Parallel sparse matrix vector multiplications and models for efficient parallelization

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Outline

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- Row parallel
- Column parallel
- Row-column parallel

Bypergraphs and hypergraph partitioning

- Hypergraph models for row-parallel SpMxV
- Hypergraph models for column-parallel SpMxV
- Hypergraph models for row-column-parallel SpMxV
- Some other partitioning problems

4 Summary and concluding remarks

Sparse matrices

A sparse matrix is a matrix with a lot of zero entries.

More importantly: all or some zeros are not stored.

$$\mathbf{A} = \begin{bmatrix} 1.1 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.2 & 0.0 & 2.4 & 0.0 \\ 3.1 & 0.0 & 3.3 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 4.4 & 0.0 \\ 0.0 & 5.2 & 0.0 & 5.4 & 5.5 \end{bmatrix}$$

Sparse matrices are abound in scientific computing: \blacktriangleright large scale optimization, \blacktriangleright chemical process simulation, \blacktriangleright computational fluid dynamics, \blacktriangleright numerical solution of partial differential equations, \blacktriangleright web information retrieval (e.g., Google's page rank),...

Sparse matrices: Coordinate format

There are many ways to store a sparse matrix.

We will look at three standard representations which store only the nonzero entries.

1.1	0.0	0.0	0.0	0.0]	
0.0	2.2	0.0	2.4	0.0	
3.1	0.0	3.3	0.0	0.0	
0.0	0.0	0.0	4.4	0.0	
0.0	5.2	0.0	5.4	5.5	

Со	Coordinate (Triplet) format														
Τw doι	Two integer arrays (irn, jcn) and a double array A:														
irn	=	[1	2	2	3	3	4	5	5	5]			
jcn	jcn = [1 2 4 1 3 4 2 4 5]														
A	=	[1	.1	2.2	2.4	3.1	3.3	4.4	5.2	5.4	5.5	1			

The kth entry a_{ij} is stored as irn[k] = i, jcn[k] = j, $a[k] = a_{ij}$.

Let τ denote the number of nonzeros, then the storage is 2τ integer and τ double (or single or complex). In general, $\tau = O(m + n)$.

Sparse matrices: Compressed row storage

There are many ways to store a sparse matrix.

We will look at three standard representations which store only the nonzero entries.

1.1	0.0	0.0	0.0	0.0
0.0	2.2	0.0	2.4	0.0
3.1	0.0	3.3	0.0	0.0
0.0	0.0	0.0	4.4	0.0
0.0	5.2	0.0	5.4	5.5

Co	m	pre	ss	sed	row	sto	rage	e				
Tw doi	o ub	int le	te ar	ger ray	arra A:	iys ((ia,	jcn)	an	d a		
ia	=	[1	2		4		6	7		10]
jcn	=	[1	2	4	1	3	4	2	4	5]	
A	=	[1	. 1	2.2	2.4	3.1	3.3	4.4	5.2	5.4	5.5]	

The nonzeros of the *i*th row are stored at the ia[i]... ia[i+1]-1 positions of jcn and A.

For example the 3rd row: starts at ia[3] = 4 and finishes at ia[3+1]-1=5. The column indices are therefore jcn[4,5]=1.3 and values are A[4,5]=3.1.3.3.

Sparse matrices: Compressed row storage

There are many ways to store a sparse matrix.

We will look at three standard representations which store only the nonzero entries.

1.1	0.0	0.0	0.0	0.0	1
0.0	2.2	0.0	2.4	0.0	
3.1	0.0	3.3	0.0	0.0	
0.0	0.0	0.0	4.4	0.0	
0.0	5.2	0.0	5.4	5.5	

Co	Compressed row format														
Τw doι	Two integer arrays (ia, jcn) and a double array A:														
ia	=	[1	2		4		6	7		1	10	נ		
jcn	=	[1	2	4	1	3	4	2	4	5]			
A	=	[1	. 1	2.2	2.4	3.1	3.3	4.4	5.2	5.4	5.5]			

The nonzeros of the *i*th row are stored at the ia[i]...ia[i+1]-1 positions of jcn and A.

Let matrix be of size $m \times n$, and τ be the number of nonzeros, then the storage is $m + 1 + \tau$ integer and τ double (or single or complex).

Sparse matrices: Compressed column storage

There are many ways to store a sparse matrix.

We will look at three standard representations which store only the nonzero entries.

1.1	0.0	0.0	0.0	0.0
0.0	2.2	0.0	2.4	0.0
3.1	0.0	3.3	0.0	0.0
0.0	0.0	0.0	4.4	0.0
0.0	5.2	0.0	5.4	5.5

Со	Compressed column storage													
Τw doι	Two integer arrays (irn, ja) and a double array A:													
ja	=	C	1		3		5	6			9		10]
irn	=	[1	3	2	5	3	2	4	5	5]		
A	=	[1	. 1	3.1	2.2	5.2	3.3	2.4	4.4	5.4	5.5]		

The nonzeros of the *j*th column are stored at the ja[j]...ja[j+1]-1 positions of irn and A.

For example the 2nd col: starts at ja[2] = 3 and finishes at ja[2+1]-1=4. The row indices are therefore im[3,4]=2.5 and values are A[3,4]=2.25.2.

Sparse matrices: Compressed column storage

There are many ways to store a sparse matrix.

We will look at three standard representations which store only the nonzero entries.

1.1	0.0	0.0	0.0	0.0	
0.0	2.2	0.0	2.4	0.0	
3.1	0.0	3.3	0.0	0.0	
0.0	0.0	0.0	4.4	0.0	
0.0	5.2	0.0	5.4	5.5	

Coi	Compressed column format														
Τw doι	Two integer arrays (irn, ja) and a double array A:														
ja	=	[1		3		5	6			9		10]	
irn	=	[1	3	2	5	3	2	4	5	5]			
A	=	[1.	. 1	3.1	2.2	5.2	3.3	2.4	4.4	5.4	5.5]			

The nonzeros of the *j*th column are stored at the ja[j]... ja[j+1]-1 positions of irn and A.

