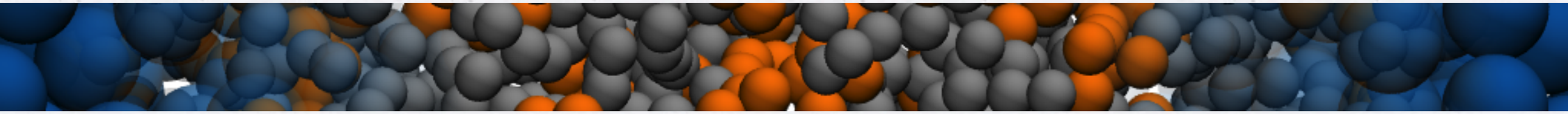


ADAPTIVE RESOLUTION SIMULATION METHODS

Raffaello Potestio

Max Planck Institute for Polymer Research

ESPResSo Summer School 2013

Stuttgart, October 10th, 2013

Motivation

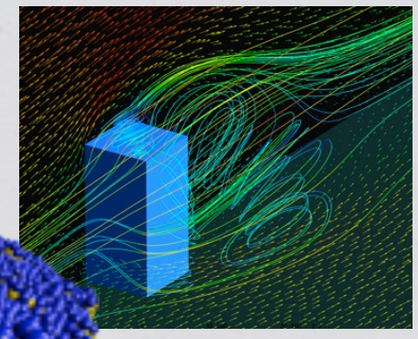
Time (sec)

1

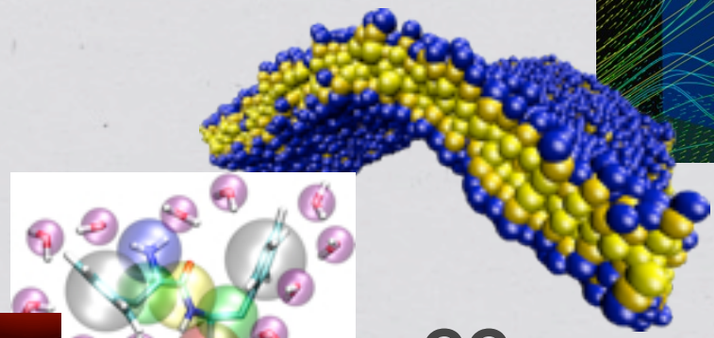
10^{-8} - 10^{-4}

10^{-10}

Soft matter systems cover a broad range of time- and length-scales

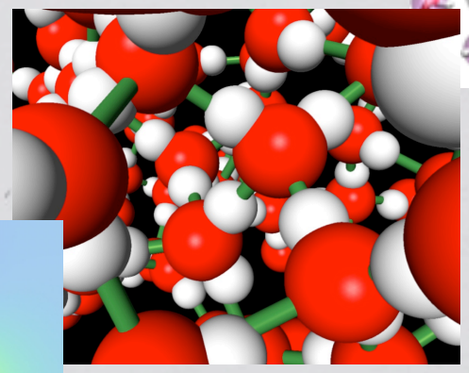


continuum models

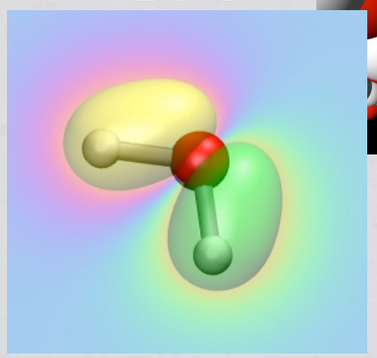


CG models

MD



DFT



Tailored methods have been developed to tackle specific cases

1 - 10

10 - 100

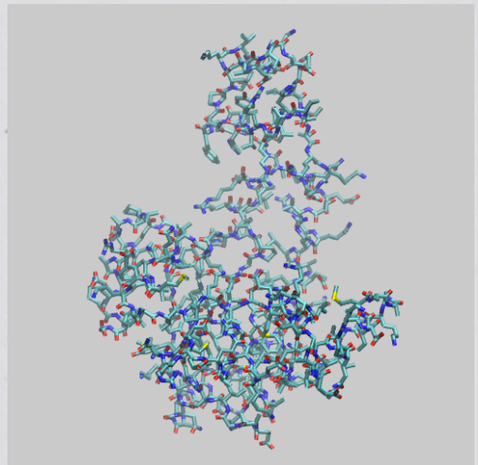
100 - 1000

Length (Å)

The resolution of a simulation is chosen based on the process of interest

Chemistry-specific interactions

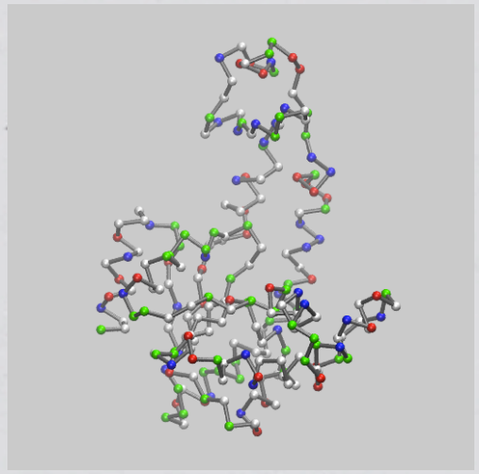
All-atom force-fields, DFT



Expensive

Large-scale properties, conformational transitions, phase ordering

Coarse-grained models

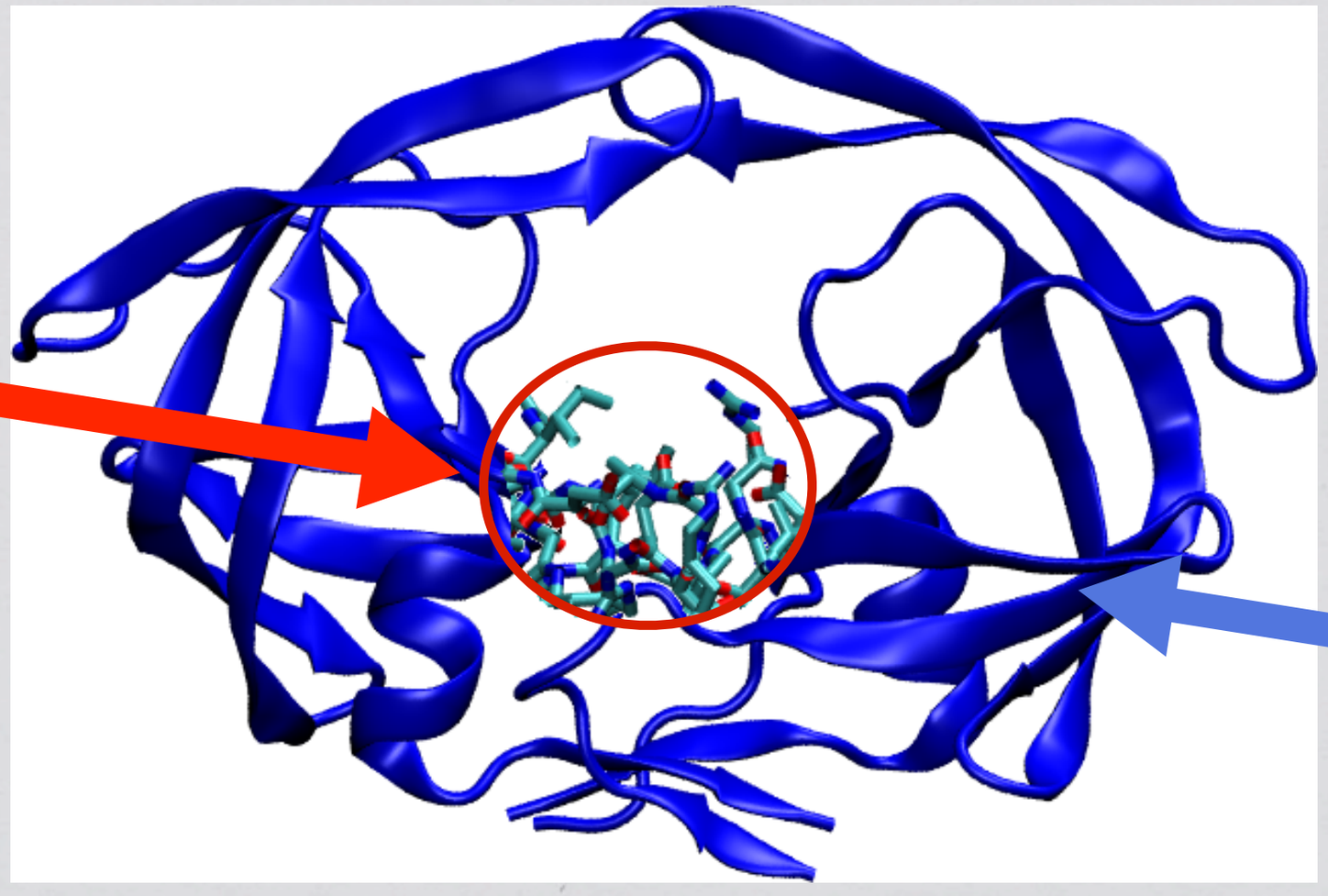


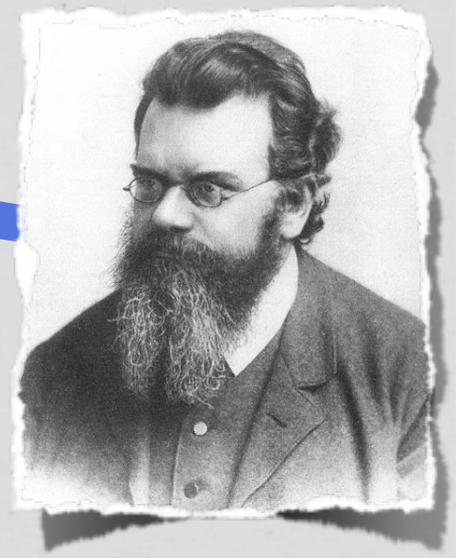
No detail

Dual resolution simulations: concurrent use of different resolutions in separate regions of the simulation domain

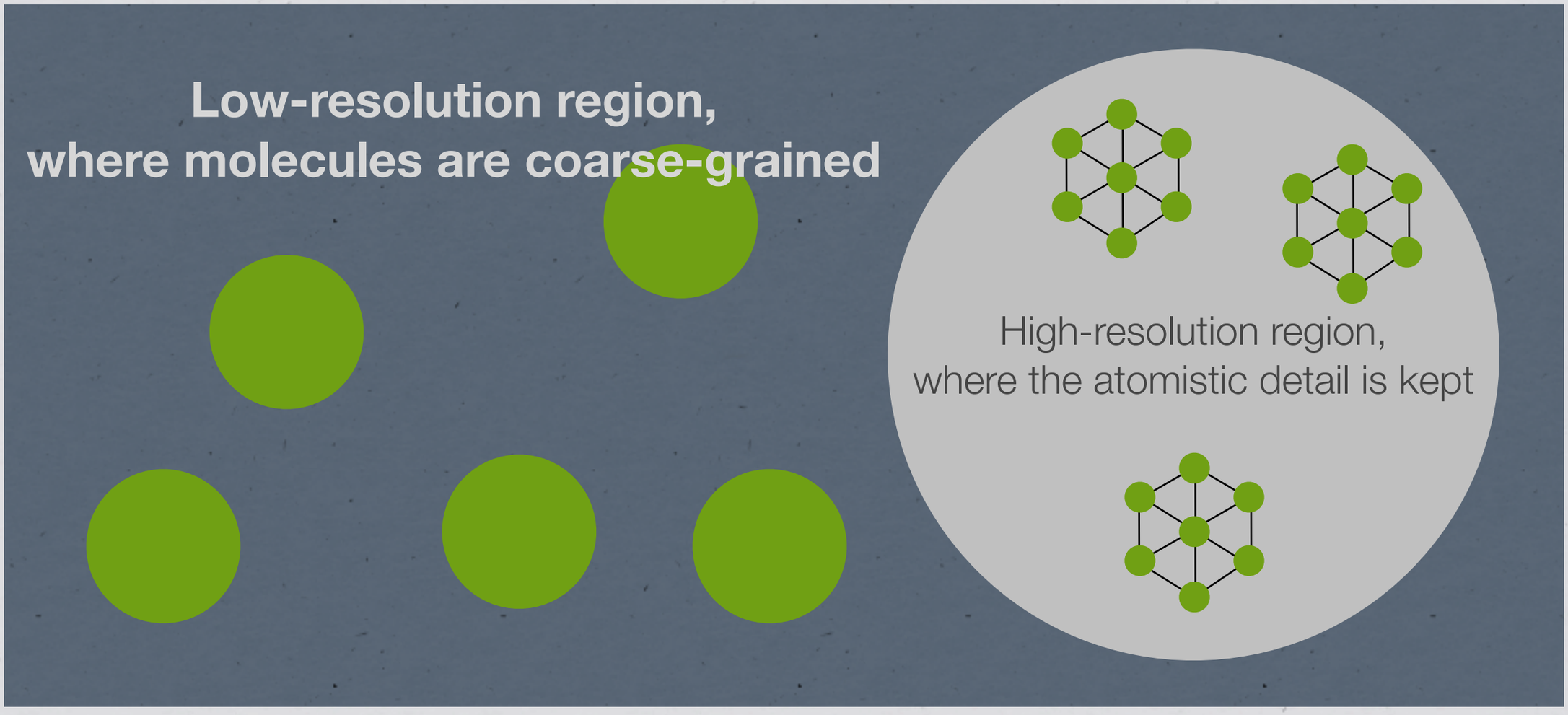
Example: QM/MM simulation methods

A small region is treated at the quantum level, the rest with classical force fields





Dual resolutions of soft matter: atomistic and coarse-grained



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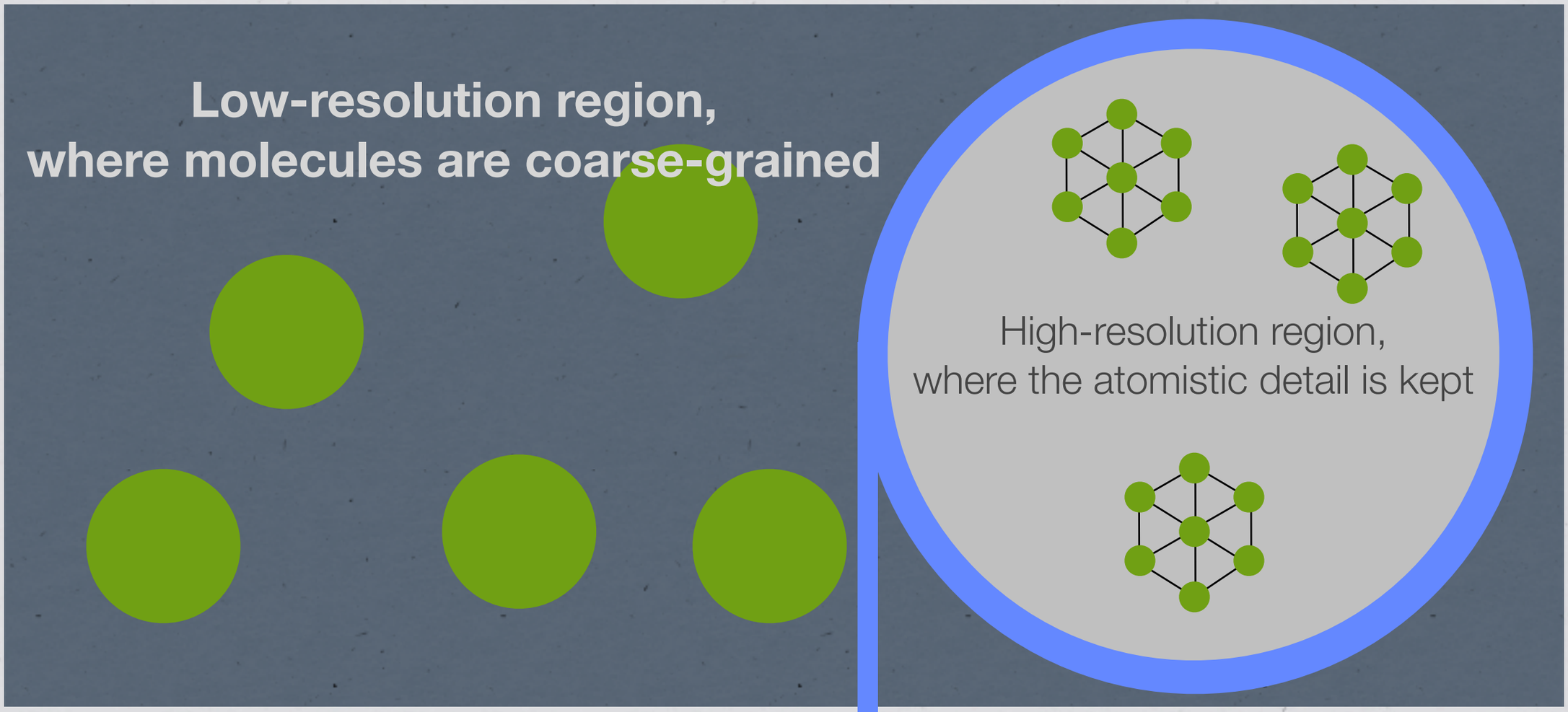
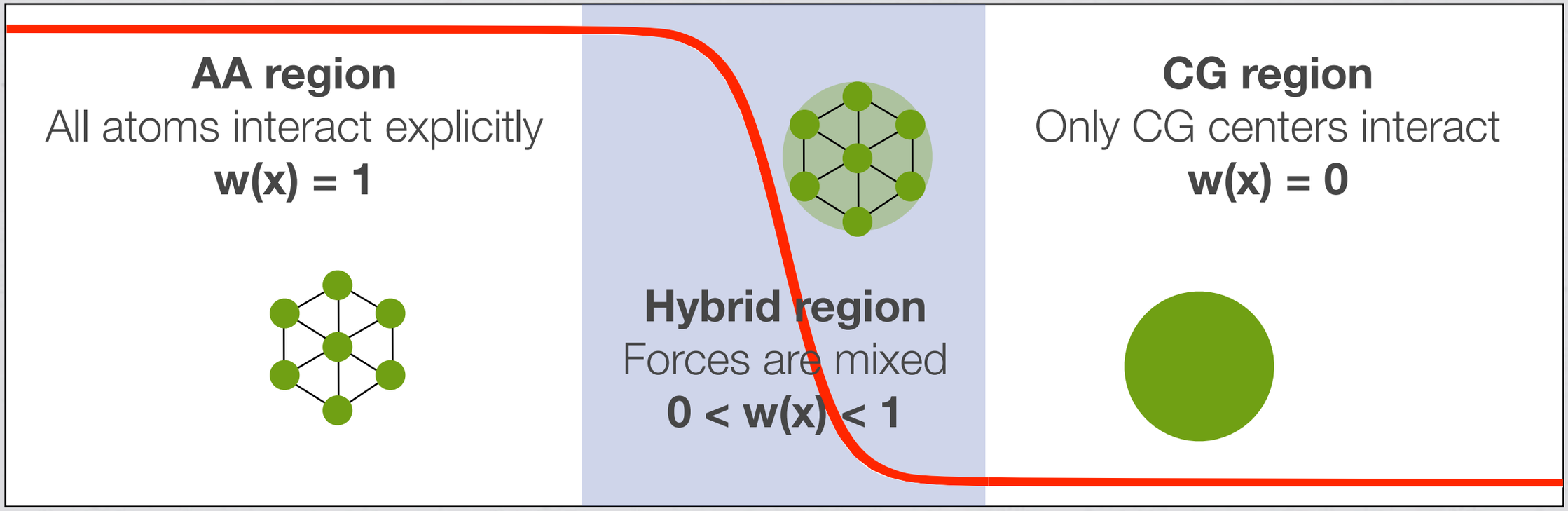


