**Performance of Block Jacobi-Davidson EigenSolver Algorithms**

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**Numerical method**

**Eigenvalue problem definition**

- Calculate a small number of extremal eigenpairs \((\lambda, \mathbf{x})\) for a sparse, large matrix \(A\) if \(A\) is Hermitian.
- With an unshifted basis \(Q = \{\mathbf{q}_1, \ldots, \mathbf{q}_n\}\), each \(A\)-invariant subspace \(V = \text{span}(\mathbf{v}_1, \ldots, \mathbf{v}_m)\) one obtains the same stable block framework: \(AQ = QD\).

**Block correction equation**

- For more than 20 eigenpairs, the block Jacobi-Davidson method may be beneficial.

**Block vector operations**

- Required in each inner iteration (iterative solver for the block correction equation).
- Calculate block vector \(y\) for given \(X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}\) with \(Ay = \lambda y\).
- Shifted sparse matrix–multiple-vector multiplication (spMMVM) can be applied in one step.

**Applications from quantum physics**

**Spin matrices**

- Generic benchmark problem from quantum physics.
- Chain of \(J\)-electron spins \((s = 1/2)\) closed to a ring (Fig. 6).
- Computational representation of Hamilton operator in terms of bit patterns & bit swap/flip operations.
- Block vectors required as input to the spin vector.

**References**


**Software**

- **ESSEX (General Hybrid Optimized Sparse Toolkit)**
  - General hybrid optimized sparse toolkit
  - High-level parallel programming model for scalable and efficient sparse matrix computations
  - Support for CUDA, OpenMP, Pthreads, etc.

- **PHYSICS**
  - Electronic structure and quantum chemistry applications
  - Large-scale quantum chemistry problems

- **GHOST**
  - General hybrid optimized sparse toolkit
  - High-level parallel programming model for scalable and efficient sparse matrix computations
  - Support for CUDA, OpenMP, Pthreads, etc.

- **SGHOST**
  - High-level parallel programming model for scalable and efficient sparse matrix computations
  - Support for CUDA, OpenMP, Pthreads, etc.

**Setup**

- Spin matrices and vectors distributed on a cluster of 16 nodes (using MPI)
- Dual socket nodes with 10 cores per socket using OpenMP parallelization
- Intel Xeon E5-2660 v2 CPU (8 cores) at 2.20 GHz

**Results**

- Significant speedup of Jacobi-Davidson through blocking in contrast to the conclusion [1];
- For more than 20 eigenpairs blocking may be beneficial.
- Experimentation with different block sizes (2-4) and different numbers of MPI processes.
- Performance improvements for blocking numbers.

**Future work**

- Further research on the performance of the Jacobi-Davidson method by blocking.
- Use of hybrid parallelization strategies in the future.

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**Performance engineering of key operations**

**Jacobi-Davidson operator**

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- Shifted sparse matrix–multiple-vector multiplication (spMMVM) can be applied in one step.

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**Spin**

- Single-electron spin operators.
- Computational representation of Hamilton operator in terms of bit patterns & bit swap/flip operations.
- Block vectors required as input to the spin vector.

**Applications from quantum physics**

**Spin matrices**

- Generic benchmark problem from quantum physics.
- Chain of \(J\)-electron spins \((s = 1/2)\) closed to a ring (Fig. 6).
- Computational representation of Hamilton operator in terms of bit patterns & bit swap/flip operations.
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**References**

