Accelerating Configuration Interaction Calculations for Nuclear Structure

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June 22, 2008

Eigenvalue Computation by Implicitly Restarted Lanczos

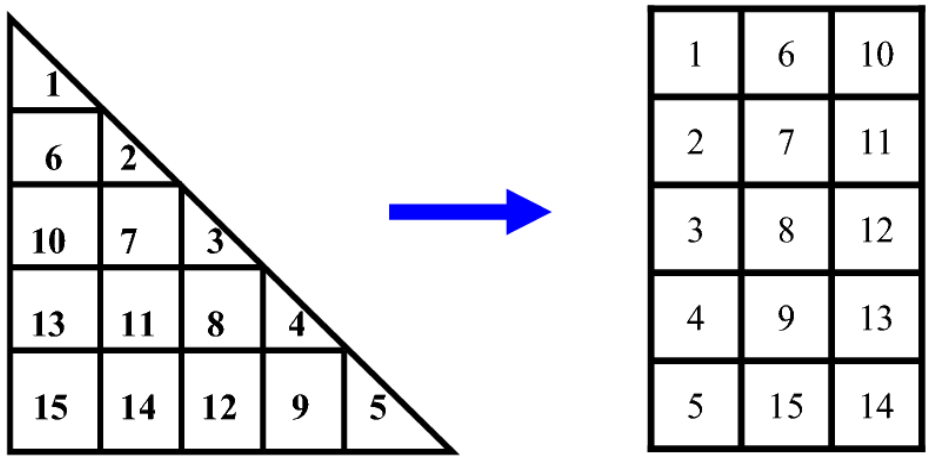
- How it works
  1. Lanczos factorization: $HV_{k+p} = V_{k+p}T_{k+p} + fe_{k+p}^T$
  2. Implicit restart: $H(V_{k+p}Q) = (V_{k+p}Q)(Q^T T_{k+p}Q) + fe_{k+p}^T Q$
  3. Expand: $HV_{k+p}^+ = V_{k+p}^+ T_{k+p}^+ + f^+ e_{k+p}^T$
- Why it works
  1. Similar to the implicit QR algorithm for dense eigenvalue problems
  $$Q = Q_1 Q_2 \cdots Q_p, \quad H - \mu_i I = Q_i R_i$$
  2. $V_{k+p}^+ e_1 = p(H)V_{k+p}e_1$, where
  $$p(\lambda) = (\lambda - \mu_1)(\lambda - \mu_2)\cdots(\lambda - \mu_p).$$
  3. Choices of k and p: k number of desired eigenvalues; $p = k$ or $p = 20$ (it is the degree of the filtering polynomial)

Parallelization

- Source of parallelism
  1. Matrix vector multiplication (MATVEC), application dependant: $y \leftarrow Hx$
  2. Orthogonalization $f \leftarrow (I - VV^T)y$
- Processor to matrix mapping
  - Hamiltonian: triangular processor grid
  - Lanczos vectors: remap to a rectangular grid

d **diagonal** processors

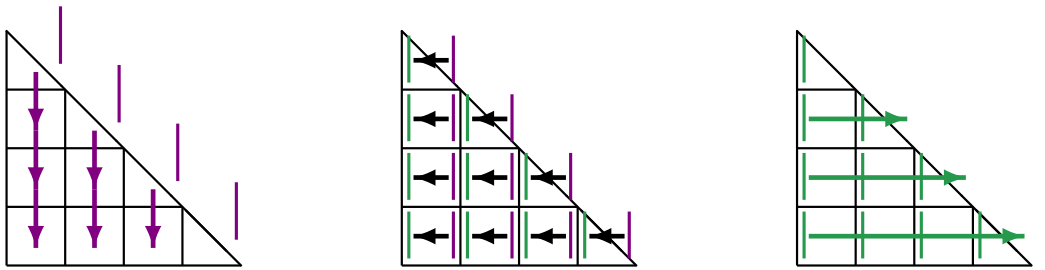
$d(d+1)/2$ total processors



Parallel Matrix-Vector Multiply

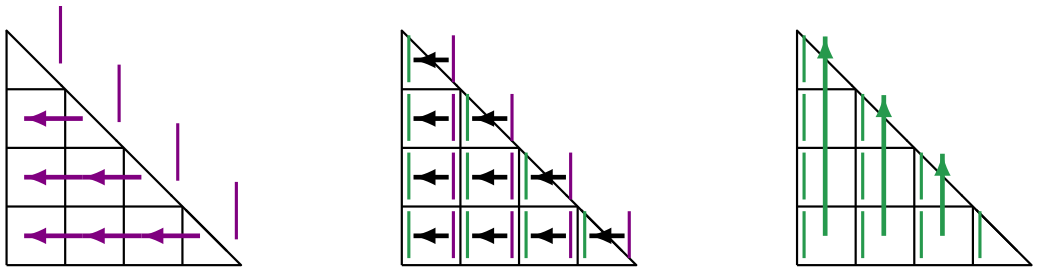
Steps for MATVEC: input (x) and output (y) vectors are stored on diagonal processors

1.



