ExaNLA Survey Response Report

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Submission Details

Library Name: DFTB+
Version: 24.1
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Organization: The University of Strathclyde

Selected NLA Operations

1. Other NLA Operation
2. Symmetric/Hermitian Eigenvalue Problems

1. Codes Information

Basic information about your application/simulation codes.

Library Name:
DFTB+

Current Version:
24.1

Contact Information:
Not specified

Name:
Ben Hourahine

Email:
benjamin.hourahine@strath.ac.uk

Organization:
The University of Strathclyde

Application Domain:
Not specified

What is the primary application domain of your codes?:
Materials Science, Other: Materials science, but also quantum chemistry, condensed matter

Materials Science:
Not specified

What are the main functionalities of your code?:
Ground state DFT, Time-dependent DFT, Molecular dynamics, Quantum transport, Excited-state dynamics, Surface science, Defect calculations, Other

If you selected "Other", please specify::
Semi-empirical (density-functional based tight binding) but close to DFT with some differences (smaller basis, trivial equation set-up time). Note this code is more heavily used for quantum chemistry than materials science, but also has condensed matter and engineering applications.

Climate/Weather Modeling:
Not specified

What are the main functionalities of your code?:
Not specified

If you selected "Other", please specify::
Not specified

Fluid Dynamics:
Not specified

What are the main functionalities of your code?:
Not specified

If you selected "Other", please specify::
Not specified

Other Domain Functions:
Not specified

What are the main functionalities of your code?:
Not specified

Use Case Information:
Not specified

Does your codes have multiple distinct use cases?:
Yes, multiple distinct use cases

Which use case are you describing in this submission?:
Ground state calculation code path

Library Description:
Electronic structure for non- and self-consistent models that are derived from DFT, but tabulated (with the addition of long-rage electrostatics if self-consistent). The ground state calculations, for reasonably large systems, spending ~90 of time in solving the generalised eigen-problem and another 10% in forming the density matrix via dsyrk / zherk operations. Or using some specialised solvers, directly from the starting matrices to the density matrix. The conventional solver route uses dense matrices, currently with BLACS decomposition, the direct solvers are either BLACS or a mixture of sparse formats (a form of CSR and also code specific). We may need to solve either real of complex cases and either a single set of eigen problems, or a coupled set over an index (spin and/or k-points). Note for the eigen-solution, we have not tested our Required tolerance/precision recently (possibly use of weaker tolerance for that stage of the calculation could be made, but we seem to need double precision for the self-consistency mixing of past solutions).

2. Other NLA Operation

Other NLA Operation:
Yes

Please specify your NLA operation:
Rank k-update (xSYRK / xHERK). Could use GEMM, but this is slightly faster and lower memory.

3. Generalized Eigenvalue Problems (Ax = »Bx)

Symmetric/Hermitian A, SPD B

Matrix Structure:
A is dense, B is dense, A is sparse, B is sparse, Complex valued, Real valued, Other: Internal storage in sparse format, then conversion for interfacing with solver(s)

Reduction to Standard Eigenproblem (using B):
Not specified

Reduction to Standard Eigenproblem:
Yes, always

Reduction Method:
Cholesky factorization of B (B = LLW or B = L*L)

Matrix Properties:
Not specified

Eigenvalue distribution:
Mix of clustered and separated

Problem Scale:
Large (10,000 - 100,000)

Computation Requirements:
Not specified

Percentage of eigenvalues:
All eigenvalues

What to compute:
Eigenvalues and eigenvectors

Eigenvalue location:
All eigenvalues

Required tolerance/precision:
Not specified

Residual tolerance type:
Absolute residual (||Ax - »x||)

Absolute residual tolerance:
High (10^-9)

Relative residual tolerance:
Not specified

Hybrid residual tolerance:
Not specified

Orthogonality tolerance:
High (10^-9)

Working Precision:
Double precision (64-bit)

Workload Characteristics:
Not specified

Computation Pattern: capability or capacity:
Repeated similar-sized problems (e.g., time evolution or parameter sweeps), Large-scale single problems (e.g., one large generalized eigenproblem at a time, using significant computational resources)

Distributed-Memory NLA Library Usage:
Not specified

Distributed-Memory Dense Linear Algebra:
ScaLAPACK, ELPA

Iterative Eigensolvers:
Not specified

High-Level & Interface Libraries:
ELSI – Abstraction layer for eigenvalue solvers (e.g., used by SIESTA, FHI-aims)

Are there any NLA libraries you are interested in using (but have not yet adopted)?:
EigenExa, ChASE, FEAST, SLATE

Benchmarking Requirements:
Not specified

Benchmark Input Types:

Real matrices from application workloads, Mini-apps or extracted kernels from real applications

Can You Provide Data or Mini-apps?:

Yes, both matrices and mini-apps

Scaling Requirements:

Weak scaling (fixed problem size per process/node), Both strong and weak scaling needed