Newton Homotopies for Sampling Stationary Points of Potential Energy Landscapes

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One of the most challenging and frequently arising problems in many areas of science is to find solutions of a system of multivariate nonlinear equations. There are several numerical methods that can find many (or all if the system is small enough) solutions but they each exhibit characteristic problems. Moreover, traditional methods can break down if the system consists of singular solutions. Here, we propose an efficient implementation of Newton homotopies, which can sample a large number of the stationary points for complicated many-body potentials. We demonstrate how the procedure works by applying it to the nearest-neighbor ϕ^4 model and atomic clusters.

Introduction: Solving nonlinear equations is one of the most frequently arising problems in physics, chemistry, mathematical biology and many areas of engineering. In particular, finding stationary points (SPs) of a potential energy function $V(\mathbf{x})$ provides the foundations for global optimisation [1–3], thermodynamic sampling to overcome broken ergodicity [4–7], as well as rare event dynamics [8–15] within the general framework of potential energy landscape theory [16]. Here, the SPs of $V(\mathbf{x})$, which is a real-valued function from $\mathbb{R}^n$ to $\mathbb{R}$, are defined as the simultaneous solutions of the system of equations $f_i(\mathbf{x}) = \partial V(\mathbf{x})/\partial x_i = 0$, for all $i = 1, \ldots, n$. The SPs can be employed to analyze many different properties of a diverse range of physical, chemical and biological systems, including metallic clusters, biomolecules, structural glass formers, coarse-grained models of soft and condensed matter, etc. [16, 17].

Since nonlinear equations are generally difficult to solve, it is usually not possible to find all the SPs analytically and one must resort to numerical methods. For example, in the Newton-Raphson (NR) approach one refines an initial guess via successive iterations in the hope of converging to a solution. Unfortunately, unless the initial guess is sufficiently close to a solution, the NR method may converge slowly or fail to converge at all. Furthermore the NR method is also notorious for its erratic behavior near "irregular" singular solutions, e.g., see [18]. An alternative method to find stationary points is the gradient-square minimization method which solves $f_i(\mathbf{x}) = \mathbf{0}$ by minimizing the sum of squares $W = \sum_{i=1}^{N} f_i(\mathbf{x})^{\mathbf{2}}$ using traditional numerical minimization methods, such as conjugate gradient [19, 20]. However, the number of minima with $W > 0$, which are not the solutions of $f_i(\mathbf{x})$, generally outweighs the number of minima with $W = 0$, and these non-solutions also have an additional zero eigenvalue, making the minimization problem ill-conditioned [21, 22], and very inefficient in practice [21, 23]. A more systematic approach was proposed in Refs. [21, 23] based on eigenvector-following, as implemented in the `OPTIM` package. This program includes many other geometry optimization techniques, such as a modified version of the limited-memory Broyden–Fletcher–Goldfarb–Shanno (LBFGS) algorithm [24, 25], single- and double-ended [26] transition state searches via a variety of gradient-only and second derivative-based eigenvector-following techniques [27, 28], and hybrid eigenvector-following methods [29, 30, 52]. The recently described biased gradient squared descent framework [53] may provide a useful alternative, which merits investigation in future work. Recently, a completely different approach based on algebraic geometry, namely the numerical polynomial homotopy continuation (NPHC) method, has been used to find all the solutions of various models with polynomial-like nonlinearity [31, 33]. After estimating an upper bound on the number of isolated complex solutions of the given equations, a different system consisting of the same variables and having exactly the same number of solutions as the estimated upper bound is constructed. Then, each solution of the new system is tracked towards the original system via a single parameter. This method can identify *all* isolated complex solutions (which include real solutions) of the original system (see e.g., Refs. [32–34] for more details). When the number of complex solutions is very large but the number of real solutions is very small, computing all of the real solutions using the NPHC method can be a computationally expensive task. Another approach to find all the solutions of a system of nonlinear equations is the interval based method [35], but it has only proved successful for a very small number of atoms and SPs so far, because it is based on bisections of the ranges.

