Applications of Distance Geometry Algorithms to Atomistic Simulation of Polymer Systems

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R. V. N. Melnik,* A. Uhlherr,† J. H. Hodgkin‡ and F. de Hoog§

Abstract

In solving molecular conformation problems, stochastic methods based on Molecular Dynamics and Monte-Carlo simulations have become quite popular amongst the researchers. Despite recent progress, these methods are still computationally very demanding and the success of their applications to realistic polymer systems relies heavily on the choice of initial conformation. In this talk we argue that moving towards atomistic simulations of complex polymer systems and composites, another group of stochastic search methods, known under its generic name as distance geometry (DG), will play an increasingly important role. Formulating the general distance geometry problem in atomistic simulation of materials as an optimisation problem, we apply two distance geometry algorithms to its solution and analyse their performance for bulk decane molecules. The comparative analysis of the described algorithms in applications to cross-linked polymeric structures is a natural extension of the presented work.

Key words: distance geometry algorithms, polymer systems.

AMS subject classifications: 82D60, 65C20, 73S10.

1 Introduction

Polymeric materials and polymer-based composites became an intrinsic part of many new industrial materials technologies where structural engineering and material engineering research go hand in hand [17]. This research relies heavily on the fact that the material from which the end-use structure is made can be "designed" in principle and adapted to suit specific engineering purposes. A core component in this research, both from the technological and theoretical point of view, is to be able to extract the information about the macroscopic (thermomechanical, structural) properties of polymers from their microscopic (atomistic) constitution [7].

Since microscopic, atomistically detailed models of materials provide a key to a better understanding of their behaviour at the macroscopic level, the development of such models and algorithms for their implementation become an important activity in industrial materials research, in particular in polymer and composite sciences. The computer-aided molecular design of structures using effective algorithms leads to the situation where compounds and composites worthy of actual synthesis can be effectively identified.

The main focus of this paper is the application of two distance geometry algorithms to atomic-level simulations of polymer structures and the analysis of these algorithms in terms of their performance in molecular conformation problems. The potential of such algorithms in predictions of detailed atomic-level structures, and ultimately, of properties of the material, provides the real opportunity to design, characterise and optimise polymers before undertaking

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expensive experimental work. Reflecting industrial trends in widening those areas where polymeric materials and polymer-based composites displace metals, ceramics and glass, atomistic models and effective algorithms for their implementation will play an increasingly important role.

2 Distance Geometry as a Natural Approach to Atomistic Simulations of Complex Polymer Systems and Composites

A general approach to atomistic simulations of polymeric structures is based on a blend of quantum mechanics (QM) and molecular dynamics (MD) methodologies. By using methods of quantum mechanics we can compute first principles force fields and then, by using the latter, we can apply molecular dynamics techniques to calculate trajectories which will allow to extract the information on the macroscopic properties of the material. Unfortunately, the application of this straightforward procedure to realistic polymers leads to considerable difficulties. Indeed, to describe partially crystalline polymers one needs $\sim 10^6$ atoms per unit cell, which makes the use of classical *ab initio* methods of quantum chemistry such as pseudospectral or cell multipole methods highly problematic. A standard simplification of the above approach consists of averaging electronic degrees of freedom into force fields and charges. This simplification opens the door for applications of MD and Monte Carlo (MC) simulation methods. Although quantum mechanical calculations can provide potential surfaces for small molecules, empirical energy functions of the molecular mechanics type become the only possible source of such information for proteins and the surrounding solvent, for polymeric materials, as well as for complex composite structures [11].

Despite recent progress in the computational-cost-reduction program, MD simulation techniques applied to real polymeric systems are still computationally very demanding [10]. Moreover, since polymers are characterised by a wide-range hierarchy of different length and time scales, in MD simulations of a long-chain polymer the large-scale conformational characteristics of the system are given too little time to evolve. As a result, the system often remains trapped within the neighbourhood of the initial configuration which leads to insufficient sampling of the configuration space and unreliable estimations of the dynamic and structural properties of the polymer. These two factors retard a wider applicability of the MD technique to realistic polymer structure and lead to an increase of interest in alternative approaches. When static thermodynamic properties of the material (rather than the dynamics) are of the main concern, Monte Carlo algorithms provide a viable alternative to the MD methodology. Moreover, after relaxing the system with an effective MC algorithm, the study of the system with the MD methodology can help to extend the simulation time to longer scales [14].

