

FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
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Lehrstuhl für Informatik 10 (Systemsimulation)



**Multigrid accelerated Poisson-Solver for ab initio Molecular dynamic
Applications**

Rochus Schmid, Harald Köstler and Ulrich Rüde

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Rochus Schmid

Ruhr-University Bochum

Lehrstuhl fuer Anorganische Chemie II
Organometallics and Materials Chemistry
Bochum, Germany

Harald Köstler and Ulrich Rude

University of Erlangen-Nuremberg

Department of Computer Science 10
Erlangen, Germany

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Abstract

In this paper we present an application for a Poisson multigrid solver in 3D to solve the Coulomb problem for the charge self interaction in a quantum-chemical program used to perform ab initio molecular dynamics. Techniques such as Mehrstellendiscrretization and τ -extrapolation are used to improve the discretization error. The results show that the expected convergence rates of the multigrid solver are achieved. Within the applied Car-Parrinello Molecular Dynamics scheme the quality of the solution also determines the accuracy in energy conservation. All forms of discretization employed lead to energy conserving dynamics. However, in case of τ -extrapolation only a red-black smoother leads to the expected results, whereas a lexical smoother gives substantial deviations from energy conservation.

1 Introduction

The development of efficient tools to calculate the electronic structure of molecules as well as extended systems on an ab initio level greatly enlarged the importance of theoretical simulation methods for fields like new materials research, catalysis or nanotechnology. The majority of modern computer codes for large scale systems are based on the expansion of electronic wavefunctions and densities in terms of plane waves (PW). However, since some of the necessary integrals are evaluated in Fourier space but others can only be calculated in real space (RS) the 3D-FFT is heavily used to transform back and forth. This leads to complications for the parallelization of the approach for massively parallel computer systems as the 3D-FFT involves a global communication step [1]. In addition, the intrinsic periodicity of PW limits the application to interesting systems with reduced dimensionality as e.g. 2D periodic surfaces of high interest in various areas of research. As a consequence, more recently Real Space methods have been developed, where all quantities are described on a real space mesh and FFT is no longer necessary, all communication operations are local and arbitrary and complex boundary conditions (as 2D periodicity) are simply realized [2, 3]. In the more traditional forms of electronic structure calculations with spherical atom centered basis functions for finite systems or PW based methods for periodic systems, which have originally been developed mostly within the theoretical chemistry and physics community, to some extent the knowledge of the solution has been used to make the calculation tractable. In contrast to that the grid based approach is much more similar to grid based methods used in many other fields of science like for example fluid dynamics or astronomy. An advantage is now the simplicity of the algorithms. However, the knowledge and competence of the Computational Science community, which developed very efficient grid based methods to solve arbitrary partial differential equations, will have to be exploited in much greater extent than before. It is the intent of this contribution to present first results of our joint effort in this direction.

2 Ab initio Car-Parrinello Molecular Dynamics

Within the so called Kohn-Sham Density Functional Theory (KS-DFT) [4, 5] the quantum states of the electrons in a molecular system can be found by solving the eigenvalue equation (for a system with $2n$ paired electrons) for the n lowest eigenvalues ϵ_i :

$$(T_e + V_{ne}(\mathbf{R}) + V_{ee} + V_{xc}) |\psi_i\rangle = \epsilon_i |\psi_i\rangle \quad (1)$$

The KS-Operator consists of the kinetic energy operator $T_e = -\frac{1}{2}\nabla^2$ and the potentials of electron nuclei interaction (V_{ne}), electron-electron self-interaction (V_{ee}) and the non-classical and non-linear exchange-correlation potential V_{xc} [6, 7]. The one electron wave functions ψ_i must fulfill the orthogonality constraint $S_{ij} = \langle \psi_i | \psi_j \rangle = \delta_{ij}$. The nuclei potential $V_{ne}(\mathbf{R})$ depends only on the nuclei positions \mathbf{R} , but V_{ee} and V_{xc} depend on the electron density, which is given by the sum of the squares of the occupied wavefunctions according to $\rho = 2 \sum_i^n \psi_i^2$. Due to the dependence of the operator on the density, the non-linear equations have to be solved iteratively. The corresponding Kohn-Sham energy functional is given by (with the E being the corresponding energies to the potentials V):

