Biosystems

Presented by

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Biosciences Division

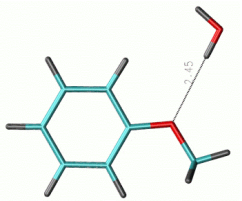
Simulation model of lignocellulose

1 nm

Length-scale

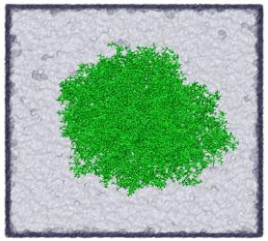
1 µm

Atomic*

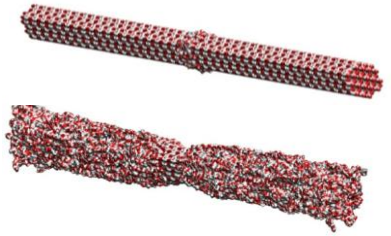


Model compounds:
force field of lignin

Molecular†

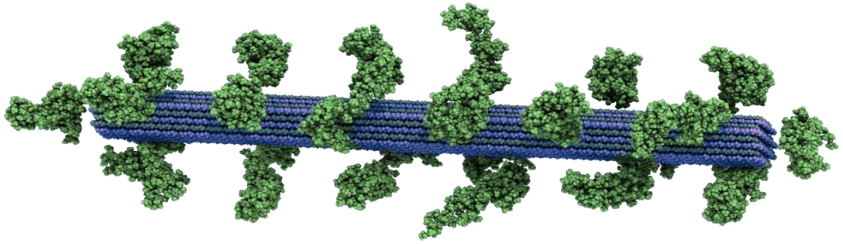


Lignin



Cellulose

Supramolecular‡



Lignin and cellulose

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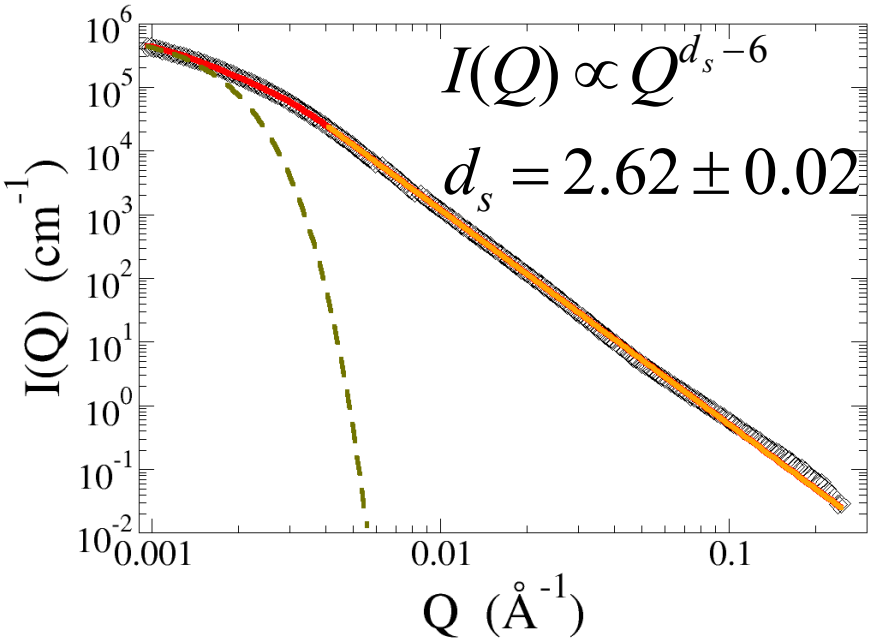
* L. Petridis and J. C. Smith (2009), "A molecular mechanics force field for lignin," *Journal of Computational Chemistry* **30** 457−467

† L. Petridis, J. Xu, M. F. Crowley, J. C. Smith, X. Cheng (in print), "Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes," in *Computational Modeling in Lignocellulosic Biofuel Production* (eds.: M. R. Nimlos, M. F. Crowley), ACS

