Innovative ideas in Life Sciences

MDStudio: Molecular Dynamics workflows made easy

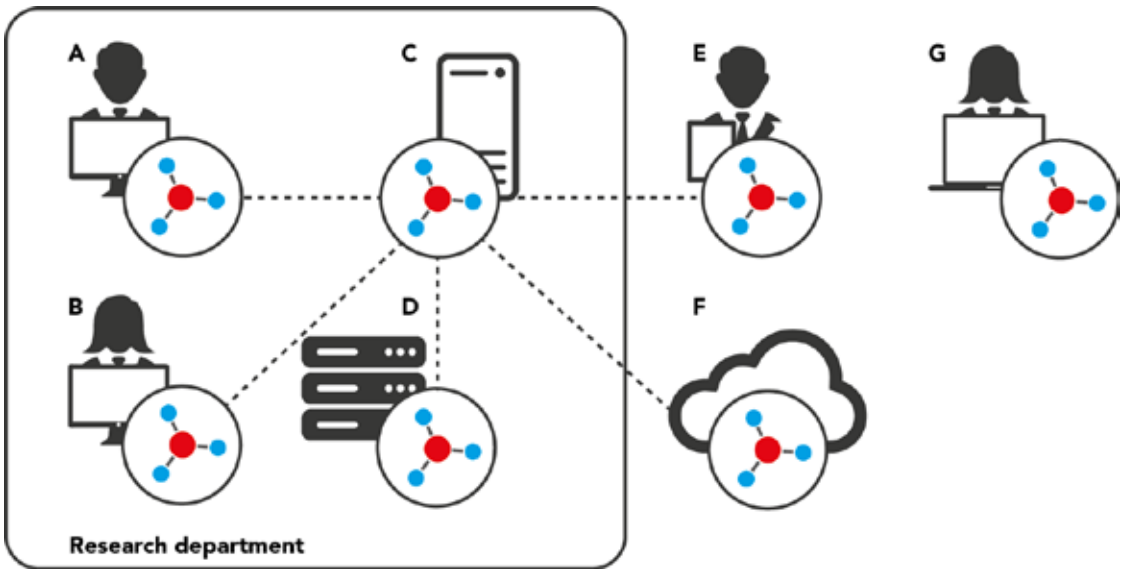
Molecular Dynamics (MD) simulations can directly aid to drug design and development, bioengineering, understanding drug resistance, or other (bio)molecular-oriented R&D.

To fill the current gap that prevents wide-spread application of MD-based methods in applied settings we have launched the MDStudio software initiative with three main ideas in mind:

(i) developing a software platform to let the user focus on science, not IT
(ii) integration of MD-based workflows
(iii) involving the community.

With MDStudio we will directly contribute to the straightforward application of MD-based methods in drug design and research. Furthermore, we envision that our platform will function as a catalyst for the further development and use of state-of-the-art MD methods in academia and industry.

MDStudio development is coordinated by Daan Geerke (PI) and Marc van Dijk (senior scientist), on the right- and leftbackcorners of the enclosed picture, which shows the Geerke group (together with collaborator Bill Swope, IBM Research).



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