$$E_{DFT}[\{\psi_i\}, \mathbf{R}_n] = \sum_i^n 2 \langle \psi_i | -\frac{1}{2}\nabla^2 | \psi_i \rangle + E_{ne}[\rho, \mathbf{R}_n] + E_{ee}[\rho] + E_{xc}[\rho] + E_{nn}(\mathbf{R}_n) \quad (2)$$

For the application to molecular dynamics Carr and Parrinello have recast the problem in their seminal paper of 1985 into a joint dynamic of both nuclei and wavefunction degrees of freedom, which is called Car-Parrinello Molecular Dynamics (CP-MD) [8]. For the fictitious dynamic of the wavefunction ψ_i a wave function mass parameter μ_e is introduced, which must be chosen large enough to allow stable integration of the Newtonian dynamics equations, but small enough to let the electronic degrees freedom follow the nuclei quasi instantaneous. This joint dynamic is defined by the Lagrangian

$$\mathcal{L}_{CP} = \frac{1}{2} \sum_n M_n \dot{\mathbf{R}}_n^2 + \sum_i \mu_e \langle \dot{\psi}_i | \dot{\psi}_i \rangle - E_{DFT}[\{\psi_i\}, \mathbf{R}_n] + \sum_{ij} \Lambda_{ij} (S_{ij} - \delta_{ij}) \quad (3)$$

The Lagrange parameters Λ_{ij} have to be determined each time step to maintain orthogonality of the wavefunctions. The advantage of CP-MD over the standard ab initio MD approach is, that the KS equations (Eq. 1) do not have to be solved accurately at every timestep in order to achieve good energy conservation. Even though a smaller timestep must be chosen for CP-MD in order to be able to integrate also the wavefunction dynamics, a smaller numerical effort is necessary to reach energy conserving dynamics [9]. This approach has originally been introduced and widely used in the context of a plane wave (PW) expansion of the single particle wavefunctions ψ_i and pseudopotentials to describe V_{ne} in an efficient way [9]. One of us has recently shown that this approach can also be used in the context of the recently established real space (RS) methods [3], where the wavefunctions ψ_i and the density ρ are discretized on a real space grid [10, 11]. The advantage here is of course the locality of all operations allowing an efficient and straight forward parallelization, as well as the ability to choose the boundary conditions for the wavefunctions in a much more flexible way as opposed to PW methods, which are intrinsically periodic [2].

However, a major drawback of the RS method is the fact that the Hartree potential V_{ee} can not be calculated in an analytic fashion like in the Fourier space representation, which is used in the PW methods. Instead, an iterative solution of the Poisson equation on the numeric grid must be employed. It should be pointed out, that the potential V_{ee} acts directly as a force on the wavefunctions within the CP-MD approach and must therefore be the exact derivative of the corresponding energy term E_{ee} with respect to the density in order not to violate energy conservation. It was found that this redetermination of the potential V_{ee} at each timestep represents the major computational bottleneck of the approach.

3 Numerical solution of the Poisson equation

3.1 Discretization

In the current implementation the Poisson equation

$$\nabla^2 V_{ee} = -4\pi\rho \quad (4)$$

is discretized with finite differences (cf. [12], p.57) on a rectangular domain in 3D with meshsize h . Besides the standard 7-point stencil for the Laplacian (cf. [13], p.71) that leads to a discretization error of order $\mathcal{O}(h^2)$ (abbreviated as FD1 in the following) we use the so-called Mehrstellen-discretization (cf. [13], p.xx) given by the stencil