Let matrix be of size $m \times n$, and τ be the number of nonzeros, then the storage is $n + 1 + \tau$ integer and τ double (or single or complex).

Reminder: Dense matrix vector multiplication

Need to compute $y \leftarrow Ax$ for an $m \times n$ dense B matrix A and suitable dense vectors y and x.

Row major order

for
$$i = 1$$
 to m do
 $y[i] \leftarrow 0.0$
for $j = 1$ to n do
 $y[i] \leftarrow y[i] + A[i,j] * x[j]$

Column-major order

for i = 1 to m do $y[i] \leftarrow 0.0$ for j = 1 to n do for i = 1 to m do $y[i] \leftarrow y[i] + A[i, j] * x[j]$

Sparse matrices: Sparse matrix vector multiplies

Need to compute $y \leftarrow Ax$ for an $m \times n$ sparse matrix A and suitable dense vectors y and x.

Coordinate format with τ nonzeros (irn, jcn, A) for i = 1 to m do $y[i] \leftarrow 0.0$ for k = 1 to τ do $y[irn[k]] \leftarrow y[irn[k]] + A[k] * x[jcn[k]]$

Sparse matrices: Sparse matrix vector multiplies

Need to compute $y \leftarrow Ax$ for an $m \times n$ sparse matrix A and suitable dense vectors y and x.

Compressed row storage	Compressed column storage
(ia, jcn, A)	(ja, irn, A)
for $i = 1$ to m do $val \leftarrow 0.0$ for $k = ia[i]$ to $ia[i + 1] - 1$ do $val \leftarrow val + A[k] * x[jcn[k]]$ $y[i] \leftarrow val$	for $i = 1$ to m do $y[i] \leftarrow 0.0$ for $j = 1$ to n do $xval \leftarrow x[j]$ for $k = ja[j]$ to $ja[j+1] - 1$ do $y[irn[k]] \leftarrow y[irn[k]] + A[k] * xval$

- Characterizes a wide range of applications with irregular computational dependency.
 - reduction operation from inputs (here entries of *x*) to outputs (here entries of *y*)
- A fine grain computation: each nnz is read/operated on once. Guaranteeing efficiency will guarantee efficiency in applications with a coarser grain computation.

Sparse matrices: Sparse matrix vector multiplies

SpMxV's of the form $y \leftarrow Ax$ are the computational kernel of many scientific computations

- Solvers for linear systems, linear programs, eigensystems, least squares problems,
- Repeated SpMxV with the same large sparse matrix A,
- The matrix A can be symmetric, unsymmetric, rectangular,
- Sometimes multiplies are of the form y ← ADA^Tz with a diagonal
 D (in interior point methods for linear programs).
 - computation proceeds (why?) as $w \leftarrow \mathbf{A}^T z$, then $x \leftarrow \mathbf{D} w$, then $y \leftarrow \mathbf{A} x$
- Sometimes we have multiplies with A and A^T independent; y ← Ax and w ← A^Tz (QMR, CGNE, and CGNR methods with square unsymmetric A; rectangular A in Lanczos method).
- Most of the time the SpMxV's are of the form y ← AM⁻¹x (called preconditioning).

Iterative solvers: How do they look?

Basic form

while not converged do computations check convergence

Computations are of the form:

Linear vector operations

 $x \leftarrow x + \alpha y$ $\blacktriangleright x_i = x_i + \alpha y_i$

Inner products

 $\alpha \leftarrow (\mathbf{x}, \mathbf{y}) \qquad \blacktriangleright \alpha = \sum \mathbf{x}_i \mathbf{y}_i$

• Sparse matrix vector multiplies $y \leftarrow \mathbf{A} \underline{x}$

$$y \leftarrow \mathbf{A}^T x$$

The Conjugate Gradient method

Compute $r_0 := b - Ax_0, p_0 := r_0$. For j = 0, 1, ..., until convergence $\alpha_j := (r_j, r_j)/(Ap_j, p_j)$ $x_{j+1} := x_j + \alpha_j p_j$ $r_{j+1} := r_j - \alpha_j Ap_j$ $\beta_j := (r_{j+1}, r_{j+1})/(r_j, r_j)$ $p_{j+1} := r_{j+1} + \beta_j p_j$ EndDo

With certain types of preconditioners, we have SpMxV with another matrix **M** and/or \mathbf{M}^{T} . Replace $\mathbf{A}_{p_{j}}$ with $\mathbf{AM}_{p_{j}}$.

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4 Summary and concluding remarks

We restrict ourselves to the distributed memory setting.

- nonzeros in A are distributed,
- the input vector entries, x_js, are distributed,
- the ouput vector entries, *y_i*s, are distributed (that is, the responsibility of storing them is decided).

What are the aims of a distribution?

- load balance among processors: equal number of a_{ij} per processor,
- reduced communication requirement:
 - a_{ij} is to be multiplied by x_j ; these two should meet at a processors;
 - the scalar product $a_{ij}x_j$ is a contribution to y_i ; the result of the product $a_{ij}x_j$ and the vector entry y_i should meet at a processor.

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Row parallel Column parallel Row-column parallel

Parallelization objectives

Achieve load balance

Load of a processor: number of nonzeros.

 \Rightarrow assign almost equal number of nonzeros per processor.

Minimize communication cost

Communication cost is a complex function (depends on the machine architecture and problem size):

- total volume of messages,
- total number of messages,
- max. volume of messages per processor (sends or receives, both?),
- max. number of messages per processor (sends or receives, both?).

We restrict ourselves to the distributed memory setting.

What are the aims of a distribution?

- load balance among processors: equal number of aij per processor,
- reduced communication requirement: a_{ij} is to be multiplied by x_j; these two should meet at a processors; the scalar product a_{ij}x_j is a contribution to y_i; the result a_{ij}x_j and y_i should meet at a processor.

