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Application of the Fast Automatic Differentiation for Calculation of Gradients of Material's Bulk Modulus and Shear Modulus

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Abstract. In computer modeling of crystal structures the gradient optimization methods are often used. This raises the need to calculate the exact gradients of the Bulk modulus and the Shear modulus of materials. With help of the Fast Automatic Differentiation the formulas that allow the calculation of the exact above-mentioned gradients were derived in the case where the total interatomic energy of the system is determined by Tersoff's Potential.

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1 Introduction and problem formulation

When modeling many solid atomic structures, such as carbon, silicon, germanium, and their compounds, the Tersoff's Potential is often used (see [1]). It is an example of the multiparticle potential based on concepts of link order: the interaction between two atoms depends on the local surrounding. The Tersoff Potential consists of ten parameters specific to the modeling material.

Various mathematical models are used to study materials of atomic structures. Some parameters of these models are unknown. They should be identified from the condition that the calculated properties of the modeled material are close to its properties, which were found experimentally. In [2] was considered an optimization problem of minimizing the following cost function

$$f(\xi) = \sum_{i=1}^{m} \omega_i (y_i(\xi) - \widetilde{y_i})^2 \tag{1}$$

where ω_i is the weight factor; $\widetilde{y_i}$ is the value of the i-th material characteristic obtained experimentally, and $y_i(\xi)$ is the value of the same material characteristic calculated using Tersoff Potential with ξ parameters ($\xi \in R^m$ are vector parameters to be identified). The solution of the problem is looked for on the set $X \subseteq R^m$, which is a parallelepiped. Its boundaries are chosen so that it obviously contained the admissible range of parameters. The quantity of items in formula (1) varies depending on the studied material. A required set of parameters has to provide the minimum deviation of the calculated characteristics of material from the known

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experimental values, thereby most precisely describing the modeled properties of a crystal. For numerical solution of this problem the gradient minimization methods are often used. There exists the need to calculate the exact value of the objective function gradient efficiently.

These derivatives are often calculated (in particular, see [2]) using the finite difference method. Studies have shown that finite difference method does not allow to calculate the gradient of the cost function with acceptable accuracy and requires $(m+1)$ times to calculate the value of the function.

One of the terms in formula (1) is the total energy of the system of atoms. As the interatomic potential energy, the Tersoff Potential was choosen. In [3], using the Fast Automatic Differentiation (see [4]), formulas to calculate the exact gradient of the total energy with respect to parameters of Tersoff Potential (specific for modeled substance) were received.

The other two terms in formula (1) are the Bulk modulus of elasticity (it relates to how the volume of a piece of material changes when exposed to a uniform change in pressure) and the Shear modulus. They are proportional to $B(E)$ — the second derivative of the total energy with respect to length of crystal lattice. Note that in [2] $B(E)$ is also calculated using the finite difference method.

In this paper, we build a multistep algorithm to calculate the exact value of $B(E)$ in the case where the total energy of the system is determined by Tersoff Potential. With the help of Fast Automatic Differentiation we derived formulas to calculate the gradient of $B(E)$ with respect to Tersoff parameters with machine precision.

2 Calculation of second derivative of total energy with respect to atomic lattice coefficient

Let a be the initial length of the edges of the lattice of atoms; $\widetilde{a} = \alpha a$ $(\alpha \in R)$ — length of the edges of the lattice of atoms after deformation; $\rho = \widetilde{a} - a$ — deformation parameter. Then $\dfrac{a+\rho}{a} = \left(1 + \dfrac{\rho}{a}\right) a$. If $\overline{r}_k = (x_{k1}, x_{k2}, x_{k3})$ are the coordinates of some lattice atom before deformation and $\widetilde{\overline{r}}_k = (\widetilde{x}_{k1}, \widetilde{x}_{k2}, \widetilde{x}_{k3})$ are its coordinates after deformation, then $\widetilde{x}_{k1} = \left(1 + \dfrac{\rho}{a}\right) x_{k1},\ \widetilde{x}_{k2} = \left(1 + \dfrac{\rho}{a}\right) x_{k2},\ \widetilde{x}_{k3} = \left(1 + \dfrac{\rho}{a}\right) x_{k3}$.

Let $E(\overline{r}_1, \overline{r}_2, ..., \overline{r}_I)$ be the total energy of atoms' system before deformation. Then $E(\widetilde{\overline{r}}_1, \widetilde{\overline{r}}_2, ..., \widetilde{\overline{r}}_I) = E\left[\left(1 + \dfrac{\rho}{a}\right)\overline{r}_1, \left(1 + \dfrac{\rho}{a}\right)\overline{r}_2, ..., \left(1 + \dfrac{\rho}{a}\right)\overline{r}_I\right]$ is the total energy of atoms' system after deformation. The Bulk modulus and the Shear modulus of the material are proportional to $B(E)$, that can be calculated by the formula:

$$B(E) = \frac{\partial^2}{\partial \rho^2} E\left[\left(1 + \frac{\rho}{a}\right)\overline{r}_1, \left(1 + \frac{\rho}{a}\right)\overline{r}_2, ..., \left(1 + \frac{\rho}{a}\right)\overline{r}_I\right]\Big|_{\rho=0}.$$

