Parallel QR Algorithm with Aggressive Early Deflation

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Trogir, October 2011
• Dense linear eigenvalue problems
  
  – Standard eigenvalue problem (SEP): $Ax = \lambda x$
  – Generalized eigenvalue problem (GEP): $Ax = \lambda Bx$

Sometimes **ALL** eigenvalues are needed.
Achieved via Schur decomposition: $A = QTQ^H$ or $(A, B) = (QSZ^H, QTZ^H)$. 
Modern QR Algorithm

- QR algorithm:
  1. (optional) Balancing (isolating and scaling)
  2. Hessenberg reduction ($A \rightarrow H$)

```
+---+    +---+  
|   |    |   |  
|   |    +---+  
```

3. Repeat
   Aggressive early deflation
   Multi-shift QR sweep (bulge-chasing)
   Until converge ($H \rightarrow T$)

```
+---+    +---+  
|   |    |   |  
|   |    |   |  
```

4. (optional) Backward transformation.
• Aggressive early deflation (AED)

\[
\begin{align*}
H &= \begin{pmatrix}
1 & H_{11} & H_{12} & H_{13} \\
H_{21} & H_{22} & H_{23} & 0 \\
0 & H_{32} & H_{33} & 0
\end{pmatrix}, \\
U &= \begin{pmatrix}
I & 1 \\
1 & V
\end{pmatrix}, \\
U^H H U &= \begin{pmatrix}
H_{11} & H_{12} & H_{13} V \\
H_{21} & H_{22} & H_{23} V \\
0 & s & S
\end{pmatrix}, \\
S &= V^H H_{33} V = \square.
\end{align*}
\]

– If the last entry of the vector \(s\) is small enough, we can deflate an eigenvalue.
– Otherwise, the undeflatable eigenvalue is moved up.
– Reduce back to Hessenberg form after all eigenvalues are tested.
– Undeflatable eigenvalues can be used as shifts in the next QR sweep.
- Software structure

**PDHSEQR**
Entry routine for new parallel QR algorithm.

**PDLAQR1**
Modified version of ScaLAPACK's current implementation of the parallel QR algorithm.

**PDLAQR0**
New parallel QR algorithm.

**PDLAQR3**
Aggressive early deflation and shift computation.

**PDLAQR5**
Multishift QR iteration based on chains of tightly coupled bulges.
Parallel QR Algorithm

- Parallel bulge-chasing algorithms
  (on distributed-memory systems)

ScaLAPACK 1.8.0

New algorithm

PDLAQR1()  BLAS-1  loosely coupled

PDLAQR5()  BLAS-3  tightly coupled
• Local bulge chasing

Several chains of tightly coupled bulges are chased simultaneously.
• Cross border chasing

Odd-numbered windows

Even-numbered windows
• Aggressive early deflation
  – Schur decomposition for a smaller matrix
    Several possible choices: recursion, (modified) ScaLAPACK solver, or even LAPACK solver.
    Depends on the size of AED window, as well as the number of processors.
  – We need to take care of eigenvalue reordering (PBDTRORD).
  – Usually the AED phase is slow since the submatrix (AED window) is not large enough.
    Sometimes we need to redistribute the submatrix to a subset of processors.
  – We prefer QR sweep since it scales better than AED. So the threshold (NIBBLE) for skipping a QR sweep is larger than that used in LAPACK.
A 16000 × 16000 dense eigenvalue problem with 100 processors

\[ H \rightarrow T = Q^T HQ \]

- ScaLAPACK
- New software
Profile of the total execution time ($A \rightarrow H \rightarrow T$)
$(4000 \times 4000 \text{ per core})$
A $100,000 \times 100,000$ Dense Eigenvalue Problem

<table>
<thead>
<tr>
<th># Procs</th>
<th>16 x 16</th>
<th>24 x 24</th>
<th>32 x 32</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Time</td>
<td>5.87 hrs</td>
<td>3.97 hrs</td>
<td>3.07 hrs</td>
</tr>
<tr>
<td>Balancing</td>
<td>0.24 hrs</td>
<td>0.24 hrs</td>
<td>0.24 hrs</td>
</tr>
<tr>
<td>Hess. red.</td>
<td>2.92 hrs</td>
<td>1.78 hrs</td>
<td>1.08 hrs</td>
</tr>
<tr>
<td>QR+AED</td>
<td>2.72 hrs</td>
<td>1.95 hrs</td>
<td>1.75 hrs</td>
</tr>
<tr>
<td>AED/(QR+AED)</td>
<td>44%</td>
<td>44%</td>
<td>42%</td>
</tr>
<tr>
<td>shifts per eig</td>
<td>0.30</td>
<td>0.22</td>
<td>0.16</td>
</tr>
</tbody>
</table>
Concluding Remarks

- New issues in the parallel QR algorithm
  - multiple chains of shifts
  - crossover points for different algorithms
  - shifting strategy
  - data redistribution
- The software will be released soon.
- Future work
  faster, faster, and even faster . . .
  (perhaps less and less energy consumption in the future)
Thank you!