High-Performance Matrix Computations
Final Projects

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Deadline: Midnight, the evening before your oral exam

- Routines

  r1. Generalized eigensolvers $\begin{cases} \texttt{xSYGV, xSYGVD, xSYGVX} & \texttt{x} \in \texttt{[s|d]} \\ \texttt{xHEGV, xHEGVD, xHEGVX} & \texttt{x} \in \texttt{[c|z]} \end{cases}$

  r2. Dense eigensolvers $\begin{cases} \texttt{xSYEVR, xSYEV, xSYEVD, xSYEVX} & \texttt{x} \in \texttt{[s|d]} \\ \texttt{xHEEVR, xHEEV, xHEEVD, xHEEVX} & \texttt{x} \in \texttt{[c|z]} \end{cases}$

  r3. Tridiagonal eigensolvers `xSTEMR, xSTEQR, xSTEDC, xSTEVX` $\texttt{x} \in \texttt{[s|d]}$

- Matrix size

  n1. $n \in [10, \dots, 200]$
  n2. $n \in [200, \dots, 1500]$
  n3. $n \in [1500, \dots, N]$

$$N = \begin{cases} 10000 & \text{for r3} \\ 7000 & \text{for r2} \\ 4000 & \text{for r1} \end{cases}$$

- Matrix types

  t1. Random entries, uniform distribution (0,1)
  t2. Random entries, std normal distribution
  t3. Random eigenvalues, uniform (0,1)
  t4. Random eigenvalues, std normal distr.
  t5. Uniform eigenvalue distribution*
  t6. Geometric eigenvalue distribution*
  t7. $n-1$ eigvalues are ϵ, one is 1
  t8. one eigvalue is ϵ, $n-1$ are 1
  t9. Matrix 1-2-1*
  t10. Wilkinson-type matrix*
  t11. Clement-type matrix*
  t12. Legendre-type matrix*
  t13. Laguerre-type matrix*
  t14. Hermite-type matrix*

$*$: See page 119 of `http://arxiv.org/pdf/1401.4950v1.pdf`

Eigensolver study

Consider the eigensolvers in the group [r?] for datatype [?].

r1: $Az = \lambda Bz$ r2: $Ay = \lambda y$ r3: $Tx = \lambda x$

Q1. Compare the eigensolvers in terms of accuracy, performance and scalability, over a set[1] of matrices of type [t?] and different size [n?]. Document and report.

Q2. For each solver, give one or more indicative breakdowns of the computation time in terms of the calls directly within the routine. Repeat for 1 and ≥ 8 cores. Identify the bottleneck(s).

QB. **Bonus** (difficult): Assess the rate at which the flops of the tridiagonal solvers are performed. Compare with the TPP.

Q3. **Groups r1 and r2**: Optimize the blocksize `NB` of the reduction to tridiagonal form. Repeat with 1 and ≥ 8 cores.

Q4. **Group r1**: Relate the accuracy of each generalized solver to that of the corresponding dense and tridiagonal ones.

Q5. **Everybody**: You are given a sequence of at least 50 random symmetric tridiagonal matrices (type t1) of fixed size[2]. The solver of choice is xSTEDC.
What is the best way to make use of the available cores? Motivate your reasoning.

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[1] At least 6 matrices per matrix type.

[2] Fix a size $\bar{n} \in$ [n?].

How to build a matrix M with a given eigenspectrum?[3]

- The idea is to use similarity transformations, as they preserve the eigenspectrum.
  If Q is a dense orthogonal matrix, then
  $A := Q * \Lambda * Q^H$ is dense and $\lambda(A) = \lambda(\Lambda)$.

- For a dense eigenproblem, first construct Λ and then compute A.

  In order to create a dense orthogonal matrix Q,
  compute the QR factorization of a random matrix M.

- For a generalized eigenproblem, first build a dense problem,
  then construct an SPD matrix B, compute its Cholesky factor L,
  and $A := L * A * L^H$.

Accuracy for a generalized eigenproblem

- The eigenvectors X of the generalized eigenproblem $Ax = \lambda Bx$ are B-orthogonal:
  $X^H * B * X = I$.

[3] See attached file.

Rules and Submission

- Execute on one of the compute nodes of RZ's cluster:
  `https://doc.itc.rwth-aachen.de/display/CC/Hardware+of+the+RWTH+Compute+Cluster`
- Possible approaches are manual instrumentation, ELAPS, profilers and tools such as gprof and VTune, and any combination of them.
- Submit all your work, code, scripts, makefiles.
- For Q1, submit the tridiagonal representation of the matrices used.
- Prepare a report (pdf,org,html). Describe mathematically your computations.
- Archive the files: `your_name.tgz` or `your_name.zip`
- Submission by email to `pauldj@aices.rwth-aachen.de`
- Email's subject: ''`HPMC-15 Project your_last_name`''
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