In this contribution, we use an efficient, robust, and highly parallel implementation of *Newton homotopies* (NH), a previously underutilized approach for finding SPs. Unlike the NPHC and the minimization based methods, the NH approach has the benefit of directly targeting the real SPs. When compared to the NR method, our approach for NH is more effective at finding singular solutions and also capable of finding multiple solutions starting from a single point. Numerical experiments with Nearest-Neighbor 2D ϕ^4 models and atomic clusters suggest that NH is an efficient and effective method capable of finding a large number of SPs within a reasonable amount of time, and has great potential for use in a wide range of other applications.

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Newton Homotopy: The fundamental goal is to find solutions $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ to a **target system** consisting of n equations $\mathbf{F}(x_1, \ldots, x_n) = \mathbf{F}(\mathbf{x}) = \mathbf{0}$. The general idea of homotopy continuation is to deform the target system into a different one, the starting system, for which solutions are easier to compute. In this article, we focus on deforming using a Newton Homotopy developed in [36–38] which is given by $\mathbf{H} : \mathbb{R}^{n+1} \to \mathbb{R}$ with

$$\mathbf{H}(\mathbf{x}, t) := \mathbf{F}(\mathbf{x}) - t\mathbf{F}(\mathbf{a}) \tag{1}$$

for some chosen $\mathbf{a} \in \mathbb{R}^n$. Clearly, it is a homotopy between the target system $\mathbf{H}(\mathbf{x}, 0) \equiv \mathbf{F}(\mathbf{x})$ and the starting system $\mathbf{H}(\mathbf{x}, 1) \equiv \mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{a})$ when we restrict the t to $[0, 1]$. The system of equations $\mathbf{H}(\mathbf{x}, t) = \mathbf{0}$ represents a family of equations parameterized by t containing the target system $\mathbf{F}(\mathbf{x}) = \mathbf{0}$, which we aim to solve. We can consider $\mathbf{H}(\mathbf{x}, t) = \mathbf{0}$ as a system of n equations defining a solution set $\mathcal{V}(\mathbf{H}) := \{(\mathbf{x}, t) \in \mathbb{R}^{n+1} \ : \ \mathbf{H}(\mathbf{x}, t) = \mathbf{0}\}$ containing the target solution set of $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ as a cross-section at $t = 0$. While the structure of $\mathcal{V}(\mathbf{H})$ can be complicated, depending on the choice of $\mathbf{a}$, certifiable methods for numerically tracking along curves in $\mathcal{V}(\mathbf{H})$ are provided in [39, 40].

If the Jacobian matrix $\mathbf{J_H}(\mathbf{a}, 1)$ of $\mathbf{H}$ at $(\mathbf{a}, 1)$ has rank n, then $(\mathbf{a}, 1)$ is a smooth point of an irreducible curve contained in $\mathcal{V}(\mathbf{H})$. Locally, this curve is smooth so that one may track along it in a neighborhood. To simplify the situation, assume that the Newton homotopy (1) satisfies the smoothness assumption, namely $\mathbf{J_H}(\mathbf{x}, t)$ has rank n for all $(\mathbf{x}, t) \in \mathcal{V}(\mathbf{H})$. Thus, $\mathcal{V}(\mathbf{H})$ is the union of disjoint smooth curves in $\mathbb{R}^{n+1}$ with one passing through $(\mathbf{a}, 1)$. By tracking along this curve, one may locate points in $\mathcal{V}(\mathbf{H}) \cap \{(\mathbf{x}, t) \in \mathbb{R}^{n+1} : t = 0\}$ corresponding to the real solutions of $\mathbf{F}(\mathbf{x}) = \mathbf{0}$. Figure 1 depicts this situation.

