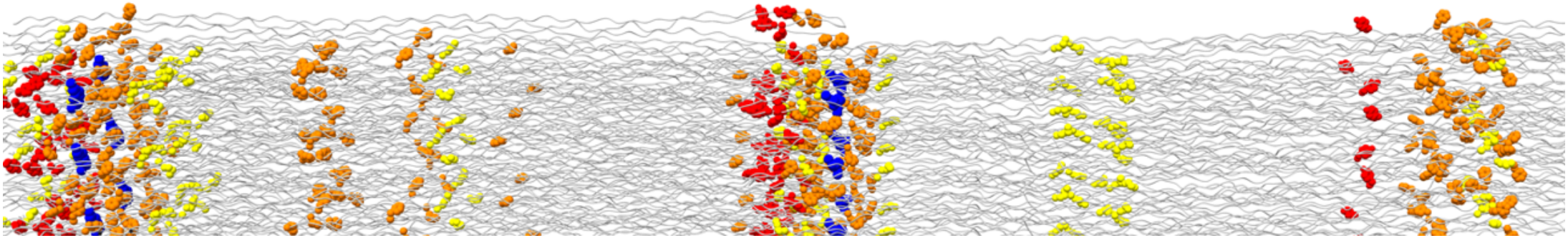
Heidelberg Institute for Theoretical Studies

HITS

IWR Interdisciplinary Center for Scientific Computing

HPC for biomaterials: Why does it hurt to play soccer (and baseball)?

Frauke [フラウケ] Gräter, 02/2019

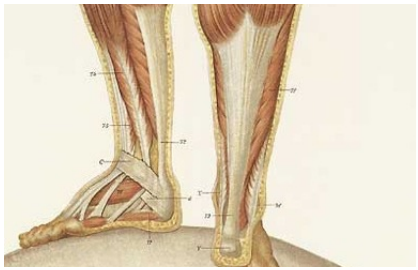



UEFA
RIONS

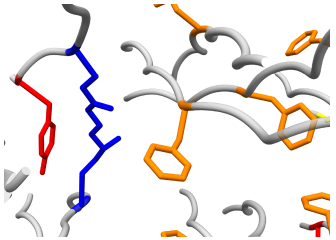

LG G3

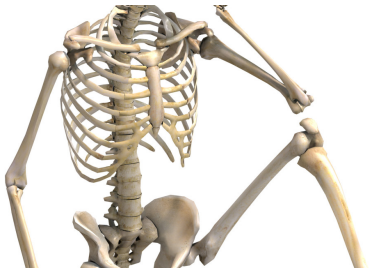
MOLECULAR (bio)mechanics – why?

≈

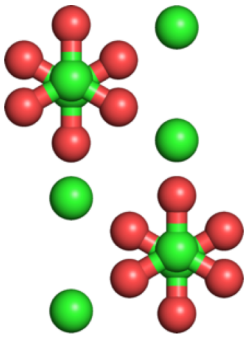


collagen





mineralized tissue



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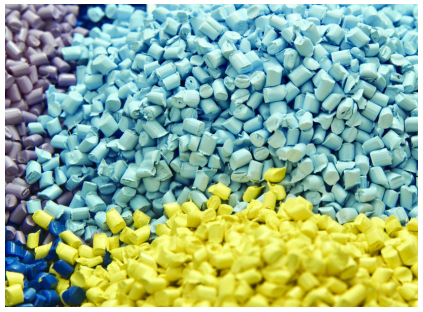
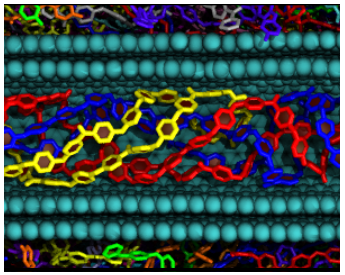


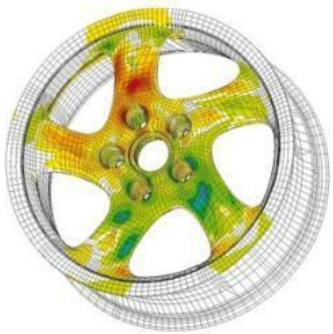
polymer



Strain and fracture: force distribution

conventional design tools:
force distribution

in constructions, cars ...



macroscopic structures:
meters

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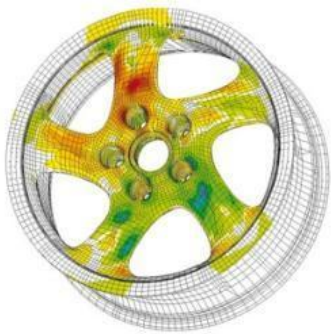
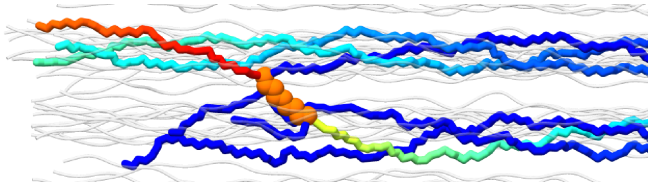


macroscopic structures:
meters

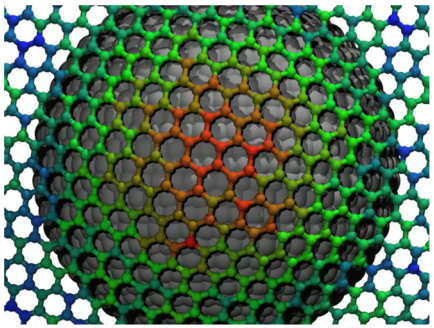
new:
force distribution in (bio)molecules

