

*12 March 2019*

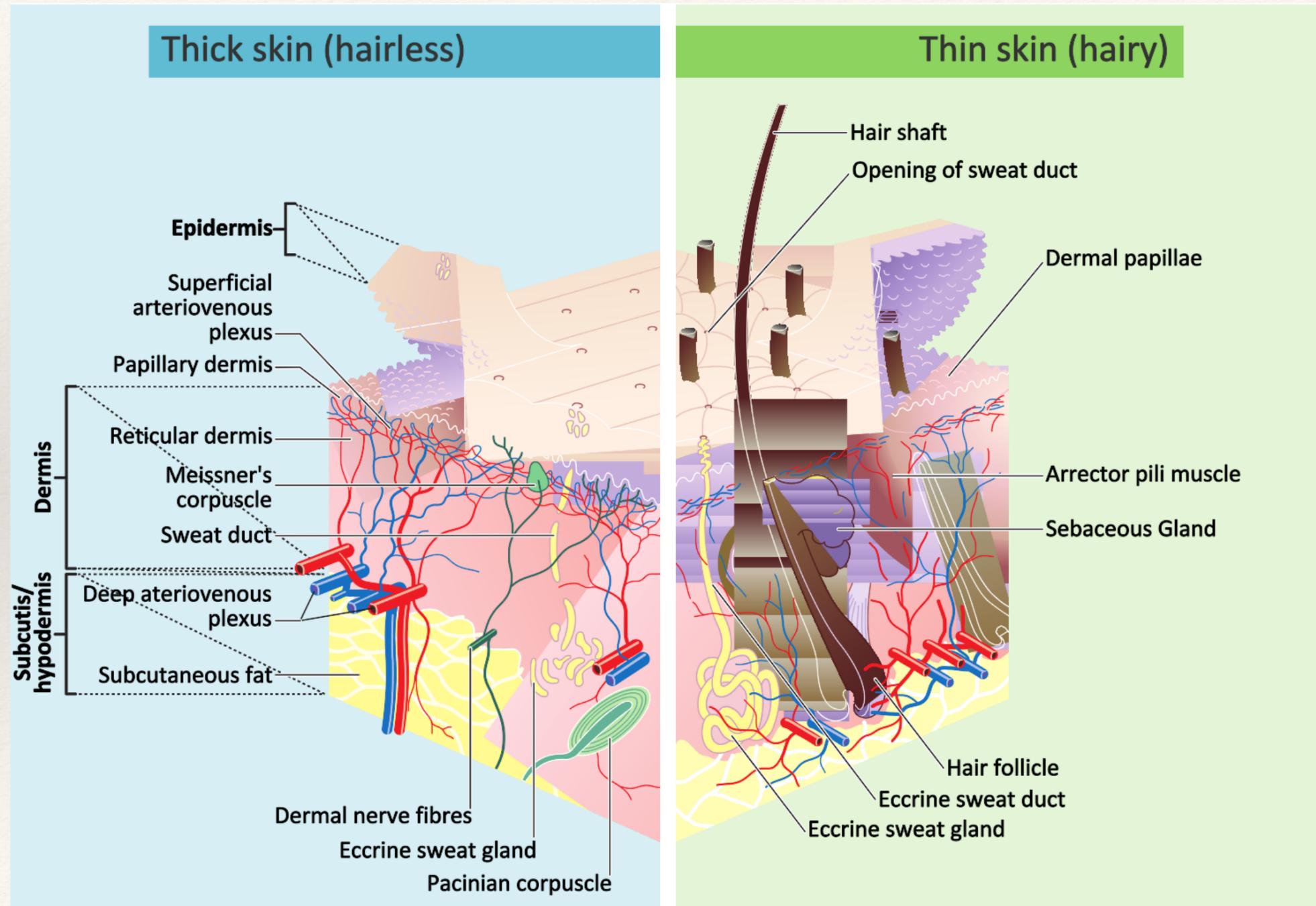
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**Skin Simulations**  
**Challenges for High Performance**  
**Computing**