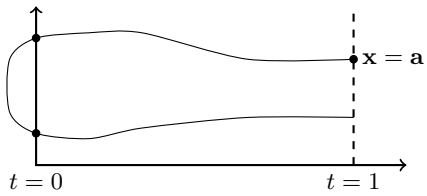

Figure 1: A smooth curve defined by $\mathbf{H}(\mathbf{x}, t) = \mathbf{0}$

This setup suggests a practical numerical method for locating solutions of the system $\mathbf{F}(\mathbf{x}) = \mathbf{0}$: starting at the point $(\mathbf{a}, 1)$, trace the curve defined by $\mathbf{H}(\mathbf{x}, t) = \mathbf{0}$ in $\mathbb{R}^n \times \mathbb{R}$ via an efficient and reliable numerical methods. A solution to the target system is produced each time the curve passes through the hyperplane defined by $t = 0$. Since we will not test if the smoothness assumption holds, we will simply track along the curve locating real solutions of $\mathbf{F} = \mathbf{0}$ until singularities arise. Remark 1 discusses some options for tracking through singularities.

Tracing smooth curves: By the smoothness assumption, the zero set $\mathcal{V}(\mathbf{H})$ of $\mathbf{H}$ consists of smooth curves. Let γ be the unique curve containing $(\mathbf{a}, 1)$. The numerical Newton homotopy continuation method revolves around the procedure of "tracing" the curve γ from $(\mathbf{a}, 1)$. Here we brief outline one basic method and refer to standard references such as [32, 41–43] for other variations.

The smooth curve γ is naturally parametrized by arc length. For convenience, let $\mathbf{y} = (\mathbf{x}, t)$ and write $\mathbf{H}(\mathbf{x}, t) = \mathbf{H}(\mathbf{y})$. Given any $(\mathbf{a}, t) \in \gamma$, an arc-length parametrization of γ at $(\mathbf{a}, t)$ is a smooth function $\mathbf{y} : \mathbb{R}^+ \to \gamma$ such that $\mathbf{y}(0) = (\mathbf{a}, t)$, $\mathbf{H}(\mathbf{y}(s)) = \mathbf{0}$, and $\|\dot{\mathbf{y}}(s)\|_2 = 1$ for all $s \in \mathbb{R}^+$. Clearly, parametrizations satisfying these conditions are not unique: there at least two different arc-length parametrizations going in opposite directions. Therefore, to trace along a curve without backtracking, one must be able to determine and maintain a consistent orientation: Since, $\mathbf{H}(\mathbf{y}(s)) = \mathbf{0}$, we necessarily have $\mathbf{J_H}(\mathbf{y}(s))\, \dot{\mathbf{y}}(s) = \mathbf{0}$, where $\mathbf{J_H}(\mathbf{y}(s))$ is the Jacobian matrix of $\mathbf{H}$ at $\mathbf{y}(s)$. That is, $\dot{\mathbf{y}}(s)$ generates the one dimensional null space of $\mathbf{J_H}(\mathbf{y}(s))$. Therefore, the $(n+1) \times (n+1)$ square matrix $\begin{bmatrix} \mathbf{J_H}(\mathbf{y}(s)) \\ \dot{\mathbf{y}}(s) \end{bmatrix}$ is never singular, i.e. its determinant never vanishes and hence maintains a consistent sign. Consequently this sign determines the *orientation* of the parametrization. Once an orientation $\sigma_0 = \pm 1$ is chosen, one must keep the orientation consistent while tracing the curve to prevent backtracking. With the additional orientation constraint, the arc-length parametrization for γ at $(\mathbf{a}, 1)$ is characterized by

$$\begin{aligned} \mathbf{J_H}(\mathbf{y}(s))\, \dot{\mathbf{y}}(s) &= \mathbf{0} \\ \operatorname{sgn} \det \begin{bmatrix} \mathbf{J_H}(\mathbf{y}(s)) \\ \dot{\mathbf{y}}(s) \end{bmatrix} &= \sigma_0 \\ \|\dot{\mathbf{y}}(s)\| &= 1 \\ \mathbf{y}(0) &= (\mathbf{a}, 1) \end{aligned} \quad . \tag{2}$$

