Multi-scale Modeling using the Adaptive Resolution Scheme

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Coworkers

A lot of people have contributed to AdResS:

- Cecilia Clementi (Rice University, Texas)
- Luigi Delle Site (MPI-P $\rightarrow$ FU Berlin)
- Sebastian Fritsch (MPI-P)
- Kurt Kremer (MPI-P)
- Brad Lambeth (Rice University, Texas)
- Debashish Mukherji (MPI-P)
- Patrick Kiley (University of Cambridge)
- Simón Poblete (MPI-P $\rightarrow$ FZ Jülich)
- Adolfo Poma (MPI-P $\rightarrow$ Sapienza University of Rome)
- Matej Praprotnik (MPI-P $\rightarrow$ National Institute of Chemistry, Slovenia)
- Stac Bevc (National Institute of Chemistry, Slovenia)

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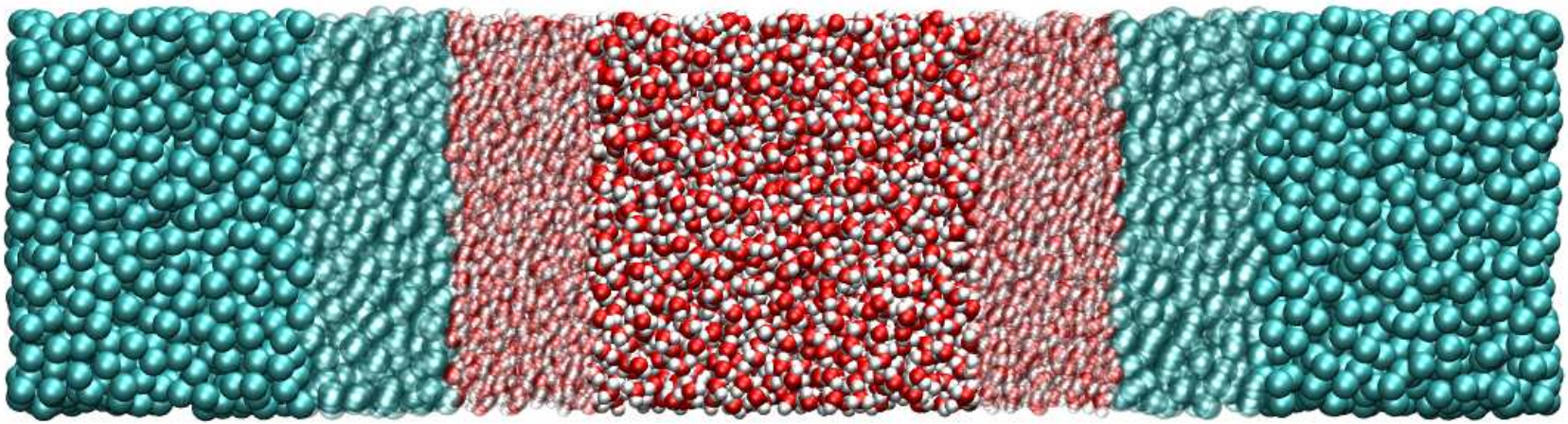
Introduction

The Adaptive Resolution Scheme (AdResS)



The big idea[1]

- Coupling of two resolutions (AA and CG) by a force interpolation:

$$\vec{F}_{\alpha\beta} = w_\alpha w_\beta \vec{F}^{\mathrm{AA}}_{\alpha\beta} + [1 - w_\alpha w_\beta]\, \vec{F}^{\mathrm{CG}}_{\alpha\beta} \ ,$$

