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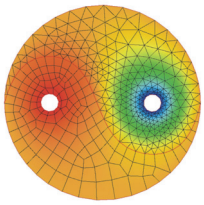

FITTING REACTIVE FORCE FIELDS USING GENETIC ALGORITHMS

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Abstract

With reactive force fields it is possible to perform atomistic simulations that join the accuracy of quantum chemical treatments (including bond breaking and formation) with the ability to treat hundreds of thousands of atoms on time scales well into the nanosecond regime. To utilize this power in everyday applications requires (I) the assembly of a suitable reference data set of sufficient quality, and (II) a reliable fit of the huge and complex parameter set of a general reactive force field to these reference data. In this contribution, we show that genetic algorithms can be used to achieve goal (II). We discuss algorithm design and implementation aspects (including parallelization) and present an application to azobenzene as real-life example.

Key words: genetic algorithms, global optimization, azobenzene

1. INTRODUCTION

Hot topics of current research in chemistry include smart materials (Murphy & Wudl, 2010; Sun et al., 2012) that change their properties upon external stimuli and molecular machines (Browne & Feringa, 2006; Shirai et al., 2006) that perform mechanical tasks at the nanoscale. Applications of this kind hinge upon fine control of molecular actions over long time scales, compared to the ultrafast regime of elementary reaction steps. Hence, theoretical simulations in such areas require reactive molecular dynamics (MD) of many thousands of atoms for many nanoseconds. Such a feat is currently impossible with desirable approaches like quantum chemical direct dynamics, and this will remain so for the next decades. There is, however, an alternative viable today: classical-mechanical MD with reactive force fields.

Reactive force fields have accompanied MD simulations since its beginnings (Alder & Wainwright, 1959; Karplus et al., 1965; Verlet, 1967). Only in recent decades, non-reactive biochemistry force fields have taken over the majority of MD applications. Despite this trend, reactive force fields have been used for special purposes. Well-known examples include the Brenner potential for hydrocarbons (Brenner, 1990), the empirical valence bond (EVB) approach (Warshel & Bromberg, 1970; Warshel & Weiss, 1980; Kamerlin & Warshel, 2010) and its re-invention as multiconfigurational molecular mechanics (MCMM) (Kim et al., 2000). 12 years ago, the ReaxFF potential was added to this list (van Duin et al., 2001). Since then, it has been made available for many systems of current interest, including difficult ones like e.g. transition-metal catalysis of organic reactions, and it has seen many applications in recent years. Therefore, we have chosen ReaxFF for the present contribution.

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Differing binding propensities of different atoms in different oxidation states and molecular neighborhoods need to be properly represented in any force field. Traditional biochemical force fields use atom types for this purpose. They make it possible to describe chemically relevant propensities of atoms in very specific situations (e.g., an sp^2 hybridized carbon atom bound to another sp^2 carbon atom, to a hydroxyl group and to a methyl group) with relatively few parameters (about a dozen), which are comparatively easy to determine from fitting to a limited reference data set, which in turn is relatively easy to establish since it needs to be representative only for this very specific situation. The price for these simplifications is the inability to switch from one atom type to another, and even if this were possible, to determine when to do so, how fast, and to which other atom type.

Hence, reactive force fields typically have no atom types. Therefore, they need to represent a given atom in all of its possible surroundings. For this, many more parameters per atom are necessary. Likewise, the reference data set needs to encompass all situations relevant to determining all of these parameters (and all combinations of them) uniquely. At the same time, the character of the fitting process changes from a rather simple, well-behaved case (often amenable to standard local optimization algorithms) into a difficult multi-minima situation. In this contribution, we demonstrate that such a difficult optimization task can be treated successfully with modern global optimization tools, specifically with Genetic Algorithms (GA), as shown here for the ReaxFF force field. At the beginning of this project, this was a new idea. While we were establishing its realization, Pahari and Chaturvedi (2012) published a small study on GA-optimization of ReaxFF parameters. As the authors admit, however, the reference data set they employed was very limited (comprising the equilibrium structures of only five molecules), and the main aim of the study was to use statistical methods to find a set of parameters to optimize, rather than establishing a suitable reference data set for general purposes or a good strategy for parameter optimization in a real-life application setting, with many parameters and a large set of reference data. This is provided by the present work.