by  
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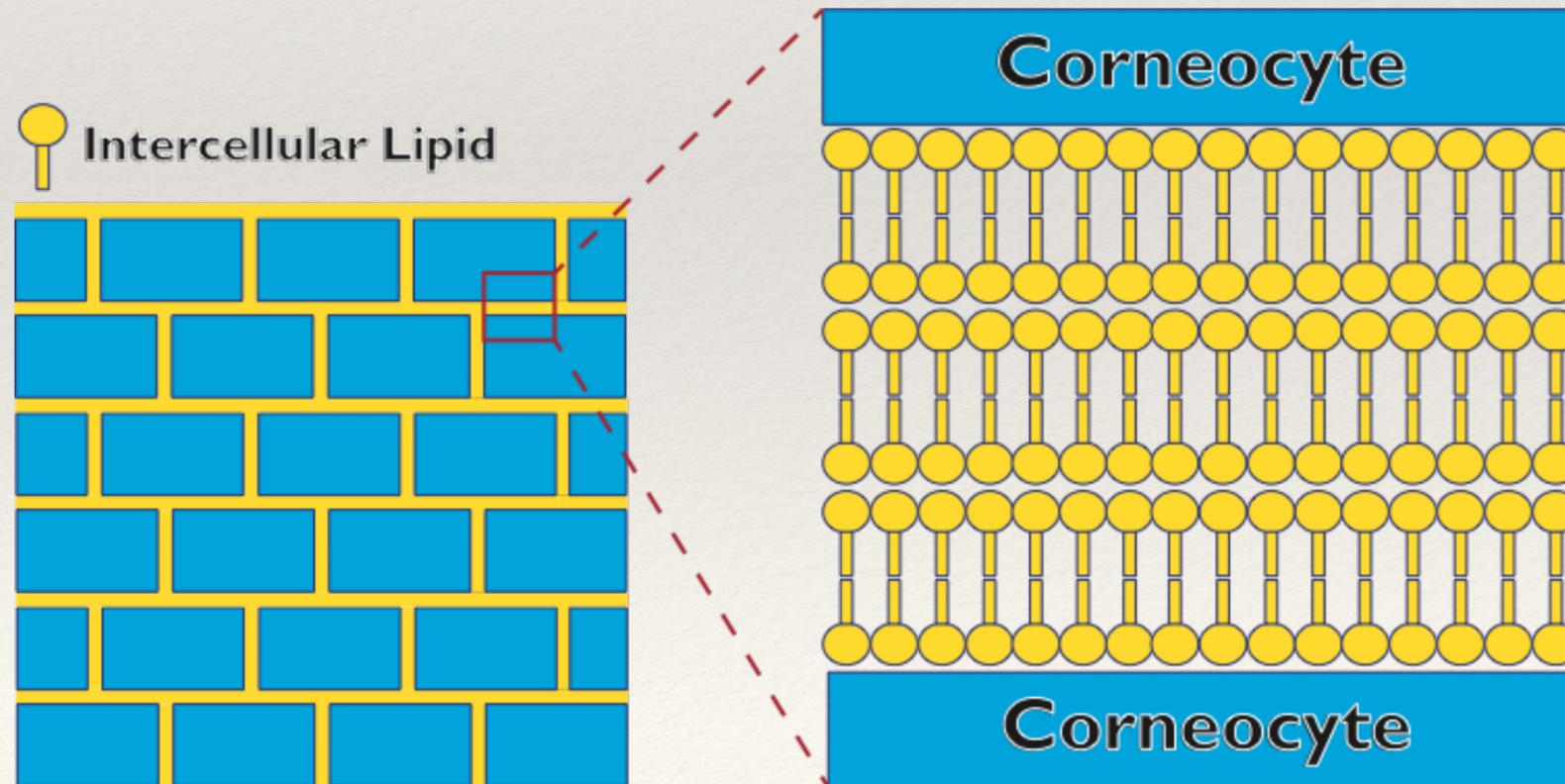
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# Skin



# Skin

Skin is crucial in maintaining the homeostasis of the organism. A healthy skin is a barrier that is difficult to breach unless the integrity of the stratum corneum is compromised.



