ExaNLA Survey Response Report

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Submission Details

Library Name: Quantum ESPRESSO
Version: 7.5
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Selected NLA Operations

1. QR Factorization
2. Matrix-Matrix Multiplication (GEMM)
3. Cholesky Factorization

1. Codes Information

Basic information about your application/simulation codes.

Library Name:
Quantum ESPRESSO

Current Version:
7.5

Contact Information:
Not specified

Name:
Pietro Delugas

Email:
pdelugas@sissa.it

Organization:
SISSA

Application Domain:
Not specified

What is the primary application domain of your codes?:
Materials Science

Materials Science:
Not specified

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

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?:
Not specified

Use Case Information:
Not specified

Does your codes have multiple distinct use cases?:
No, single primary use case

Which use case are you describing in this submission?:
Ground state DFT calculations

Library Description:
Basic DFT code with ground state calculations, static perturbations (e.g. phonons, static dielectric constants), excitation spectra with TDDFT (e.g. Optical Spectra, EELS spectra, Magnons)

2. QR Factorization

QR Factorization (A = QR):
Yes

Matrix Properties:
Dense, Complex valued

Matrix Distribution:
Block cyclic distribution (e.g., ScaLAPACK style)

Matrix Storage Format:
Dense (column-major/row-major)

Matrix Properties:
Not specified

Condition Number:
Varies significantly

Matrix Dimensions:
Medium (1,000 - 10,000)

Matrix Shape:
Varies by application

Computation Requirements:
Not specified

What to Compute:
QR with column pivoting, Q factor only

Q Factor Handling:
Explicit Q matrix

Accuracy Requirements:
Not specified

Q Orthogonality:
High accuracy (10^-9)

Factorization Accuracy:
High accuracy (10^-9)

Working Precision:
Double precision (64-bit)

Workload Characteristics:
Not specified

Computation Pattern: capability or capacity:
Large-scale single factorizations (e.g., one large matrix at a time, using significant computational resources)

Distributed-Memory Dense Linear Algebra:
Not specified

Currently Used Libraries:
ScaLAPACK, ELPA

Interested in Using:
SLATE, DPLASMA

Specialized Libraries (Sparse/Structured/Hierarchical):
Not specified

Currently Used Libraries:
Other: none at the moment

Interested in Using:
Other: none at the moment

Benchmarking Requirements:
Not specified

Benchmark Input Types:
Mini-apps or extracted kernels from real applications

Can You Provide Data or Mini-apps?:
Yes, both matrices and mini-apps

Scaling Requirements:
Both strong and weak scaling needed

3. Matrix-Matrix Multiplication (GEMM)

Matrix-Matrix Multiplication (GEMM):
Yes

Matrix Properties:
Not specified

Matrix Structure:
Dense matrices

Matrix Distribution:
Block cyclic distribution (e.g., ScaLAPACK style), Block row/column distribution

Matrix Storage Format:
Dense (column-major/row-major)

Which types of matrix multiplications do you perform?:
Full GEMM (±AB + ^{2}C), Transpose multiplication (A@B, AB@),
multiplication (A†B, AB†), Standard multiplication (AB)

Typical Dimensions:
Not specified

Matrix Size Range:
Large (1,000 - 10,000)

Typical Matrix Shapes:
Square matrices (m "H n "H k), Tall-skinny matrices (m >>

Batch Size:
Small (< 10), Medium (10 - 100)

Distributed-Memory NLA Library Usage:
Not specified

General Distributed Memory Libraries (CPU/GPU):
ScaLAPACK, ELPA

Special/Advanced Implementations:
Other: none at the moment

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

Future Requirements:
Not specified

Desired Features:
Auto-tuning capabilities, Hardware-specific optimizations, Better mixed precision support, More flexible memory layouts, More efficient batched operations

Benchmarking Requirements:
Not specified

Benchmark Input Types:
Mini-apps or extracted kernels from real applications

Can You Provide Data or Mini-apps?:
Yes, mini-apps only, Yes, both matrices and mini-apps

Scaling Requirements:
Both strong and weak scaling needed

Working Precision:
Double precision (64-bit)

4. Cholesky Factorization

Cholesky Factorization (A = LL^T):
Yes

Diagonal Dominance:
Not diagonally dominant

Condition Number:
Varies widely / Not known

Matrix Properties and Structure:
Dense

Matrix Distribution:
Block row/column distribution, Block cyclic distribution (e.g., ScaLAPACK style)

Matrix Storage Format:
Dense (column-major/row-major)

Matrix Dimensions:
Medium (1,000 – 10,000)

Factorization Tolerance:
Very high accuracy (10^-12)

Working Precision:
Double precision (64-bit)

Workload Characteristics:
Not specified

Computation Pattern: capability or capacity:
Large-scale single factorizations (e.g., one large matrix at a time, using significant computational resources)

Distributed-Memory Dense NLA Library Usage:
Not specified

Currently Used Libraries:
ScaLAPACK, Other: Internal routines of Quantum ESPRESSO in LAXlib, ELPA

Interested in Using, but not currently using:
DLA-Future

Specialized Libraries (Sparse/Structured/Hierarchical):
Not specified

Currently Used Libraries:
Other: no specialized libraries

Interested in Using, but not currently using:
Other: no interest at the moment

Benchmarking Requirements:
Not specified

Benchmark Input Types:
Mini-apps or extracted kernels from real applications

Can You Provide Data or Mini-apps?:
Yes, both matrices and mini-apps

Scaling Requirements:
Both strong and weak scaling needed

5. Generalized Eigenvalue Problems (Ax = »Bx)

Symmetric/Hermitian A, SPD B

Matrix Structure:
A is dense, B is dense, Complex valued, Real valued

Reduction to Standard Eigenproblem (using B):
Not specified

Reduction to Standard Eigenproblem:
Yes, sometimes (depends on solver or problem)

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:
Medium (1,000 - 10,000)

Computation Requirements:
Not specified

Percentage of eigenvalues:
50-90%

What to compute:
Eigenvalues and eigenvectors

Eigenvalue location:
Smallest eigenvalues

Required tolerance/precision:
Not specified

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

Absolute residual tolerance:
Very high (10^-12)

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:
Large-scale single problems (e.g., one large generalized eigenproblem at a time, using significant computational resources), Many independent smaller problems (e.g., batch processing multiple generalized eigenproblems simultaneously)

Distributed-Memory NLA Library Usage:
Not specified

Distributed-Memory Dense Linear Algebra:
ScaLAPACK, ELPA, DLA-Future

Iterative Eigensolvers:
Other: KS solvers within Quantum ESPRESSO distribution

High-Level & Interface Libraries:
Not specified

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

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, mini-apps only

Scaling Requirements:
Both strong and weak scaling needed