One of the main disadvantages of the MD algorithms (as well as of the MC algorithms) is the requirement of one conformation as a starting point. Therefore, a real challenge for these types of algorithms is to build plausible initial configurations which can then be relaxed effectively [13]. For complex polymeric systems and composites, this has often proved to be a difficult task. Even if the initial conformation is found, the computer time required for full conformational search by the MD and MC algorithms and many other stochastic search methods (genetic algorithms, e.g.) is often hardly feasible for real polymeric systems and composites. The situation is not better for the majority of deterministic methods that, due to their exhaustive search of the conformational space, are becoming less feasible computationally when designing complex new material structures. Taking this into account, it is natural to seek such methods that (1) do not need any starting conformation; (2) do not need force field parameters, (3) allow us to determine quickly the existence of a model that satisfies our experimental constraints, (4) have good sampling properties, and (5) allow us to obtain a credible conformational profile of the system. In principle, such methods should be complimentary to MD procedures in a sense that they aim at generating complex models rapidly with little efforts and producing structures that give appropriate *starting points* for MD calculations [3]. Such calculations are often essential for comparing the models and finding the lowest energy structure, though the methods themselves may not preferentially sample low energy structures. Some very promising candidates for these types of methods can be chosen by using the *distance geometry* methodology. In the heart of this methodology is a dependency between geometric constraints on the atoms of a molecule and the structure of the molecule. The interest in distance geometry algorithms has been recently revived when it was shown that they can perform as well as many well-established techniques of conformational analysis [18].

Mathematically speaking, the problem of distance geometry applied to atomistic simulation of polymeric systems can be formulated in two parts.

Part I. Since measurements (obtained, for example, from NMR data) may introduce errors into the symmetric matrix (of measured distances) A with nonnegative entries $a_{ij} \geq 0$, $i, j = 1, ..., n$, $i \neq j$ and such that $a_{ii} = 0$, $i = 1, ..., n$, in the general case this matrix, called a dissimilarity or pre-distance matrix, will deviate from the Euclidean matrix [2]. Recall ([15], e.g.) that if for a pre-distance matrix $D = (d_{ij})_{i,j=1,...,n}$ there exist n points

$\mathbf{x}^l \in \mathbb{R}^r$, $l = 1, ..., n$ such that

$$\|\mathbf{x}^i - \mathbf{x}^j\|_2 = \delta_{i,j}, \quad (i, j) \in \mathcal{S}, \tag{1}$$

is satisfied, we call such a matrix the Euclidean distance matrix. In (1) $\delta_{ij} = \sqrt{d_{ij}}$ is the given distance between atoms i and j, $\mathcal{S}$ is a subset (say, $i, j = 1, ..., n$, $n \leq m$) of all atom pairs ($i, j = 1, ..., m$), $\mathbf{x}^k \in \mathbb{R}^r$, $k = 1, ..., m$ are the sought-for positions of the atoms in the molecular system, and r is the embedding dimension. Therefore, the first problem of distance geometry can be formulated as follows. Having a pre-distance matrix A, we have to "complete" it to a Euclidean distance matrix D. This problem is equivalent to the problem of finding such a Euclidean distance matrix D from a set of all admissible Euclidean matrices that solves the weighted Euclidean matrix optimisation problem

$$f_1(D) := \|H \circ (A - D)\|_F \to \min, \tag{2}$$

where H is the weight matrix (see [1] for a special case $H = I$), $\| \cdot \|$ denotes the Frobenius norm ($\|A\|_F = \sqrt{\mathrm{tr}A^T A}$) and $\circ$ denotes the Hadamard-Schur product (by definition, $A \circ B = (a_{ij}b_{ij})_{i,j=1,...,n}$).

Part II. Assuming that the Euclidean distance problem (or the Euclidean distance completion problem) is solved, the problem of finding positions of atoms $\mathbf{x}^l \in \mathbb{R}^r$, $l = 1, ..., n$ that satisfies (1) can be reformulated as an optimisation problem

$$f_2(\mathbf{x}) = \sum_{i,j \in \mathcal{S}} \omega_{i,j}(\|\mathbf{x}^i - \mathbf{x}^j\|_2^2 - \delta_{i,j}^2)^2 \to \min, \tag{3}$$

which is solved by such $\mathbf{x} \in \mathbb{R}^{r \times n}$ that $f_2(\mathbf{x}) = 0$. We assume that the embedding dimension is 3 and $n \geq 4$ (since $r \leq n - 1$). In reality, however, the distance matrix is given only approximately, and some elements are defined by lower and upper bounds that are not equal. As a result, the process of converting the distance bounds matrix into Cartesian coordinates becomes much more tedious. Apart from the problem of whether the structure can be determined uniquely from incomplete but exact data ([8], e.g.), this leads to the problem of finding positions $\mathbf{x}^1, ..., \mathbf{x}^n \in \mathbb{R}^3$ such that inequalities with the given lower, l_{ij}, and upper, u_{ij}, bounds on a set of distance constraints (1) with $\delta_{ij} \in [l_{ij}, u_{ij}]$ are satisfied, i.e.

