Application of the Fast Automatic Differentiation to the Computation of the Gradient of the Energy of Atoms' System with Respect to Tersoff Parameters*

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Abstract— Gradient optimization methods are often used to tackle problems of computer modeling of materials' crystal structures. This raises the need to determine the exact value of the gradient of the Tersoff potential using specific parameters of this potential for the modeled substance. Based on the technique of the Fast Automatic Differentiation the formulas that allow the calculation of the exact value of the above-mentioned gradient were derived.

Keywords—Tersoff potential; gradient; Fast Automatic Differentiation

I. INTRODUCTION

For modeling solid atomic structures the Tersoff Potential is often used ([1]). The Tersoff Potential depends on ten parameters specific to the modeling material. These parameters are usually unknown and they should be identified as the solution of the inverse problem. In [2] one possible optimization problem was considered. It consists of minimizing the following cost function

$$f(\xi) = \sum_{i=1}^{n} w_i \big(y_i(\xi) - \mathfrak{y}_i\big)^2, \qquad (1)$$

where w_i is the weight factor; $\mathfrak{y}_i$ 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 the 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. A required set of parameters has to provide the minimum deviation of the calculated characteristics of the material from the known experimental values. For numerical solution of this problem the gradient minimization methods are often used. One of the terms in formula (1) is the total energy of the system of atoms. There exists the need to calculate efficiently the exact gradient of the total energy with respect to parameters of the Tersoff Potential.

This gradient is often calculated (see, for example, [2]) using the finite difference method. Studies have shown that finite difference method does not allow to calculate the gradient of the energy of atoms' system with respect to

Tersoff parameters with acceptable accuracy and requires $(m+1)$ times to calculate the value of the function.

In this paper, we build a multistep algorithm to calculate the value of total atoms' system energy in the case where this energy is determined by Tersoff Potential and a multistep algorithm to calculate the conjugate variables, by which the value of the above-mentioned gradient is determined with machine precision on the basis of the Fast Automatic Differentiation methodology.

II. ALGORITHM FOR CALCULATION THE TOTAL ENERGY OF ATOMS' SYSTEM AND THE ADJOINT VARIABLES

Let $\bar{r}_k = (x_{k1}, x_{k2}, x_{k3})$ be the coordinates of some lattice atom. As to total energy $E(\bar{r}_1, \bar{r}_2, ..., \bar{r}_I)$ it is calculated with the help of expression $E(\bar{r}_1, \bar{r}_2, ..., \bar{r}_I) = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j \neq i}}^{I} V_{ij}$, 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:

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

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

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

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

$$b_{ij} = \big(1 + (\gamma\varsigma_{ij})^\eta\big)^{-\frac{1}{2\eta}}, \qquad \varsigma_{ij} = \sum_{\substack{k=1 \\ k \neq i,j}}^{I} f_c(r_{ik}) g_{ijk} \omega_{ijk},$$

$$\omega_{ijk} = \exp\left(\lambda^3 \tau_{ijk}\right), \qquad \tau_{ijk} = \left(r_{ij} - r_{ik}\right)^3,$$

$$g_{ijk} = g(\theta_{ijk}) = 1 + \left(\frac{c}{d}\right)^2 - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2}.$$

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 the substance. Tersoff Potential depends on these ten parameters ($m = 10$), specific to modeled substances: D_e, r_e, β, S, η, γ, λ, c, d, h.

For using the Fast Automatic Differentiation to calculate the gradient of cost function, we construct the multistep algorithm to determine 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

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

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

$$q_{ijk} = \cos(\theta_{ijk}) = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2 r_{ij} r_{ik}}.$$ For compactness further in the study we introduce vectors $\bar{u}$ and $\bar{z}$ having the following coordinates: $\bar{u}^T = [u_1, u_2, ..., u_{10}]^T$, $\bar{z}^T = [z_1, z_2, ..., z_{17}]^T$, where $u_1 = D_e$, $u_2 = r_e$, $u_3 = \beta$, $u_4 = S$, $u_5 = \eta$, $u_6 = \gamma$, $u_7 = \lambda$, $u_8 = c$, $u_9 = d$, $u_{10} = h$;

$$z_1 = \left\{ z_1^{ijk} = \sqrt{\left(x_{1i} - x_{1k}\right)^2 + \left(x_{2i} - x_{2k}\right)^2 + \left(x_{3i} - x_{3k}\right)^2} \right\},$$

$$z_2 = \left\{ z_2^{ijk} = \sqrt{\left(x_{1j} - x_{1k}\right)^2 + \left(x_{2j} - x_{2k}\right)^2 + \left(x_{3j} - x_{3k}\right)^2} \right\},$$

