MAX DRIVING THE EXASCALE TRANSITION

The DBCSR Library

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The DBCSR Library

- **Distributed**
  - **MPI** parallelization is based on the Cannon algorithm
  - On node with **OpenMP**
- **Block Compressed Sparse Row**
  - Block-sparse, where blocks correspond to atoms
- **Sparse matrix-matrix multiplication library (SpGEMM)**
  - As well as other linear algebra operations
  - And: tensor contractions framework

The DBCSR Library

- Written in Fortran
- Types supported: double
- GPU accelerated for NVIDIA & AMD via CUDA & HIP
- First written as a part of CP2K, but now released as standalone

Code snippets

- DBCSR has a Fortran API as well as a C API

Code snippets: initialize the library

```
! initialize libdbcsr
CALL dbcsr_init_lib(MPI_COMM_WORLD)

!
! the matrix will contain nblkrows_total row blocks and nblkcols_total column blocks
nblkrows_total = 4
nblkcols_total = 4

!
! set the block size for each row and column
ALLOCATE (row_blk_sizes(nblkrows_total), col_blk_sizes(nblkcols_total))
row_blk_sizes(:) = 2
col_blk_sizes(:) = 2
```

Code snippets: set row/col distributions

```
   !
   ! set the row and column distributions (here the distribution is set randomly)
   CALL random_dist(row_dist, nblkrows_total, npdims(1))
   CALL random_dist(col_dist, nblkcols_total, npdims(2))

   !
   ! set the dbcsr distribution object
   CALL dbcsr_distribution_new(dist, group=group, row_dist=row_dist, col_dist=col_dist,
reuse_arrays=.TRUE.)
```

Code snippets: create a matrix

```
!
! create the dbcsr matrices, i.e. a double precision non symmetric matrix
! with nblkrows_total x nblkcols_total blocks and
! sizes "sum(row_blk_sizes)" x "sum(col_blk_sizes)", distributed as
! specified by the dist object
CALL dbcsr_create(matrix=matrix_a, &
                  name="this is my matrix a", &
                  dist=dist, &
                  matrix_type=dbcsr_type_no_symmetry, &
                  row_blk_size=row_blk_sizes, &
                  col_blk_size=col_blk_sizes, &
                  data_type=dbcsr_type_real_8)
```

Code snippets: set up matrix elements

```
!
! set up the a matrix
CALL dbcsr_distribution_get(dist, mynode=mynode)
ALLOCATE (values(max_nze))
DO row = 1, dbcsr_nblkrows_total(matrix_a)
   DO col = MAX(row - 1, 1), MIN(row + 1, dbcsr_nblkcols_total(matrix_a))
      row_s = row; col_s = col
      CALL dbcsr_get_stored_coordinates(matrix_a, row_s, col_s, node_holds_blk)
      IF (node_holds_blk .EQ. mynode) THEN
         nze = row_blk_sizes(row_s)*col_blk_sizes(col_s)
         CALL RANDOM_NUMBER(values(1:nze))
         CALL dbcsr_put_block(matrix_a, row_s, col_s, values(1:nze))
      ENDIF
   ENDDO
ENDDO
DEALLOCATE (values)
```

Code snippets: multiply matrices

```
!
! finalize the dbcsr matrices
CALL dbcsr_finalize(matrix_a)
! b, c ...

!
! multiply the matrices
CALL dbcsr_multiply('N', 'N', 1.0D0, matrix_a, matrix_b, 0.0D0, matrix_c)

!
! print the matrices
CALL dbcsr_print(matrix_a)
! b, c ...
!
! release the matrices
CALL dbcsr_release(matrix_a)
! b, c ...
```

