CP2K

New Frontiers

in

ab initio Molecular Dynamics

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Ab Initio Molecular Dynamics

- Molecular Dynamics Sampling of classical statistical ensemble (alternatively Monte Carlo sampling). Introduces temperature and pressure into simulation, connection to experimental conditions

- Electronic Structure Theory Interaction potentials are calculated using quantum mechanics for electrons. Ab initio theory - no precomputed or empirically adjusted potential functions needed.

Ab Initio Molecular Dynamics

Applications

- Chemical reactions in solution
- Complex interfaces (liquid/vapor, solid/liquid)
- Structural phase transitions
- Proton and/or electron transfer
- etc.

Ab Initio Molecular Dynamics

Embarrassingly Parallel Sampling Approaches

Replica exchange algorithms

Multiple walker metadynamics

Free energy string methods

Time Series Generation (MD, MC)

Electronic Structure Calculation

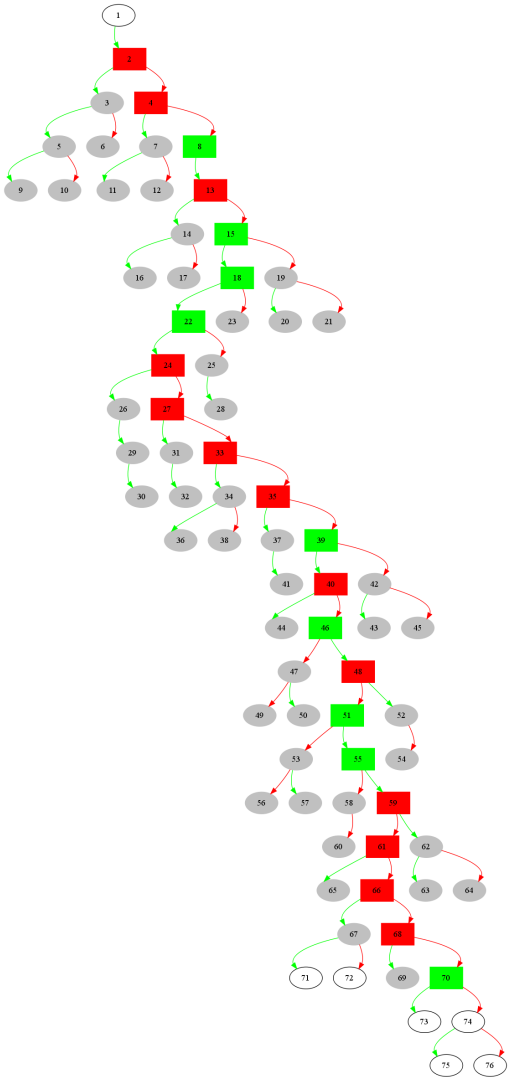
Parallel Time Series Generation

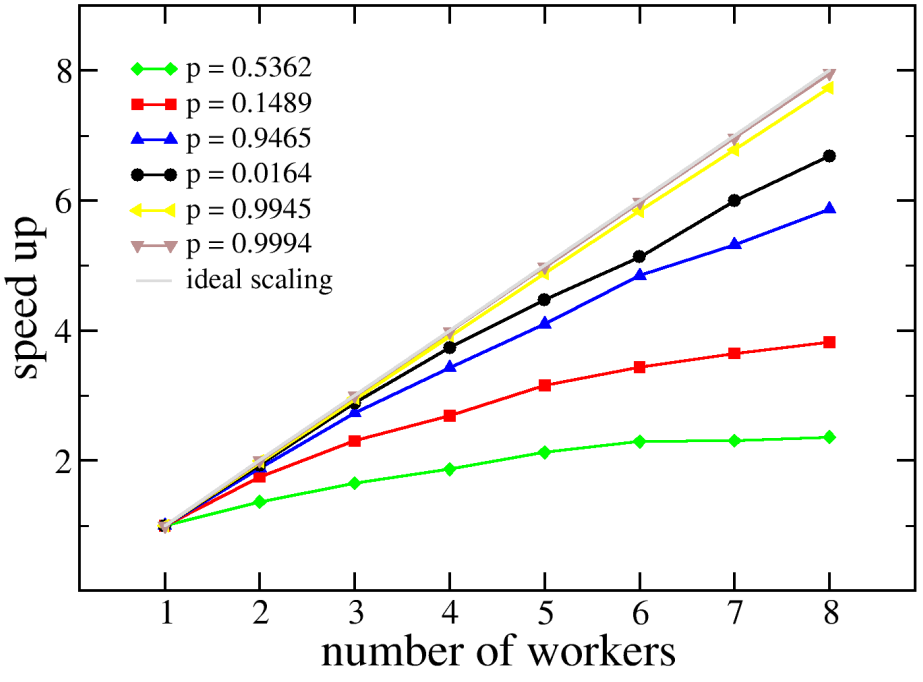
- Parallel Molecular Dynamics
  - Waveform relaxation;
    A. Bellen, M. Zennaro, J. Comput. Appl. Math. 25, 341 (1989)
  - Solar system dynamics;
    P. Saha, J. Stadel, S. Tremaine, Astron. J. 114, 409 (1997)