How are these two regions | **interfaced?**

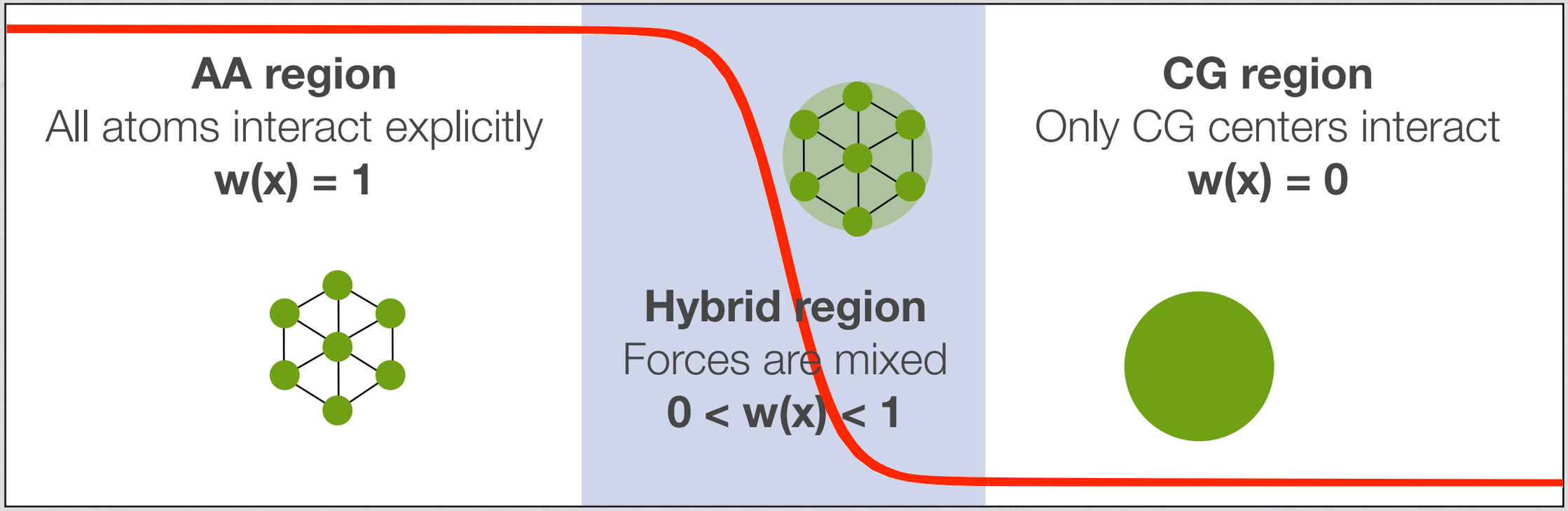
Interpolation of force-fields



Interpolation of force-fields

AdResS - Adaptive Resolution Simulation scheme

$$\mathbf{F}_{\alpha\beta} = w(X_\alpha)w(X_\beta)\mathbf{F}^{expl}_{\alpha\beta} + [1 - w(X_\alpha)w(X_\beta)]\mathbf{F}^{cg}_{\alpha\beta}$$



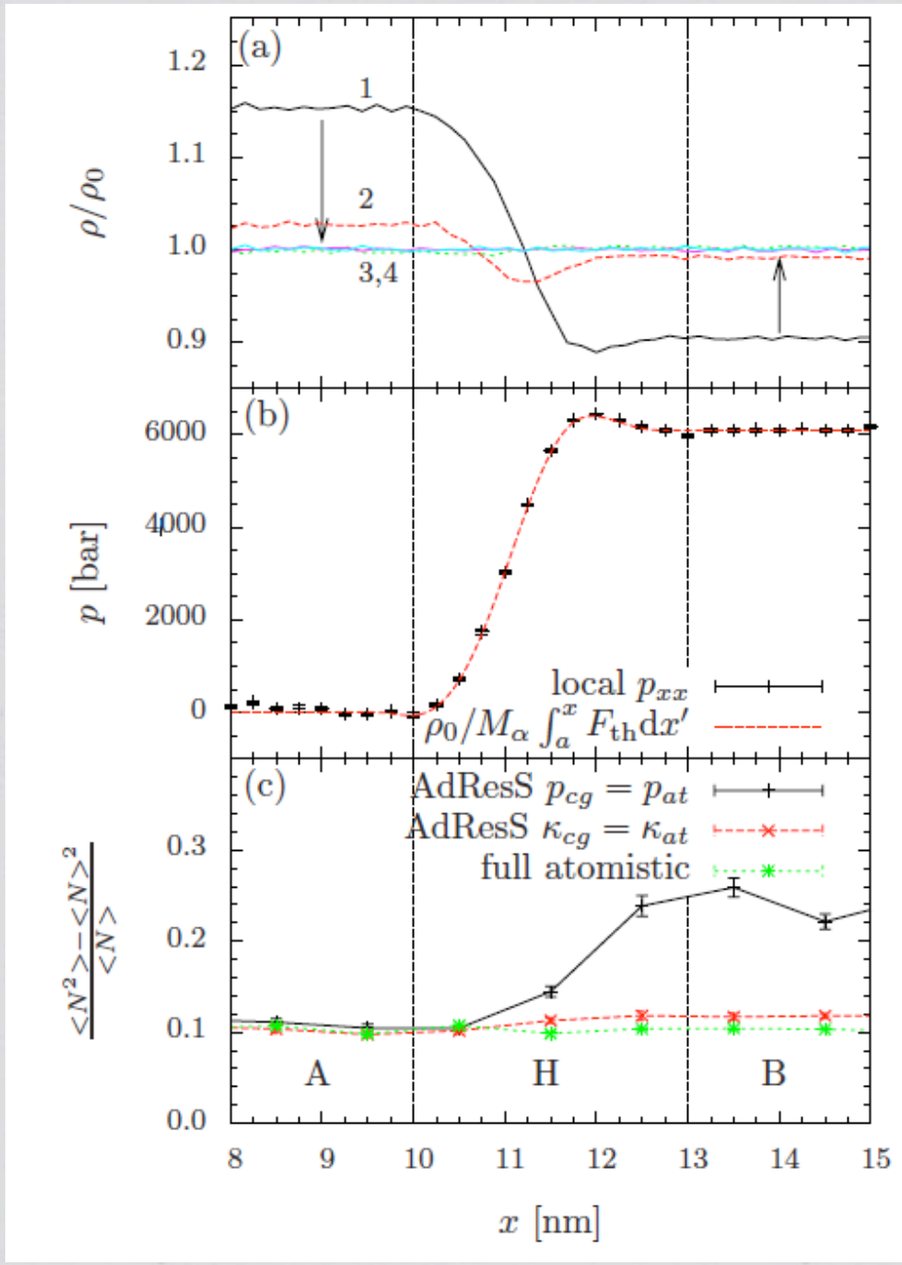
M. Praprotnik, L. Delle Site, and K. Kremer, J. Chem. Phys. 123, 2005

Control of the thermodynamics in the explicit region

Coarse-grained potentials usually don't match the atomistic system's virial pressure

The difference can be balanced via an iteratively-refined thermodynamic force [1]

$$\mathbf{F}_{th}^{i+1}(x) = \mathbf{F}_{th}^{i}(x) - \frac{M}{\rho_0^2 \kappa_T} \nabla \rho^i(x)$$



[1] S. Fritsch, S. Poblete, C. Junghans, G. Ciccotti, L. Delle Site, and K. Kremer, Phys Rev Lett 17, vol 108, 2012 [Figures from therein]

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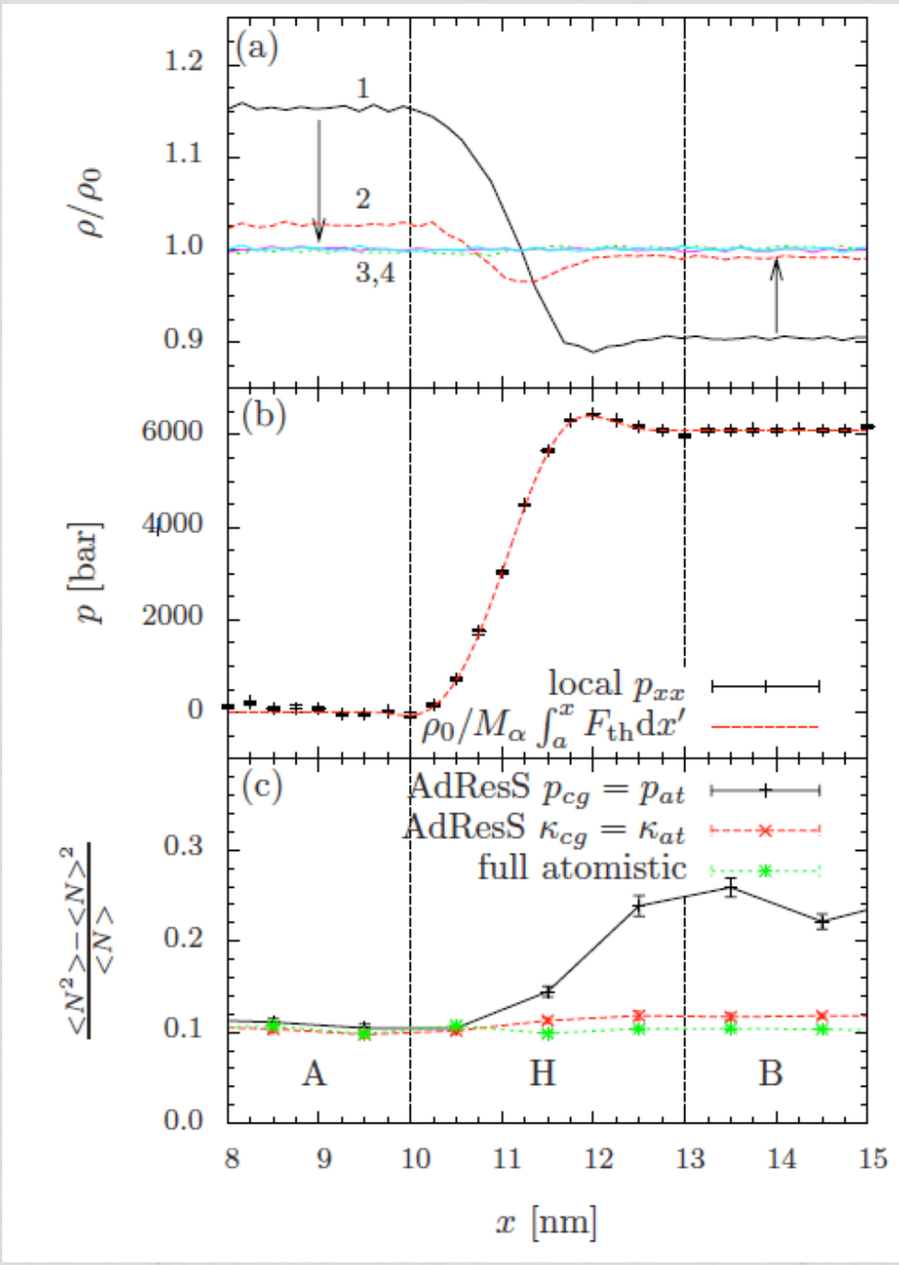

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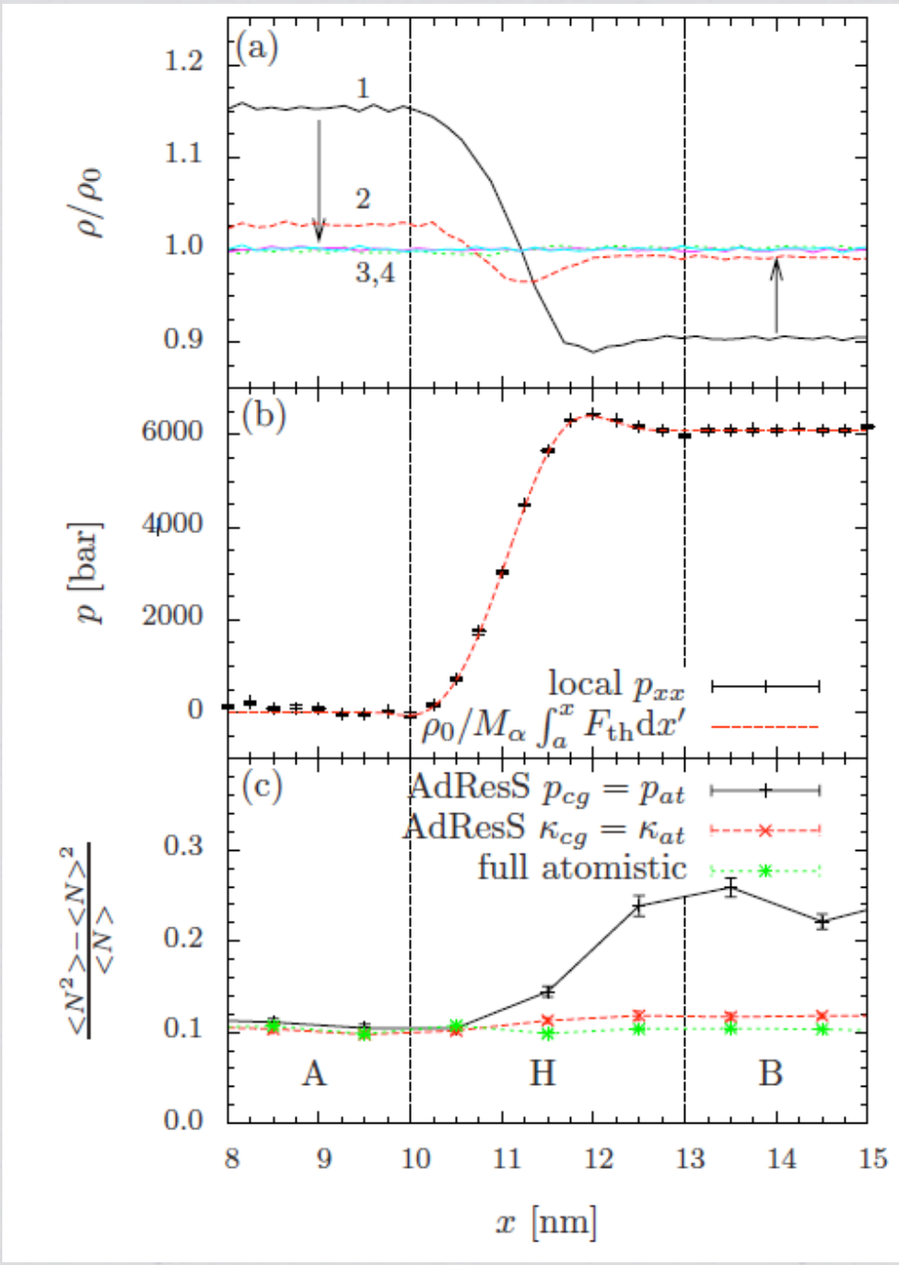
The explicit region behaves as an open system



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Validation and applications

Figure 6

(*a*) The on-the-fly interchange between the atomistic (*far-right molecule*) and coarse-grained (*far-left molecule*) levels of description. The middle hybrid molecule is a linear combination of a fully atomistic molecule with an additional center-of-mass particle representing the coarse-grained molecule. (*b*) Snapshot of the hybrid atomistic/mesoscopic model liquid with $\rho = 0.175$ and $T = 1.0$. The red molecules are the explicit atomistically resolved tetrahedral molecules, and the blue molecules are the corresponding one-particle coarse-grained molecules.

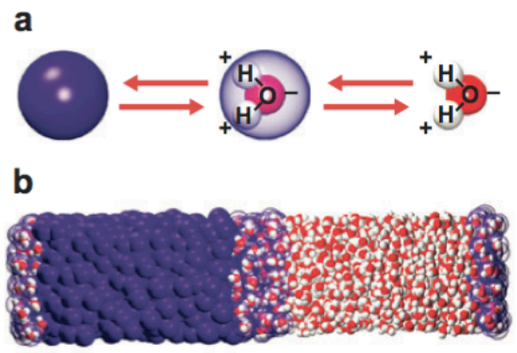


Figure 11

(*a*) On-the-fly interchange between the all-atom and coarse-grained water models. (*b*) A schematic representation of the hybrid liquid-water system.

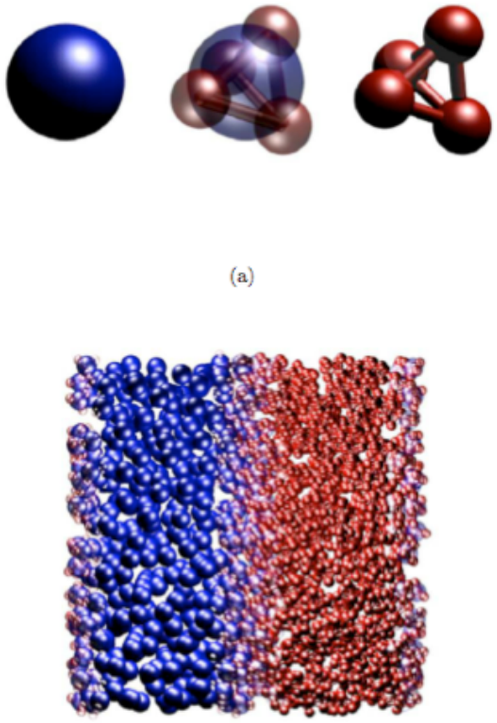


FIG. 1: (a) The on-the-fly interchange between the atomic and coarse-grained levels of description. The middle hybrid molecule is a linear combination of fully atomistic tetrahedral molecule with an additional center of mass particle representing the coarse-grained molecule. (b) Snapshot of the hybrid atomistic/mesoscopic model at $\rho^* = 0.1$ and $T^* = 1$ (LJ units). The red molecules are the explicit atomistically resolved tetrahedral molecules, the blue molecules are the corresponding one particle coarse-grained molecules.

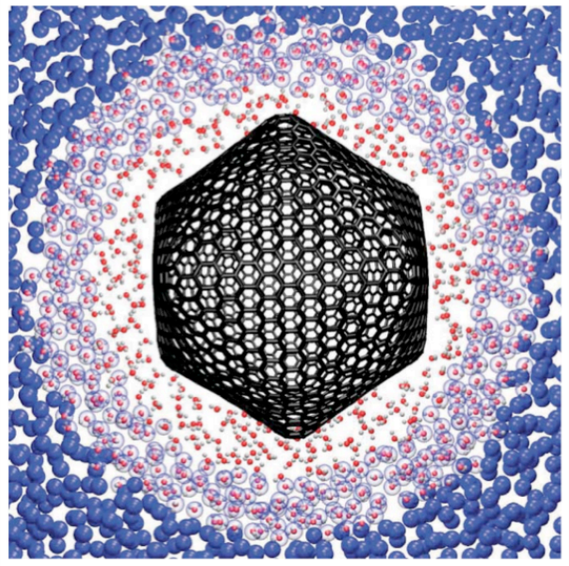


FIG. 1. Adaptive resolution simulation scheme for hydrophobic solutes, illustrated for the case of C_{2160} icosahedral fullerene.

