Performance of Block Jacobi-Davidson

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Numerical method

Eigenvalue problem definition
Calculate a small number of external eigenpairs $(1, \lambda)$ for a sparse, large matrix $A$:

$$\lambda \min_{\|y\|_2=1} \max_{x} \frac{(Ax, y)}{(x, A^\top y)}$$

With an orthonormal basis $Q = [q_i]$ for the invariant subspace $(1, \lambda)$, one obtains the more stable block formulation:

$$Q^\top A Q = \begin{bmatrix} \lambda I & B \\ B^\top & \delta A \end{bmatrix}$$

With partial Schur decomposition with $Q = [Q_j]$:

$$\begin{bmatrix} \tilde{Q} \\ \delta Q \end{bmatrix} = Q \begin{bmatrix} I & \delta Q \tilde{Q} \\ 0 & I \end{bmatrix}$$

With a block Jacobi-Davidson algorithm one calculates correction vectors $\tilde{Q}_j^\top A \tilde{Q}_j$. If $\delta A$ is small enough, $Q$ is updated by $Q_{j+1} = Q_j + \tilde{Q}_j$.

Block correction equation

In each step of a block Jacobi-Davidson algorithm one calculates correction vectors $\tilde{Q}_j^\top A \tilde{Q}_j$. Here $Q_j$ is the current approximation with $\tilde{Q}_j$ and the column vectors $1$ to $I$.

Applications from quantum physics

Spin

Spin

4

Block performance in strong scaling experiments

Regrouping for blocked iterative solvers

- Group together similar operations of different systems.
- Employ faster block sparseMM and block vector operations.
- Reduce the number of MPI messages.
- Remove converged systems.
- Employ new systems.

Blocked GMRES algorithm

- Standard GMRES method (unpreconditioned)
- Single iteration:
  - Apply operator to preconjugate basic vector $\tilde{q}_j = (1 - \beta_j) Q \tilde{Q}_j$, orthogonal $\tilde{q}_j$ with all previous vectors.
  - Perform local operations (Gauss rotations, …)
- Basic vectors stored as blocks in a ring buffer (Fig. 2).
- Individual systems can be restarted when buffer is full.

Block performance in strong scaling experiments

Setup

- Sparse matrices and vectors distributed on a cluster of 1-44 nodes (using MPI)
- Dual socket nodes with 10 cores per socket (using OpenMP parallelization)
- Intel Xeon E5-2660 v2@ 2.20 GHz with 32GB of RAM. One i7 4790K (2.0 GHz) for single vector algorithm. Epetra 3.12 for 8, 16, 24, 32 cores.

Results

- Significant speedup of Jacobi-Davidson through blocking in comparison to the conclusion in [22] will be shown.
- The hosts for strong scaling tests are on up to 1200 cores.
- Small block sizes (10 or 20) are beneficial.
- Further effects of blocking:
  - Total communication volume increases (spMVM).
  - Total work of Jacobi-Davidson decreases with the performance.
  - See [2] for a detailed discussion.

Future work

- Overlap communication and computation:
  - Increased data traffic due to blocking
  - Use accelerator hardware such as GPUs.

References