As to total energy $E(\overline{r}_1, \overline{r}_2, ..., \overline{r}_I)$ it is calculated with the help of expression

$$E(\overline{r}_1, \overline{r}_2, ..., \overline{r}_I) = \sum_{i=1}^{I} \sum_{j=1; j\neq i}^{I} V_{ij},$$

where V_{ij} is the interaction potential between atoms marked i and j (i-atom and j-atom). In present paper the Tersoff Potential is used as interaction potential:

$$V_{ij} = f_c(r_{ij})\left(V_R(r_{ij}) - b_{ij}V_A(r_{ij})\right),$$

$$f_c(r) = \begin{cases} 1, & r < R - R_{cut}, \\ \frac{1}{2}\left(1 - \sin\left(\frac{\pi(r-R)}{2R_{cut}}\right)\right), & R - R_{cut} < r < R + R_{cut}, \\ 0, & r > R + R_{cut}, \end{cases}$$

$$V_{ij}^R = V_R(r_{ij}) = \frac{D_e}{S-1}\exp\left(-\beta\sqrt{2S}(r_{ij} - r_e)\right),$$

$$V_{ij}^A = V_A(r_{ij}) = \frac{SD_e}{S-1}\exp\left(-\beta\sqrt{\frac{2}{S}}(r_{ij} - r_e)\right),$$

$$b_{ij} = \left(1 + (\gamma\zeta_{ij})^{\eta}\right)^{-\frac{1}{2\eta}}, \qquad \zeta_{ij} = \sum_{k=1;k\neq i,j}^{I} f_c(r_{ik})g_{ijk}\omega_{ijk}, \qquad \omega_{ijk} = \exp(\lambda^3\tau_{ijk}),$$

$$\tau_{ijk} = (r_{ij} - r_{ik})^3, \qquad g_{ijk} = 1 + \left(\frac{c}{d}\right)^2 - \frac{c^2}{d^2 + (h - \cos\Theta_{ijk})^2}.$$

Here I is the number of atoms in considered system; r_{ij} is the distance between i-atom and j-atom; Θ_{ijk} is the angle between two vectors, first vector begins at i-atom and finishes at j-atom, second vector begins at i-atom and finishes at k-atom; R and R_{cut} are known parameters, identified from experimental geometric properties of substance. Tersoff Potential depends on ten parameters ($m = 10$), specific to modeled substances: $D_e, r_e, \beta, S, \eta, \gamma, \lambda, c, d, h$.

Let us construct the multistep algorithm to calculate the total energy E of atoms' system (interaction potential is Tersoff Potential). The distance between i-atom and j-atom is determined by the formula:

$$r_{ij} = \sqrt{(x_{1i} - x_{1j})^2 + (x_{2i} - x_{2j})^2 + (x_{3i} - x_{3j})^2},$$

where x_{1i}, x_{2i}, x_{3i} are the Cartesian coordinates of i-atom. If Θ_{ijk} is the angle between two vectors, connecting i-atom with j-atom and k-atom respectively, then $\cos\Theta_{ijk} = q_{ijk} = \dfrac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2r_{ij}r_{ik}}$. For compactness further in the study we introduce vectors $\overline{u}$ and $\overline{z}$ having the following coordinates: $\overline{u}^T = [u_1, u_2, ..., u_{10}]^T$, $\overline{z}^T = [z_1, z_2, ..., z_{10}]^T$, where $u_1 = D_e$, $u_2 = r_e$, $u_3 = \beta$, $u_4 = S$, $u_5 =$

$\eta, \quad u_6 = \gamma, \quad u_7 = \lambda, \quad u_8 = c, \quad u_9 = d, \quad u_{10} = h;$

$$z_1 = \left\{ z_1^{ijk} = \sqrt{(x_{1i}-x_{1k})^2 + (x_{2i}-x_{2k})^2 + (x_{3i}-x_{3k})^2} \right\} \equiv F(1, Z_1, U_1),$$
$$z_2 = \left\{ z_2^{ijk} = \sqrt{(x_{1j}-x_{1k})^2 + (x_{2j}-x_{2k})^2 + (x_{3j}-x_{3k})^2} \right\} \equiv F(2, Z_2, U_2),$$
$$z_3 = \left\{ z_3^{ijk} = q_{ijk} = \frac{(z_{13}^{ij})^2 + (z_1^{ijk})^2 - (z_2^{ijk})^2}{2 z_1^{ijk} z_{13}^{ij}} \right\} \equiv F(3, Z_3, U_3),$$
$$z_4 = \left\{ z_4^{ijk} = f_c(z_1^{ijk}) \right\} \equiv F(4, Z_4, U_4),$$
$$z_5 = \left\{ z_5^{ijk} = g_{ijk} = 1 + \left(\frac{u_8}{u_9}\right)^2 - \frac{(u_8)^2}{(u_9)^2 + (u_{10} - z_3^{ijk})^2} \right\} \equiv F(5, Z_5, U_5),$$
$$z_6 = \left\{ z_6^{ijk} = \tau_{ijk} = (z_{13}^{ij} - z_1^{ijk})^3 \right\} \equiv F(6, Z_6, U_6),$$
$$z_7 = \left\{ z_7^{ijk} = \omega_{ijk} = \exp((u_7)^3 z_6^{ijk}) \right\} \equiv F(7, Z_7, U_7),$$
$$z_8 = \left\{ z_8^{ijk} = f_c(r_{ik}) g_{ijk} \omega_{ijk} = z_4^{ijk} z_5^{ijk} z_7^{ijk}) \right\} \equiv F(8, Z_8, U_8),$$
$$z_9 = \left\{ z_9^{ij} = \zeta_{ij} = \textstyle\sum_{k=1;k\neq i,j}^{I} z_8^{ijk} \right\} \equiv F(9, Z_9, U_9),$$
$$z_{10} = \left\{ z_{10}^{ij} = \gamma \zeta_{ij} = u_6 z_9^{ij} \right\} \equiv F(10, Z_{10}, U_{10}),$$
$$z_{11} = \left\{ z_{11}^{ij} = (\gamma \zeta_{ij})^{\eta} = (z_{10})^{u_5} \right\} \equiv F(11, Z_{11}, U_{11}),$$
$$z_{12} = \left\{ z_{12}^{ij} = b_{ij} = (1 + z_{11}^{ij})^{-\frac{1}{2u_5}} \right\} \equiv F(12, Z_{12}, U_{12}),$$
$$z_{13} = \left\{ z_{13}^{ij} = \sqrt{(x_{1i}-x_{1j})^2 + (x_{2i}-x_{2j})^2 + (x_{3i}-x_{3j})^2} \right\} \equiv F(13, Z_{13}, U_{13}),$$
$$z_{14} = \left\{ z_{14}^{ij} = V_{ij}^R = \tfrac{u_1}{u_4 - 1} \exp\left(-u_3 \sqrt{2u_4}(z_{13}^{ij} - u_2)\right) \right\} \equiv F(14, Z_{14}, U_{14}),$$
$$z_{15} = \left\{ z_{15}^{ij} = V_{ij}^A = \tfrac{u_1 u_4}{u_4 - 1} \exp\left(-u_3 \sqrt{\tfrac{2}{u_4}}(z_{13}^{ij} - u_2)\right) \right\} \equiv F(15, Z_{15}, U_{15}),$$
$$z_{16} = \left\{ z_{16}^{ij} = f_c(z_{13}^{ij}) \right\} \equiv F(16, Z_{16}, U_{16}),$$
$$z_{17} = \left\{ z_{17}^{ij} = V_{ij} = z_{16}^{ij}(z_{14}^{ij} - z_{12}^{ij} z_{15}^{ij}) \right\} \equiv F(17, Z_{17}, U_{17}),$$
$$\left(i = \overline{1, I}, \quad j = \overline{1, I}, \quad j \neq i, \quad k = \overline{1, I}, \quad k \neq i, j\right).$$

