b`	4	1872	1437
	16	4698	4144
	64	9214	9011
`tbdmatlab`	4	10857	10041
	16	28041	25117
	64	52467	50116
`nug30`	4	55924	47984
	16	126255	110433
	64	212303	194083
`tbdlinux`	4	30667	29764
	16	73240	68132
	64	146771	139720

Mondriaan split strategy: v1 localbest, v3 hybrid, $\epsilon = 0.03$.

Mondriaan 3.0 coming soon

- Ordering of matrices to SBD and BBD structure: cut rows are placed in the middle, and at the end, respectively.
- Visualisation through Matlab interface, MondriaanPlot, and MondriaanMovie
- Library-callable, so you can link it to your own program
- Hypergraph metrics: $\lambda - 1$ for parallelism, and cut-net for other applications
- Interface to PaToH hypergraph partitioner

Separated block-diagonal (SBD) structure

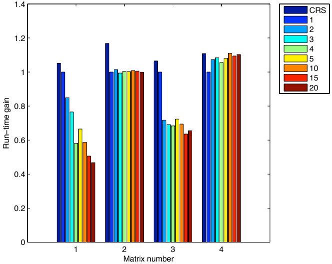


- SBD structure is obtained by recursively partitioning the columns of a sparse matrix, each time moving the cut (mixed) rows to the middle. Columns are permuted accordingly.
- The cut rows are sparse and serve as a gentle cache transition between accesses to two different vector parts.
- Mondriaan is used in one-dimensional mode, splitting only in the column direction.

Partition the columns till the end, $p = n = 59$

- The recursive, fractal-like nature makes the ordering method work, irrespective of the actual cache characteristics (e.g. sizes of L1, L2, L3 cache).
- The ordering is cache-oblivious.

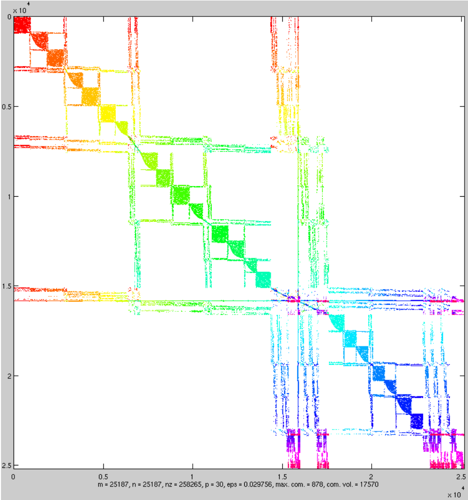
Wall clock timings of SpMV on Huygens



Splitting into 1–20 parts

- Experiments on 1 core of the dual-core 4.7 GHz Power6+ processor of the Dutch national supercomputer Huygens.
- 64 kB L1 cache, 4 MB L2, 32 MB L3.
- Test matrices: 1. `stanford`; 2. `stanford_berkeley`; 3. `wikipedia-20051105`; 4. `cage14`

Screenshot of Matlab interface



- Matrix `rhpentium`, split over 30 processors

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Where meshes meet matrices

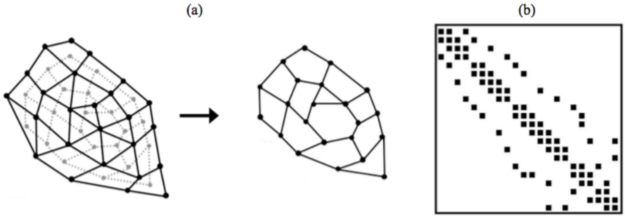


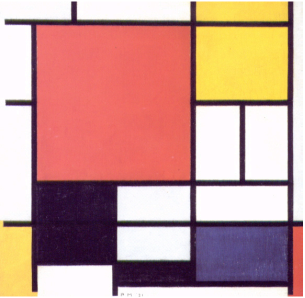
Fig. 8 Example of an unstructured grid with its associated dual graph and partitioning process (a) and the related sparse matrix (b).

- Unstructured grid and its sparse matrix
- Source: N. Gourdain et al. 'High performance Parallel Computing of Flows in Complex Geometries. Part 1: Methods' *Computational Science and Discovery* 2009.

Apply Mondriaan matrix partitioning

- Use Mondriaan in 1D mode, not in full 2D mode.
- Advantage: no need to change data structure, while still giving almost the same communication volume (for FEM matrices).
- Advantage: hypergraph partitioning leads to less ghost cells, and less communication, especially in 3D.

Apply Mondriaan matrix partitioning



- Advantage: Mondriaan is open-source, can be changed by yourself or by us for your needs, and is an ongoing research project with much attention for software engineering.
- Disadvantage: hypergraph partioner Mondriaan itself takes more time and memory than graph partitioners (such as Scotch or Metis).

Conclusions on regular meshes

- To achieve a good partitioning with a low surface-to-volume ratio, all dimensions must be cut. For regular grids in 2D, this gives square subdomains; in 3D, cubic.
- In 2D, an even better method is to use digital diamonds. This basic cell tiles a rectangular domain in a straightforward manner. Best performance is obtained for $p = 2q^2$.
- In 3D, the best method is to use truncated octahedra with WYSIWYG tie breaking at the boundaries. Best performance is obtained for $p = 2q^3$.

Conclusions on irregular meshes

- For unstructured grids, the same gains can be obtained by using hypergraph partitioning, which minimises the exact amount of communication and number of ghost cells.
- Using graph partitioning and the edge-cut metric will lead to $\sqrt{3}$ more communication and ghost memory usage.

Current/future work

- Mondriaan 3.0, to be released soon, contains improved methods for sparse matrix partitioning, which can also be used to partition meshes.
- We are working on a converter for reading meshes directly, translating them to matrices, partitioning them, and writing the result back as a mesh.
- We hope to be able to build a Mondriaan hypergraph partitioning option into AVBP.