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. 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?:
Other: Mostly quantum chemistry for this code path

Materials Science:
Not specified

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

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

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?:
Ground state DFT, Time-dependent DFT(B), Molecular dynamics, Quantum transport, Excited-state dynamics, Surface science, Defect calculations, Other

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?:
Excited state calculations

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). Excited state requires the ground state solution first at each geometry (see relevant survey entry), but the time dominate step on this code path is the excited solution stage. At the moment we have two different sub-code paths within the excited state path, the pARPACK route will probably eventually fully replace the other code path (the second is required for hybrid density-functionals as the matrices are non-symmetric in that case). I will therefore describe the ARPACK route.

2. Standard Eigenvalue Problems (Ax = »x)

Symmetric/Hermitian

Primary Use Cases:
Other: Casida (also known as Random Phase Approximation) equations from tight-binding models.

Matrix Properties and Structure:
Matrix-free (only matrix-vector products available)

Matrix Properties:
Not specified

Matrix Distribution:
Other: Matrix-vector, so not distributed, but the data to generate the action is replicated.

Matrix Storage Format:
Not specified

Positive definiteness:
Usually positive definite

Eigenvalue distribution:
Scattered/unpredictable

Problem Scale:
Large (10,000 - 100,000), Very Large (100,000 - 1,000,000)

Computation Requirements:
Not specified

Percentage of eigenvalues:
Less than 1%

What to compute:
Eigenvalues and eigenvectors

Eigenvalue location:
Smallest eigenvalues

Required tolerance/precision:
Not specified

Residual tolerance type:
Both absolute and relative

Absolute residual tolerance:
High (10^-9)

Relative residual tolerance:
High (10^-9)

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:
Large-scale single problems (e.g., one large matrix at a time, using significant computational resources)

Distributed-Memory NLA Library Usage:
Not specified

Distributed-Memory Dense Linear Algebra:
Not specified

Iterative Eigensolvers:
ARPACK – Shift-invert methods for symmetric eigenproblems

High-Level & Interface Libraries:
Other: Have tried ELSI-rci, but not currently using this.

Are there any NLA libraries you are interested in using (but have not yet adopted)?:
Not specified

Benchmarking Requirements:
Not specified

Benchmark Input Types:
Other: Probably best to generate these from the main application code efficiently on the fly (as matrix action on vector is performed so nothing stored).

Can You Provide Data or Mini-apps?:
Not specified

Scaling Requirements:
Both strong and weak scaling needed