Note that $z_3^{ijk}\left(\left(1+\frac{\rho}{a}\right) r_{ij}, \left(1+\frac{\rho}{a}\right) r_{ik}, \left(1+\frac{\rho}{a}\right) r_{jk}\right) = z_3^{ijk}(r_{ij}, r_{ik}, r_{jk});$

$$z_5^{ijk}\left(\left(1+\frac{\rho}{a}\right) r_{ij}, \left(1+\frac{\rho}{a}\right) r_{ik}, \left(1+\frac{\rho}{a}\right) r_{jk}\right) = z_5^{ijk}(r_{ij}, r_{ik}, r_{jk}).$$

The energy E of the atoms in the system with the help of new variables may be rewritten as follows:

$$E(z(u)) = \sum_{i=1}^{I} \sum_{j=1;j\neq i}^{I} z_{17}^{ij}.$$

Variables $z_1, z_2, ..., z_{17}$ (the phase variables) are determined by the specified above multistep algorithm $z_l = F(l, Z_l, U_l)$, $(l = 17)$, where Z_l is the set of elements z_n in the right part of the equation $z_l = F(l, Z_l, U_l)$, and U_l is the set of elements u_n that appear in the right side of this equation. Note that each component z_l depends on a number of other components (z_l^{ij} or z_l^{ijk}).

Let us introduce also the following designations: $\widetilde{z}_1, \widetilde{z}_2, ..., \widetilde{z}_{17}$ and $\widetilde{\widetilde{z}}_1, \widetilde{\widetilde{z}}_2, ..., \widetilde{\widetilde{z}}_{17}$, where

$$\widetilde{z}_n = \left\{ \widetilde{z}_n^{ijk} : \widetilde{z}_n^{ijk} = \left.\frac{\partial z_n^{ijk}(\widetilde{r}_{ij}, \widetilde{r}_{ik}, \widetilde{r}_{jk})}{\partial \rho}\right|_{\rho=0} = \right.$$

$$\left. = \left.\frac{\partial z_n^{ijk}\left(\left(1+\frac{\rho}{a}\right) r_{ij}, \left(1+\frac{\rho}{a}\right) r_{ik}, \left(1+\frac{\rho}{a}\right) r_{jk}\right)}{\partial \rho}\right|_{\rho=0} \right\}, \qquad n = \overline{1,8},$$

$$\widetilde{z}_n = \left\{ \widetilde{z}_n^{ij} : \widetilde{z}_n^{ij} = \left.\frac{\partial z_n^{ij}(\widetilde{r}_{ij})}{\partial \rho}\right|_{\rho=0} = \left.\frac{\partial z_n^{ij}\left(\left(1+\frac{\rho}{a}\right) r_{ij}\right)}{\partial \rho}\right|_{\rho=0} \right\}, \qquad n = \overline{9,17},$$

$$\widetilde{\widetilde{z}}_n = \left\{ \widetilde{\widetilde{z}}_n^{ijk} : \widetilde{\widetilde{z}}_n^{ijk} = \left.\frac{\partial^2 z_n^{ijk}(\widetilde{r}_{ij}, \widetilde{r}_{ik}, \widetilde{r}_{jk})}{\partial \rho^2}\right|_{\rho=0} = \right.$$

$$\left. = \left.\frac{\partial^2 z_n^{ijk}\left(\left(1+\frac{\rho}{a}\right) r_{ij}, \left(1+\frac{\rho}{a}\right) r_{ik}, \left(1+\frac{\rho}{a}\right) r_{jk}\right)}{\partial \rho^2}\right|_{\rho=0} \right\}, \qquad n = \overline{1,8},$$

$$\widetilde{\widetilde{z}}_n = \left\{ \widetilde{\widetilde{z}}_n^{ij} : \widetilde{\widetilde{z}}_n^{ij} = \left.\frac{\partial^2 z_n^{ij}(\widetilde{r}_{ij})}{\partial \rho^2}\right|_{\rho=0} = \left.\frac{\partial^2 z_n^{ij}\left(\left(1+\frac{\rho}{a}\right) r_{ij}\right)}{\partial \rho^2}\right|_{\rho=0} \right\}, \qquad n = \overline{9,17},$$

$$\left(i = \overline{1,I}, \quad j = \overline{1,I}, \quad j \neq i, \quad k = \overline{1,I}, \quad k \neq i, j\right).$$

