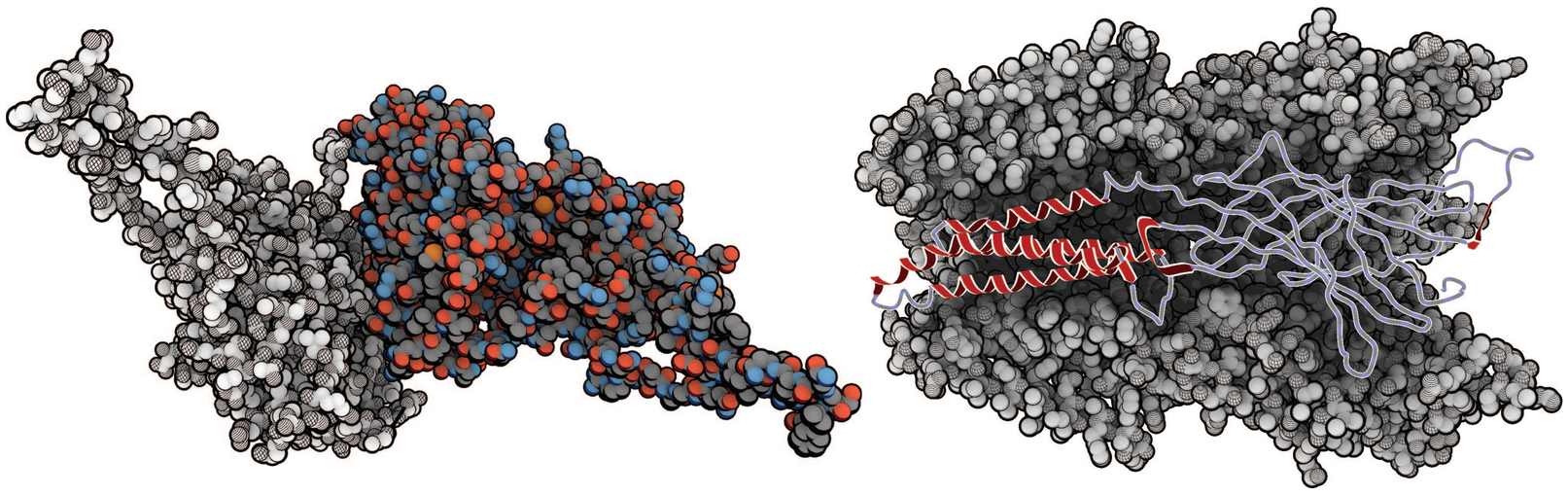
Spatially Continuous Change of Abstraction in Molecular Visualization

Wouter Lueks[1] Ivan Viola[2] Matthew van der Zwan[1] Henk Bekker[1] Tobias Isenberg[1,3]

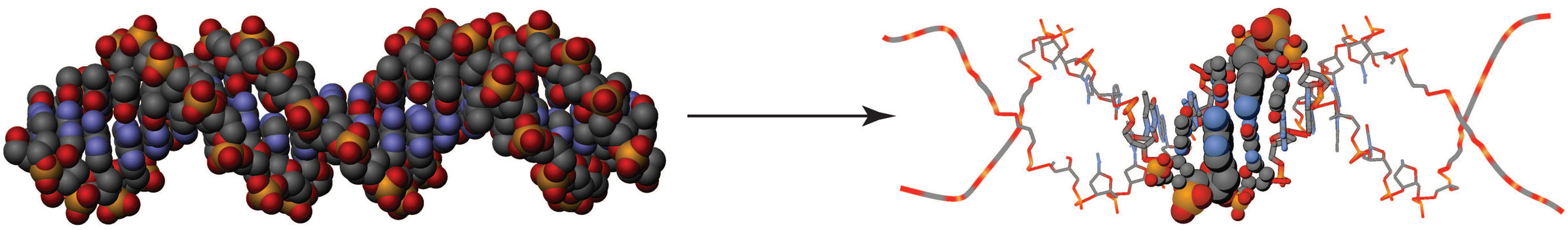
[1] University of Groningen [2] University of Bergen [3] DIGITEO/CNRS/INRIA

Starting Point: Temporally Seamless Abstraction of Molecular Models [1]

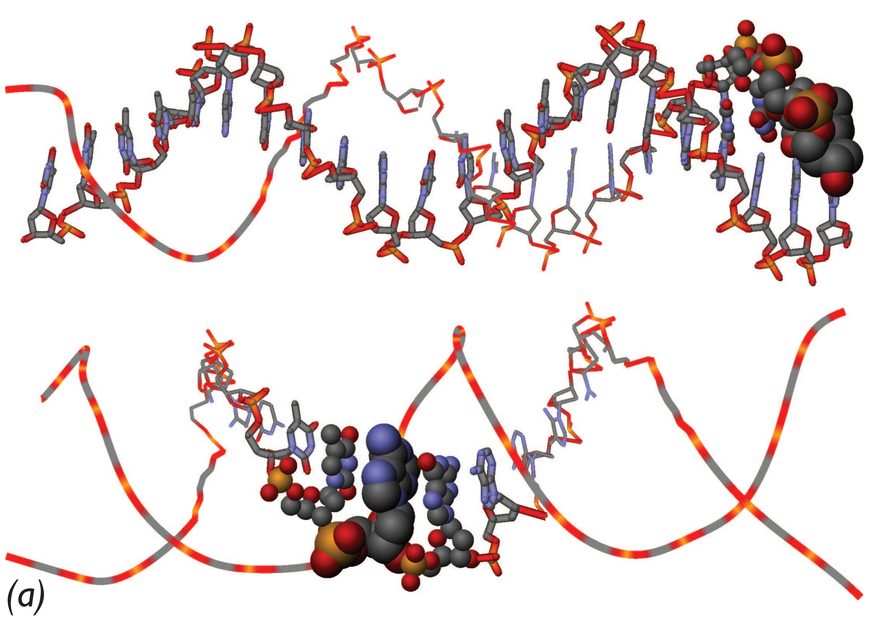


Problem: The abstraction in our original approach [1] can only be controlled interactively per strand or for the molecule as a whole. This means that the structural abstraction or the 'illustrativeness' cannot be changed depending on the location within the molecule. Thus, different levels of abstraction could not be used at the same time, resulting in a need for an improved molecular abstraction technique.

