DRIVING THE EXASCALE TRANSITION

Pushing FLEUR to the limits: Large magnetic setups

Uliana Alekseeva

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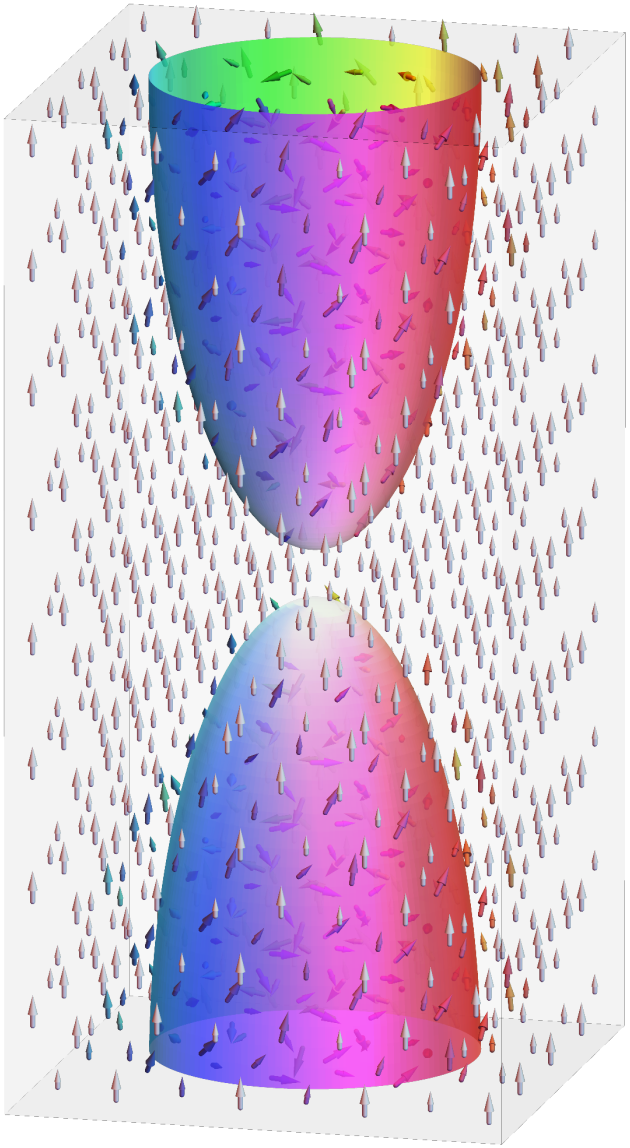
Outline