Assume there are no operations between x and y of the SpMxV $y \leftarrow Ax$ after the multiply operation.

In half of the cases(!), the input vector x and the output vector y undergo vector operations (such as $x \leftarrow x + \beta y$, or $\gamma \leftarrow x^T y$), in such cases it is better to have the same partition on x and y —we will come to this later.

Parallel sparse matrix vector multiplies: Variants

We classify parallel SpMxV algorithms into three groups (according to the distribution on the matrix)

- Row-parallel algorithm: all nonzeros in a row of the matrix is assigned to the same processor (a_{ij} and a_{ik} are in the same processor),
- Column-parallel algorithm: all nonzeros in a column of the matrix is assigned to the same processor (*a_{ij}* and *a_{kj}* are in the same processor).
- Row-column parallel algorithm: many possibilities
 - each nonzero is assigned to a processor on its own (*a_{ij}* and *a_{ik}* can be in different processors; *a_{ij}* and *a_{kj}* can be in different processors),
 - the nonzeros in a row and/or column are assigned to a small set of processors (e.g., assume a 2D mesh of processors and distribute the nonzeros in a row of A among the processors of a row of the mesh).

Row parallel

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Summary and concluding remarks

Row parallel

Parallel SpMxV: Row-parallel

The rows and columns of an $m \times n$ matrix **A** are permuted into a $K \times K$ block structure

$$A_{BL} = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1K} \\ A_{21} & A_{22} & \cdots & A_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ A_{K1} & A_{K2} & \cdots & A_{KK} \end{bmatrix}$$

for rowwise partitioning, where K is the number of processors.

- Block $\mathbf{A}_{k\ell}$ is of size $m_k \times n_\ell$, where $\sum_k m_k = m$ and $\sum_\ell n_\ell = n$.
- Processor P_k holds the kth row stripe $[\mathbf{A}_{k1} \cdots \mathbf{A}_{kK}]$ of size $m_k \times n$.
- Load balance: The row stripes should have nearly equal number of nonzeros for having the computational load balance among processors.

Row parallel Column parallel Row-column parallel

Parallel SpMxV: Row-parallel

In $y \leftarrow Ax$, y and x are column vectors of size m and n; A is partitioned as shown in the previous slide.

- A rowwise partition of matrix **A** defines a partition on the output vector *y*.
- The input vector x is assumed to be partitioned conformably with the column permutation of matrix **A**.
- y and x vectors are partitioned as $y = [y_1^T \cdots y_K^T]^T$ and $x = [x_1^T \cdots x_K^T]^T$, where y_k and x_k are column vectors of size m_k and n_k , respectively.
- processor P_k holds x_k and is responsible for computing y_k .

Row parallel Column parallel Row-column parallel

Parallel SpMxV: Row-parallel

Matrix is partitioned rowwise among 4 processors.



- row stripes are assigned to processors.
- virtual column stripes shows the assignment of x vector entries.
- The columns of the matrix are permuted according to the partition on *x*.

25 nonzeros in the 1st row stripe (assigned to processor P_1) 26 nonzeros in the 2nd row stripe (assigned to processor P_2) 25 nonzeros in the 3rd row stripe (assigned to processor P_3) 25 nonzeros in the 4th row stripe (assigned to processor P_4)

Parallel SpMxV: Row-parallel algorithm

Executes the following steps at each processor P_k :

- For each nonzero off-diagonal block A_{ℓk}, send sparse vector x̂^ℓ_k to processor P_ℓ, where x̂^ℓ_k contains only those entries of x_k corresponding to the nonzero columns in A_{ℓk}.
- Ompute the diagonal block product y^k_k ← A_{kk} × x_k, and set y_k = y^k_k.
- For each nonzero off-diagonal block $\mathbf{A}_{k\ell}$, receive \hat{x}_{ℓ}^{k} from processor P_{ℓ} , then compute $y_{k}^{\ell} \leftarrow \mathbf{A}_{k\ell} \times \hat{x}_{\ell}^{k}$, and update $y_{k} \leftarrow y_{k} + y_{k}^{\ell}$.

In Step 1, P_k might be sending the same x_k -vector entry to different processors according to the sparsity pattern of the respective column of **A**. This multicast-like operation is called the expand operation.

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Parallel SpMxV: Row-parallel

Matrix is partitioned rowwise among 4 processors. y vector entries are partitioned according to the rowwise partition of **A**; assume the x vector entries are partitioned and the columns of **A** are permuted.

				P_{I}			1	P_2				P_{3}			P_4	
				x_{I}				x_2				<i>x</i> ₃			x_4	
			- ∩ ∾	4 ₪	6	დე	10	12	13	14	15 16	17 18	19 20	21 22	23 24	25 26
P_{I}	<i>y</i> ₁	1 2 3	× × × × × × ×	× × × × ×	× × ×								×××			× ×
<i>P</i> ₂	<i>y</i> ₂	4 5 6 7 8	~ ~ ~	×	× × ×	× × × × × ×	× × × × ×	××××	×	× × ×			××			
P_{3}	<i>y</i> ₃	9 10 11 12						×	×	× ×	× × × × ×	× × × × ×	× × × × × × ×			×× ×
<i>P</i> ₄	<i>Y</i> ₄	13 14 15 16			× ×			×					×	× × × × × × ×	× × × × × × × ×	× × × × × ×

- 1. Expand x vector (sends/receives)
- 2. Compute with diagonal blocks
- Receive x and compute with offdiagonal blocks

Row parallel Column parallel Row-column paralle

Row-parallel SpMxV: Communication requirements



- Expand x vector (sends/receives)
- 2. Compute with diagonal blocks
- Receive x and compute with offdiagonal blocks

Fact 1: Number of messages sent by P_k

The number of messages sent by processor P_k is equal to the number of nonzero off-diagonal blocks in the *k*th virtual column stripe of **A**.

