MaX DRIVING THE EXASCALE TRANSITION

Software engineering towards exascale: domain specific libraries, communication optimality, and machine learning

J. VandeVondele, A. Kozhevnikov, M. Kabic,
S. Jakobovits, S. Pintarelli, S. Frasch, M. Taillefumier
CSCS, ETH Zurich

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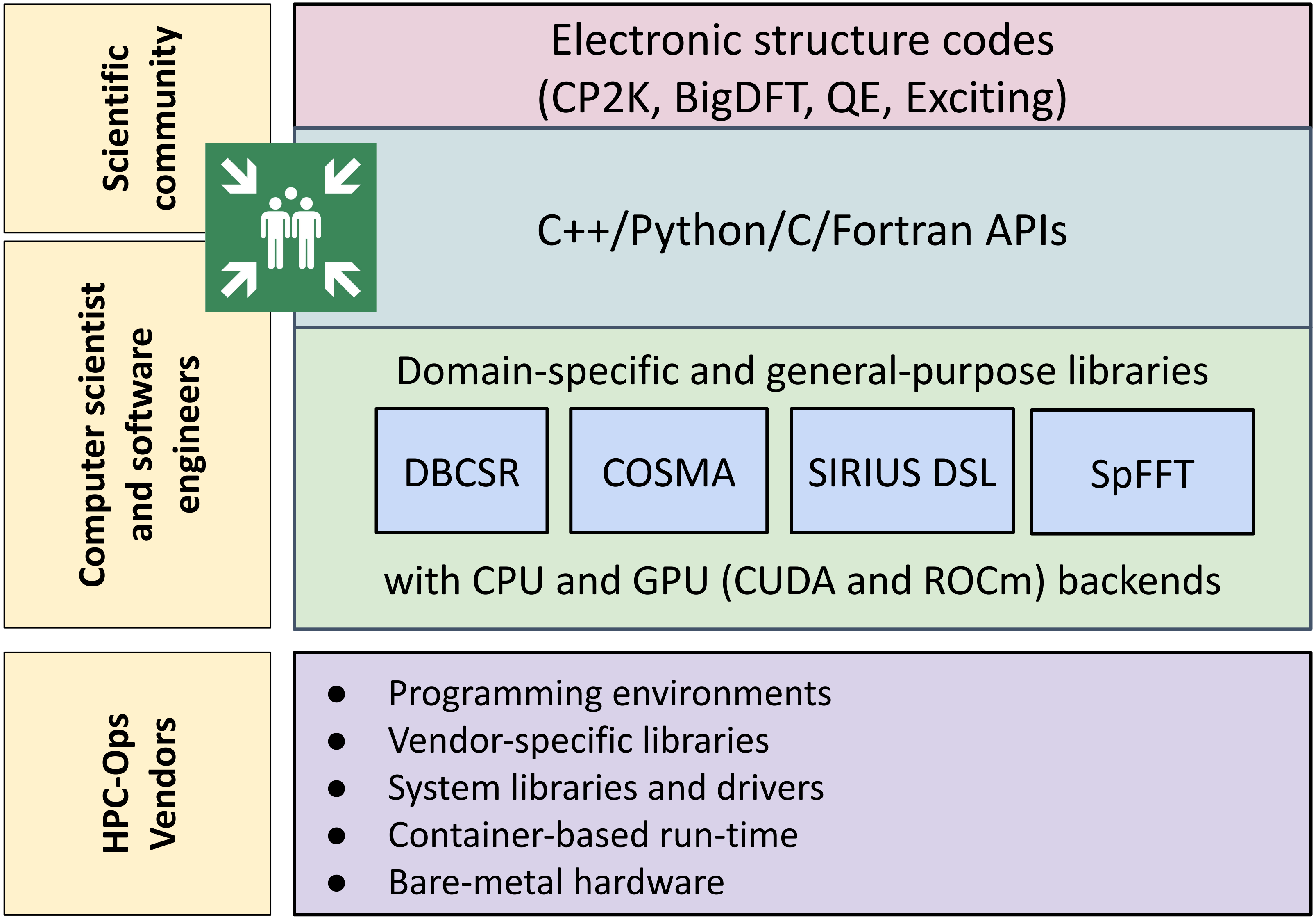
Overview

within MaX2, ETH Zurich delivers and promotes:

