Partitioning for applications

Rob H. Bisseling, Albert-Jan Yzelman, Bas Fagginger Auer

Mathematical Institute, Utrecht University
Rob Bisseling: also joint Laboratory CERFACS/INRIA, Toulouse, May–July 2010

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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.

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

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

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**.
Relation operator–matrix

\[
A = \begin{bmatrix}
-4 & 1 & 1 & . & . & . & . & . & . \\
1 & -4 & 1 & 1 & . & . & . & . & . \\
. & 1 & -4 & . & 1 & . & . & . & . \\
1 & . & . & -4 & 1 & 1 & . & . & . \\
. & 1 & . & 1 & -4 & 1 & 1 & . & . \\
. & . & 1 & . & 1 & -4 & . & 1 & . \\
. & . & . & 1 & . & . & -4 & 1 & . \\
. & . & . & . & 1 & 1 & -4 & 1 & . \\
. & . & . & . & . & 1 & 1 & . & -4 \\
\end{bmatrix}
\]

\[
u = A v \iff \Delta_{i,j} = x_{i-1,j} + x_{i+1,j} + x_{i,j+1} + x_{i,j-1} - 4x_{i,j}, \text{ for } 0 \leq i, j < k.
\]
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:

- 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,
  \[ T_{\text{comm}, \text{strips}} = 2kg. \]

- (b) Boundary corrections improve load balance.
- (c) Partition into square blocks: shorter borders,
  \[ T_{\text{comm}, \text{squares}} = \frac{4k}{\sqrt{p}} g \quad (\text{for } p > 4). \]
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?

The high-level object of our study
Blocks are nice, but diamonds . . .

Digital diamond, or closed \( l_1 \)-sphere, defined by

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

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

\( B_r(c) \) is the set of points with Manhattan distance \( \leq r \) to the central point \( c \).
Points of a diamond

- The number of points of $B_r(c)$ is
  
  $$1 + 3 + 5 + \cdots + (2r - 1) + (2r + 1) + (2r - 1) + \cdots + 1 = 2r^2 + 2r + 1.$$

- 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
Tile the whole sky with diamonds

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

- Total computation: 672 flops. Avg 84. Max 90.
- Total time: \( 90 + 14g = 90 + 14 \cdot 10 = 230 \) (ignoring \( 2l \)).
- 8 rectangular blocks of size 6 × 3 blocks: time is \( 87 + 15 \cdot 10 = 237 \).
 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 $\epsilon = 10\%$.)
- Total time: $91 + 16g = 91 + 16 \cdot 10 = 251$.  

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

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Communication cost (in g) for a Laplacian operation on a grid. Mondriaan with $\epsilon = 10\%$. 
Parallel sparse matrix–vector multiplication $\mathbf{u} := \mathbf{A}\mathbf{v}$

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

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

4 supersteps: communicate, compute, communicate, compute
Divide evenly over 4 processors
Mondriaan block partitioning of $60 \times 60$ matrix $\text{prime60}$ with 462 nonzeros, for $p = 4$

- $a_{ij} \neq 0 \iff i|j$ or $j|i$ \hspace{1cm} (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.
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 $\mathcal{H} = (\mathcal{V}, \mathcal{N})$ ⇒ exact communication volume in sparse matrix–vector multiplication.

- Columns ≡ Vertices: 0, 1, 2, 3, 4, 5, 6.
  Rows ≡ 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 \(\times\) 138 symmetric matrix bcsstk22, \(nz = 696\), \(p = 8\)
- Reordered to Bordered Block Diagonal (BBD) form
- Split of row \(i\) over \(\lambda_i\) processors causes a communication volume of \(\lambda_i - 1\) data words
Row split has \textbf{unit cost}, irrespective of $\lambda_i$
Mondriaan 2D matrix partitioning

- $p = 4$, $\epsilon = 0.2$, global non-permuted view
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 $p \neq 2^q$. 
Splitting the $3937 \times 3937$ sparse matrix $\text{lns3937}$ into 5 parts.
Recursive, adaptive bipartitioning algorithm

MatrixPartition\((A, p, \epsilon)\)

*input:* \(p = \text{number of processors}, \ p = 2^q\)
\(\epsilon = \text{allowed load imbalance, } \epsilon > 0.\)

*output:* \(p\)-way partitioning of \(A\) with imbalance \(\leq \epsilon\).

if \(p > 1\) then

\[ q := \log_2 p; \]
\[ (A_0^r, A_1^r) := h(A, \text{row, } \epsilon/q); \text{ hypergraph splitting} \]
\[ (A_0^c, A_1^c) := h(A, \text{col, } \epsilon/q); \]
\[ (A_0^f, A_1^f) := h(A, \text{fine, } \epsilon/q); \]
\[ (A_0, A_1) := \text{best of } (A_0^r, A_1^r), (A_0^c, A_1^c), (A_0^f, A_1^f); \]

\[ \maxnz := \frac{\text{nz}(A)}{p} (1 + \epsilon); \]
\[ \epsilon_0 := \frac{\maxnz}{\text{nz}(A_0)} \cdot \frac{p}{2} - 1; \text{ MatrixPartition}(A_0, p/2, \epsilon_0); \]
\[ \epsilon_1 := \frac{\maxnz}{\text{nz}(A_1)} \cdot \frac{p}{2} - 1; \text{ MatrixPartition}(A_1, p/2, \epsilon_1); \]

else output \(A\);
### Mondriaan version 1 vs. 3 (Preliminary)

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</table>

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
Matrix rhpentium, split over 30 processors
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
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.
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.