A Vectorized Sparse Matrix Multiply for Compressed Row Storage Format

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ICCS 2005
May 23, 2005

This research supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL). This work was performed using resources at the National Center for Computational Sciences at ORNL, which is supported by the U.S. Department of Energy under Contract Number DE-AC05-00OR22725.

Important kernel: Solve sparse linear systems

- Bulk of time spent solving, large, sparse linear systems $Ax = b$
- Can solve with direct methods (Gaussian-elimination)
  - Guaranteed to find solution
  - But hard to scale to large systems, many processors
- Iterative methods practical for large problems
  - Can scale to large problem sizes; easy to parallelize
  - Require less time to find solution

Problem for users of Cray-X1 and other vector machines:

- Modern iterative solver packages designed for scalar architectures
  - Out-of-box performance is terrible due to short vector lengths!
- We describe a vectorized sparse mat-vec,
  a vital component of Krylov subspace methods

Outline

- Review sparse matrix storage formats, mat-vec algorithms
- Describe CSRPERM algorithm
  - With vectorization of CSR data in place
  - With rearrangement using ELLPACK storage
- Initial performance results on the Cray-X1 at NCCS/ORNL, using CSRPERM matrix implementation in PETSc

Compressed Sparse Row (CSR)

- CSR is most widely-used format for general sparse matrices
- Stores matrix in three arrays:
  - val: nonzero elements in row-by-row fashion
  - col_ind: column index of each element of val
  - row_ptr: points to beginning of each row in val

$$A = \begin{pmatrix} 11 & 0 & 0 & 14 & 0 \\ 21 & 22 & 0 & 24 & 0 \\ 32 & 0 & 33 & 34 & 35 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{pmatrix}$$

val	11	14;	21	22	24;	31	33	34	35;	43	44;	55
col_ind	1	4;	1	2	4;	1	3	4	5;	3	4;	5

row_ptr	1	3	6	10	12	13

- Mat-vec proceeds directly through val, operating row-by-row.
- Poor performance on vector machines b/c of short row vectors
  - 1st order star-type FD stencil: 5 elements per row in 2D, 7 elements in 3D

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ELLPACK/ITPACK Format (ELL)

- If all rows have similar # nonzeros, can use ELLPACK format
- Uses two N x NZMAX arrays constructed by:
  - Shifting all nonzeros left
  - Columns of shifted "matrix" stored consecutively in val
  - Corresponding col_ind array stores column indices

$$A = \begin{pmatrix} 11 & 0 & 0 & 14 & 0 \\ 21 & 22 & 0 & 24 & 0 \\ 32 & 0 & 33 & 34 & 35 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{pmatrix}$$

val(:,1)	11	14	0	0
val(:,2)	21	22	24	0
val(:,3)	31	33	34	35
val(:,4)	43	44	0	0
val(:,5)	55	0	0	0

col_ind(:,1)	1	4	0	0
col_ind(:,2)	1	2	4	0
col_ind(:,3)	1	3	4	5
col_ind(:,4)	3	4	0	0
col_ind(:,5)	5	0	0	0

- Mat-vecs proceed along columns of val
- Long vectors + regular access yields good compiler vectorization

Jagged Diagonal Format (JAD)

- Jagged Diagonal (JAD) storage eliminates zero padding of ELL.
- To construct:
  - Permute matrix, ordering rows by decreasing number of nonzeros
  - First JAD: leftmost nonzeros of row 1, row2, etc. of *PA*
  - Second JAD: next nonzeros from row 1, row2, etc.

$$PA = \begin{bmatrix} 32 & 0 & 33 & 34 & 35 \\ 21 & 22 & 0 & 24 & 0 \\ 11 & 0 & 0 & 14 & 0 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{bmatrix}$$

jdiag	31	21	11	43	5;	33	22	14	44;	34	24;	35
col_ind	1	1	1	3	5;	3	2	4	4;	4	4;	5

jd_ptr	1	6	10	12

perm	3	2	1	4	5

- Mat-vecs proceed along jagged diagonals; yields long vector lengths
- Significant memory traffic to repeatedly read/write result vector y