The remainder of this paper is organized as follows: In section 2, technical details of our approach are specified, including computer implementation aspects. Results are presented in section 3, where a brief overview of test cases is followed by a more detailed report on an application to azobenzene. The paper concludes with a summary in section 4.

2. METHODS AND TECHNIQUES

The basic ideas of the GA approach go back at least to Holland (1975). Since then, this approach has grown into a research field of its own, with many ramifications (Goldberg, 1989; Goldberg, 2002; Weise, 2012). GAs belong to the class of stochastic-heuristic global optimization methods. As such, they turn out to be applicable successfully to large instances of difficult, multi-modal, non-convex optimization problems that take far too long to treat with deterministic methods. This becomes possible by abandoning the premise of covering all search space, directly or by estimations. The price for this practical advantage is that in GA applications there never is any certainty about having found a globally optimal solution; hence there also is no convergence criterion.

Very briefly, in a GA, a pool of trial solutions ("individuals") is iteratively improved upon by two basic mechanisms: Information is interchanged between individuals via "crossover" in a "mating" process (two new individuals are generated from two old ones). Single individuals are modified by "mutation", i.e., by changing part of the individual by some amount. Using a fitness function, the current performance of the individuals is measured (relative to each other, or relative to a known goal). The better ones get better chances to enter new rounds of mating, while the worse ones are eventually deleted from the pool. Accepted proofs for the performance of GAs are lacking, as well as a precise understanding for why they work as well as they do in practice.

Applications of GAs in various branches of chemistry and other fields have been reviewed several times (Hartke, 2002; Johnston, 2004; Hartke, 2011). Among these, global optimization of cluster structures (Hartke, 1993; Hartke, 1999) has grown into a research field of its own. Optimization efficiency was enhanced considerably by the phenotype approach (Deaven & Ho, 1995), in which crossover and mutation do not act on an abstract string representation of the atomic coordinates but rather directly on the cluster structures themselves. This automatically solves the "linkage problem" (which coordinates should be grouped with which others, to retain meaningful building blocks upon which the GA can operate) and also allows for chemical insight in the construction of new GA operators to

further enhance search efficiency (Hartke, 2000; Schulz & Hartke, 2002; Hartke, 2003; Takeuchi, 2006).

In contrast to the applications mentioned in the previous paragraph, here we have a considerably more abstract global optimization problem. Hence, no phenotype operators are possible, and we fall back upon more traditional representations and definitions of crossover and mutation operators: One individual is represented within the GA as a decimal string of values for all parameters to be optimized. Crossover is realized as simple one-point crossover between two parent strings, at a randomly chosen boundary between two parameter values. Mutation is realized as normal-distributed random deviation from the previous parameter value. As usual, the user sets a percentage value for crossover to happen, relative to all matings. In matings without crossover, both children are mutated. An additional GA control parameter determines how many parameters are mutated in such a case.

In order to optimize force field parameters, a set of reference data items is needed, which can consist of experimental data, calculated results, or a mixture of both. These data are then re-calculated employing the ReaxFF force field with a given set of force field parameters. As criterion for optimization, the usual sum of squared deviations between these two data sets is employed (called "error sum" for short in the following). Since the reference data usually vary wildly in character and importance, each entry additionally carries a weight factor that also enters into the sum (and formally makes it dimensionless). Since these weights are quite arbitrary, error sums cannot be compared across different data sets, and not even within the same data set if the weights are varied. The only strictly meaningful application of an error sum value is its relative minimization within one series of optimization runs, for one and the same reference data set.