M. Praprotnik, L. Delle Site, K. Kremer, Phys. Rev. E 73, 2006

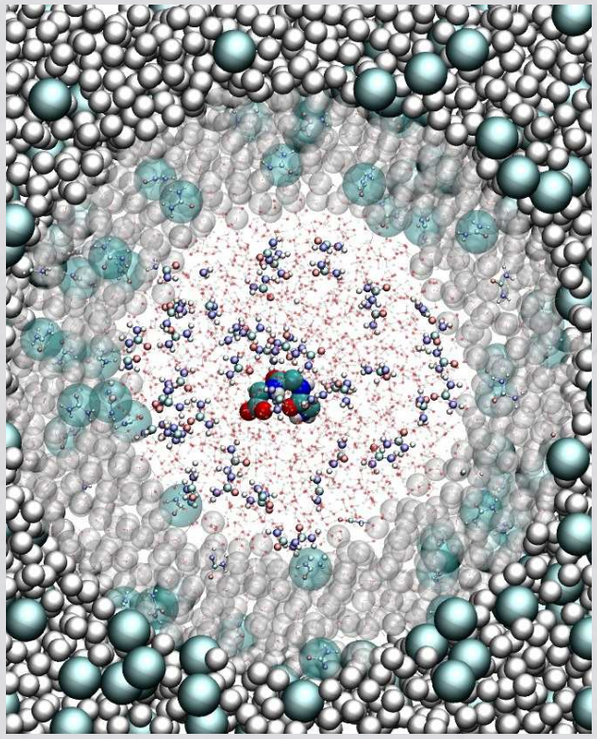
M. Praprotnik, L. Delle Site , K. Kremer, Annu. Rev. Phys. Chem. 59, 2008

B.P. Lambeth, Jr., C. Junghans, K. Kremer, C. Clementi, L. Delle Site, J. Chem. Phys. 133, 2010

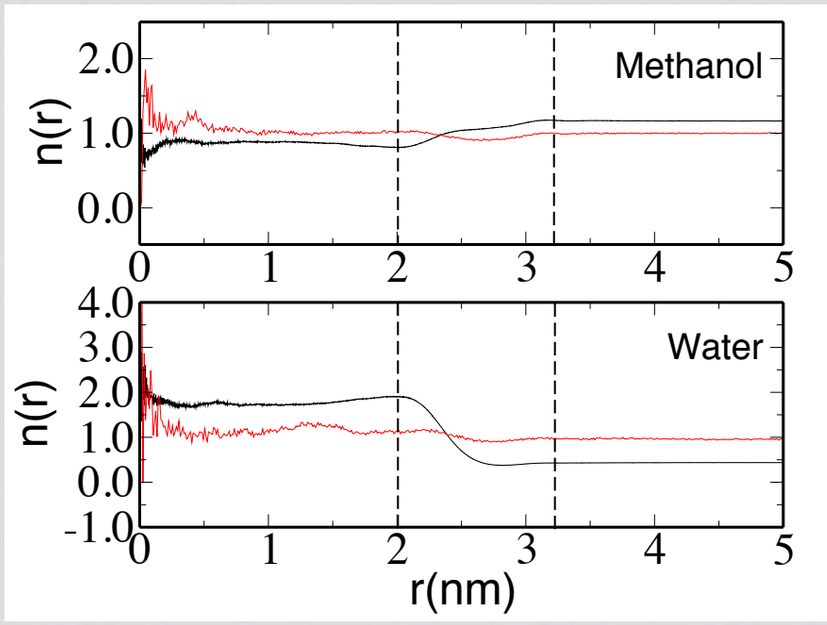
Application of AdResS for "open-boundaries" simulations

When the correct particle fluctuations are important large simulation boxes are needed

Triglycine solvated in aqueous urea



Example of density correction in a methanol-water mixture



A two-component solvent requires two thermodynamic force terms

D. Mukherji, N. F. A. van der Vegt, K. Kremer, and L. Delle Site, JCTC. 8, 375 (2012)
D. Mukherji, N. F. A. van der Vegt, and K. Kremer, JCTC 8, 3536 (2012)

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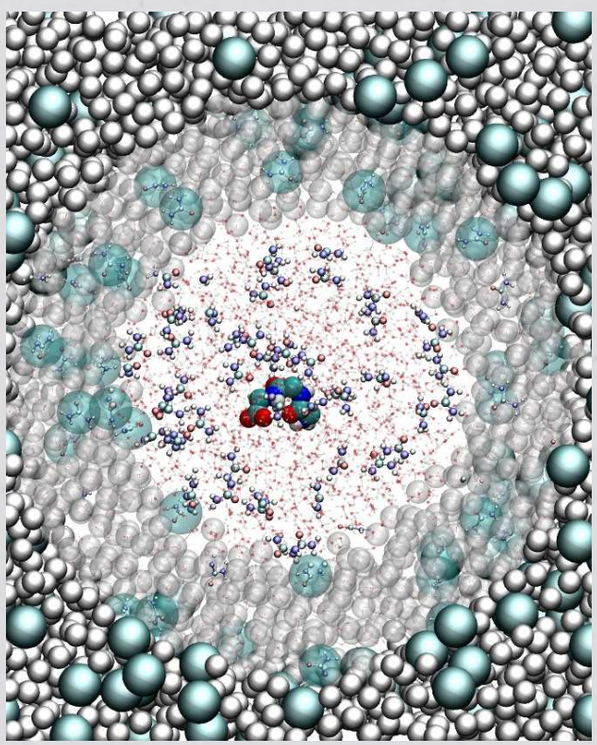

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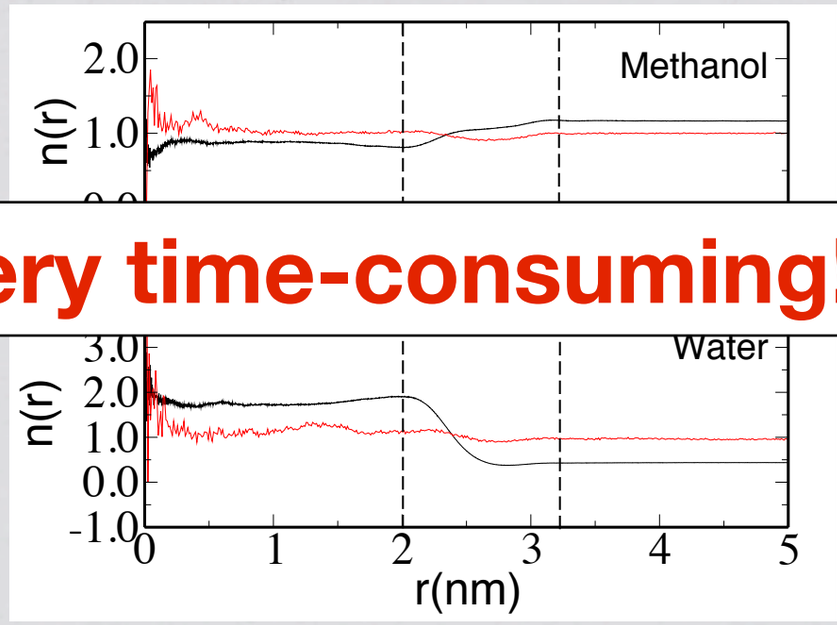

Very time-consuming! :(

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Pros and cons of the force-based approach

A force-based mixing was chosen over an energy-based mixing

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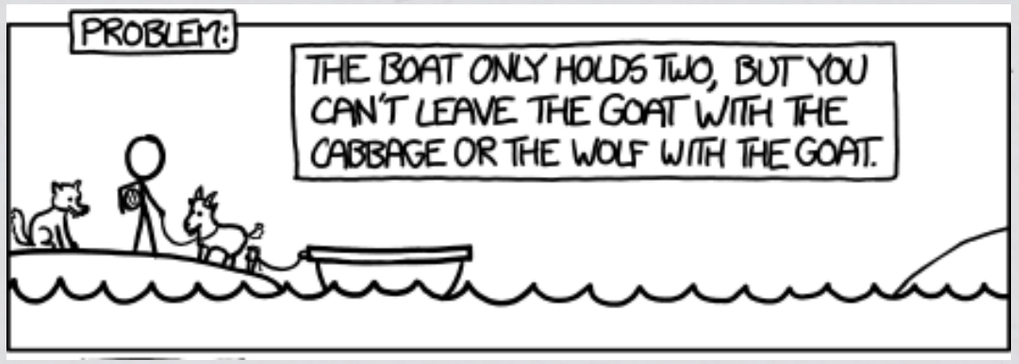

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xkcd.com

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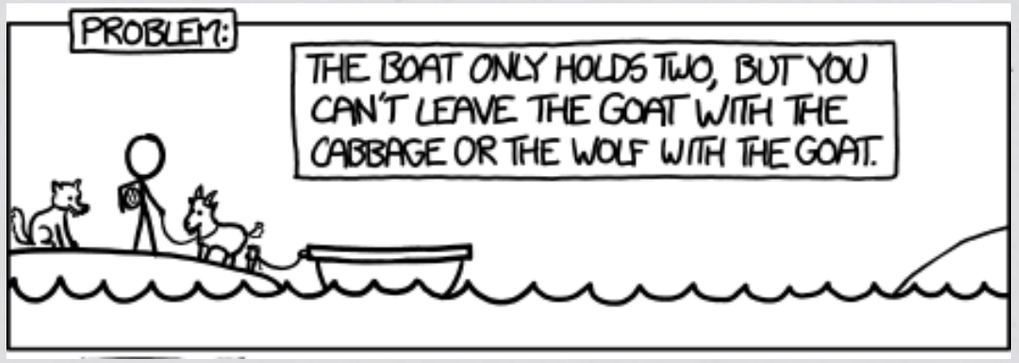

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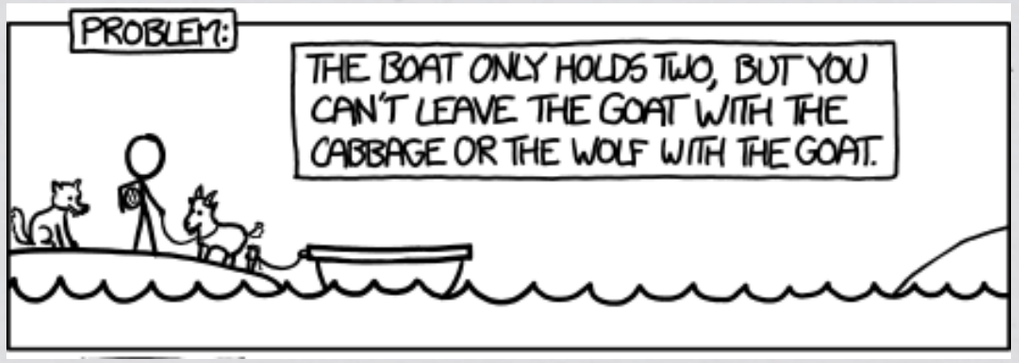

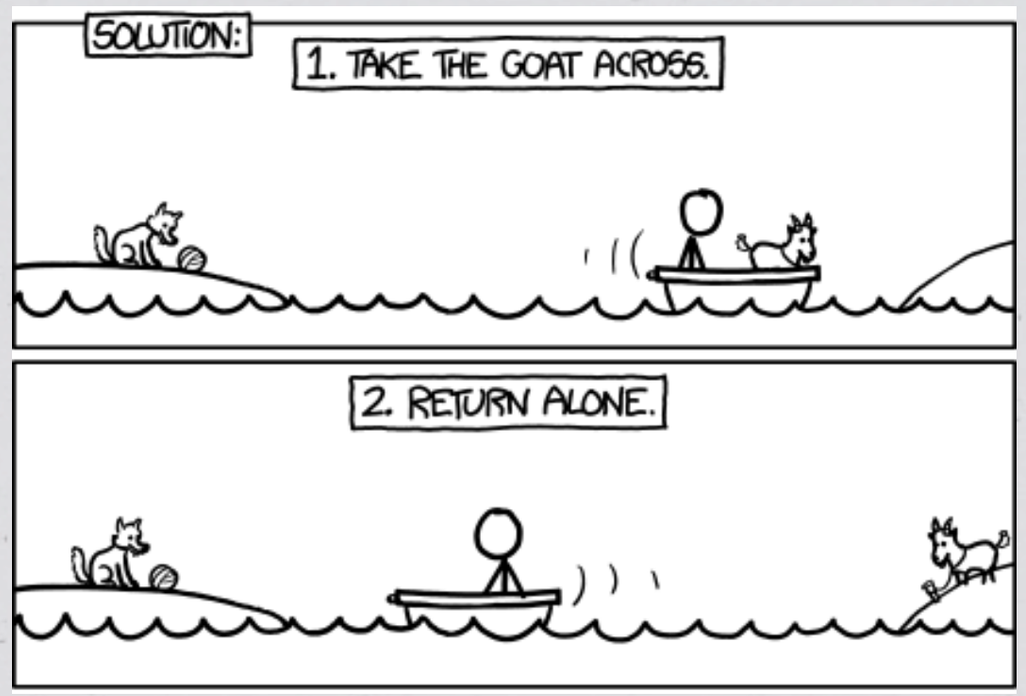

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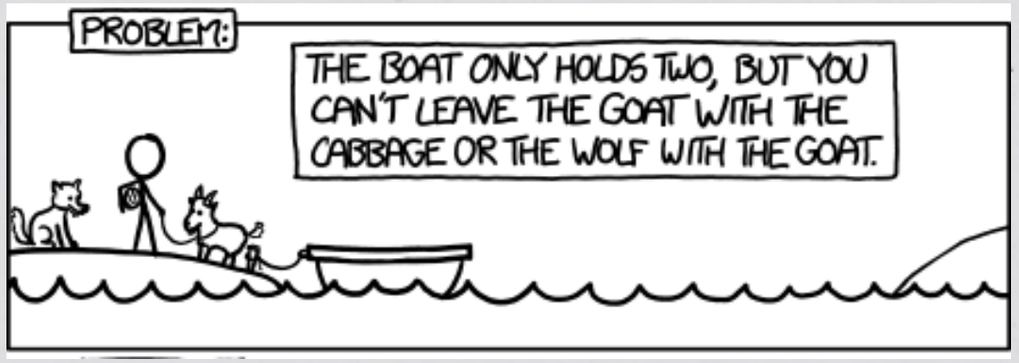

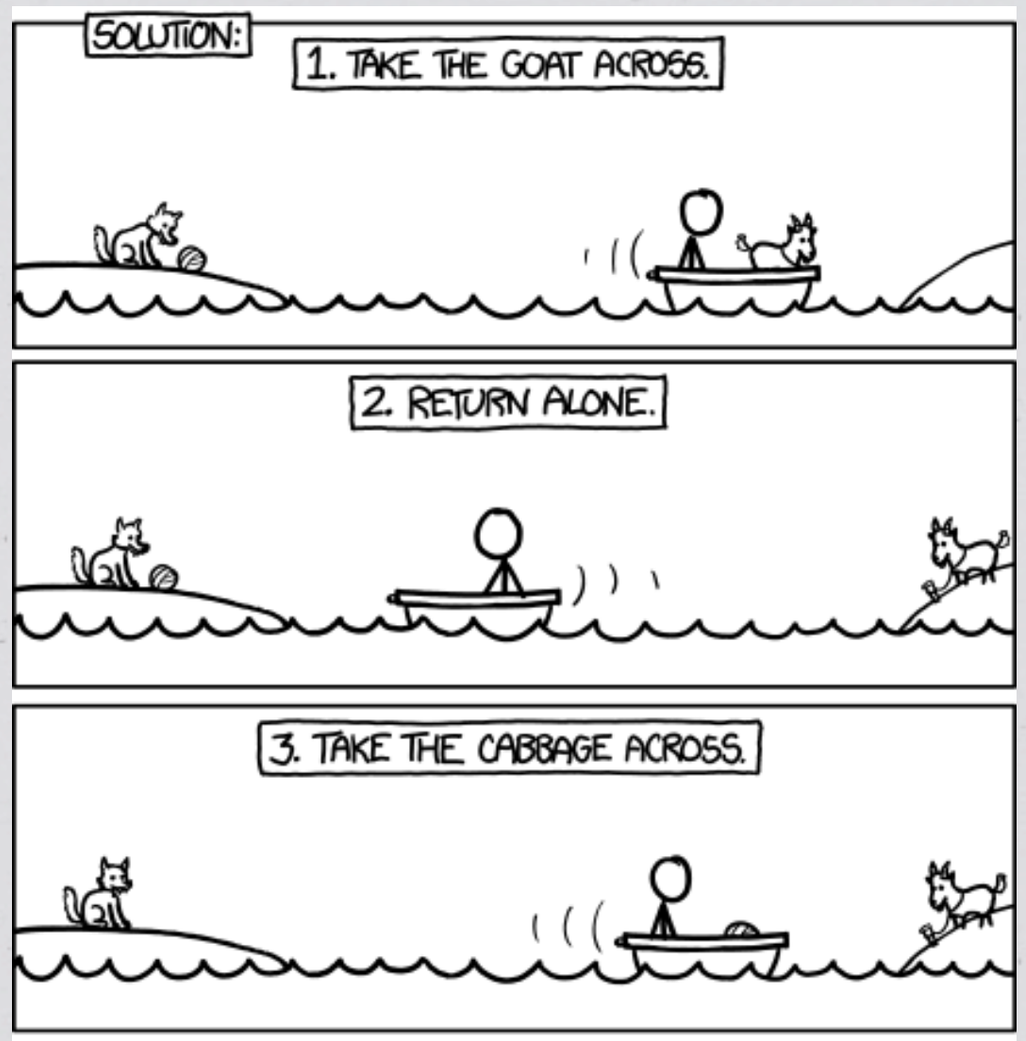

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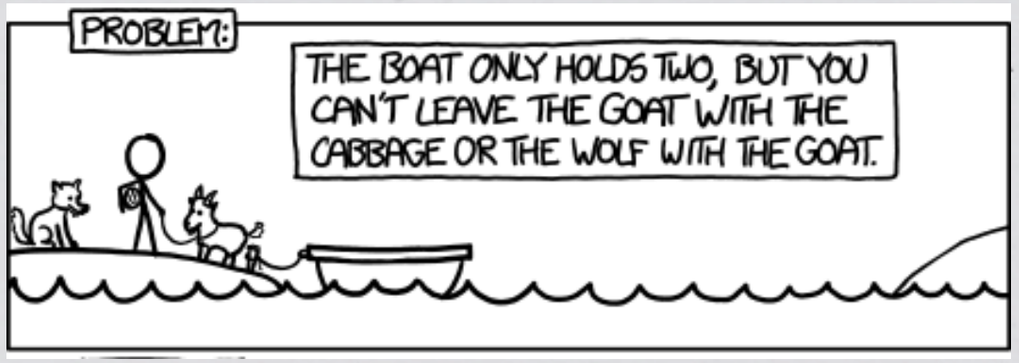