- P₂, sends x[12:14] to P₃—nonzero columns 12, 13, and 14 in A₃₂.
- P_2 sends x[12] to P_4 —nonzero column 12 in A_{42} .
- The number of messages sent by P_2 is 2.

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Row-parallel SpMxV: Communication requirements



- Expand x vector (sends/receives)
- Compute with diagonal blocks
- Receive x and compute with offdiagonal blocks

Fact 2: Volume of messages sent by P_k

The volume of messages sent by P_k is equal to the sum of the number of nonzero columns in each off-diagonal block in the *k*th virtual column stripe of **A**.

- P₂, sends x[12:14] to P₃—(size 3).
- P_2 sends x[12] to P_4 —(size 1).
- The volume of messages sent by P_2 is 4.

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Row-parallel SpMxV: Communication requirements



- Expand x vector (sends/receives)
- Compute with diagonal blocks
- Receive x and compute with offdiagonal blocks

Fact 3: Total volume and number of messages

- The total volume of messages is equal to the number of nonzero columns in off-diagonal blocks.
- The total number of messages is equal to the number of nonzero off-diagonal blocks.
- Total volume of messages is 13. Total number of messages is 9.

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Parallel SpMxV: Column-parallel

The rows and columns of an $m \times n$ matrix **A** are permuted into a $K \times K$ block structure

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1K} \\ A_{21} & A_{22} & \cdots & A_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ A_{K1} & A_{K2} & \cdots & A_{KK} \end{bmatrix}$$

for columnwise partitioning, where K is the number of processors.

- Block $\mathbf{A}_{k\ell}$ is of size $m_k \times n_\ell$, where $\sum_k m_k = m$ and $\sum_\ell n_\ell = n$.
- Processor P_k holds the *k*th column stripe $[\mathbf{A}_{1k}^T \cdots \mathbf{A}_{Kk}]^T$ of size $m \times n_k$.
- Load balance: The column stripes should have nearly equal number of nonzeros for having the computational load balance among processors.

Column paralle

Parallel SpMxV: Column-parallel

In $y \leftarrow Ax$, y and x are column vectors of size m and n; A is partitioned as shown in the previous slide.

- A columnwise partition of matrix A defines a partition on the input-vector \mathbf{x} .
- The output vector y is assumed to be partitioned conformably with the row permutation of matrix A.
- y and x vectors are partitioned as $y = [y_1^T \cdots y_{\kappa}^T]^T$ and $x = [x_1^T \cdots x_{\kappa}^T]^T$, where y_k and x_k are column vectors of size m_k and n_k , respectively.
- processor P_k holds x_k and is responsible for computing y_k .

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Parallel SpMxV: Column-parallel

Matrix is partitioned columns among 4 processors.



- column stripes are assigned to processors.
- virtual row stripes shows the assignment of *y* vector entries.
- The rows of the matrix are permuted according to the partition on *y*.
- Load balance achieved:
 25 nonzeros assigned to processor P₁;
 26 nonzeros assigned to processor P₂;
 25 nonzeros assigned to processor P₃;
 25 nonzeros assigned to processor P₄.

Parallel SpMxV: Column-parallel algorithm

Executes the following steps at each processor P_k :

- For each nonzero off-diagonal block A_{ℓk}, form sparse vector ŷ^k_ℓ which contains only those results of y^k_ℓ = A_{ℓk} × x_k corresponding to the nonzero rows in A_{ℓk}. Send ŷ^k_ℓ to processor P_ℓ.
- Ocompute the diagonal block product y^k_k ← A_{kk} × x_k, and set y_k = y^k_k.
- For each nonzero off-diagonal block $\mathbf{A}_{k\ell}$ receive partial-result vector \hat{y}_k^{ℓ} from processor P_{ℓ} , and update $y_k \leftarrow y_k + \hat{y}_k^{\ell}$.

In Step 3, the multinode accumulation on the y_k -vector entries is called the fold operation.

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Parallel SpMxV: Column-parallel

Matrix is partitioned columnwise among 4 processors. x vector entries are partitioned according to the columnwise partition of **A**; assume the y vector entries are partitioned and the rows of **A** are permuted.



- Compute with off diagonal blocks; obtain partial y results, issue sends/receives
- 2. Compute with diagonal block
- Receive partial results on y for nonzero off-diagonal blocks and add the partial results

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Column-parallel SpMxV: Communication requirements



Fact 1: Number of messages sent by P_k

The number of messages sent by processor P_k in column-parallel $y \leftarrow Ax$ is equal to the number of nonzero off-diagonal blocks in the *k*th column stripe of **A**.

- P₃ sends a message to P₂ for y vector entries y[12, 13, 14] and to P₄ for y[25, 26].
- P_4 sends messages to P_1 P_2 and P_3 .

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Column-parallel SpMxV: Communication requirements



Fact 2: Volume of messages sent by P_k

- The volume of messages sent by P_k is equal to the sum of the number of nonzero rows in each off-diagonal block in the kth column stripe of **A**.
 - P₃ sends a message to P₂ for y vector entries y[12, 13, 14] and another one to P₄ for y[25, 26].
 - P₃ sends 5 units of messages.

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Column-parallel SpMxV: Communication requirements



- Compute with off diagonal blocks; obtain partial y results, issue sends/receives
- 2. Compute with diagonal block
- Receive partial results on y for nonzero off-diagonal blocks and add the partial results

Fact 3: Total volume and number of messages

- The total volume of messages is equal to the number of nonzero rows in off-diagonal blocks. (13)
- The total number of messages is equal to the number of nonzero off-diagonal blocks. (9)

Row parallel Column parallel Row-column parallel

Parallel SpMxV: Row parallel and column parallel algorithms



The communication patterns of column parallel $y \leftarrow \mathbf{A}^T x$ and row parallel $y \leftarrow \mathbf{A} x$ are duals of each other (the columnwise partition on \mathbf{A}^T is equal to the rowwise partition on \mathbf{A}).