In many applications, GA is hybridized with local search, often in such a way that after mating each child is locally optimized. In such hybrid algorithms, local optimization takes up 85-95% of the overall computational burden. Therefore, a very efficient local optimization is necessary, which can be realized employing standard local optimization algorithms like conjugate gradients or quasi-Newton methods, in combination with analytical derivatives with respect to the parameters to be optimized. Here, however, no analytical derivatives of the error sum with respect to the force field parameters are available, since the reference data set may encompass a broad variety of items, ranging from simple entries like relative energies to more complex items like atomic or molecular charges and minimum-energy geometrical data (distances, bond angles, dihedral angles), both of which are determined by iteratively convergent ReaxFF evaluation cycles while calculating the error sum.

It is common wisdom that replacing non-existent analytic derivatives in iterative optimization algorithms with numerical ones is inefficient, compared to iterative optimization algorithms not requiring derivatives. Hence, we have tested several algorithms of the latter type (Larsson et al., 2012). Our best choice for routine application is BOBYQA (Powell, 2009), which has the added benefit of respecting upper and lower bounds on all parameters, the specification of which is necessary for proper functioning of the GA anyway. In addition, mainly for postprocessing, we use NEWUOA (Powell, 2008), a predecessor of BOBYQA without constraints, to check if further optimization of a solution candidate is possible by relaxing the pre-set bounds.

The remainder of our GA setup follows the standard GA specified by Goldberg (1989). The only important deviation is that we do not use the generational paradigm but instead employ a steady-state / pool concept, since this incurs the benefit of seamless parallelizability across individuals without serial bottlenecks (Bandow & Hartke, 2006). In addition to this parallelization option, two further ones are available: across reference data set items, and across beyond-cutoff atoms at the level of ReaxFF energy/force calculations. The first two options are particularly attractive as they involve independent entities with little need for communication (embarrassing parallelism), allowing for near-ideal scaling. The latter option has already been implemented upon incorporation of ReaxFF into the ADF/SCM program suite (Yakovlev et al., 2012). To keep our initial implementation simple, we have switched off this energy/force based parallelism, and we have not made use of parallelization across individuals. We have, however, implemented reference data item parallelization, via explicit MPI calls at the source code level. For this, we have realized a strongly decoupled master-slave model: Only the master walks through all GA-related subroutines, while all slave processes wait for the master inside the subroutine where current ReaxFF values are generated for all reference data set items. There, in a straightforward loop with automatic load balancing (Gropp

et al., 1999), the master hands out job tickets for these items, which are then worked upon by the slaves in parallel. The master collects the results and, after leaving this code section, computes the total error sum for the present individual, which then enters into the usual GA scheme via an exponential fitness function. This reflects the actual work load rather well, since real-life tests proved that a speedup maximum could be achieved with a few dozen slave processes (Larsson et al., 2012).

3. RESULTS

3.1. Overview

To establish and test our GA approach to optimizing ReaxFF force field parameters, we have used three published test cases, provided by the main ReaxFF author Adri van Duin, with a given set of reference data items, with given selection of parameters to be optimized, and with given upper and lower bounds for each of them (which were modified in later stages of the optimization process).

The simplest one of these is the **Co** set (LaBrosse et al., 2010), with 12 parameters to be optimized and 147 reference data items. The best error sum van Duin's group could achieve is 1443.72. Without using any information from that solution, our best value is 1439.84. We consider this case to be trivial.

We have used the second set, **SiOH** (van Duin et al., 2003), for extensive testing; a detailed account of this testing will be published elsewhere (Larsson et al., 2012). This set contains 67 parameters to be optimized and 304 reference data set entries. Typical single GA runs for this set take 2-3 days real time (without local optimization) on 12-24 processes in parallel. Our best error sum for the original setup is 3196; when taking additional parameters into the optimization (bringing up the total to 93) we can even get down to 2807. The official best result from the van Duin group is 6455; preliminary results from our side prompted further optimization runs on their side, bringing their result down to just below 4000.