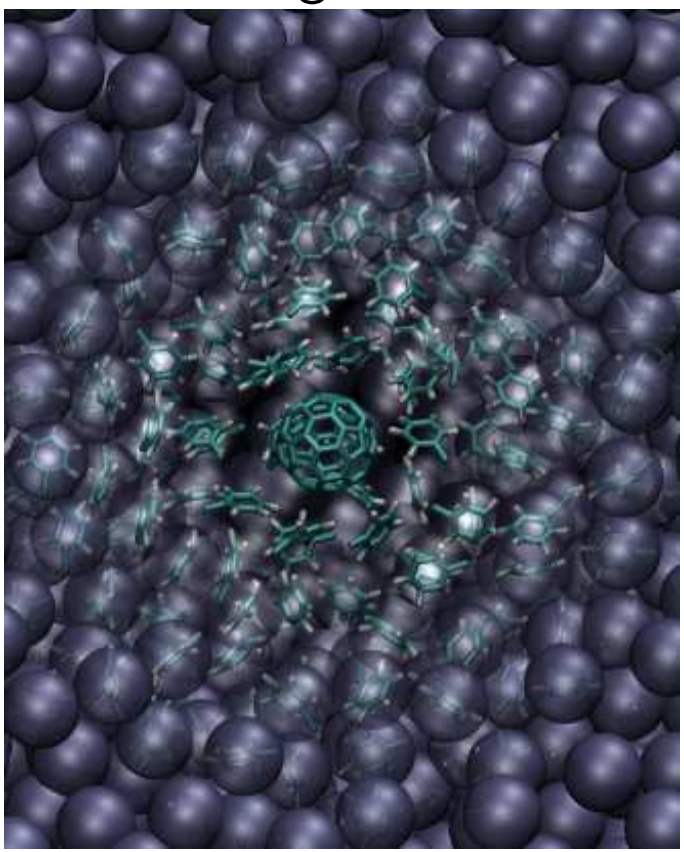
where α and β are molecules

[1] M. Praprotnik, L. Delle Site, and K. Kremer, JCP **123**, 224106 (2005).