Pushing FLEUR to the limits

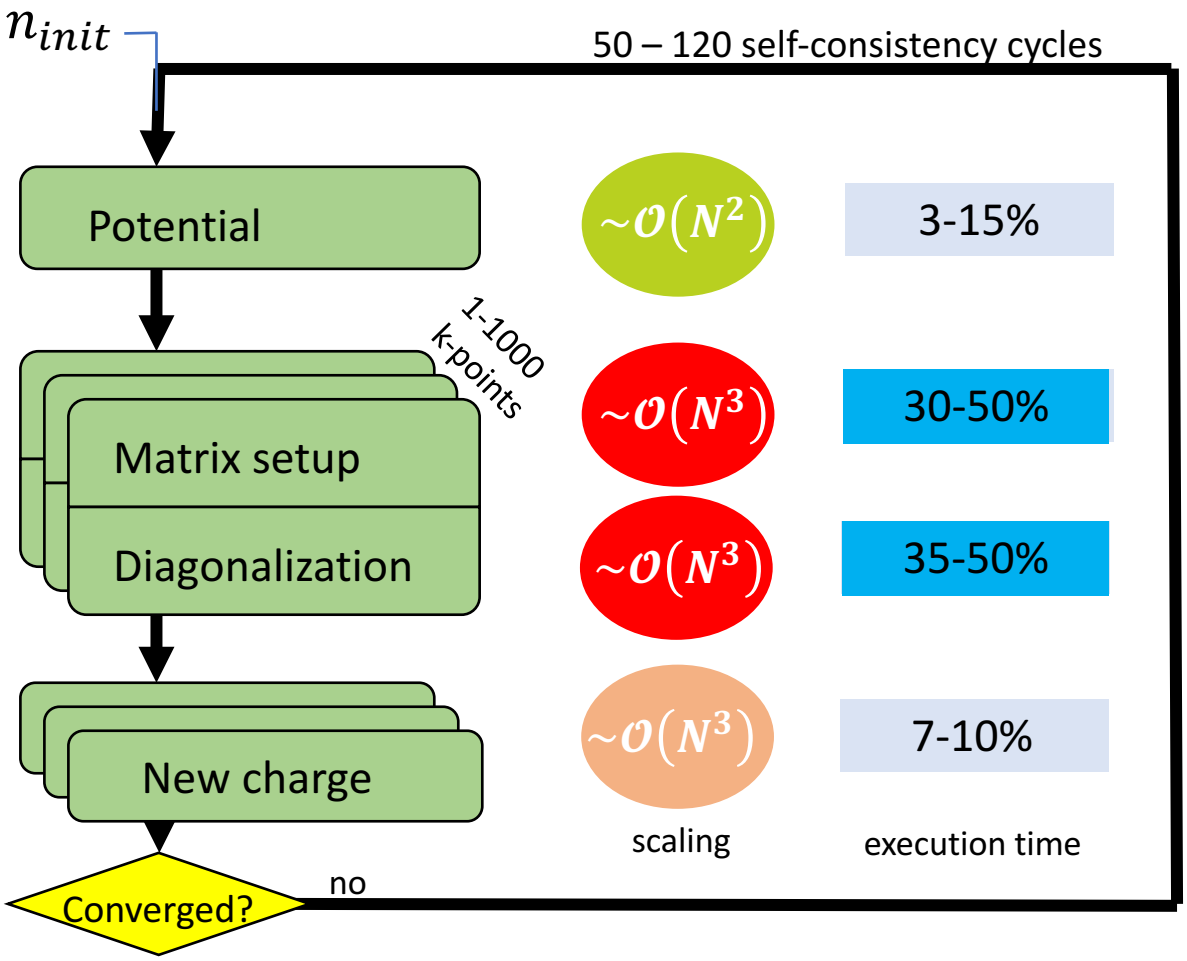


- Parallelization and optimization

Large magnetic setups

- Simulations of complex magnetic objects

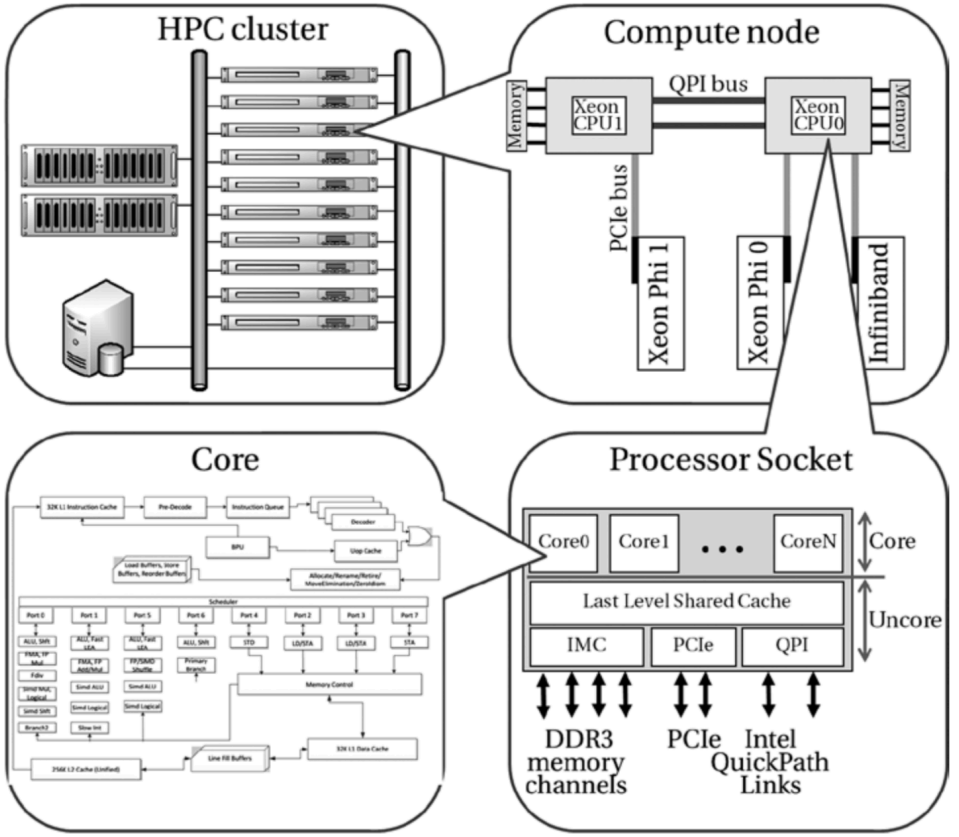
Computationally intensive parts of FLEUR



Parallelization

Levels of parallelization:

- MPI over k-points
- MPI eigenvector parallelization
- OpenMP parallelization
- SIMD Vectorization



Supalov, Semin, Klemm, Dahnken
"Optimizing HPC applications with Intel Cluster Tools"

Parallelization

Levels of parallelization:

- **MPI over k-points**
- MPI eigenvector parallelization
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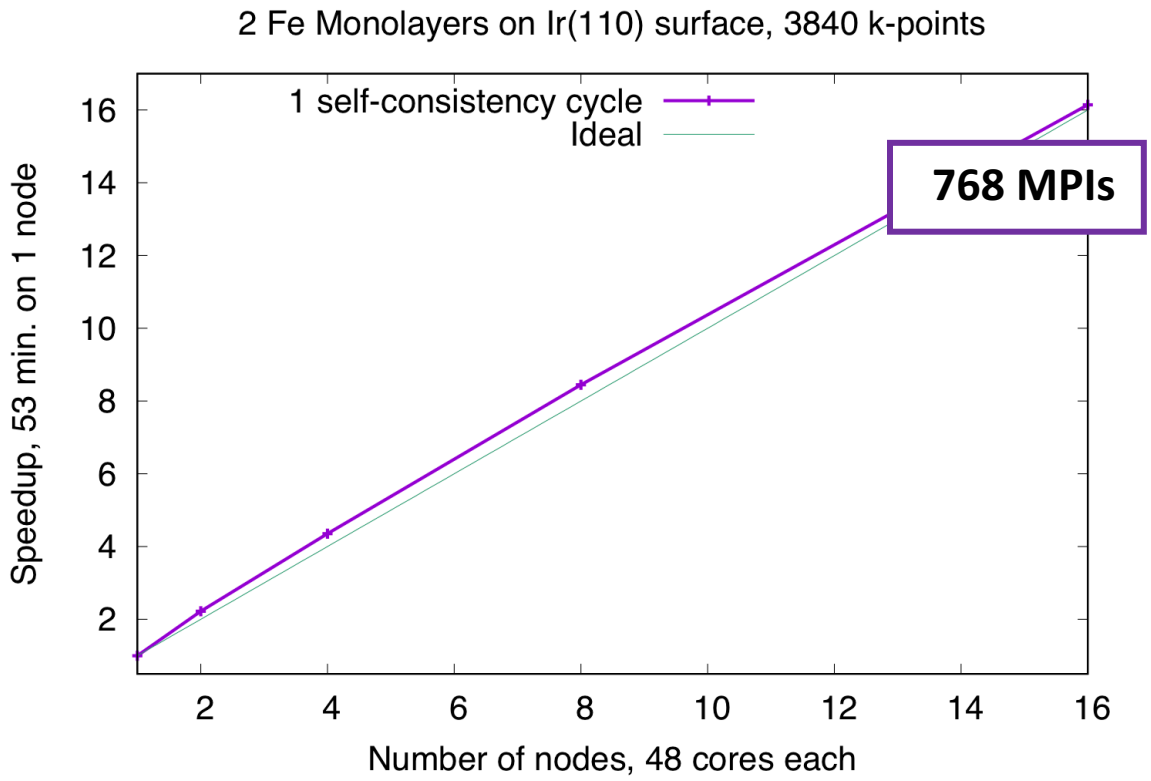
- most time-consuming part of the code are independent for different k-points
- FLEUR will distribute k-points to maximize the load balance