This provides ample proof that an unbiased global GA search can indeed produce better results in these complicated, high-dimensional optimization tasks than traditional, sequential-local optimizations (van Duin et al., 1994) backed up with extensive experience.

For a third set, **Gly** (Rahaman et al., 2011), GA work is currently in progress. This set contains 299 parameters and 2049 reference items. Not surprisingly, it turns out to be more challenging than the other two.

3.2. Azobenzene

The cases listed in the previous subsection were artificial in at least two respects: (1) All information needed to directly start the GA parameter optimization was given, in particular including several non-trivial items: the reference data set, the set of parameters to be optimized, and upper and lower bounds for these parameters; (2) performance on the reference data set (i.e., the error sum) was taken as the only indicator for suitability of newly generated force field parameter sets. In a more typical real-life application scenario, all this will be different: The reference data set will have to be established first, a reasonable subset of force field parameters will have to be selected for optimization (as opposed to leaving them at values taken from other force field optimization cases), and boundaries for these parameters will have to be set. Cross checks will have to be made to determine whether variations in the parameters chosen for optimization are actually covered by the reference data. Finally, after one round of GA optimizations, the best resulting new force fields will undergo exemplary applications beyond the reference data set, which may then lead to its extension, and to further repetitions of the cycle.

As a test case for checking the performance of our GA approach to ReaxFF optimization in this extended sense we have selected azobenzene. This system is the paradigmatic case of a molecular photoswitch, as its cis↔trans conversion can be triggered by light of suitable wavelengths. We have recently examined the photochemical properties of some of its derivatives (Carstensen et al., 2010; Carstensen et al., 2011). From these studies, we had access to a fast but accurate quantum-chemical method, specifically tuned to azobenzene: floating-occupation configuration-interaction based on semiempirical Austin-method-1 orbitals (FOCI-AM1; for details see Carstensen et al., 2010, and references therein). This proved to be ideal for the quick generation of reliable reference data. For the present initial tests, however, we restricted our attention to thermal dynamics of azobenzene in its electronic ground state.

Hence, a first version of a reference data set was generated by extracting 2000 snapshots from classical-mechanical 3 ps ground-state trajectories of cis- and trans-azobenzene at 300 K, with forces deter-

mined from FOCI-AM1. The error sum for this reference set consisted of equally weighted contributions from the deviations between FOCI-AM1 and ReaxFF energies at these snapshot geometries (without geometry optimizations in either case). In order to establish a suitable set of ReaxFF parameters to optimize, and to find upper and lower bounds to them, we extracted information from the previously used test cases (Co, SiOH and Gly). In addition, we had to define parameters for the HCCN, CNNC and NNCC dihedral angles, which were not present in those test cases but are of prime importance for the cis-trans-isomerization of azobenzene (Carstensen et al., 2011). This lead us to a set of 162 parameters to be optimized via our GA approach.

In this context, a minimum requirement for a good force field parameter set should be the ability to *qualitatively* reproduce the MD trajectories from which the reference data set was extracted. Hence, after a first round of GA optimizations, we used the best resulting new force fields in MD production runs, starting from cis-azobenzene, at 300 K. The resulting behavior was obviously very wrong, in a qualitative way: We observed very unchemical fusions and dissociations, occurring very quickly. Figure 1 shows exemplary snapshots for this behavior. Obviously, this initially chosen reference data set was not sufficient to ensure suitable behavior in these MD runs, despite the extraction of the reference data from MD runs with the very same initial conditions.

The obvious reason for this finding is that the ReaxFF force field is too flexible to be reliably determined by relative energies of the molecular geometries actually visited during such MD runs. Instead, additional information on the potential energy surface beyond these areas appears to be needed.