Installation & Requirements

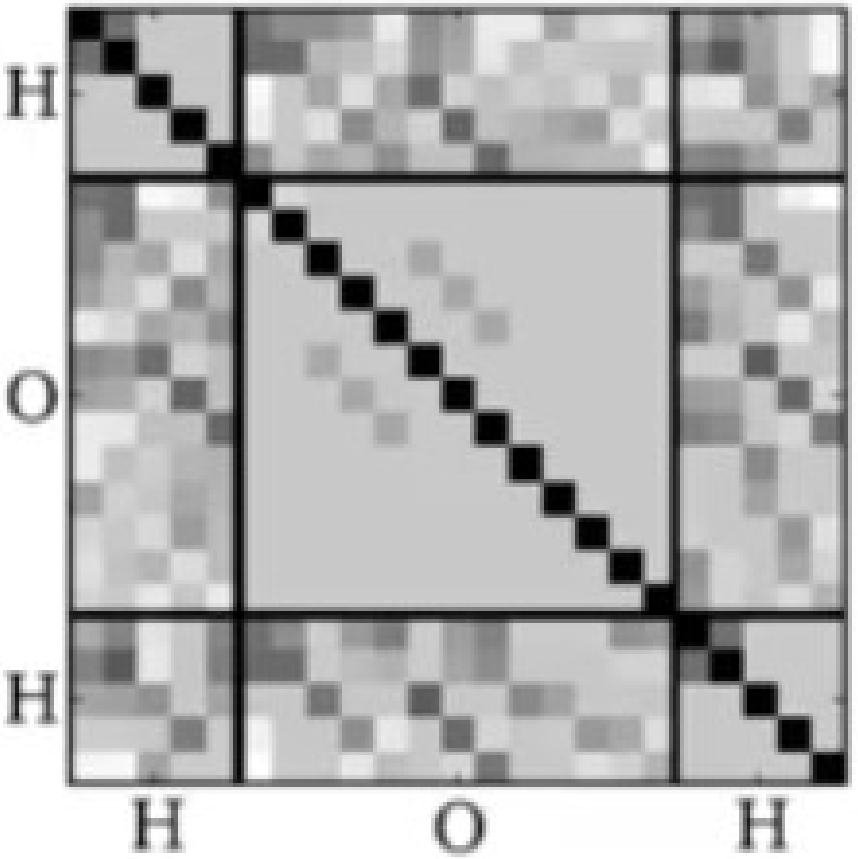
- Requirements
  - Cmake and GNUmake, Ninja
  - A BLAS + LAPACK implementation
  - (Optional: libxsmm)