$$l_{ij} \leq \|\mathbf{x}^i - \mathbf{x}^j\| \leq u_{ij}, \quad (i, j) \in \mathcal{S}. \tag{4}$$

Following the approach originally proposed in [4], we are looking for the solution(s) of the following problem

$$\tilde{f}_2(\mathbf{x}) \to \min, \quad \mathbf{x} \in \mathbb{R}^{3n}, \tag{5}$$

where $f(\mathbf{x})$ can be thought as the potential function. We aim at the construction of an efficient algorithm to find a representative sample of local minimisers for such an objective function. The choice of the potential function $f(\mathbf{x})$ is not unique and can influence the computational effectiveness of the DG algorithm associated with such a choice.

3 Distance Geometry Algorithms with Smooth and Non-Smooth Potential Functions

Since their first appearance in problems of computational chemistry, distance geometry algorithms have been extensively developed to provide better initial trial coordinates as well as better error refinement [18]. These algorithms have often been quoted in the context with methodologies for compound structure determination such as nuclear-magnetic resonance (NMR) technique, in particular, the approximate solution conformations of protein and peptides from NMR data [4, 9, 18]. They appeared to be a viable tool in the solution of the central problem of molecular biophysics, namely the determination of the time-average conformations of biological macromolecules. Today, the DG algorithms boast a wide variety of techniques such as metric matrix method, embedding algorithm, torsional space method (as well as their modifications), and provide a powerful tool in molecular modelling applications ranging from conformational analysis of small molecules and pharmacophore modelling to drug-receptor docking and constructing genetic maps [3, 16]. However, it would be fair to say that for many years such algorithms have been traditionally applied predominantly to small molecules where they usually perform as well as other sampling procedures.

Due to their computational effectiveness and the ability to provide results compatible with well-established techniques [18], the DG algorithms become very attractive candidates for applications to more complex structures such

as polymeric systems and composites. It should be borne in mind, however, that since DG algorithms do not use interatomic potentials, after their application to high density structures refinement with molecular dynamics or energy minimisation is typically required [19]. This approach allows us to extract physico-mechanical properties of a range of technologically interesting polymers [6, 7].

Since there is no ideal conformational sampling procedure that is optimal, in some sense, for all cases, the choice of the objective function in the solution of problem (4)–(5) and the procedure for tracing local minimisers of this function deserve much more attention than they were accounted in the past.

We consider two possible avenues in the analysis of DG algorithms.

First is a simple approach (called here DG1) consisting of a generation of minimising the error function by generating random conformers and then of the refinement of the obtained coordinates against an error function [4, 3]. Typically, the objective function in this case is the double sum $\sum_{i=1}^{n-1} \sum_{j=i+1}^{n}$ of one of the following error functions:

$$(6) \quad \epsilon_{ij}^1 = \max[0, (d_{ij}^2 - u_{ij}^2)^2] + \max[0, (l_{ij}^2 - d_{ij}^2)^2], \quad \epsilon_{ij}^2 = \max\left[0, \left(\frac{d_{ij}^2}{u_{ij}^2} - 1\right)^2\right] + \max\left[0, \left(\frac{l_{ij}^2}{d_{ij}^2} - 1\right)^2\right],$$

$$(7) \quad \epsilon_{ij}^3 = \max\left[0, \left(\frac{d_{ij}^2}{u_{ij}^2 - 1}\right)^2\right] + \max\left[0, \left(\frac{2l_{ij}^2}{l_{ij}^2 + d_{ij}^2} - 1\right)^2\right], \quad \epsilon_{ij}^4 = \max(l_{ij} - d_{ij}, d_{ij} - u_{ij}).$$