- Speculative Monte Carlo
  - Similar to branch prediction in CPUs
  - Effective if generation of states much cheaper than calculation of state energy.

Wasteful algorithms: Efficiency $\approx 0.2 - 0.6$

Speculative Monte Carlo





Electronic Structure Calculations

Kohn-Sham Density Functional Theory

- Nonlinear Schrödinger equation

$$\downarrow \qquad \text{basis set expansion}$$

Nonlinear generalized eigenvalue equation

$$\mathbf{H}[\mathbf{C}]\mathbf{C} = \mathbf{S}\mathbf{C}E$$

- Basis: Atom-centered Gaussian functions

$$\varphi(r) = Y_{lm}(\hat{r})\ \exp[-\alpha(r-A)^2]$$

Key Algorithms

- Gaussian to plane wave transform

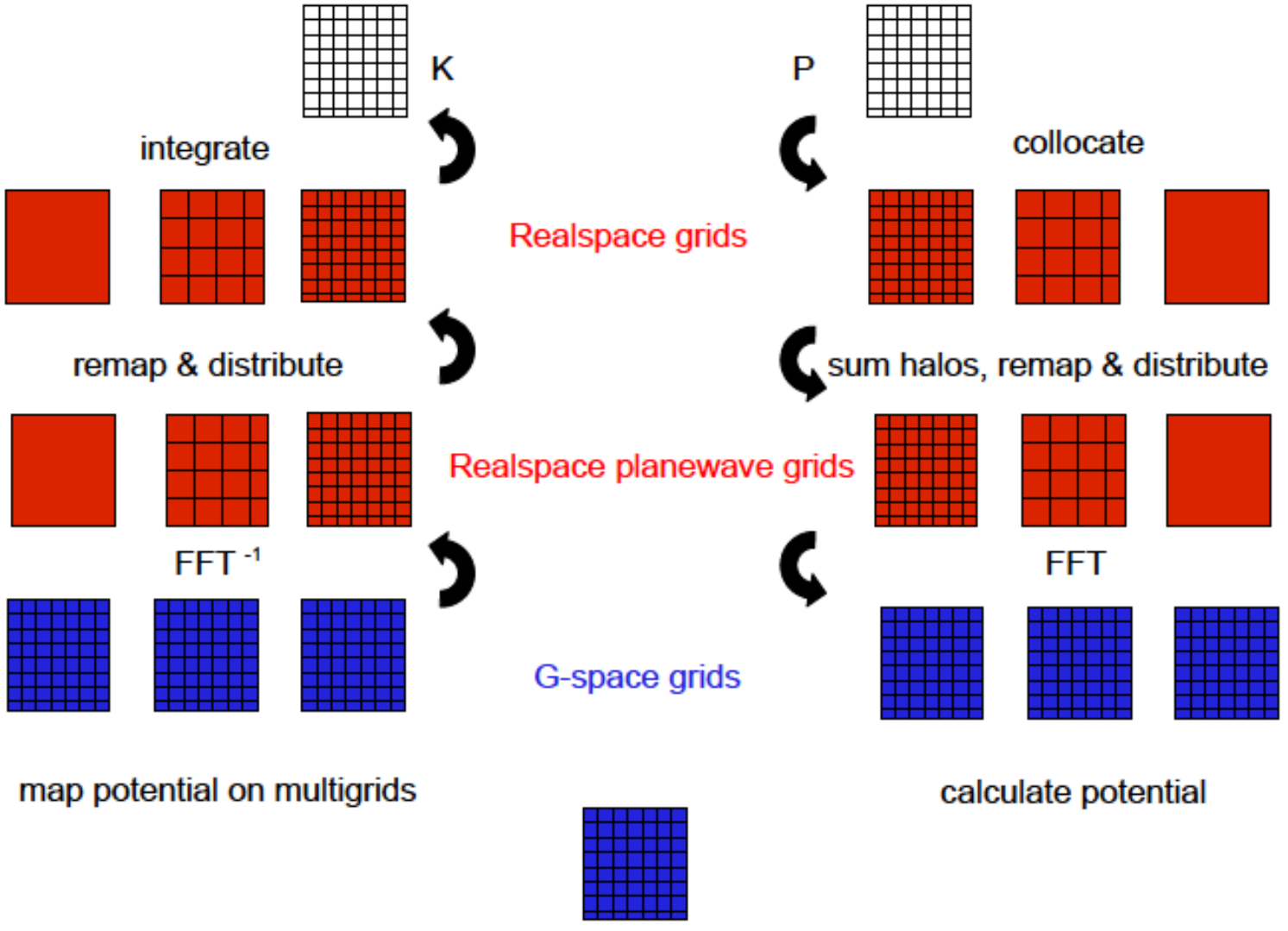
$$H^c_{\alpha\beta} = \sum_{\gamma\delta} P_{\gamma\delta} I_{\alpha\beta,\gamma\delta} = \sum_G (\alpha\beta, G) \frac{4\pi}{G^2} \left[\sum_{\gamma\delta} P_{\gamma\delta} (\gamma\delta, G) \right]$$

