



MultiXscale

EuroHPC JU Centre of Excellence

Matej Praprotnik

National Institute of Chemistry, Ljubljana, Slovenia

MultiXscale Hackathon, SLING days, Ljubljana



**Co-funded by
the European Union**

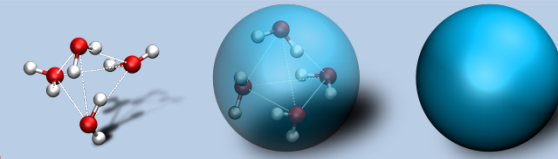


EuroHPC
Joint Undertaking

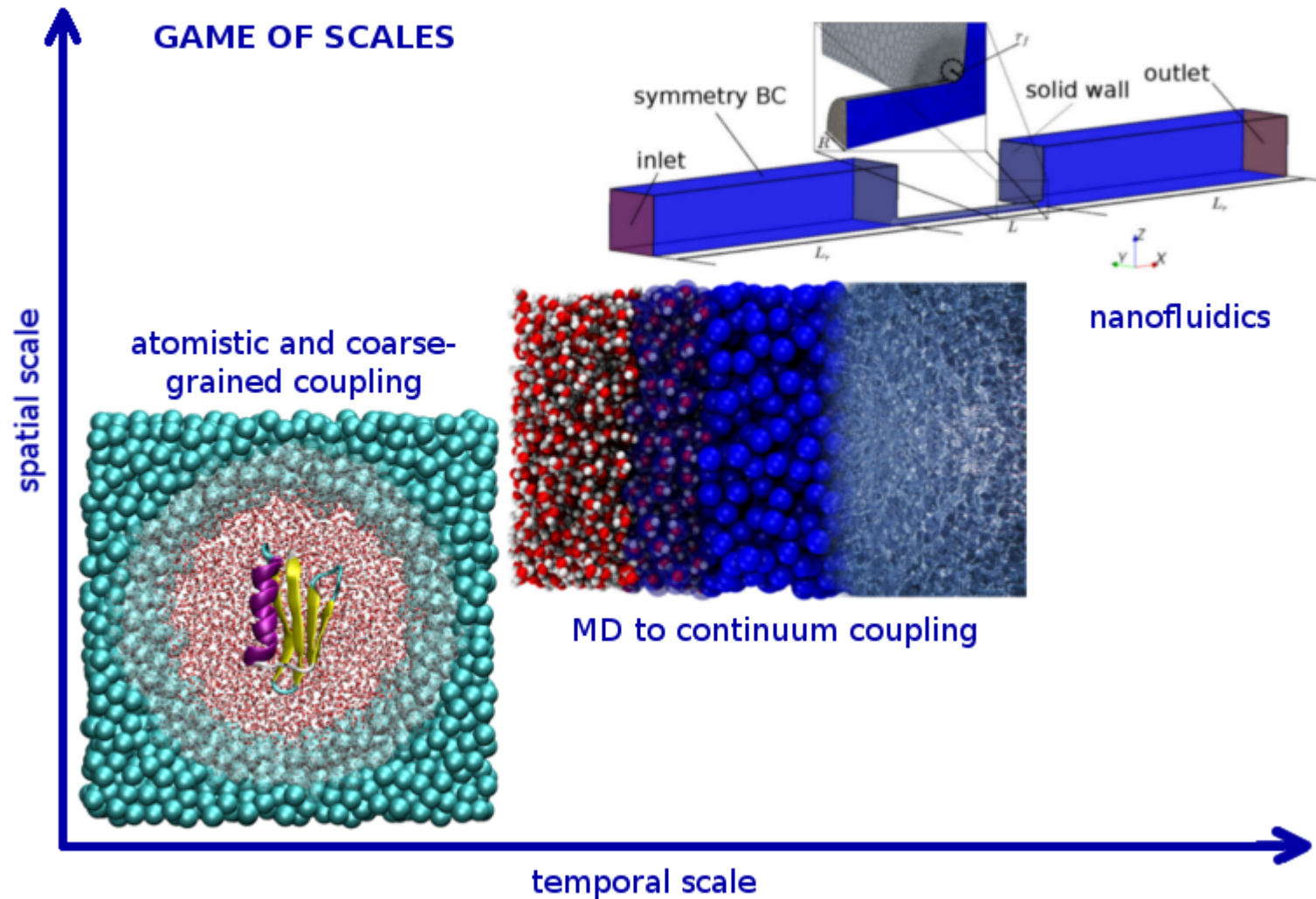


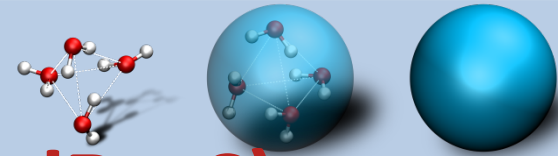
3.12.2024

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European High Performance Computing Joint Undertaking (JU) and countries participating in the project. Neither the European Union nor the granting authority can be held responsible for them.