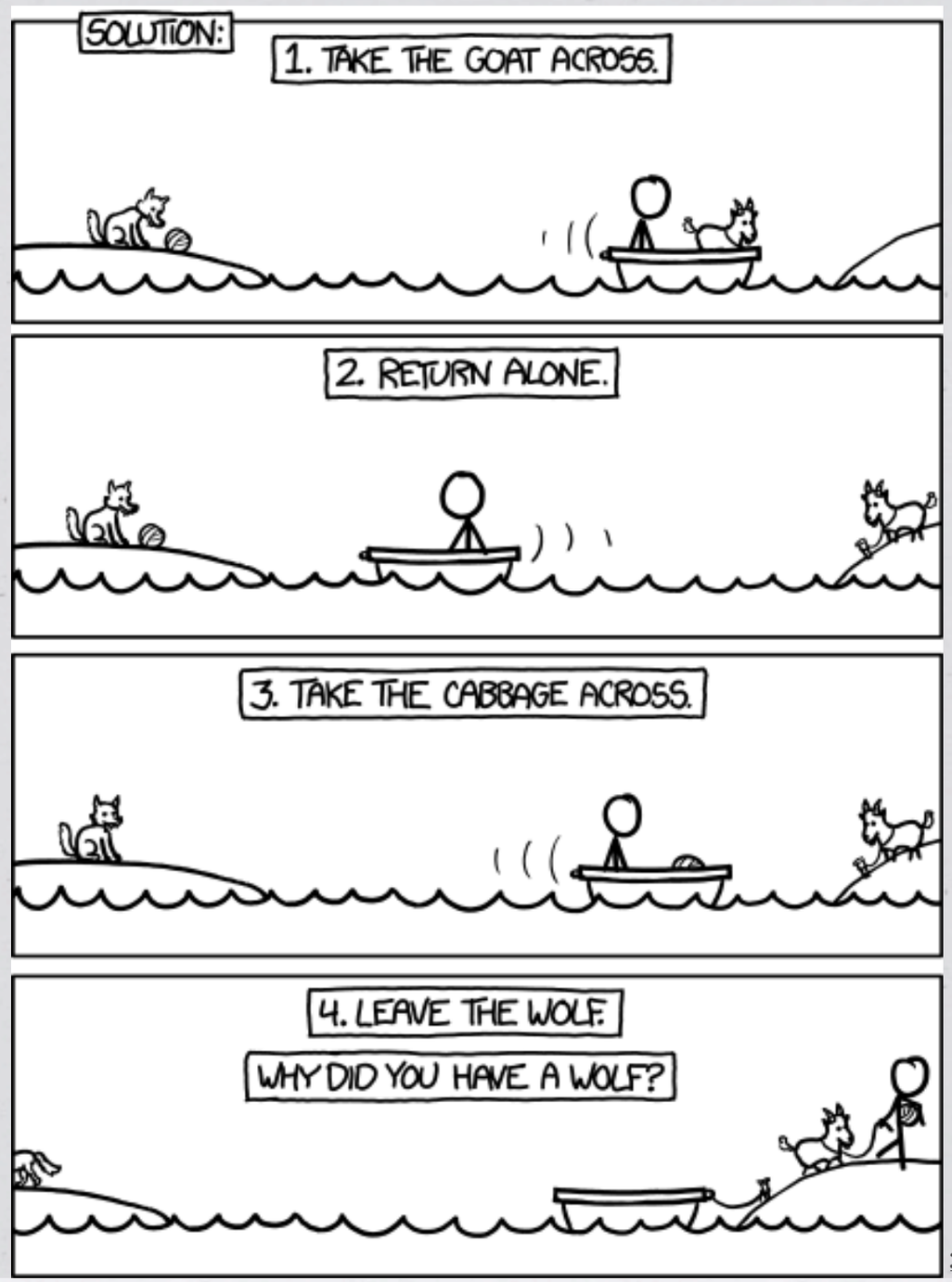

xkcd.com

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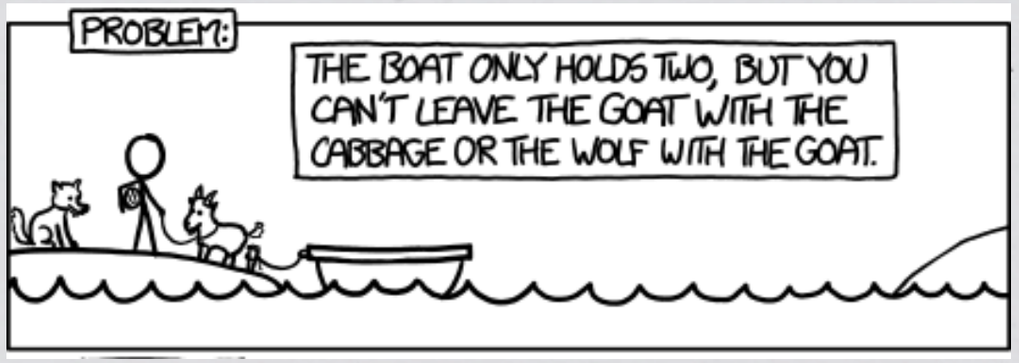

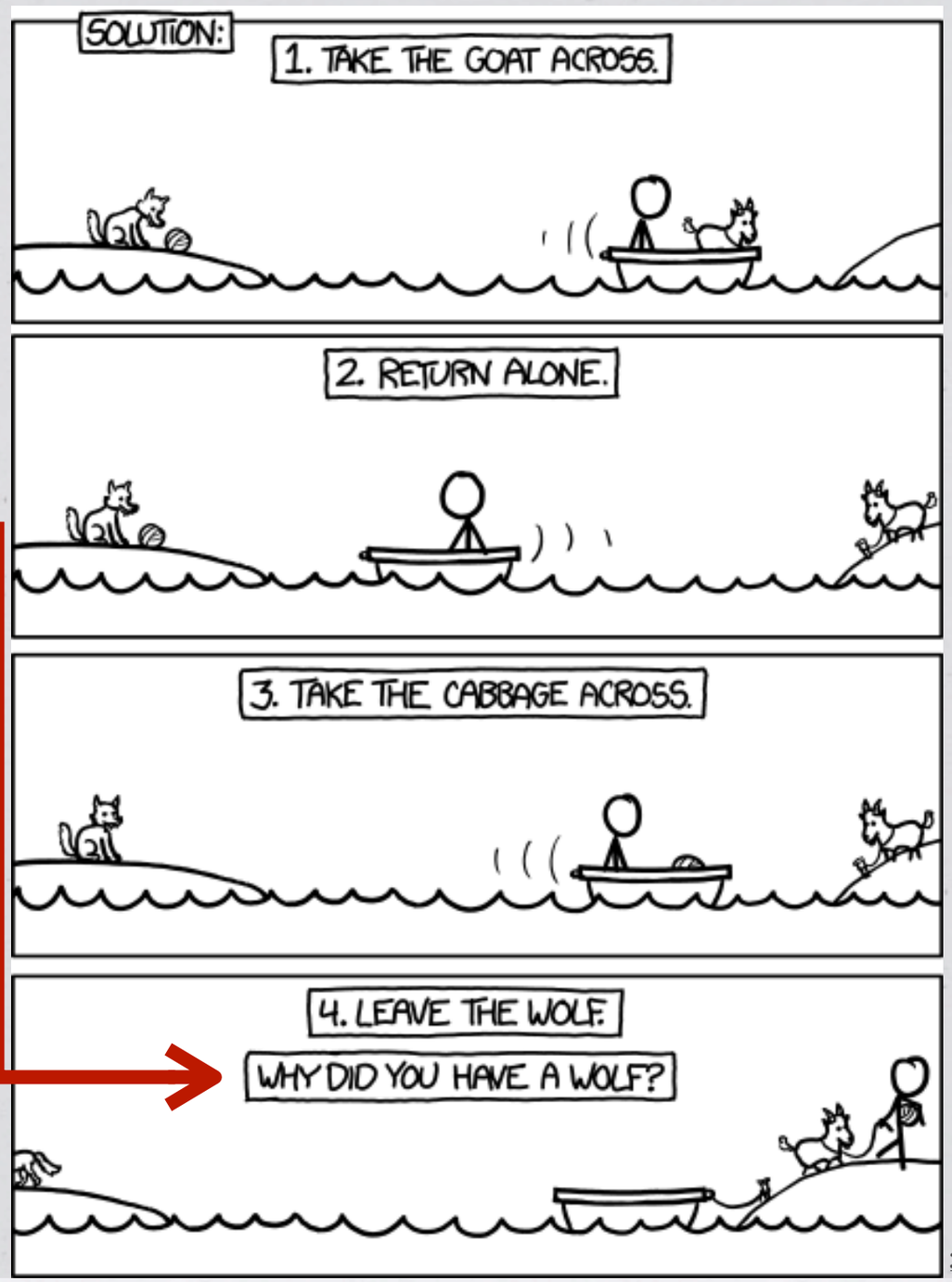

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The H-AdResS method

$$H = \mathcal{K} + V^{int} + \sum_{\alpha} \{\lambda_\alpha V_\alpha^{AA} + (1-\lambda_\alpha) V_\alpha^{CG}\}$$

$$V_\alpha^{\mathrm{AA}} \equiv \frac{1}{2} \sum_{\beta,\beta\neq\alpha}^{N} \sum_{ij} V^{AA}(|\mathbf{r}_{\alpha i} - \mathbf{r}_{\beta j}|)$$

$$V_\alpha^{\mathrm{CG}} \equiv \frac{1}{2} \sum_{\beta,\beta\neq\alpha}^{N} V^{CG}(|\mathbf{R}_\alpha - \mathbf{R}_\beta|)$$

$$\lambda_\alpha = \lambda(\mathbf{R}_\alpha)$$

RP, S. Fritsch, P. Español, R. Delgado-Buscalioni, K. Kremer, R. Everaers and D. Donadio, Phys. Rev. Lett. 110, 108301 (2013)

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The total energies of the molecules are weighted by the switching function

RP, S. Fritsch, P. Español, R. Delgado-Buscalioni, K. Kremer, R. Everaers and D. Donadio, Phys. Rev. Lett. 110, 108301 (2013)

The H-AdResS method

$$H = \mathcal{K} + V^{int} + \sum_{\alpha} \left\{ \lambda_\alpha V_\alpha^{AA} + (1-\lambda_\alpha) V_\alpha^{CG} \right\}$$

$$\begin{aligned} \mathbf{F}_\alpha &= \mathbf{F}_\alpha^{int} + \sum_{\beta,\beta\neq\alpha} \left\{ \frac{\lambda_\alpha + \lambda_\beta}{2} \mathbf{F}_{\alpha|\beta}^{AA} + \left(1 - \frac{\lambda_\alpha + \lambda_\beta}{2}\right) \mathbf{F}_{\alpha|\beta}^{CG} \right\} \\ &- \left[V_\alpha^{AA} - V_\alpha^{CG} \right] \nabla_\alpha \lambda_\alpha \end{aligned}$$

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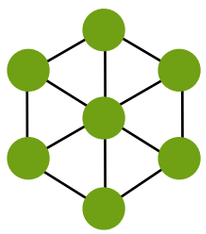
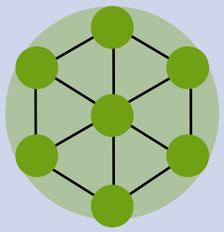
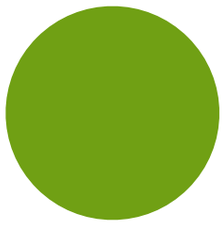


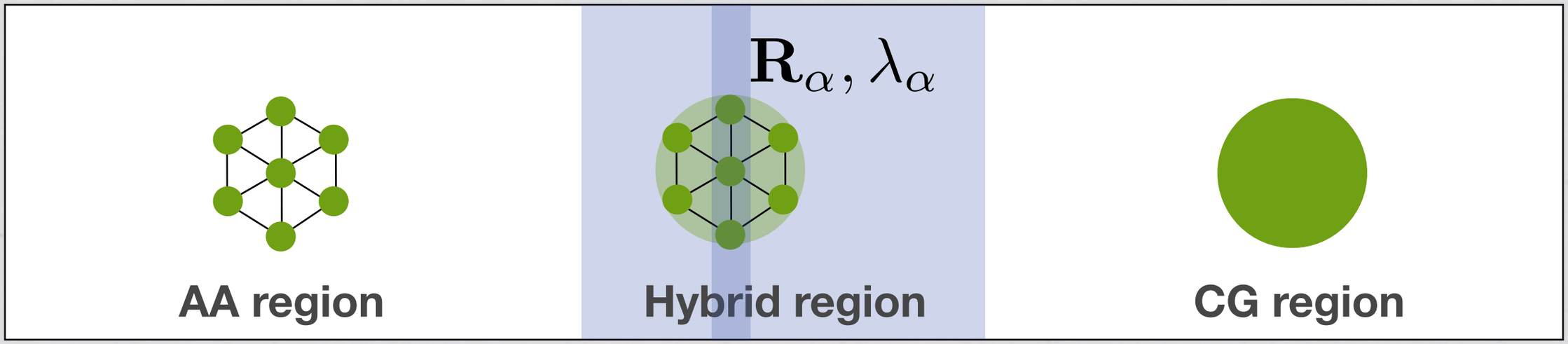
AA region



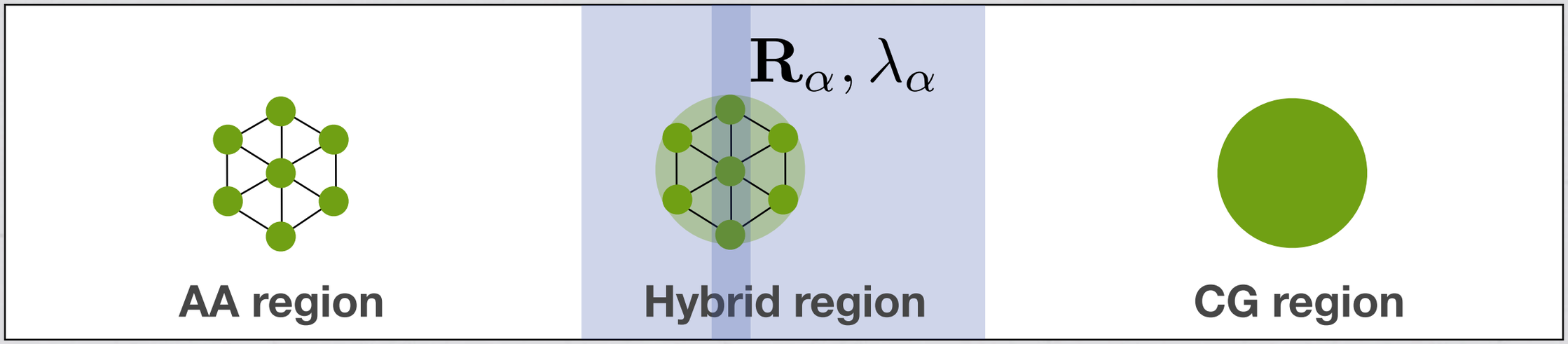
Hybrid region



CG region


$\mathbf{R}_\alpha, \lambda_\alpha$
AA region
Hybrid region
CG region

$$\left\langle \mathbf{F}_\alpha^\nabla \right\rangle = -\left\langle [V_\alpha^{AA} - V_\alpha^{CG}] \right\rangle_{\mathbf{R}_\alpha} \nabla\lambda(\mathbf{R}_\alpha)$$



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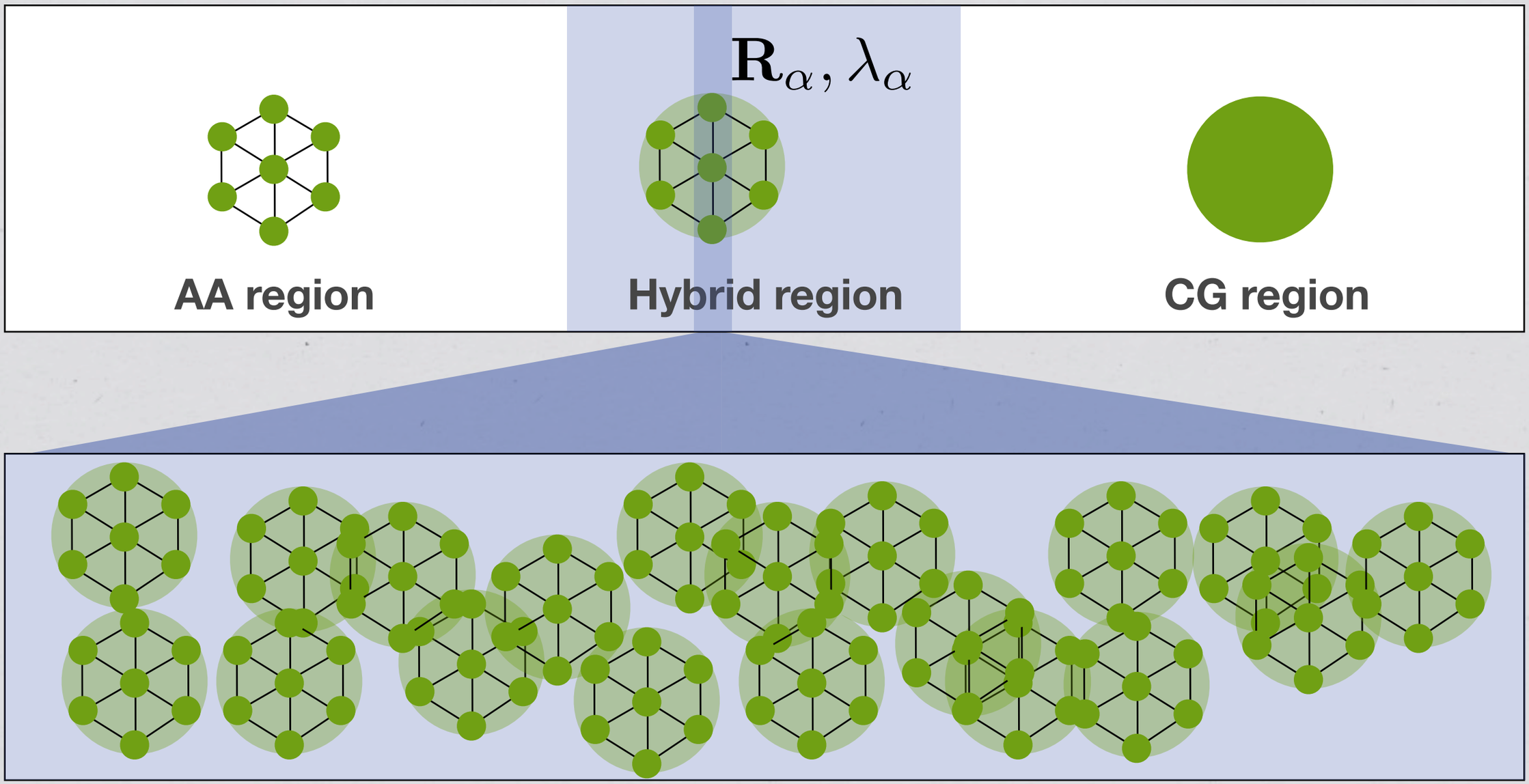

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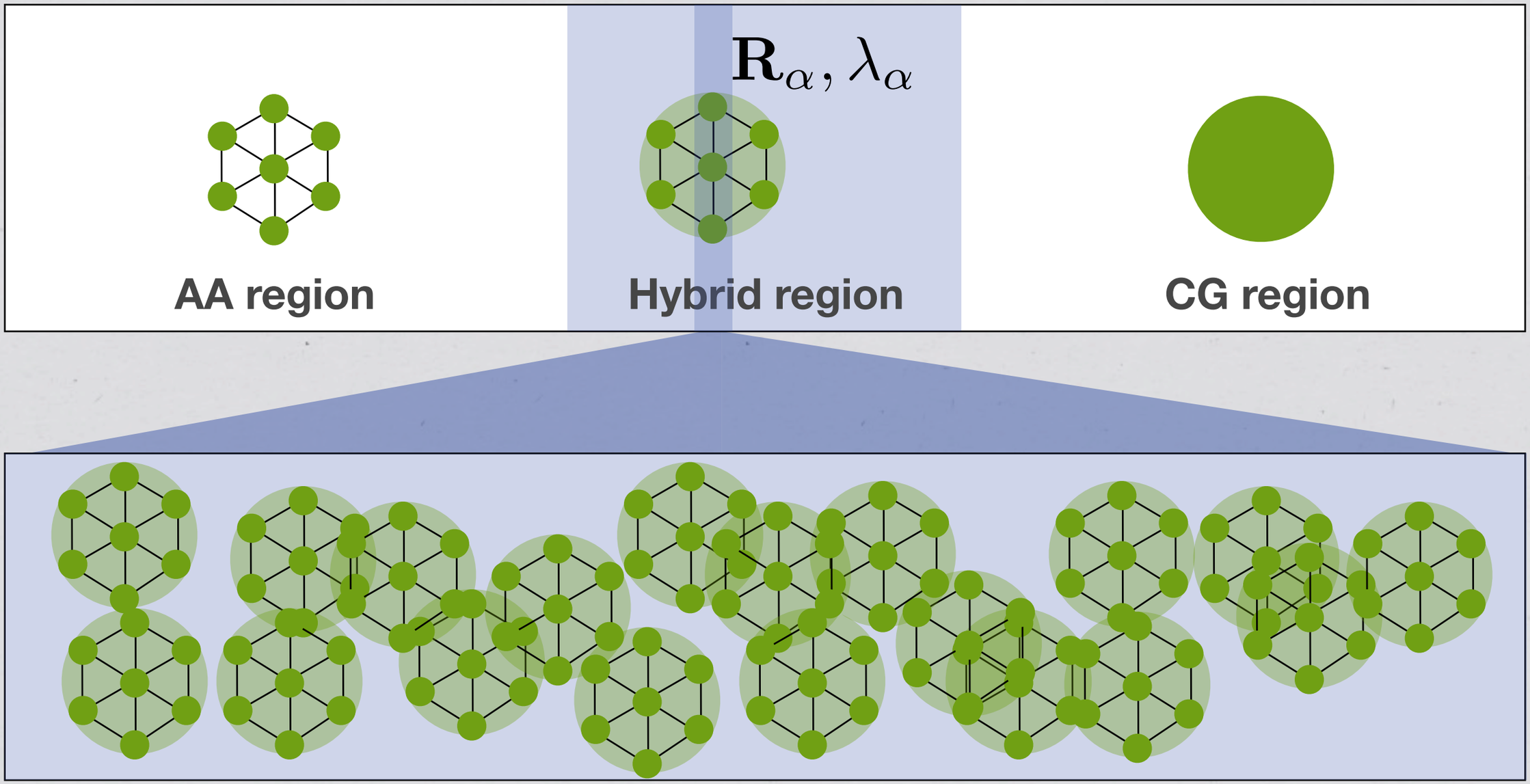