- Analytic Integrals for Hartree-Fock exchange

$$H^x_{\alpha\beta} = \sum_{\gamma\delta} P_{\gamma\delta} I_{\alpha\gamma,\beta\delta}$$

- Direct constraint subspace optimization
  Replace diagonalization by direct optimization with constraints
  Sparse matrix linear algebra

Gaussian to Plane Wave Transform



Gaussian to Plane Wave Transform

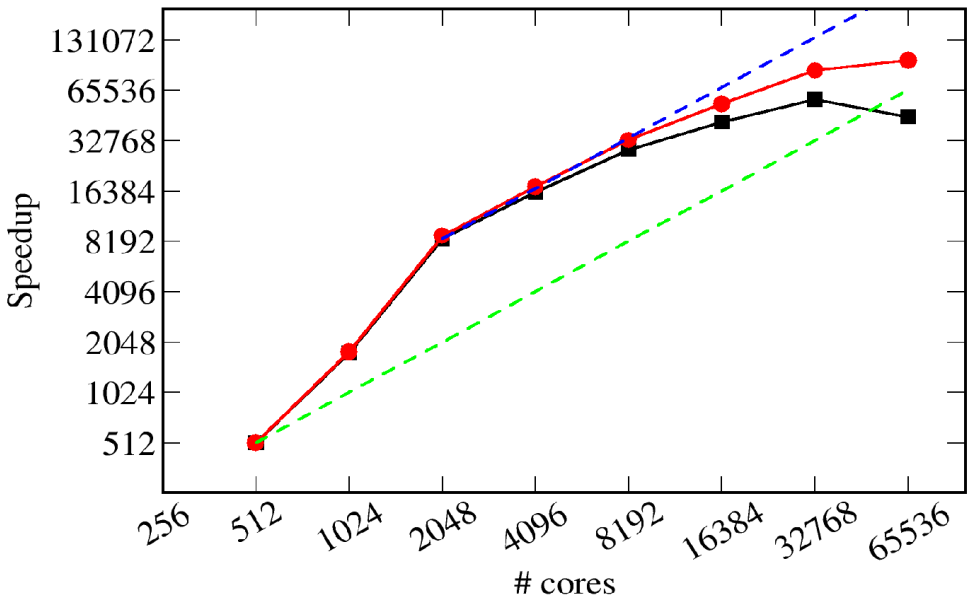
- Distributed sparse matrices and distributed grids
  Halo exchange
- 3d FFTs
- Complicated load-balancing problems
- Collaboration with EPCC Edinburgh
  MPI/OpenMP parallelization
  Target for co-array Fortran implementation