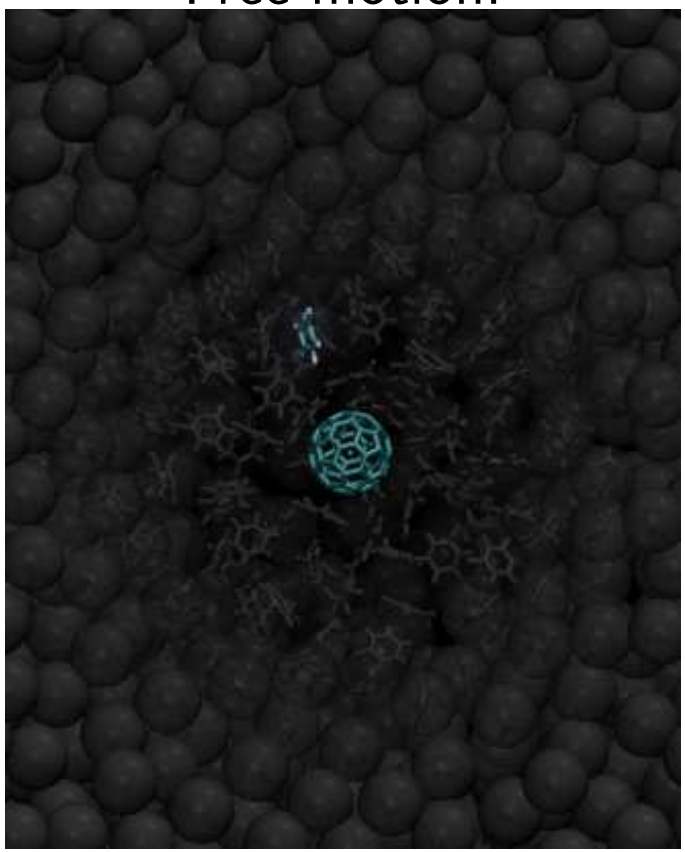
Introduction

Illustration

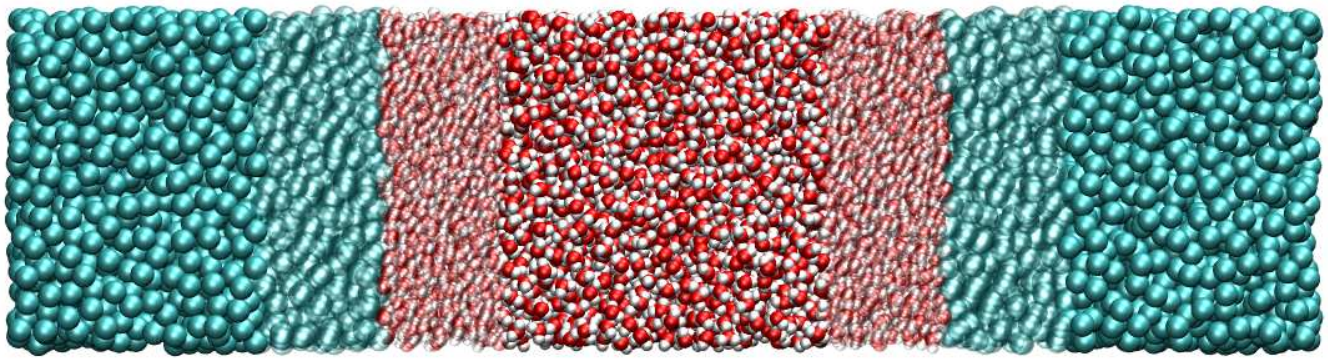
Magnifier:



Free motion:



Introduction
Motivation



Inherited from coarse-graining

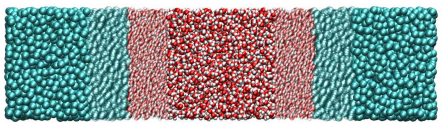
- Accessibility of bigger time- and length-scales
- Avoids sampling of unimportant degrees of freedom
- Better sampling through smoother energy landscape
- Computational speed-up

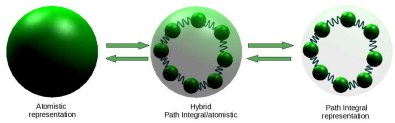
As an analysis tool

- Study influence of coarse-graining
- Replace surrounding environment

Introduction

What kind of systems can be coupled?





- Atomistic and coarse-grained representation of the same system
- Atomistic and very simplified (LJ) system
- Quantum and atomistic systems

