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Response to "Comment on 'Exploring the potential energy landscape of the Thomson problem via Newton homotopies'" [J. Chem. Phys. 143, 247101 (2015)]

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Introduction. We agree with the comment[1] that the Newton homotopy (NH) and Newton trajectory (NT) methods are closely related in that they share a common root, namely, the "Continuous Newton" method of Branin.[2,3] We elaborate on the connections and differences between the two approaches with the main focus on NH, since an overview of NT is provided in the comment.

A historical remark. The problem of finding stationary points of a potential function amounts to solving a multivariate nonlinear system of equations $\mathbf{F} = \nabla V = \mathbf{0}$. It was in this general setting that both NH and NT were first developed. Recall that starting from $\mathbf{x}_0$, Newton's method is defined by the iterative process $\mathbf{x}_{k+1} = \mathbf{x}_k - [D\mathbf{F}(\mathbf{x}_k)]^{-1}\mathbf{F}(\mathbf{x}_k)$, where $[D\mathbf{F}(\mathbf{x}_k)]^{-1}$ is the inverse of the Jacobian matrix of $\mathbf{F}$ at $\mathbf{x}_k$. It may be interpreted as the numerical integration, using Euler's method with step size 1, of

$$\dot{\mathbf{x}}(t) = \pm[D\mathbf{F}(\mathbf{x}(t))]^{-1}\mathbf{F}(\mathbf{x}(t)), \tag{1}$$

with $\mathbf{x}(0) = \mathbf{x}_0$. Here "±" reflects the flexibility in choosing the flow direction. This flow was exploited by Branin[2,3] to find solutions of $\mathbf{F}(\mathbf{x}) = \mathbf{0}$. The procedure has been referred to as the *Continuous Newton* method, similar to the *Global Newton* method.[4] One can easily verify that along a solution curve $\mathbf{F}(\mathbf{x}(t))$ points to a fixed direction. Taking this as the defining feature, a geometric formulation of NT[5,6] is developed in the context of *Newton leaves*, providing a much richer structure than Branin's approach.[7]

The ordinary differential equation (ODE), Eq. (1), has singularities wherever $D\mathbf{F}$ is singular. To "extend over" such singularities, it is customary to replace $D\mathbf{F}^{-1}$ in Eq. (1) by the adjugate matrix $\mathrm{adj}\, D\mathbf{F}(\mathbf{x})$ of $D\mathbf{F}(\mathbf{x})$.[2,3] This modification can be understood as a reparametrization of the trajectory of Eq. (1). Though useful as a theoretical tool, this augmented flow can be difficult to compute and numerically unstable[8,9] (according to Ref. 10, "[...] near such singular points [of Eq. (1)], the evaluation of the right hand side remains numerically unstable"). Moreover, *extraneous singularities* (as defined by Branin[2]) where $\mathbf{F}(\mathbf{x}) \neq \mathbf{0}$ but $(\mathrm{adj}\, D\mathbf{F}(\mathbf{x}))\mathbf{F}(\mathbf{x}) = \mathbf{0}$ may be introduced.[11,12] As noted in the comment, a substantial body of work is devoted to the handling of these singularities and computational issues, with much success[12,13] and with applications of NT in chemistry.[6,14–18]

NH was originally proposed as an alternative approach for resolving the problems caused by a singular $D\mathbf{F}$. It was observed by Keller[8] and, independently, by Garcia and Gould[10,19,20] that a solution curve of Eq. (1) can be realized as a projection of the curve implicitly defined by the homotopy function

$$\mathbf{H}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x}) - t\mathbf{F}(\mathbf{x}_0). \tag{2}$$

That is, under certain smoothness assumptions, the solution set of $\mathbf{H}(\mathbf{x}, t) = \mathbf{0}$ consists of curves in the one-higher dimension (due to introduction of the additional variable t), and their projections onto the $\mathbf{x}$-space (by simply erasing t-values) coincide with the phase portrait of the continuous Newton method defined by the ODE Eq. (1) away from its singularities. Thus, a key feature of the NH method is the "lifting" of the flow defined by Eq. (1) into a space of one-higher dimension via the new variable t. It is only the projection onto the $\mathbf{x}$-space that coincides with NTs.

Contemporary NH formulation. The comment suggests that by proceeding in the reverse direction of the NH approach and treating the variables $\mathbf{x} = (x_1, \ldots, x_n)$ in Eq. (2) as functions of t, one obtains exactly the basic form of the continuous Newton method Eq. (1) of Branin. In this view, there will be no intrinsic difference between NH and NT: they would simply be different definitions of the same curves, one algebraic, one analytic, though some subtle but important differences were explored in Ref. 13.