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# Simulations vs. Experiments

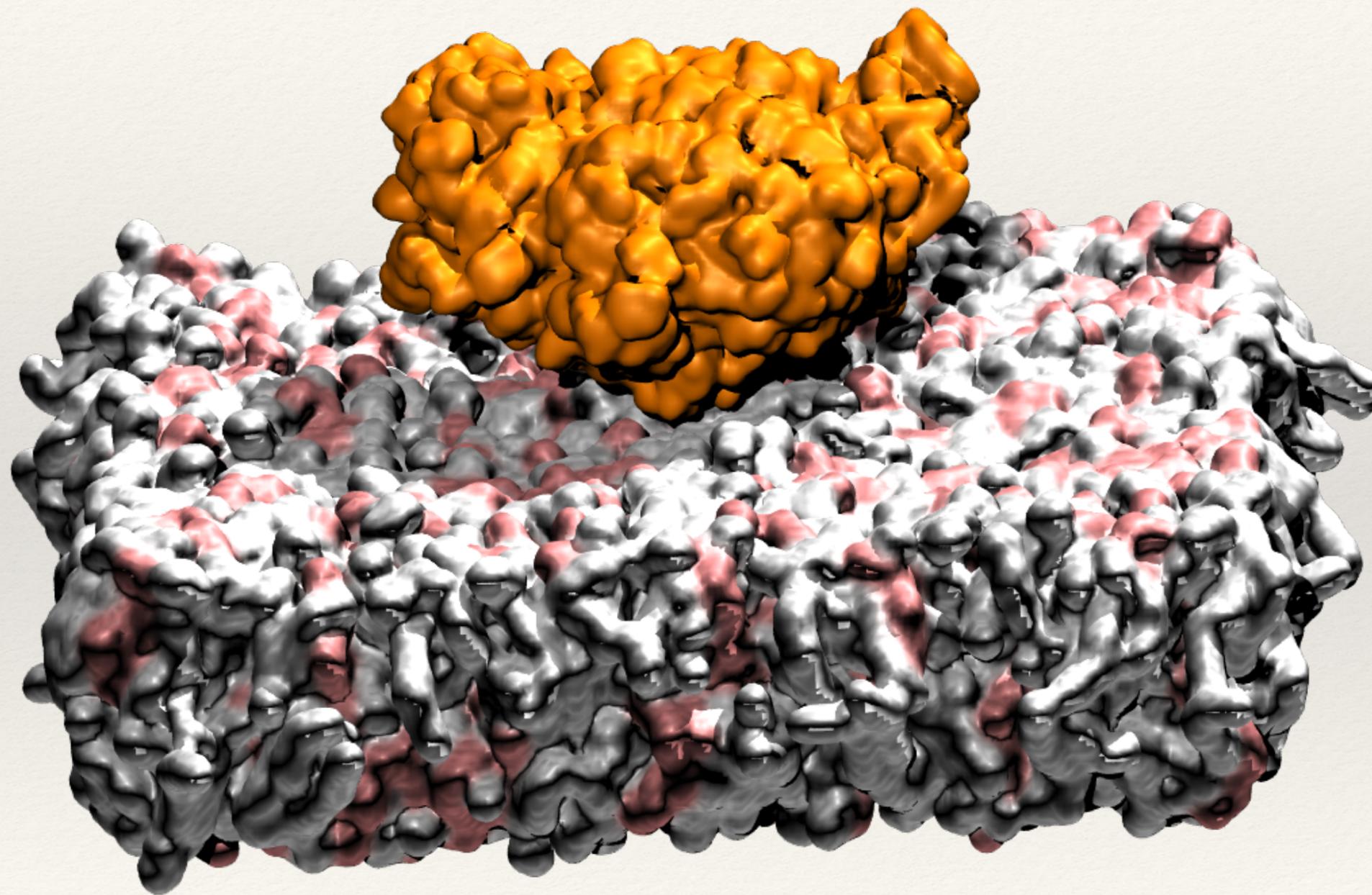
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Molecular dynamics can meaningfully complement experimental data because they allow for fine control and tuning of the “experiment”.