Locally, at any fixed s and its corresponding $\mathbf{y}(s)$, the tangent vector $\dot{\mathbf{y}}(s)$ can be computed efficiently via numerical methods. In particular, the null space of $\mathbf{J_H}(\mathbf{y}(s))$, which contains $\dot{\mathbf{y}}(s)$, can be computed via QR-decomposition of the transpose matrix $\mathbf{J_H}(\mathbf{y}(s))^T$. Under the smoothness condition, the null space is one-dimensional and contains exactly two vectors of unit length. Utilizing the information produced during the QR-decomposition the correct choice of $\dot{\mathbf{y}}(s)$ can be made, as a by-product, with at most $O(n)$ extra floating point operations. Globally, in principle, any ordinary differential equation solver capable of integrating the above system can be used to trace the curve and potentially obtain a solution to the target system point at $t = 1$. Numerical methods based on this idea are generally referred to as "global Newton methods" [37]. Our implementation employs a "prediction-correction scheme" due to numerical stability concerns [38].

Remark 1. *We should note that the numerical method described in this section is actually capable of handling cases where the Newton homotopy defines curves with isolated "simple branch points", such as points at which two curves intersect transversally. More advanced techniques for handling singularities can be found in [42, 44–47, 54].*

An Example System: Consider the system

$$\begin{cases} \frac{29}{16}x^3 - 2xy & = 0, \\ y - x^2 & = 0, \end{cases} \tag{3}$$

from [18]. This system has only one solution in $\mathbb{R}^2$, namely $(0, 0)$, which has multiplicity 3. It is shown in [18] that

starting from almost every point in $\mathbb{R}^2 \setminus \{(0,0)\}$, the NR method will diverge. In other words, the NR method will almost surely never find the solution of this system. Figure 2 shows that the Newton homotopy (1) was successful at locating the solution for many starting points (x_0, y_0).

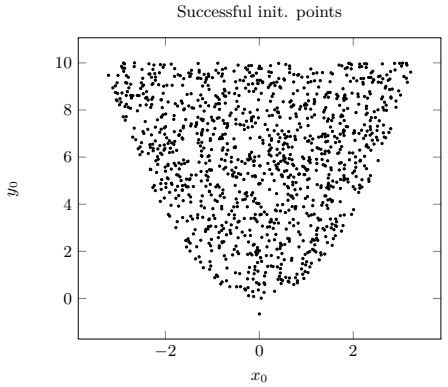

Figure 2: Scatter plot of some starting points (x_0, y_0) for which the NH (1) was successful in obtaining the singular solution $(0, 0)$ of the system (3) within machine precision.

The Nearest-Neighbor Two-dimensional ϕ^4 Model: We consider a model from theoretical physics called the two-dimensional nearest-neighbor ϕ^4 model. It has been widely studied because it is one of the simplest models with a continuous configuration space that exhibits a phase transition in the same universality class as the two-dimensional Ising model. For an $N \in \mathbb{Z}^+$ and $J, \lambda, \mu \in \mathbb{R}$ the model, in N^2 variables $\mathbf{x} = (x_{11}, x_{12}, \ldots, x_{NN})$, is $V(\mathbf{x})$ given by

$$V(\mathbf{x}) = \sum_{(i,j)\in\Lambda} \left(\frac{\lambda}{4!} x_{ij}^4 - \frac{\mu^2}{2} x_{ij}^2 + \frac{J}{4} \sum_{(k,l)\in\mathcal{N}_{(i,j)}} (x_{ij} - x_{kl})^2 \right) \quad (4)$$

where $\Lambda \subset \mathbb{Z}^2$ is the standard square lattice with N^2 lattice-sites and $\mathcal{N}_{(i,j)} \subset \Lambda$ is the four nearest-neighbor sites of (i, j). The N^2 stationary equations are given by

$$\frac{\partial V(\mathbf{x})}{\partial x_{ij}} = \frac{\lambda}{3!} x_{ij}^3 + (4J - \mu^2) x_{ij} - \sum_{(k,l)\in\mathcal{N}_{(i,j)}} J x_{kl} = 0. \quad (5)$$

for each pair of $i, j = 1, \ldots, N$. Given the physical context, only real solutions are needed. We use periodic boundary conditions, $\lambda = 3/5$ and $\mu^2 = 2$.