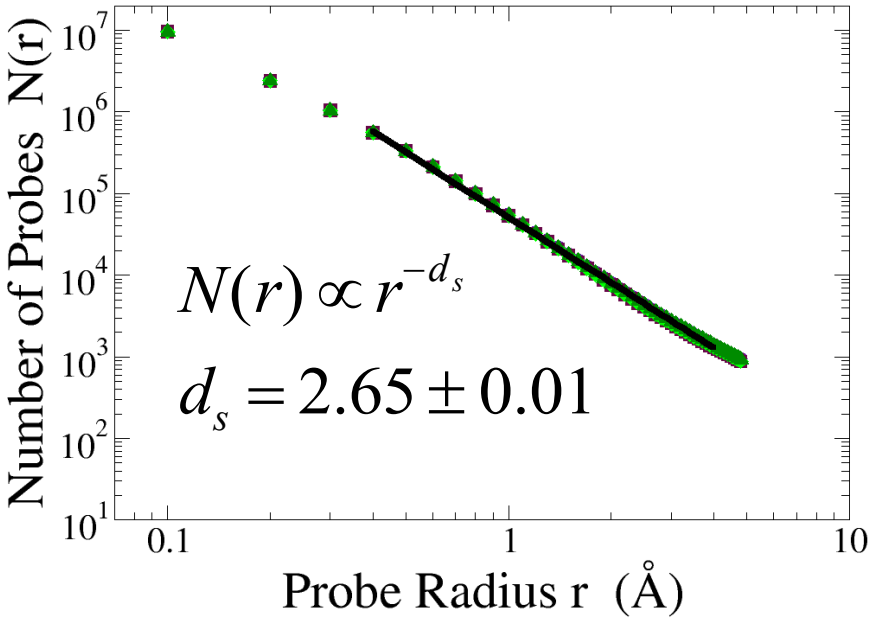
‡ R. Shulz, B. Lindner, L. Petridis, J. C. Smith (in print), "Scaling of Multimillion-Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer," *Journal of Chemical Theory and Computation*, DOI: 10.1021/ct900292r

Comparison of small angle neutron scattering (SANS) and MD simulation

Experimental SANS



Molecular Dynamics



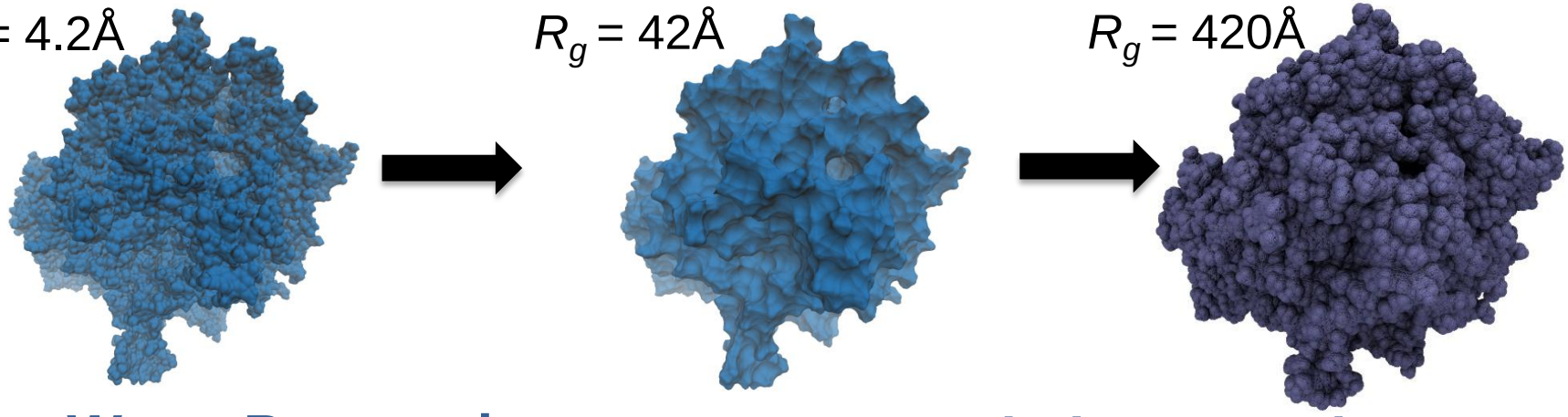
L. Petridis, S.V. Pingali, V. Urban, W. Heller, H.M. O'Neil, M. Foston, A. Ragauskas, J.C. Smith, "Self-Similar Multiscale Structure of Lignin Revealed by Neutron Scattering and Molecular Dynamics Simulation", submitted for publication