- Build

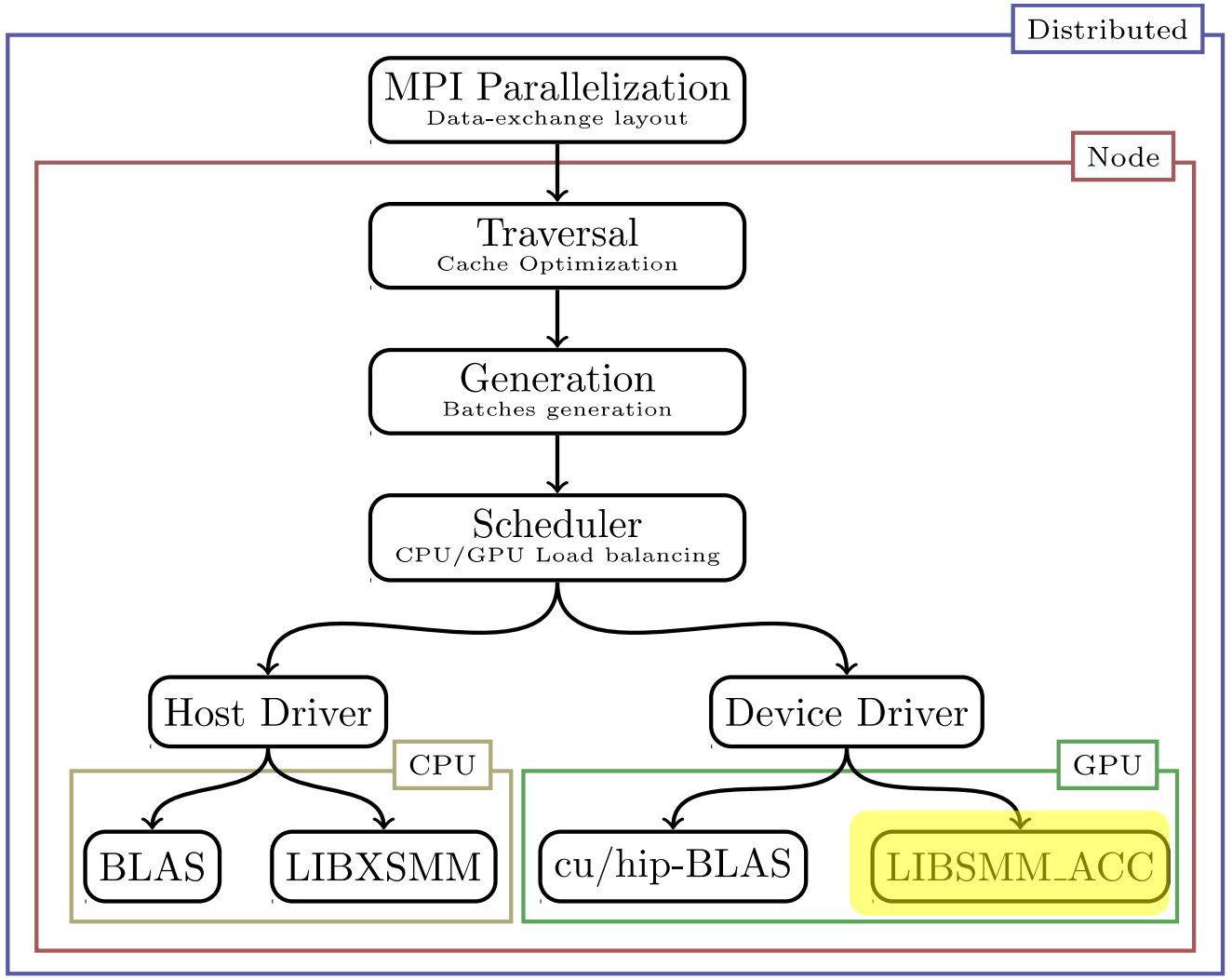
```
cmake .. \
      -DUSE_MPI=<ON|OFF> -DUSE_OPENMP=<ON|OFF>
      -DUSE_SMM=<blas|libxsmm>
      -DUSE_CUDA=<OFF|ON> -DUSE_HIP=<OFF|ON>
      -DWITH_GPU=<P100|K20X|K40|K80|V100|Mi50>
```