$$-\Delta_h = \frac{1}{6h^2} \left[\left[\begin{array}{ccc} 0 & -1 & 0 \\ -1 & -2 & -1 \\ 0 & -1 & 0 \end{array} \right]_h \left[\begin{array}{ccc} -1 & -2 & -1 \\ -2 & 24 & -2 \\ -1 & -2 & -1 \end{array} \right]_h \left[\begin{array}{ccc} 0 & -1 & 0 \\ -1 & -2 & -1 \\ 0 & -1 & 0 \end{array} \right]_h \right] \quad (5)$$

that leads to a discretization error of order $\mathcal{O}(h^4)$ (abbreviated as MSD). For the Mehrstellen-discretization we also have to change the right hand side of the Poisson equation by the stencil

$$f_h = \frac{1}{12} \left[\left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{array} \right]_h \left[\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 6 & 1 \\ 0 & 1 & 0 \end{array} \right]_h \left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{array} \right]_h \right]. \quad (6)$$

After the discretization we have to solve the linear system

$$\vec{A}_h \vec{u}_h = \vec{f}_h \quad (7)$$

3.2 Multigrid

One of the most efficient iterative methods to solve the resulting sparse linear system is Multigrid. Its complexity is linear in the number of unknowns. A good introduction but also some useful hints for the advanced user of multigrid methods can be found in [13]. The multigrid efficiency is achieved through the combination of a smoothing procedure on a fine grid that reduces the high frequency error components of the solution and a correction step that uses information from coarser grids to reduce the low frequency error components.

We have implemented both a lexical and a red-black Gauss-Seidel smoother for the FD1 and MSD operators and use linear interpolation \mathcal{I}_H^h and its transpose, the full-weighting \mathcal{I}_h^H , for restriction. The coarse grid operator is a simple 7-point stencil for the Laplacian on all levels, even if we have discretized it by the Mehrstellen-discretization on the finest level. In case of the MSD discretization on the finest level the interpolated correction from the second finest level is scaled by a factor of 1.25. This was found to give the fastest convergence rate for this mixed scheme (MSD on the finest level and FD1 on the coarser grids) by trial and error.

The above components are linked together to a V- or a W-Cycle. In the following we write e.g. V(2,1) in order to indicate that we use 2 presmoothing steps and 1 postsmoothing step on every level in the V-Cycle.

4 τ -Extrapolation

Extrapolation is another possibility to improve the discretization error to order $\mathcal{O}(h^4)$ that is less computational expensive than the Mehrstellen-discretization. Standard extrapolation techniques such as the Richardson Extrapolation can be used if there exist asymptotic expansions of the discretization error (cf. [14]). In this case the solutions of different mesh sizes can be combined to eliminate the lower order terms.

In contrast to that τ -Extrapolation is a multigrid specific technique that works only on a single grid (abbreviated as TAU). It is based on the principle of **defect correction** and has been first mentioned by BRANDT (cf. [15], see also HACKBUSCH [16], pp.278).

In the CS(correction scheme)-Multigrid algorithm two different iterations are used alternately, the smoother and the coarse grid correction (cf. [13]). These two iterations have a common fixed

point described by $\vec{f}_h - \vec{A}_h \vec{u}_h = 0$ (cf. [17], p. 17f). As mentioned above the smoother converges fast for certain (usually the high frequency) solution components, but converges only slowly for the remaining (low frequency) modes. The coarse grid correction behaves vice versa. If these complementary properties are combined the typical multigrid efficiency is obtained.

Now we follow the idea of **double discretization**, i.e. in the coarse grid correction process higher order discretizations are used. Using a correction of the form

$$\vec{u}_h^{(k+1)} = \vec{u}_h^{(k)} + \vec{e}_h^{(k)} , \quad (8)$$

where $\vec{e}_h^{(k)}$ is computed as a coarse grid correction

$$\vec{e}_h^{(k)} = \mathcal{I}_H^h \vec{A}_H^{-1} \widehat{\mathcal{I}}_h^H (\vec{f}_h - \vec{A}_h \vec{u}_h^{(k)}) , \quad (9)$$

would lead to a standard multigrid method. τ -extrapolation consists in using a linear combination of fine and coarse grid residual to construct an extrapolated correction

$$\widehat{\vec{u}}_h^{(k+1)} = \vec{u}_h^{(k)} + \mathcal{I}_H^h \vec{A}_H^{-1} \left(\frac{4}{3} \widehat{\mathcal{I}}_h^H (\vec{f}_h - \vec{A}_h \vec{u}_h^{(k)}) - \frac{1}{3} (\widehat{\mathcal{I}}_h^H \vec{f}_h - \vec{A}_H \mathcal{I}_h^H \vec{u}_h^{(k)}) \right) . \quad (10)$$