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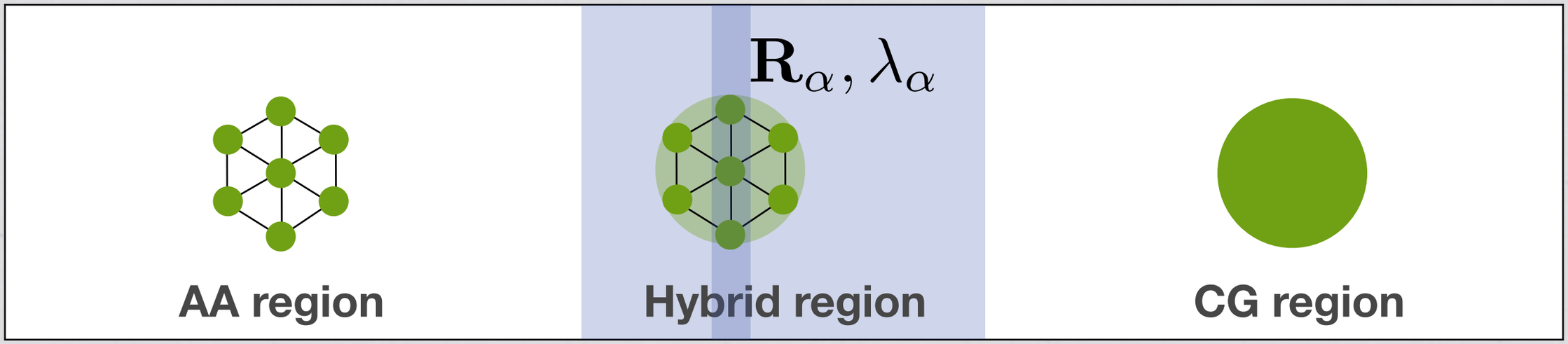

The force in the hybrid region is proportional to the difference of Helmholtz free energy between AA and CG models

Modify the Hamiltonian introducing a compensation term

$$H_\Delta = H - \sum_{\alpha=1}^{N} \Delta H(\lambda(\mathbf{R}_\alpha))$$

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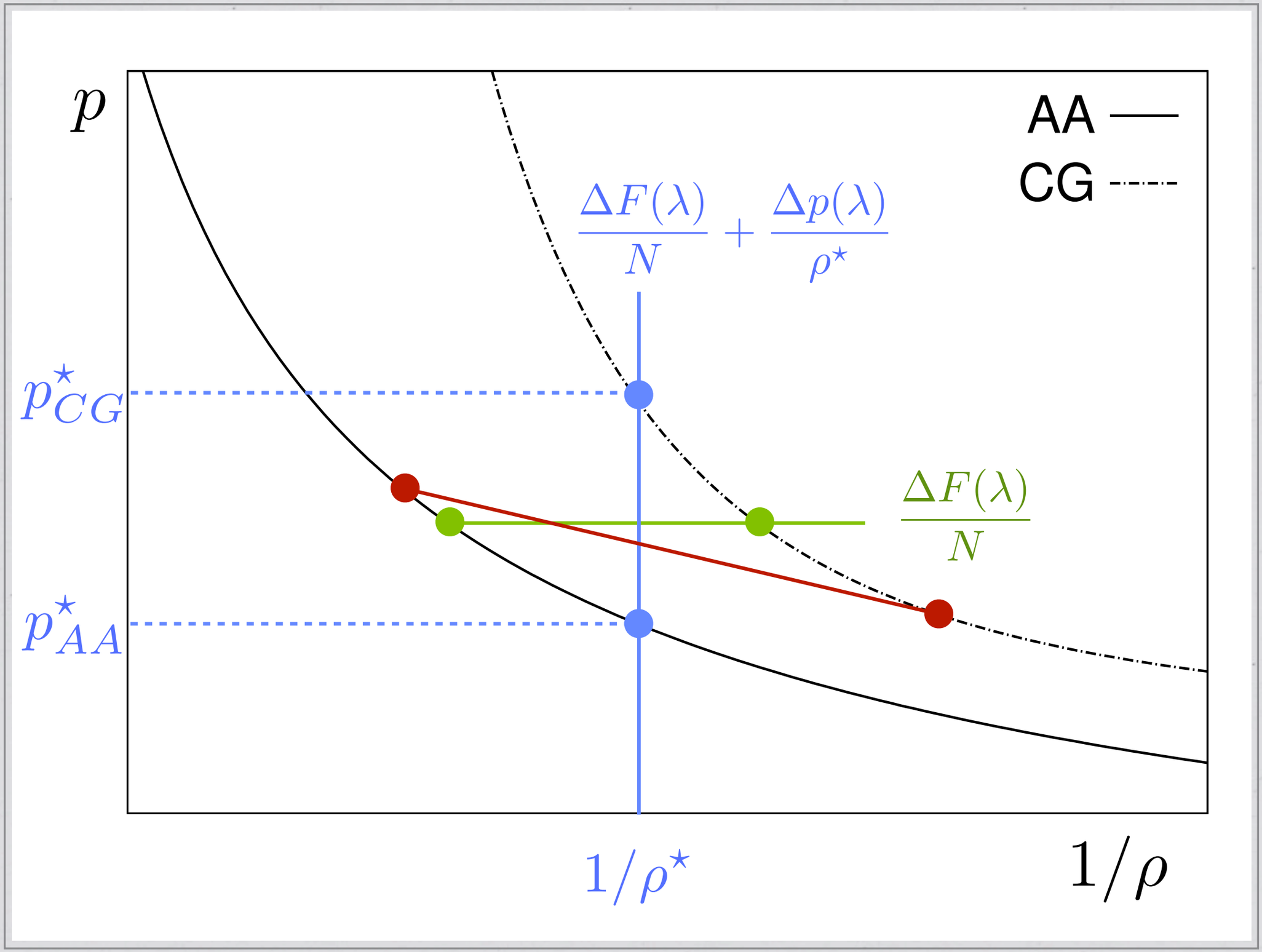
To remove the pressure imbalance between AA and CG we employ **Gibbs free energy** difference:

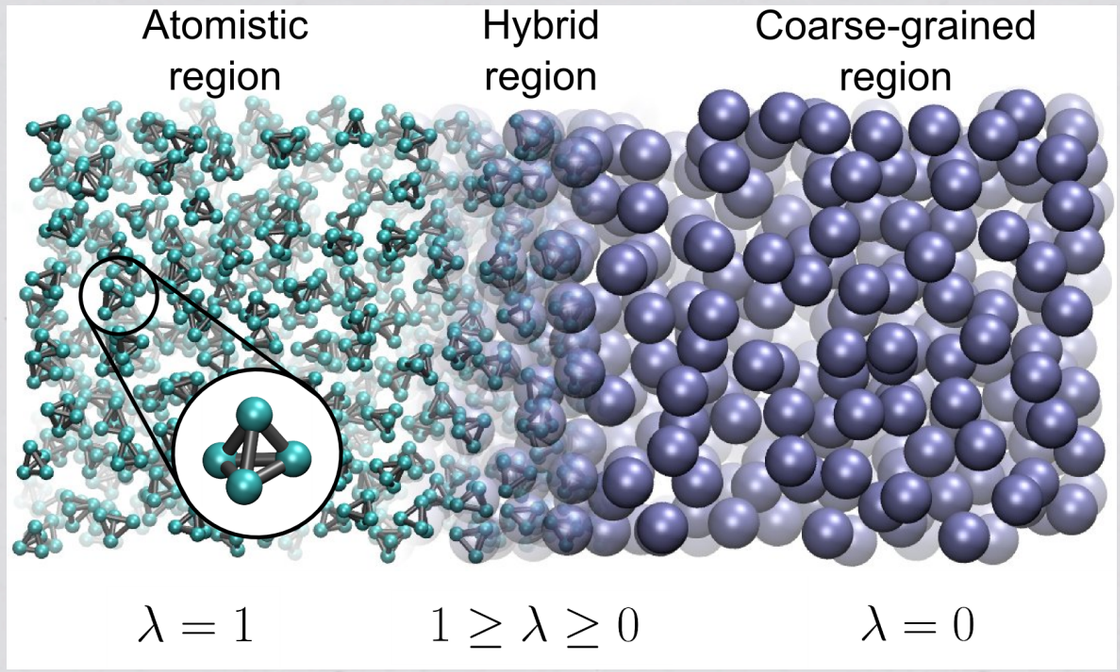
$$\Delta H(\lambda) \equiv \Delta\mu(\lambda) = \frac{\Delta F(\lambda)}{N} + \frac{\Delta p(\lambda)}{\rho^\star}$$

The big picture

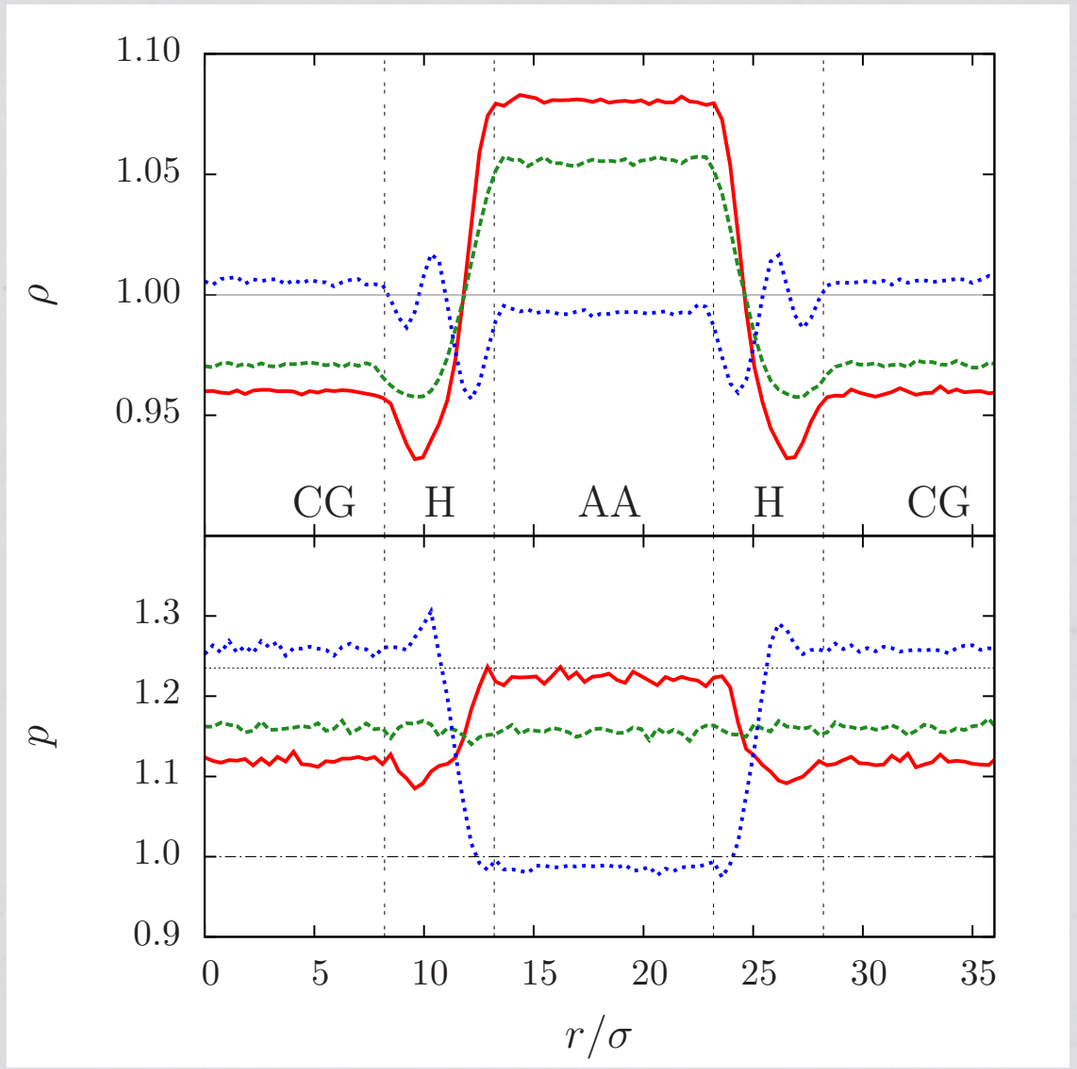


MicroCanonical simulations

Energy-conserving simulations of a simple toy model system



- Tetrahedral purely-repulsive molecules
- The CG potential is NOT parametrized on the AA system



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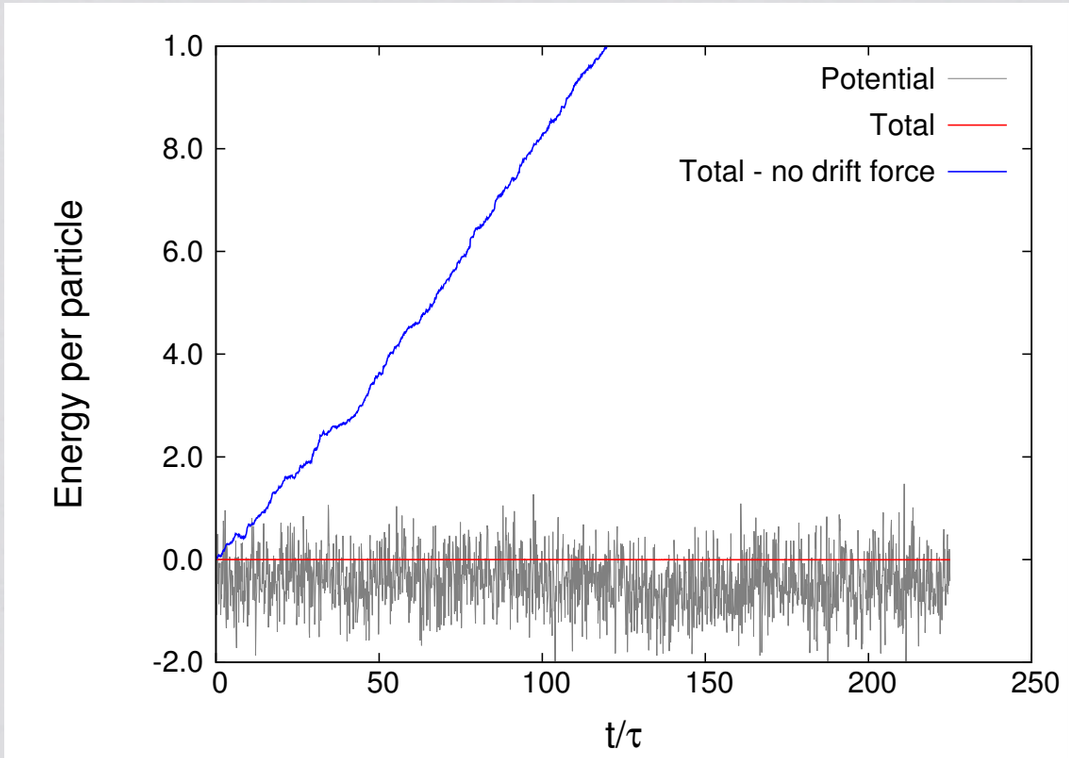

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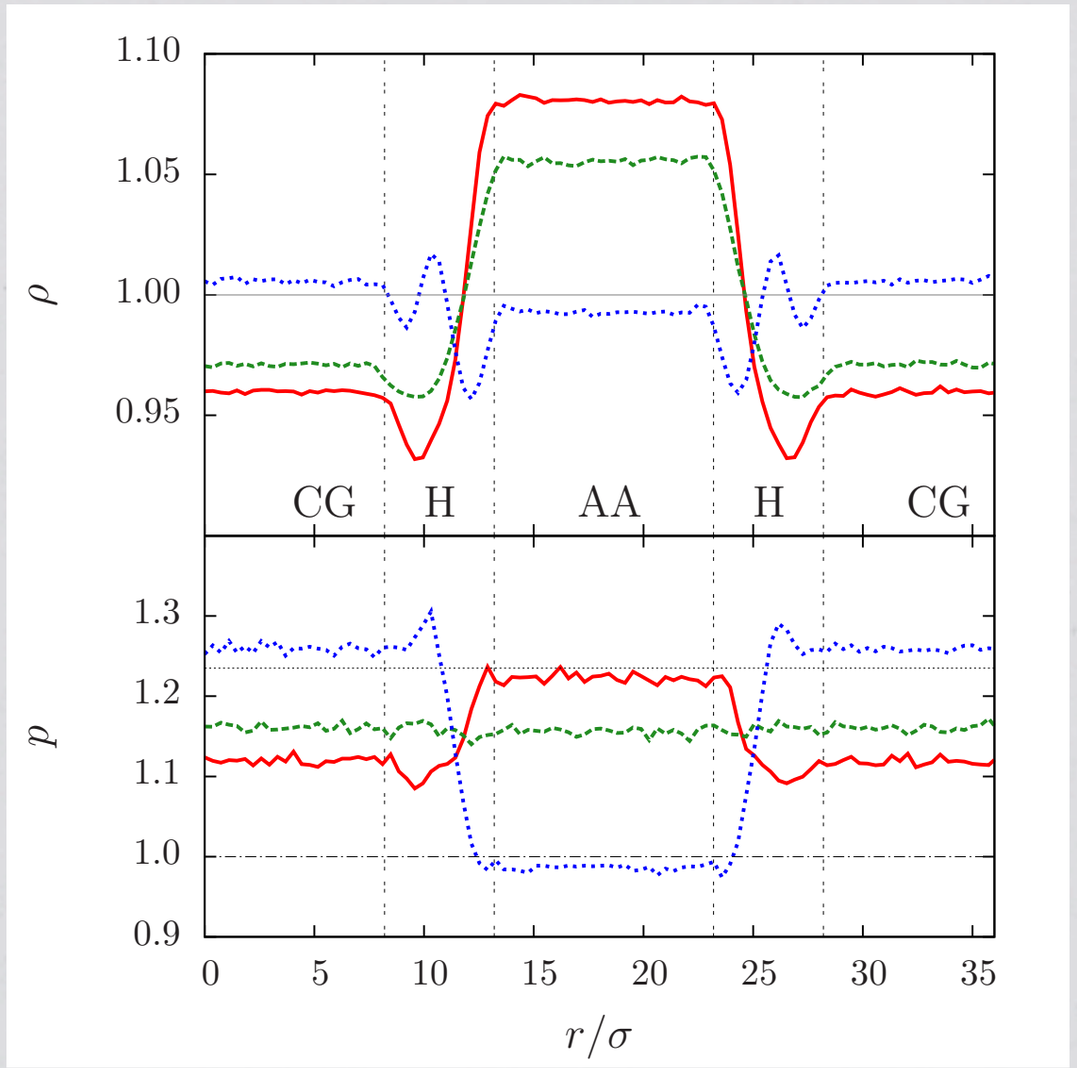
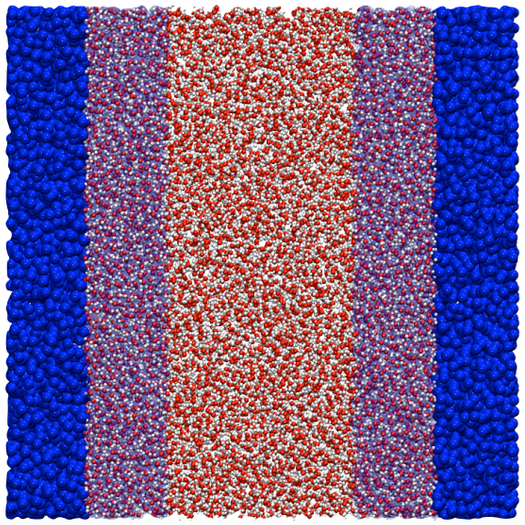
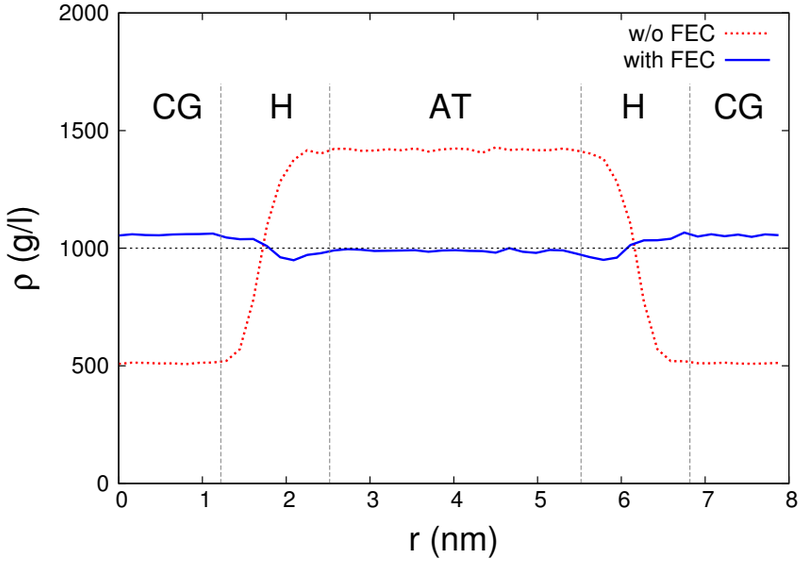
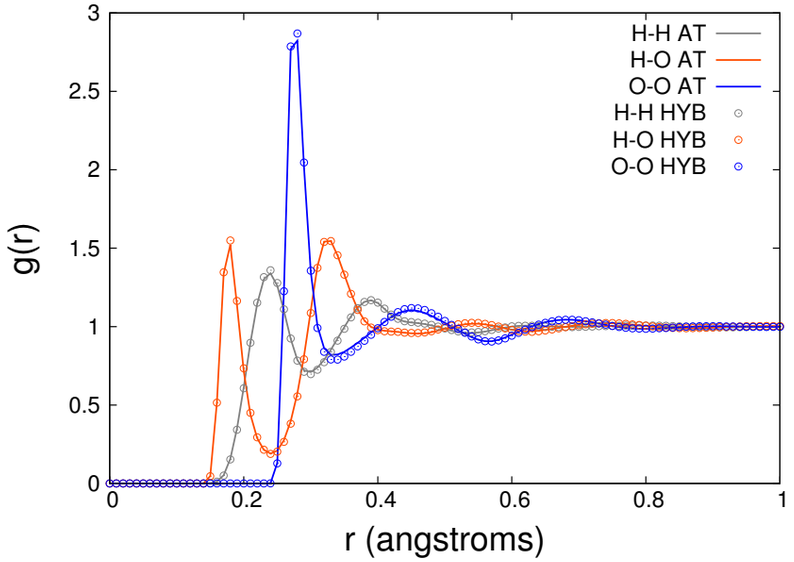