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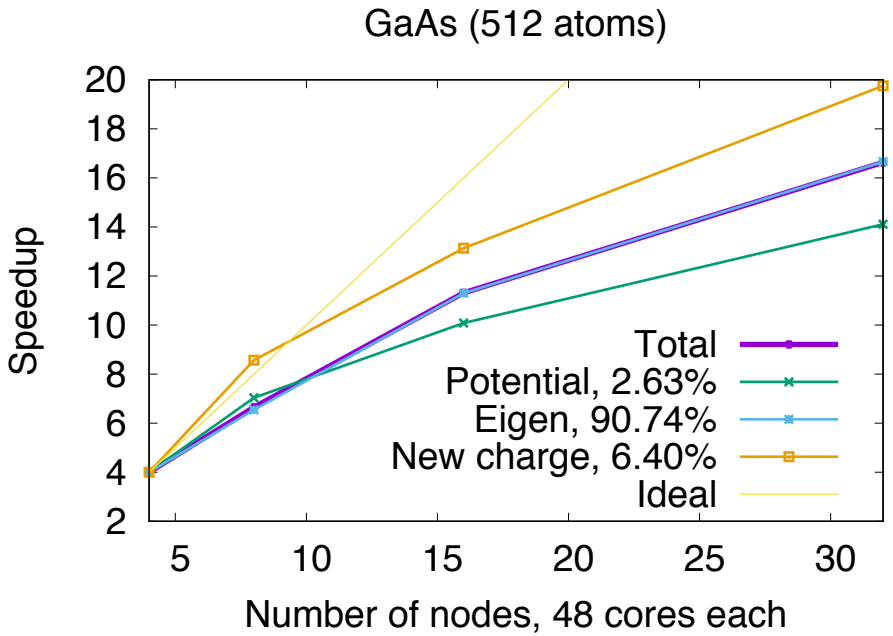

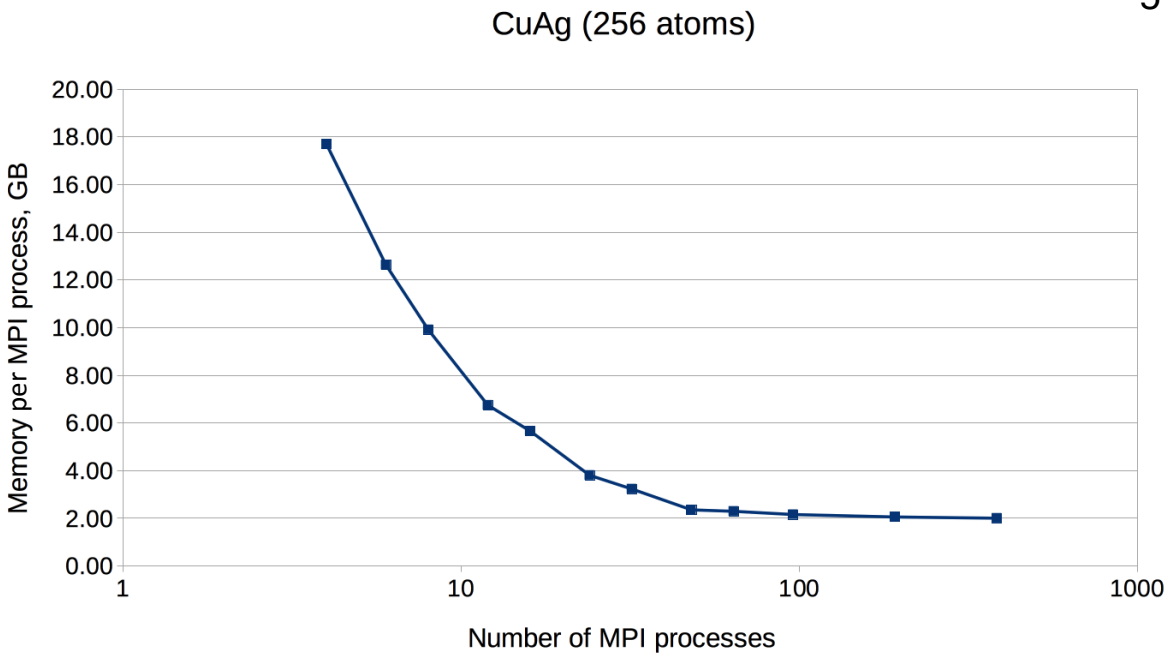

- gives an additional speedup
- allows to tackle larger systems by reducing the memory usage per MPI process

Parallelization

Levels of parallelization:

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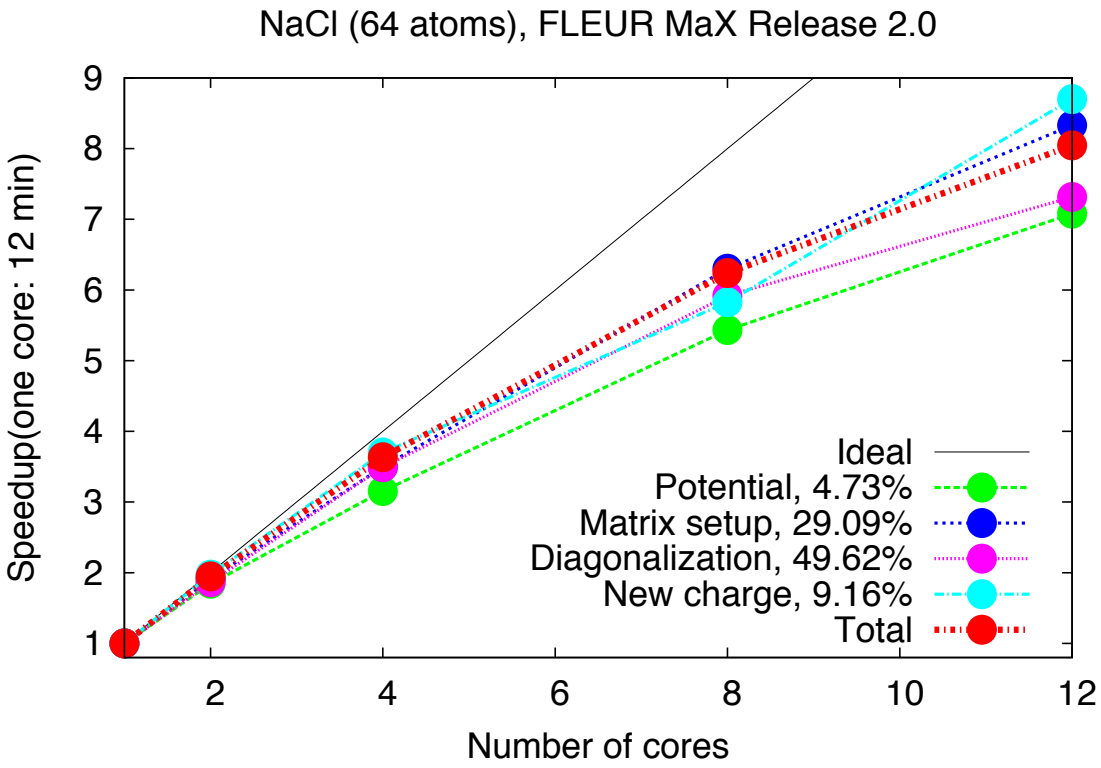
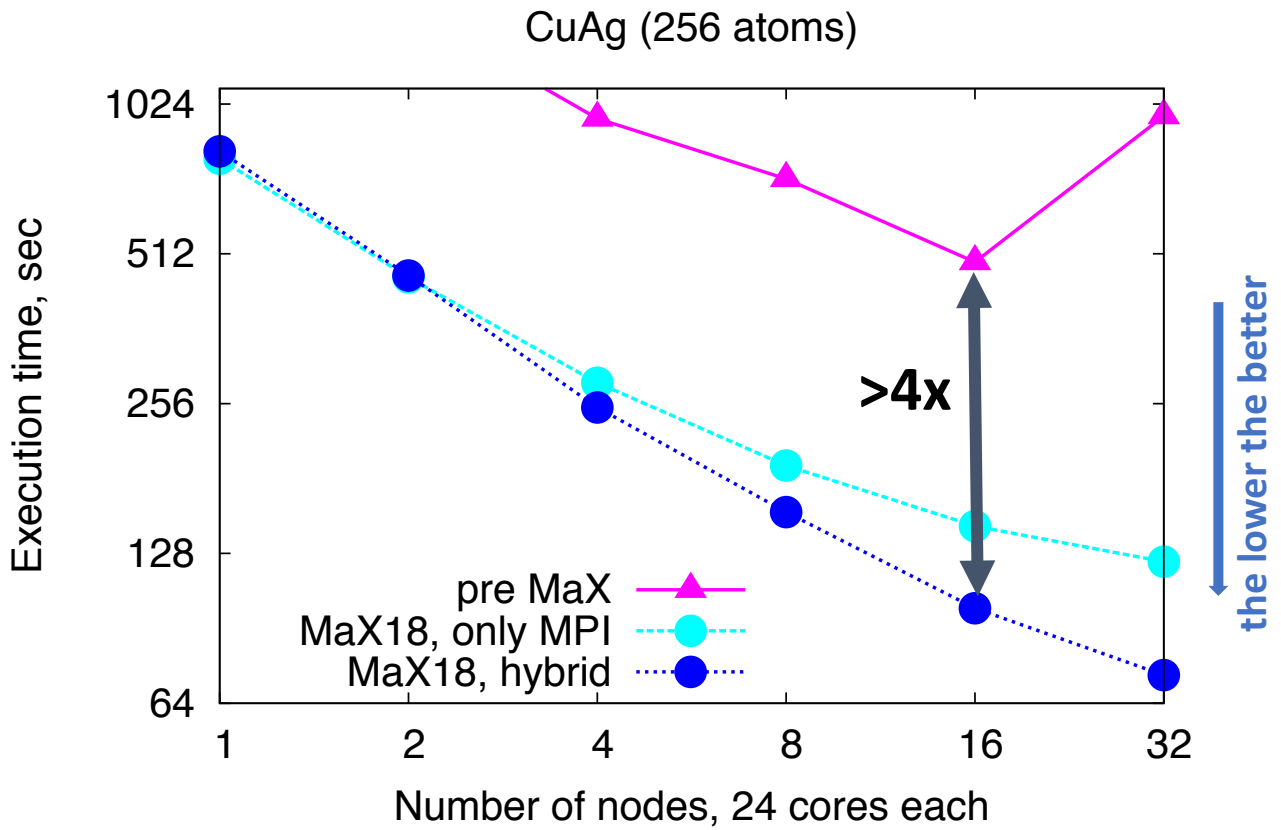
- MPI eigenvector parallelization
- **OpenMP parallelization**
- SIMD Vectorization