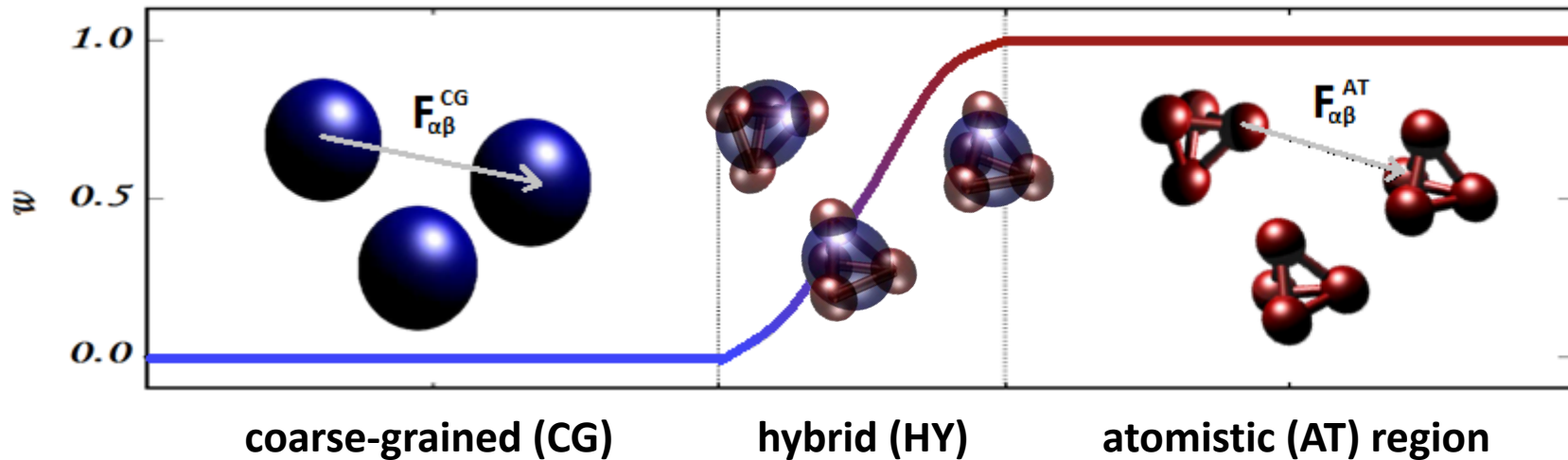


Multiscale modeling & simulation





Adaptive Resolution Scheme (AdResS)



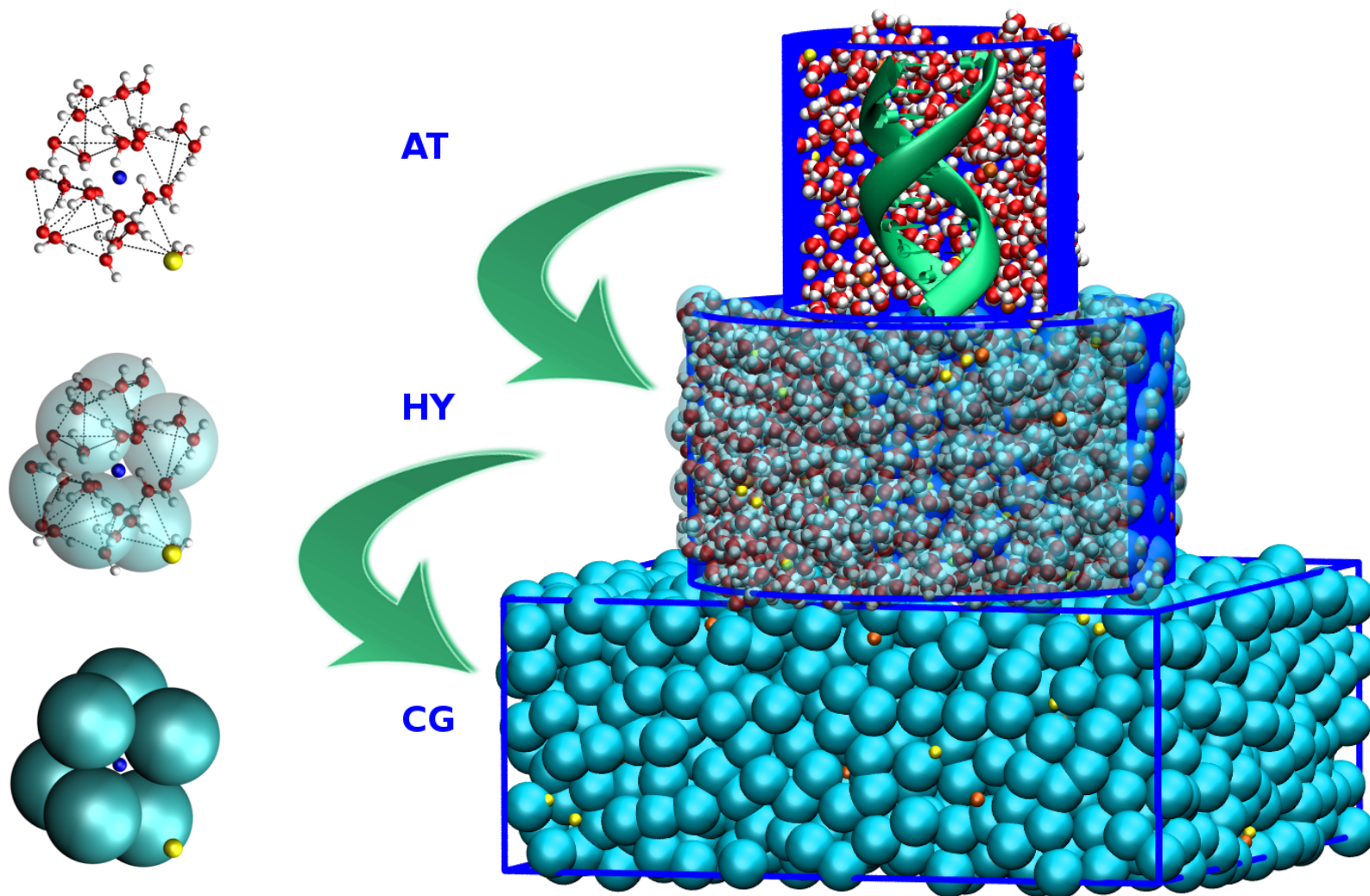
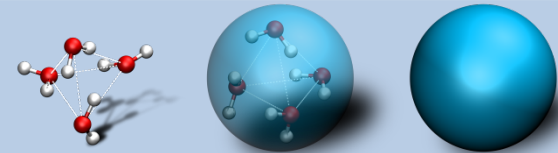
➤ force between particle α and β :

$$F_{\alpha}^{AdResS} = \sum_{\beta \neq \alpha} w(|R_{\alpha} - R|) w(|R_{\beta} - R|) F_{\alpha\beta}^{AT} + \sum_{\beta \neq \alpha} \left[1 - w(|R_{\alpha} - R|) w(|R_{\beta} - R|) \right] F_{\alpha\beta}^{CG} - F_{\alpha}^{TD}(|R_{\alpha} - R|)$$