NVT simulations

Thermostated simulation of a water system







The CG potential is NOT parametrized on the AA system

Extension to multicomponent systems

Hamiltonian of a binary mixture

$$
\begin{aligned}
H^{MIX} &= \mathcal{K} + V^{int} \\
&+ \sum_{a \in A} \left[\lambda_a V_a^{AT} + (1 - \lambda_a) V_a^{CG} \right] \\
&+ \sum_{b \in B} \left[\lambda_b V_b^{AT} + (1 - \lambda_b) V_b^{CG} \right]
\end{aligned}
$$

How can we control the thermodynamics of both species?

Extension to multicomponent systems

$$H_{\Delta}^{MIX} = H^{MIX} - \sum_{a \in A} \Delta H_A(\lambda_a) - \sum_{b \in B} \Delta H_B(\lambda_b)$$

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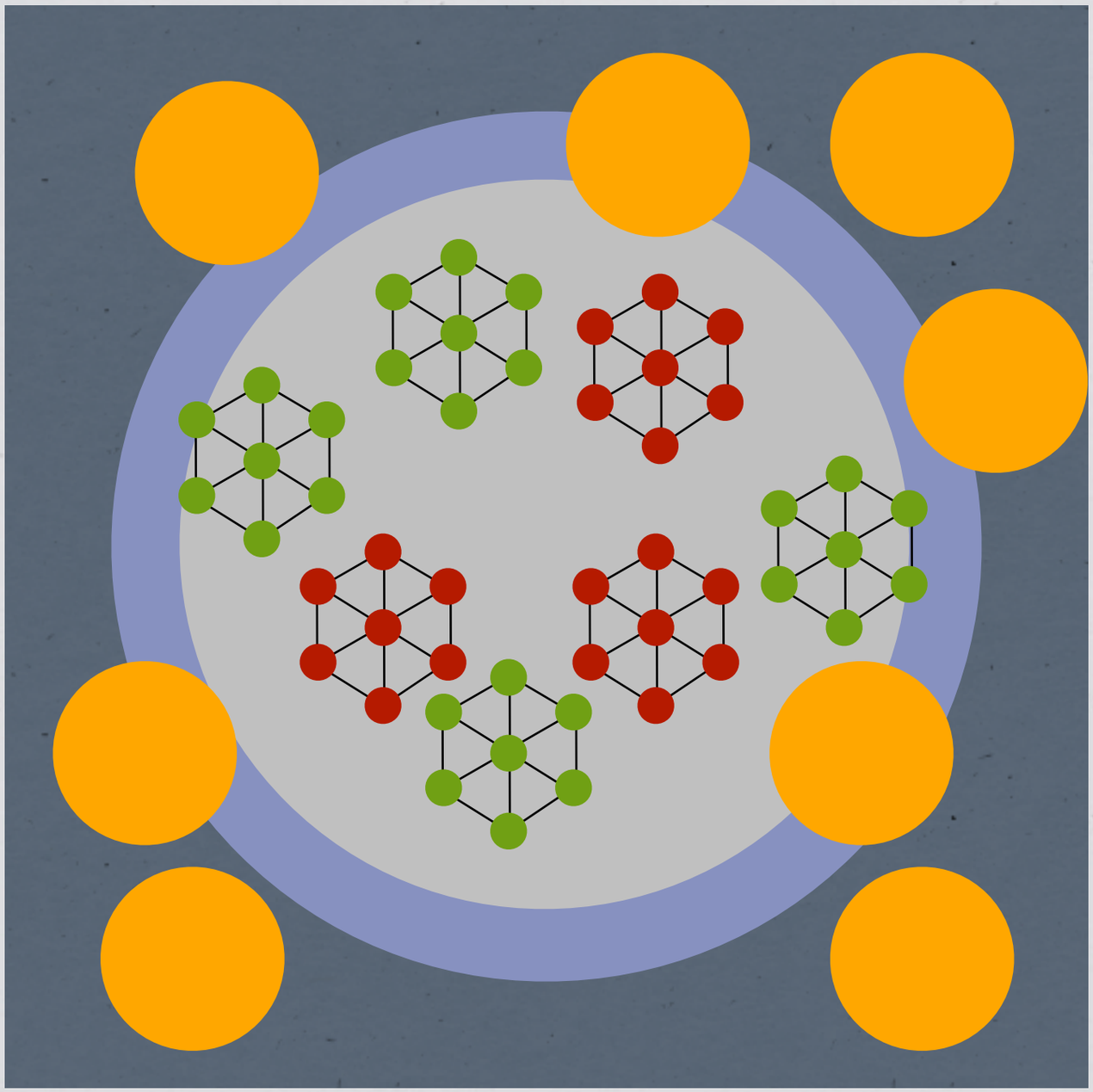
All compensation terms are computed with
a single Kirkwood Thermodynamic Integration

The Free Energy Compensation method as a replacement for coarse-graining



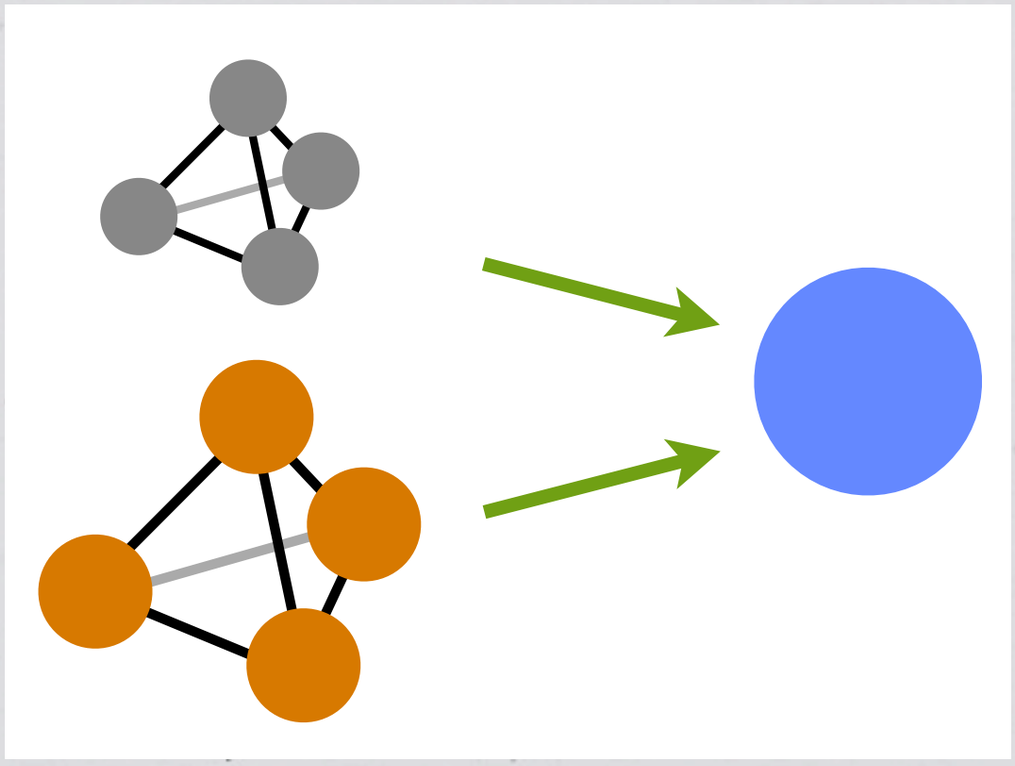
The hybrid region can interface **arbitrarily different models** while preserving the equilibrium properties of the high-resolution region

A problem-specific CG interaction can be chosen at will

Accurate coarse-graining of the high-resolution system is thus not necessary

Monte Carlo simulation of a binary mixture - Case I

Binary mixture composed by two DIFFERENT species in EQUAL proportions



The SAME coarse-grained model is used for both

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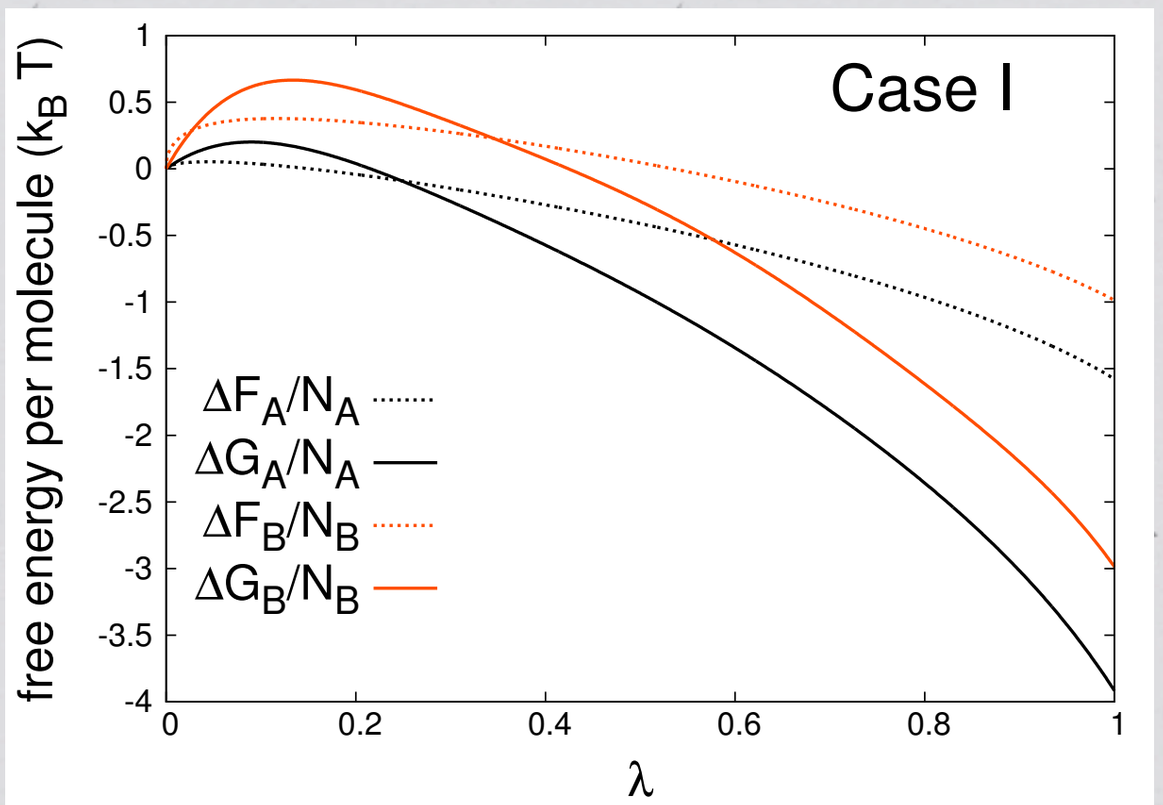

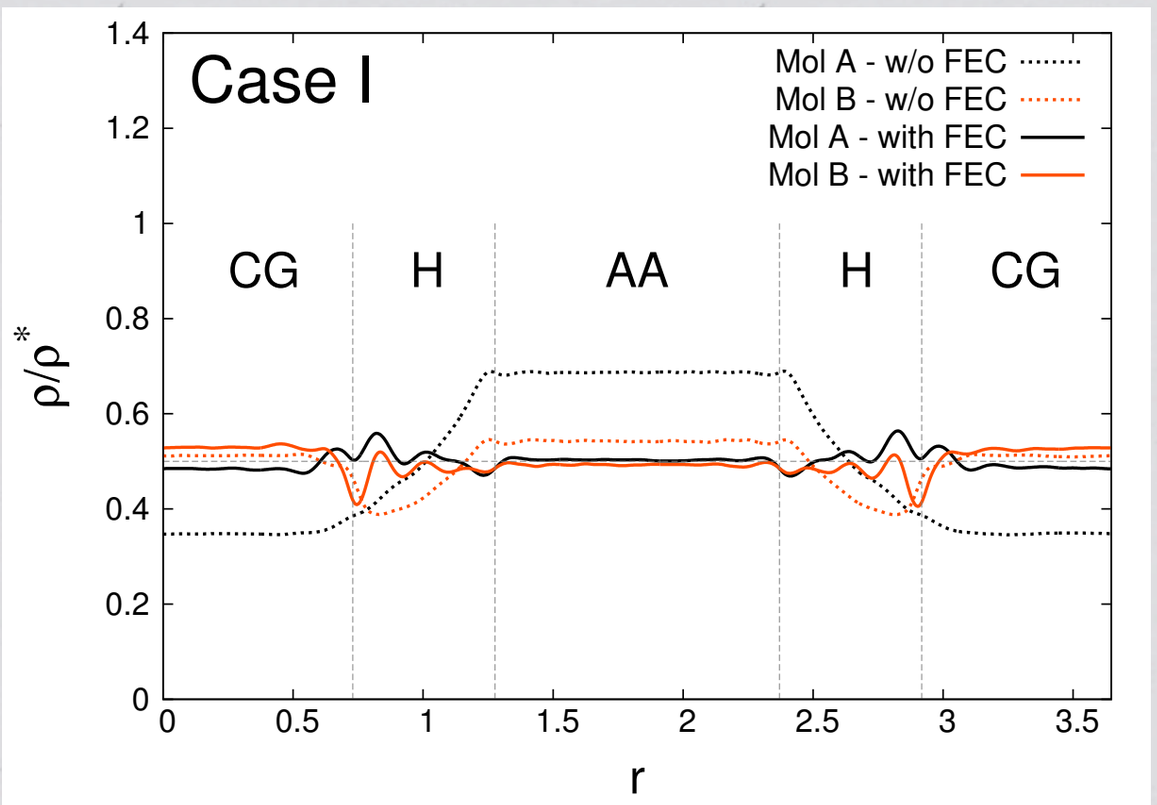

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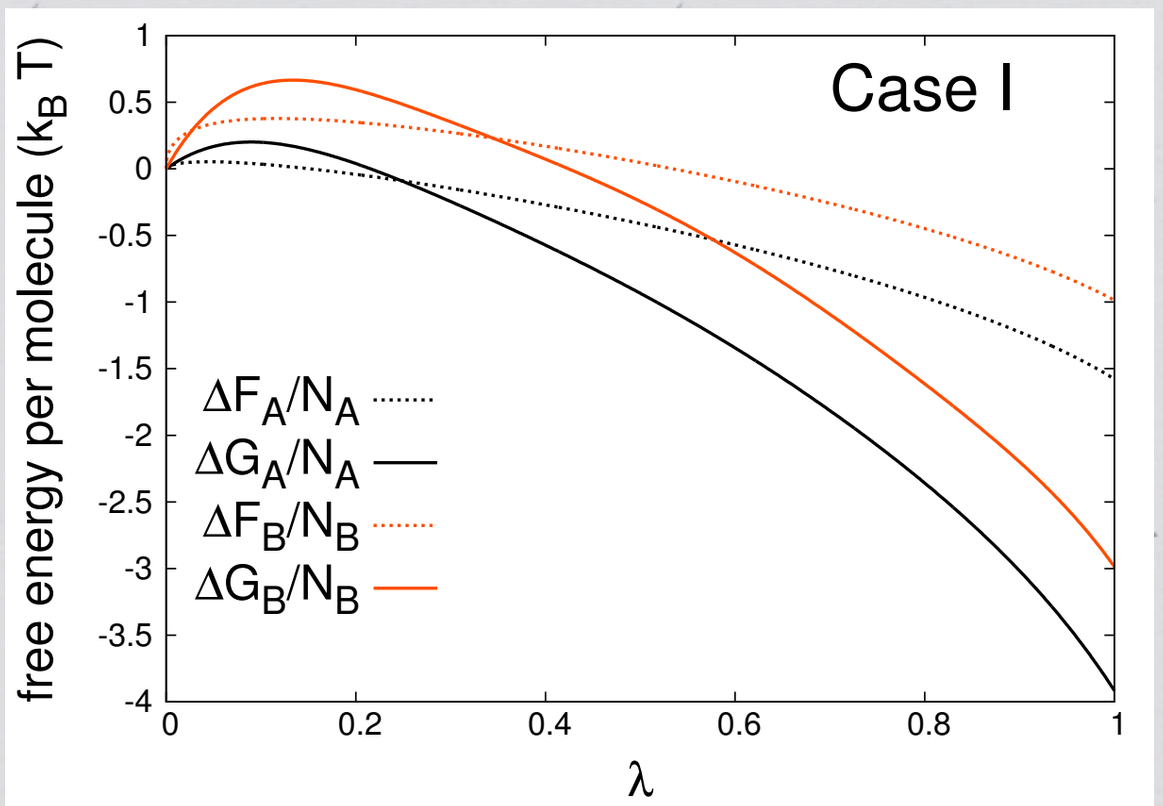