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Summary and concluding remarks

Parallel SpMxV: Row-column parallel algorithm

Consider $y \leftarrow Ax$, where y and x are column vectors of size m and n, respectively, and the matrix is partitioned in two dimensions among K processors.

- The vectors y and x are partitioned as $y = [y_1^T \cdots y_K^T]^T$ and $x = [x_1^T \cdots x_K^T]^T$, where y_k and x_k are column vectors of size m_k and n_k , respectively. As before we have $\sum_k m_k = m$ and $\sum_\ell n_\ell = n$.
- Processor P_k holds x_k and is responsible for computing y_k .
- Nonzeros of a processor P_k can be visualized as a sparse matrix \mathbf{A}^k

$$\mathbf{A}^{k} = \begin{bmatrix} \mathbf{A}_{11}^{k} & \cdots & \mathbf{A}_{1k}^{k} & \cdots & \mathbf{A}_{1K}^{k} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{A}_{k1}^{k} & \cdots & \mathbf{A}_{kk}^{k} & \cdots & \mathbf{A}_{kK}^{k} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{A}_{K1}^{k} & \cdots & \mathbf{A}_{Kk}^{k} & \cdots & \mathbf{A}_{KK}^{k} \end{bmatrix}$$

of size $m \times n$, where $\mathbf{A} = \sum \mathbf{A}^k$ (here \mathbf{A}^k s are disjoint).

Row parallel Column parallel Row-column parallel

Parallel SpMxV: Row-column parallel algorithm

 P_k has \mathbf{A}^k , holds x_k and is responsible for y_k .

$$\mathbf{A}^{k} = \begin{bmatrix} A_{11}^{k} & \cdots & A_{1k}^{k} & \cdots & A_{1K}^{k} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ A_{k1}^{k} & \cdots & A_{kk}^{k} & \cdots & A_{kK}^{k} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ A_{K1}^{k} & \cdots & A_{Kk}^{k} & \cdots & A_{KK}^{k} \end{bmatrix}$$

- The blocks in row-block stripe $A_{k*}^{k} = [A_{k1}^{k}, \cdots, A_{kk}^{k}, \cdots, A_{kK}^{k}]$ have row dimension of size m_{k} .
- The blocks in column-block stripe $A_{*k}^k = [A_{1k}^k, \cdots, A_{kk}^k, \cdots, A_{Kk}^k]$ have column dimension of size n_k .
- The x-vector entries that are to be used by processor P_k are represented as x^k = [x^k₁, · · · , x^k_k, · · · , x^k_k], where x^k_k corresponds to x_k and other x^k_ℓ are belonging to some other processor P_ℓ.
- The y-vector entries for which processor P_k computes partial results are represented as y^k = [y^k₁, ..., y^k_k, ..., y^k_K], where y^k_k corresponds to y_k and other y^k_ℓ are to be sent to some other processor P_ℓ.

Parallel SpMxV: Row-column parallel algorithm

Executes the following steps at each processor P_k :

- **9** For each $\ell \neq k$ having nonzero column-block stripe \mathbf{A}_{*k}^{ℓ} , send sparse vector \hat{x}_{μ}^{ℓ} to processor P_{ℓ} , where \hat{x}_{μ}^{ℓ} contains only those entries of x_k corresponding to the nonzero columns in A_{*k}^{ℓ} .
- **2** Compute the column-block stripe product $y^k \leftarrow \mathbf{A}_{*k}^k \times x_k^k$.
- Solution For each nonzero column-block stripe $\mathbf{A}_{\ell,\ell}^k$, receive \hat{x}_{ℓ}^k from processor P_{ℓ} , then compute $y^k \leftarrow y^k + \mathbf{A}_{*\ell}^k \times \hat{x}_{\ell}^k$, and set $y_k = y_k^k$.
- For each nonzero row-block stripe $A_{\ell_*}^k$, form sparse partial-result vector \hat{y}_{ℓ}^{k} which contains only those results of $y_{\ell}^{k} = \mathbf{A}_{\ell*}^{k} \times x^{k}$ corresponding to the nonzero rows in $\mathbf{A}_{\ell_*}^k$. Send \hat{y}_{ℓ}^k to processor P_{ℓ_*} .
- So For each $\ell \neq k$ having nonzero row-block stripe A_{k*}^{ℓ} receive partial-result vector \hat{y}_{k}^{ℓ} from processor P_{ℓ} , and update $y_{k} \leftarrow y_{k} + \hat{y}_{k}^{\ell}$.

Row parallel Column parallel Row-column parallel

Parallel SpMxV: Row-column parallel algorithm



Expand x vector Scalar multiply and add $(\mathbf{y}_{i} \leftarrow \mathbf{a}_{ii} \mathbf{x}_{i} + \mathbf{a}_{ik} \mathbf{x}_{k})$ 3. Fold on v vector (send and receive partial results)

Load balance is achieved by assigning almost equal number of nonzeros to the processors.

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Row parallel Column parallel Row-column parallel

Row-column-parallel SpMxV: Communication requirements

• Communication on *x* (expand operations)

Same as that in the row-parallel algorithm

• Communication on y (fold operations)

Same as that in the column-parallel algorithm

Row parallel Column parallel Row-column parallel

Running time comparisons

from Vastenhouw and Bisseling'05

Table 5.8 Communication volume (in data words) and time (in ms) of parallel sparse matrixvector multiplication on an SGI Origin 3800. The lowest volume and time are marked in boldface.