The above values are calculated by the formulas:

$$\widetilde{z}_1^{ijk} = r_{ik}/a; \qquad \widetilde{z}_2^{ijk} = r_{jk}/a; \qquad \widetilde{z}_3^{ijk} = 0; \qquad \widetilde{z}_4^{ijk} = \left.\frac{\partial f_c\left(\left(1+\frac{\rho}{a}\right) r_{ik}\right)}{\partial \rho}\right|_{\rho=0};$$

$$\widetilde{z}_5^{ijk} = 0; \qquad \widetilde{z}_6^{ijk} = 3z_6^{ijk}/a; \qquad \widetilde{z}_7^{ijk} = 3z_6^{ijk} z_7^{ijk} (u_7)^3/a;$$

$$\widetilde{z}_8^{ijk} = z_5^{ijk}(\widetilde{z}_4^{ijk} z_7^{ijk} + z_4^{ijk} \widetilde{z}_7^{ijk}); \qquad \widetilde{z}_9^{ij} = \sum_{k=1, k\neq i,j}^{I} \widetilde{z}_8^{ijk}; \qquad \widetilde{z}_{10}^{ij} = \widetilde{z}_9^{ij} u_6;$$

$$\widetilde{z}_{11}^{ij} = \widetilde{z}_{10}^{ij} u_5 (z_{10}^{ij})^{u_5 - 1}; \qquad \widetilde{z}_{12}^{ij} = -\frac{1}{2} u_5 \widetilde{z}_{11}^{ij} (1 + z_{11}^{ij})^{-\frac{1}{2u_5} - 1}; \qquad \widetilde{z}_{13}^{ij} = z_{13}^{ij}/a;$$

$$\widetilde{z}_{14}^{ij} = -\frac{u_3 \sqrt{2u_4} z_{13}^{ij} z_{14}^{ij}}{a}; \quad \widetilde{z}_{15}^{ij} = -\frac{u_3 \sqrt{2/u_4} z_{13}^{ij} z_{15}^{ij}}{a}; \quad \widetilde{z}_{16}^{ij} = \left.\frac{\partial f_c\left(\left(1+\frac{\rho}{a}\right) r_{ij}\right)}{\partial \rho}\right|_{\rho=0};$$

$$\widetilde{z}_{17}^{ij} = \widetilde{z}_{16}^{ij} z_{14}^{ij} - \widetilde{z}_{16}^{ij} z_{12}^{ij} z_{15}^{ij} + \widetilde{z}_{14}^{ij} z_{16}^{ij} - \widetilde{z}_{12}^{ij} z_{16}^{ij} z_{15}^{ij} - \widetilde{z}_{15}^{ij} z_{16}^{ij} z_{12}^{ij};$$

$$\widetilde{\widetilde{z}}_1^{ijk} = \widetilde{\widetilde{z}}_2^{ijk} = \widetilde{\widetilde{z}}_3^{ijk} = \widetilde{\widetilde{z}}_5^{ijk} = 0; \qquad \widetilde{\widetilde{z}}_4^{ijk} = \left.\frac{\partial^2 f_c\left(\left(1+\frac{\rho}{a}\right) r_{ik}\right)}{\partial \rho^2}\right|_{\rho=0};$$

$$\widetilde{\widetilde{z}}_6^{ijk} = 6z_6^{ijk}/a^2; \qquad \widetilde{\widetilde{z}}_7^{ijk} = \tfrac{3}{a^2} z_6^{ijk} z_7^{ijk} (u_7)^3 (3z_6^{ijk} (u_7)^3 + 2);$$

$$\widetilde{\widetilde{z}}_8^{ijk} = z_5^{ijk}(\widetilde{\widetilde{z}}_4^{ijk} z_7^{ijk} + 2\widetilde{z}_4^{ijk}\widetilde{z}_7^{ijk} + z_4^{ijk}\widetilde{\widetilde{z}}_7^{ijk}); \qquad \widetilde{\widetilde{z}}_9^{ij} = \sum_{k=1;k\neq i,j}^{I} \widetilde{\widetilde{z}}_8^{ijk};$$

$$\widetilde{\widetilde{z}}_{10}^{ij} = \widetilde{\widetilde{z}}_9^{ij} u_6; \qquad \widetilde{\widetilde{z}}_{11}^{ij} = u_5(u_5-1)(\widetilde{z}_{10}^{ij})^2(z_{10}^{ij})^{u_5-2} + u_5(\widetilde{\widetilde{z}}_{10}^{ij})(z_{10}^{ij})^{u_5-1};$$

$$\widetilde{\widetilde{z}}_{12}^{ij} = \frac{1+2u_5}{4u_5}(\widetilde{z}_{11}^{ij})^2(1+z_{11}^{ij})^{-\frac{1}{2u_5}-2} - \frac{1}{2u_5}\widetilde{\widetilde{z}}_{11}^{ij}(1+z_{11}^{ij})^{-\frac{1}{2u_5}-1}; \qquad \widetilde{\widetilde{z}}_{13}^{ij} = 0;$$

$$\widetilde{\widetilde{z}}_{14}^{ij} = \frac{2(u_3)^2u_4(z_{13}^{ij})^2 z_{14}^{ij}}{a^2}; \quad \widetilde{\widetilde{z}}_{15}^{ij} = \frac{2(u_3)^2(z_{13}^{ij})^2 z_{15}^{ij}}{a^2 u_4}; \quad \widetilde{\widetilde{z}}_{16}^{ij} = \left.\frac{\partial^2 f_c\left(\left(1+\frac{\rho}{a}\right) r_{ij}\right)}{\partial \rho^2}\right|_{\rho=0};$$

$$\widetilde{\widetilde{z}}_{17}^{ij} = \widetilde{\widetilde{z}}_{16}^{ij} z_{14}^{ij} + 2\widetilde{z}_{16}^{ij}\widetilde{z}_{14}^{ij} - \widetilde{\widetilde{z}}_{16}^{ij} z_{12}^{ij} z_{15}^{ij} - 2\widetilde{z}_{16}^{ij}\widetilde{z}_{12}^{ij} z_{15}^{ij} - 2\widetilde{z}_{16}^{ij} z_{12}^{ij}\widetilde{z}_{15}^{ij} +$$
$$+ \widetilde{\widetilde{z}}_{14}^{ij} z_{16}^{ij} - \widetilde{\widetilde{z}}_{12}^{ij} z_{16}^{ij} z_{15}^{ij} - 2\widetilde{z}_{15}^{ij} z_{16}^{ij}\widetilde{z}_{12}^{ij} - \widetilde{\widetilde{z}}_{15}^{ij} z_{16}^{ij} z_{12}^{ij}.$$

