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 $\det \mathbf{G}$ (Sloan, Womersley, 2004).

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

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

  where $\mathbf{p} := \mathbf{P_n^{(1,0)}}$ is a Jacobi polynomial of degree $\mathbf{n}$.
- $\mathbf{G}$ is symmetric non-negative definite.
- If $\mathbf{G}$ is non-singular then $\{\mathbf{x_1}, \ldots, \mathbf{x_m}\}$ uniquely interpolates all spherical polynomials to degree $\mathbf{n}$.

Optimization using L-BFGS-B

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

- 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 $\mathbf{f = \log\det G}$ is obtained from the Cholesky decomposition $\mathbf{G = LL^T}$ via

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

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

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

  where $\mathbf{X_{k,i} := (x_i)_k}$, $\mathbf{k = 1, 2, 3}$, $\mathbf{(DG)_{i,j} := \frac{n+1}{4\pi} p'(x_i \cdot x_j)}$ 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 $\mathbf{f}$ and $\nabla\mathbf{f}$,
  3. Control process calls L-BFGS-B with $\mathbf{f}$ and $\nabla\mathbf{f}$,
  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 $\mathbf{G}$ is a function of the current point set $\mathbf{X}$.
  - Only $\mathbf{X}$ needs to be distributed per step.
  - Each process creates its own local parts of $\mathbf{G}$ and $\mathbf{DG}$.
- 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**

	0	0	1	1	0	0	1	1
0	$G_{1,1}$	$G_{1,2}$	$G_{1,3}$	$G_{1,4}$	$G_{1,5}$	$G_{1,6}$	$G_{1,7}$	$G_{1,8}$
0	$G_{2,1}$	$G_{2,2}$	$G_{2,3}$	$G_{2,4}$	$G_{2,5}$	$G_{2,6}$	$G_{2,7}$	$G_{2,8}$
1	$G_{3,1}$	$G_{3,2}$	$G_{3,3}$	$G_{3,4}$	$G_{3,5}$	$G_{3,6}$	$G_{3,7}$	$G_{3,8}$
1	$G_{4,1}$	$G_{4,2}$	$G_{4,3}$	$G_{4,4}$	$G_{4,5}$	$G_{4,6}$	$G_{4,7}$	$G_{4,8}$
0	$DG_{1,5}$	$DG_{1,6}$	$DG_{1,7}$	$DG_{1,8}$	$G_{5,5}$	$G_{5,6}$	$G_{5,7}$	$G_{5,8}$
0	$DG_{2,5}$	$DG_{2,6}$	$DG_{2,7}$	$DG_{2,8}$	$G_{6,5}$	$G_{6,6}$	$G_{6,7}$	$G_{6,8}$
1	$DG_{3,5}$	$DG_{3,6}$	$DG_{3,7}$	$DG_{3,8}$	$G_{7,5}$	$G_{7,6}$	$G_{7,7}$	$G_{7,8}$
1	$DG_{4,5}$	$DG_{4,6}$	$DG_{4,7}$	$DG_{4,8}$	$G_{8,5}$	$G_{8,6}$	$G_{8,7}$	$G_{8,8}$

APAC SC nodes and interconnect

Australian Partnership for Advanced Computing (APAC) National Facility SC cluster(2001 to 2005):

- 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

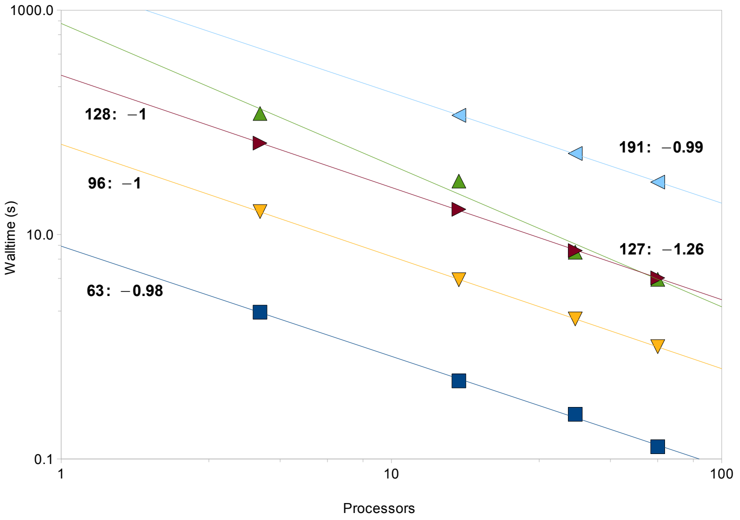
- Quadrics Elan3 interconnect:
  - MPI latency of $< 5\ \mu s$
  - MPI bandwidth of 250 Mbyte/s bidirectional

