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Application of GRID resource for modeling charge transfer in DNA

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Recently, at the interface of physics, chemistry and biology, a new and rapidly developing research trend has emerged concerned with charge transfer in biomacromolecules. Of special interest to researchers is the electron and hole transfer along a chain of base pairs, since the migration of radicals over a DNA molecule plays a crucial role in the processes of mutagenesis and carcinogenesis. Moreover, understanding the mechanism of charge transfer is necessary for the development of a new field, concerned with charge transfer in organic conductors and their possible application in computing technology.
To use biomolecules as conductors, one should know the rate of charge mobility. We calculate theoretical values of charge mobility on the basis of a quantum-classical model of charge transfer in various synthesized polynucleotides at varying temperature T of the environment. To take into account temperature fluctuations, a random force with specified statistical characteristics was added in the classical equations of site motion (Langevin force). (See e.g.: V.D.Lakhno, N.S.Fialko. Hole mobility in a homogeneous nucleotide chain // JETP Letters, 2003, v.78 (5), pp.336-338; V.D.Lakhno, N.S.Fialko. Bloch oscillations in a homogeneous nucleotide chain // Pisma v ZhETF, 2004, v.79 (10), pp.575-578).
As is known, the results of most biophysical experiments are averaged (for example, in our case, over a great many DNA fragments in a solution) values of macroscopic physical parameters. When modeling charge transfer in a DNA at finite temperature, calculations should be carried out for a great many realizations so that to find average values of macroscopic physical parameters. This formulation of the problem enables paralleling of the program by realizations such as “one processor –one realization”.
A sequential algorithm is used for individual realizations. Initial values of site velocities and displacements are preset randomly from the requirement of equilibrium distribution at a given temperature. In calculating individual realizations, at each step a random number with specified characteristics is generated for the Langevin term.
To make the problem of modeling of the charge transfer in a given DNA sequence at a prescribed temperature suitable to be calculated using GRID resource, the original program was divided into 2 parts.
The first program calculates one realization for given parameters. At the input it receives files with parameters and initial data. The peculiarity of the task is that we are interested in dynamics of charge transfer, so at the program output we get several dozens Mb results.
Using a special script, 100-150 copies of the program run with the same parameters and random initial data. Upon completion of the computations, the files of results are compressed and transmitted to a predefined SE.
When an appropriate number of realizations is calculated, the second program runs

once. It must calculate average values for charge probabilities, for site displacements from the equilibrium, etc.
A special script is sent to calculate this program on WN. This WN takes from SE files with results of realizations in series of 10 items. For each series the averaging program runs (at the output one gets the data averaged over 10 realizations). If the output file of a current realization is absent or defective, it is ignored, and the next output file is taken. The files obtained are processed by this averaging program again. This makes our results independent of chance failures in calculations of individual realizations.
Using GRID resource by this method, we have carried out calculations of the hole mobility at different temperatures in the range from 10 to 300 K for (GG) and (GC) polynucleotide sequences (several thousands realizations).

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