It can be shown that this modification of the coarse grid correction leads to a numerical error of order $\mathcal{O}(h^4)$ (cf. [18]). The modified coarse grid correction is only applied on the finest grid once per V-cycle. Additionally we have to take care when choosing the restriction and the interpolation operators. Normally trilinear interpolation for \mathcal{I}_H^h , full weighting for $\widehat{\mathcal{I}}_h^H$ and injection for \mathcal{I}_h^H is used, but this can vary from problem to problem. One has also to pay attention not do too many post smoothing steps and to choose the right smoother, otherwise the higher accuracy can be destroyed. A concise analysis of the τ -extrapolation is e.g. found in [18].

5 Results

5.1 Details of the Calculations

We have tested the different implementations of the Poisson-Solver with a similar testcase already employed before in Ref. [10]. A nitrogen molecule is positioned in a simulation box of 47x47x47 grid points (49x49x49 points including boundary points) using a grid spacing of $h = 0.3 \text{ bohr}$, which is sufficient to describe the valence wave functions appropriately. Further details on the exact implementation of the energy functional and the pseudo-potentials used (to efficiently describe the nuclei electron interactions) can be found in Ref. [10]. In contrast to the previous work Gaussian type compensation charges were employed to remove all the long range electrostatic interactions of the atoms [19]. The Poisson equation is actually solved only for the deformation density given by the full density minus the compensation charge. Thus, the potential of this deformation charge can be taken to be zero at the boundary of the simulation domain. Electronic and nuclei degrees of freedom are propagated with a second order Verlet propagator. In case of optimizations a special friction dynamics scheme was used to minimize the energy.

The point of interest is now the iterative calculation of V_{ee} via a solution of Eq. (4). The corresponding electrostatic self interaction of the electron cloud is calculated in our approach via a simple trapezoidal rule integration given by:

$$E_{ee} = \frac{1}{2} h^3 \sum V_{ee} \rho \quad (11)$$

Since the density is not known analytically but only on the discrete grid points there is also no accurate analytic “reference solution”. Thus, the quality of discretization must just be sufficient to give a physically correct representation of the Coulomb problem, which essentially means its discretization error must be comparable to the discretization errors for the integrals of the other energy terms. For the CP-MD dynamics, however, the potential V_{ee} is taken to be the exact derivative $\partial E_{ee} / \partial \rho$ (as a partial derivative due to the discretization). Even for slight deviations from this equality a deviation from energy conservation can be observed. It was already shown that energy conservation critically depends on the quality of the boundary conditions for V_{ee} and on the convergence. It is important to note that due to the small timestep the changes in the density ρ

	E_{DFT} [ha]	E_{ee} [ha]	HOMO [eV]	d(N-N) [Å]
FD1	-19.905108	0.100242	-10.422	1.0845
TAU	-19.906913	0.099943	-10.440	1.0835
MSD	-19.909161	0.099027	-10.469	1.0823

Table 1: Parameters of the optimized nitrogen molecule using different discretization strategies for the Poisson equation.

and thus on V_{ee} are only modest. Thus the problem to be tackled is a repeated reoptimization of the potential V_{ee} starting from a very good initial guess from the previous timestep. In addition, the initial solution can be improved further by a second order extrapolation from the previous timesteps. As a stopping criterion for the Poisson solver we tested whether the root mean square residual (divided by the number of grid points) is below 10^{-10} . In case of the τ -extrapolation the residual is meaningless and we tested whether the resulting E_{ee} changed by less than 10^{-8} a.u. between consecutive V-cycles, which was tested to give roughly equal convergence. For the multigrid V-cycles a V(4,1) strategy was used throughout with 4 grid levels. In the free dynamics simulations a timestep of $\Delta t = 5$ a.u. was used for the propagation.