- exploits the intra-node parallelism
- makes simulations of large unit cells feasible

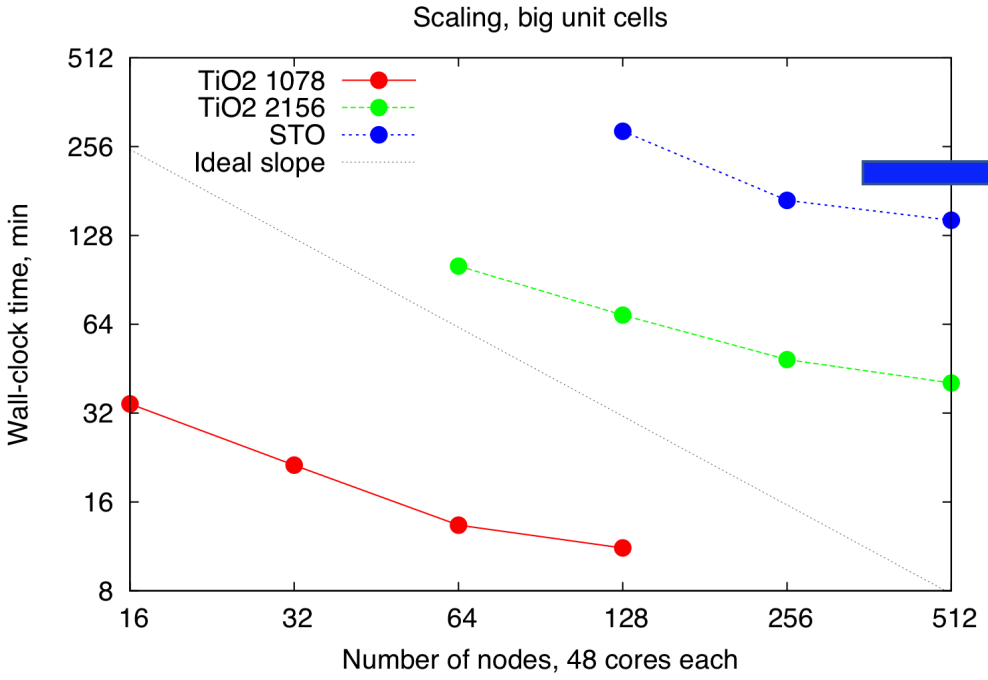


Performance optimization during MaX project



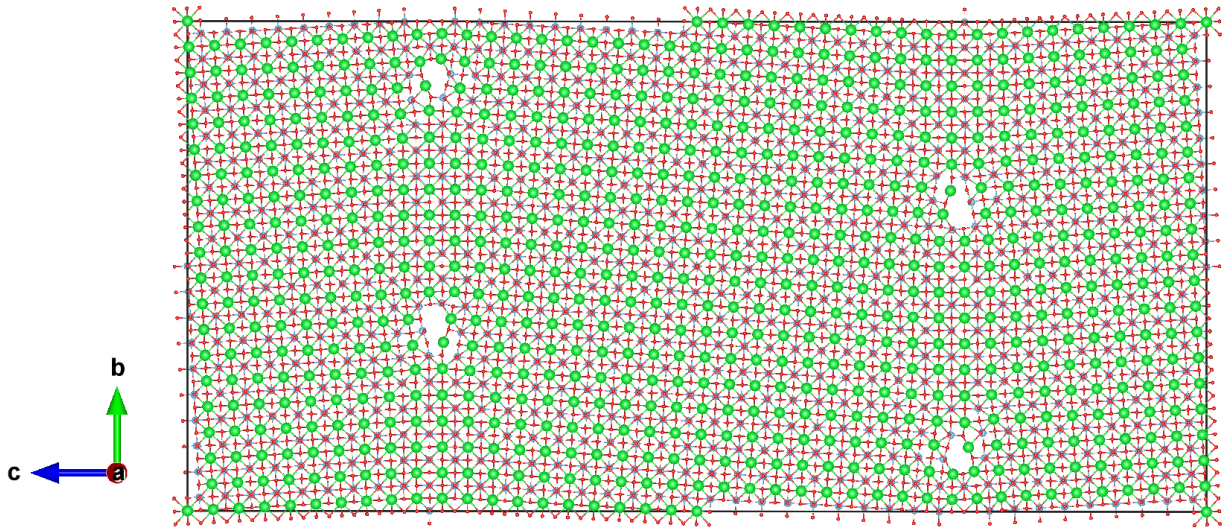
U. Alekseeva, G. Michalicek, D. Wortmann, S. Blügel (2018)
https://doi.org/10.1007/978-3-319-96983-1_52

FLEUR simulations with large unit cells



$SrTiO_3$, 3750 atoms, 4 k-points

- 1024 nodes (Intel, 48 cores)
- Size of the matrices:
  345k x 345k (dense Hermitian)
- 100 minutes/ iteration
- 45 iterations to convergence
  (800k core-hours)