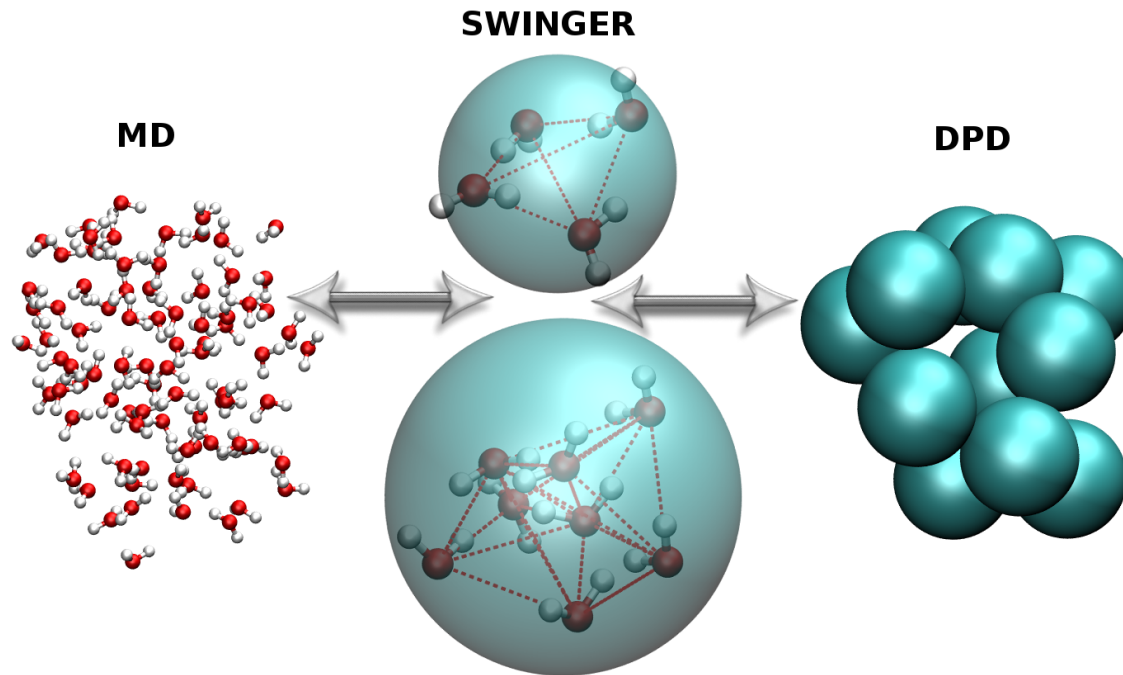
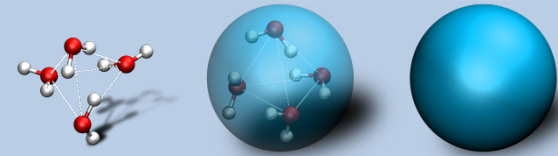
$w(r)$... position dependent weighting function

➤ above force coupling scheme obeys Newton's third law

DNA molecule in bundled-SPC/MARTINI salt solution



MD/DPD water



MD:

$$\mathbf{F}_{ij}^{MD,C}(\mathbf{r}_{ij}) = -\frac{\partial U^{MD}}{\partial \mathbf{r}_{ij}}$$

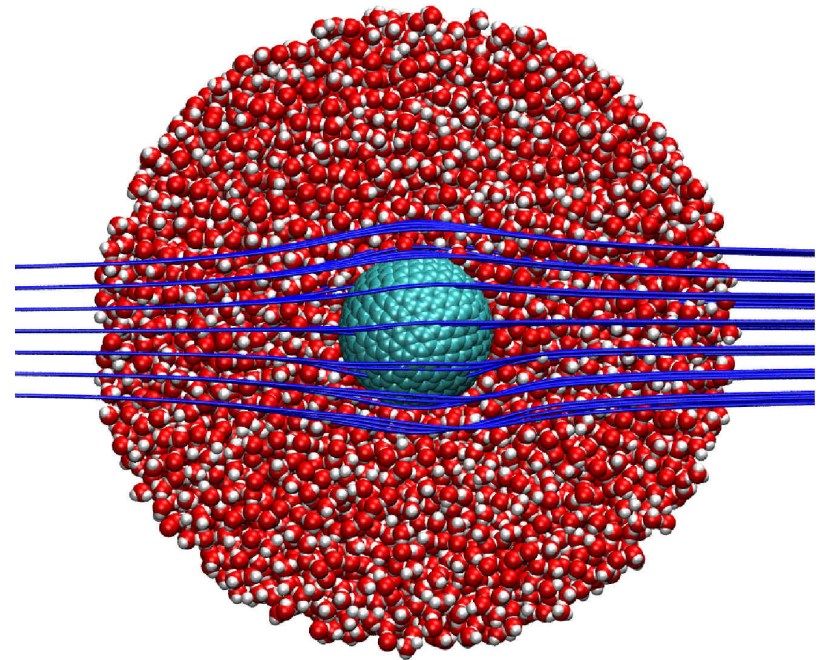
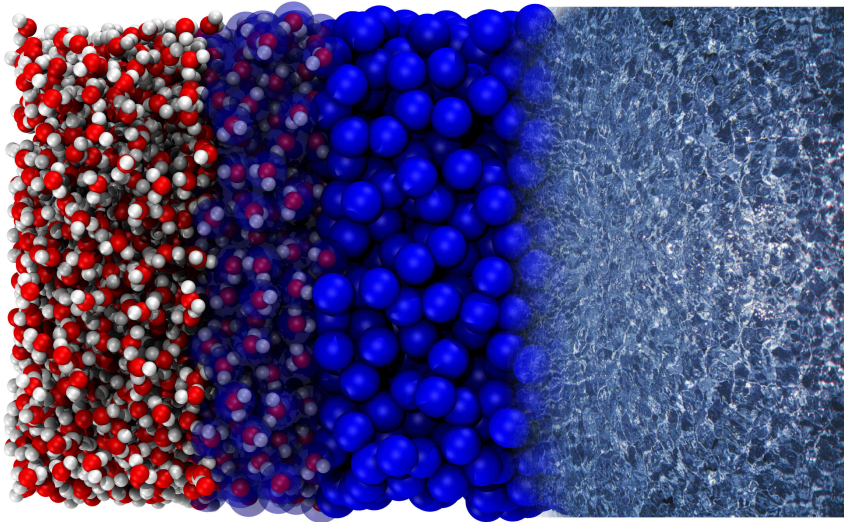
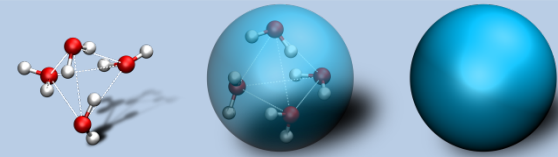
DPD:

$$\mathbf{F}_{\alpha\beta}^{DPD,C}(\mathbf{R}_{\alpha\beta}) = a_{\alpha\beta}(1 - R_{\alpha\beta}/R_c)\hat{\mathbf{R}}_{\alpha\beta}$$

$$\mathbf{F}_{\alpha\beta}^{DPD,R}(\mathbf{R}_{\alpha\beta}) = \sqrt{2\gamma_{\alpha\beta}k_B T}(1 - R_{\alpha\beta}/R_c)\zeta_{ij}\hat{\mathbf{R}}_{\alpha\beta}$$