Shape of surface invariant under change of scale

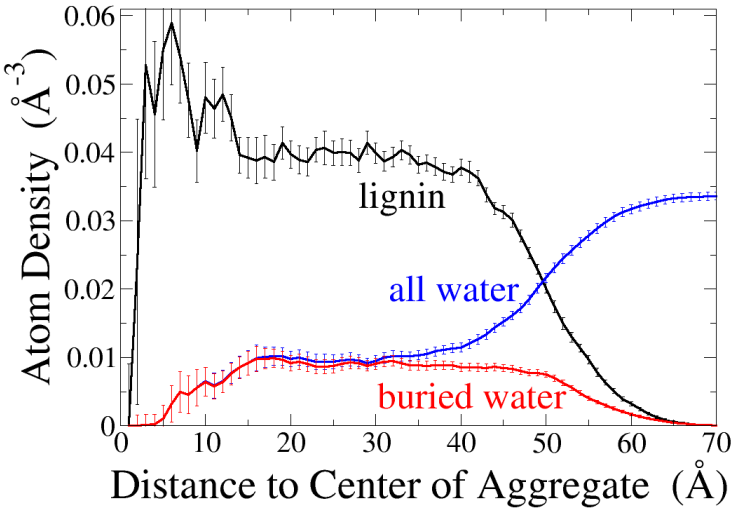
MD:
R_g = 4.2Å

MD&SANS:
R_g = 42Å

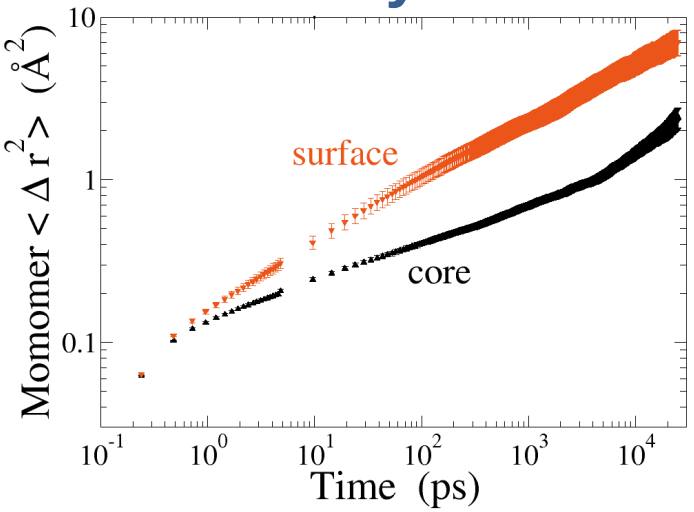
SANS:
R_g = 420Å



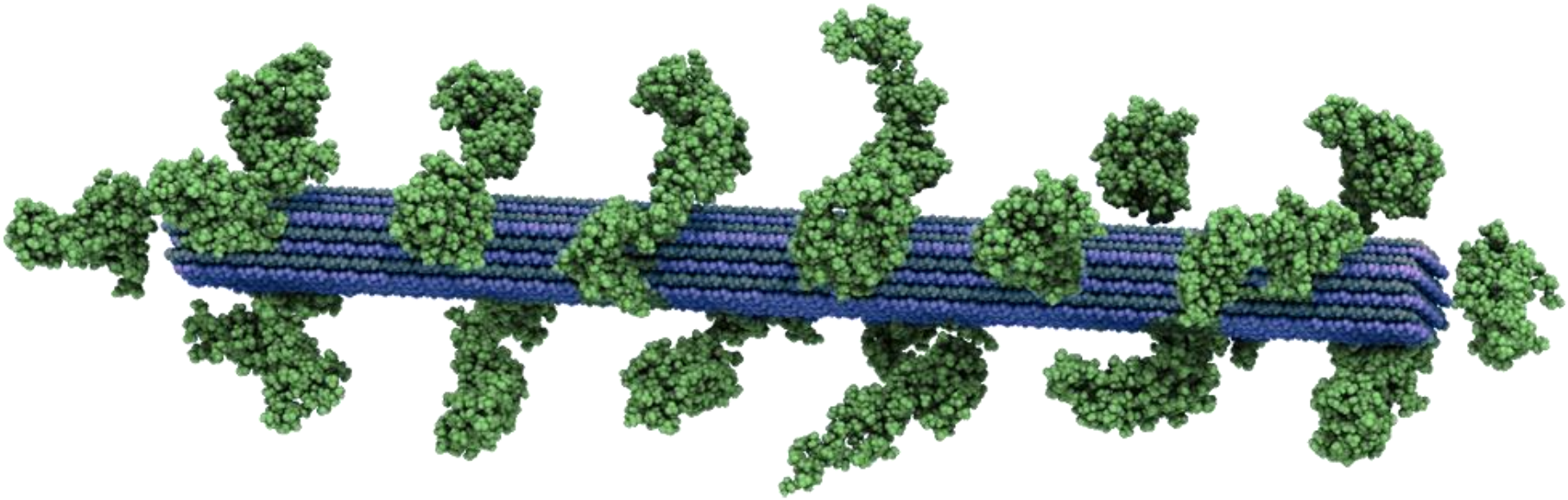
Water Penetration



Chain Dynamics



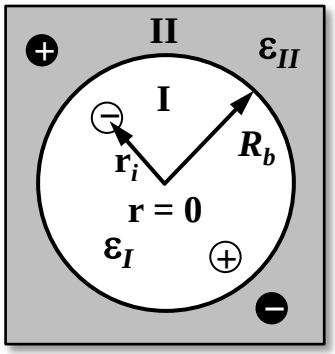