- The principle of separation of concerns
- general-purpose and domain specific libraries
  - NVIDIA GPU and AMD GPU hardware readiness
  - Communication-optimal algorithms
  - Machine-learning techniques for the performance
- Access to novel architectures and programming paradigms
- Knowledge transfer on the topics of HPC and HTC

Current software stack



Scientific community

Computer scientist and software engineers

HPC-Ops Vendors

Electronic structure codes
(CP2K, BigDFT, QE, Exciting)

C++/Python/C/Fortran APIs

Domain-specific and general-purpose libraries

DBCSR

COSMA

SIRIUS DSL

SpFFT

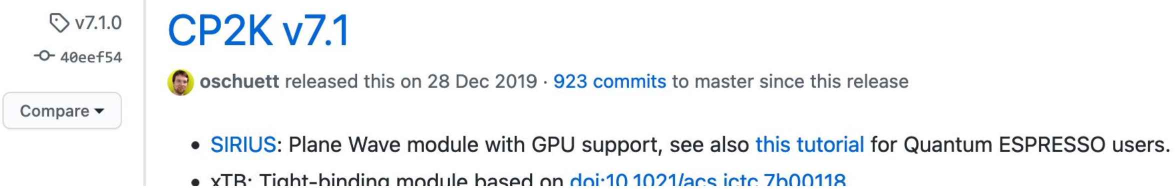
with CPU and GPU (CUDA and ROCm) backends

- Programming environments
- Vendor-specific libraries
- System libraries and drivers
- Container-based run-time
- Bare-metal hardware

SIRIUS DSL | Overview

SIRIUS is a domain specific library for electronic structure calculations, and is designed for GPU acceleration of popular community codes such as BigDFT, CP2K, Exciting, Elk and Quantum ESPRESSO

- MPI and OpenMP parallel
- Nvidia and AMD GPUs
- Fully featured



CP2K v7.1

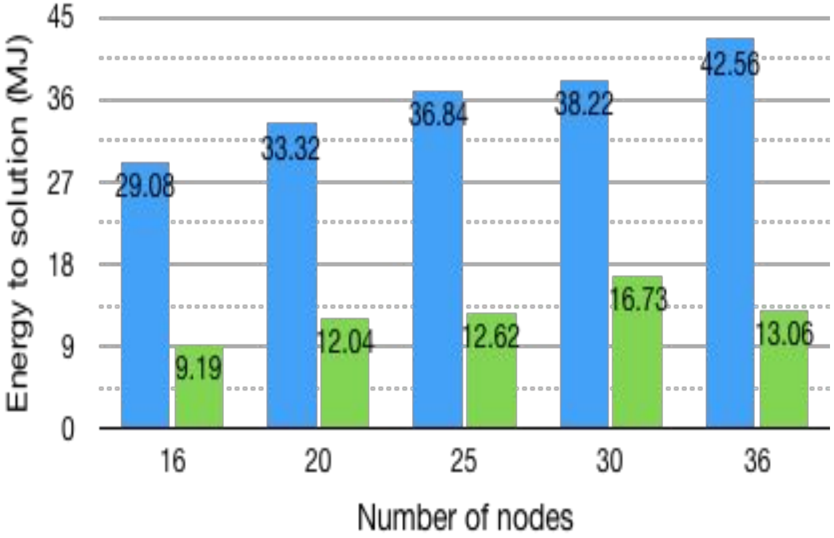
oschuett released this on 28 Dec 2019 · 923 commits to master since this release

- SIRIUS: Plane Wave module with GPU support, see also this tutorial for Quantum ESPRESSO users.
- xTB: Tight-binding module based on doi:10.1021/acs.jctc.7b00118

