Porting a sphere optimization program from LAPACK to ScaLAPACK

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Outline of talk

► The problem: maximizing a Gram determinant

► The approach: optimization using L-BFGS-B

► Converting the serial optimization code to ScaLAPACK

► Performance of the resulting parallel code
Maximizing a Gram determinant

Maximize the Gram determinant $\det G$ (Sloan, Womersley, 2004).

- Gram matrix $G$ of degree $n$ is a function of a set of points $\{x, \ldots, x_m\}$ on the unit sphere $S^2$, where $m = (n + 1)^2$.

  $$ G_{i,j} := \frac{n + 1}{4\pi} p(x_i \cdot x_j), $$

  where $p := P_n^{(1,0)}$ is a Jacobi polynomial of degree $n$.

- $G$ is symmetric non-negative definite.

- If $G$ is non-singular then $\{x_1, \ldots, x_m\}$ uniquely interpolates all spherical polynomials to degree $n$. 

Optimization using L-BFGS-B

Sphere optimization program SPHOPT uses L-BFGS-B to obtain a local maximum of $\det G$.

- L-BFGS-B (Zhu, Byrd, Lu, Nocedal, 1994)
  - Based on Limited Memory BFGS (Nocedal, 1980; Liu, Nocedal, 1989),
  - Based on BFGS (Broyden-Fletcher-Goldfarb-Shanno, 1970) quasi-Newton optimization method.

- L-BFGS-B needs the function value and gradient at each step.
SPHOPT function value and gradient

- **Function value** $f = \log \det G$ is obtained from the Cholesky decomposition $G = LL^T$ via

$$f = 2 \sum_{i=1}^{m} \log L_{i,i}.$$

- **Gradient** $\nabla f$ where $(\nabla f)_{k,i} := \frac{\partial f}{\partial X_{k,i}}$ is computed by

$$\nabla f = 2X \ (DG \bullet G^{-1}),$$

where $X_{k,i} := (x_i)_k$, $k = 1, 2, 3$, $(DG)_{i,j} := \frac{n+1}{4\pi} p'(x_i \cdot x_j)$ and $\bullet$ is the Hadamard product.

- SPHOPT uses LAPACK for Cholesky decomposition (DPOTRF), inverse (DPOTRI) and multiply (DSYMM).
ScaLAPACK

- Distributed memory parallel linear algebra (Choi, Dongarra, Pozo, Walker, 1992; Blackford et al. 1997).
- Distributed memory versions of LAPACK linear algebra routines, eg. dense solves, matrix inversion, eigensystems.
- Uses Block Cyclic data layout.
- Parallel Basic Linear Algebra Subroutines (PBLAS) includes matrix-vector and matrix-matrix products.
- Basic Linear Algebra Communications Subsystem (BLACS).
- Often implemented using Message Passing Interface (MPI) (Dongarra, Hempel, Hey, Walker, 1993).
PSPHOPT code structure using ScaLAPACK

- All processes run from the beginning of the one program.
- BLACS calls enable broadcast communication and synchronization between processes.
- To control loops and branches the PSPHOPT program:
  1. Sends all relevant data to a control process,
  2. Makes the decision in the control process,
  3. Broadcasts the decision.
- L-BFGS-B runs in the control process.
  1. Control process broadcasts the current point set $\mathbf{X}$,
  2. PSPHOPT uses ScaLAPACK to obtain $f$ and $\nabla f$,
  3. Control process calls L-BFGS-B with $f$ and $\nabla f$,
  4. L-BFGS-B calculates a new $\mathbf{X}$, or stops.
PSPHOPT code structure using ScaLAPACK

- ScaLAPACK calls need synchronization between processes.
- Structure of ScaLAPACK use is:
  1. Distribute operands,
  2. Synchronize,
  3. Operate,
  4. Distribute results.
- Gram matrix $G$ is a function of the current point set $X$.
  - Only $X$ needs to be distributed per step.
  - Each process creates its own local parts of $G$ and $DG$.
- PSPHOPT uses ScaLAPACK for Cholesky decomposition (PDPOTRF), inverse (PDPOTRI) and multiply (PDSYMM).
Compressed block cyclic storage

- ScaLAPACK uses Block Cyclic data distribution to store arrays.
- ScaLAPACK routines on symmetric matrices touch only one triangle.
- PSPHOPT uses a square processor array. This simplifies storage and addressing of symmetric matrices $G$ and $DG$.
- PSPHOPT uses the unused triangle of $G$ to store most cycles of $DG$. The diagonal cycles of $DG$ are stored in a separate array.
### Compressed block cyclic storage of $G$ and $DG$

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APAC SC nodes and interconnect


- Compaq AlphaServer SC45 with 127 nodes each containing:
  - 4 × 1 GHz ev68 (Alpha 21264C) cpus
  - L1 cache (on chip): 64 kbytes (I) + 64 Kbytes (D)
  - L2 cache (off chip): 8 Mbytes per cpu
  - between 4 and 16GB of RAM

- Quadrics Elan3 interconnect:
  - MPI latency of < 5 \( \mu s \)
  - MPI bandwidth of 250 Mbyte/s bidirectional
APAC AC nodes and interconnect

APAC National Facility AC cluster (2005 to present):

- SGI Altix 3700 Bx2 cluster with 30 nodes each containing:
  - 64 × 1.6 GHz Itanium2 cpus with:
    - L1 cache: 16 kbytes (D) + 16 kbytes (I). Cache line 64bytes
    - L2 cache: 256 kbytes. Cache line 128 bytes
    - L3 cache: 6 Mbytes. Cache line 128 bytes
  - between 128 GB and 384 GB of RAM

- SGI NUMAlink4 interconnect within and between nodes:
  - MPI latency of < 2 $\mu$s
  - Bandwidth of 3.2 Gbytes/s bidirectional
APAC SC: Gram matrix time

![Graph showing the relationship between Walltime (s) and Processors for different data points.

- Data points for 128, 96, and 63 processors with corresponding Walltimes: -1, -1, and -0.98, respectively.
- Another data point at 191 processors with a Walltime of -0.99.
- A data point at 127 processors with a Walltime of -1.26.

The graph indicates a decreasing trend in Walltime as the number of Processors increases.]
## APAC SC: Cholesky factor (PDPOTRF) time

<table>
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<tr>
<th>Processors</th>
<th>Walltime (s)</th>
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<tr>
<td>96</td>
<td>-0.77</td>
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<td>-0.61</td>
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<td>191</td>
<td>-0.89</td>
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<tr>
<td>127</td>
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![Graph showing the relationship between walltime and processors for Cholesky factor (PDPOTRF) with points at (128, -0.84), (96, -0.77), (63, -0.61), (191, -0.89), (127, -0.98).](image)
APAC SC: Cholesky inverse (PDPOTRI) time

Processors
Walltime (s)
128: −0.99
96: −0.91
63: −0.69
191: −0.87
127: −0.98
APAC SC: Total $f$ and $\nabla f$ time

![Graph showing the relationship between processors and walltime, with various points indicating different walltimes at different number of processors.]
APAC AC: Total L-BFGS-B, $f$ and $\nabla f$ time

![Graph showing walltime (s) against processors with two distinct lines, one with points at 96: -0.81 and 127: -0.94.](chart.png)