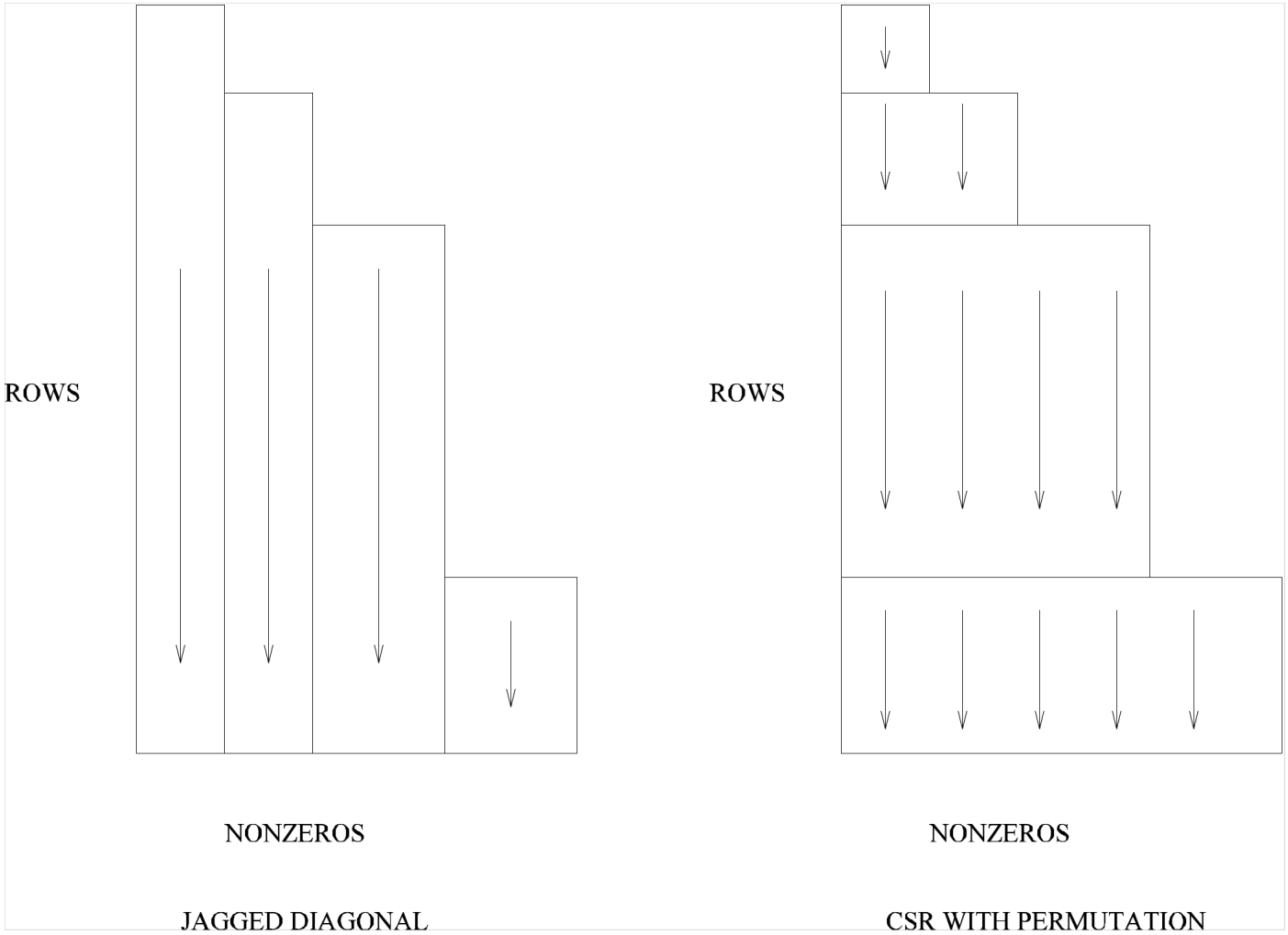
CSR with permutation (CSRPERM)

- Like JAD, sort (permute) rows based on # nonzeros
- Construct groups of rows w/ same # nonzeros

- Mat-vec computed one group at a time:
  - Performs mat-vec for a group in same manner as ELLPACK
  - No zero padding b/c of sorting
- Reduced memory bandwidth requirements compared to JAD

- Can leave CSR data in place (CSRP):
  - Only need O(N) extra storage for permutation
  - Irregular memory access to `val` array
- Or, can copy groups into ELLPACK format (CSRPELL):
  - Better memory access pattern
  - But storage requirements doubled