A variety of computational tools have been used to study this model. In particular, the NPHC method has found all the SPs for $N = 3, 4$ in a previous study [48, 49]. However, this family of problems poses a particularly tough challenge to methods that find all complex solutions, since the total number of solutions in $\mathbb{C}^{N^2}$, counting multiplicity, is always equal to its total degree (the Bezout bound) 3^{N^2}, which grows quickly as N increases. Direct computation of all complex solutions is clearly unfeasible with current technology for large values of N. However, by varying the parameter J from 0 to 1, one can go from the case when all the solutions are real to only an extremely small fraction are real. For the latter, the method of Newton homotopy, which directly targets the real solutions, has a clear advantage over methods that compute all complex solutions.

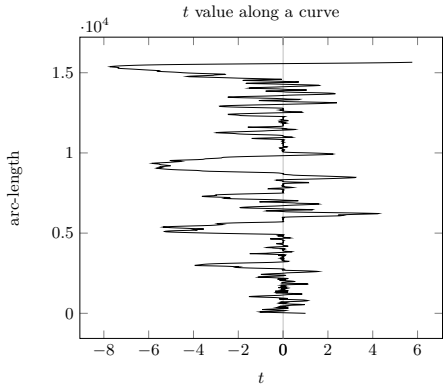

Figure 3: The t value along a curve defined the Newton homotopy for (5) for $N = 6$ and $J = 0.9$.

In our numerical experiments, Newton homotopies (1) were applied to (5) with varying values for N and J. From a *single* randomly chosen starting point multiple real solutions were obtained. Table I summarizes the ability and efficiency of Newton homotopy in finding the real solutions for a range of N and J values. Indeed, *all real solutions were found in many cases.* For example, with $N = 3$, in the case of $J = 0.9, 0.8, 0.7, 0.6, 0.5$, and 0.4, our Newton homotopy implementation was able to obtain *all* of them with a single randomly chosen starting point. The CPU time information in the table corresponds to a workstation with a 3.4 GHz Intel Core i5-3570K processor. The results highlight the strength of the Newton homotopy: it is capable of finding a large number of real solutions very quickly. The efficiency is particularly noteworthy in the case of $N = 7$ and $N = 8$. With a total of more than 10^{23} and 10^{30} complex solutions, respectively, any approach involving finding all complex solutions is clearly impractical. In contrast, with $J = 0.9$ Newton homotopy was able to obtain 358 and 1522 real solutions, for the cases of $N = 7, 8$ respectively, using a *single* starting point *within 1 minute.*

N	J	No. of SPs	% of total SPs found	Time
3	0.90	3	(All) 100%	0.008s
	0.70	3	(All) 100%	0.012s
	0.50	171	(All) 100%	0.999s
	0.30	1121	99.1%	2.001s
4	0.90	83	(All) 100%	0.903s
	0.60	199	68.4%	1.371s
	0.30	40225	40.6%	59.27s
5	0.90	102	-	2.009s
	0.60	679	-	49.50s
6	0.90	208	-	23.95s
	0.60	959	-	52.37s
7	0.90	358	-	29.66s
	0.60	3266	-	37.25s
8	0.90	674	-	43.12s
	0.60	1538	-	55.99s

Table I: The number of real solutions of (5) found using Newton homotopy with *one* starting point. The percentages are computed with respect to all SPs [48, 49].