Name	p		Volume			Time	
		1D row	1D col	2D	1D row	1D col	2D
tbdmatlab	1	0	0	0	5.74	5.71	5.77
	2	5056	6438	5056	3.28	3.31	3.20
	4	14650	14949	11005	2.08	2.06	1.95
	8	30982	26804	17792	1.62	1.40	1.34
	16	56923	42291	27735	1.34	1.19	1.17
	32	98791	62410	40497	1.77	1.58	1.70
tbdlinux	1	0	0	0	67.55	67.61	74.15
	2	15764	24463	15764	36.65	32.26	32.16
	4	42652	54262	30444	14.06	12.22	12.14
	8	90919	96038	49120	6.49	6.35	6.62
	16	177347	155604	75884	5.22	4.22	4.20
	32	297658	227368	106563	4.32	4.08	3.23
bcsstk30	1	0	0	0	50.99	50.96	56.18
	2	948	948	940	28.37	28.24	26.04
	4	2099	2099	2124	6.00	6.03	5.83
	8	5019	5019	4120	2.87	2.90	2.88
	16	9344	9344	8491	1.53	1.56	1.64
	32	15593	15593	14771	1.08	1.12	1.17

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Parallelization objectives

Achieve load balance

Load of a processor: number of nonzeros.

 \Rightarrow assign almost equal number of nonzeros per processor.

Minimize communication cost

Communication cost is a complex function (depends on the machine architecture and problem size):

- total volume of messages,
- total number of messages,
- max. volume of messages per processor (sends or receives, both?),
- max. number of messages per processor (sends or receives, both?).

The common metric in different works: total volume of communication.

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Hypergraphs: Definitions

A hypergraph is two-tuple $\mathcal{H} = (\mathcal{V}, \mathcal{N})$ where \mathcal{V} is a set of vertices and \mathcal{N} is a set of hyperedges.

A hyperedge $h \in \mathcal{N}$ is a subset of vertices. We call them nets for short.

A cost c(h) is associated with each net h.

A weight w(v) is associated with each vertex v.

An undirected graph can be seen as a hypergraph where each net contains exactly two vertices.

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Hypergraphs: Example

$$\begin{aligned} \mathcal{H} &= (\mathcal{V}, \mathcal{N}) \text{ with } \mathcal{V} = \{1, 2, 3, 4, 5\} \ \mathcal{N} = \{n_1, n_2, n_3\} \text{ where } \\ n_1 &= \{1, 3, 4\} \quad n_2 = \{1, 2, 3, 4\} \quad n_3 = \{2, 5\} \end{aligned}$$



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Hypergraphs: Partitioning

Partition

- $\Pi = \{\mathcal{V}_1, \mathcal{V}_2, \dots, \mathcal{V}_K\} \text{ is a } K\text{-way vertex partition if }$
 - $\mathcal{V}_k \neq \emptyset$,
 - parts are mutually exclusive: $\mathcal{V}_k \cap \mathcal{V}_\ell = \emptyset$,
 - parts are collectively exhaustive: $\mathcal{V} = \bigcup \mathcal{V}_k$.

In Π , a net connects a part if it has at least one vertex in that part, i.e., h connects \mathcal{V}_k if $h \cap \mathcal{V}_k \neq \emptyset$.

The connectivity $\lambda(h)$ of a net is equal to the number of parts connected by h.

Objective: minimize cutsize(Π)	Constraint: balanced part weights					
$\sum_{h} c(h)(\lambda(h)-1),$	$\sum_{v\in\mathcal{V}_k} \mathbf{w}(v) \leq (1+\varepsilon) \frac{\sum_{v\in\mathcal{V}} \mathbf{w}(v)}{\kappa}.$					
Hypergraph partitioning problem is NP-complete.						

Parallel sparse matrix vector multiplications

Hypergraphs partitioning: Example

 $\mathcal{H} = (\mathcal{V}, \mathcal{N})$ with 10 vertices and 4 nets, partitioned into four parts. $V_1 = \{4,5\}$ $V_2 = \{7,10\}$ $V_3 = \{3,8,9\}$ $V_4 = \{1,2,6\}$



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Hypergraphs: Partitioning tools and applications

Tools

hMETIS (Karypis and Kumar, Univ. Minnesota),

MLPart (Caldwell, Kahng, and Markov, UCLA/UMich),

Mondrian (Bisseling and Meesen,

Utrecht Univ.),

Parkway (Trifunovic and Knottenbelt,

Imperial Coll. London),

PaToH (Çatalyürek and Aykanat, Bilkent Univ.),

Zoltan-PHG (Devine, Boman, Heaphy,

Bisseling, and Çatalyürek, Sandia National Labs.).

Applications

- VLSI: circuit partitioning,
- Scientific computing: matrix partitioning, ordering, cryptology, etc.,
- Parallel/distributed computing: volume rendering, data aggregation, scheduling, declustering/clustering,
- Software engineering, information retrieval, processing spatial join queries, etc.

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Hypergraph models for matrix partitioning for parallel computations

In all of the cases we will see, we will have unit net-costs, that is c(h) = 1 The objective function becomes

$$\sum_{h} (\lambda(h) - 1)$$

- Make the data to be partitioned as vertices of the hypergraph.
- Assign weights to the vertices.
- Put nets to represent dependencies of computations to the input data; and dependencies of output data into computations.
- Partition into K parts, each V_k holds the data of a processor.
- Load balance would be achieved if part weights are balanced.
- Total volume of communication would be equivalent to the cut-size.

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Hypergraph models for row-parallel SpMxV

- Three entities to partition y, rows of A, and x three types of vertices y_i, r_i, and x_j
- Assign vertex weights weight of r_i is equal to the number of nnz in row i. weight of y_i and x_i can be set to zero.
- y_i is computed by a single row, that is r_i represent the dependency of y_i on r_i
- x_j is a data source; r_i s where $a_{ij} \neq 0$ need x_j connect x_i and all such r_i

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Row-parallel SpMxV: Communication requirements



Total volume and number of messages

The total volume of messages is equal to the number of nonzero columns in off-diagonal blocks. Here, the total volume of messages is 13.

Hypergraph models for row-parallel SpMxV

Hypergraph models for row-parallel SpMxV



Partition the vertices into K parts (partition the data among K processors)

Part weights=processor's loads in terms of nnz.