Simulation of cellulose-lignin system



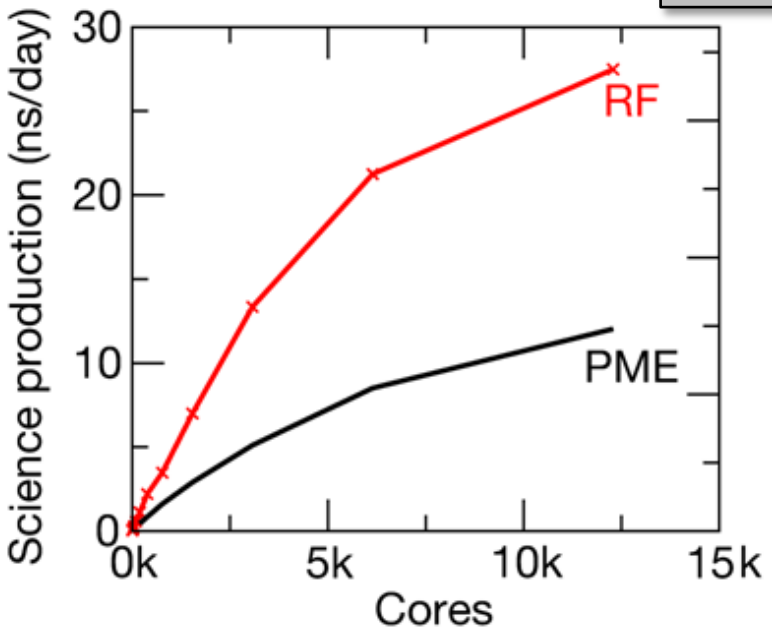
- Cellulose (blue)
- Lignin molecules (green)
  chemical composition: NREL and GATech
- Water (not shown)

Scalable code development

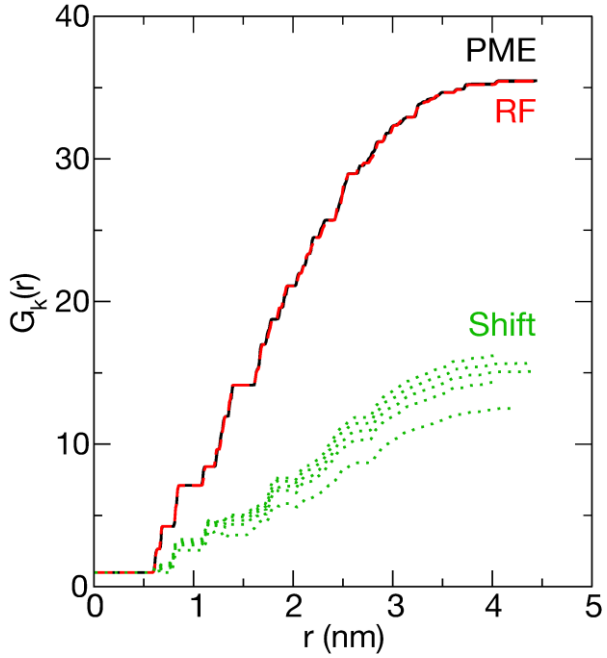
Reaction field (RF) for electrostatics calculations