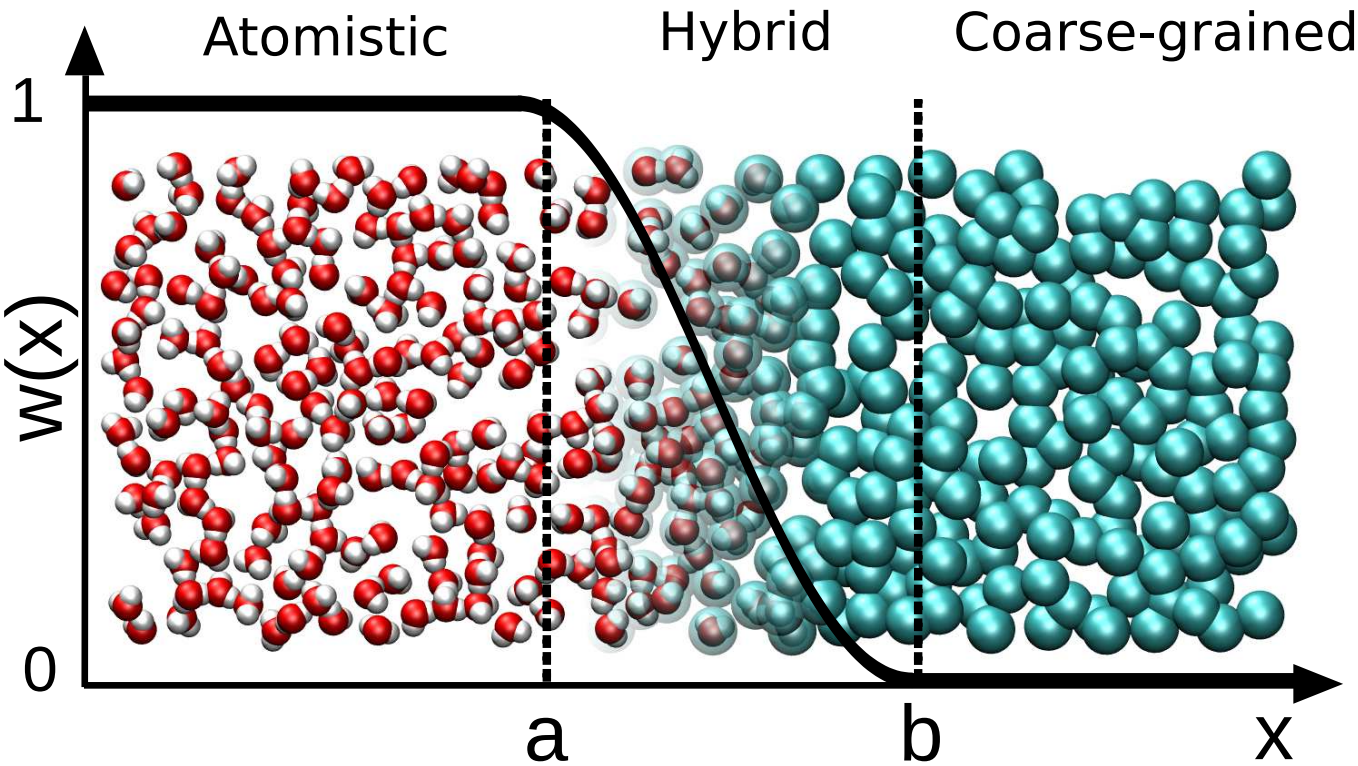
Coupling conditions[2]

$$\rho^{\mathrm{at}} = \rho^{\mathrm{cg}}, \quad T^{\mathrm{at}} = T^{\mathrm{cg}}, \quad (p^{\mathrm{at}} = p^{\mathrm{cg}})$$

[2] M. Praprotnik, L. Delle Site and K. Kremer; Annu. Rev. Phys. Chem. **59** 545 (2008).

