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Recent PETSc Functionality in Linear Operators and Solvers

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PETSc linear operators and solvers for extreme-scale computing

- **Sparse Matrix-Matrix Operations**
  - Computational kernels
    - Matrix product would be denser -

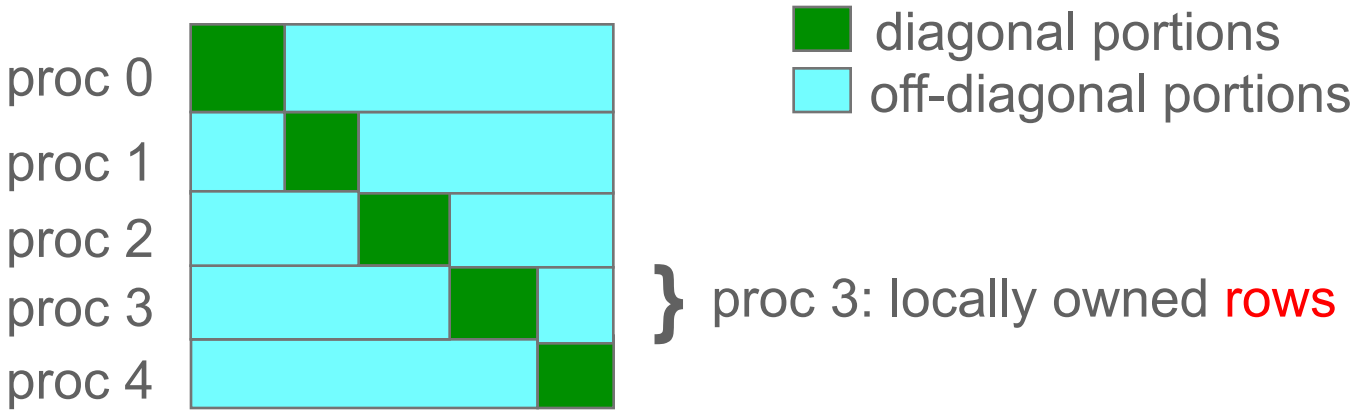
      avoid using these operations if possible
  - GAMG preconditioner requires these operations to be scalable to 10k+ processor cores
- **Krylov Solvers**
  - Fundamental sparse linear solvers
  - Global inner product (via MPI_Allreduce) is a major bottleneck for extreme-scale computing

Sparse Matrix-Matrix Operations (PETSc-3.3)

- C=AB (MatMatMult):
  - New parallel implementations, '-matmatmult_scalable'
- C=A^TB (MatTransposeMatMult):
  - sequential and parallel
- C=AB^T (MatMatTransposeMult):
  - sequential, '-matmattransmult_color'
- C=RAR^T (MatRARt):
  - sequential
- C=P^TAP (MatPtAP):
  - '-matptap_sparseaxpy 2' : slower, but uses a tmp array of local size (ptap->rmax) instead of global P->cmap->N.
- AB and P^TAP run smoothly on 13,824 cores in GAMG

PETSc Parallel Sparse Matrix (MATMPIAIJ)

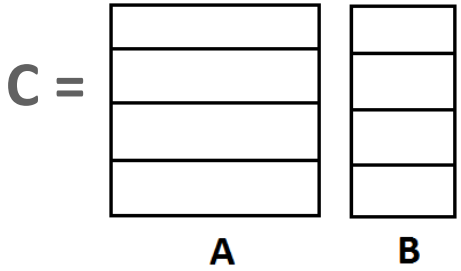
- Each process locally owns a submatrix of contiguously numbered global rows.
- Each submatrix consists of **diagonal** and **off-diagonal** parts.



Sparse Matrix-Matrix Operations (seqential)

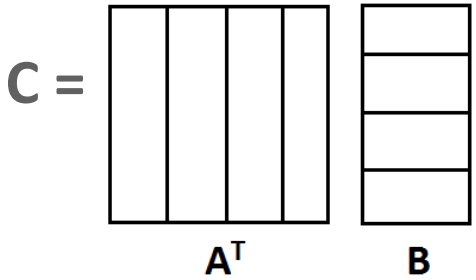
- **C=AB**

  O(Anz*Bnzi)



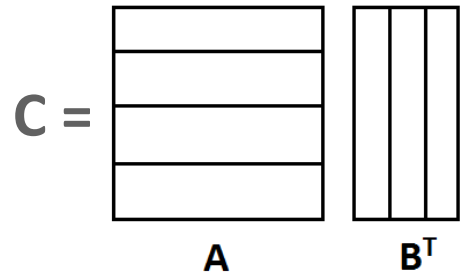
- **C=A^{T}B**

  O(Anz*Bnzi)



