ExaNLA Survey Response Report

Generated on: 10/17/2025 at 12:49:18 PM

Submission Details

Library Name: Principle modes
Version: No released version
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Organization: The University of Strathclyde

Selected NLA Operations

1. Other NLA Operation
2. Matrix-Matrix Multiplication (GEMM)

1. Codes Information

Basic information about your application/simulation codes.

Library Name:
  Principle modes

Current Version:
  No released version

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: Macroscopic Maxwell equations sover, using a semi-analytical method on the boundary of systems and expanding the field in a basis of multipoles. https://doi.org/10.1364/OE.19.021432

  Materials Science:
    Not specified

    What are the main functionalities of your code?:

    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?:
Frequency domain calculation of electromagnetic modes. These can then be used to evaluate various properties (absorption, scattering, q-factors non-linear effects, ...).

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?:
Ben Hourahine

Library Description:
Solves the electromagnetic modes of nanostructures in the frequency domain. Mathematical operation is equivalent to a least squares solution, A X = B, with a very poor condition number for A. But this approach uses the nature of the differential equations and their boundary conditions to write well conditioned equations on the interface between two sub-spaces of the system (and then evaluates principal angles and principal modes).

2. Other NLA Operation

Other NLA Operation:
Yes

Please specify your NLA operation:
Singular value decomposition, mostly for tall skinny matrices (>10K, ~1K) shape for a single particle. Multiparticle probably can be solved more efficiently, but naive solutions multiply these numbers by particle count.

3. Matrix-Matrix Multiplication (GEMM)

Matrix-Matrix Multiplication (GEMM):
Yes

Matrix Properties:
Not specified

Matrix Structure:
Dense matrices, Tall-and-skinny matrices, Other: Multiple indepdendent calculations at different frequencies, but if phase coherence is required there is an inter-frequency set of SVD problems.

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

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

Which types of matrix multiplications do you perform?:
Hermitian multiplication (A†B, AB†)

Typical Dimensions:
Not specified

Matrix Size Range:
Very Large (10,000 - 100,000)

Typical Matrix Shapes:
Tall-skinny matrices (m >> k, n small)

Batch Size:
Not specified

Distributed-Memory NLA Library Usage:
Not specified

General Distributed Memory Libraries (CPU/GPU):
ScaLAPACK

Special/Advanced Implementations:
Not specified

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

Future Requirements:
Not specified

Desired Features:
Auto-tuning capabilities, Other: Hybrid CPU-GPU

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?:
Not sure yet

Scaling Requirements:
Weak scaling (fixed problem size per process/node)

Working Precision:
Double precision (64-bit)