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# Molecular Dynamics

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# Molecular Dynamics

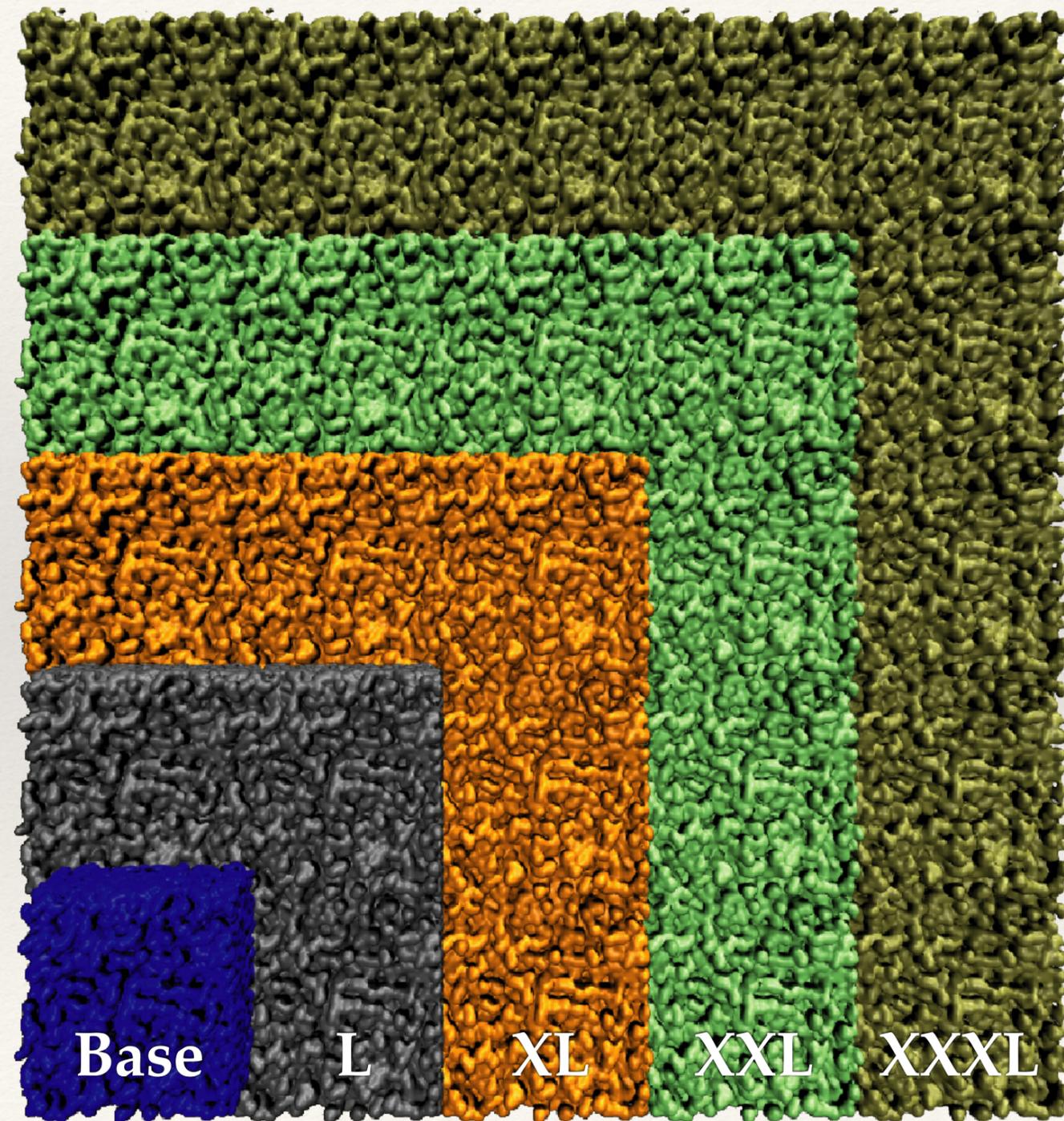
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A set of parameters describing bonded and non-bonded interactions is used to solve Newtonian equations of motion.