To compute the second derivative of a function $f_c(r)$ there is a need for smoothing this function. It is proposed to replace the function $f_c(r)$ as follows:

$$f_c(r) = \begin{cases} 0, & r \geq R + R_{cut}, \\ 1, & r \leq R - R_{cut}, \\ C \cdot (f_*)^{\varphi(r)}, & R \leq r < R + R_{cut}, \\ C \cdot \left(2f_* - (f_*)^{\psi(r)}\right), & R - R_{cut} < r \leq R, \end{cases}$$

where $C = \dfrac{1}{2f_*}$, $f_* = \exp(-\dfrac{3}{2})$, $\varphi(r) = \dfrac{R_{cut}^2}{(r-R-R_{cut})^2}$, $\psi(r) = \dfrac{R_{cut}^2}{(r-R+R_{cut})^2}$.
Derivatives of function $f_c(r)$ with respect to ρ are calculated by the formulas:

$$\left.\frac{\partial f_c\left(\left(1+\frac{\rho}{a}\right) r\right)}{\partial \rho}\right|_{\rho=0} = \begin{cases} 0, & r \geq R + R_{cut}, \\ 0, & r \leq R - R_{cut}, \\ C \cdot (f_*)^{\varphi(r)} \ln(f_*) \cdot \widetilde{\varphi}(r), & R \leq r < R + R_{cut}, \\ C \cdot (f_*)^{\psi(r)} \ln(f_*) \cdot \widetilde{\psi}(r), & R - R_{cut} < r \leq R, \end{cases}$$

$$\left.\frac{\partial^2 f_c\left(\left(1+\frac{\rho}{a}\right) r\right)}{\partial \rho^2}\right|_{\rho=0} = \begin{cases} 0, & r \geq R + R_{cut}, \\ 0, & r \leq R - R_{cut}, \\ C \cdot (f_*)^{\varphi(r)} \ln(f_*) \left[\ln(f_*)\widetilde{\varphi}^2(r) + \widetilde{\widetilde{\varphi}}(r)\right], & R \leq r < R + R_{cut}, \\ -C \cdot (f_*)^{\psi(r)} \ln(f_*) \left[\ln(f_*)\widetilde{\psi}^2(r) + \widetilde{\widetilde{\psi}}(r)\right], & R - R_{cut} < r \leq R, \end{cases}$$

where $\quad \widetilde{\varphi}(r) = \dfrac{-2rR_{cut}^2}{a(r-R-R_{cut})^3}, \qquad \widetilde{\psi}(r) = \dfrac{-2rR_{cut}^2}{a(r-R+R_{cut})^3},$

$$\widetilde{\widetilde{\varphi}}(r) = \frac{6r^2R_{cut}^2}{a^2(r-R-R_{cut})^4}, \qquad \widetilde{\widetilde{\psi}}(r) = \frac{6r^2R_{cut}^2}{a^2(r-R+R_{cut})^4}.$$

Thus, $B(E)$ is calculated by the formula

$$B(E) = \sum_{i=1}^{I} \sum_{i=1; j \neq i}^{I} \widetilde{\widetilde{z}}_{17}^{ij},$$

where the variables $z_1, z_2, ..., z_{17}$, $\widetilde{z}_1, \widetilde{z}_2, ..., \widetilde{z}_{17}$, $\widetilde{\widetilde{z}}_1, \widetilde{\widetilde{z}}_2, ..., \widetilde{\widetilde{z}}_{17}$ are determined by mentioned above multistep algorithm.

3 Determining the adjoint variables and gradient

We represent the general formulas of Fast Automatic Differentiation below, which will be used to calculate the gradient of function $B(E)$ with respect to parameters of Tersoff Potential specific to modeled substance. Let vectors $z \in R^n$ and $u \in R^m$ satisfy the following system of nonlinear scalar equations (multistep process):

$$z_i = F(i, Z_i, U_i), \qquad 1 \leq i \leq n \tag{2}$$

where Z_i is the set of vectors z_j, that appear at the right part of equality (2), and U_i is the set of vectors u_j, that appear at the right part of the same equality (2). Usually the vectors $z \in R^n$ and the vectors $u \in R^m$ are called dependent (phase) and independent (control) variables respectively. Let differentiable function $W(z, u)$ define mapping $W : R^n \times R^m \longrightarrow R^1$. Then the composite function $\Omega(u) = W(z(u), u)$ is differentiable, and its gradient with respect to the independent variables u_i is given by the formula

$$\frac{\partial \Omega}{\partial u_i} = W_{u_i}(z, u) + \sum_{q \in \overline{K}_i} F_{u_i}(q, Z_q, U_q) p_q. \tag{3}$$

The multipliers $p_i \in R^n$ are the adjoint variables that are defined by the following system of linear algebraic equations:

$$p_i = W_{z_i}(z, u) + \sum_{q \in \overline{Q}_i} F_{z_i}(q, Z_q, U_q) p_q, \tag{4}$$

where $\overline{Q}_i$ and $\overline{K}_i$ are the index sets:

$$\overline{Q}_i = \{j : 1 \leq j \leq n, \quad z_i \in Z_j\} \qquad \overline{K}_i = \{j : 1 \leq j \leq n, \quad u_i \in U_j\}.$$

In accordance to (4), for all $i = \overline{1, I}$, $j = \overline{1, I}$, $j \neq i$, $k = \overline{1, I}$, $k \neq i, j$ adjoint variables corresponding to the phase variables $z_1, z_2, ..., z_{17}$, $\widetilde{z}_1, \widetilde{z}_2, ..., \widetilde{z}_{17}$,