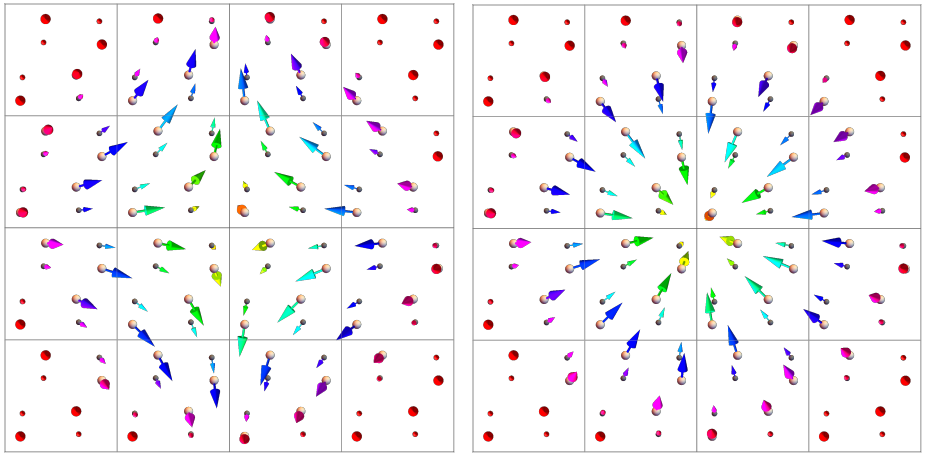
Extended defect in STO

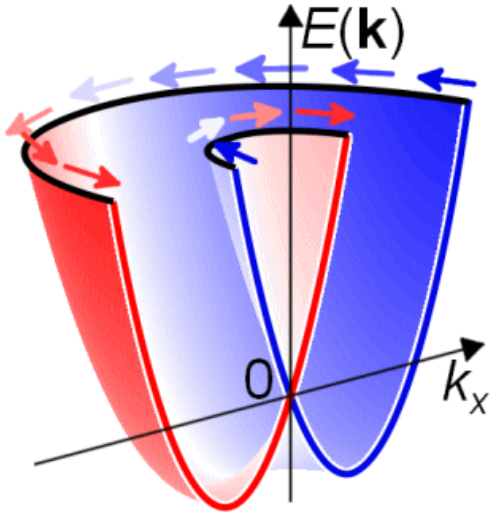
FLEUR simulations with magnetic setups

FLEUR is the code to simulate

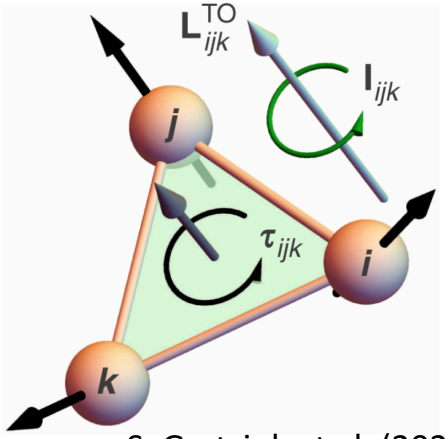
complex magnetic phenomena:

- Relativistic effects
- Spin-orbit coupling
- Non-collinear magnetic systems
- Crystals and thin films
- Spin-spirals