e.g. in collagen



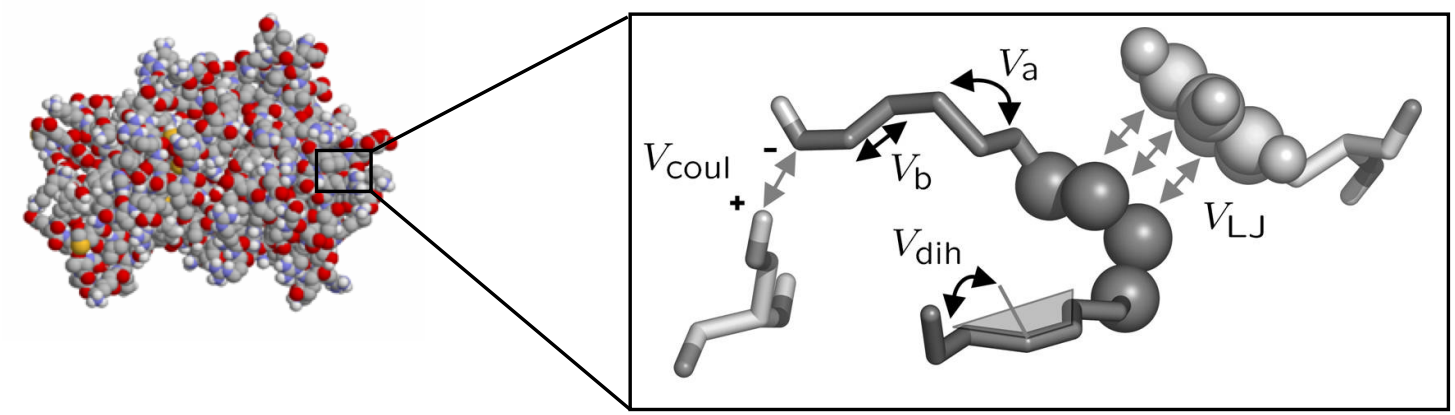
microscopic structures:
~ 10^{-9} meters

in graphene



W. Stacklies, et al, PLoS Comp Biol, 2009
Costescu et al, BMC Biophys, 2012

Forces from classical Molecular Dynamics

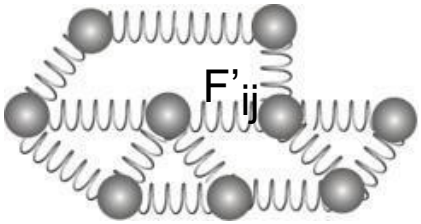


$$
\begin{aligned}
E \;=\; & \sum_{bonds} \frac{k_i}{2}(l_i - l_{i,0})^2 \\
& + \sum_{angles} \frac{k_i}{2}(\Theta_i - \Theta_{i,0})^2 \\
& + \sum_{torsions} \frac{V_n}{2}(1 + cos(n\omega - \gamma)) \\
& + \sum_{i=1}^{N} \sum_{j=i+1}^{N} (4\epsilon_{ij}((\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}) + (\frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}))
\end{aligned}
$$

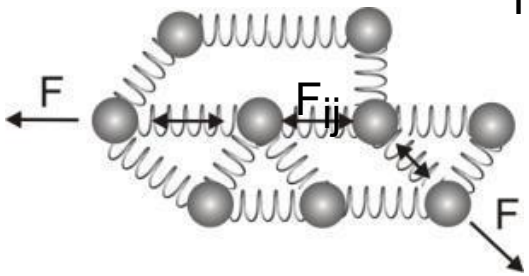
bonded interactions

non-bonded interactions

Forces from classical Molecular Dynamics



F'_{ij} force between atom i and j in relaxed state

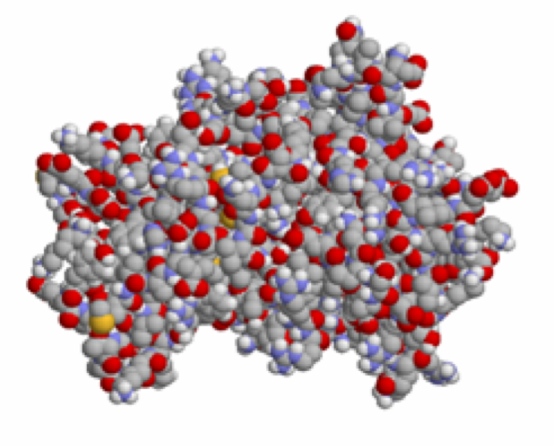


F_{ij} force between atom i and j in stretched state

change in pairwise forces

$$\Delta F_{ij} = F_{ij} - F'_{ij}$$

Proteins: a jiggling and wiggling (Feynman)



Mean velocity:

$$\hat{v} = \sqrt{\frac{2RT}{M}}$$

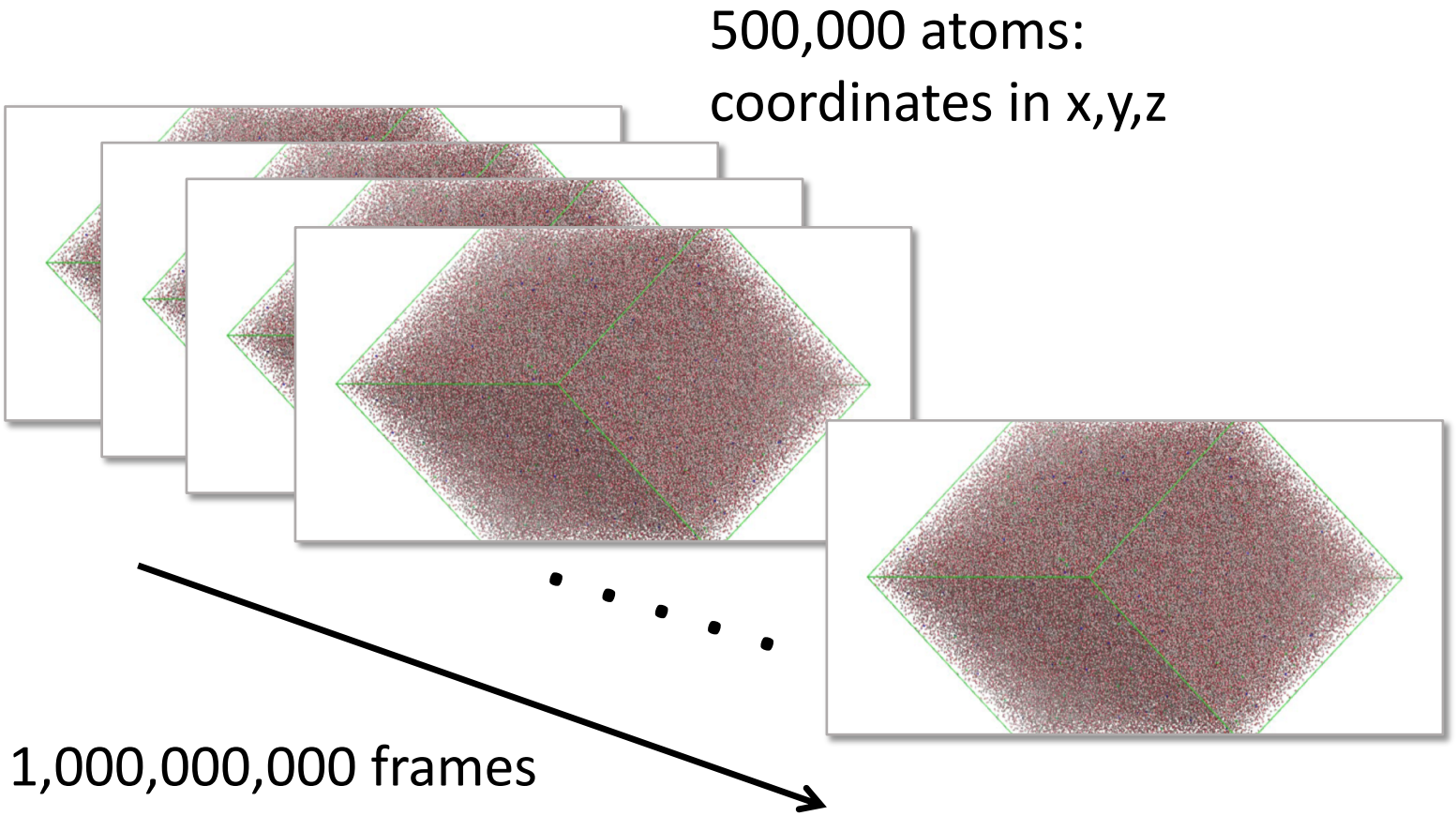
R: gas constant

T: temperature

M: molar mass

-> roughly 100-1000 m/s

Molecular Dynamics



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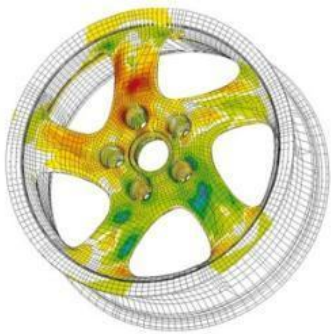

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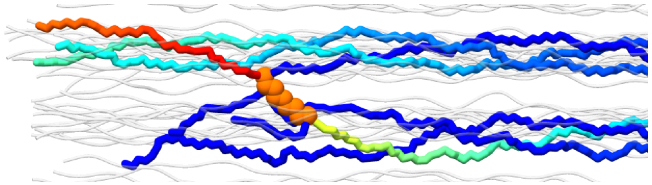

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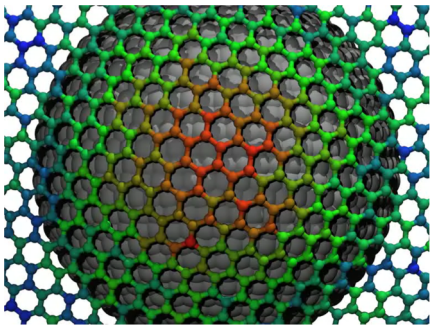