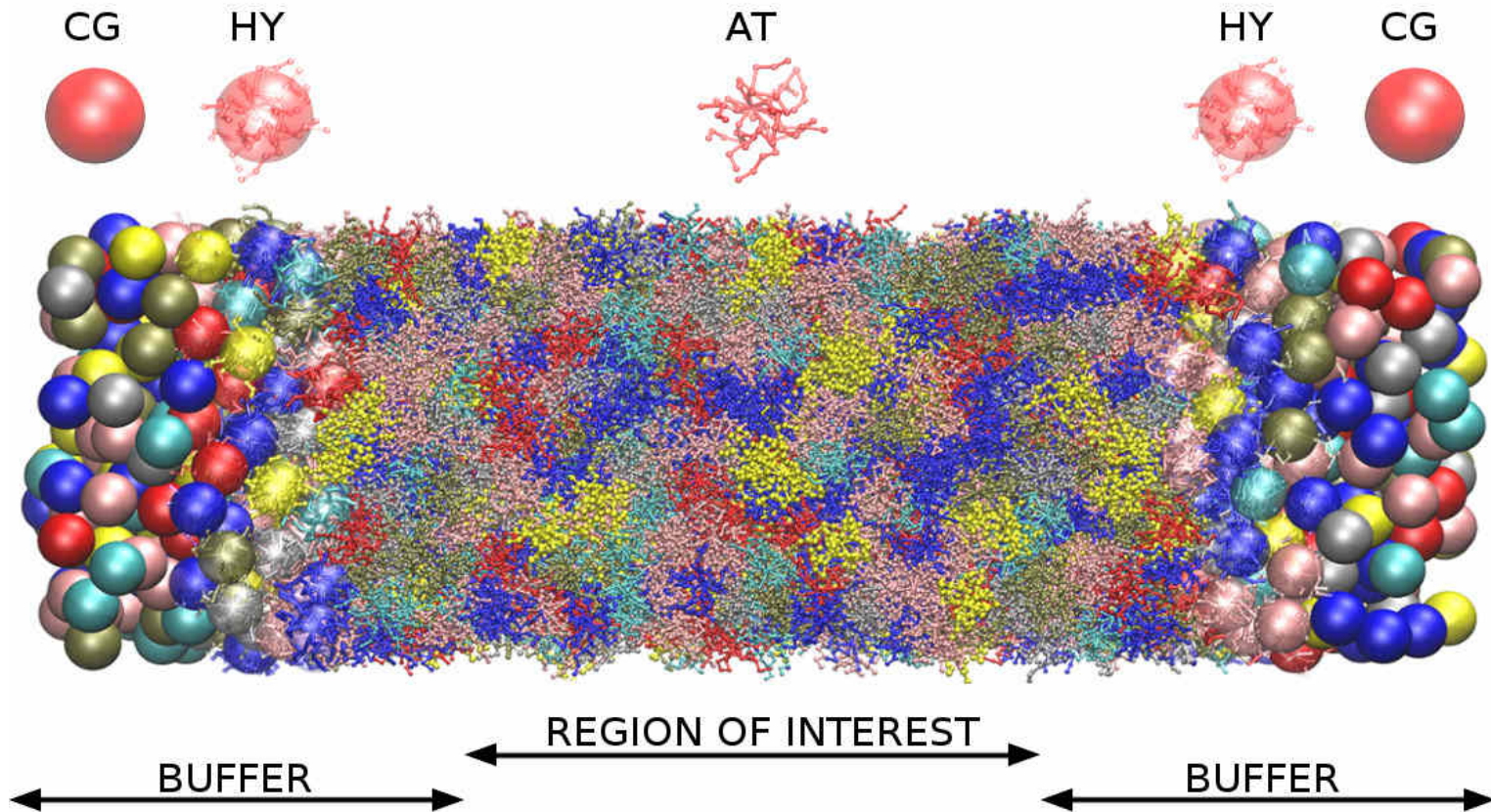
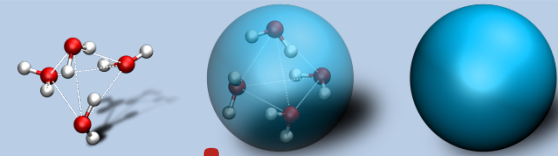
$$\mathbf{F}_{\alpha\beta}^{DPD,D}(\mathbf{R}_{\alpha\beta}) = -\gamma_{\alpha\beta}(1 - R_{ij}/R_c)^2(\hat{\mathbf{R}}_{\alpha\beta} \cdot \mathbf{V}_{\alpha\beta})\hat{\mathbf{R}}_{\alpha\beta}$$

Coupling to CFD



Delgado-Buscalioni, Sablić, Praprotnik; *Eur. Phys. J. Special Topics* (2015)
Walther et al.; *J. Comput. Phys.* (2012)

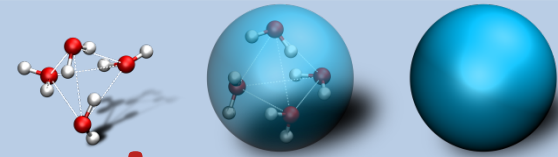
Open Boundary Molecular Dynamics



Delgado-Buscalioni, Sablić, Praprotnik; *Eur. Phys. J. Special Topics* (2015)

Sablić, Praprotnik, Delgado-Buscalioni; *Soft Matter* (2016)

Delle Site, Praprotnik; *Phys. Rep.* (2017)



Open Boundary Molecular Dynamics

➤ system exchanges mass, momentum, and energy with its surroundings

1. Insertion of molecules: $\Delta N_B = \frac{\Delta t}{\tau_r} (\alpha \langle N_B \rangle - N_B)$
2. Multiscale buffers -> facilitates insertion

