The mathematical modeling of grouping the dipole water clusters

V. SHAIDUROV ¹, Viktoriya KORNIENKO ², A. VYATKIN ¹

¹ Institute of Computational Modeling of Russian Academy of Sciences, Krasnoyarsk, Russia,

E-mail: shaidurov04@mail.ru

² Siberian Federal University, Krasnoyarsk, Russia
E-mail: vika-svetlakova@yandex.ru

Abstract: In the paper, a physical-mathematical model and a computational algorithm implementing the model are proposed to study the behavior of particles having an electric dipole moment in an external electric field. Computational experiments demonstrate the orientation dynamics of water clusters with the increase of the generated field. The dipole properties of some water clusters were previously determined using Hyperchem program.

Keywords: electric dipole, water clusters, physical-mathematical model, computational experiment, Runge-Kutta methods

2010 Mathematics Subject Classification: 93A30, 70-08

References

- [1] T. Miyake, M. Aida. H-bond patterns and structure distributions of water octamer (H₂O)₈ at finite temperatures. *Chemical Physics Letters.* **424**, 215–220 (2006).
- [2] R.P. Feynman, R.B. Leighton, M. Sands. The Feynman Lectures on Physics. Vol. 2. London, Addison-Wesley Publishing Company (1964).
- [3] Ch. Kittel. Introduction to Solid State Physics. Wiley (2004).
- [4] A. Vyatkin. Analyzing the Behavior of the Explicit Runge-Kutta Methods at the Singular point in the Two-body Problem. *Automation and Remote Control.* **74**(2), 325–330 (2013).