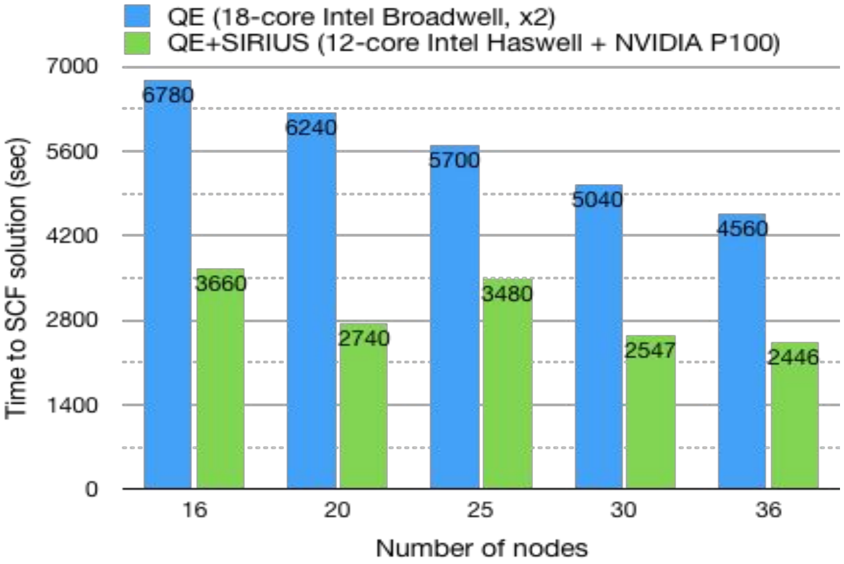
Features		
Pseudopotential	Full-potential	Common
● NC/US/PAW pseudopotentials ● Collinear and non-collinear magnetism ● Hubbard U correction ● Spin-orbit coupling ● Stress tensor ● Atomic forces ● Verification of S-operator matrix ● Iterative Davidson and exact diagonalization solvers	● L(A)PW+lo method with arbitrary number of local orbitals ● Collinear and non-collinear magnetism with second variational approach ● Iterative Davidson and exact diagonalization solvers ● Spin-orbit coupling ● Atomic forces	● Python frontend ● Symmetrization of lattice-periodic functions and on-site matrices (using symmetries from *spglib*) ● Generation of **k**-point mesh using *spglib* ● Run-time control of the eigenvalue solvers (Lapack / MAGMA / ScaLAPACK / ELPA) ● Run-time control of the BLAS provider (CPU BLAS / cuBlas / cuBlasXt)

SIRIUS DSL | GPU (NVIDA and AMD) backend for Quantum ESPRESSO

ENERGY TO SOLUTION



TIME TO SOLUTION

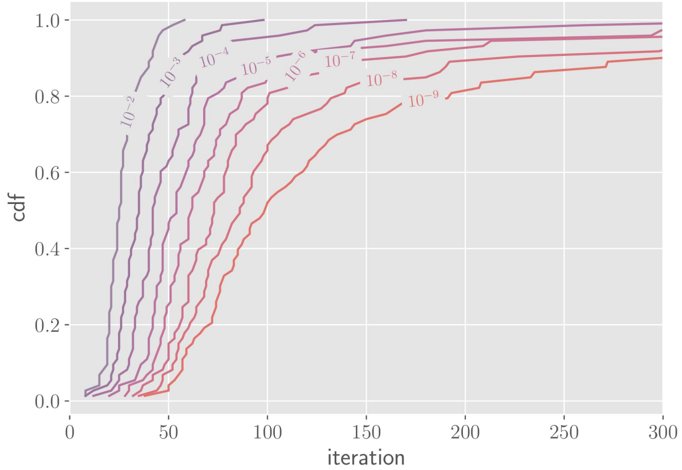


A single GPU node of Piz Daint outperforms a multicore node, in both time and energy to solution by 200% - 300%

443-atom unit cell of IrC

Enables high throughput computing (HTC) with robust methods

- The standard SCF cycle often fails to converge
- Direct minimization algorithms provide a robust alternative method
- Enable Exascale-level HTC calculations based on the AiiDA framework.