DBCSR: Use cases and Matrix Types

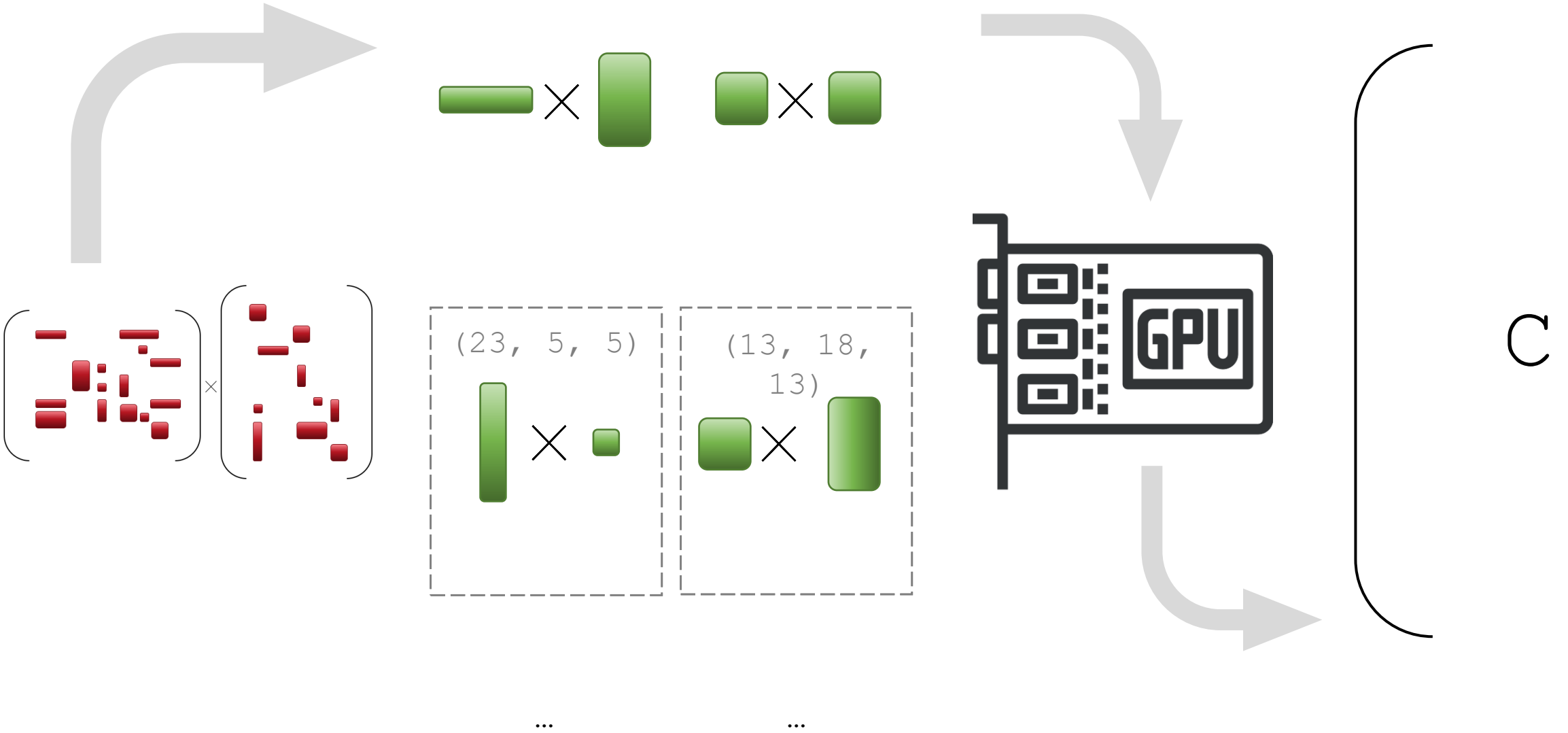
- Natural use case: Electronic Structure
- Application-specific sparsity patterns
- DBCSR is based on blocked structure
  - Non-zero elements are small dense blocks
    - typically 13x13, 23x23, …
  - Take full advantage of the block structured sparse nature of the matrices
  - Each block corresponds to the interaction between two atoms