Compare RF and commonly used PME method for 3.3M atom lignocellulose



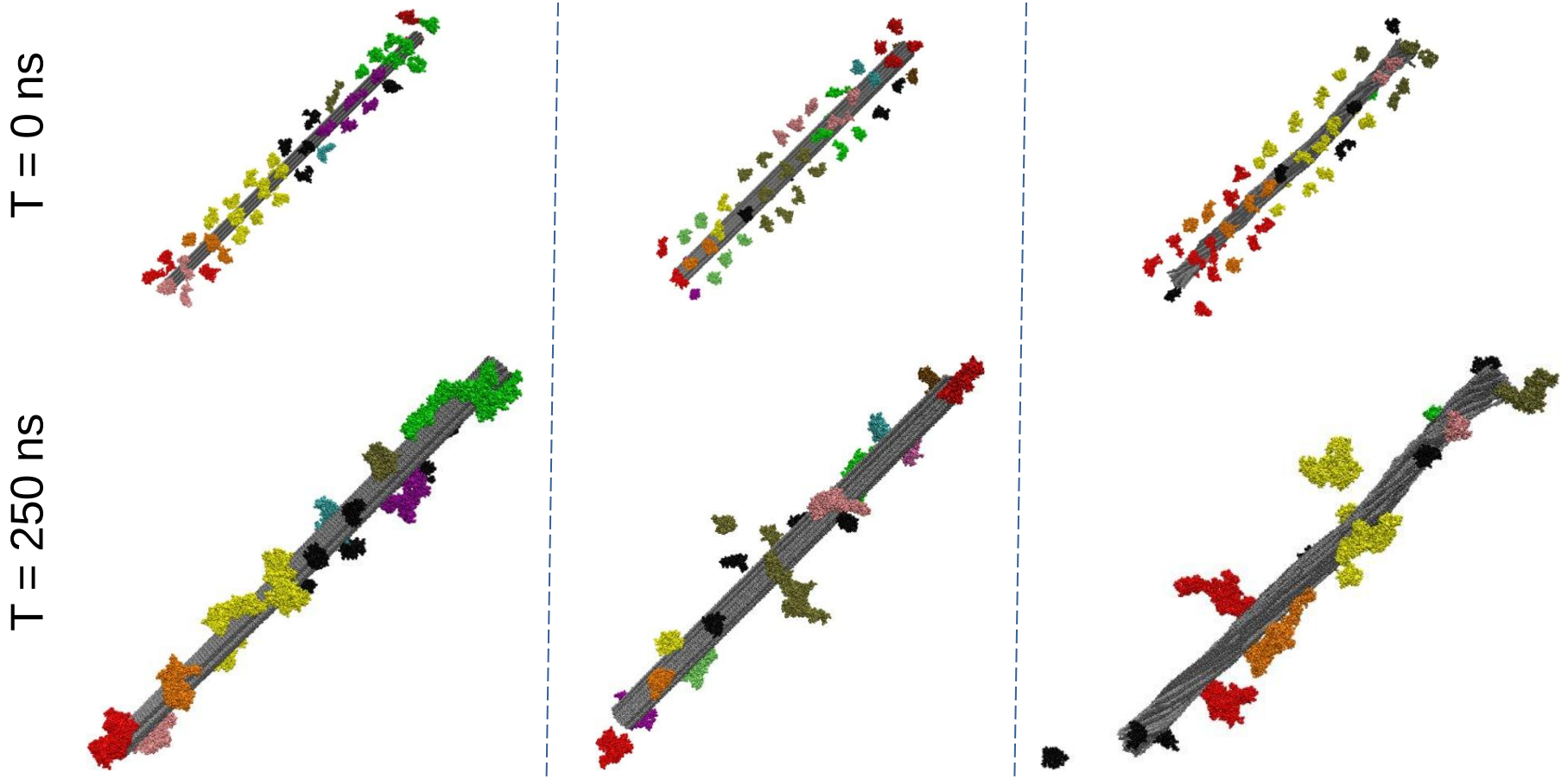
Improved scaling



Same accuracy: Cellulose dipole correlations

‡ R. Shulz, B. Lindner, L. Petridis, J. C. Smith (2009), *J. Chem. Theory Comput.*, DOI: 10.1021/ct900292r

Lignin aggregation and precipitation onto cellulose



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