Hartree-Fock Exchange

- Large structured matrix vector multiply

$$H^x_{\alpha\beta} = \sum_{\gamma\delta} P_{\gamma\delta} I_{\alpha\gamma,\beta\delta}$$

- Current implementation:
  Distributed matrix ($I_{\alpha\gamma,\beta\delta}$), replicated vectors ($P_{\gamma\delta}$, $H^x_{\alpha\beta}$)



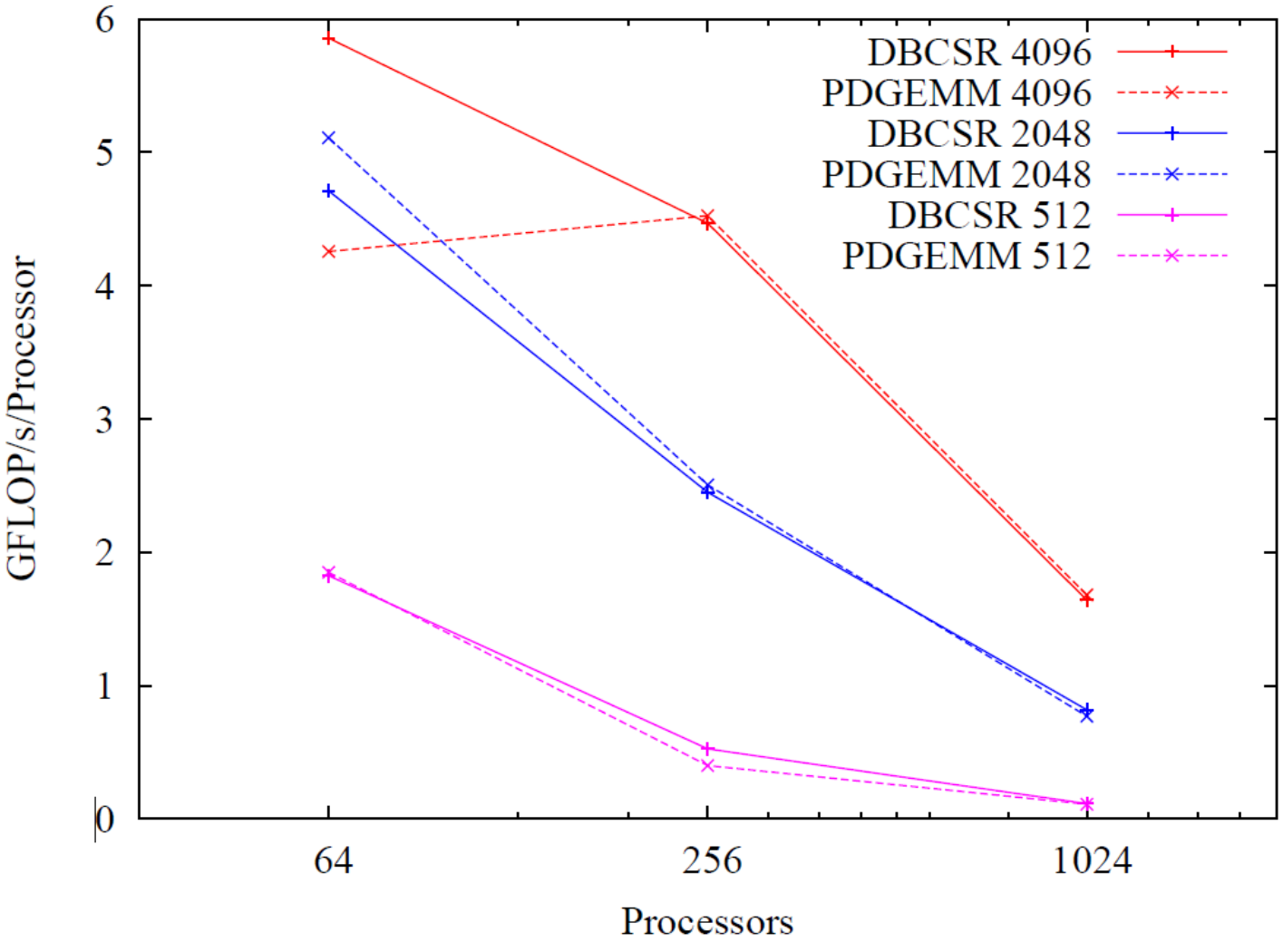
Sparse Linear Algebra

- Optimization (= solving the nonlinear eigenvalue equation) is mapped to matrix multiplications
- Old code: sparse matrices (operators) and dense matrices (solution vectors)
  Basic operation: sparse $\times$ dense matrix multiplication
- Linear scaling algorithms require
  Code refactoring: All matrices are of sparse type
- DBCSR library
  Distributed Block Compressed Sparse Row matrix format