Methodic Details

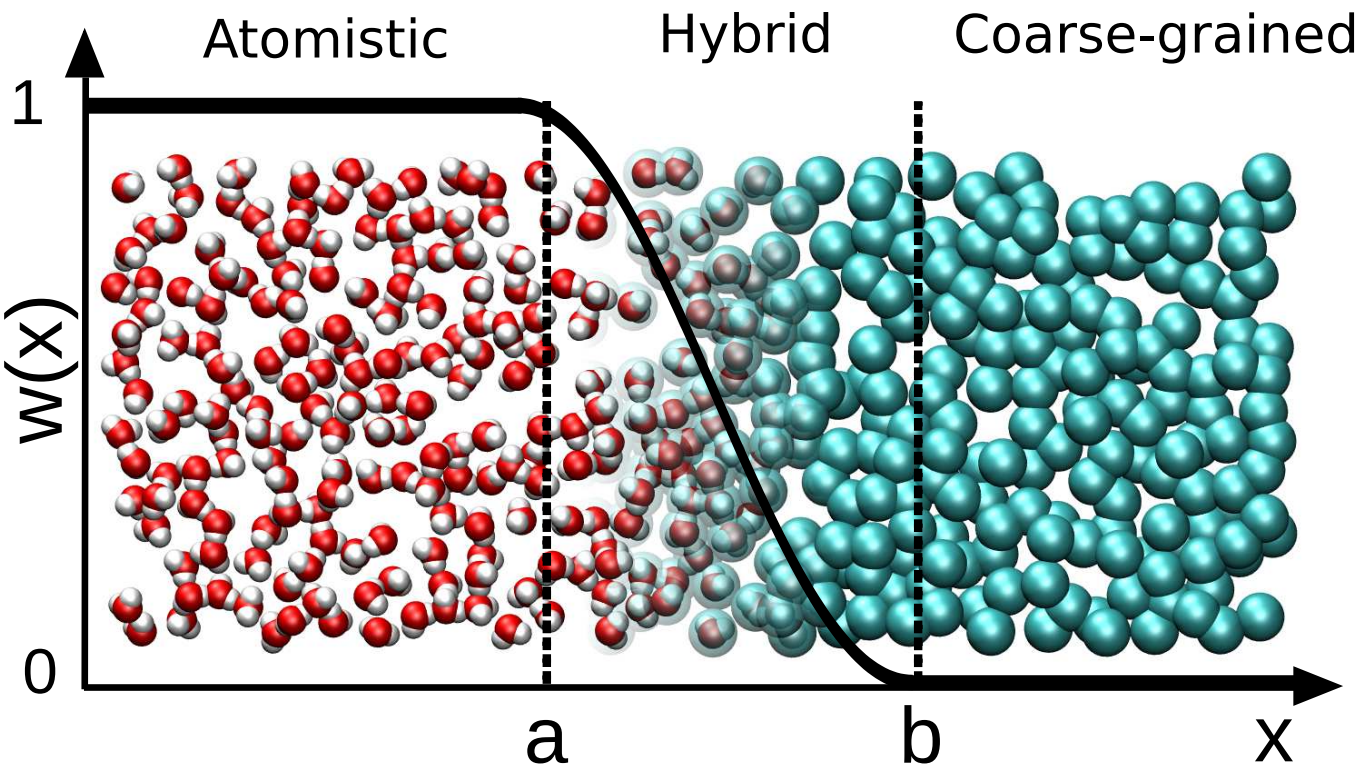
The Weighting Function I



$$w(x) = \begin{cases} 1 & : \text{atomistic/explicit region} \\ 0 < w < 1 & : \text{hybrid region} \\ 0 & : \text{coarse-grained region} \end{cases}$$