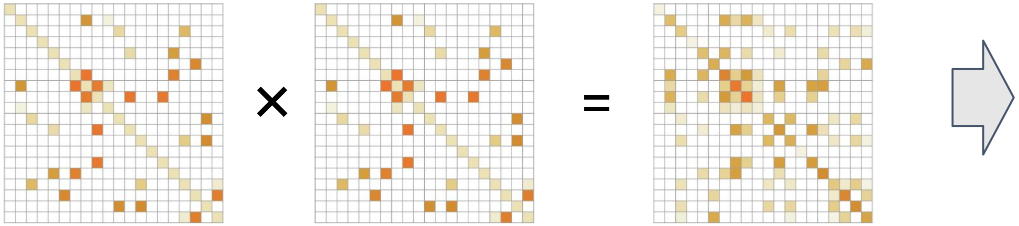


100 metallic (magnetic) systems failing to converge with the SCF cycle. Recent tests carried out by Marnik Bercx from EPFL yielded a 98% success rate with tolerance 10^{-10} (NC pseudos). Results for the ultrasoft case are in preparation.

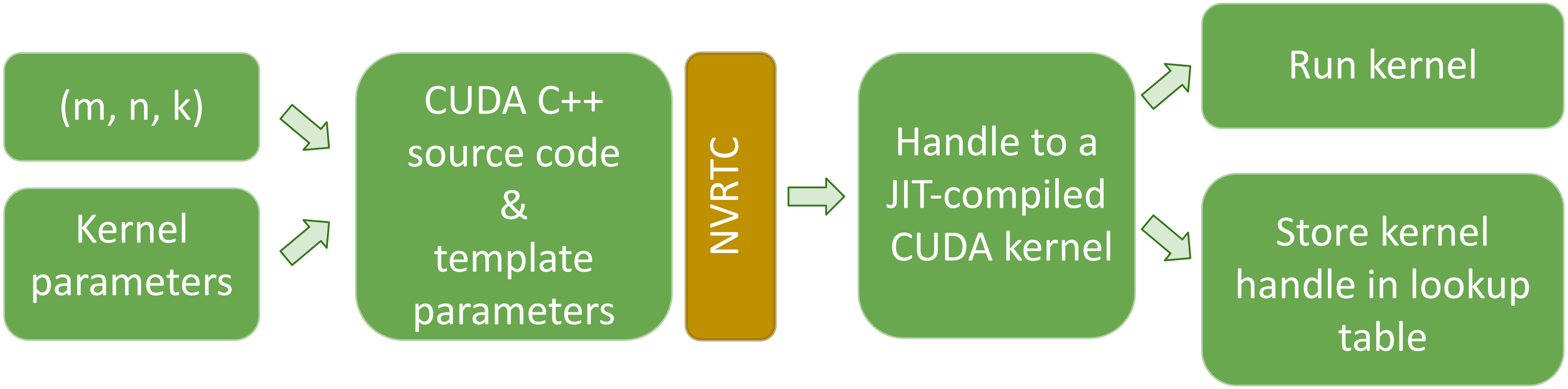
- Robust optimization is implemented in the SIRIUS python module or in C++ library
- Performance portability (Nvidia or AMD gpus) via Kokkos and GPU BLAS/LAPACK libraries
- In SIRIUS enabled QuantumESPRESSO

DBCSR library | Overview

DBCSR is a highly optimized library designed to perform sparse matrix-matrix multiplication at scale.



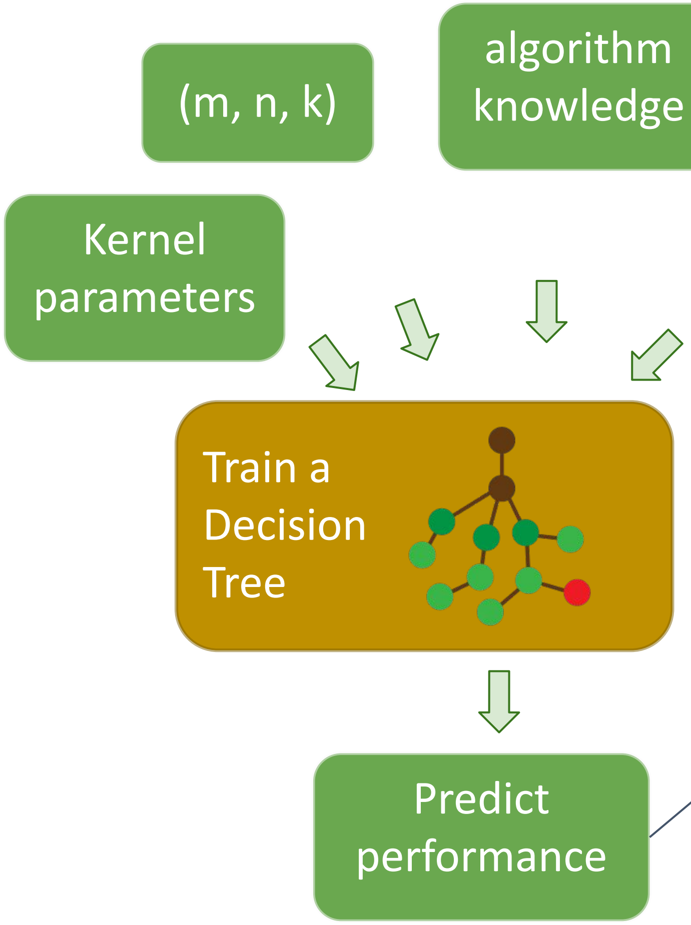
broken down into small dense blocks, run on GPU