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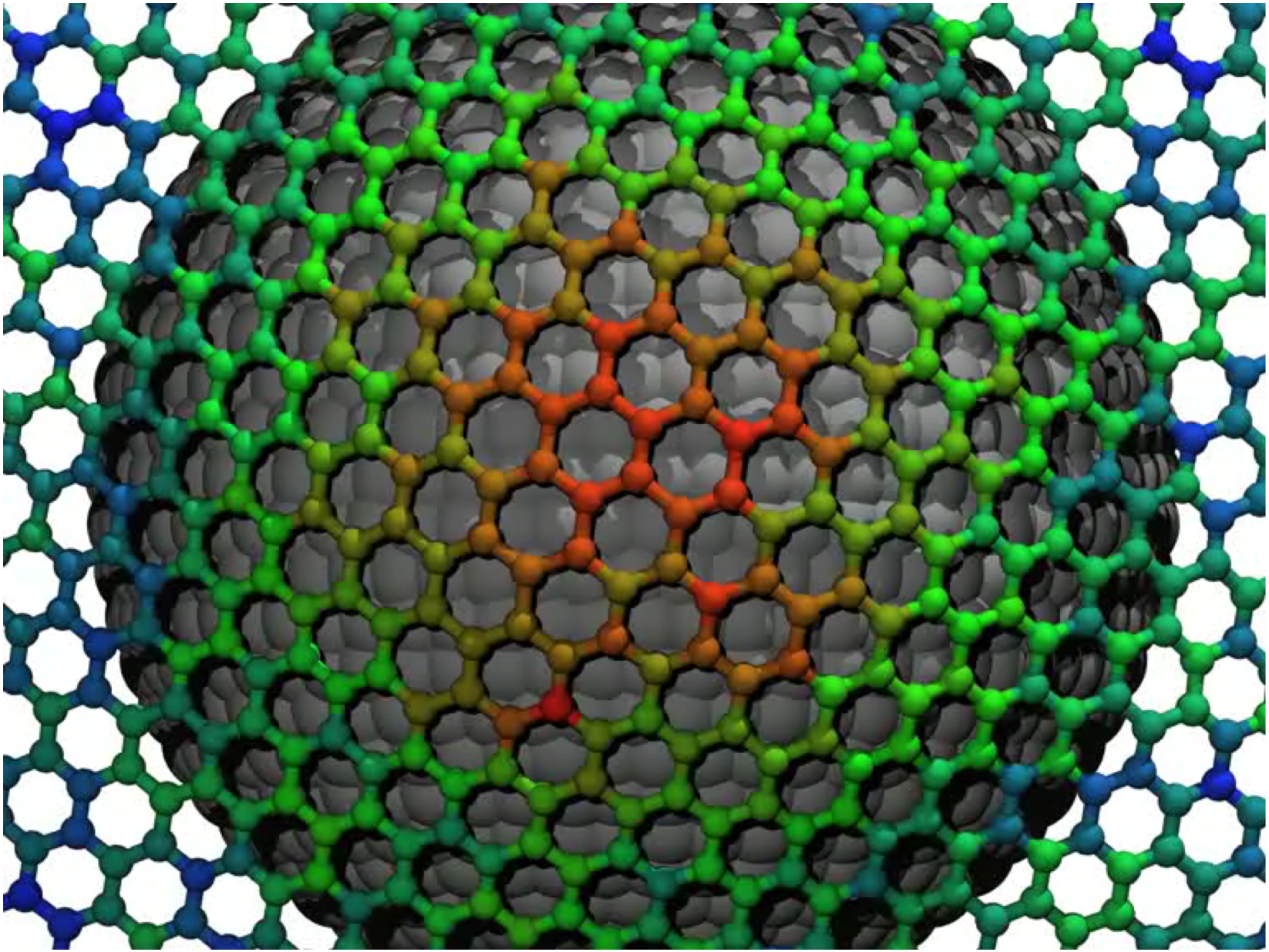
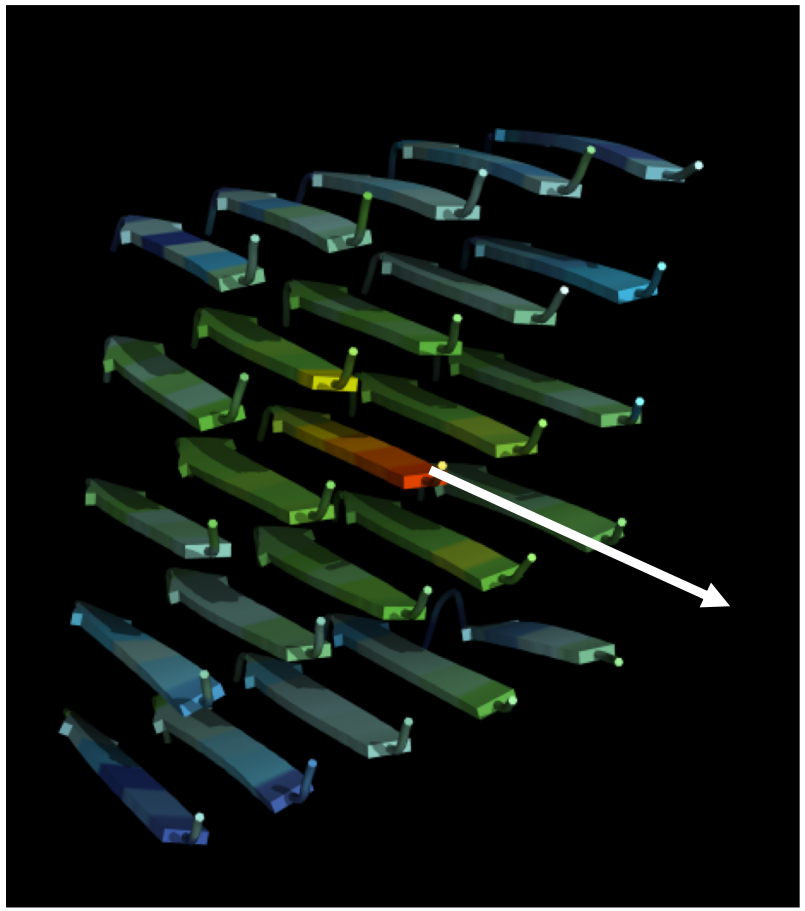
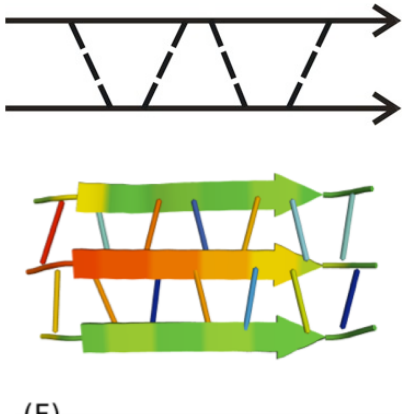
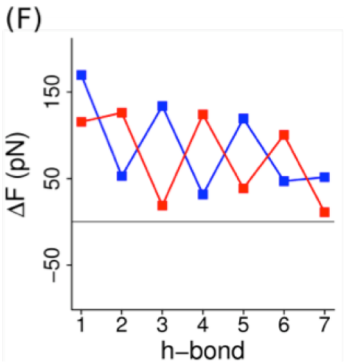