APAC AC nodes and interconnect

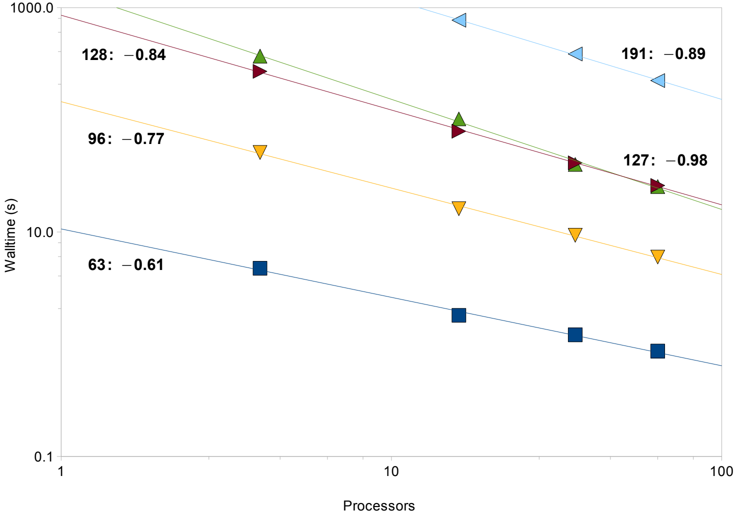
APAC National Facility AC cluster (2005 to present):

- SGI Altix 3700 Bx2 cluster with 30 nodes each containing:
  - 64 $\times$ 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

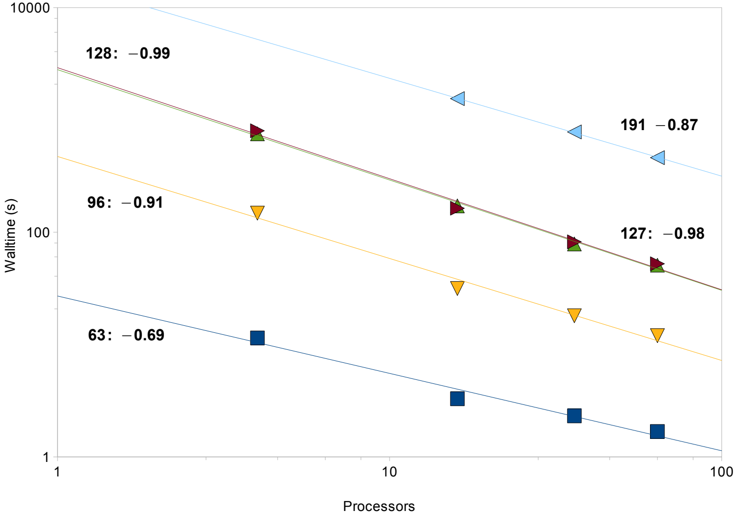
APAC SC: Gram matrix time



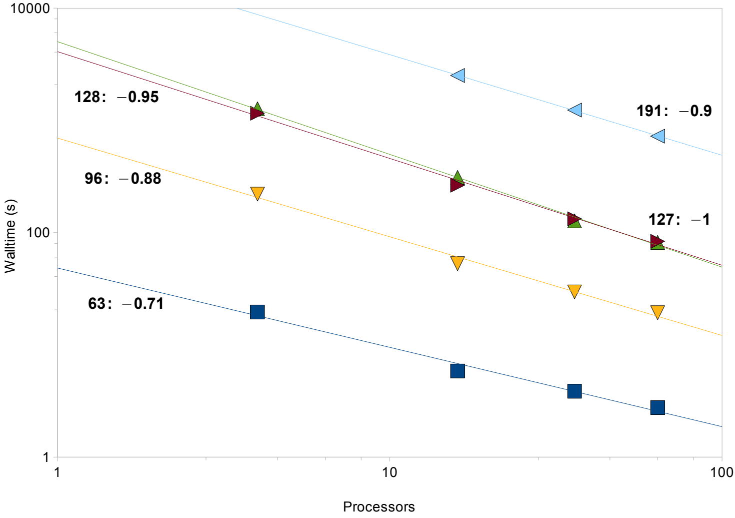
APAC SC: Cholesky factor (PDPOTRF) time



APAC SC: Cholesky inverse (PDPOTRI) time



APAC SC: Total $\mathbf{f}$ and $\nabla\mathbf{f}$ time



APAC AC: Total L-BFGS-B, $\mathbf{f}$ and $\nabla\mathbf{f}$ time