This view, however, does not reflect current implementations nor the original intention of the NH method. As emphasized in Refs. 21 and 22, generally the variables $\mathbf{x} = (x_1, \ldots, x_n)$ in Eq. (2) cannot be treated as differentiable functions of t and hence $d\mathbf{x}/dt$ is not meaningful. For the simple example of $F(x) = x^3/2 + 1/2$, starting from $x(0) = 1$, the trajectory of Eq. (1) is given by $x(t) = \sqrt[3]{2t-1}$. When t reaches $1/2$, x will reach 0 at which $DF = 0$, and both DF^{-1} and dx/dt become undefined: the trajectory encounters a singularity. Instead, $\mathbf{x}$ and t are considered as independent

variables in NH. Indeed, earlier homotopy continuation methods[23] developed in the 1970s had already adopted the view that homotopy paths should be parametrized by intrinsic parameters rather than the parameter t of the homotopy function (see Ref. 24 for an NT version). The most basic choice is the parametrization by the arc length s. That is, one ought to consider $\mathbf{x}$ and t both as differentiable functions of s, $\mathbf{x}(s)$ and $t(s)$ respectively, where s indicates the arc length along a curve implicitly defined by Eq. (2). With this formulation, the tangent vector at a point is characterized by the system[23,25]

$$\begin{aligned} D\mathbf{F}(\mathbf{x}(s))\frac{d\mathbf{x}}{ds} - \mathbf{F}(\mathbf{x}_0)\frac{dt}{ds} &= \mathbf{0}, \\ \operatorname{sgn}\det\begin{bmatrix} D\mathbf{F}(\mathbf{x}(s)) & -\mathbf{F}(\mathbf{x}_0) \\ \dfrac{d\mathbf{x}}{ds} & \dfrac{dt}{ds} \end{bmatrix} &= \pm 1, \\ \left\|\frac{d\mathbf{x}}{ds}\right\|^2 + \left|\frac{dt}{ds}\right|^2 &= 1, \quad \mathbf{x}(0) = \mathbf{x}_0,\ t(0) = 1. \end{aligned} \tag{3}$$

Note that this is just a standard formulation of the curve tangent direction, and we refer to Ref. 10 for the long list of different possibilities. Reference 26 presents an application of NH in this field, and our contributions[21,22] serves to extend the versatility of the NH method.

As noted in Refs. 21 and 22, the ability to handle *turning points* without extra effort is crucially important, and this formulation "resolves" the singularities of Eq. (1) caused by turning points. Slightly more complicated are the singularities of Eq. (1) caused by points where two curves intersect transversally. Techniques based on studies of *bifurcation equations*[25] allow one to "jump over" such crossings or "switch branches." Alternatively, such crossings can be handled from an algebraic point of view.[27] Under the mild condition that Equation (2) is locally holomorphic (complex differentiable) near a singularity, higher order bifurcations can readily be handled. For instance, the local geometry of such a bifurcation is analyzed in Ref. 28 from the homotopy side. The NT method has been investigated against valley-ridge inflection points.[29–31]

The conceptual difference. The physical interpretation of NH as given in Sec. IV, Ref. 21 is closely related to the approach of *mechanochemical transformations*.[32] While NT constructs pathways *on* the potential energy landscape (PEL), NH deforms PEL itself by exerting a mechanical force and keeps track of the movement of the critical points. These alternative viewpoints may enable us to further exploit geometric structure of the PELs.

Synergistic interactions. For NH, much powerful machinery can be put to use if one allows the path parameter s to be a complex variable and recognizes that the real solution curves defined by Eq. (2) are actually embedded in the complex solution curves defined by the same equation in complex variables. The *Cauchy integral* technique[33] can be used to accurately approximate the bifurcation points, the *Monodromy* technique[33] allows one to go through a bifurcation point indirectly by taking a "detour" through complex numbers, and Smale's alpha-theory can certify individual homotopy paths and solutions.[34–36] These tools may be carried over from NH to NT.

Conclusion. Our conclusion is nicely captured in Ref. 13, which we quote verbatim: "*Although in some cases the paths of trajectory methods can be interpreted as projections of paths generated by suitable homotopy methods (cf. Newton-homotopy vs Newton trajectories) onto the domain space one should keep the different philosophies of the two approaches in mind. And generally, if a method can be viewed in both ways, these two viewpoints can each contribute to the understanding of what goes on.*"

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