It can be seen from (6)–(7) that objective functions are often chosen as a sum of terms, one for each constraint, such that the term is zero if the constraint is satisfied or monotonically increasingly positive as the violation of the constraint increases. DG1 has been used to produce better starting conformations, in the sense that subsequent minimisation of the error function more often succeeds in reaching a value close to zero [5]. Results reported in this talk were obtained with the function $\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \epsilon_{ij}^4$. Of course, this function is non-differentiable and in the general case may have too many minimisers. Since bound-smoothing procedures increase the number of effective constraints and decrease the regularity properties of this function, no bound-smoothing technique has been implemented in this algorithm to keep it computationally effective. Recall that in the standard metric matrix DG algorithms we obtain a trial metric matrix which corresponds to some conformation in $\mathbb{R}^n$. Then the nearest rank 3 matrix (built up out of the 3 largest positive eigenvalues and corresponding eigenvectors of the trial metric matrix) is converted into a set of atomic trial coordinates in $\mathbb{R}^3$. These trial coordinates might not obey the original geometric constraints. Then, refined coordinates are found by local minimisation of the constraint violations as a function of atomic coordinates starting from the trial coordinates. In our DG1 algorithm we avoided the procedure of using such time-consuming steps as the determination of the three largest eigenvalues of the metric matrix and their corresponding eigenvectors. When we want to ensure the "best" possible random sampling of conformational space, smoothing can be easily implemented via different versions of the metrisation procedure (see [3], e.g.). In particular, the smoothing procedure can be applied to lower some (unrealistic) default upper bounds in our constraints with the triangle inequality and to raise some (unrealistic) default lower bounds with the inverse triangle inequality. Note that other rules such as tetrangle (the more so, pentangle) inequality will lead to the deterioration of computational effectiveness of the DG method since they require n^4 arithmetic operations. In constructing the DG1 code, we assumed that atoms in different molecules can be treated as hard spheres and they have a minimum separation corresponding to a non-overlap condition. This gives the obvious condition for default lower bounds. To choose default upper bounds, we assumed that all random points are confined to an "amorphous" cube (the half of its diagonal will give the required bound) and we measured other effective distances via elementary chemical geometry. No smoothing procedure for the objective function has been implemented in this case.

The second approach (called DG2) is based on the Moré-Wu methodology consisting of a transformation of the original objective function to a smoother function that have smaller number of local minimisers, and then of tracing back those minimisers to the original objective function [15]. In this case, the potential function in (4)–(5) is defined as

$$(8) \quad \tilde{f}_2(\mathbf{x}) = \sum_{(i,j)\in\mathcal{S}} p_{ij}(\mathbf{x}^i - \mathbf{x}^j) \quad \text{where} \quad p_{ij} : \mathbb{R}^n \to \mathbb{R}, \quad \text{defined by} \quad p_{ij}(\mathbf{x}) = h_{ij}(\|\mathbf{x}\|),$$

that is

$$(9) \qquad \tilde{f}_2(\mathbf{x}) = \sum_{(i,j) \in \mathcal{S}} h_{ij}(d_{ij}), \quad \text{where as before,} \quad d_{ij} = \|\mathbf{x}^i - \mathbf{x}^j\|.$$

For example, for distances function (3) in a special case where $\omega_{ij} = 1$, we have

$$(10) \qquad h_{ij}(d_{ij}) = (d_{ij}^2 - \delta_{ij}^2)^2,$$

while for bounds on distances it has the form

$$(11) \qquad h_{ij}(d_{ij}) = \min\left[\left(\frac{d_{ij}^2}{l_{ij}^2} - 1\right)^2, 0\right] + \max\left[\left(\frac{d_{ij}^2}{u_{ij}^2} - 1\right)^2, 0\right].$$

The coordinates $\mathbf{x}^1, ..., \mathbf{x}^m$ from the representative sample we mentioned above should satisfy the following inequalities

$$(12) \qquad \left|\|\mathbf{x}^i - \mathbf{x}^j\| - \delta_{ij}\right| \le \epsilon, \quad (i,j) \in \mathcal{S}.$$

For fixed $\epsilon > 0$ this leads to the problem of finding ϵ-optimal solutions to our distance geometry problem.

With the Gaussian transform $g \in \mathbb{R}^n \to \mathcal{G}^\lambda(f) \in \mathbb{R}$

$$(13) \qquad \mathcal{G}^\lambda(g) = \frac{1}{\pi^{n/2}\lambda^n} \int_{\mathbb{R}^n} g(\mathbf{y}) \exp\left(-\frac{\|\mathbf{y} - \mathbf{x}\|^2}{\lambda^2}\right) d\mathbf{y}$$

we transform the original function f to a smoother function (with controlled degree of smoothing) with fewer local minimisers, apply an optimisation algorithm to the transformed function, and trace the minimisers back to the original function [15]. For the function $\tilde{f}_2$ (9) we have (see [15] and references therein)

$$(14) \qquad \mathcal{G}^\lambda(\tilde{f}_2) = \sum_{(i,j) \in \mathcal{S}} \frac{1}{\sqrt{2\pi}d_{ij}} \int_{-\infty}^{+\infty} (d_{ij} + \lambda s) h_{ij}(d_{ij} + \lambda s) \exp(-s^2/2) ds.$$

