Progress Towards Optimizing the PETSc Numerical Toolkit on the Cray X-1

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Deterministic solution of PDEs

- Many scientific codes simulate systems by solving PDEs.
- Typically:
  - Discretize system: Consider finite number of points
  - Obtain linear systems $Ax = b$

- Bulk of time spent solving large, sparse linear systems.
- Can solve with direct methods (Gaussian-elimination)
  - Guaranteed to find solution
  - But hard to scale to large systems, many processors
- Iterative methods are an increasingly popular alternative
  - Can scale to large problem sizes
  - Easy to parallelize
  - Require less time to find solution

Unfortunately...

- Modern iterative solver packages designed for scalar architectures!
  - Out-of-box performance is terrible!
- We describe ongoing work to provide vectorized PETSc kernels.

PETSc:

  - Object-oriented framework for scalable solution of PDEs
  - Several iterative (linear & nonlinear) solvers & preconditioners
  - Seamless interface w/ other packages (e.g. SuperLU, Hypre)
  - Shields user from complicated data structures, communication

- Initial work has focused on sparse matrix-vector multiply, 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
- Construction of CSRPERM matrix class into PETSc
  - Seamless integration to fully take advantage of PETSc
- Initial performance results on the X1

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

$$A = \begin{pmatrix} 11 & 0 & 0 & 14 & 0 \\ 21 & 22 & 0 & 24 & 0 \\ 31 & 0 & 33 & 34 & 35 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{pmatrix}$$

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

$$A = \begin{pmatrix} 11 & 0 & 0 & 14 & 0 \\ 21 & 22 & 0 & 24 & 0 \\ 31 & 0 & 33 & 34 & 35 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{pmatrix}$$

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

- 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.

$$PA = \begin{pmatrix} 31 & 0 & 33 & 34 & 35 \\ 21 & 22 & 0 & 24 & 0 \\ 11 & 0 & 0 & 14 & 0 \\ 0 & 0 & 43 & 44 & 0 \\ 0 & 0 & 0 & 0 & 55 \end{pmatrix}$$

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

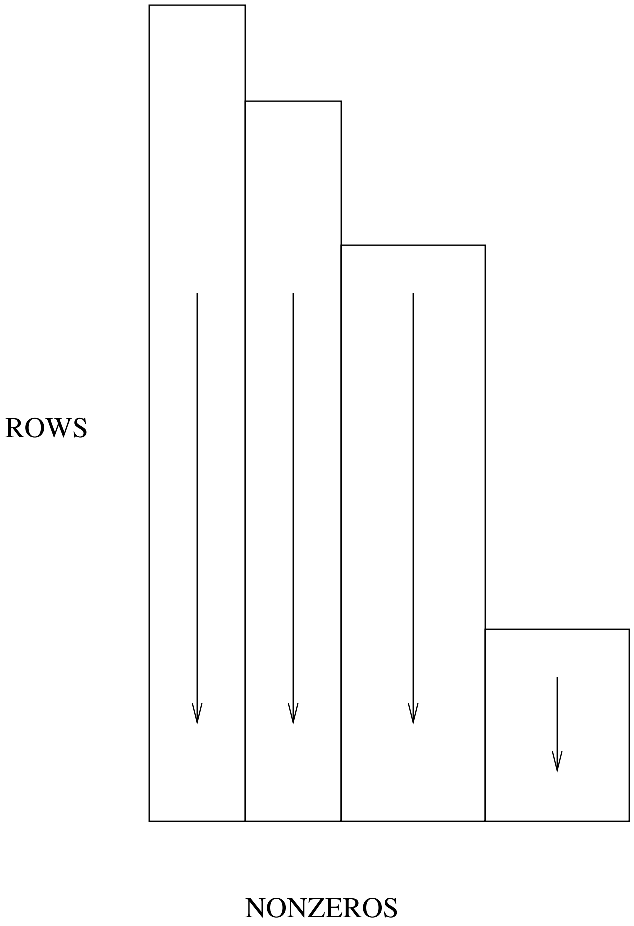
CSR with permutation (CSRPERM)