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# Thinking Big

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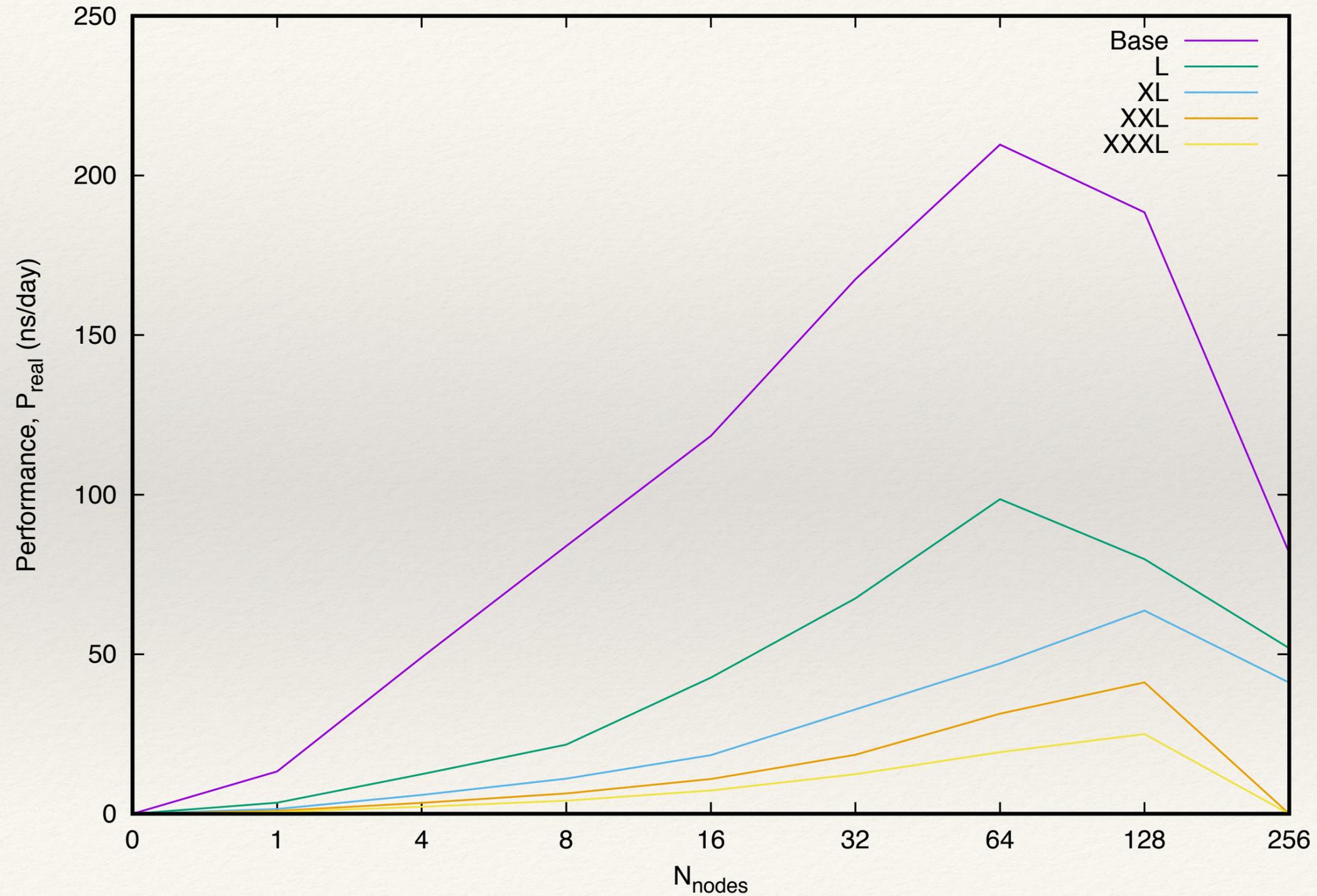
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# Importance of Benchmarks