- **C=AB^T**

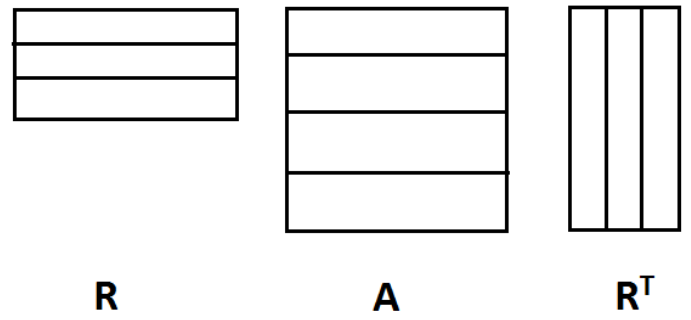
  O(Cnz *(Anzi + Bnzi))



Sparse Matrix-Matrix Operations (seq)

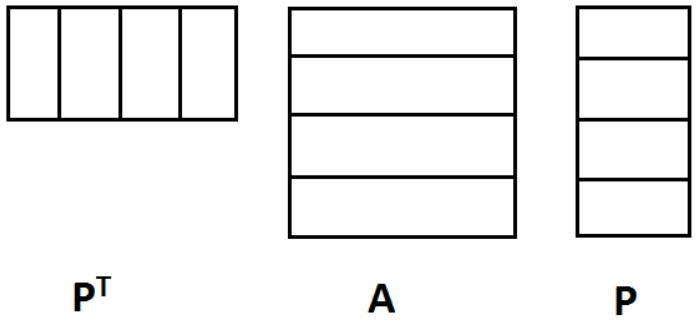
- **$C=RAR^T$**

  O(2Rnz*Anzi + Rm*Anzi*Anzi)



- **$C=P^TAP$**

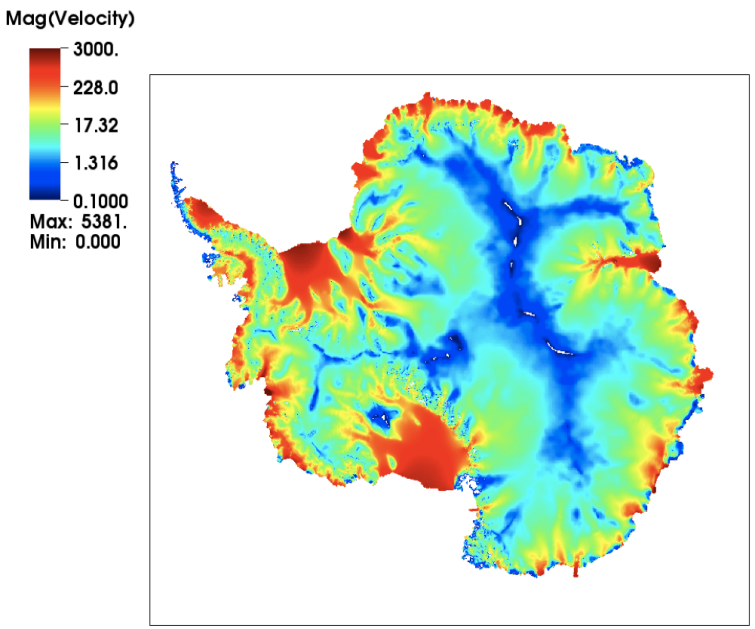
  O(2Anz*Pnzi)

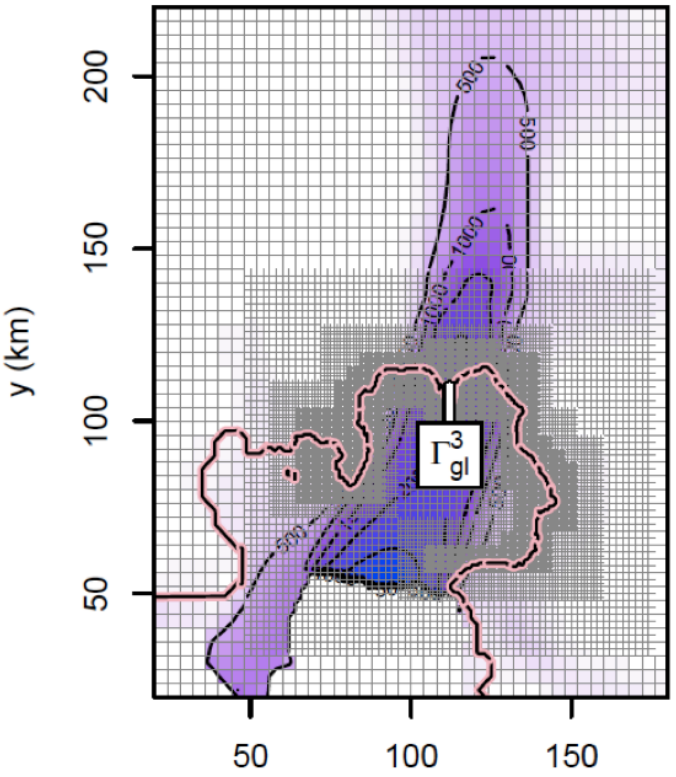


Sparse outer-product is preferable to sparse inner-product

GAMG (geometric algebraic multigrid)