Mechanics of silk fibers

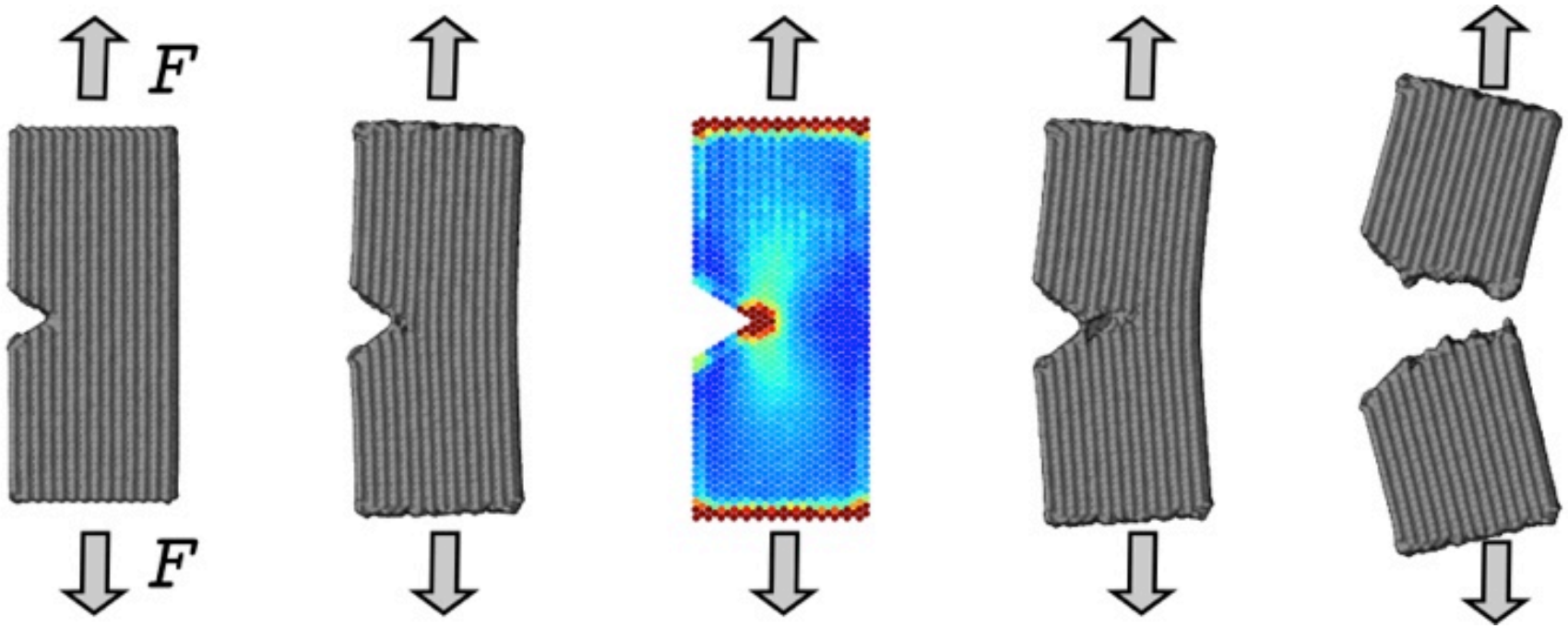


zigzag pattern of
hydrogen bonds
crucial for stabilization

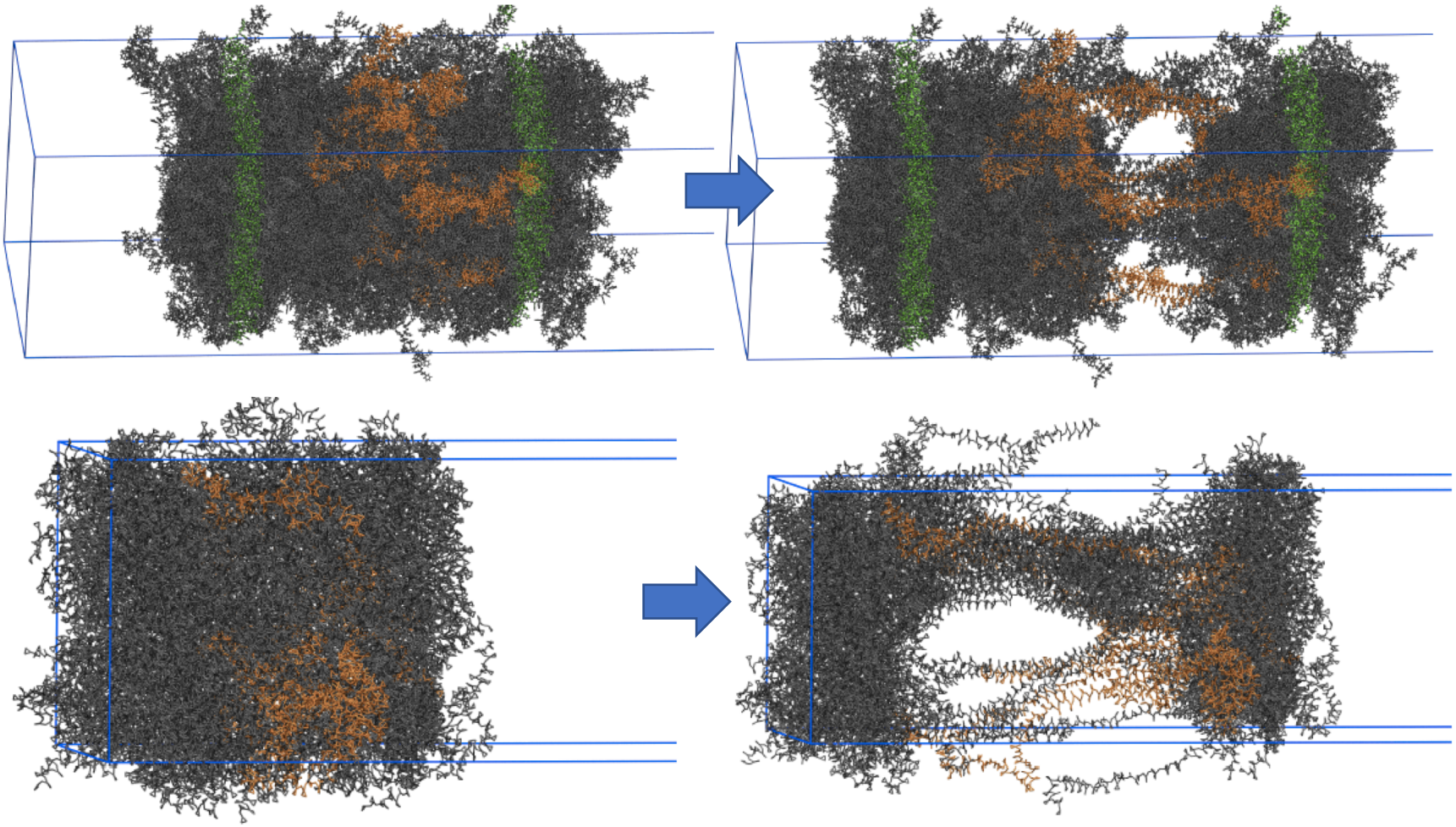




Mechanics of bone & teeth:
Rupture mechanisms and stress concentration of flawed biominerals



Mechanics of polymer nanocomposites



Gromacs: fast, free, and flexible

- up to hundreds of millions of particles
- *extremely high performance* compared to all other MD programs.
- innermost loops are written in C using intrinsic functions that the compiler transforms to SIMD machine instructions