DBCSR Software Structure



libsmm_acc: library for small matrix-matrix multiplications on accelerators



libsmm_acc: parametrized CUDA kernels

- grouping
- number of CUDA threads
- minblocks
- tile_m, tile_n
- P_a, P_b

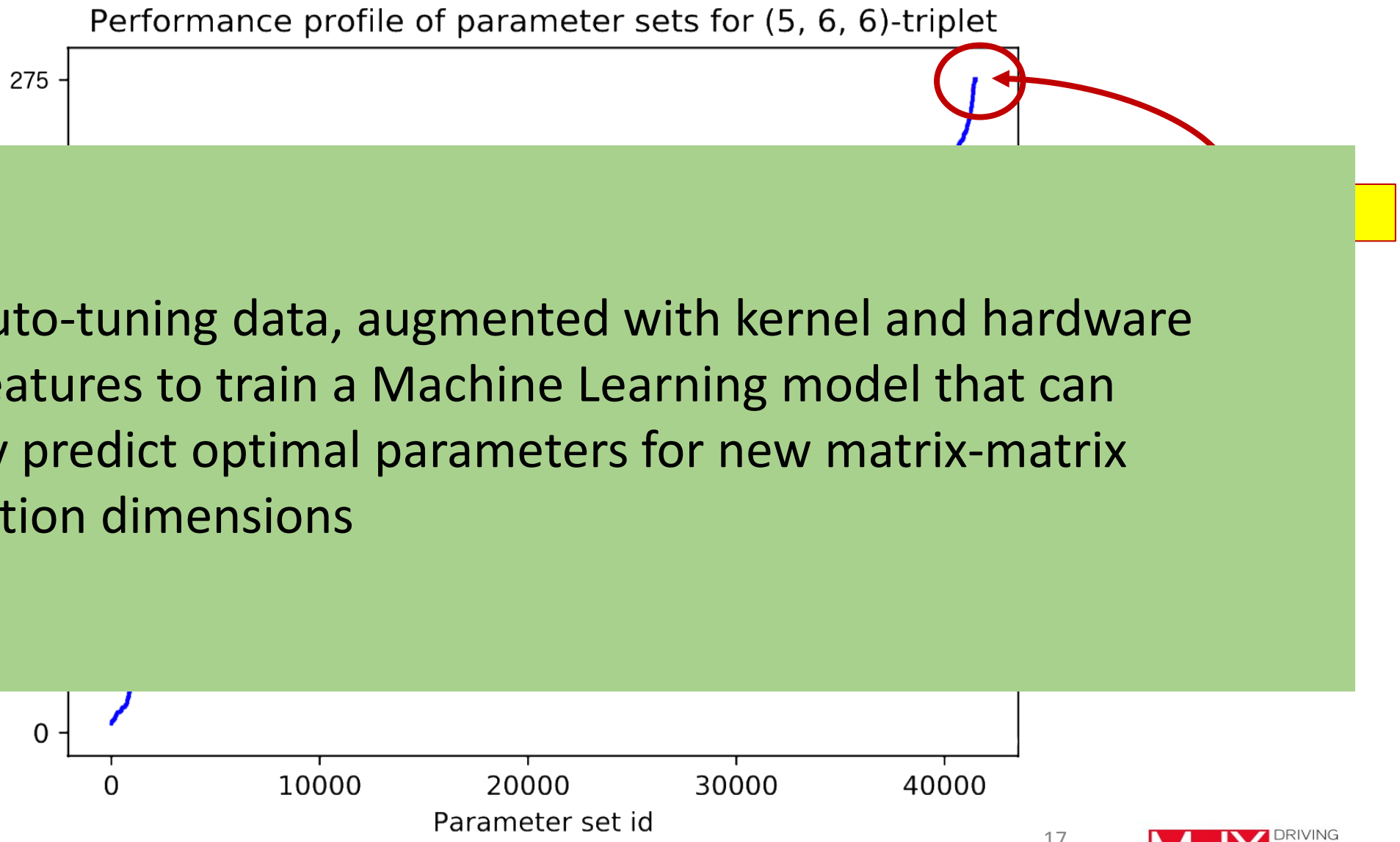
  +

- algorithm

} 7 parameters

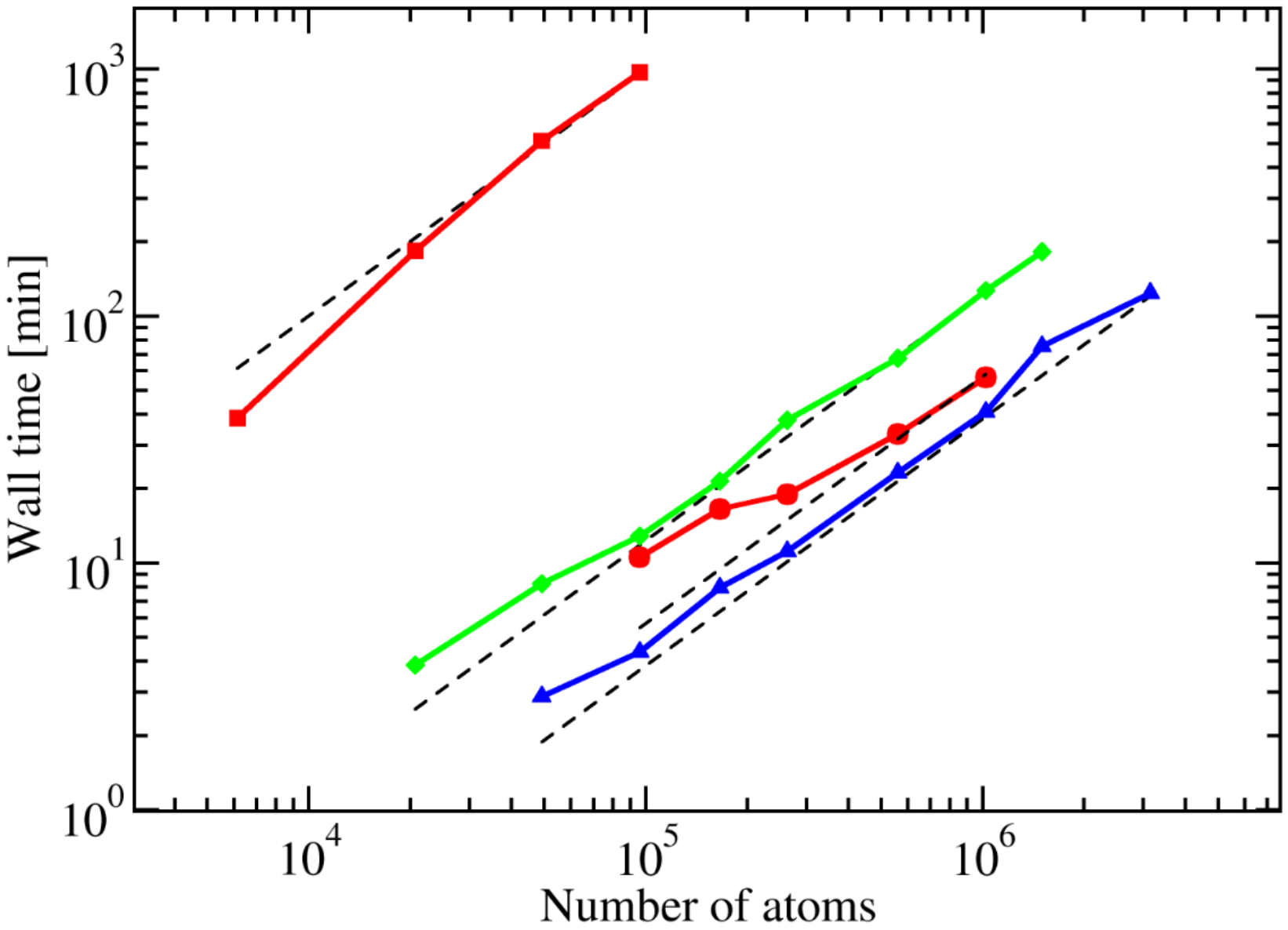
- Performance is difficult to model
- There are tradeoffs and interactions between parameters