In order to assess the saving in CPU time achieved by the MG solver in comparison to the previously used SOR solver with an overrelaxation parameter $\omega = 1.7$ we used a larger test system of 8 silicon atoms optimizing the bond length in a cubic structure. Again a grid spacing of $h = 0.3$ a.u. was used and the box consisted of $71 \times 71 \times 71$ points ($73 \times 73 \times 73$ including boundary values for V_{ee}).

5.2 Optimization of a Nitrogen Molecule

First we optimized both wavefunctions and nuclei of the nitrogen molecule using the three different forms of discretization FD1, TAU and MSD in Eq. (7) in order to investigate the effect on physical quantities of the solution. In Tab. 1 a selection of the resulting parameters are given. The self energy E_{ee} differs by less than 1% for the different operators. The value resulting for the τ -extrapolation lies as expected between the ones for FD1 and MSD. Note, that we actually calculate only the self energy of the difference between the true valence electron density and the gaussian type reference density, which leads to rather small absolute values of E_{ee} . As a consequence the changes for the total energy are modest. Also the eigenvalues of the highest occupied KS-Orbital (HOMO) are nearly identical and also the equilibrium bond length only weakly depends on the quality of the discretization of the Poisson equation. However, MSD is of course more accurate for the price of a higher numerical effort. Thus, the TAU approach is without any doubt an improvement over FD1 with a comparably small extra effort necessary for the calculation of the τ -extrapolation (Eq. (10)).

5.3 Free Dynamics for a Nitrogen Molecule: Energy Conservation

Now we verified the quality of energy conservation for the different discretizations. For this purpose we first optimized just the wavefunction at a constrained bond length of $d(\text{N-N}) = 1$ Å. Then we performed a free dynamic for 2000 timesteps starting from this situation. In Fig. 1 both potential, kinetic and conserved energies for the example of FD1 are shown relative to the initial values. The N_2 molecule oscillates around its equilibrium bond length (see Tab. 1). The wavefunction moves along with the nuclei and the energy is nicely conserved. In Fig. 2 only the conserved energies for the three operators are compared in a finer scale. Despite the small oscillations no significant drift for none of the three cases can be observed. However, FD1 and MSD show a very similar pattern, whereas the TAU extrapolation slightly differs. It should be noted, that both FD1 and MSD lead to identical results for a given convergence threshold irrespective of the type of the smoother or the V-cycle chosen. In contrast to that the results of the TAU extrapolation depend on the number of post smoothing steps on the finest level. Interestingly we observed a very important effect when using a lexical and not a red-black GS smoother in the V-cycle. The symmetry breaking introduced by the lexical GS smoother to some extent remains in the final solution of the TAU extrapolation, which is not the case for the non-symmetry breaking red-black smoother. In case of FD1 and MSD this does not make a difference. However, for the TAU extrapolation only with the red-black