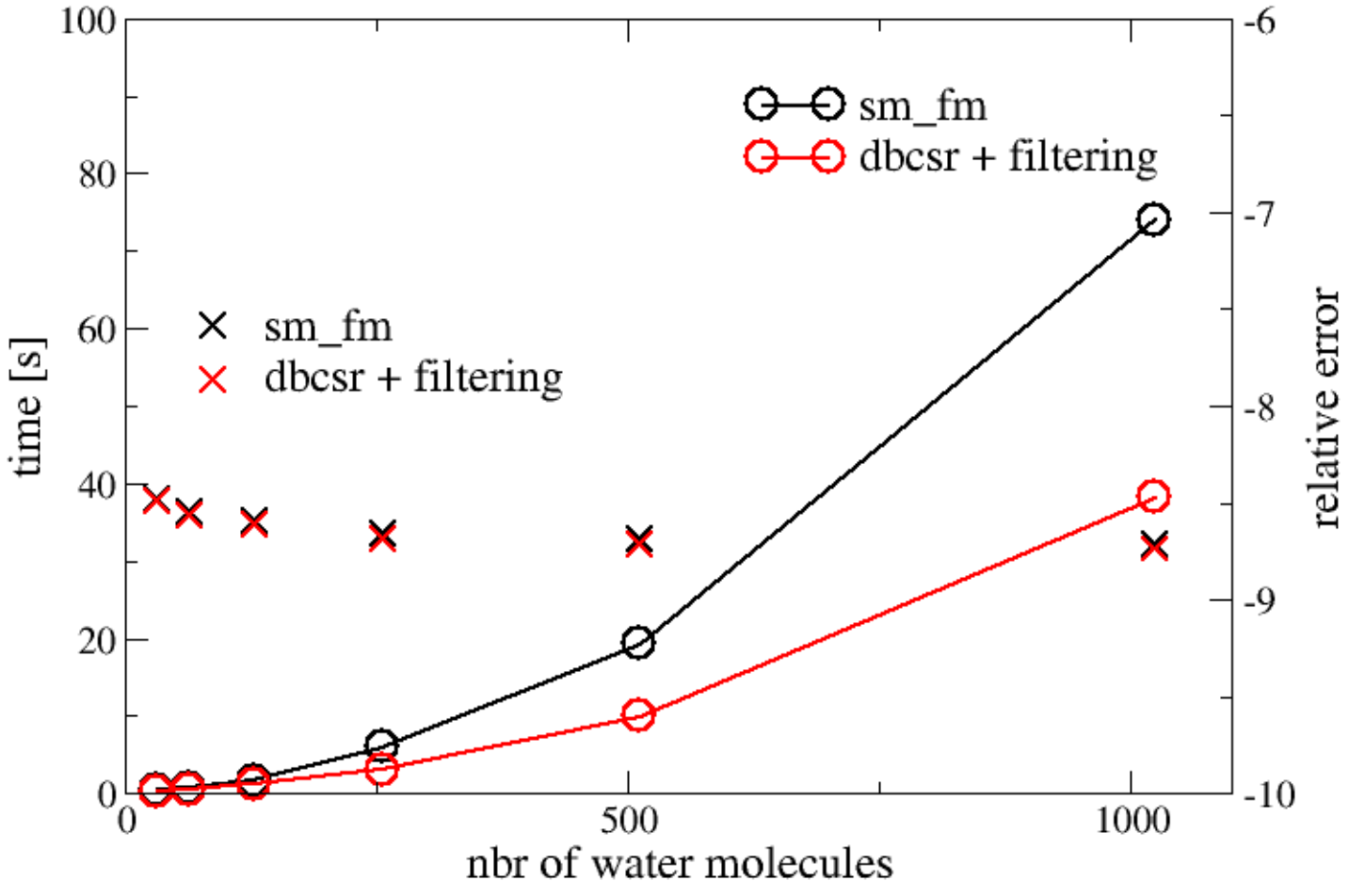
DBCSR Library

- ca. 50'000 lines Fortran 95
- Extensive functionality (single/double real/complex)
- Sparse-sparse matrix multiplication
  filtering, predetermined sparsity pattern
- Interface to ScaLapack
- MPI/OpenMP parallelization