$$z_3 = \left\{ z_3^{ijk} = q_{ijk} = \frac{(z_{13}^{ij})^2 + (z_1^{ijk})^2 - (z_2^{ijk})^2}{2 z_{13}^{ij} z_1^{ijk}} \right\},$$

$$z_4 = \left\{ z_4^{ijk} = f_c(z_1^{ijk}) \right\},$$

$$z_5 = \left\{ z_5^{ijk} = g_{ijk} = 1 + \left(\frac{u_8}{u_9}\right)^2 - \frac{(u_8)^2}{(u_9)^2 + (u_{10} - z_3^{ijk})^2} \right\},$$

$$z_6 = \left\{ z_6^{ijk} = \tau_{ijk} = \left(z_{13}^{ij} - z_1^{ijk}\right)^3 \right\},$$

$$z_7 = \left\{ z_7^{ijk} = \omega_{ijk} = \exp\left((u_7)^3 z_6^{ijk}\right) \right\},$$

$$z_8 = \left\{ z_8^{ijk} = f_c(r_{ik}) g_{ijk} \omega_{ijk} = z_4^{ijk} z_5^{ijk} z_7^{ijk} \right\},$$

$$z_9 = \left\{ z_9^{ij} = \varsigma_{ij} = \sum_{k=1, k \neq i, j}^{I} z_8^{ijk} \right\},$$

$$z_{10} = \left\{ z_{10}^{ij} = \gamma \varsigma_{ij} = u_6 z_9^{ij} \right\},$$

$$z_{11} = \left\{ z_{11}^{ij} = (\gamma \varsigma_{ij})^{\eta} = (z_{10}^{ij})^{u_5} \right\},$$

$$z_{12} = \left\{ z_{12}^{ij} = b_{ij} = (1 + z_{11}^{ij})^{-\frac{1}{2u_5}} \right\},$$

$$z_{13} = \left\{ z_{13}^{ij} = \sqrt{\left(x_{1i} - x_{1j}\right)^2 + \left(x_{2i} - x_{2j}\right)^2 + \left(x_{3i} - x_{3j}\right)^2} \right\},$$

$$z_{14} = \left\{ z_{14}^{ij} = V_{ij}^R = \frac{u_1}{u_4 - 1} \exp\left(-u_3 \sqrt{2u_4}(z_{13}^{ij} - u_2)\right) \right\},$$

$$z_{15} = \left\{ z_{15}^{ij} = V_{ij}^A = \frac{u_1 u_4}{u_4 - 1} \exp\left(-u_3 \sqrt{\frac{2}{u_4}}(z_{13}^{ij} - u_2)\right) \right\},$$

$$z_{16} = \left\{ z_{16}^{ij} = f_c(z_{13}^{ij}) \right\},$$

$$z_{17} = \left\{ z_{17}^{ij} = V_{ij} = z_{16}^{ij}(z_{14}^{ij} - z_{12}^{ij} z_{15}^{ij}) \right\},$$

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

The total energy of the atoms' system with the help of new variables may be rewritten as follows: $E(z(u)) = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j \neq i}}^{I} z_{17}^{ij}$.

Variables $z_1, z_2, ..., z_{17}$ (the phase variables) are determined by the specified above multistep algorithm $z_l = F(l, Z_l, U_l)$, ($l = \overline{1, 17}$), 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}).

Below are represented the general formulas of the Fast Automatic Differentiation (see [3]). They will be used later to calculate the gradient of the total energy E of atoms' system with respect to parameters of the Tersoff Potential.

Let vectors $z \in R^n$ and $u \in R^m$ satisfy the following system of nonlinear scalar equations (multistep process):

$$z_i = F(i, Z_i, U_i), \qquad 1 \le i \le n, \qquad (2)$$

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 vectors $z \in R^n$ and vectors $u \in R^m$ are called dependent (phase) and independent (control) variables respectively. Let differentiable function $W(z,u)$ define mapping $W : R^n \times R^m \to R^1$. 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

$$\frac{d\Omega}{du_i} = W_{u_i}(z,u) + \sum_{q \in \overline{K}_i} F_{u_i}^T(q, Z_q, U_q) p_q . \qquad (3)$$

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

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

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

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

The partial derivatives of function $\Omega(u) = E(z(u)) = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j \ne i}}^{I} z_{17}^{ij}(u)$ with respect to independent variables u_m, $(m = \overline{1,10})$ (components of gradient), according to equations (3), (4) are determined by the relations:

$$\frac{\partial \Omega}{\partial u_m} = \sum_{q \in \overline{K}_m} F_{u_m}^T(q, Z_q, U_q) p_q, \overline{K}_m = \{j : \ u_m \in U_j\},$$
$$m = \overline{1,10},$$

where the conjugate variables p_i are defined by the following system of linear algebraic equations:

$$p_l = E_{z_l}(z) + \sum_{q \in \overline{Q}_l} F_{z_l}^T(q, Z_q, U_q) p_q, \qquad (5)$$

$$\overline{Q}_l = \{j : \ z_l \in Z_j\}, \qquad (l = \overline{1,17}).$$

Note that $E_{u_m}(z(u)) = 0$ because function $E(z(u))$ clearly does not depend on the vector components $\overline{u}$.