- excellent CUDA-based GPU acceleration
- tailored towards bio-simulations, but increasingly used in the materials science domain

*Abraham, et al. (2015) SoftwareX **1-2** 19-25*
GROMACS benchmarking: *Kutzner, et al. (2015) J. Comput. Chem., **36** 1990-2008*

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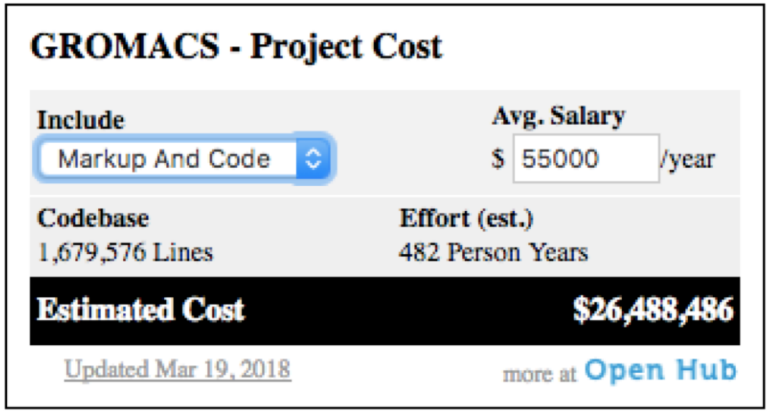

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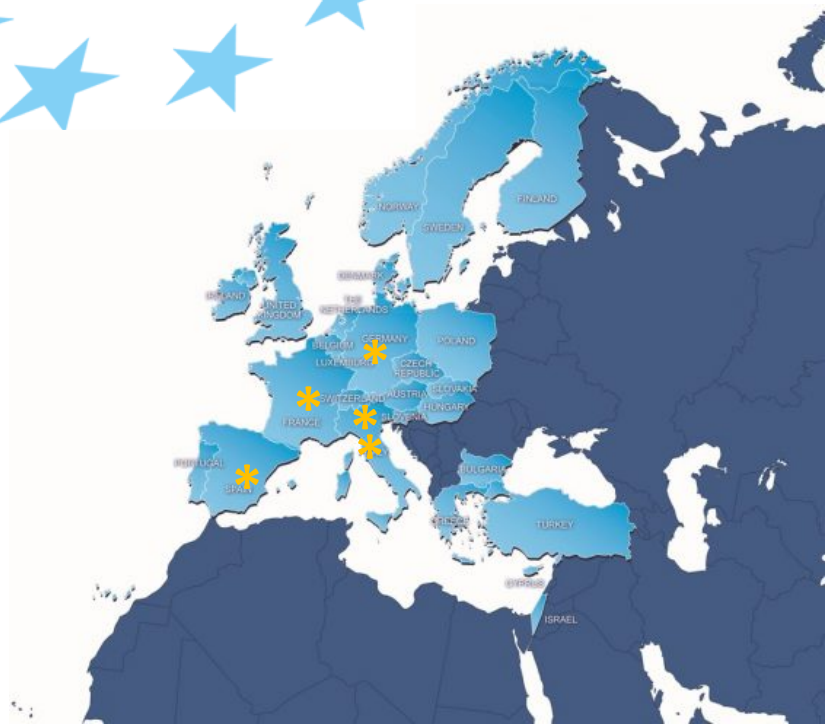
Molecular Dynamics & HPC

