Parallel Eigensolver Performance on High Performance Computers

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Summary

• (Briefly) Introduce parallel diagonalization methods
  – Application Background
  – Numerical Library Routines

• Parallel (MPI) Performance Analysis
  – For
    • Applications
    • Eigensolver methods
    • High-end Architectures

• Petascaling strategies
Interest in Eigensolver Performance

• Demand for efficient eigensolver performance
  – Traditionally a huge computational bottleneck
    • Especially Electronic Structure codes, Atomic Molecular Codes, large-scale problems.
      – At STFC this includes PRMAT, CRYSTAL, GAMESS-UK, KPPW
    • Large amounts of memory, cpu time and communication required
  – Researchers are not always using most efficient methods
    • Several methods to choose from
      – New developments with Divide and Conquer and Multiple Relatively Robust Representations
    • Performance is application dependent (differs from linear systems)
      – $\alpha O(n^3)$, where $\alpha$ can vary
Standard Eigenvalue problem

Standard Eigenvalue Problem:

\[ \mathbf{A} \mathbf{x} = \lambda \mathbf{x} \]

… where \( \mathbf{A} \) is a dense real matrix and \( \lambda \) is an eigenvalue corresponding to eigenvector \( \mathbf{x} \).

Diagonalization:

\[ \mathbf{A} = \mathbf{S} \Lambda \mathbf{S}^{-1} \]

… where the columns of matrix \( \mathbf{S} \) are represented by the eigenvectors of \( \mathbf{A} \) and the diagonal matrix \( \Lambda \) represents the associated eigenvalues.

If \( \mathbf{A} \) is symmetric, then:

\[ \mathbf{A} = \mathbf{Q} \Lambda \mathbf{Q}^T \]
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If \( \mathbf{A} \) is symmetric, then:

\[ \mathbf{A} = \mathbf{Q} \Lambda \mathbf{Q}^T \]

\( \Lambda \) captures key characteristics of \( \mathbf{A} \)
Underlying Equations

Solve the non-relativistic Schrodinger equation:

\[ \hat{H} \Psi = E \Psi \]

**PRMAT - Atomic & Molecular Physics Application Code**

- R-matrix based atomic scattering calculations
- Baluja-Burke-Morgan approach - Diagonalize Representative of the Green’s function \( (\hat{H} + \hat{L} - E \hat{I})^{-1} \) within a basis (Hamiltonian Matrix)

**CRYSTAL - Electronic Structure of Periodic Systems Code**

- Diagonalization of the effective one electron Hamiltonian gives the eigenstates and associated energies that the electrons may occupy
- Periodic Hartree-Fock or density functional Kohn-Sham Hamiltonian matrix
- Eigensolver often part of iterative process
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Solving the Symmetric Standard Eigenvalue Problem

The solution to the real symmetric Eigensolver problem usually takes place via three main steps

1. Reduction of the matrix to tri-diagonal form, typically using the Householder Reduction. \(O(n^3)\)

2. Solution of the real symmetric tri-diagonal Eigenproblem via one of the following methods:
   - Bisection for the Eigenvalues and inverse iteration for the Eigenvectors, up to \(O(n^3)\)
   - QR algorithm, up to \(O(n^3)\)
   - Divide & Conquer method (D&C), up to \(O(n^3)\)
   - Multiple Relatively Robust Representations (MRRR algorithm). \(O(nk)\)

3. Back transformation to find Eigenvectors for the full problem. \(O(n^3)\)

Other Methods
- Jacobi Method \(O(n^3)\)
- Symmetric Subspace Decomposition Algorithm
Parallel Real Symmetric Eigensolver Routines

**Scalapack**
- drivers for solving standard and generalized dense symmetric or dense Hermitian Eigenproblems.
- PDSYEV (QR Method) (Scalapack 1.5) *(all eigenpairs only)*
- PDSYEVX (Bisection & Inverse Iteration) (Scalapack 1.5) *(all/subset of eigenpairs)*
- PDSYEVD (D&C Method) (Scalapack 1.7) *(all eigenpairs)*
- PDSYEVR (MRRR Method) Scalapack *(1.9?)* - current version **under development** *(all/subset of eigenpairs) (Voemel et al.)*
- Memory overheads all $\sim O(n^2)$ except PDSYEVR $O(n)$ (in theory)

**Peigs**
- General symmetric and standard symmetric eigenproblems
  - PDSPEV (Bisection & Inverse Iteration) *(all/subset of eigenpairs)*

**Plapack**
- QR method *(all eigenpairs only)*
- MRRR ’Multiple Relatively Robust Representations’ *(all/subset of eigenpairs)*
Test Matrices

PRMAT
- Sector Hamiltonian matrices from external region Fe+ calculations
Matrix Characteristics
- Real, Symmetric
- Relatively well distributed eigenvalues
Matrix Sizes
- Dimension 10032, 20064, 35904, 63504