In accordance to (5), for all $i = \overline{1,I}, \ j = \overline{1,I}, j \ne i, k = \overline{1,I}, k \ne i, j$ conjugate variables corresponding to the phase variables $z_1, z_2, ..., z_{17}$ are defined by the equations:

$$p_1^{ijk} = \frac{(z_1^{ijk})^2 - (z_{13}^{ij})^2 + (z_2^{ijk})^2}{2(z_1^{ijk})^2(z_{13}^{ij})} p_3^{ijk} +$$
$$+ \frac{\tilde{df}_{ijk}}{dz_1^{ijk}} p_4^{ijk} - 3(z_{13}^{ij} - z_1^{ijk})^2 p_6^{ijk},$$

$$p_2^{ijk} = -\frac{z_2^{ijk}}{z_1^{ijk} z_{13}^{ij}} p_3^{ijk}, \quad p_3^{ijk} = -\frac{2u_8^2(u_{10} - z_3^{ijk})}{\left(u_9^2 + (u_{10} - z_3^{ijk})^2\right)^2} p_5^{ijk},$$

$$p_4^{ijk} = z_5^{ijk} z_7^{ijk} p_8^{ijk}, \qquad\qquad p_5^{ijk} = z_4^{ijk} z_7^{ijk} p_8^{ijk},$$

$$p_6^{ijk} = u_7^3 \exp(z_6^{ijk} u_7^3) p_7^{ijk}, \qquad p_7^{ijk} = z_4^{ijk} z_5^{ijk} p_8^{ijk},$$

$$p_8^{ijk} = p_9^{ij}, \qquad p_9^{ij} = u_6 p_{10}^{ij}, \qquad p_{10}^{ij} = u_5 \left(z_{10}^{ij}\right)^{u_5 - 1} p_{11}^{ij},$$

$$p_{11}^{ij} = -\frac{1}{2u_5}\left(1 + z_{11}^{ij}\right)^{-1/(2u_5) - 1} p_{12}^{ij}, \quad p_{12}^{ij} = -z_{15}^{ij} z_{16}^{ij} p_{17}^{ij},$$

$$p_{13}^{ij} = \sum_{\substack{k=1, \\ k \ne i, j}}^{I} \left(\frac{(z_{13}^{ij})^2 - (z_1^{ijk})^2 + (z_2^{ijk})^2}{2(z_1^{ijk})(z_{13}^{ij})^2} p_3^{ijk} \right) +$$

$$+ \sum_{\substack{k=1, \\ k \ne i, j}}^{I} \left(3(z_{13}^{ij} - z_1^{ijk})^2 p_6^{ijk} \right) + \frac{df_{ij}}{dz_{13}^{ij}} p_{16}^{ij} -$$

$$- \frac{u_1 u_3 \sqrt{2u_4}}{u_4 - 1} \exp\left(-u_3\sqrt{2u_4}(z_{13}^{ij} - u_2)\right) p_{14}^{ij} -$$

$$- \frac{u_1 u_3 u_4 \sqrt{2/u_4}}{u_4 - 1} \exp\left(-u_3\sqrt{2/u_4}(z_{13}^{ij} - u_2)\right) p_{15}^{ij},$$

$$p_{14}^{ij} = z_{16}^{ij} p_{17}^{ij}, \qquad\qquad p_{15}^{ij} = -z_{12}^{ij} z_{16}^{ij} p_{17}^{ij},$$

$$p_{16}^{ij} = (z_{14}^{ij} - z_{12}^{ij} z_{15}^{ij}) p_{17}^{ij}, \qquad p_{17}^{ij} = 1.$$

The conjugate variables are calculated in the following order: $p_{17}, p_{16}, ..., p_1$.

III. DETERMINING THE COMPONENTS OF THE GRADIENT

Partial derivatives of the function $\Omega(u) = E(z(u))$ with respect to independent variables u_m, $(m = \overline{1,10})$ are determined by these relations:

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

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

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

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

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

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

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

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

$$\frac{\partial \Omega}{\partial u_6} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j \neq i}}^{I} \left(z_9^{ij} \; p_{10}^{ij} \right), \qquad\qquad (6)$$

$$\frac{\partial \Omega}{\partial u_7} = \sum_{i=1}^{I} \sum_{\substack{j=1 \\ j \neq i}}^{I} \left(\sum_{k=1, k \neq i, j}^{I} \left(3 z_6^{ij} z_7^{ij} u_7^2 \; p_7^{ijk} \right) \right),$$

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

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

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

The received formulas for calculation of the gradient of the total energy of atoms' system with respect to Tersoff parameters are quite complex and bulky. Therefore, there is a natural question whether it would be better to use simpler approaches to calculate the gradient of the function $\Omega(u) = E(z(u))$, for example, finite difference method.