Conceptual comparison between JAD and CSRP

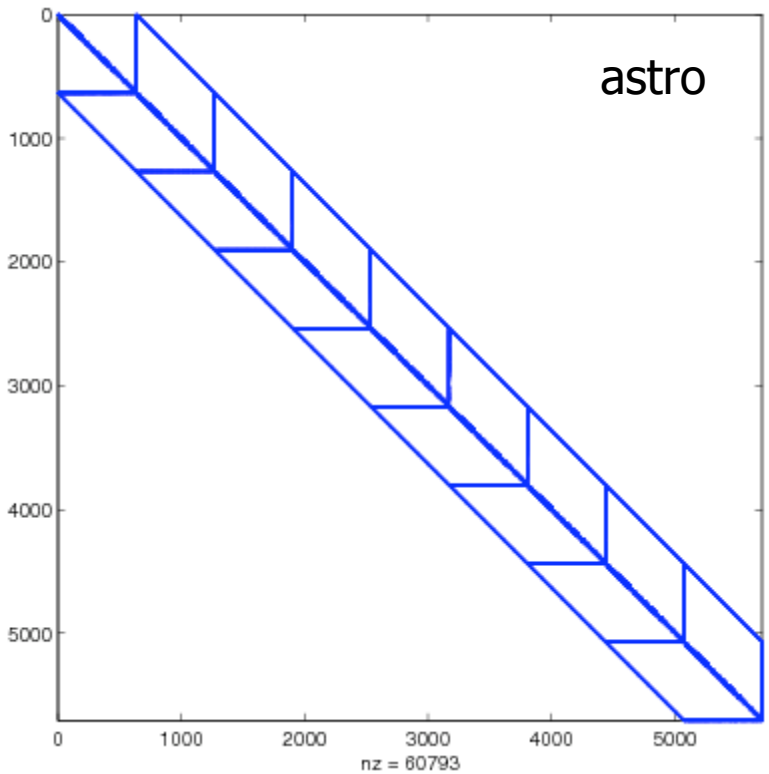


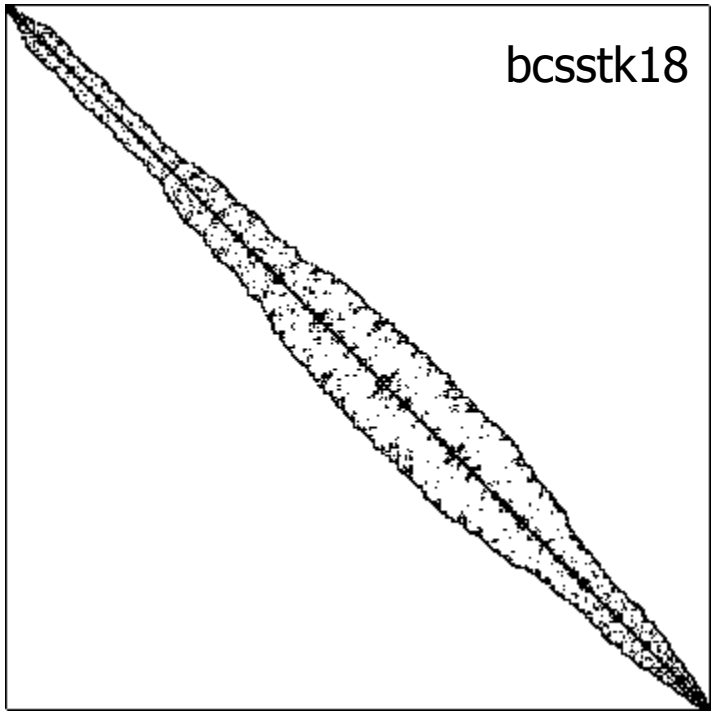
Performance results on the Cray-X1

- Implemented our CSRP kernel as a class in the PETSc framework
- Cray-X1:
  - Each node has four Multi-streaming Processors (MSPs)
  - Each MSP consists of 4 Single-streaming processors (SSPs)
  - Each SSP has 16 KB L1 and 2 MB L2 cache
  - Vector clock 800MHz, scalar clock 400 MHz
  - Memory-cache bandwidth: 34.1 GB/s, cache-cpu: 76.8 GB/s
  - MSP: 8 vector registers, each holding 64 elements of 64bit data

Performance: Sparse mat-vec

Name	N	Nonzeros	Description
Astro	5706	60793	Nuclear astrophysics problem
bcsstk18	11948	80519	Stiffness matrix from Ha rwell -Boeing library
7pt	110592	760320	7-pt stencil in 48 x 48 x 48 grid
7pt_blk	256000	7014400	4x4 blocks 7 -pt stencil in 40 x 40 x 4 0 grid