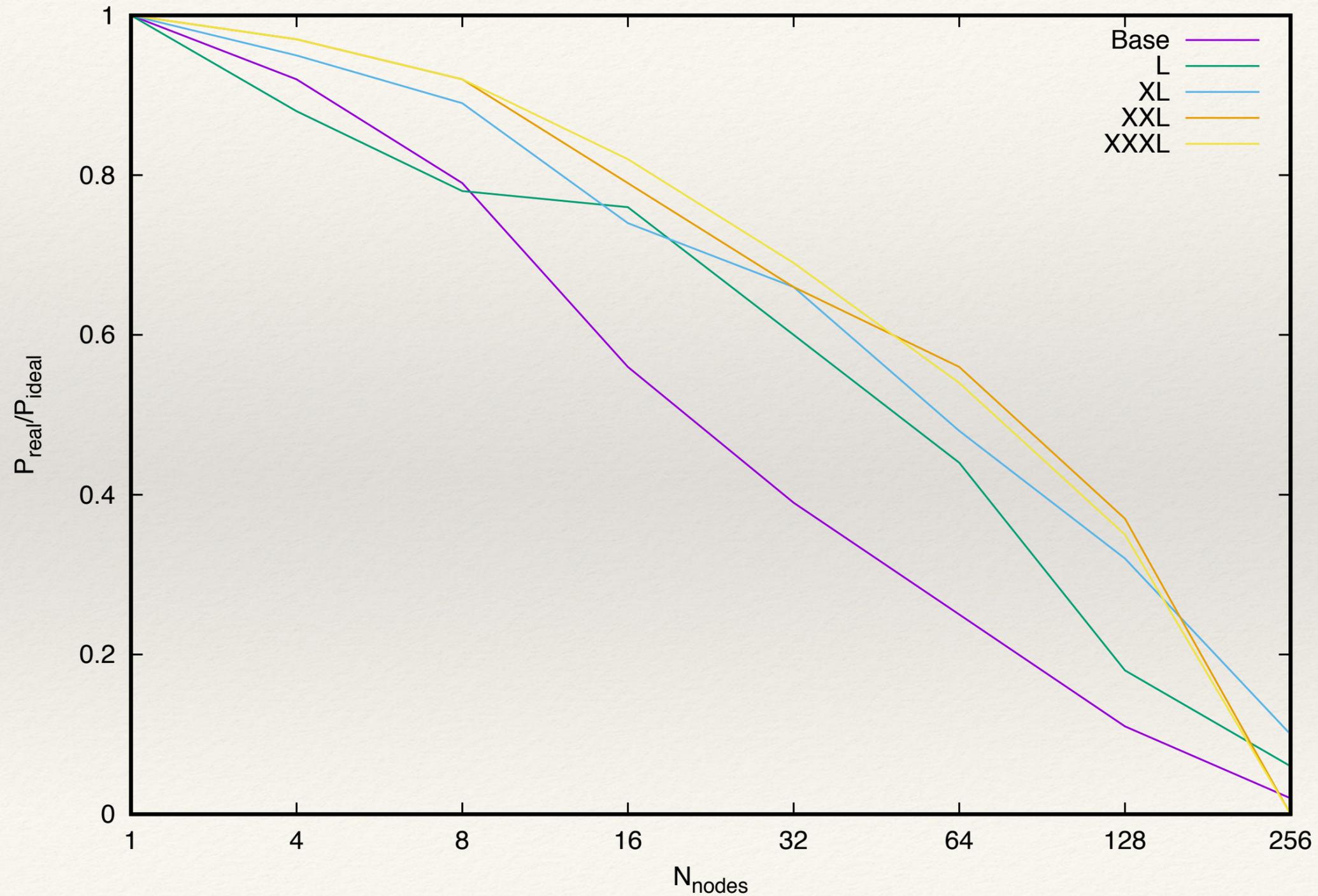
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More Nodes == More Performance

# Importance of Benchmarks



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# Importance of Benchmarks

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Depends.