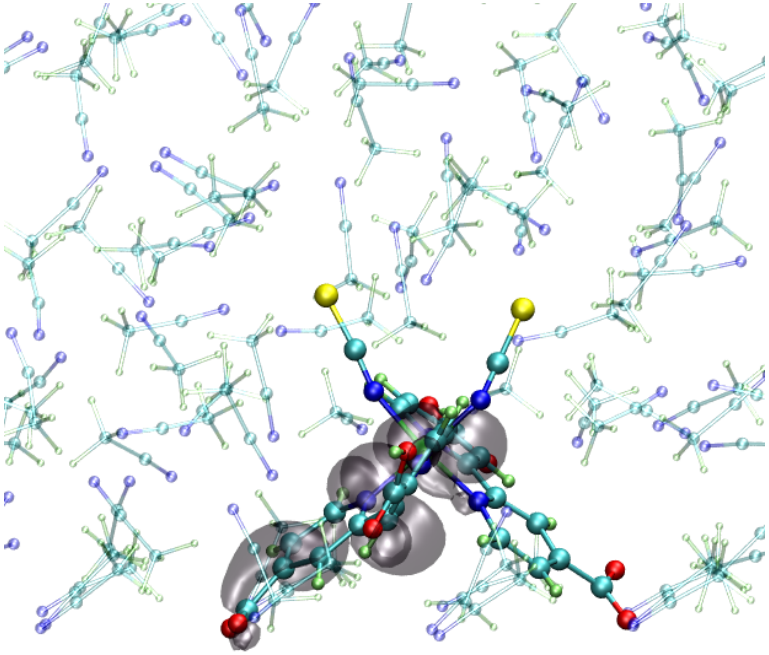
DBCSR vs. PDGEMM



DBCSR: Sparse-Dense Matrix Multiplication



State of the Art Application



- 1319 atoms, 5890 electrons, 15733 bsf
- Optimization: Function of 46 Mio. variables
- 4000 derivatives of the energy function
- 60s/MD step on 512 cores Cray XT-5
- 5 ps dynamics/week

Target Application Scenarios

- Small system - Very extensive sampling
  200-500 atoms – $10^7 - 10^9$ force evaluations
  2.1 Mio threads = 64 (replica exchange) $\times$ 16 (speculative MC) $\times$ 128 (MPI) $\times$ 16 (OpenMP)
- Medium system - Extensive sampling
  1000-5000 atoms – $10^5 - 10^6$ force evaluations
  524'288 threads = 32 (string method) $\times$ 1024 (MPI) $\times$ 16 (OpenMP)
- Large system - Minimal sampling
  10'000-100'000 atoms – $10^3 - 10^4$ force evaluations
  262'144 threads = 16384 (MPI) $\times$ 16 (OpenMP)

CP2K: Software Engineering

- $\approx$ 900'000 lines Fortran 95
  machine generated $\approx$ 200'000 lines
- Explicit subroutine interfaces- strong type checking
- Templates
- $\approx$ 1600 regression tests
  all commits are automatically tested
- External libraries: Lapack/BLAS, ScaLapack/BLACS, MPI, OpenMP, FFTW, libint

Refactoring

- Separate code into independent libraries (e.g. DBCSR)
- Use more unit testing (vs. regression testing)
- Extended OpenMP fine grain parallelization
- Identify code segments for heterogenous computing (GPGPU)
- Parallel I/O (MPI)
- Fault tolerance (MPI)

CP2K Universe

- GPL code
- Open CVS development (`cp2k.berlios.de`)
- User community (Google group, 250 members)
- Developers
  UZH, PNNL, LLNL, PSI, U Bochum, U Minnesota,
  IBM Research
- EPCC Edinburgh
  dCSE Grant: OpenMP parallelization
  Software Sustainability Institute
  Exascale Technology Centre

CP2K HP2C Team

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