This integral can be easily approximated with the Gauss-Hermite approximation

$$(15) \qquad \mathcal{G}^\lambda(\tilde{f}_2) \approx \mathcal{G}^{\lambda,q}(\tilde{f}_2) = \sum_{(i,j) \in \mathcal{S}} \frac{1}{d_{ij}} \sum_{k=1}^{q} \omega_k (d_{ij} + \lambda s_k) h_{ij}(d_{ij} + \lambda s_k),$$

where ω_k and s_k, $k = 1, ..., q$ are weights and nodes, respectively, for the Gaussian quadrature for the integral

$$(16) \qquad I(g) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(s) \exp(-s^2/2) ds.$$

To determine local minimisers of $\tilde{f} = \mathcal{G}^{\lambda_k,q}(\tilde{f}_2)$, $k = 0, 1, ..., p$ such that $\lambda_0 > \lambda_1 > ... > \lambda_p$ (recall that the original function is recovered in the limit $\lambda \to 0^+$) we follow [15] and use a quasi-Newton-type algorithm. We judge the result upon the following error functions

$$(17) \qquad \epsilon_l = \min\left(\frac{d_{ij}}{l_{ij} - 1}, 0\right), \quad \epsilon_u = \max\left(\frac{d_{ij}}{u_{ij} - 1}, 0\right), \quad \epsilon_l^u = \max(\epsilon_l, \epsilon_u),$$

and the value of the objective function $\sum_{(i,j) \in \mathcal{S}} h_{ij}(d_{ij})$.

The comparison of the performance of algorithms DG1 and DG2 for conformation of decane in the bulk liquid phase is currently under way and the results of this comparison, demonstrated by end-to-end distributions, radii of gyration, and radial distribution functions, will be presented during the talk. Our computation has been performed at constant decane density taken as 0.73 g/cm^3. Although the algorithm DG2 proves to be reliable in finding sample conformations in our experiments with decane molecules, it is quite expensive computationally. On the other hand, the algorithm DG1 has a definite advantage in computational cost, at least at the initial stage of polymer relaxation. Moreover, initial experiments suggest that the speed of the DG1 is dependent much more on total numbers of atoms than on chain lengths, although this dependence requires further investigation. We believe that a combination of features present in both of the algorithms described above would provide a powerful tool for building approximate models of complex polymer structures in conformational analysis.

4   Optimisation and Extension of Distance Geometry Algorithms to Modelling Cross-Linked Polymeric Structures

From a mathematical point of view the problem (4)–(5) is a NP problem [15, 8]. Therefore, the success of the modelling enterprise in the case of complex polymer structures and composites is determined by the economical use of computational resources. Since for molecular systems with n atoms there would be $\approx \frac{1}{2}(n-1)n$ non-bonded terms to evaluate (which require $2n^2$ memory in using DG algorithms), in our computations we restrict the number of non-bonded distances and take into account only those pairs of atoms that are not more than three bonds away from each other. We also assume that all bonds and angles are constrained and that only the torsional degrees of freedom in a chain dominate in determining its overall conformation [10].

Since in designing new materials cross-linking brings a significant change in skeletal structure which in turn leads to major differences in thermo-visco-mechanical properties of the material, an important extension of the presented work is the application and the analysis of performance of the DG algorithms described here to different nonlinear polymers including those that are created by linking together (or cross-linking) pre-existing chains of linear polymers (as in thermoset epoxy polymers), as well as those that are created by simultaneous chain growth and cross-linking.

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$$\rho\left[\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right] = -\vec{\nabla}p + \mu\vec{\nabla}^2\vec{v} + \rho\vec{f}$$

$$\rho\left[\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right] = -\vec{\nabla}p + \rho\vec{f}$$

$$p + \rho g z + \rho\frac{v^2}{2} = C$$

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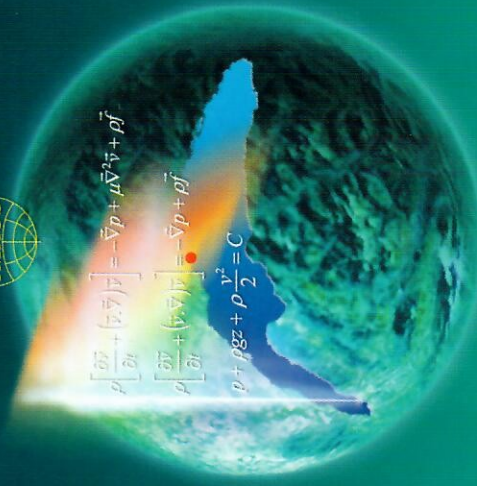Mario Romanò
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