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# Conclusion

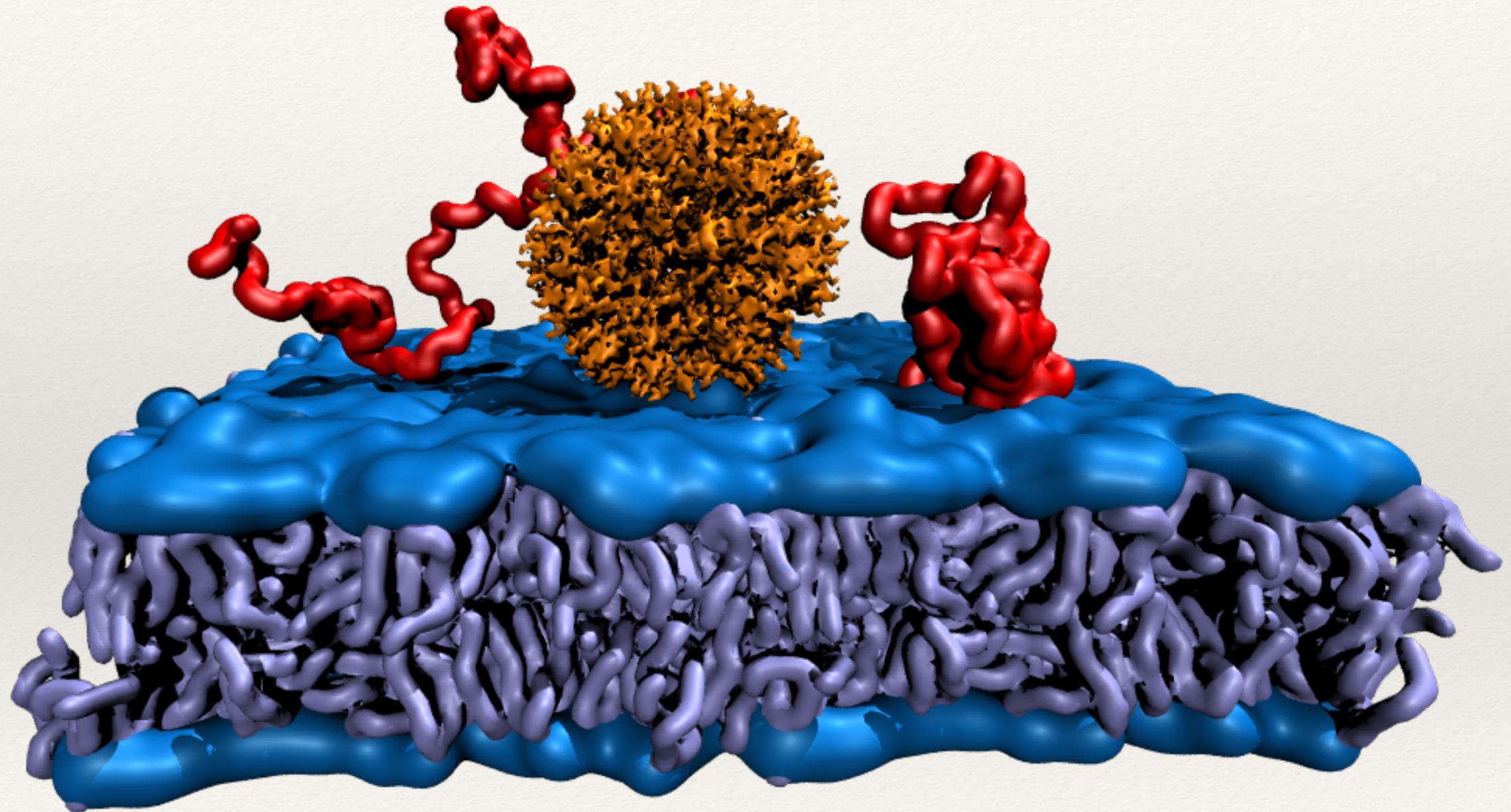
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- to simulate really big systems benchmarks are necessary
- more nodes may not lead to better performance

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# Big Picture

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# Acknowledgements

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