To supply this information, we built a new reference data set upon scans of selected internal coordinates. The most important internal coordinate for azobenzene is the CNNC dihedral angle, since the equilibrium structures for cis- and trans-azobenzene differ mainly in this coordinate. Hence, 88 structures were extracted from a relaxed scan of this angle (between 5° and 180°) at the FOCI-AM1 level. The error sum contributions for these reference data items were based on geometry deviations of corresponding ReaxFF relaxed scans, which are more compute-intensive but turned out to be more effective than comparing energies. In a similar fashion, 60 structures from relaxed CNN angle scans (100°-158°) and 86 structures from relaxed NNCC dihedral angle scans (0°-90°) were added to the reference data set. Finally, energies from rigid scans of several angles and C-C bond distances for out-of-plane deformations of the phenyl rings were also supplied.

Results from an initial round of GA runs for this new reference data set were filtered according to their performance in MD test runs. Those with the best MD results were used as initial pool for further GA runs. For good results from this second stage, figure 2 shows exemplary snapshots from MD runs,

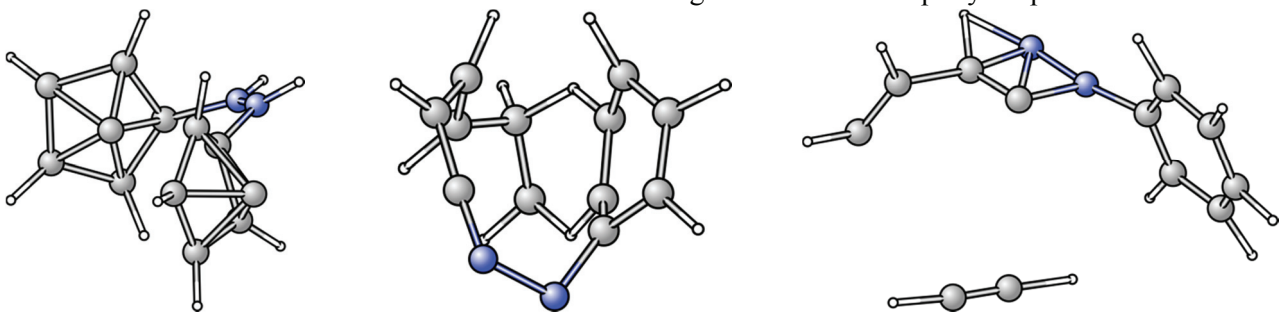

Fig. 1. *Snapshots from azobenzene MD trajectories, showing unchemical fusion and dissociation behavior.*

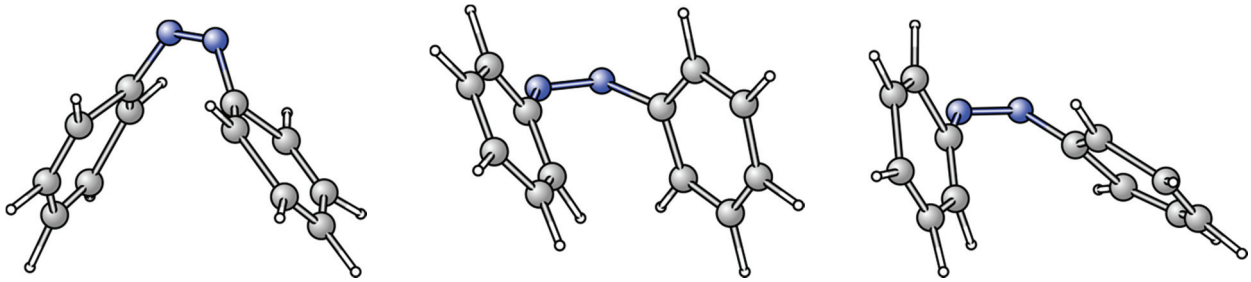

Fig. 2. *MD trajectory snapshots for cis-azobenzene at 300 K, using one of the best second-stage force fields resulting from GA optimization of ReaxFF.*

demonstrating qualitatively good behavior, comparable to what is seen at the FOCI-AM1 level.

For further characterization, in figure 3 two internal coordinate scans are shown, comparing FOCI-AM1 results with those from the unmodified Gly ReaxFF force field and from our GA-optimized ReaxFF force field. Obviously, our GA optimization has introduced drastic qualitative improvements. Some quantitative deviations, however, are also still visible, indicating that our reference data set, and possibly also our selection of ReaxFF parameters to optimize, are not yet optimal. This supports our finding that the correlation between small error sums and MD performance also is not perfect yet.