Methodic Details

The Weighting Function II

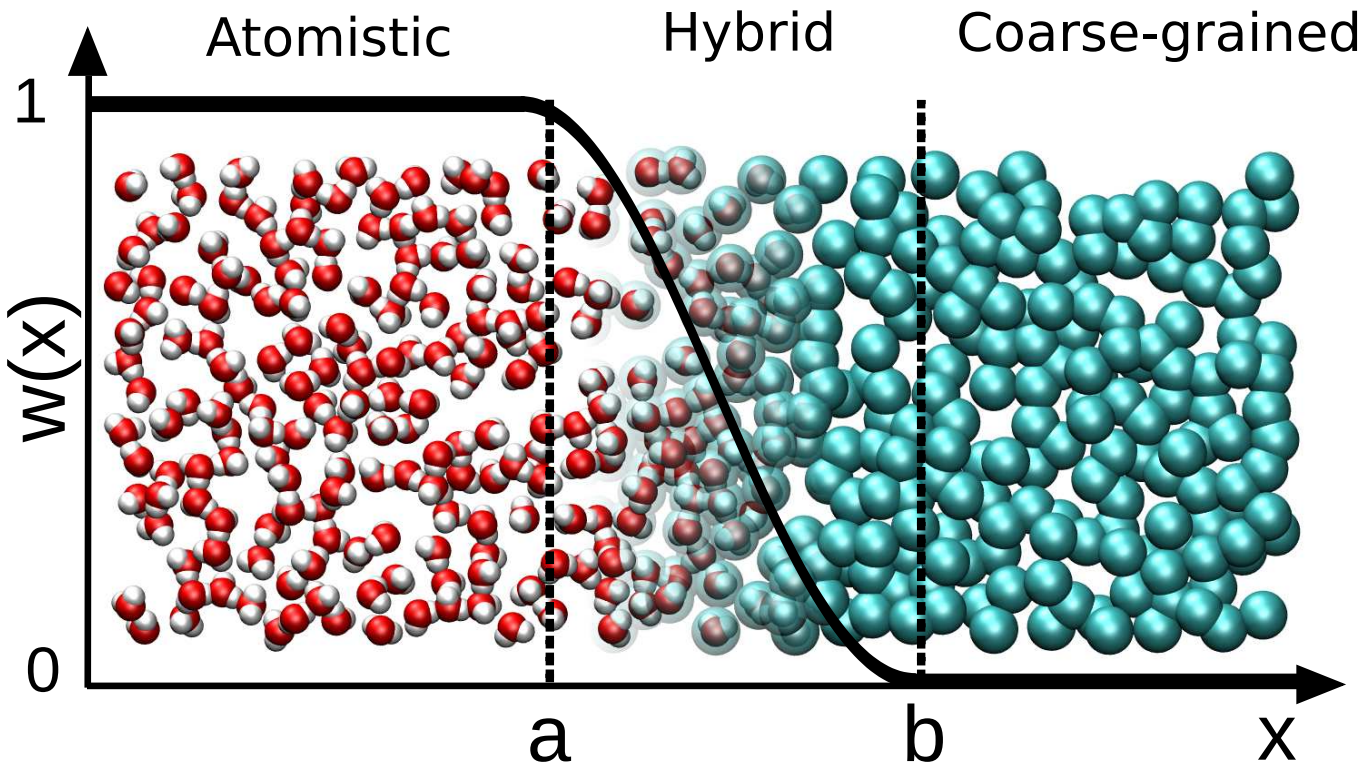


Boundary conditions

- Monotonic $\rightarrow$ No artificial barriers
- $w'(d_{ex}) = 0 = w'(d_{ex} + d_{hy}) \rightarrow$ smooth free energy transition