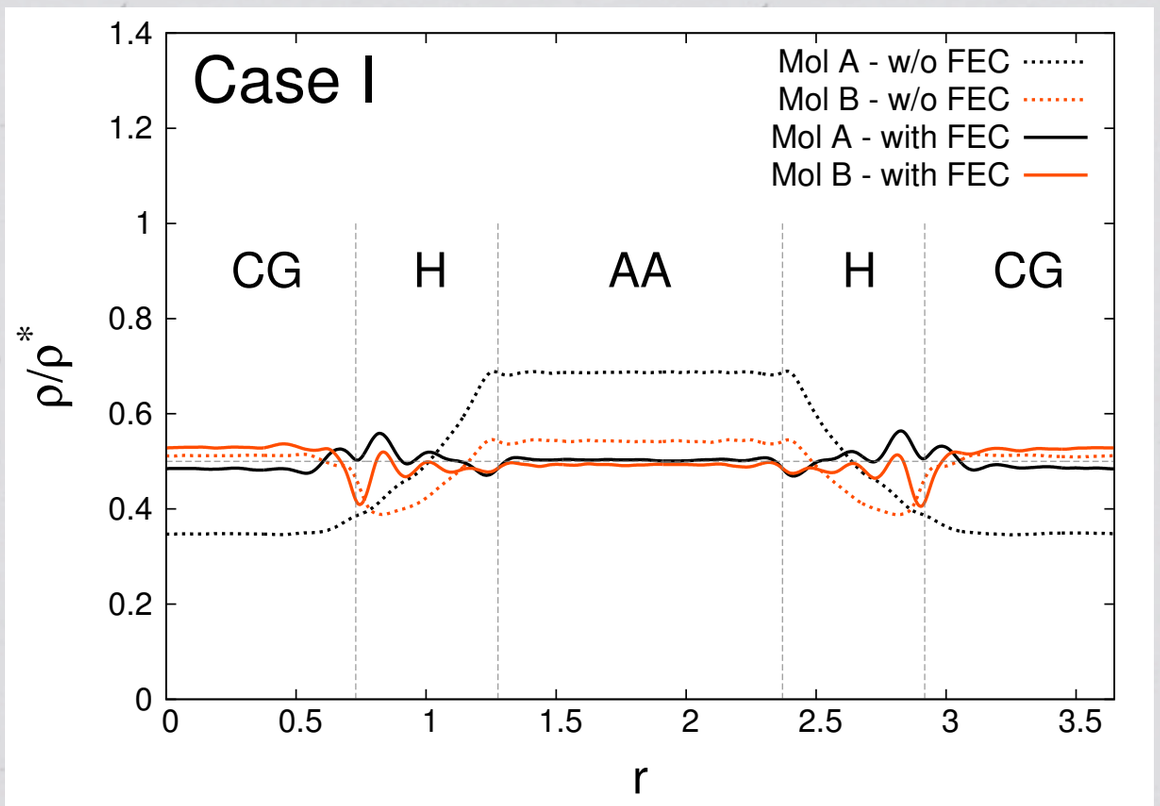

The reference density is preserved

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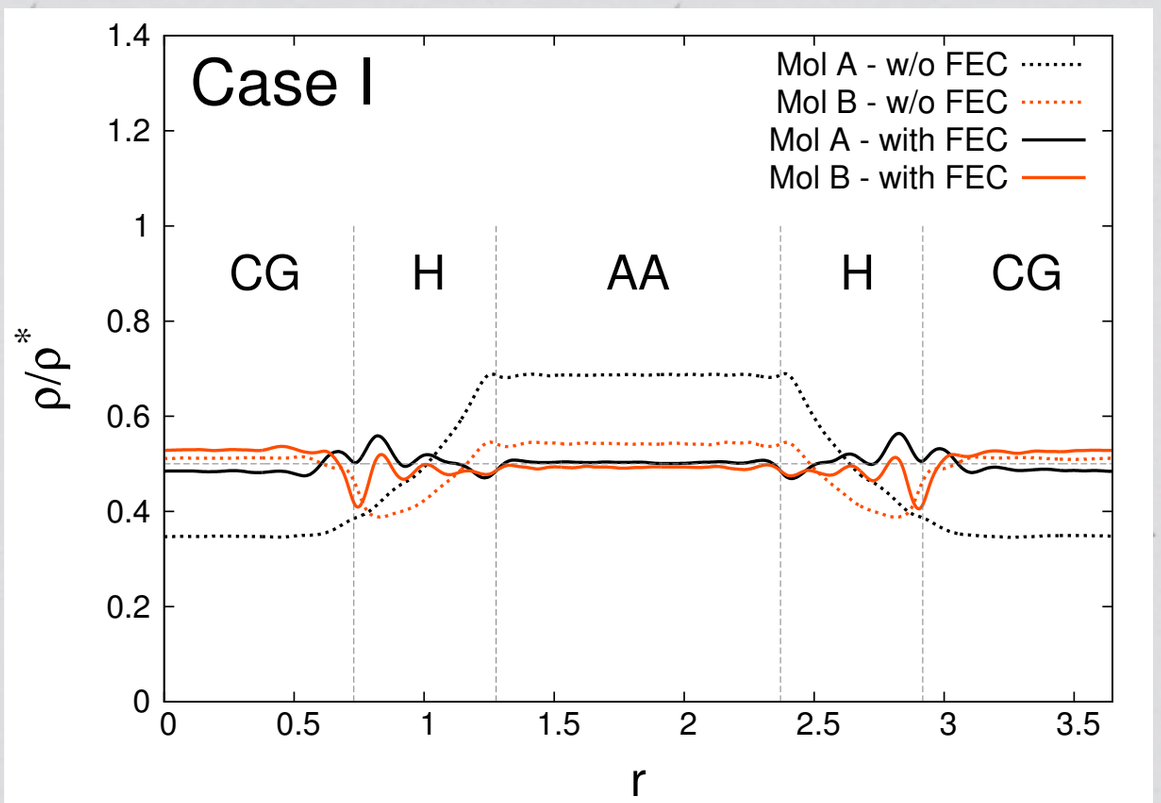

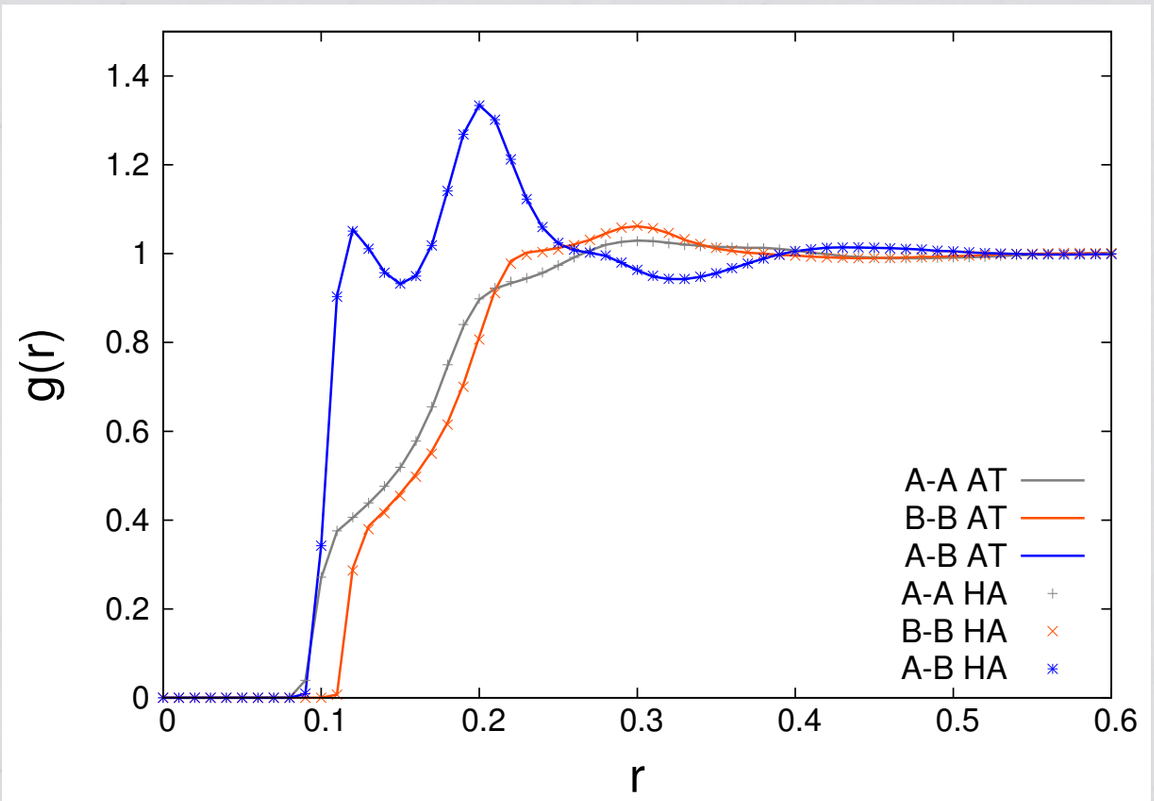

- ☑ **The reference density is preserved**
- ☑ **The pairwise structure is preserved**

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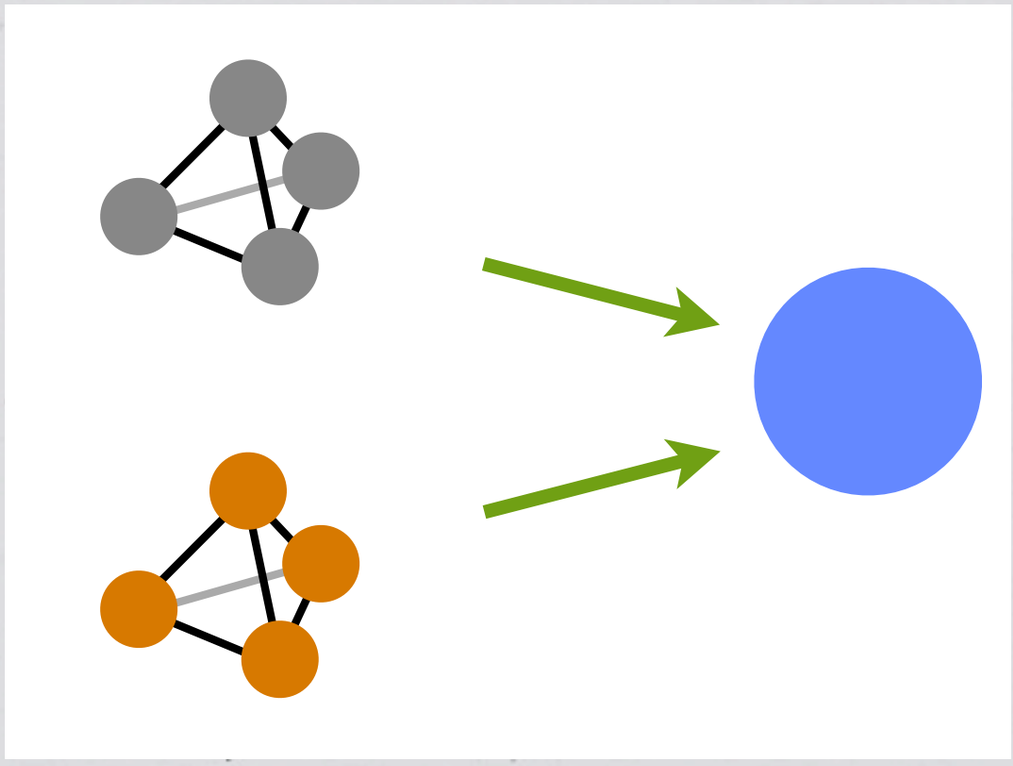
Monte Carlo simulation of a binary mixture - Case II

Binary mixture composed by two EQUAL species in DIFFERENT proportions



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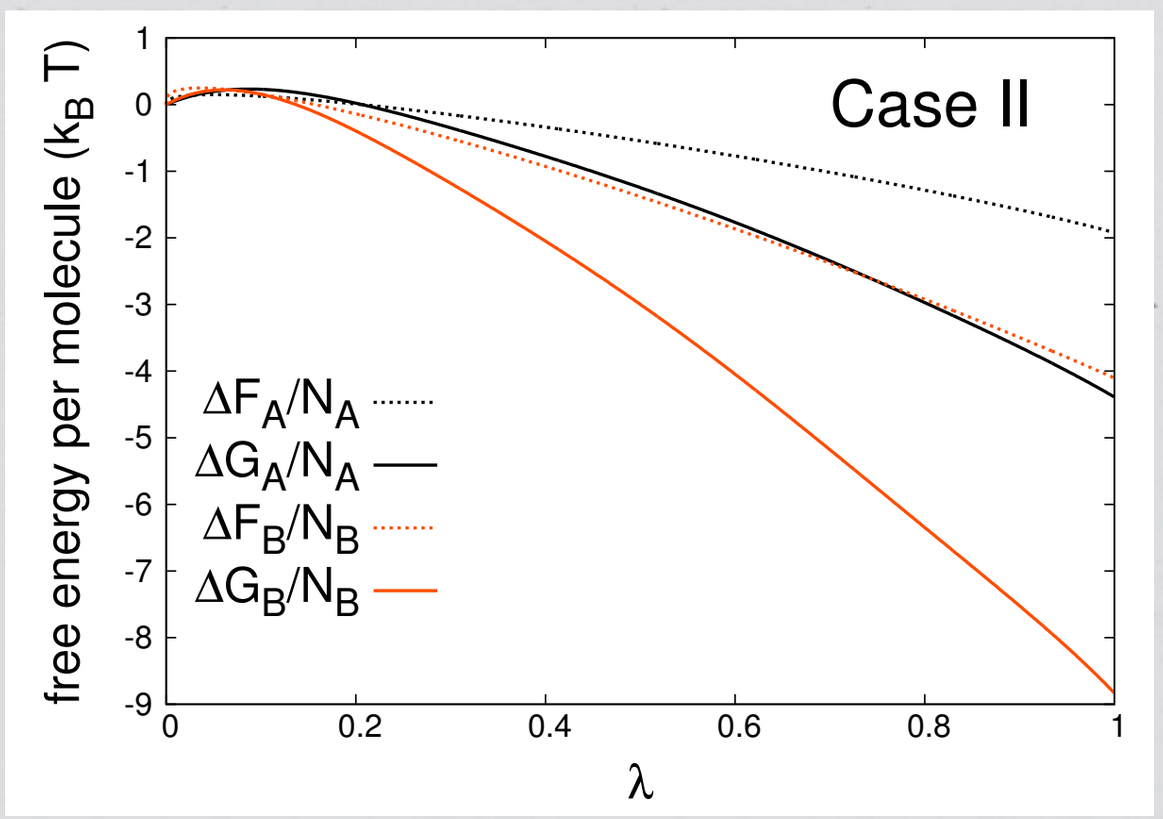

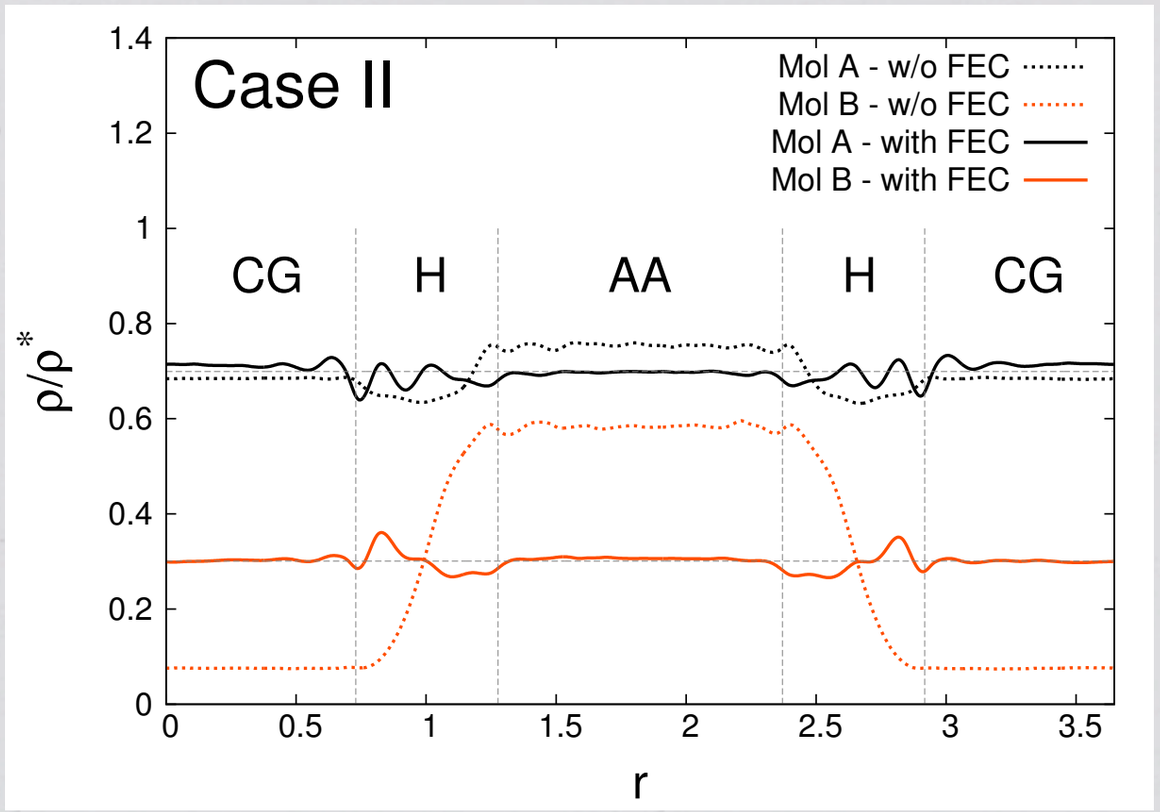

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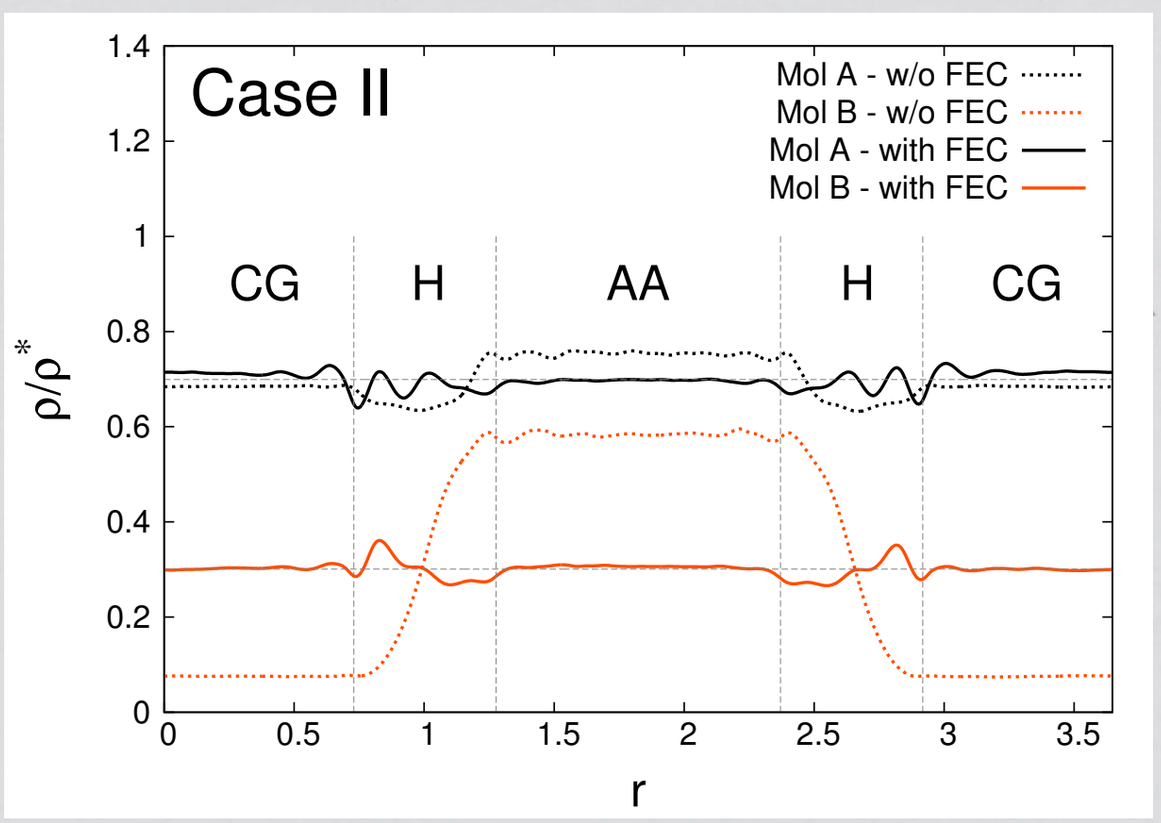