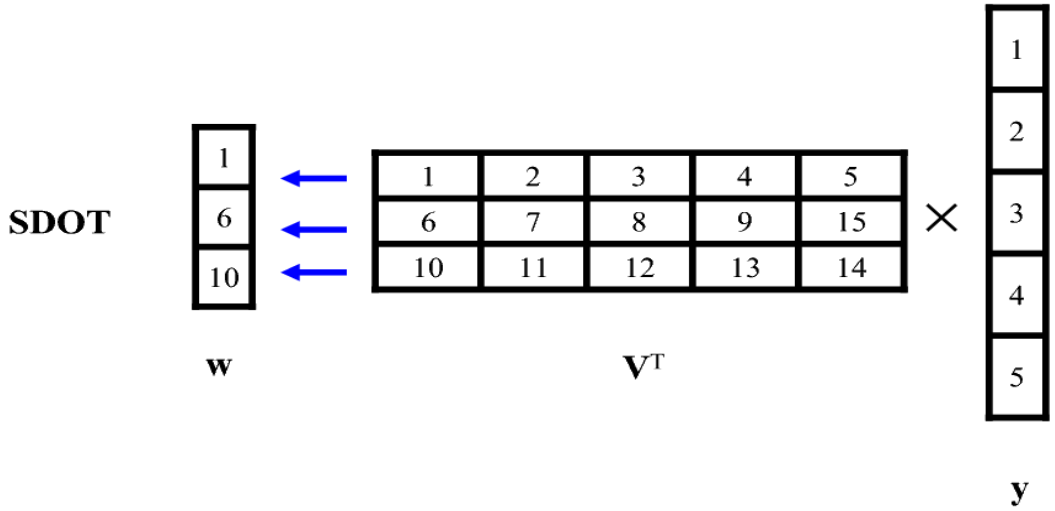
BCast(x) $y \leftarrow Ax$ Reduce(y)

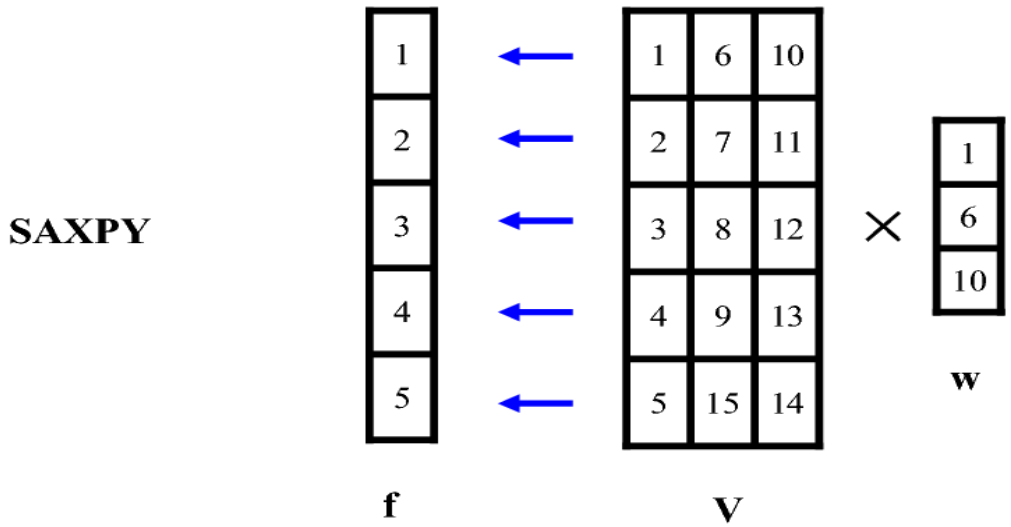
2.



BCast(x) $y \leftarrow A^T x$ Reduce(y)

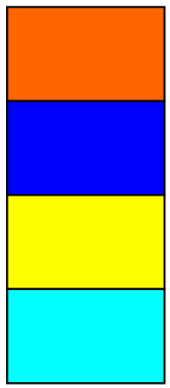
Parallel Orthogonalization $f \leftarrow V(V^T y)$



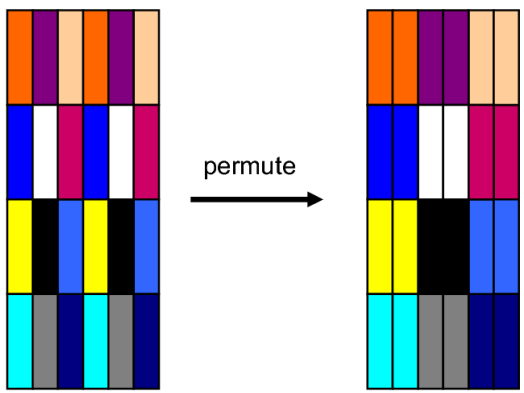


2D distributed PARPACK

- The official release of PARPACK partitions and distributes Lanczos vectors by rows. Orthogalization becomes costly when ncpus is large



- 2D cyclic distribution



ARPACK Modification

- Introduce two additional communicators
  1. All processor group
  2. Row group
  3. Column group
- Factorization and extend using 2D cyclic distribution along column groups

$$H(V_{k+p}P) = (V_{k+p}P)(P^T T_{k+p})P + fe_{k+p}^T P$$

- Implicit restart

$$H(V_{k+p}PQ) = (V_{k+p}PQ)[(PQ)^T T_{k+p}(PQ)] + fe_{k+p}^T (PQ)$$

Performance Improvement for Li^6

Problem size, proc used	1D PARPACK	2D PARPACK
Nmax=6, ncpus = 45	211	199
Nmax=8, ncpus = 496	342	287

Conclusions and Future Work

- Nuclear structure calculation is computationally demanding (large memory usage, irregular sparsity pattern, integer arithmetic);
- The ordering of MB basis states is crucial for achieving good load balance;
- Multi-level blocking is essential for efficient Hamiltonian construction; optimal partitions and levels?
- Alternative Hamiltonian ordering scheme for improving the locality of the data?
- Explore multi-core architecture to reduce memory usage