➤ external boundary condition

1. Linear momentum conservation

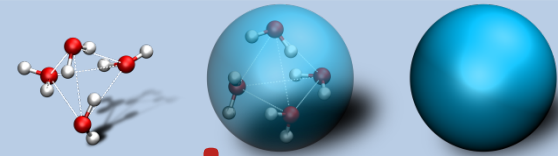
2. Additional force in buffers: $F^{ext} = J \cdot n_B A + \frac{P_{out} - P_{in}}{\Delta t} + \sum_{\alpha} F_{\alpha}^{TD}$

➤ DPD thermostat: $F_{\alpha}^{thermo} = \sum_{i \in \alpha, j \in \beta, \alpha \neq \beta} \sigma \omega^R(r_{ij}) \zeta_{ij} \hat{r}_{ij} - \gamma \omega^D(r_{ij}) (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij}$

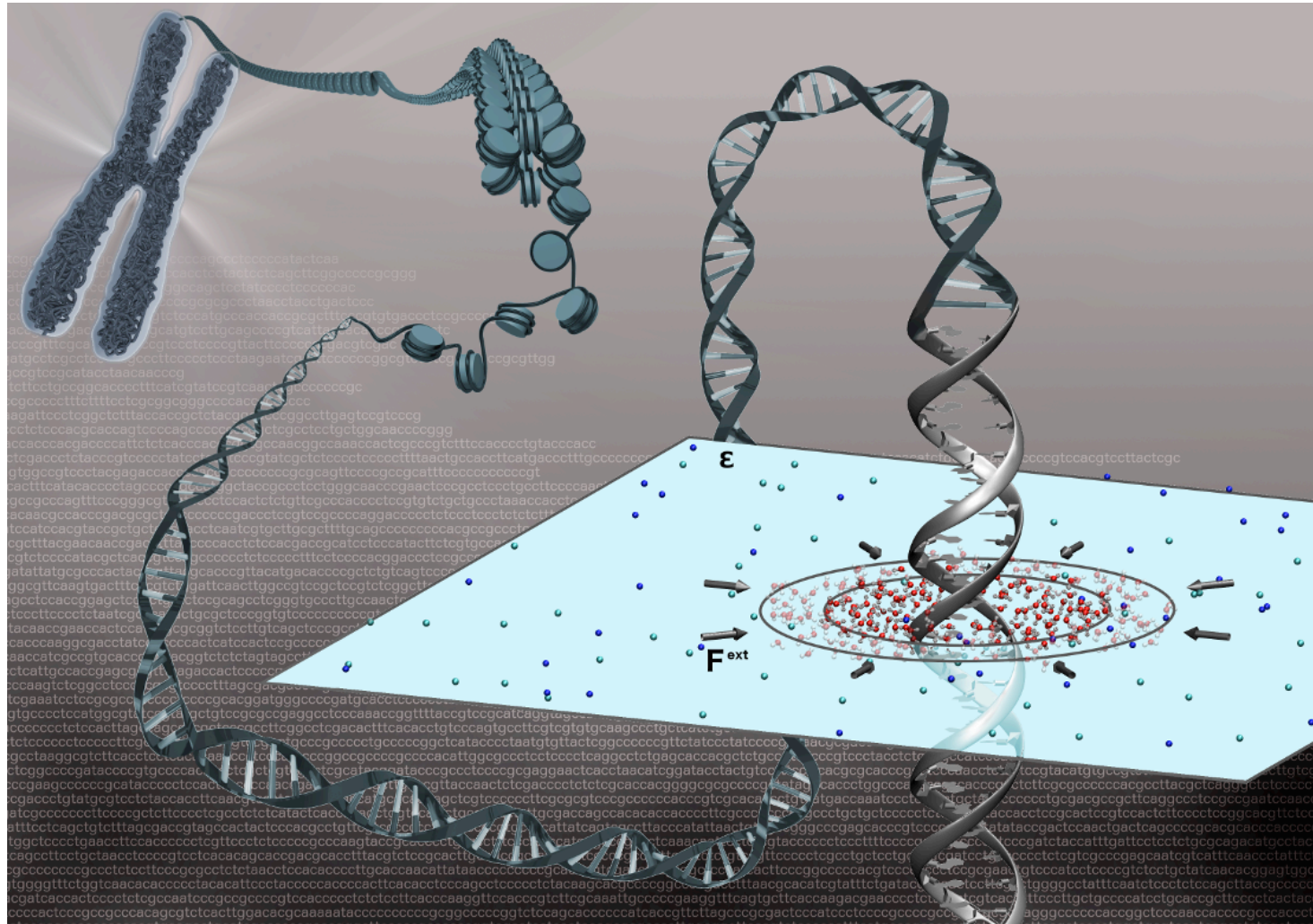
➤ total force on each particle:

$$\omega^D(r_{ij}) = \left[\omega^R(r_{ij}) \right]^2 \sigma^2 = 2k_B T \gamma$$

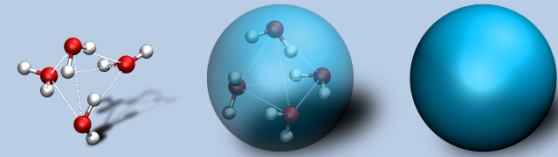
$$F_{\alpha} = F_{\alpha}^{AdResS} + F_{\alpha}^{ext} + F_{\alpha}^{thermo}$$



