SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems

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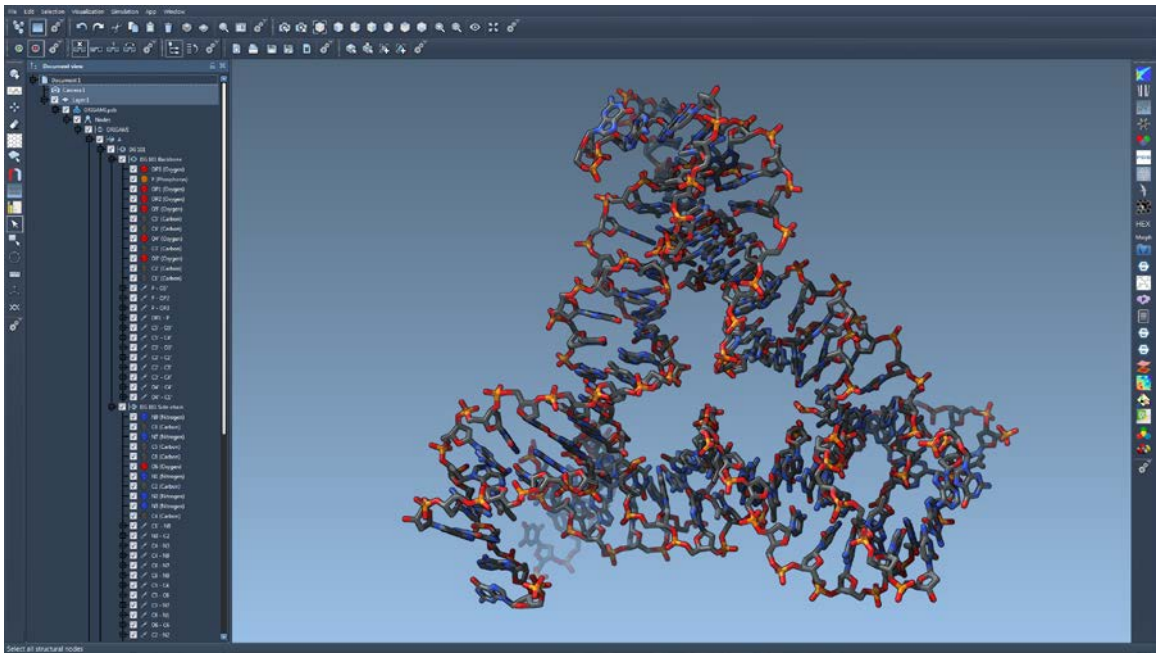
SAMSON is a software platform for computational nanoscience that can be downloaded from SAMSON Connect at https://www.samson-connect.net.

SAMSON integrates modeling and simulation to aid in the analysis and design of molecular systems. For example, as-rigid-as-possible algorithms make it easy to produce large-scale deformations of DNA strands and protein structures. Force fields and minimization algorithms help users produce realistic models, and interactive simulations help users precisely control the shapes they want to produce. Furthermore, adaptive simulation algorithms make it easy to focus calculations on the most relevant part to increase performance [1-6].

Most important, a Software Development Kit allows developers to extend SAMSON's functionality by developing SAMSON Elements (modules for SAMSON), including e.g. new interaction models, editors, apps, wrappers or interfaces to existing software, connectors to web services, etc. SAMSON Connect is open for developers and users to share SAMSON Elements.

We will present SAMSON and its general design principles, as well as specific applications to structural biology and materials science.



[1] S. Artemova and S. Redon, Physical Review Letters, 109:19, 2012
[2] M. Bosson et al, Journal of Computational Physics, 231:6, 2012
[3] M. Bosson et al, Journal of Computational Chemistry, 34:6, 2013
[4] K. K. Singh and S. Redon, Modelling and Simulation in Materials Science and Engineering, 2017
[5] S. Edorh and S. Redon, Journal of Computational Chemistry, 2018
[6] K. K. Singh and S. Redon, Journal of Computational Chemistry, 39:8, 2018