libsmm_acc: parametrized CUDA kernels



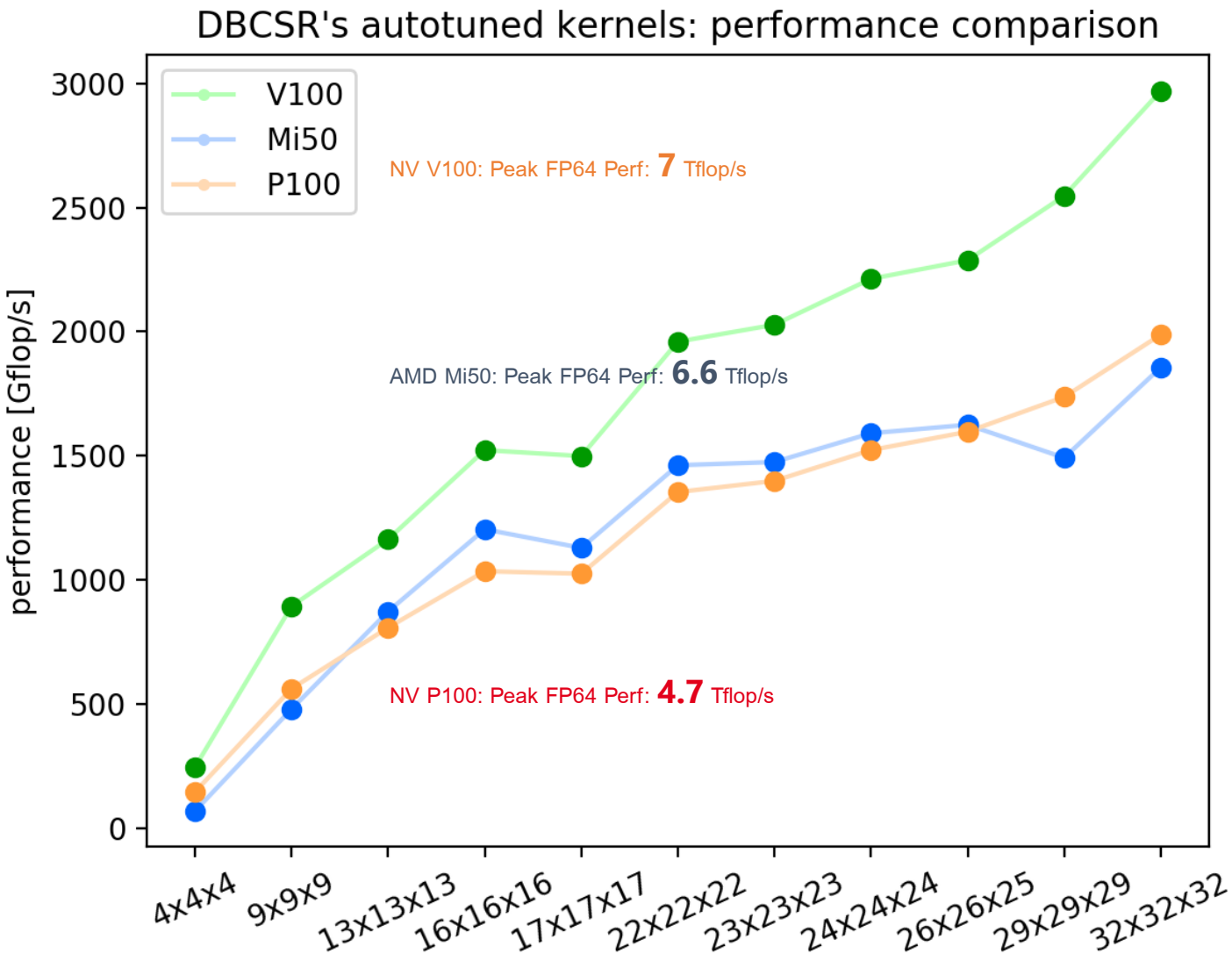
We use auto-tuning data, augmented with kernel and hardware derived features to train a Machine Learning model that can accurately predict optimal parameters for new matrix-matrix multiplication dimensions

Linear SCF scaling



Linear Scaling Self-Consistent Field Calculations with Millions of Atoms in the Condensed Phase
Joost VandeVondele, Urban Borštnik, and Jürg Hutter
Journal of Chemical Theory and Computation **2012** *8* (10), 3565-3573
DOI: 10.1021/ct200897x

GPU back end performance



Use DBCSR

- Available as a standalone
  - Github: actively developed
  - Documentation
  - Easy to use & install

Number of lines of code ~75k
Languages: 82% Fortran,
8% Python, 5% C++
License: GPL-2.0

https://github.com/cp2k/dbcsr

- Also delivered automatically with any CP2K installation, so if you're running CP2K, you're also running DBCSR (perhaps without knowing it)

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THANKS

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