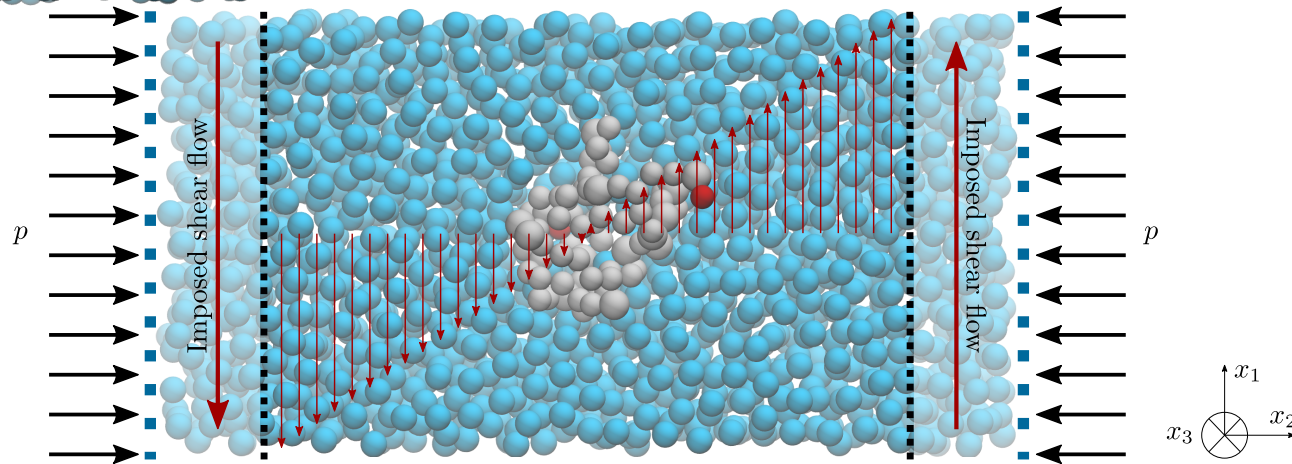
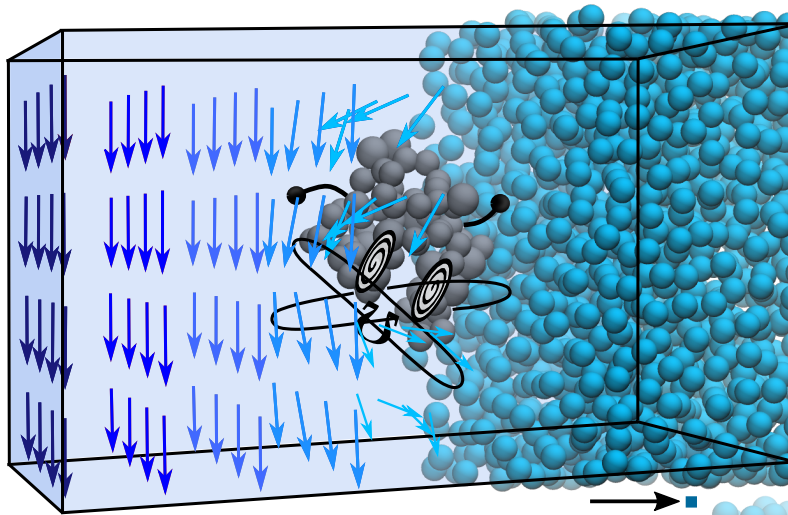
Open Boundary Molecular Dynamics



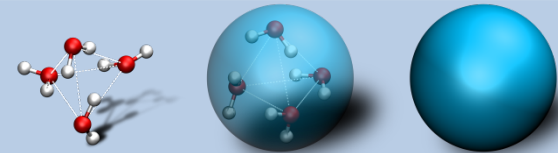
Zavadlav, Sablić, Podgornik, Praprotnik; *Biophys. J.* (2018)



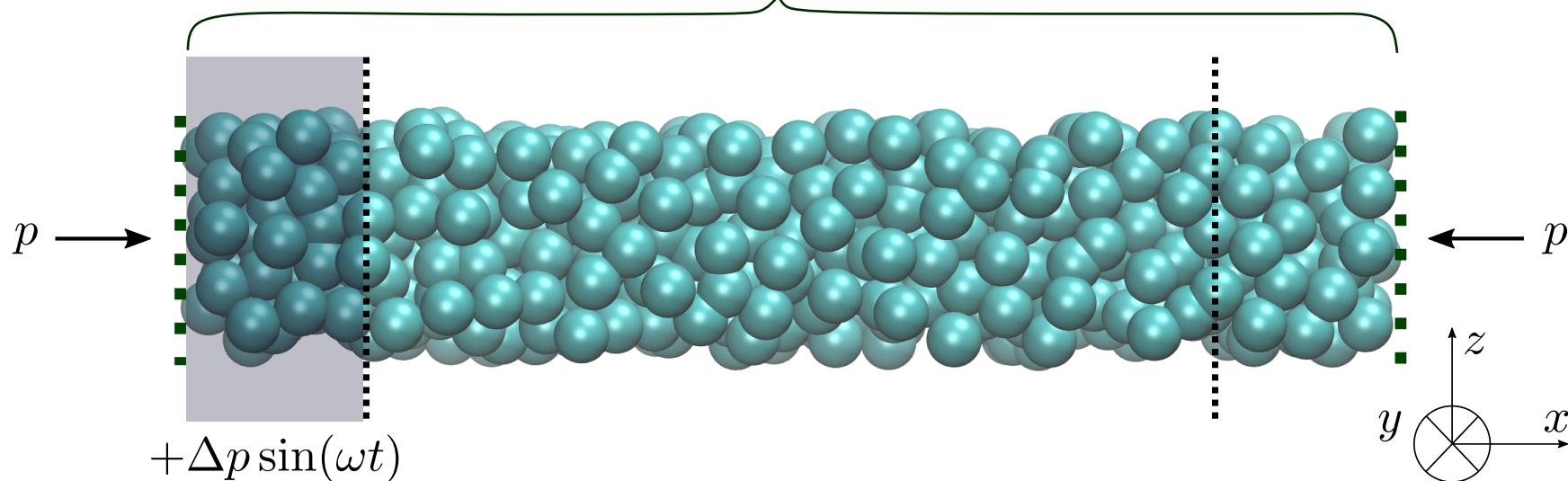
Rotational dynamics of a protein under shear flow