$\tilde{\tilde{z}}_1, \tilde{\tilde{z}}_2, ..., \tilde{\tilde{z}}_{17}$ are defined by the equations:

$$p_5^{ijk} = (\tilde{\tilde{z}}_4^{ijk} z_7^{ijk} + 2\tilde{z}_4^{ijk}\tilde{z}_7^{ijk} + z_4^{ijk}\tilde{\tilde{z}}_7^{ijk})\tilde{\tilde{p}}_8^{ijk} + (\tilde{z}_4^{ijk} z_7^{ijk} + z_4^{ijk}\tilde{z}_7^{ijk})\tilde{p}_8^{ijk} + z_4^{ijk} z_7^{ijk} p_8^{ijk};$$

$$p_7^{ijk} = \tilde{\tilde{z}}_4^{ijk} z_5^{ijk}\tilde{\tilde{p}}_8^{ijk} + \tilde{z}_4^{ijk} z_5^{ijk}\tilde{p}_8^{ijk} + z_4^{ijk} z_5^{ijk} p_8^{ijk} +$$
$$+\frac{3}{a^2} z_6^{ijk}(u_7)^3(3z_6^{ijk}(u_7)^3 + 2)\tilde{\tilde{p}}_7^{ijk} + \frac{3}{a} z_6^{ijk}(u_7)^3\tilde{p}_7^{ijk};$$

$$p_8^{ijk} = p_9^{ij}; \qquad p_9^{ij} = u_6 p_{10}^{ij};$$

$$p_{10}^{ij} = \Big[u_5(u_5-1)(u_5-2)(z_{10}^{ij})^{u_5-3}(\tilde{z}_{10}^{ij})^2 + u_5(u_5-1)(z_{10}^{ij})^{u_5-2}\tilde{\tilde{z}}_{10}^{ij}\Big]\tilde{\tilde{p}}_{11}^{ij} +$$
$$+u_5(u_5-1)(z_{10}^{ij})^{u_5-2}\tilde{z}_{10}^{ij}\tilde{p}_{11}^{ij} + u_5(z_{10}^{ij})^{u_5-1}p_{11}^{ij};$$

$$p_{11}^{ij} = -\frac{(1+4u_5)(1+2u_5)}{8(u_5)^3}(1+z_{11}^{ij})^{-\frac{1}{2u_5}-3}(z_{11}^{ij})^2\tilde{\tilde{p}}_{12}^{ij} + \frac{(1+2u_5)}{4(u_5)^2}(1+z_{11}^{ij})^{-\frac{1}{2u_5}-2}\times$$
$$\times\tilde{\tilde{z}}_{11}^{ij}\tilde{\tilde{p}}_{12}^{ij} + \frac{(1+2u_5)}{4(u_5)^2}(1+z_{11}^{ij})^{-\frac{1}{2u_5}-2}\tilde{z}_{11}^{ij}\tilde{p}_{12}^{ij} - \frac{1}{2u_5}(1+z_{11}^{ij})^{-\frac{1}{2u_5}-1}p_{12}^{ij};$$

$$p_{12}^{ij} = (-\tilde{\tilde{z}}_{16}^{ij} z_{15}^{ij} - 2\tilde{z}_{15}^{ij}\tilde{z}_{16}^{ij} - z_{16}^{ijk}\tilde{\tilde{z}}_{15}^{ij})\tilde{\tilde{p}}_{17}^{ij};$$

$$p_{14}^{ij} = \tilde{\tilde{z}}_{16}^{ij}\tilde{\tilde{p}}_{17}^{ij} + \frac{2(u_3)^2 u_4 (z_{13}^{ij})^2}{a^2}\tilde{\tilde{p}}_{14}^{ij} - u_3\sqrt{2u_4}\frac{z_{13}^{ij}}{a}\tilde{p}_{14}^{ij};$$

$$p_{15}^{ij} = (-\tilde{\tilde{z}}_{16}^{ij} z_{12}^{ij} - 2\tilde{z}_{12}^{ij}\tilde{z}_{16}^{ij} - z_{16}^{ij}\tilde{\tilde{z}}_{12}^{ij})\tilde{\tilde{p}}_{17}^{ij} + \frac{2(u_3)^2(z_{13}^{ij})^2}{a^2 u_4}\tilde{\tilde{p}}_{15}^{ij} - \sqrt{2/u_4}\frac{u_3 z_{13}^{ij}}{a}\tilde{p}_{15}^{ij};$$

$$p_{16}^{ij} = (\tilde{\tilde{z}}_{14}^{ij} - \tilde{\tilde{z}}_{12}^{ij} z_{15}^{ij} - 2\tilde{z}_{12}^{ij}\tilde{z}_{15}^{ij} - z_{12}^{ij}\tilde{\tilde{z}}_{15}^{ij})\tilde{\tilde{p}}_{17}^{ij}; \qquad p_{17}^{ij} = 0;$$

$$\tilde{p}_7^{ijk} = 2\tilde{z}_4^{ijk} z_5^{ijk}\tilde{\tilde{p}}_8^{ijk} + z_4^{ijk} z_5^{ijk}\tilde{p}_8^{ijk}; \qquad \tilde{p}_8^{ijk} = \tilde{p}_9^{ij};$$

$$\tilde{p}_9^{ij} = u_6\tilde{p}_{10}^{ij}; \qquad \tilde{p}_{10}^{ij} = 2u_5(u_5-1)(z_{10}^{ij})^{u_5-2}\tilde{\tilde{p}}_{11}^{ij} + u_5(z_{10}^{ij})^{u_5-1}\tilde{z}_{10}^{ij}\tilde{p}_{11}^{ij};$$

$$\tilde{p}_{11}^{ij} = \frac{(1+2u_5)}{2(u_5)^2}(1+z_{11}^{ij})^{-1/(2u_5)-2}\tilde{z}_{11}^{ij}\tilde{\tilde{p}}_{12}^{ij} - \frac{(1+z_{11}^{ij})^{-1/(2u_5)-1}}{2u_5}\tilde{p}_{12}^{ij};$$

$$\tilde{p}_{12}^{ij} = -2(\tilde{z}_{16}^{ij} z_{15}^{ij} + \tilde{z}_{15}^{ij} z_{16}^{ij})\tilde{\tilde{p}}_{17}^{ij}; \qquad \tilde{p}_{14}^{ij} = 2\tilde{z}_{16}^{ij}\tilde{\tilde{p}}_{17}^{ij};$$