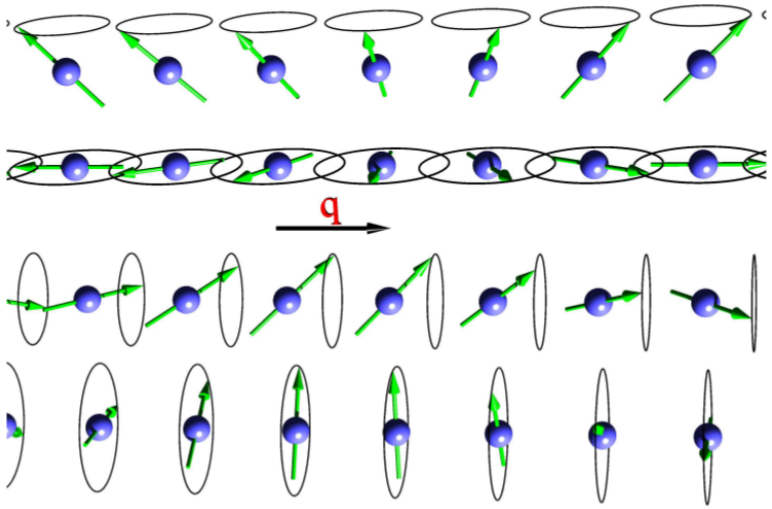




http://ishizaka.t.u-tokyo.ac.jp



S. Grytsiuk et al. (2020)



Ph. Kurz PhD Thesis, RWTH Aachen

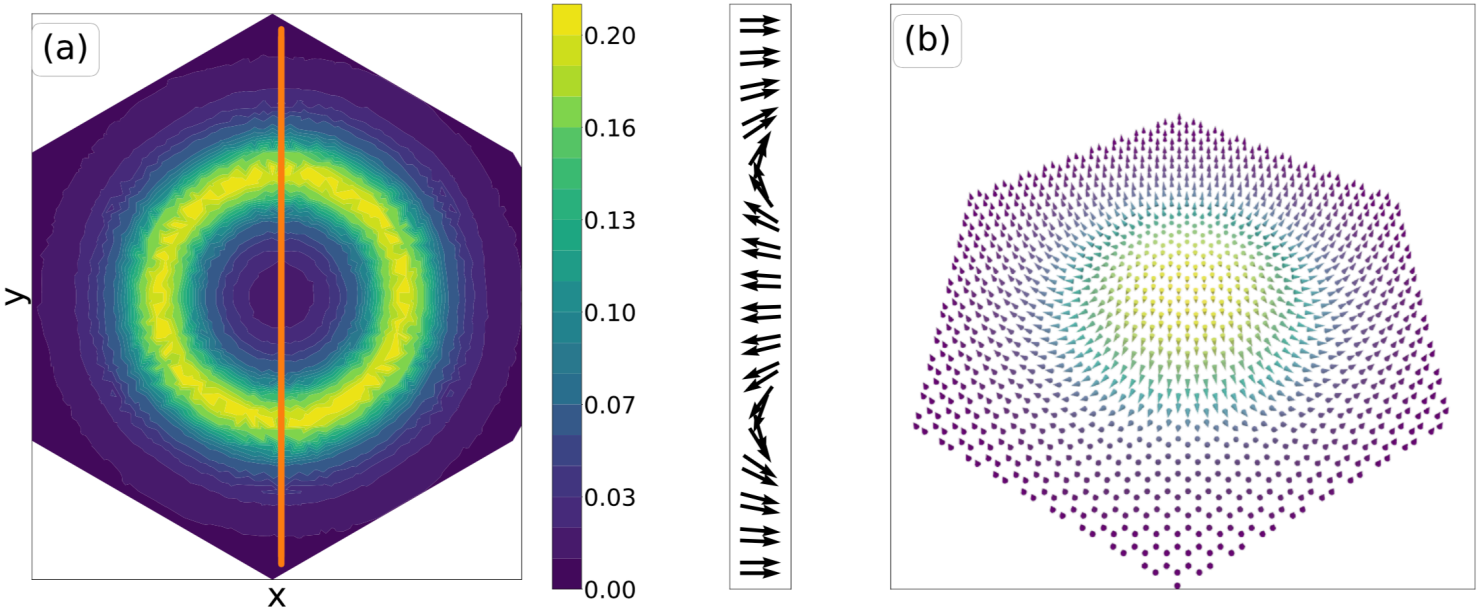
MAX DRIVING THE EXASCALE TRANSITION

Simulations of nano-sized magnetic objects

Multiscale approach:

1. ab initio calculations of fundamental material properties:
   - exchange parameters
   - Anisotropy constants
   - Dzyaloshinskii–Moriya interaction
2. spin-dynamic simulations

But:
spin-dynamic simulations do not take into account the dependence of the electronic structure from the magnetic structure



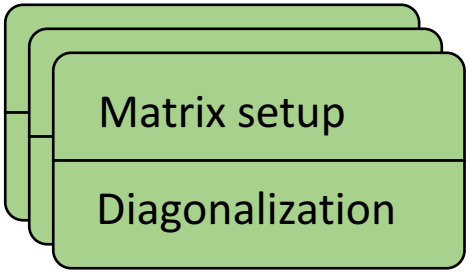
M.Redies, Masterthesis 2019 RWTH

FLEUR simulations with large magnetic setups

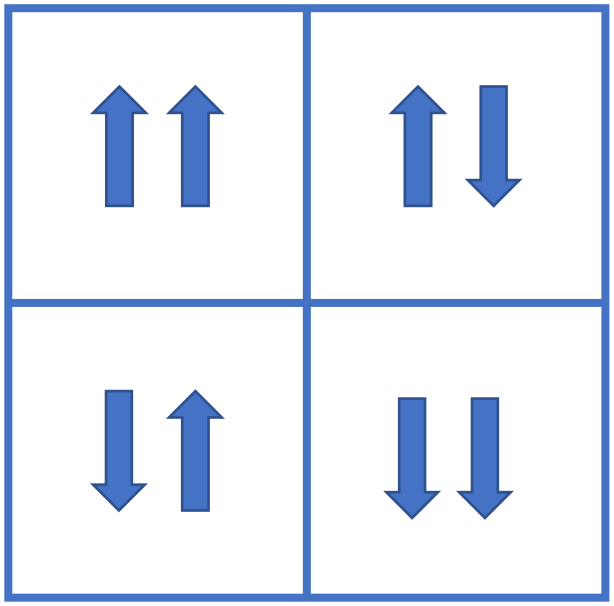
Simulations with FLEUR

- high order interactions
- long range interactions in transition metals
- validation of magnetic models

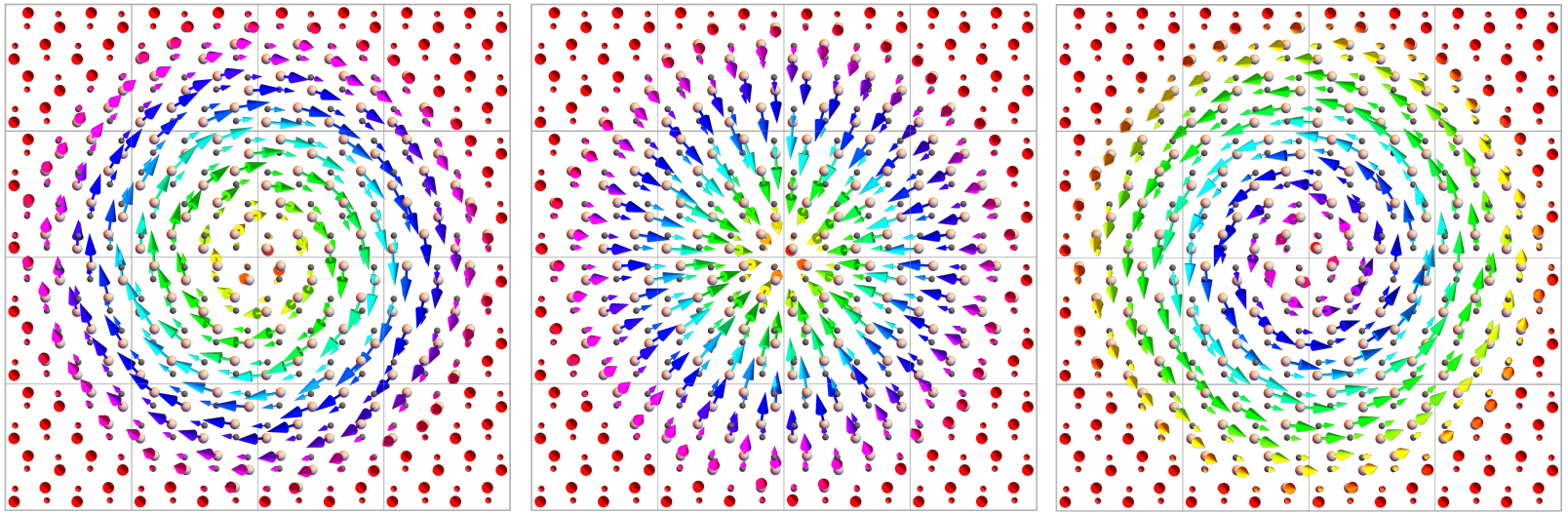
Most computationally intensive parts:



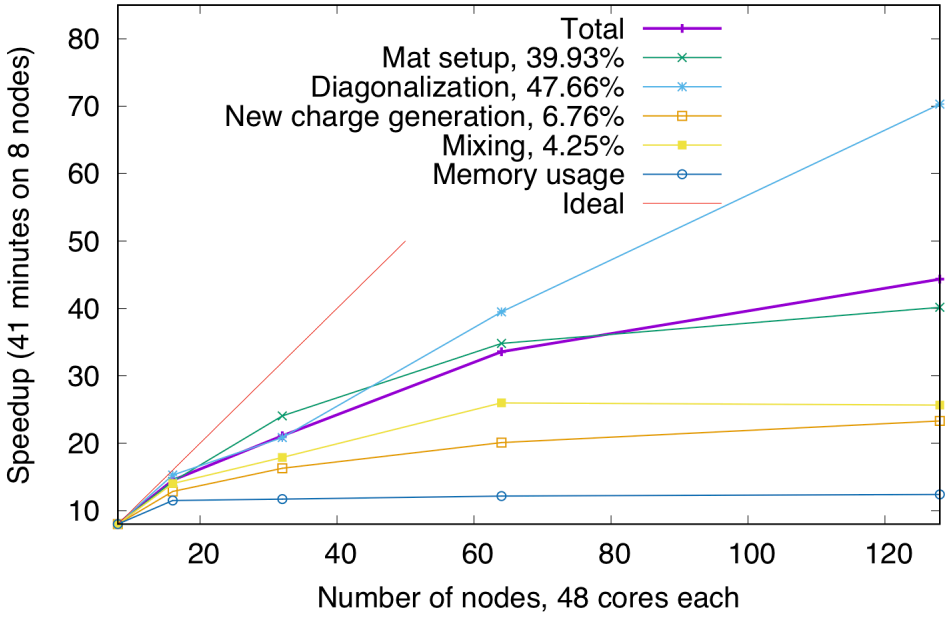
Hamiltonian:



Large magnetic setups: skyrmion tubes



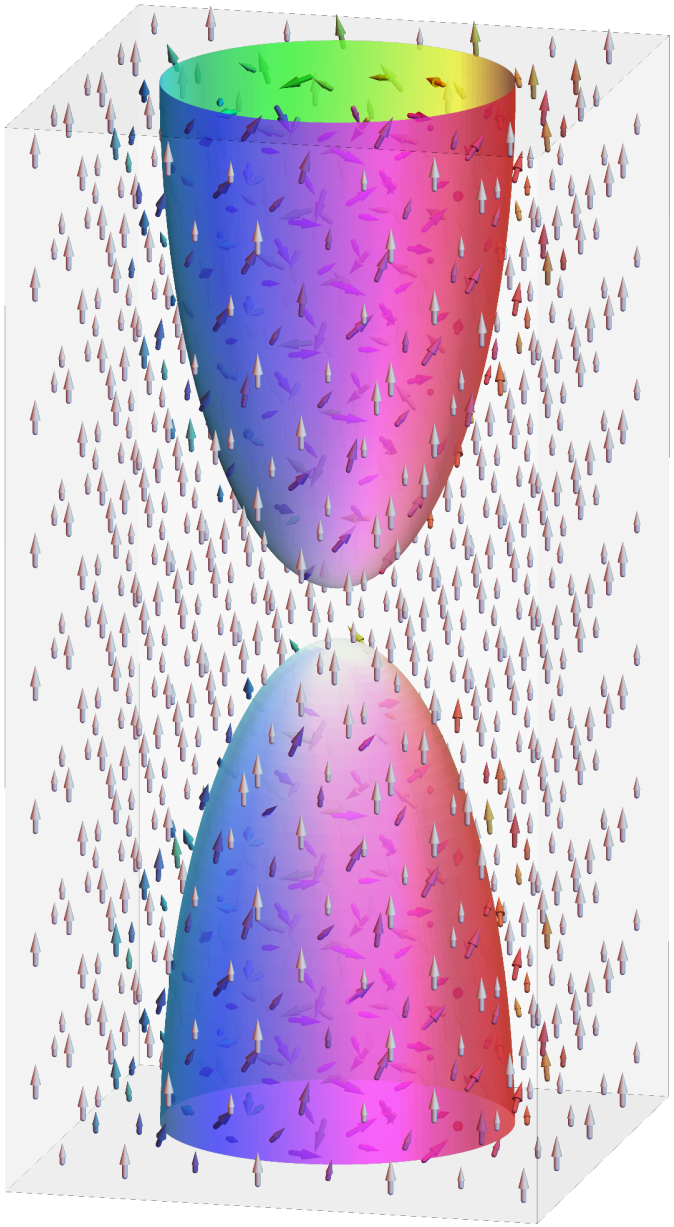
MnGe 8x8x1 (512 atoms), SuperMUC-NG



MnGe Supercell 8x8x1, 512 atoms, 4 k

- 256 nodes (64 nodes/ k-point)
- Size of the matrices:
  78k x 78k (dense Hermitian)
- 10 min/ iteration
- 66 iterations to convergence
  (135k core-hours)

Large magnetic setups: a globule



MnGe Supercell 4x4x8, 1024 atoms, 1 k-point

- 256 nodes (Intel, 48 cores)
- Size of the matrices:
  156k x 156k (dense Hermitian)
- 25 minutes / iteration
- 100 iterations to convergence
  (2 Mio core-hours)

Summary

Optimization for HPC computers

- hybrid (MPI+OpenMP) parallelization
- unit cells with >1000 atoms

HPC examples

- simulations of large magnetic setups