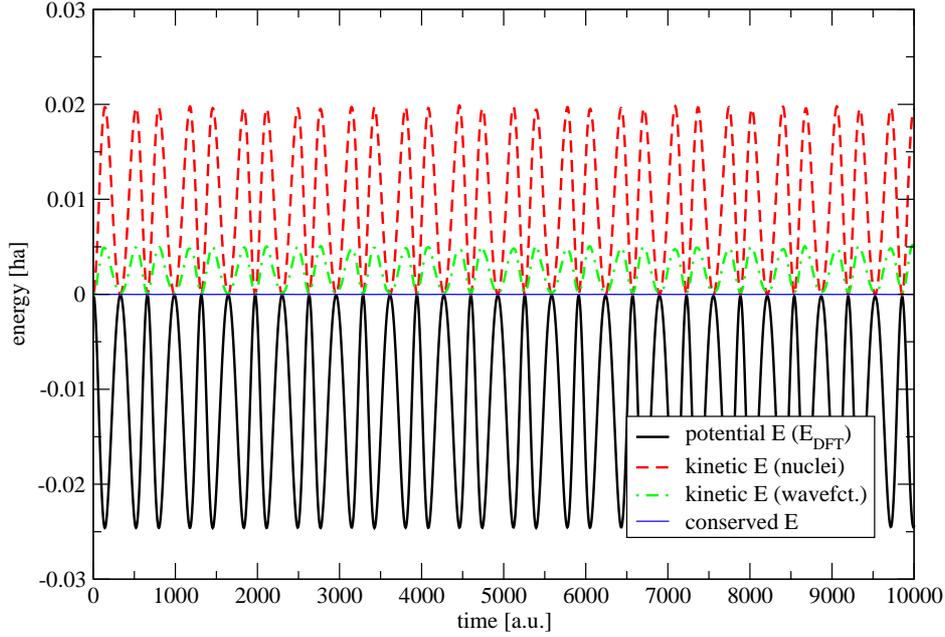


Figure 1: Energies for a free dynamics of a Nitrogen molecule (FD1). Energies in atomic units (Hartree) relative to the initial value.

GS energy conserving dynamics can be achieved, whereas for the lexical GS a strong deviation is observed as shown in Fig. 3.

5.4 Optimization of a Si_8 cluster: Numerical efficiency

In the first step of the optimization there is no guess for V_{ee} and the Poisson solver starts from zero. Here the largest number of cycles are necessary to reach convergence. In the further process the changes in the density become smaller and smaller and less steps are necessary to reach convergence. In Fig. 4 the convergence for the first step is shown comparing the SOR with the MG solver. It should be noted that only the number of fine grid cycles (5 per V(4,1) cycle) are plotted in case of MG. Due to the overhead for restriction, interpolation and the coarse grid iterations the comparison is not fair in terms of CPU time. In Tab. 2 the CPU time for the recalculation of V_{ee} per step on a typical LINUX workstation is given for the first step and as an average over the whole optimization. The timings clearly demonstrate the advantage of the MG scheme over SOR especially for the first

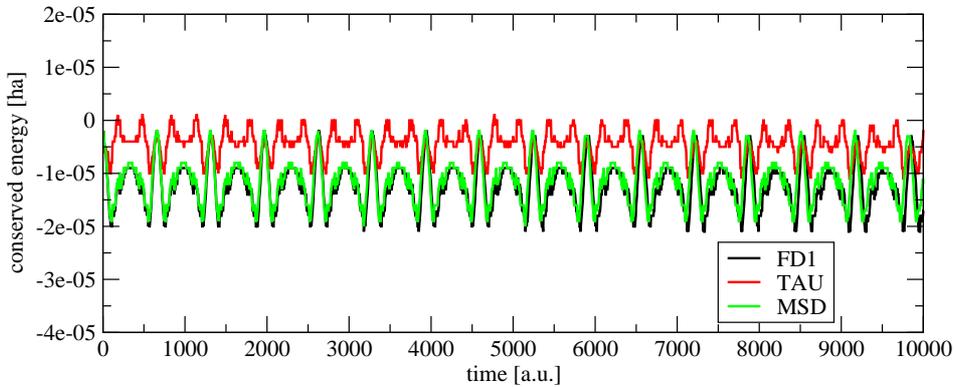


Figure 2: Conserved energies for the different operators (red-black smoother) relative to the initial value.