European partnership for HPC

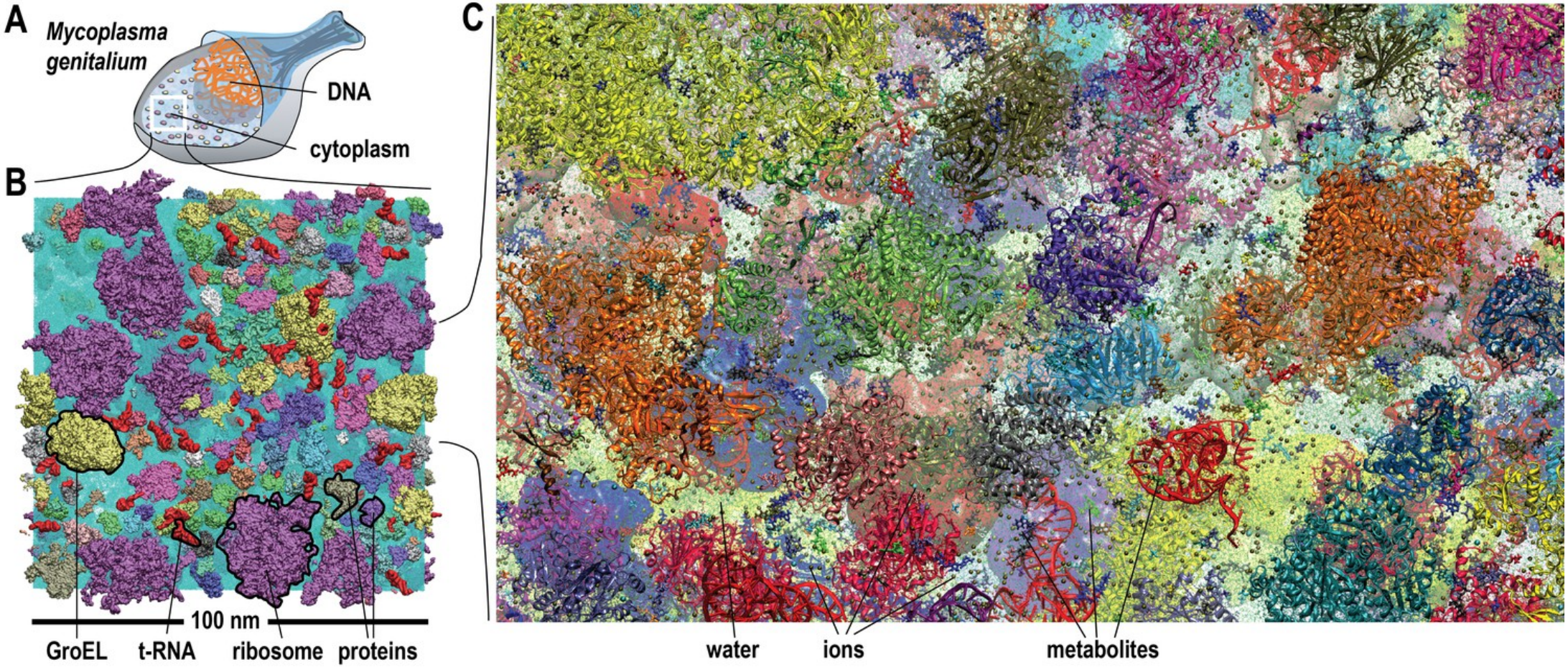
PRACE



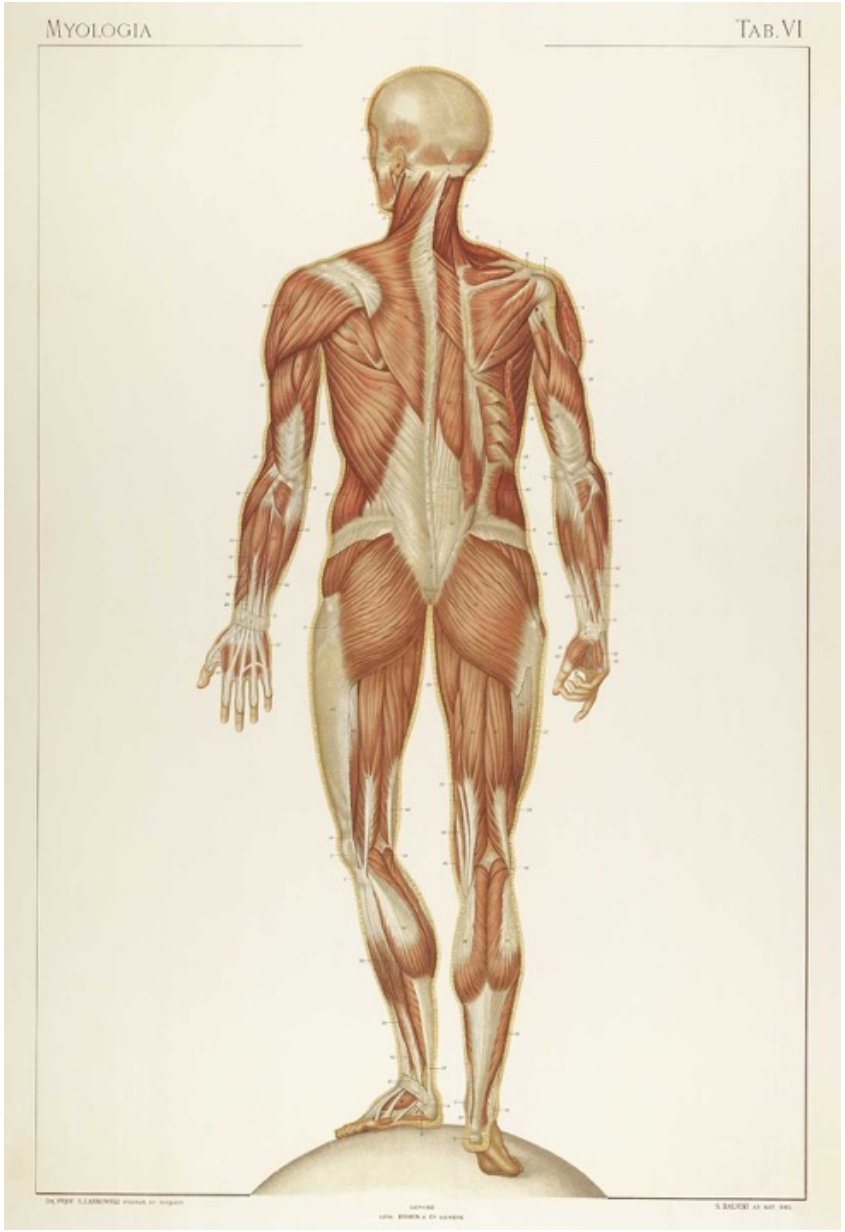
Molecular Dynamics & HPC

among the largest Molecular Dynamics simulations of a biological system

Yuji Sugita, Michael Feig and co-workers at RIKEN, on K-Computer

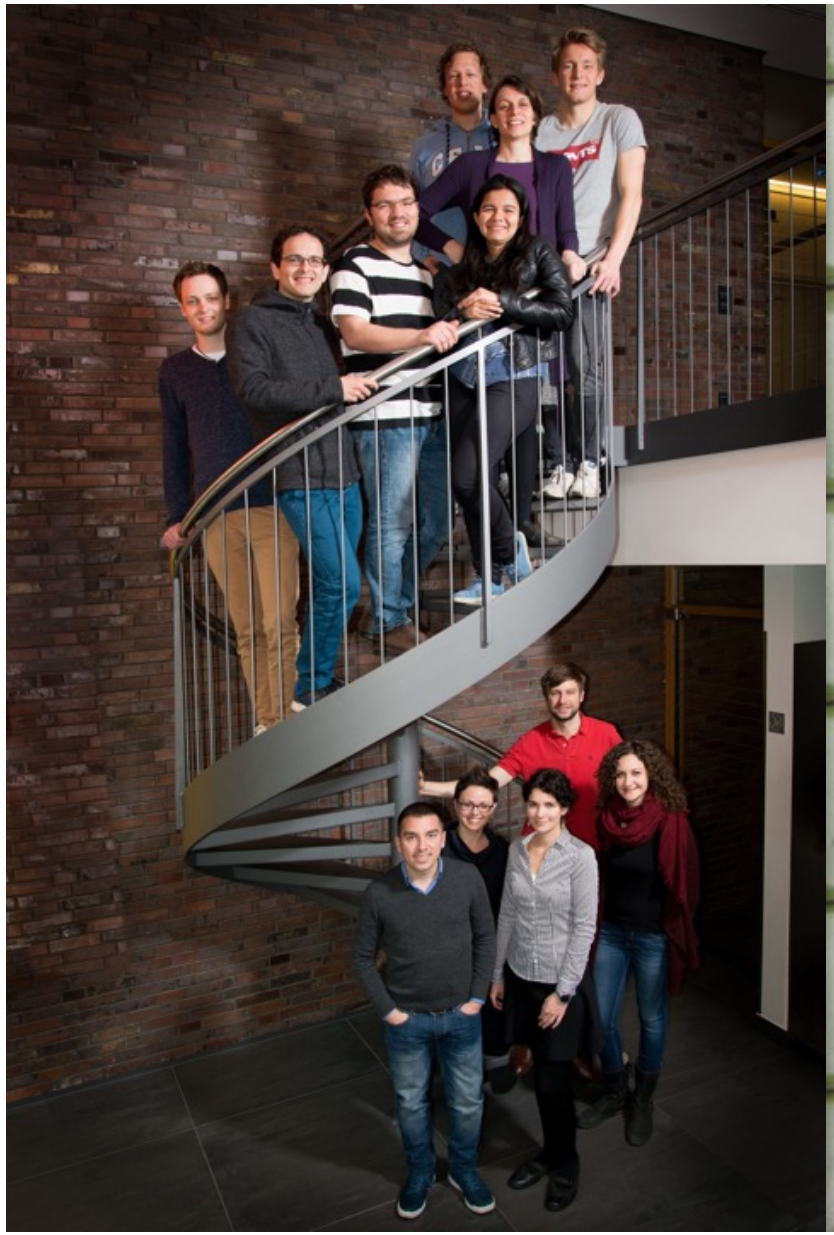



UEFA
RIONS



Collagen: major load-bearing structure of the body

Anatomic plate from Laskowski's "Anatomie normale du corps humain" (1894), illustrations by Sigismond Balicki



Molecular Biomechanics

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Agniezska Obarska-Kosinski
Tobias Jäger
Fan Jin
Benedikt Rennekamp

$$:
Klaus Tschira foundation
DFG, Volkswagen Foundation,
AvH,
Toyota