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Hypergraph models for row-parallel SpMxV



Number of nonzeros columns in off-diagonal blocks is 5. Total volume is 5.



Column-net c_{14} connects 2 parts; c_5 connects 3 parts; c_{12} connects 2 parts; c_{13} connects 2 parts. Cut-size is 5.

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Hypergraph models for row-parallel SpMxV

What about load balance?



There are 12 nnz in the first row stripe.



Each row-vertex gets a weight equivalent to the number of nonzeros in the associated row of **A**.

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Hypergraph models for column-parallel SpMxV

- Three entities to partition y, columns of **A**, and x three types of vertices y_i, c_j, and x_j
- Assign vertex weights weight of c_j is equal to the number of nnz in column j. weight of y_i and x_j can be set to zero.
- x_j is needed by a single column, that is c_j represent the need of c_j on x_j
- y_i is computed by contributions from different columns; each column c_j with a_{ij} ≠ 0 contributes to y_i connect y_i and all such c_j

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Column-parallel SpMxV: Communication requirements



- Compute with off diagonal blocks; obtain partial y results, issue sends/receives
- 2. Compute with diagonal block
- Receive partial results on y for nonzero off-diagonal blocks and add the partial results

Total volume and number of messages

The total volume of messages is equal to the number of nonzero rows in off-diagonal blocks. (13)

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 $n_i(w,r)$

 $n_k(w, r)$

 $n_i(w, r)$

Hypergraph models for column-parallel SpMxV

For column-parallel $w \leftarrow Az$ computations.



Elementary hypergraph model for 1D colwise partitioning.

Combine c_j and z_j ; one column needs only one *z*-vector entry.

Partition the vertices into K parts (partition the data among K processors). Part weights=processor loads in terms of number of nonzeros.

WL

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Hypergraph models for column-parallel SpMxV

The computation is $w \leftarrow Az$



Number of nonzeros rows in off-diagonal blocks is 5. Total volume is 5.



Row-net r_{13} connects 2 parts; r_1 connects 2 parts; r_9 connects 2 parts; r_4 connects 3 parts. Cut-size is 5.

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Hypergraph models for column-parallel SpMxV

What about load balance?



There are 11 nonzeros in the second column stripe.



Each column-vertex gets a weight equal to the number of nonzeros in the associated column of **A**.

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Hypergraph models for row column-parallel SpMxV

- Three entities to partition y, nonzeros of **A**, and x three types of vertices y_i, c_j, and a_{ij}
- Assign vertex weights weight of a_{ij}-vertex is equal to 1. weight of y_i and x_j can be set to zero.
- *x_j* is needed by all *a_{ij}* ≠ 0 connect *x_j* and all such *a_{ij}*
- *y_i* is computed by contributions from different different nonzeros; each *a_{ij}* ≠ 0 contributes to *y_i* connect *y_i* and all such *a_{ij}*

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Parallel SpMxV: Row-column parallel algorithm



- . Expand x vector
- 2. Scalar multiply and add
 - $(y_i \leftarrow a_{ij} x_j + a_{ik} x_k)$
 - Fold on y vector (send and receive partial results)
- Communication on x (expand operations): Same as that in the row-parallel algorithm.
- Communication on y (fold operations): Same as that in the column-parallel algorithm.

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Hypergraph models for row column-parallel SpMxV

For row-column-parallel $y \leftarrow Ax$ computations.



Elementary hypergraph model for row-column-parallel algorithm

Partition the vertices into K parts (partition the data among K processors). Part weights=processor loads in terms of nonzeros.

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Hypergraph models for row column-parallel SpMxV

For row-column-parallel $y \leftarrow Ax$ computations.



[Part of the fine grain model on the board....]

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The approach

- Put vertices to represent the data items to partition
- Put nets to represent dependencies and needs
- Assign weights to vertices to have load balance
- Try to simplify (not lose the flexibility) by
 - if two data items want to be in the same processors, amalgamate the vertices
 - if there are nets of size 1, remove them.
- We can specify, for a set of vertices to which part it should be assigned; if this is imposed by the problem that we want to parallelize.

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The approach on row parallel algorithm: Symmetric partitioning wanted



 y_i and r_i wants to be in the same part processor (owner computes rule—avoids communication).

net $n_y(i)$ has size 1 after amalgamation; remove it from the model. Some $n_x(i)$ may have single vertex (in which case?)—they can be removed too.

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Problem 1

Problem

Describe a hypergraph model which can be used to partition the matrix **A** rowwise for the $y \leftarrow Ax$ computations under given, possibly different, partitions on the input and output vectors x and y.

A parallel algorithm that carries out the $y \leftarrow Ax$ computations under given partitions of x and y should have a communication phase on x, a computation phase, and a communication phase on y.

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Solution to Problem 1

Problem

Describe a hypergraph model which can be used to partition the matrix **A** rowwise for the $y \leftarrow Ax$ computations under given, possibly different, partitions on the input and output vectors x and y.

Solution

Take the elementary model and fix the vertices x_j and y_i to the parts as specified by the given partitions.



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Problem 2

Problem

Describe a hypergraph model to obtain **the same partition** on the input and output vectors x and y which is **different** than the **partition on the rows** of **A** for the $y \leftarrow \mathbf{A}x$ computations.

The previous parallel algorithm will be used.

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Solution to Problem 2

Problem

Describe a hypergraph model to obtain the same partition on the input and output vectors x and y which is different than the partition on the rows of **A** for the $y \leftarrow \mathbf{A}x$ computations.

Solution

Take the elementary model and amalgamate the vertices x_i and y_i





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Problem 3

Problem

Describe a hypergraph model to obtain different partitions on x and on the rows of **A**, where y is partitioned conformably with the rows of **A** under the owner-computes rule for computations of the form $y \leftarrow \mathbf{A}x$ followed by $x \leftarrow x + y$.