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	SSP			MSP		
Problem	CSR	CSRP	CSRPELL	CSR	CSRP	CSRJAE
astro	26	163	311	14	214	655
bcsstk18	28	315	340	15	535	785
7pt	12	259	295	8	528	800
7pt_blk	66	331	345	63	918	1085

Performance of sparse mat-vec in MFlops/s

Performance: PETSc example codes

Run two PETSc examples on 1 MSP:

- ksp_ex2: Solves 2D Laplace problem w/ 5-pt FD stencil, 300x300 grid

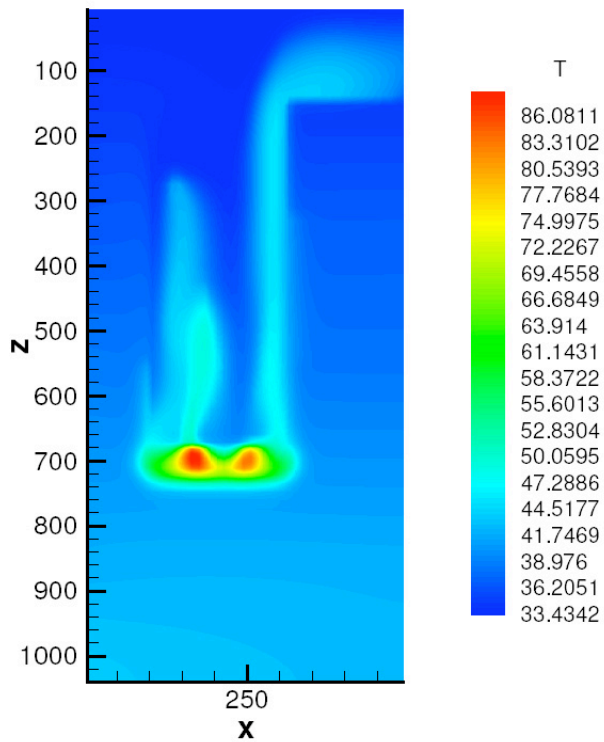
	total	MatMult	PCApply
plain, GMRES+ILU(0)	451.3	218.9	227.6
vec, GMRES+ILU(0)	235.8	1.6	229.5
vec, GMRES+Jacobi	36.9	14.6	1.1
plain, GMRES+Jacobi	1423	1400.0	1.1

- snes_ex14: 3D fuel ignition via Newton-Krylov, 7pt FD, 32x32x32 grid

	total	MatMult	PCApply
plain, GMRES+ILU(0)	26.1	10.5	11.3
vec, GMRES+ILU(0)	15.5	0.07	11.0
vec, GMRES+Jacobi	5.3	0.7	0.1
plain, GMRES+Jacobi	36.5	32.6	0.1

Performance: PFLOTRAN

- PFLOTRAN: Parallel, fully implicit, multiphase groundwater flow and transport code; coauthored w/ Peter Lichtner at LANL
- Run 3D flow + heat transport problem from NTS on 512 SSP's
- 95 x 65 x 50 grid, 3 degrees of freedom per node



	total	MatMult	PCApply
plain, GMRES+ILU(0)	26.9	4.7	6.2
vec, GMRES+ILU(0)	22.2	1.8	6.2
vec *, GMRES+Jacobi	33.7	10.3	0.3
plain, GMRES+Jacobi	54.0	30.5	0.3

* Case encountered "NO FORWARD PROGRESS" error; execution time may be unfairly long

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Performance: M3D

- M3D: 3D resistive MHD code from PPPL.
- Run on 16 MSPs w/ on a tearing-mode case.

	total	MatMult	PCApply
plain, GMRES+ILU(0)	42.0	7.8	17.1
vec, GMRES+ILU(0)	37.3	0.9	17.1
vec, GMRES+Jacobi	41.8	6.58	0.6
plain, GMRES+Jacobi	94.3	57.3	0.6

- Can't improve time w/ Jacobi,
  but note that 21-22 minutes spent in GMRES orthogonalization!
- PPPL currently uses GMRES basis size of 1000!
- Might be a win if we use TFQMR, Bi-CGSTAB… or simply a smaller GMRES basis size!