- Unstructured Geometric-Algebraic Multigrid (GAMG)
- Complex geometries demand algebraic multigrid (AMG)
- Common parallel primitives for AMG:
  - $A_{i+1} = P^T A_i P$
  - $P = (I - \omega D^{-1} A) P_0$
  - …



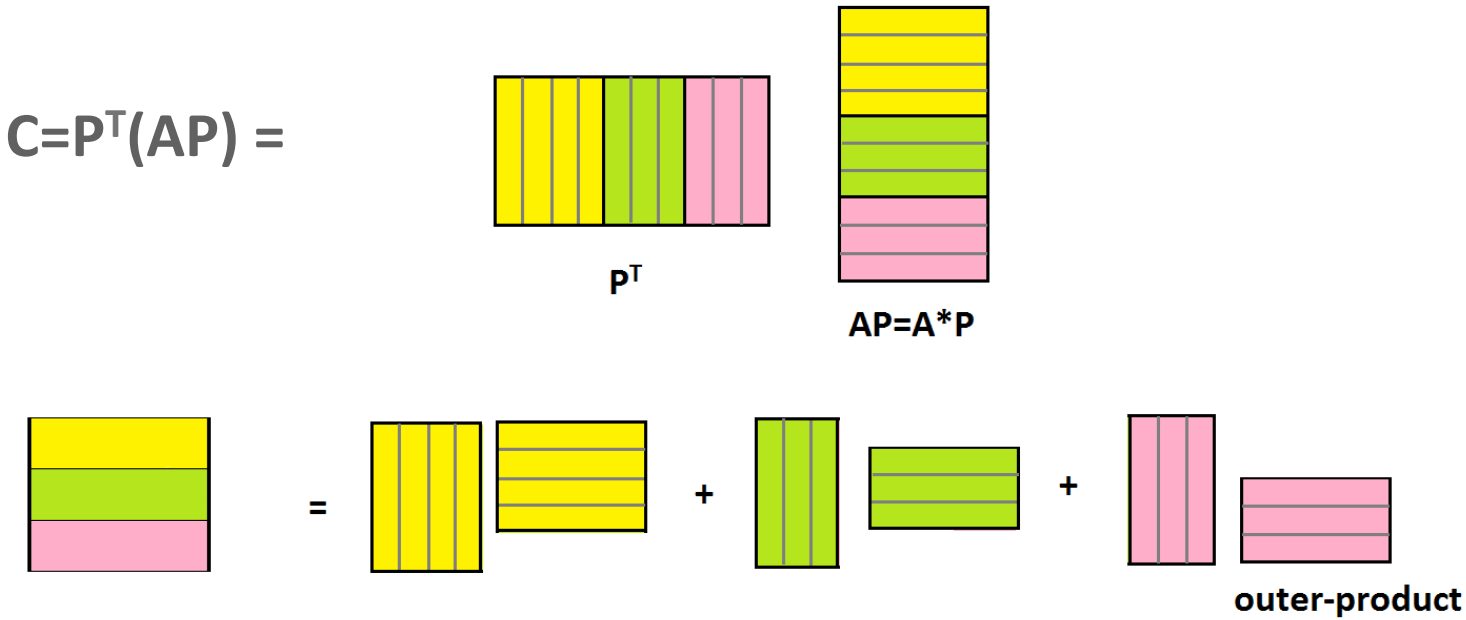


Weak Scalability of P^TAP
on Hopper@NERSC

# cores	27	216	1728	13,824
Solve time	13.2	17.2	19.5	
Setup	13.6	15.2	18.4	
P^TAP (5)	21.8	22.2	23.0	27.6
AB (5)				3.4
Iterations	39	50	55	
MFlops/core (solve)	248	245	241	

- AB only takes 12% of P^TAP execution time on 13,824 cores!

Sparse Matrix-Matrix Operations (parallel)



- Assembly C requires extensive inter-processor communications

Approach (suggested):

1. $R=P^T$ or user creates R
2. C=R*A*P

Sparse Matrix-Matrix Operations (parallel)

Trade-off between memory scalability and speed:

Example: C=A*P: C[i,:] = A[i,:] *Pseq

- '-matmatmult_scalable'

```
/* perform sparse axpy: apa_sparse: tmp array of local size Aloc_rmax*Ploc_rmax */
for (k=0; nextp<pnz; k++) {
      if (apJ[k] == pj[nextp]) { /* column of AP == column of P */
        apa_sparse[k] += valtmp*pa[nextp++];
      }
 }
```

- faster, but non-scalable:

```
/* perform dense axpy:  apa_dense: tmp array of global size PN */
for (k=0; k<pnz; k++){
      apa_dense[pj[k]] += valtmp*pa[k];
 }
```