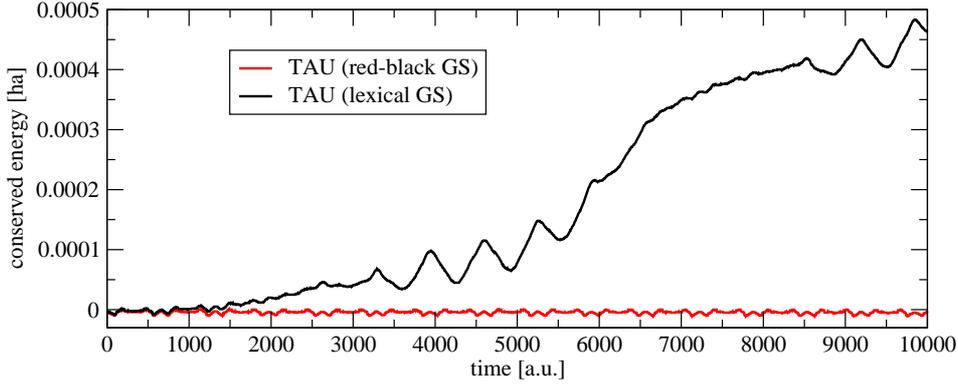


Figure 3: Comparison of the conserved energies for TAU with a lexical and a red-black Gauss-Seidel smoother.

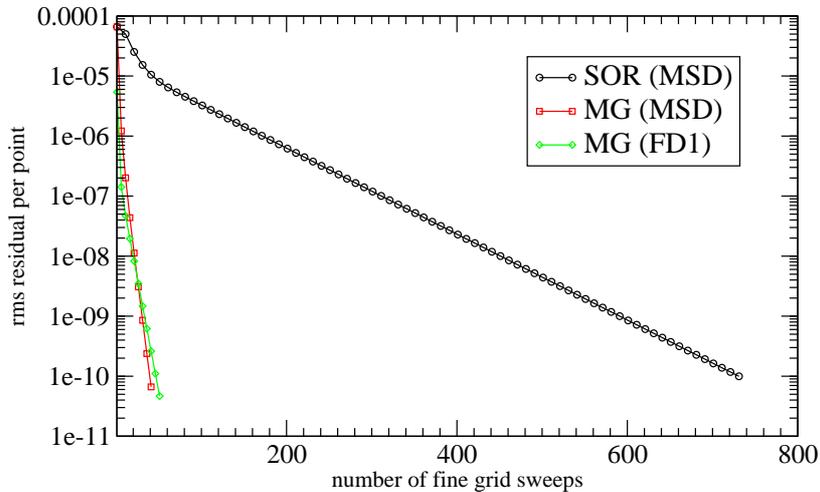


Figure 4: Convergence of the rms residual in the first step of the optimization for SOR vs. MG

step. However, also during the whole optimization the MG scheme converges faster than SOR. Interestingly, the MSD scheme (with the FD1 operator on the coarser grid levels) converges with less V-cycles as compared to FD1. As a consequence, despite the larger numerical effort for the Mehrstellen-discretization, MSD performs best.

6 Conclusions

The MG scheme is found to substantially improve the convergence speed of a Poisson solver used within a recently developed Car-Parrinello real-space electronic structure code. This holds despite the fact that a frequent redetermination of the solution for a slightly changed right hand side has to be performed. All implemented strategies were proven to yield energy conserving ab initio molecular dynamics. Interestingly, for the τ -extrapolation this was, however, only the case if a red-black

		SOR (MSD)	MG (MSD)	MG (FD1)
1. Step	CPU time [s]	21.9	2.28	2.38
Average	CPU time [s]	3.37	0.644	0.750

Table 2: CPU time for the solution of the Poisson problem in the optimization of the Si_8 system.

GS solver was employed, whereas a lexical solver led to a large deterioration of the energy conservation. Concerning the discretization accuracy the τ -extrapolation was found to lie between the Mehrstellen-discretization and the standard finite difference 7-point stencil. The effect on structural properties and electronic properties of an optimized nitrogen molecule are, however, modest. In case of the MSD scheme, the finite difference stencil was used for the coarse grid iterations and the finest grid correction was scaled by a factor of 1.25 leading to the fastest convergence of this startegy in terms of the number of V-cycles. Altogether, this combined approach was therefore most accurate and fastest in terms of CPU time. It represents a significant improvement in the code in comparison with the previously used SOR solver.

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