$$\tilde{p}_{15}^{ij} = -2(\tilde{z}_{16}^{ij} z_{12}^{ij} + \tilde{z}_{12}^{ij} z_{16}^{ij})\tilde{\tilde{p}}_{17}^{ij}; \qquad \tilde{p}_{16}^{ij} = 2(\tilde{z}_{14}^{ij} - \tilde{z}_{12}^{ij} z_{15}^{ij} - \tilde{z}_{15}^{ij} z_{12}^{ij})\tilde{\tilde{p}}_{17}^{ij};$$

$$\tilde{p}_{17}^{ij} = 0; \qquad \tilde{\tilde{p}}_7^{ijk} = z_4^{ijk} z_5^{ijk}\tilde{\tilde{p}}_8^{ijk}; \qquad \tilde{\tilde{p}}_8^{ijk} = \tilde{\tilde{p}}_9^{ij}; \qquad \tilde{\tilde{p}}_9^{ij} = u_6\tilde{\tilde{p}}_{10}^{ij};$$

$$\tilde{\tilde{p}}_{10}^{ij} = u_5(z_{10}^{ij})^{u_5-1}\tilde{\tilde{p}}_{11}^{ij}; \qquad \tilde{\tilde{p}}_{11}^{ij} = -\frac{(1+z_{11}^{ij})^{-1/(2u_5)-1}}{2u_5}\tilde{\tilde{p}}_{12}^{ij};$$

$$\tilde{\tilde{p}}_{12}^{ij} = -z_{15}^{ij} z_{16}^{ij}\tilde{\tilde{p}}_{17}^{ij}; \qquad \tilde{\tilde{p}}_{14}^{ij} = z_{16}^{ij}\tilde{\tilde{p}}_{17}^{ij};$$

$$\tilde{\tilde{p}}_{15}^{ij} = -z_{12}^{ij} z_{16}^{ij}\tilde{\tilde{p}}_{17}^{ij}; \qquad \tilde{\tilde{p}}_{16}^{ij} = (z_{14}^{ij} - z_{12}^{ij} z_{15}^{ij})\tilde{\tilde{p}}_{17}^{ij}; \qquad \tilde{\tilde{p}}_{17}^{ij} = 1;$$

The adjoint variables are calculate in the following order:

$$\widetilde{\widetilde{p}}_{17}^{ij}, \widetilde{\widetilde{p}}_{16}^{ij}, ..., \widetilde{\widetilde{p}}_{7}^{ij}, \widetilde{p}_{17}^{ij}, ..., \widetilde{p}_{7}^{ij}, p_{17}^{ij}, ..., p_{5}^{ij}.$$

Those adjoint variables, whose formulas for calculation aren't provided above, aren't used for calculation of the components of the gradient.

The partial derivatives of function

$$\Omega(\overline{u}) = B(E(\overline{u})) = \sum_{i=1}^{I} \sum_{j=1;j\neq i}^{I} \widetilde{\widetilde{z}}_{17}^{ij}$$

with respect to independent variables u_m, $(m = \overline{1,10})$ (components of gradient), according to equation (3), are determined by the relations:

$$\frac{\partial \Omega}{\partial u_1} = \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(\frac{z_{14}^{ij}}{u_1} p_{14}^{ij} + \frac{z_{15}^{ij}}{u_1} p_{15}^{ij} \right);$$

$$\frac{\partial \Omega}{\partial u_2} = \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(z_{14}^{ij} u_3 \sqrt{2u_4} p_{14}^{ij} + z_{15}^{ij} u_3 \sqrt{2/u_4} p_{15}^{ij} \right);$$

$$\frac{\partial \Omega}{\partial u_3} = \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(z_{14}^{ij} \left(-\sqrt{2u_4}(z_{13}^{ij} - u_2) \right) p_{14}^{ij} + z_{15}^{ij} \left(-\sqrt{2/u_4}(z_{13}^{ij} - u_2) \right) p_{15}^{ij} \right) +$$

$$+ \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(\frac{4u_3 u_4 (z_{13}^{ij})^2 z_{14}^{ij}}{a^2} \widetilde{\widetilde{p}}_{14}^{ij} - \frac{\sqrt{2u_4} z_{13}^{ij} z_{14}^{ij}}{a} \widetilde{p}_{14}^{ij} \right) +$$

$$+ \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(\frac{4u_3 (z_{13}^{ij})^2 z_{15}^{ij}}{a^2 u_4} \widetilde{\widetilde{p}}_{15}^{ij} - \frac{z_{13}^{ij} z_{15}^{ij}}{a} \sqrt{2/u_4} \widetilde{p}_{15}^{ij} \right);$$

$$\frac{\partial \Omega}{\partial u_4} = \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(\left(-\frac{z_{14}^{ij}}{u_4 - 1} - 0.5 u_3 \sqrt{2/u_4}(z_{13}^{ij} - u_2) z_{14}^{ij} \right) p_{14}^{ij} \right) +$$

$$+ \sum_{i=1}^{I} \sum_{\substack{j=1\\ j\neq i}}^{I} \left(\left(-\frac{z_{15}^{ij}}{u_4(u_4 - 1)} + 0.5(u_3/u_4) \sqrt{2/u_4}(z_{13}^{ij} - u_2) z_{15}^{ij} \right) p_{15}^{ij} \right) +$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(-\frac{u_3}{2a}\sqrt{2/u_4}z_{13}^{ij}z_{14}^{ij}\right)\widetilde{p}_{14}^{ij}+\left(\frac{2(u_3)^2(z_{13}^{ij})^2}{a^2}z_{14}^{ij}\right)\widetilde{\widetilde{p}}_{14}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(\frac{u_3}{2au_4}\sqrt{2/u_4}z_{13}^{ij}z_{15}^{ij}\right)\widetilde{p}_{14}^{ij}-\left(\frac{2(u_3)^2(z_{13}^{ij})^2}{a^2(u_4)^2}z_{15}^{ij}\right)\widetilde{\widetilde{p}}_{15}^{ij}\right);$$