(m, n, k)
Kernel parameters
CUDA C++ source code & template parameters
NVRTC
Handle to a JIT-compiled CUDA kernel
Run kernel
Store kernel handle in lookup table

10’000s of kernels each with 10’000s of possible parameters
Predict optimal implementations of all kernels using ML!

DBCSR library | Machine Learning for optimal compute kernel parameters

Finds near-optimal kernels within 2% of best possible performance



(m, n, k)

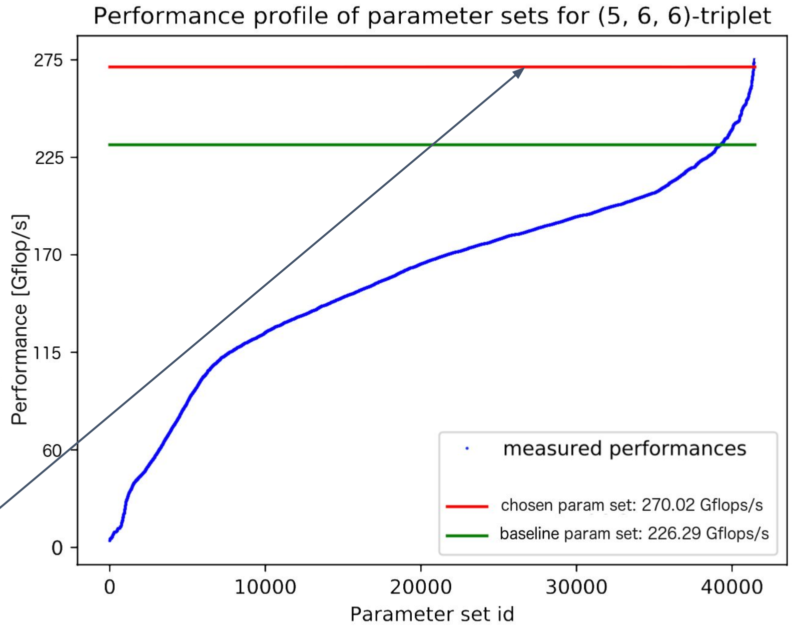
algorithm knowledge

Kernel parameters

hardware knowledge

Train a Decision Tree

Predict performance



Performance profile of parameter sets for (5, 6, 6)-triplet

CUDA / ROCm and OpenCL backends are implemented!

COSMA library | Motivation

Achieve communication-optimality in matrix-matrix multiplication, 50 years of algorithmic progress!