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

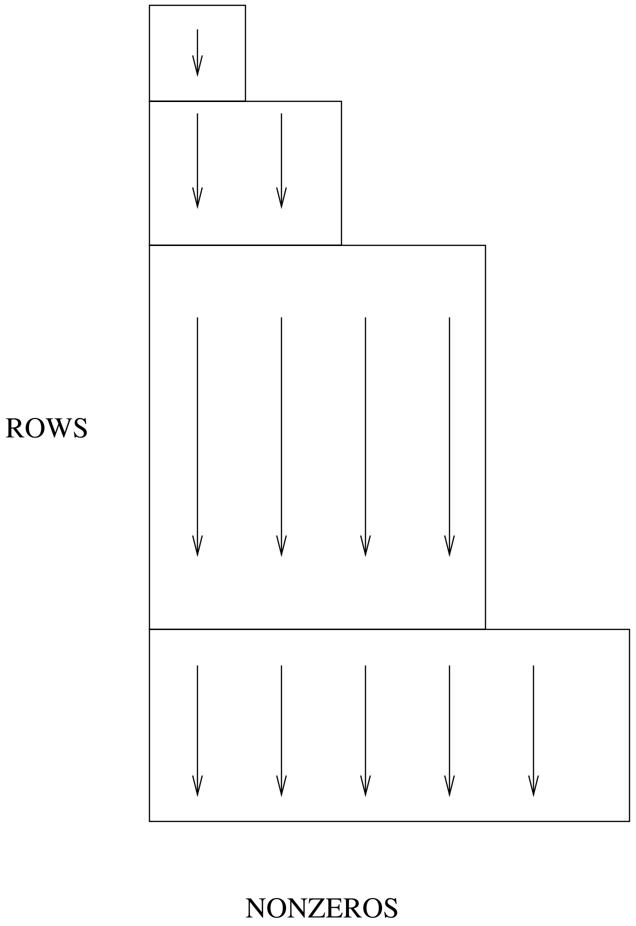
- Mat-vec computed one group at a time:
  - Performs mat-vec for a group in same manner as ELLPACK
  - No zero padding b/c of sorting
- Reduced memory bandwidth requirements compared to JAD

- 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



JAGGED DIAGONAL



CSR WITH PERMUTATION

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.

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.

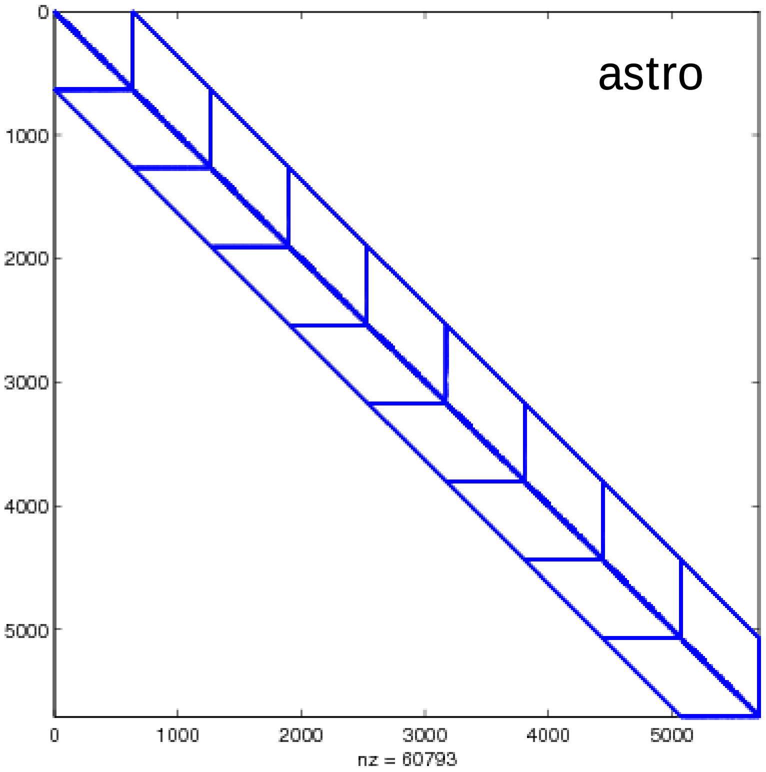
So why bother writing all this glue code?

