Keating potential minimization algorithms

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Currently, the development of new materials for optoelectronic devices used heterostructures "Ge-Si" with germanium quantum dots [1, 2]. To simulate the interactions between atoms in such hybrid materials used Keating's potential function [3], in which the relationship energy can be written as:

$$E = \sum_{i=1}^{n} \left[\frac{3}{16} \sum_{j=1}^{4} \frac{\alpha_{ij}}{d_{ij}^2} \left\{ (r_i - r_j)^2 - d_{ij}^2 \right\}^2 + \right.$$

$$+ \frac{3}{8} \sum_{j=1}^{4} \sum_{k=j+1}^{4} \frac{\beta_{ijk}}{d_{ij} \cdot d_{ik}} \left\{ (r_i - r_j) \cdot (r_i - r_k) + \right.$$

$$\left. \left. + \frac{d_{ij} \cdot d_{ik}}{3} \right\}^2 \right]$$

Here:
n - the number of atoms in lattice;
d_{ij},d_{ik}, α_{ij}, β_{ijk} - given constants;
$r_i = (x_{1i}, x_{2i}, x_{3i})$,
$r_j = (x_{1j}, x_{2j}, x_{3j})$,
$r_k = (x_{1k}, x_{2k}, x_{3k})$ - optimized variables.

Thus, Keating potential minimization problem can be reduced to the standard form:

$$f(x) \to min.$$

This minimization of potencial is necessary to simulate the properties of designed materials because it provides a steady state of a physical medium (lattice).

To solve the problems of minimizing functions developed many methods and approaches, but the high requirements to the solutions of problems of Keating potential minimization, unfortunately, not able to directly apply the known methods. The problems, which now is under consideration, have a higher dimension (at least 10^5 variables; current practical problems has about 10^6 atoms in lattice and respectively above $3 \cdot 10^6$ variables) and in addition, the solution must be obtained with an accuracy comparable to machine ε ($\approx 10^{-20}$ for double).

The paper deals with the some minimization methods, adapted to the task. These include: the method of Cauchy, conjugate gradient methods, conjugate gradient method of Nesterov [4], and a modification of Newton's method. For the conjugate gradient method has been tested 24 different modifications described in [5]. Also for conjugate gradient method was created special one-dimensional search method, based on using approximation original function of Keating potential by the fourth-degree polynomial. Newton's method is presented as a special modification, based on the using of sparse matrix technology, as a direct application of it is impossible due to physical memory limitations of modern computer systems to the size of the Hessian matrix. The proposed scheme of storing sparse matrix allows to perform minimization of the Keating potential for tasks with dimensions about 10^7 variables on modern workstations with 6 - 8 Gb RAM (full Hessian matrix for such dimensions has size above 700 Tb). For solve linear algebra task in Newton method used conjugate gradient method [6], which was modified to be be applicable in case when determinant is not positive. Unfortunately the current implementation of Newton's method is sufficiently sensitive to algorithmic parameters, and requires a rather careful adjustment to obtain the desired result. For all described methods used analytical first and second derivatives. All these methods have shown their applicability in solving problems of minimization of the potential Keating, though differ in performance (rate of convergence)

and reliability.

The implementation of the algorithms created with C language and tested on Linux OS (32- and 64-bit kernels) with different versions of GCC and ICC compilers. To increase compute speed used OpenMP [7] and CUDA [8, 9] technologies. The computational experiments carried out on SMP multiprocessor system based on Intel Xeon X5670 CPU, and Nvidia GeForce GTX580 GPU. Developed algorithms allow to solve several actual problems of minimize the Keating potential, the maximum dimension was 10535424 variables, the solution time was 43 hours.

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