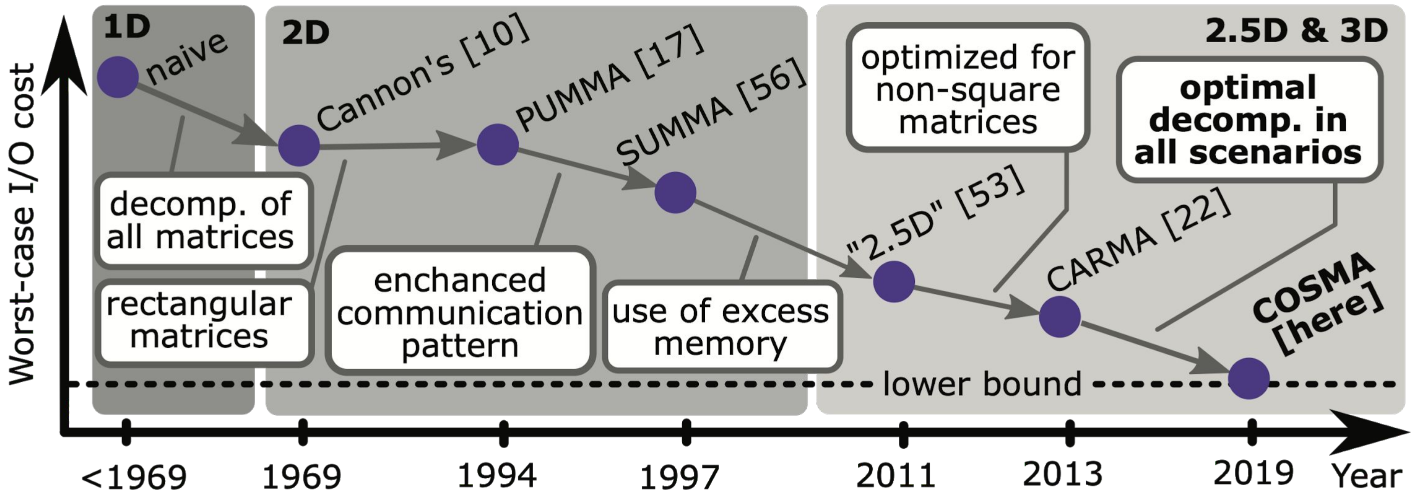
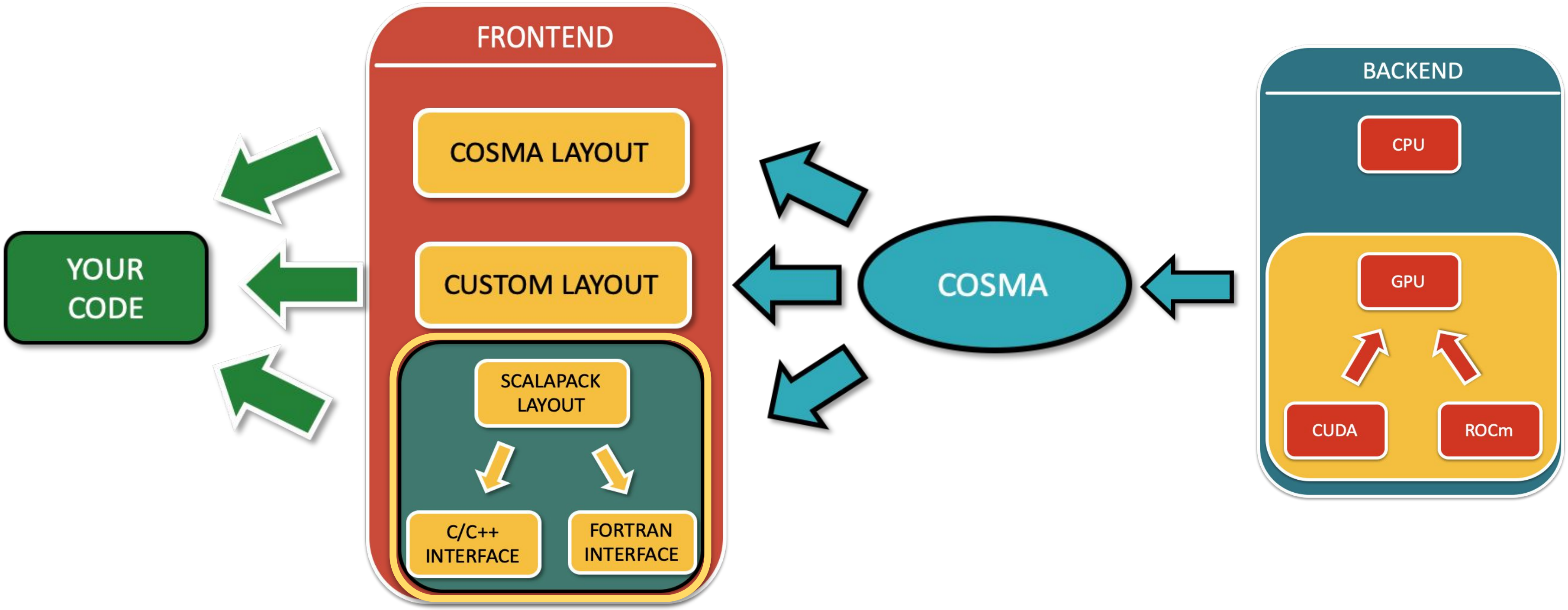


Figure 2: Illustratory evolution of MMM algorithms reaching the I/O lower bound.