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Solution to Problem 3



(a) Elementary model for $y \leftarrow \mathbf{A}x$



(c) Owner computes rule for $x_i \leftarrow x_i + y_i$



(b) New vertices for $x_i \leftarrow x_i + y_i$ and the dependencies for them.



(d) Owner computes rule for y_i

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Problem 4: Preconditioned iterative methods

- Iterative methods may converge slowly, or diverge
- transform Ax = b to another system that is easier to solve
- Preconditioner is a matrix that helps in obtaining desired transformation

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Problem 4: Preconditioned iterative methods

- We consider parallelization of iterative methods that use approximate inverse preconditioners
- Approximate inverse is a matrix **M** such that $\mathbf{AM} \approx I$
- Instead of solving Ax = b, use right preconditioning and solve

AMy = b

and then set

 $x = \mathbf{M}y$

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Problem 4: Preconditioned iterative methods

- Additional SpMxV operations with M never form the matrix AM; perform successive SpMxVs
- Parallelizing a full step in these methods requires efficient SpMxV operations with A and M partition A and M
- A blend of dependencies and interactions among matrices and vectors

partition A and M simultaneously

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Problem 4: Preconditioned iterative methods

- Partition A and M simultaneously
- Figure out partitioning requirements through analyzing linear vector operations and inner products

Reminder: never communicate vector entries for these operations

• Different methods have different partitioning requirements

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Problem 4: Preconditioned iterative methods



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Problem 4: Preconditioned BiCG-STAB

 \Rightarrow *p*, *r*, *v*, *s*, *t*, and, *x* should be partitioned conformably

What remains?



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Problem 4: Preconditioned BiCG-STAB

- We use the previously proposed models
 - define operators to build composite models



Rowwise model (y=Ax)



Colwise model (w=Mz)

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Problem 4: Preconditioned BiCG-STAB

- Nevel amalgamate/unify nets of individual hypergraphs
- combine vertices of individual hypergraphs, and connect the composite vertex to the nets of the individual vertices

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- define multiple weights for vertices, if the multiply operations are separated by global synchronization type of operations; individual vertex weights are not added up.
- need to decide how to partition matrices (lets say A rowwise and M columnwise
 - generate column-net model for the matrices to be partitioned rowwise
 - generate row-net model for the matrices to be partitioned columnwise
 - apply vertex amalgamation to respect the partitioning requirement (**PAQ**^T and **QMP**^T or **PAMP**^T).

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Problem 4: Preconditioned BiCG-STAB

BiCG-STAB requires PAMP^T —

 Reminder: rows of A and columns of M; columns of A and rows of M

• A rowwise (y=Ax), M columnwise (w=Mz)



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Problem 4: Preconditioned BiCG-STAB

columns of A and rows of M



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Problem 4: Preconditioned BiCG-STAB

Rows of A and columns of M



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Problem 4: Preconditioned BiCG-STAB

Parallel speed-up values

-	8-way					16-way				
	Volu	ime	Mes	sage	Sp.	Volume		Message		Sp.
Matrix	tot	max	tot	max	up	tot	max	tot	max	up
	CR									
Zhao1-A	4098	746	32.2	5.7	6.2	6444	586	96.7	9.3	8.7
Zhao1-M	3514	694	32.2	5.6		5478	551	97.0	9.3	
big-A	1032	201	31.4	5.7	5.7	1581	156	73.2	7.5	7.3
big-M	989	191	31.9	5.6		1527	150	75.3	7.5	
cage11-A	24424	4144	54.6	7.0	5.5	34835	3314	201.2	14.8	8.1
cage11-M	14663	2439	55.1	7.0		21010	1917	208.9	15.0	
cage12-A	87542	14306	56.0	7.0	5.9	122878	11925	230.3	15.0	9.4
cage12-M	50962	7839	56.0	7.0		71066	6136	233.1	15.0	
epb2-A	2326	429	39.0	6.4	6.4	3357	371	102.8	9.6	8.6
epb2-M	2242	438	35.0	6.5		3335	335	84.7	8.4	
epb3-A	2354	442	23.9	4.3	7.3	3971	393	66.0	6.5	12.4
epb3-M	3003	536	23.9	4.3		5023	496	66.3	6.5	
mark3_060-A	5249	960	35.2	6.3	5.8	9370	786	115.0	11.3	8.7
mark3_060-M	6323	1182	32.2	6.0		10287	964	105.3	11.0	
olafu-A	3908	960	25.8	5.0	6.7	6489	781	66.2	6.8	10.6
olafu-M	6749	1449	28.0	5.4		11258	1285	77.8	7.8	
stomach-A	14614	2815	21.1	4.0	7.1	24436	2351	67.2	7.0	14.1
stomach-M	16193	3206	21.4	4.0		28014	2652	67.8	7.1	
xenon1-A	10848	2037	36.2	6.5	6.7	15998	1496	113.2	11.3	11.2
xenon1-M	14437	2523	37.7	6.7		21459	2032	117.8	11.8	

Outline

Introduction

2 Parallel SpMxV

- Row parallel
- Column parallel
- Row-column parallel

Hypergraphs and hypergraph partitioning

- Hypergraph models for row-parallel SpMxV
- Hypergraph models for column-parallel SpMxV
- Hypergraph models for row-column-parallel SpMxV
- Some other partitioning problems

4 Summary and concluding remarks

Summary

A sparse matrix is a matrix with a lot of zero entries.

More importantly: all or some zeros are not stored.

Parallel SpMxV is an important computational kernel in many problems; furthermore it characterizes a wide range of applications with irregular computational dependency.

Row-parallel, column-parallel and row-column-parallel algorithms.

Hypergraph models can quite handy in modeling different kind of problems.

Vertex weights are used to have load balance; nets are used to encode data dependencies. Cut size corresponds to the total communication volume.

Thanks!

Thanks for your attention.

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Some of the material are from papers by Aykanat, Çatalyürek, Bisseling.