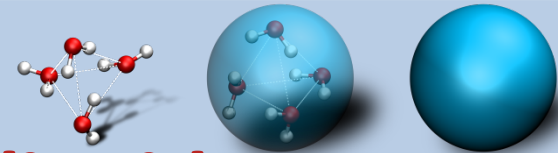


Virtual ultrasound machine

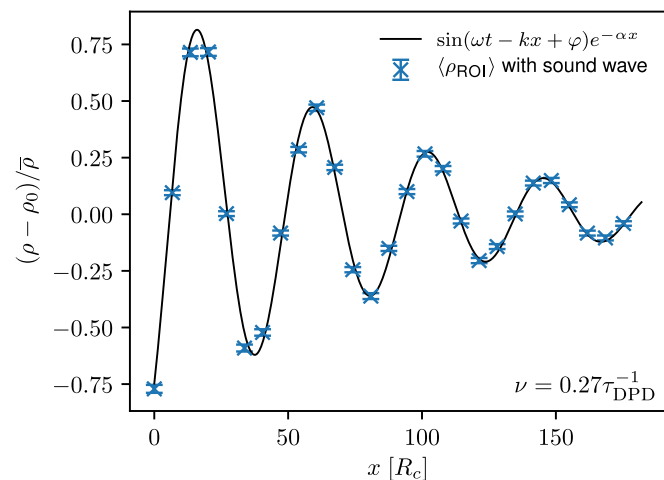
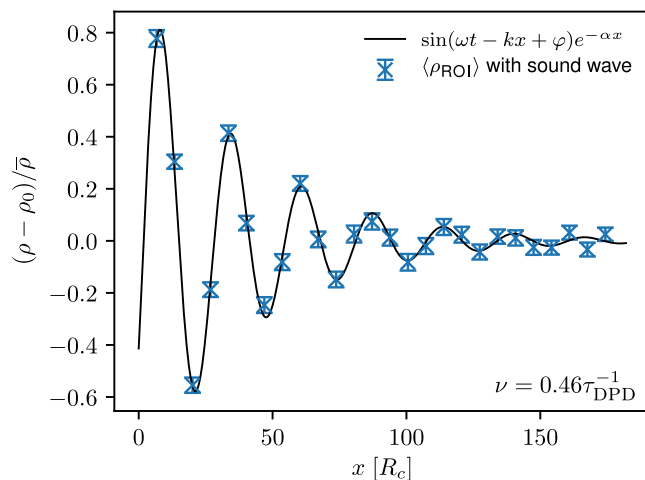
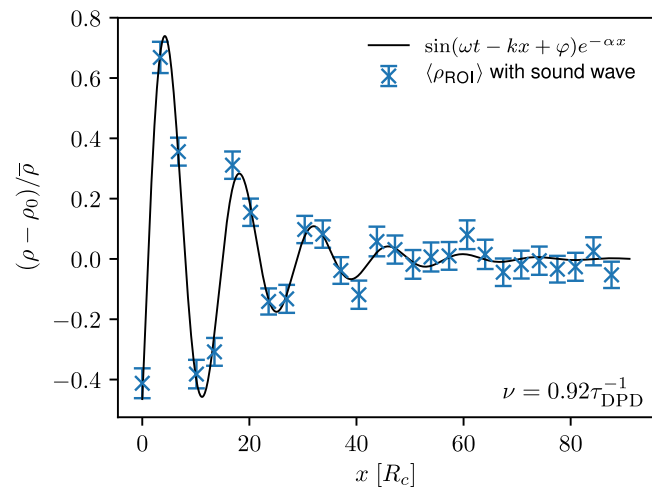
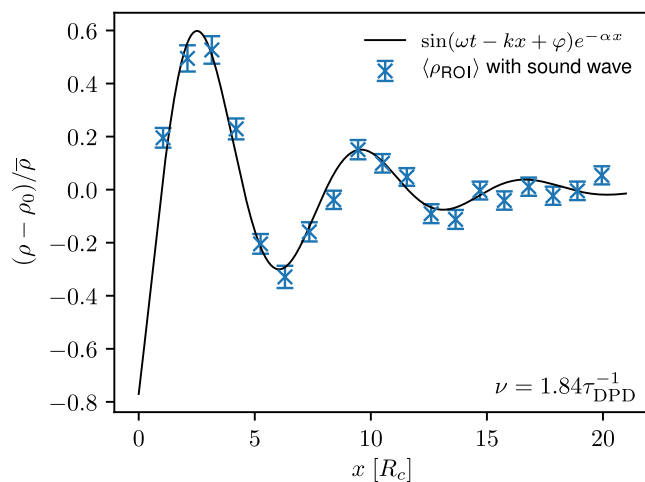


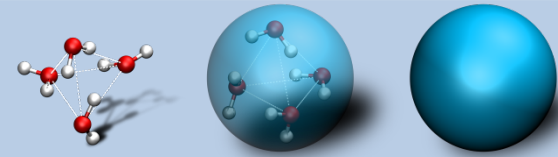
DPD and TDPD thermostat
 $\gamma_{\parallel}, \gamma_{\perp}$