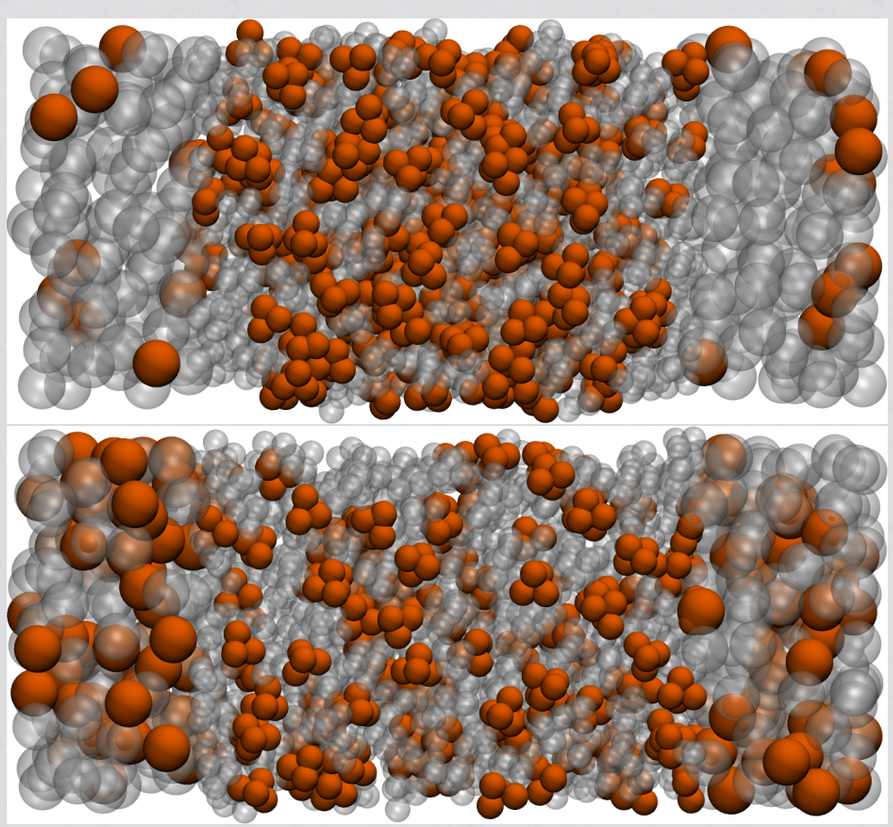

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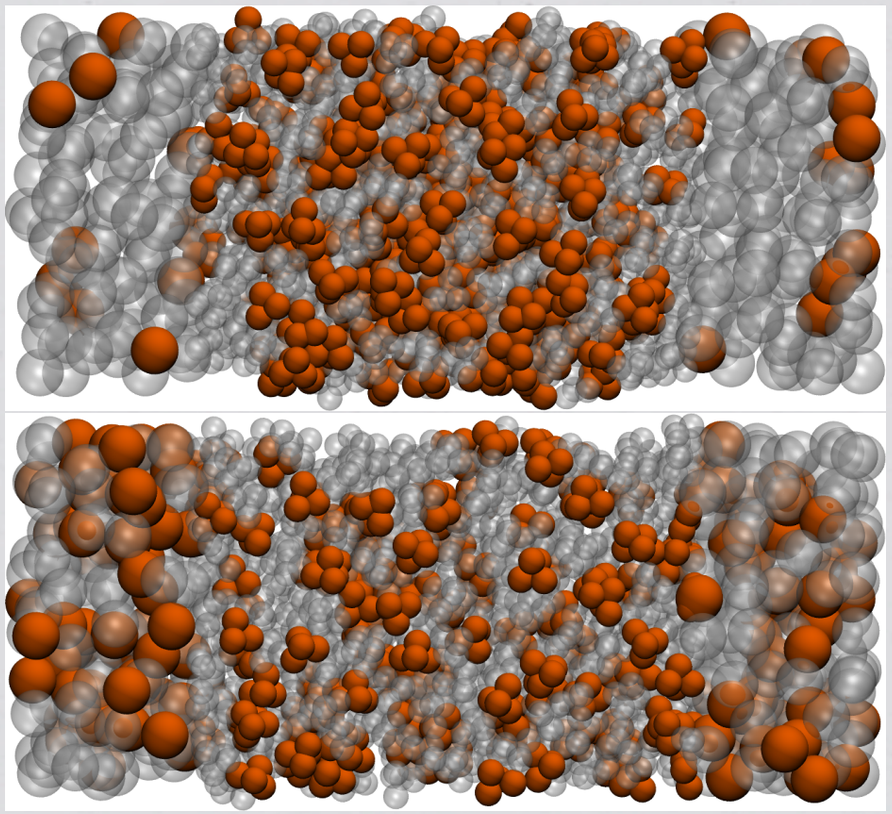

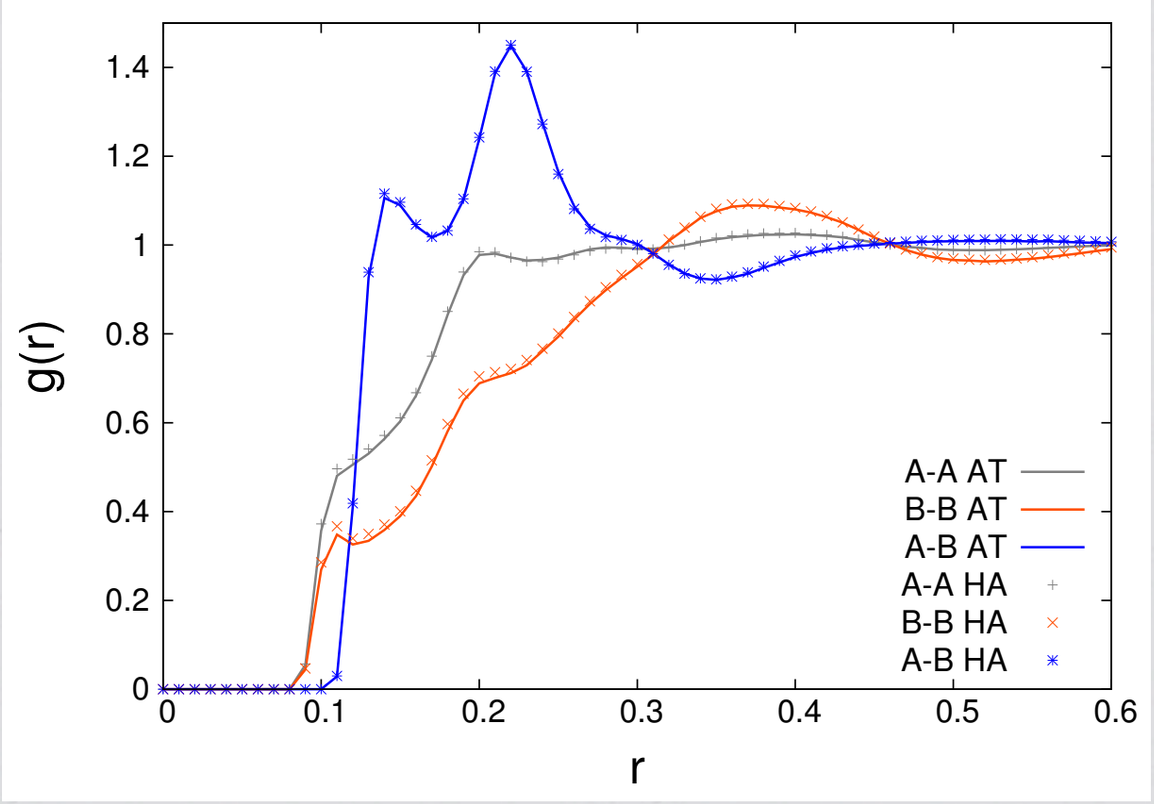

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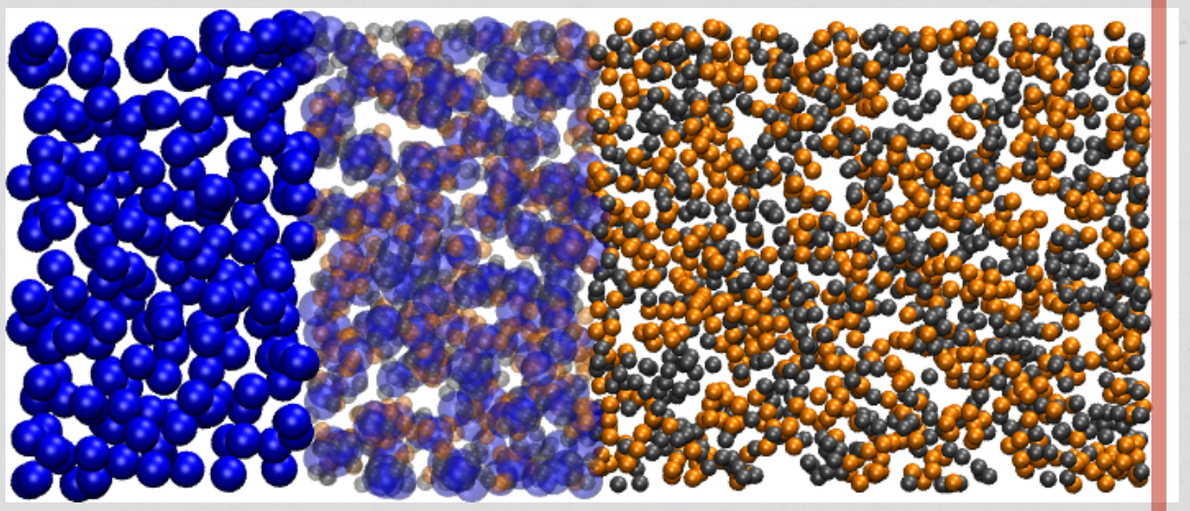
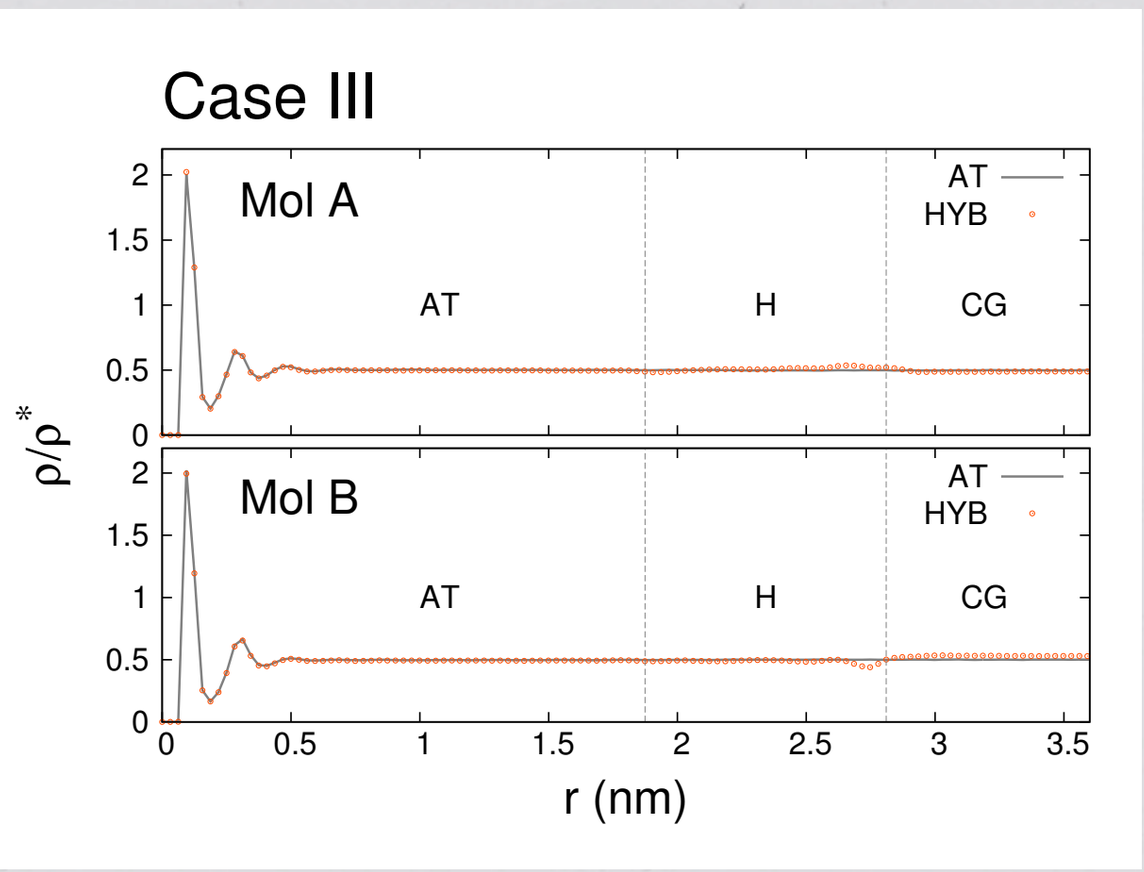
Monte Carlo simulation of a binary mixture - Case III

Binary mixture in contact with an attractive wall

- Different species in equal proportions
- All atoms interact with the wall through a LJ potential





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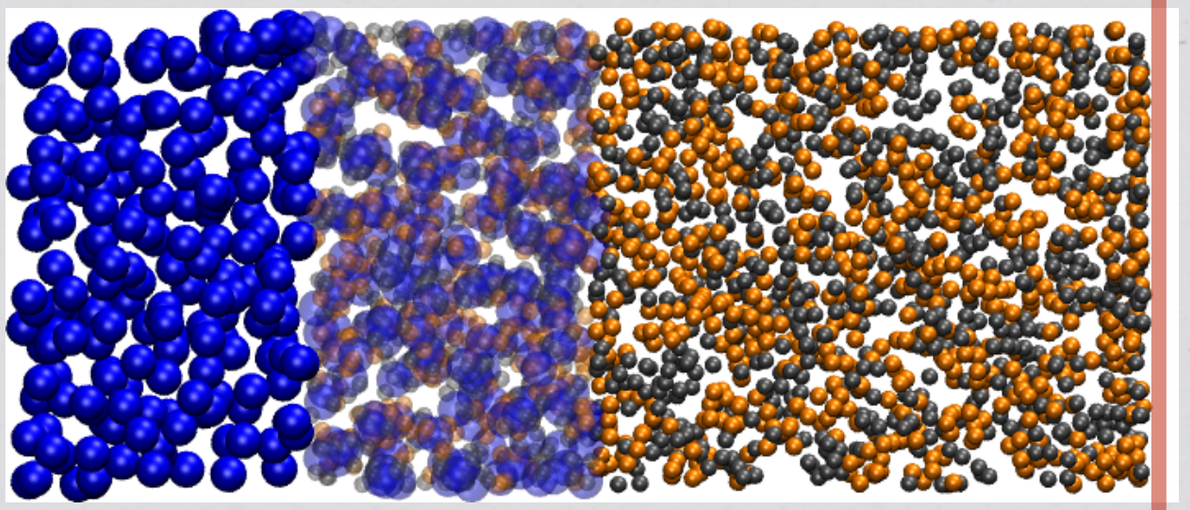

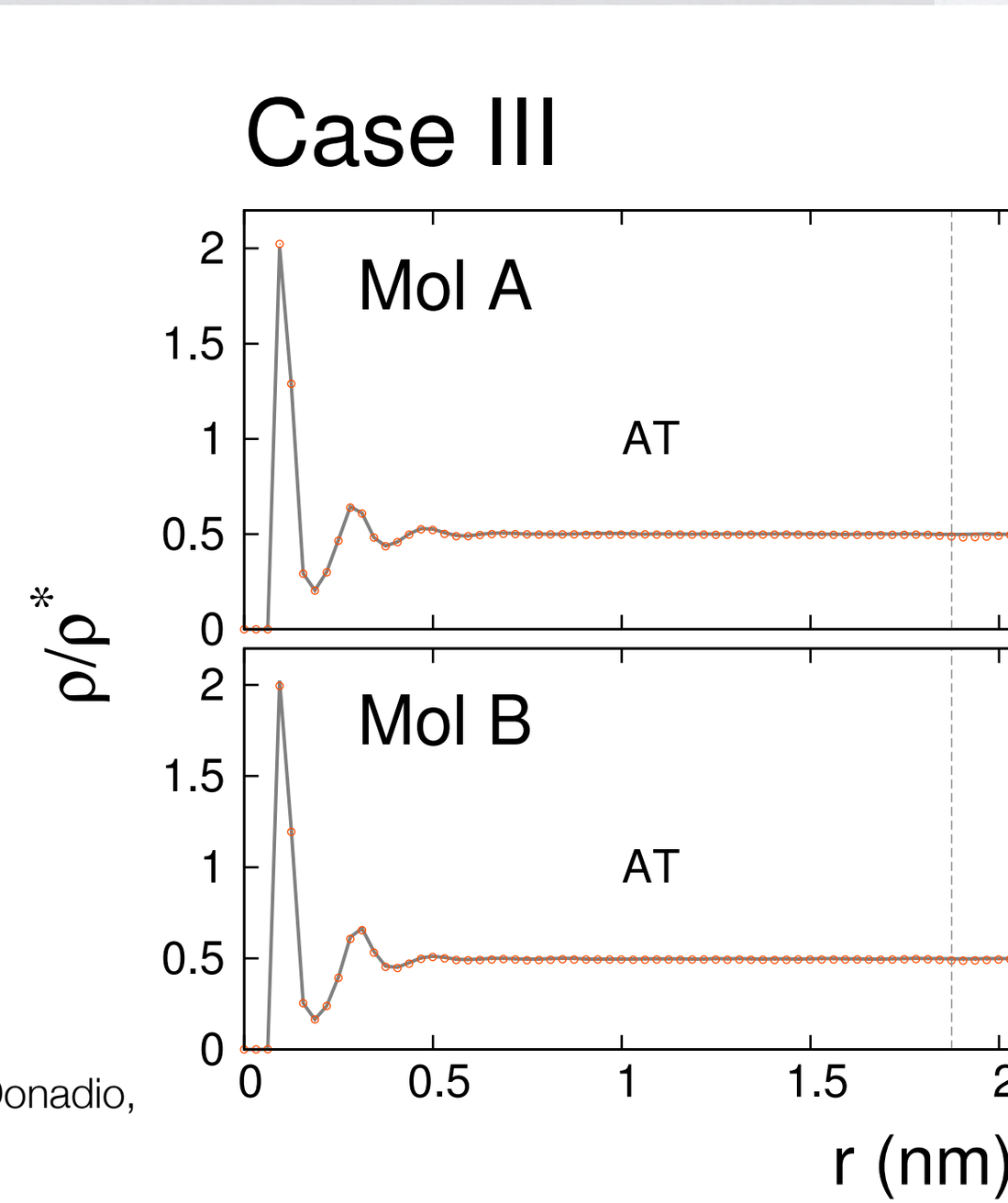

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Take-home message

- AdResS / H-AdResS: force-based or energy-based dual resolution simulation methods
- The force-based approach preserves Newton^3 exactly, but it's not conservative (a local thermostat is needed)
- The energy-based approach is Hamiltonian, but in the hybrid region Newton^3 is satisfied only on average
- Pros of having a Hamiltonian: NVE and MC possible, efficient Free Energy Compensation calculation, arbitrary CG model
- **Applications** in accretion processes (crystal growth, self-assembly), free energy calculations, classical/QM coupling (Path Integrals)

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Both AdResS and H-AdResS are implemented in Espresso++!!!

Acknowledgments

* Davide Donadio
* Sebastian Fritsch
* Kurt Kremer
* Rafael Delgado-Buscalioni
* Pep Español
* Ralf Everaers
* Max Planck Institute for Polymer Research
* Kavli Institute for Theoretical Physics

THANK YOU!