Summary and Future Directions

- Presented the CSRP mat-vec algorithm
  - Promotes long vector lengths
  - Can work well w/ CSR data left in-place
  - Implemented CSRPERM matrix type in PETSc

Preconditioning still presents a big hurdle:

- Could try to speed up triangular solves for ILU
  - Multicoloring can work, but degrades preconditioner quality
  - Block-recursive formulation yielding series of mat-vecs
  - Take first few terms of Neumann expansion of factorization
- Don't use incomplete factorizations?
  - Sparse approximate inverses
  - Polynomial preconditioners

Creating a CSRPERM matrix class for PETSc

- PETSc is written in C, but uses an object-oriented design:
  - Has its own function tables, dispatch mechanism
  - Employs data encapsulation, polymorphism, inheritance
- All PETSc objects are derived from an abstract base type
  - Mat is the base matrix type
  - MATAIJ is the standard CSR-format instantiation

- We seamlessly integrate support for out CSRP algorithm into PETSc, creating a CSRPERM matrix type derived from AIJ.
- We inherit most methods from AIJ;
  only a few select methods must be overridden.

Matrix creation method

- In PETSc, a Mat object A is built into a particular type by MatSetType(Mat mat, MatType Type)
- If Type is MATSEQCSRPERM, then PETSc calls our internal routine:

```
1 PetscErrorCode MatCreate_SeqCSRPERM(Mat A)
2 {
3   PetscObjectChangeTypeName((PetscObject)A,MATSEQCSRPERM);
4   MatSetType(A,MATSEQAIJ);
5   MatConvert_SeqAIJ_SeqCSRPERM(A,MATSEQCSRPERM,MAT_REUSE_MATRIX,&A);
6   return(0);
7 }
```

- Line 4 builds an empty MATSEQAIJ matrix.
- Line 5 converts that to object to our MATSEQCSRPERM type.

MatConvert Routine

```
 1 PetscErrorCode MatConvert_SeqAIJ_SeqCSRPERM(Mat A,MatType type,
 2    MatReuse reuse,Mat *newmat)
 3 {
 4   Mat             B = *newmat;
 5   Mat_SeqCSRPERM *csrperm;
 6   ...
 7   ierr = PetscNew(Mat_SeqCSRPERM,&csrperm);CHKERRQ(ierr);
 8   B->spptr = (void *) csrperm;
 9   ...
10   /* Set function pointers for methods that we inherit from AIJ but
11    * override. */
12   B->ops->duplicate   = MatDuplicate_SeqCSRPERM;
13   B->ops->assemblyend = MatAssemblyEnd_SeqCSRPERM;
14   B->ops->destroy     = MatDestroy_SeqCSRPERM;
15   B->ops->mult        = MatMult_SeqCSRPERM;
16   B->ops->multadd     = MatMultAdd_SeqCSRPERM;
17
18   ierr = PetscObjectChangeTypeName((PetscObject)B,MATSEQCSRPERM);CHKERRQ(ierr);
19   *newmat = B;
20   PetscFunctionReturn(0);
21 }
```

- Lines 7-8 allocate CSRPERM data structure, stash it in `spptr`.
- Lines 12-16 set pointers for AIJ methods we override.

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Assembly of the CSRP matrix

- In PETSc, assemblyend finalizes construction of matrix data structure
- Creating CSRPERM proceeds from AIJ data structure, so use AIJ assemblyend and then proceed from there

```
PetscErrorCode MatAssemblyEnd_SeqCSRPERM(Mat A, MatAssemblyType mode)
{
  PetscErrorCode ierr;
  Mat_SeqCSRPERM *csrperm = (Mat_SeqCSRPERM*) A->spptr;
  Mat_SeqAIJ     *a = (Mat_SeqAIJ*)A->data;
...
  a->inode.use = PETSC_FALSE;
  (*csrperm->AssemblyEnd_SeqAIJ)(A, mode);

  /* Now calculate the permutation and grouping information. */
  ierr = SeqCSRPERM_create_perm(A);
  PetscFunctionReturn(0);
}
```

Parallel (MPI) CSRPERM class

- What I've shown so far is for the sequential CSRPERM instantiation.

- Implementing the parallel MATMPICSRPERM class is trivial!
- MPIAIJ is simply a collection of SeqAIJs storing local matrix portions
- Similarly, MPICSRPERM a collection of SeqCSRPERMs:
  - MPICSRPERM inherits from MPIAIJ;
    changes the type for local mats from SeqAIJ to SeqCSRPERM.

So why bother writing all this glue code?

- Use CSRP kernels without modification to existing codes
  - Register CSRPERM class with PETSc
  - Use PETSc's options database to select appropriate routines: "-mat_type csrperm"
  - Use options database to set CSRPERM options (e.g., copy groups to ELLPACK format or not)

- Get CSRPERM accepted into the official PETSc source
  - Now a supported matrix class
  - Available in petsc-dev now; should be in next public release