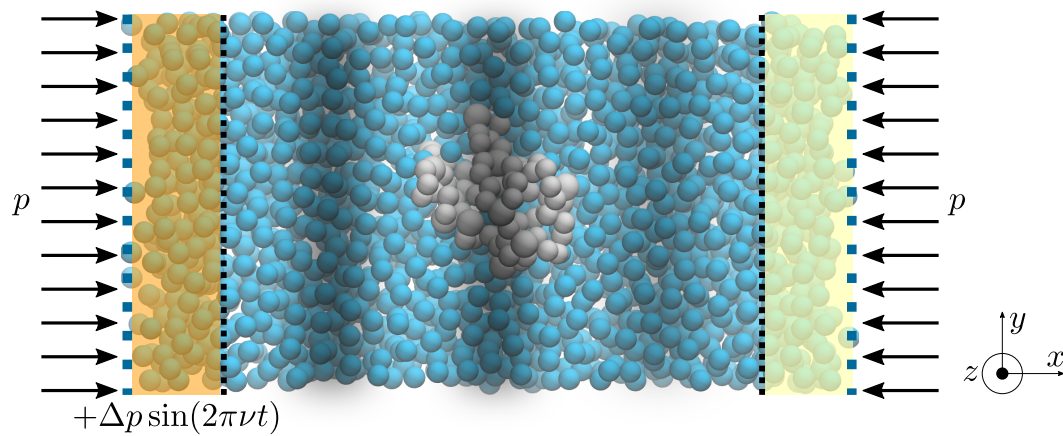


Ultrasound propagation through liquid water



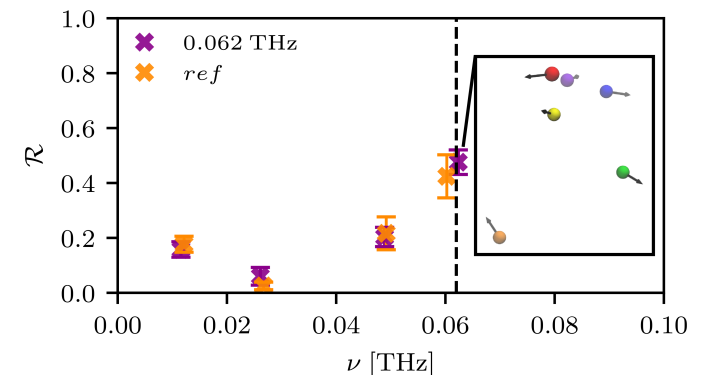
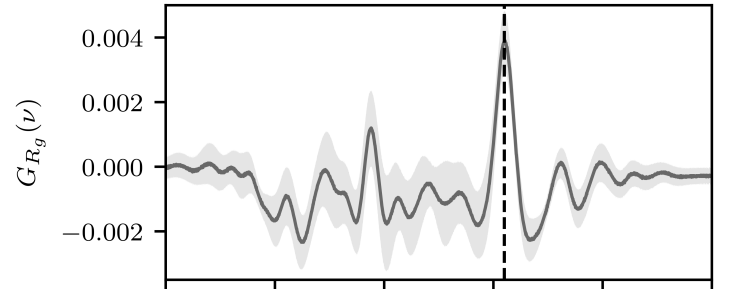
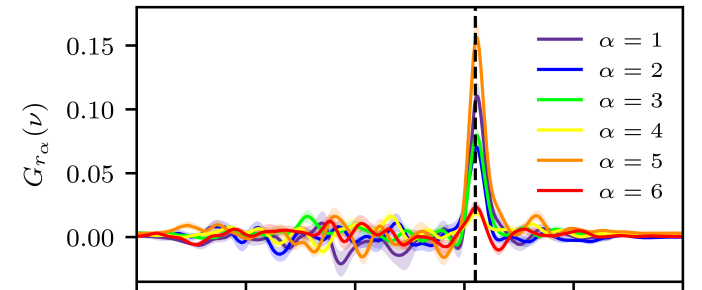


Sub-THz acoustic excitation of protein motion

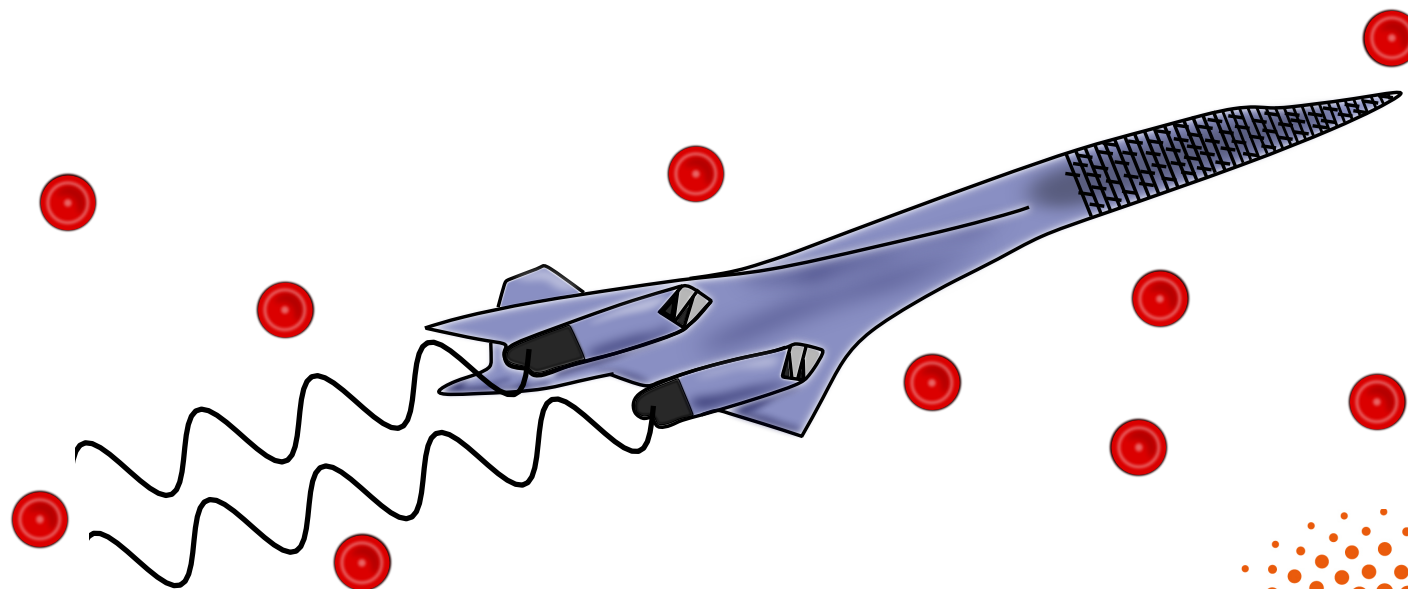
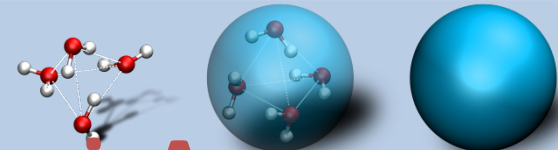


$$g_{R_g/r_\alpha}(\nu) = \frac{1}{2\pi} \int \int V_{g/\alpha}(\tau + t) V_{g/\alpha}(\tau) d\tau e^{i2\pi\nu t}$$

$$G_{R_g/r_\alpha}(\nu) = g_{R_g/r_\alpha}(\nu) - g_{R_g/r_\alpha}^0(\nu)$$



ERC AdG 2019: MULTraSonicA

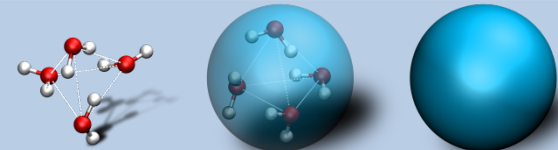


NATIONAL INSTITUTE OF CHEMISTRY

European Research Council

Established by the European Commission

Acknowledgements



- **Julija Zavadlav**; TUM, Germany
- **Jurij Sablič**; CECAM, Switzerland
- **Petra Papež**; National Institute of Chemistry, Slovenia
- **Franci Merzel**; National Institute of Chemistry, Slovenia
- **Tilen Potisk**; National Institute of Chemistry, Slovenia

- **Slovenian Research Agency** for funding

MultiXscale

Web page: www.multixscale.eu

Facebook: MultiXscale

X: @MultiXscale

LinkedIn: multixscale

YouTube: @MultiXscale



Co-funded by
the European Union



EuroHPC
Joint Undertaking



UNIVERSITAT DE
BARCELONA



Universität
Stuttgart



SORBONNE
UNIVERSITÉ



Université
de Toulouse



Consiglio Nazionale
delle Ricerche



MAX-PLANCK-GESSELLSCHAFT



Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and countries participating in the project under grant agreement No 101093169.