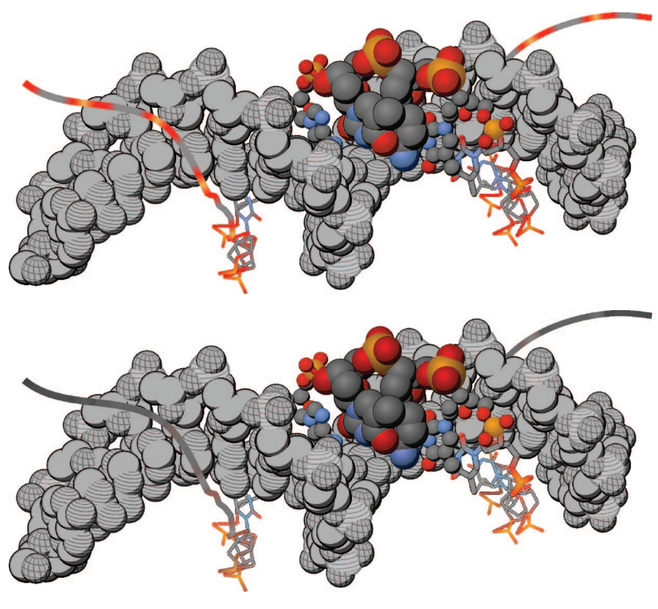
Solution: Spatially Continuous and Explicit Control of Abstraction

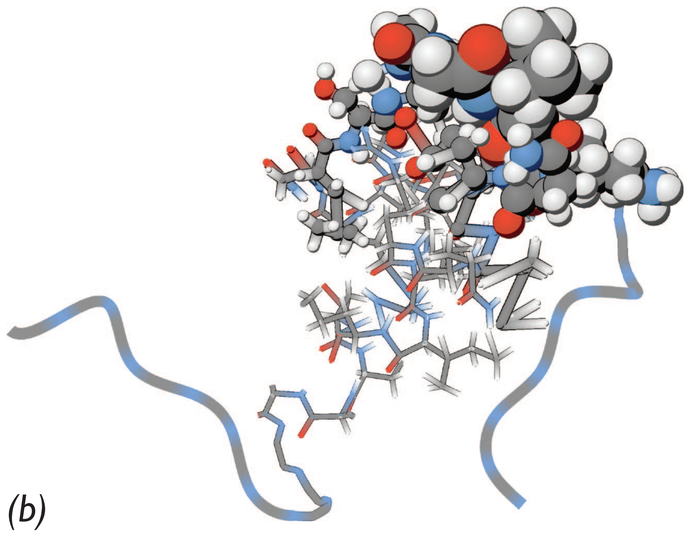


Application: Local Emphasis & Detail for Molecular Structures

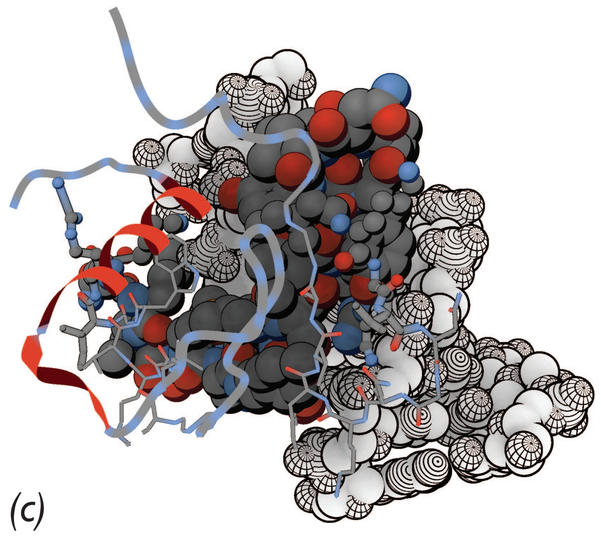


(a)





(b)



(c)

(a) *DNA:* Local abstraction is well suited for structures like DNA. DNA has a repetitive linear character so detail in one part of the visualization is representative for the remainder of the data. Both *structural abstraction* and *'illustrativeness'* can be specified locally; abstraction through support of spatial perception has a global character and is, thus, not changed.

(b) *Protein backbones:* Other elongated structures such as protein backbones can also benefit from spatially continuous change of abstraction in a similar way as DNA.

(c) *Interactions between proteins:* The local emphasis can support the visualization of interactions between two molecules—by letting the viewer look through one of the interacting molecules (being abstracted to a high degree) as well as by emphasizing the interaction through different degrees of 'illustrativeness.'

[1] Matthew van der Zwan, Wouter Lueks, Henk Bekker, and Tobias Isenberg. *Illustrative Molecular Visualization with Continuous Abstraction.* Computer Graphics Forum, 30(3):683–690, May 2011. doi> 10.1111/j.1467-8659.2011.01917.x

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Contact:
Tobias Isenberg
isenberg@cs.rug.nl
http://www.cs.rug.nl/~isenberg/