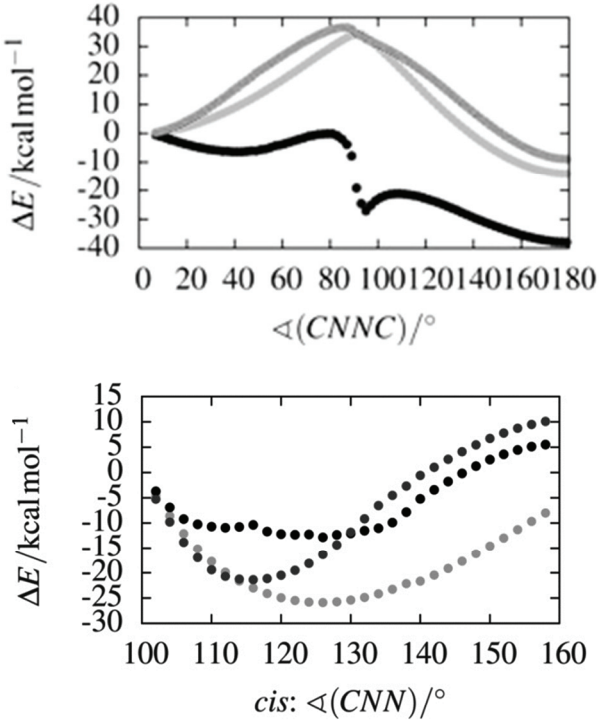

Fig. 3. *Comparison of relative energies along selected internal coordinate scans of azobenzene, between the reference level (FOCI-AM1, light grey), the Gly ReaxFF force field (black; the only available ReaxFF with fitted H,C,N atoms), and our GA-optimized ReaxFF force field (grey).*

This is, however, a drastic improvement compared to the initial results, and further iterations of the procedure described above will yield better agreement. Therefore, this suffices as proof of principle, demonstrating that our strategy of using a GA to globally optimize ReaxFF force field parameters can also be applied in realistic application cases in which initially all information on reference data, parameters to optimize and parameter ranges is missing.

4. SUMMARY AND CONCLUSIONS

We have shown that a GA approach can be used successfully to globally optimize ReaxFF force field parameters, relative to quantum-chemical reference data sets. This has been demonstrated for preselected sets of reference data and parameters, but also for a realistic system where neither a suitable set of parameters to be optimized nor a corresponding reference data set were known in advance.

We are currently working to transfer our GA optimization of ReaxFF parameters into the ADF/SCM program suite (Yakovlev et al., 2012), from where it will be publicly available.

5. ACKNOWLEDGEMENTS

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DOSTOSOWANIE PÓL SIŁ REAKCJI Z WYKORZYSTANIEM ALGORYTMÓW GENETYCZNYCH

Streszczenie

Przy pomocy pól sił reakcji możliwe jest przeprowadzenie symulacji atomowych, które łączą w sobie dokładność procesów chemii kwantowej (włączając zrywanie i tworzenie wiązań) oraz zdolność przetwarzania setek tysięcy atomów na skali czasowej w reżim nanosekundowy. Aby wykorzystać takie możliwości w powszechnych aplikacjach wymagane jest (I) zgromadzenie odpowiednich danych referencyjnych zapewniających niezawodną jakość, oraz (II) dopasowanie dużego i złożonego zestawu parametrów pola sił reakcji do tychże danych referencyjnych. W niniejszej pracy wykazujemy, że algorytmy genetyczne mogą być wykorzystane do osiągnięcia celu (II). Omówiony został wstępny algorytm oraz aspekty jego implementacji (w tym zrównoleglenie). Jako rzeczywisty przykład wykorzystania algorytmu przedstawiono jego zastosowanie w azobenzenie.

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