The problem of selection of Tersoff parameters for one-component silicon crystal was considered in [2]. To determine the initial approximations in this work an admissible set $X = [\underline{\xi}, \overline{\xi}] = \left\{ u \in R^{10} : \underline{\xi_i} \leq u_i \leq \overline{\xi_i} \right\}$ was chosen in such a way that it clearly contains all the possible values of parameters, namely:

$$\underline{\xi} = (0.5; 0.5; 0.5; 0.5; 0.1; 5 \cdot 10^{-8}; 0.5; 10000; 1; -2),$$

$$\overline{\xi} = (10; 5; 5; 5; 2; 3 \cdot 10^{-6}; 3; 200000; 30; -0.1).$$

In [4] the comparison of function gradients, calculated by the finite differences and by using Fast Automatic Differentiation formulas (6), was presented. In TABLES I and II are given the values of the gradient for two specific parameters of the simulated substance: $u_3 = \beta, \quad u_6 = \gamma$.

Input parameters $u_3 = 1.0$ and $u_6 = 10^{-7}$ were selected from the range of acceptable values. The value Δ in TABLES I and II indicates the increment of parameters u_i that were used during calculation of the gradient using the method of finite differences.

As can be seen from TABLE I, during the calculation of the third component of the gradient value $\Delta \approx 10^{-7}$ is the most suitable choice. It is about $10^{-5}\%$ from initial approximation $u_3 = 1.0$. TABLE II shows that during the calculation of the sixth component of the gradient $\Delta \approx 10^{-11}$ is the most appropriate choice. This is about $10^{-2}\%$ from the initial approximation $u_6 = 10^{-7}$. The results of the comparison are the following:

1) when computing the gradient of a 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 any parameter, if its value changed, the research must be carried out again;

4) to calculate the gradient of a complicated function using finite differences one must ($m = 10$) times calculate the value of the function itself.

TABLE I

$i = 3$ $u_3 = 1$ Δ	Gradient, calculated using the finite difference method	Gradient, calculated using the FAD-methodology
10^{-2}	$8.081747974402 \cdot 10^{+0}$	
10^{-3}	$8.113495177169 \cdot 10^{+0}$	
10^{-4}	$8.116668450269 \cdot 10^{+0}$	
10^{-5}	$8.116985761664 \cdot 10^{+0}$	$8.117021018694 \cdot 10^{+0}$
10^{-6}	$8.117017491927 \cdot 10^{+0}$	
10^{-7}	$8.117020646736 \cdot 10^{+0}$	
10^{-8}	$8.117020477982 \cdot 10^{+0}$	
10^{-9}	$8.117016392362 \cdot 10^{+0}$	
10^{-10}	$8.116973759797 \cdot 10^{+0}$	
10^{-11}	$8.116529670588 \cdot 10^{+0}$	
10^{-12}	$8.115286220800 \cdot 10^{+0}$	

TABLE II

$i = 6$ $u_6 = 10^{-7}$ Δ	Gradient, calculated using the finite difference method	Gradient, calculated using the FAD-methodology
10^{-6}	$9.846043659341 \cdot 10^{+5}$	
10^{-7}	$1.248772527026 \cdot 10^{+6}$	
10^{-8}	$1.284241101155 \cdot 10^{+6}$	
10^{-9}	$1.287911733860 \cdot 10^{+6}$	$1.288320939087 \cdot 10^{+6}$
10^{-10}	$1.288280750167 \cdot 10^{+6}$	
10^{-11}	$1.288324366744 \cdot 10^{+6}$	
10^{-12}	$1.288395748311 \cdot 10^{+6}$	
10^{-13}	$1.289073070510 \cdot 10^{+6}$	

In contrary to it, the Fast Automatic Differentiation enables us to calculate gradients of any complicated function with the machine accuracy for arbitrary number of parameters. The machine time that is needed to calculate the gradient does not exceed three times that of the calculation of the function itself (see [3]).

IV. CONCLUSION

The efficient algorithm to calculate gradients of the total energy of atoms' system with respect to Tersoff parameters is presented. The algorithm is based on the Fast Automatic Differentiation technique. The formulas to compute the gradients are derived. These formulas allow to compute the gradients with the machine accuracy and computation time that is needed to calculate the gradient does not exceed three times that of the calculation of the function itself. The following conclusion is made: the calculation of above-mentioned gradient using finite difference method is linked to substantial difficulties.

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