Application of the Fast Automatic Differentiation to the Computation of the Gradient of the Energy of Atoms System

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For modeling solid atomic structures the Tersoff Potential is often used. 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 [1] one possible optimization problem was considered. It consists 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. 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, [**?**]) 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 times to calculate the value of the function.

It should be noted that the above-mentioned optimization problem is solved with a determened, fixed position of atoms of the considered basic crystal structure. Solving the problem of parameters identifying in such a statemant, there is no certainty that the positions of basic atoms will correspond to the minimum of potential energy of the system. Therefore, the following step of studies is the optimization relatively coordinates of particles, which arranges particles to the positions, which correspond to the minimum of summary potential energy of the considered system of atoms. At this stage, there is a need to determine the gradient of the energy of atomssystem with respect to the coordinates of the atoms.

In this work, 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 gradients are determined with machine precision on the basis of the Fast Automatic Differentiation methodology.

References

1. K.K. Abgaryan and M.A. Posypkin, Optimization Methods as Applied to Parametric Identification of Interatomic Potentials, Comp. Math. and Math. Phys., vol.54, No. 12, pp. 1929-1935, 2014.