A few things I know about molecular simulation: a contribution to increase the 1% activity in applied maths on the subject

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Molecular simulation is a branch of theoretical and computational chemistry that makes it possible to use mathematical models for molecular structures and by clever discretizations allow to obtain the behaviour of electronic clouds and the structure of molecules.

Applications towards materials science, nanotechnologies and drug design are numerous. More than 30,000 research papers were produced in 2017, 25% of CPU time on scientific computing centers was used and, if necessary, the importance of the field has been attested by two the Nobel Prizes in Chemistry in 1998 and 2013.

It nevertheless appears that very few applied mathematicians have looked into the subject. Indeed, there are 100 times more MathSciNet publications that deal with fluid dynamics than with molecular simulation.

In this talk I will present some key problems of the field with achievements, intrinsically interesting and which also interest the world of computational chemistry both on ab initio simulation and molecular dynamic simulations. I think it is the right time to invest this inexhaustible source of exciting problems ….

For an introduction to the subject we can watch the videos
https://www.youtube.com/channel/UCoj8rmlGqm0q-Gq-ujPFUgA/videos

or consult the review
Cances, E., Defranceschi, M., Kutzelnigg, W., Le Bris, C., & Maday, Y. (2003). Computational quantum chemistry: a primer. *Handbook of numerical analysis*, *10*, 3-270.