These cases also showcase the ability of NH in obtaining multiple solutions using a single starting point. Figure 3

illustrates the t-value along the single curve defined by the Newton homotopy for (5) with $N = 6$ and $J = 0.9$. Here, t (horizontal axis) is plotted against the arc-length (vertical axis). Note the numerous crossings of the hyperplane at $t = 0$, represented by the light vertical line in the middle. Each crossing produces a distinct real solution for (5).

Using multiple starting points and tracing multiple curves, the likelihood for Newton homotopy to obtain many or all real solutions can be improved substantially. Note that the curve tracings are completely independent and hence can be performed in parallel. Table II summarizes the efficiency of Newton homotopy in finding a large number of real solutions for (5) using multiple randomly chosen starting points. The timing information is based on the performance on a cluster of 32 nodes, each having a quad-core Intel Xeon processor running at 2.4 GHz.

N	J	No. of Start Points	No. of SPs	% SPs	Time
4	0.90	1000	83	(All) 100%	7.15s
	0.60	1000	291	(All) 100%	110.50s
	0.30	1000	99187	(All) 100%	121.01s
5	0.90	500	243	-	99.50s
	0.60	500	1083	-	139.21s
	0.30	500	30971	-	353.97s
6	0.90	100	579	-	47.33s
	0.60	100	4172	-	329.15s
7	0.90	64	917	-	61.19s
	0.60	64	3965	-	86.31s
8	0.90	32	1522	-	58.70s
	0.60	32	5694	-	61.11s

Table II: The number and percentage of solutions for (5) found using Newton homotopy with many starting points.

Lennard-Jones Clusters: We now apply the NH method to finding SPs of atomic clusters of N atoms bound by the Lennard-Jones potential [50], which is defined as

$$V_N = 4\epsilon \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \qquad (6)$$

where ϵ is the pair well depth, $2^{1/6}\sigma$ is the equilibrium pair separation, and $r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$ is the distance between atoms i and j. We take $\epsilon = \sigma = 1$. Defined in terms of the distances, V_N is clearly invariant under rotation and translation. Therefore we can fix $x_1 = y_1 = z_1 = y_2 = z_2 = z_3 = 0$. Hence, there are in total $3N-6$ variables in V_N yielding $3N-6$ stationary equations $\nabla V_N = \mathbf{0}$. For this model, an extensive search for minima and saddle points was carried out in [21] for N up to 13, and a search for minima and saddles of index one (transition states) for $N = 14$ was presented in [51]. Table III shows the ability of Newton homotopy to find a large number of SPs for (6) for each N value. It is worth noting the data suggests that the NH approach is particularly useful in finding SPs of higher Morse indices (the number of positive eigenvalues of the Hessian matrix of V_N): among the SPs found, the majority have Morse index near the middle of the possible range (from 0 to the number of variables, $3N - 6$), which may be attributed to the fact that there are exponentially more SPs in the mid-range of the indices than at the extremes (index 0 and index $3N - 6$).

N	SPs / Distinct energy levels	local minima	transition states
3	9 / 4	3	1
4	31 / 11	3	3
5	101 / 39	1	5
6	204 / 148	2	6
7	725 / 265	4	13
8	597 / 224	8	1
9	991 / 501	16	1
10	2510 / 546	22	71
11	9940 / 552	34	83
12	20994 / 623	62	90
13	10920 / 289	73	92
14	32517 / 264	37	81

Table III: Number of SPs and distinct critical energy levels of (6) found using Newton homotopies.

Conclusion: We have developed a novel implementation of the Newton homotopy method which, in our experiments, is much more efficient at finding SPs of PELs arising in chemical physics than the usual Newton-Raphson method. Newton homotopies appear to be better behaved at possible singular SPs and our implementation does not require the inversion of large matrices. Our results suggest that the NH method has the potential to replace the NR method in many contemporary computational approaches, especially in computational chemistry.

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