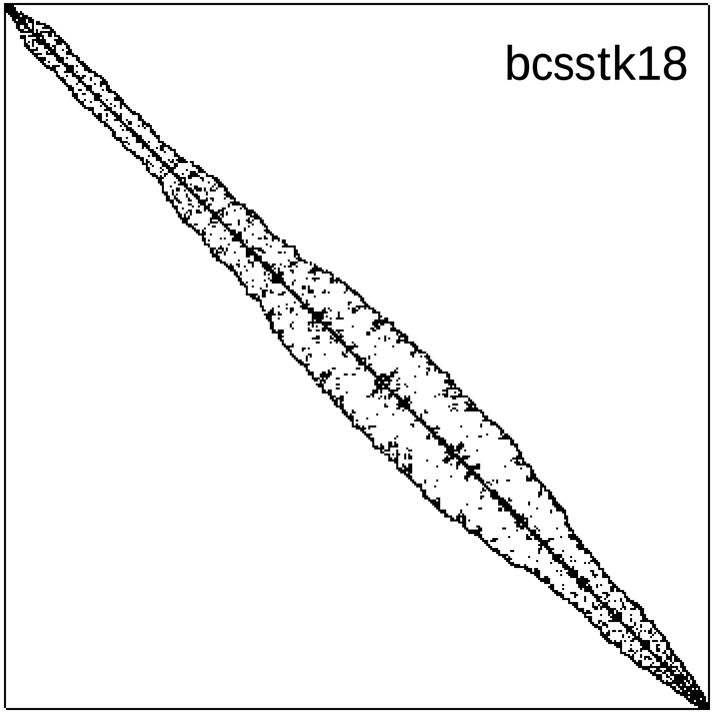
- Use CSRP kernels without modification to existing codes
  - Register CSRPERM class with PETSc
  - Use PETSc’s options database to select appropriate routines: “-mat_type csrperm”
  - Use options database to set CSRPERM options (e.g., copy groups to ELLPACK format or not)

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

Performance: Sparse mat-vec

Name	N	Nonzeros	Description
Astro	5706	60793	Nuclear astrophysics problem
bcsstk18	11948	80519	Stiffness matrix from Harwell-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 40 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

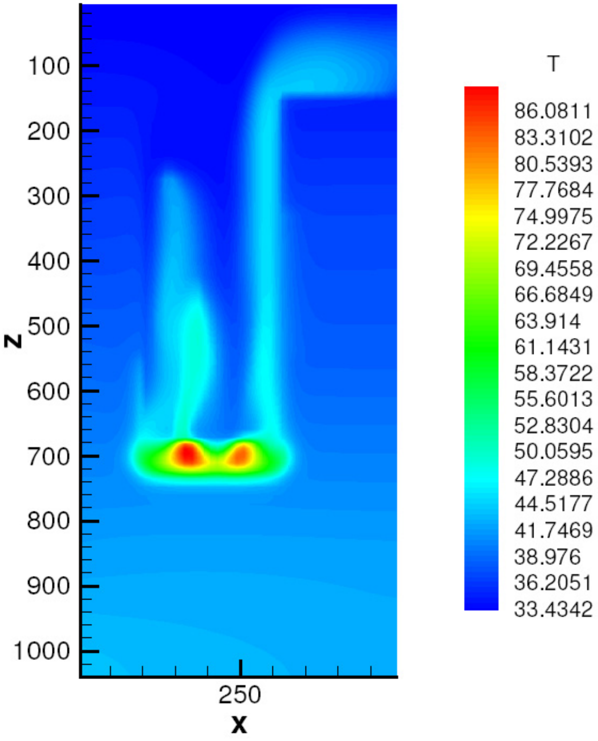
	total	MatMult	PCApply
plain, GMRES+ILU(0)	451.3	218.9	227.6
vec, GMRES+ILU(0)	235.8	1.6	229.5
vec, GMRES+Jacobi	36.9	14.6	1.1
plain, GMRES+Jacobi	1423	1400.0	1.1

- 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	0.1	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) on subdomains	26.9	4.7	6.2
vec, GMRES+ILU(0) on subdomains	22.2	1.8	6.2
vec*, GMRES+Jacobi	33.7	10.3	0.3
plain, GMRES+Jacobi	54.0	30.5	0.3

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(3) on subdomains	42.0	7.8	17.1
vec, GMRES+ILU(3) on subdomains	37.3	0.9	17.1
vec, GMRES+Jacobi	41.8	6.6	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 more reasonable 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