COSMA is communication-optimal for all combinations of matrix dimensions, number of processors and memory sizes, without the need for any parameter tuning.

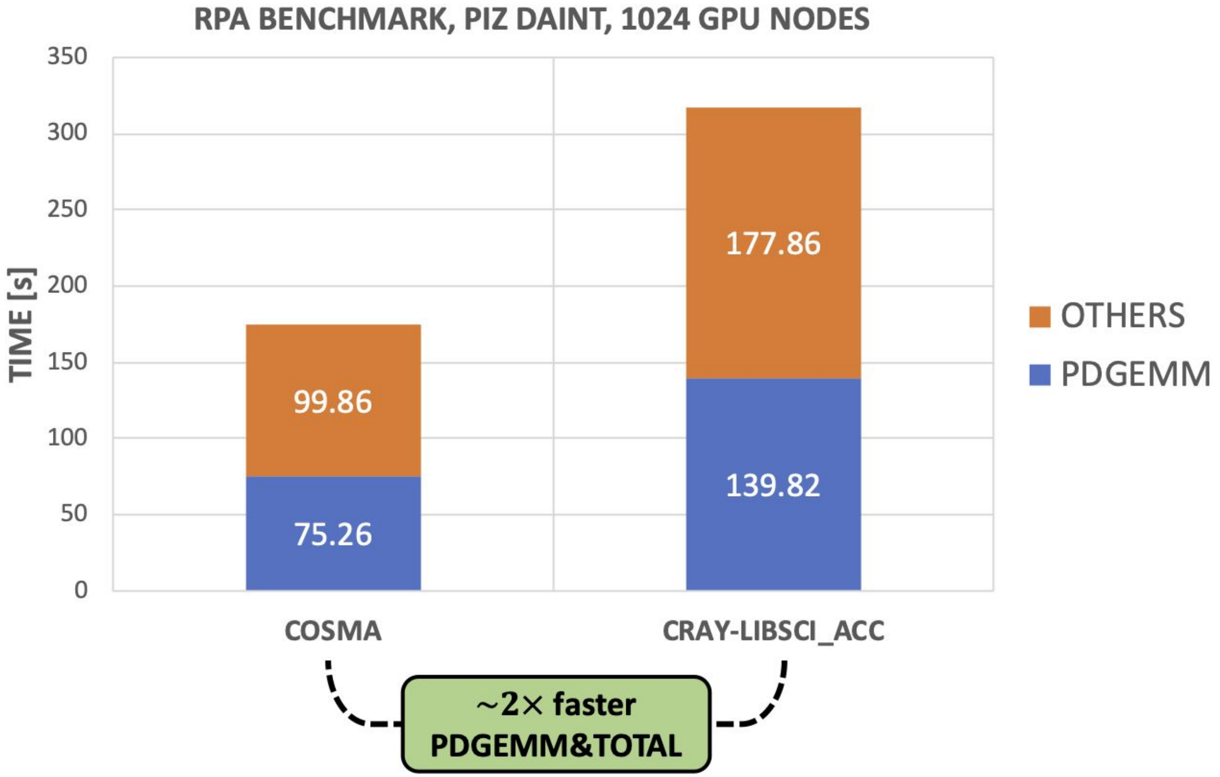
COSMA library | Overview

- MPI and OpenMP parallel
- Nvidia and AMD GPUs via CUDA and ROCm
- Drop-in replacement for ScaLAPACK, no re-coding needed



COSMA library | Performance

On 1024 nodes, the speedup becomes even very significant, outperforming vendor specific solutions significantly



~2× faster PDGEMM&TOTAL

COSMA library is fully integrated in the CP2K toolchain and used in production in order to accelerate large tall-and-skinny matrix multiplications arising in RPA calculations.

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Thanks you! Questions?

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