$$\frac{\partial\Omega}{\partial u_5}=\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left((z_{10}^{ij})^{u_5}\ln(z_{10}^{ij})p_{11}^{ij}+\frac{(1+z_{11}^{ij})^{-1/(2u_5)}}{2(u_5)^2}\ln(1+z_{11}^{ij})p_{12}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left((z_{10}^{ij})^{u_5-1}\widetilde{z}_{10}^{ij}+u_5(z_{10}^{ij})^{u_5-1}\widetilde{z}_{10}^{ij}\ln(z_{10}^{ij})\right)\widetilde{p}_{11}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left((2u_5-1)(z_{10}^{ij})^{u_5-2}+((u_5)^2-u_5)(z_{10}^{ij})^{u_5-2}\ln(z_{10}^{ij})\right)(\widetilde{z}_{10}^{ij})^2\widetilde{\widetilde{p}}_{11}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left((z_{10}^{ij})^{u_5-1}+u_5(z_{10}^{ij})^{u_5-1}\ln(z_{10}^{ij})\right)\widetilde{\widetilde{z}}_{10}^{ij}\widetilde{\widetilde{p}}_{11}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(\frac{(1+z_{11}^{ij})^{-1/(2u_5)-1}}{2(u_5)^2}-\frac{\ln(1+z_{11}^{ij})}{4(u_5)^3}(1+z_{11}^{ij})^{-1/(2u_5)-1}\right)\widetilde{z}_{11}^{ij}\widetilde{p}_{12}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(-\frac{(1+u_5)}{2(u_5)^3}(1+z_{11}^{ij})^{-1/(2u_5)-2}\right)(\widetilde{z}_{11}^{ij})^2\widetilde{\widetilde{p}}_{12}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(\frac{(1+2u_5)\ln(1+z_{11}^{ij})}{8(u_5)^4}(1+z_{11}^{ij})^{-1/(2u_5)-2}\right)(\widetilde{z}_{11}^{ij})^2\widetilde{\widetilde{p}}_{12}^{ij}\right)+$$

$$+\sum_{i=1}^{I}\sum_{\substack{j=1\\ j\neq i}}^{I}\left(\left(\frac{(1+z_{11}^{ij})^{-1/(2u_5)-1}}{2(u_5)^2}-\frac{\ln(1+z_{11}^{ij})}{4(u_5)^3}(1+z_{11}^{ij})^{-1/(2u_5)-1}\right)\widetilde{\widetilde{z}}_{11}^{ij}\widetilde{\widetilde{p}}_{12}^{ij}\right);$$

$$\frac{\partial\Omega}{\partial u_6} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \left(z_9^{ij} p_{10}^{ij} + \tilde{z}_9^{ij} \tilde{p}_{10}^{ij} + \tilde{\tilde{z}}_9^{ij} \tilde{\tilde{p}}_{10}^{ij} \right);$$

$$\frac{\partial\Omega}{\partial u_7} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \sum_{\substack{k=1 \\ k\neq i,j}}^{I} \left(3z_6^{ijk} z_7^{ijk} (u_7)^2 p_7^{ijk} + \frac{9}{a} z_6^{ijk} z_7^{ijk} (u_7)^2 \tilde{p}_7^{ijk} \right) +$$

$$+ \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \sum_{\substack{k=1 \\ k\neq i,j}}^{I} \left(\left(\frac{3z_6^{ijk} z_7^{ijk}}{a^2} \left(18 z_6^{ijk} (u_7)^5 + 6(u_7)^2 \right) \right) \tilde{\tilde{p}}_7^{ijk} \right);$$

$$\frac{\partial\Omega}{\partial u_8} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \sum_{\substack{k=1 \\ k\neq i,j}}^{I} \left(\left(\frac{2u_8}{(u_9)^2} - \frac{2u_8}{(u_9)^2 + (u_{10} - z_3^{ijk})^2} \right) p_5^{ijk} \right);$$

$$\frac{\partial\Omega}{\partial u_9} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \sum_{\substack{k=1 \\ k\neq i,j}}^{I} \left(\left(\frac{-2(u_8)^2}{(u_9)^3} + \frac{2(u_8)^2 u_9}{\left((u_9)^2 + (u_{10} - z_3^{ijk})^2 \right)^2} \right) p_5^{ijk} \right);$$

$$\frac{\partial\Omega}{\partial u_{10}} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j\neq i}}^{I} \sum_{\substack{k=1 \\ k\neq i,j}}^{I} \left(\left(\frac{2(u_8)^2 (u_{10} - z_3^{ijk})}{\left((u_9)^2 + (u_{10} - z_3^{ijk})^2 \right)^2} \right) p_5^{ijk} \right).$$

The received formulas for calculation of the gradient of function $B(E(u))$ outwardly are represented quite difficult and bulky. Therefore, there is a natural question: whether to use simpler approaches, for example, finite difference method, to calculate the gradient functions $B(E(u))$.

In [5] the comparison of function gradients, calculated by the finite differences and by using Fast Automatic Differentiation formulas (see above), was presented. The results of comparison are the following:

1) when computing the gradient of complicated function using finite differences, one must conduct researches related to the choice of suitable increments of each parameter;

2) for different parameters, the researches must be carried out independently;

3) for the same parameter, the researches must be carried out if its value changed;

4) to calculate the gradient of complicated function using finite differences one must $(m+1)$ times calculate the value of function itself.

In contrary to it, the Fast Automatic Differentiation enables us to calculate gradients of any complicated function with the machine accuracy for arbitrary parameters. The machine time that is needed to calculate the gradient does not exceed three times of calculation of the function itself.

4 Conclusion

In this work an efficient algorithm to calculate gradients of the Bulk modulus and the Shear modulus is presented. The algorithm is based on the modern Fast Automatic Differentiation technique. The formulas to compute the mentioned gradients are derived. These formulas allow us to compute the gradients with the machine accuracy. The computation time that is needed to calculate the gradient does not exceed three times of calculation of the function itself. The comparison of the proposed algorithm and finite differences method to calculate gradients of complicated function is made. The conclusion is made: the calculation of gradient of Bulk modulus and the Shear modulus using finite difference method is linked to enormous difficulties.

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