CRYSTAL
- Electronic Structure and Related properties of periodic systems
- All electron, local Gaussian basis set, DFT and Hartree-Fock
Matrix Characteristics
- Real, symmetric
- Many degeneracies - closely coupled eigenvalues.
- Varying degrees of sparsity
Matrix Sizes
- Dimension 7194, 12354, 20480 (Crystal, SCF-calc)
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Machines

Cray XT4 *HECToR*
  - DC 2.8 GHz Opterons 11328 cores
Cray XT3 *palu CSCS*
  - DC 2.6 GHz Opterons 3328 cores

IBM p5-575 *HPCx*
  - DC 1.7 GHz POWER5, HPS, 2560 cores
IBM BlueGene/P *Legion, STFC Daresbury*
  - QC PowerPC 850 MHz, 4096 cores
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Libraries

- Libsci, acml libraries
- Scalapack, pessl, essl
Parallel Performance of methods (CRYSTAL n=3888)

Parallel Diagonalizer Timings IBM p5-575
Matrix CRYSTAL n=3888

Time (seconds)

Number of Processors
Relative Scaling with Matrix Size (PRMAT)
Breakdown of Timings within the eigensolver (CRYSTAL n=12354)
Relative Scaling with Matrix Size
(PRMAT, large cases)

Number of Processors

Relative Performance

- Cray XT 4 PDSYEV n = 62304
- Cray XT 4 PDSYEV n = 35904
- Cray XT 4 PDSYEV n = 20064
- IBM p 5-575 PDSYEV n = 35904
- IBM p 5-575 PDSYEV n = 20064

n=~62K
n=~35K
n=~20K
Relative PDSYEVX Performance on HPC platforms

<table>
<thead>
<tr>
<th>Model</th>
<th>Ncpus</th>
<th>CPU</th>
<th>Interconnect</th>
<th>Site</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cray XT4</td>
<td>11328</td>
<td>Opteron 2.8 GHz</td>
<td>SeaStar</td>
<td>UoE, UK</td>
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<tr>
<td>IBM</td>
<td>2560</td>
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<td>IBM BG/P</td>
<td>4096</td>
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### Relative PDSYEVD Performance on HPC platforms

<table>
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</tbody>
</table>

**CRYSTAL matrix n=20480**
## Green Top 500 Supercomputer List

<table>
<thead>
<tr>
<th>Machine</th>
<th>Mflops/watt</th>
<th>Green Top 500 Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBM BG/P (STFC)</td>
<td>357.23</td>
<td>1</td>
</tr>
<tr>
<td>IBM BG/L (STFC)</td>
<td>215</td>
<td>6</td>
</tr>
<tr>
<td>Cray XT3 (CSCS)</td>
<td>56.58</td>
<td>145</td>
</tr>
<tr>
<td>IBM p5-575 (HPCx)</td>
<td>30.96</td>
<td>403</td>
</tr>
<tr>
<td>Cray XT4 (HECToR)</td>
<td>21.01</td>
<td>460</td>
</tr>
</tbody>
</table>

*Arbitrary, relative to BG/P 16 procs

Lower is better
Petascaling PRMAT: Partition of Configuration Space

External Region

Parallel Diagonalization of large Hamiltonian matrix required for each sector

• Sector diagonalizations can be undertaken simultaneously on sub-groups of processors.
Petascaling Diagonalization Calculations in PRMAT

Sector Hamiltonian matrices, n=20064

Parallelisation of Sector Calculations in PRMAT

Lower is better
Petascaling CRYSTAL

Graph showing the percentage execution time against the number of processors for HPCx Integrals, HECToR Integrals, HPCx Diag, and HECToR Diag.
Petascaling CRYSTAL

Possible Approaches:

• New parallel block D&C methods under development
  – Block tridiagonalization (Bai & Ward)
  – Block D&C method (Bai & Ward)
    • Possibility of trading accuracy for performance
  – Could also be in future releases of Scalapack

• Diagonalization-free methods
Conclusions (methods)

• PDSYEVD consistently the fastest parallel eigensolver (for all eigenpairs) for application matrices tested
  – particularly for degenerate eigenvalues
  – high memory overheads

• PDSYEVR performance close to matching PDSYEVD
  – final release may be even faster
  – should have lower memory overheads than PDSYEVD
  – ability to select subsets of eigenpairs

• Reduction to tridiagonal form dominates parallel performance
  – More efficient methods may be available in Scalapack 1.9?
Conclusions (machines)

- Cray XT4 / IBM Power 5 comparisons
  - Similar performance upto ~ 256 processors
  - Eigensolvers scale better on Cray XT4 on larger processor counts
    - Especially if the matrices are large

- May need new strategies for petascale architectures
  - How to scale performance upto 10000+ processors?

- Future Priorities
  - Mflops/s or Mflops/watt?
Acknowledgements

Christian Voemel, ETH Zurich
Ian Bush, Mike Ashworth, STFC Daresbury Laboratory
Technical Reports on Parallel Eigensolver Performance Analysis:

http://www.hpcx.ac.uk/research/hpc

Lapack Working Notes (LAWNS):
- Updates on parallel diagonalizer implementations in Scalapack
  http://www.netlib.org/lapack/lawns