Methodic Details

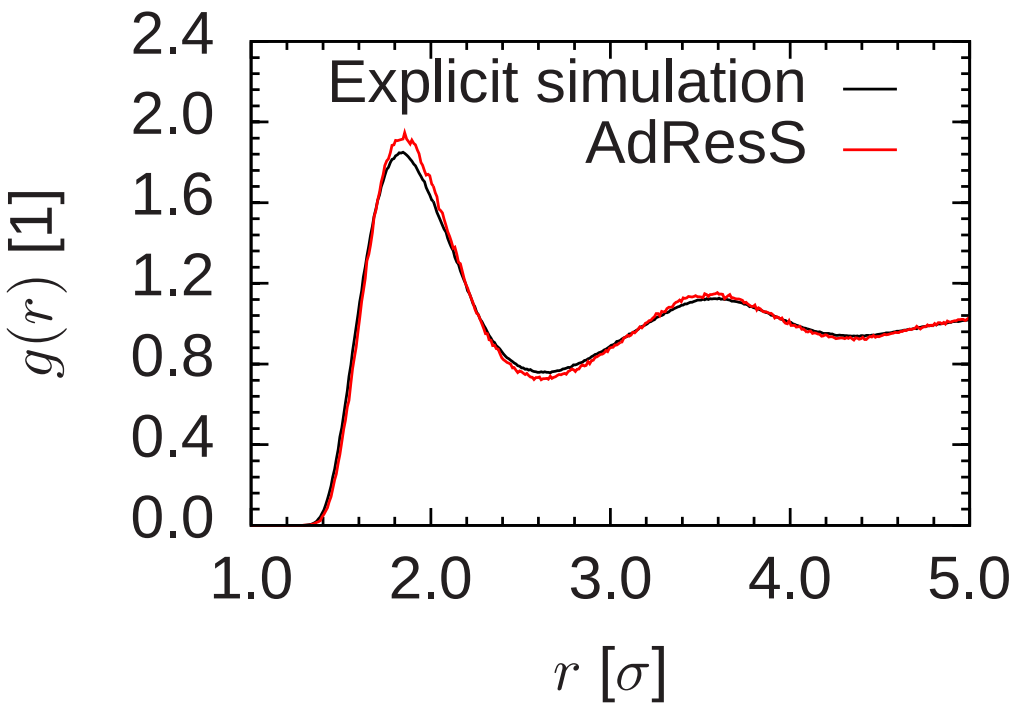
The Weighting Function III



$$w(x) = \begin{cases} 0 & : \quad x > d_{ex} + d_{hy} \\ \cos^2\left(\frac{\pi}{2d_{hy}}(x - d_{ex})\right) & : \quad d_{ex} + d_{hy} > x > d_{ex} \\ 1 & : \quad d_{ex} > x \end{cases}$$

AdResS at a First Glance

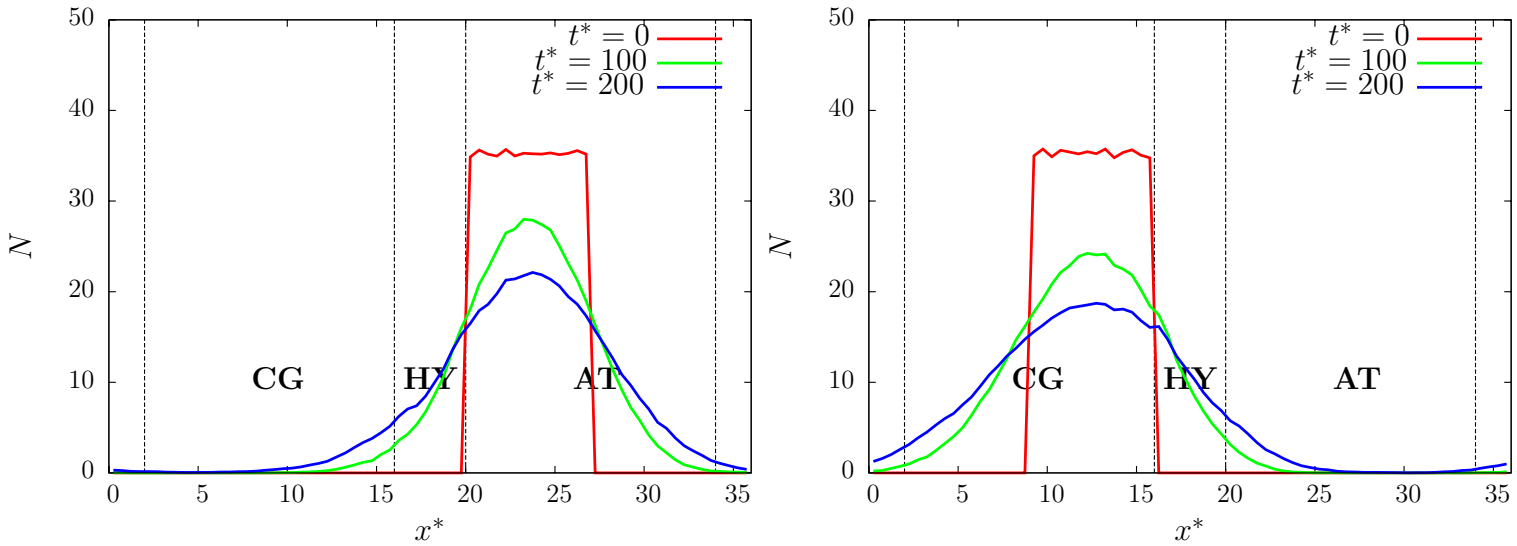
Radial Distribution Function (Tetrahedral Liquid)



- AdResS as a "magnifier" for a certain region
- RDF matches and accuracy depends more on the accuracy of the coarse-graining than on AdResS

AdResS at a First Glance

Particle Fluctuations

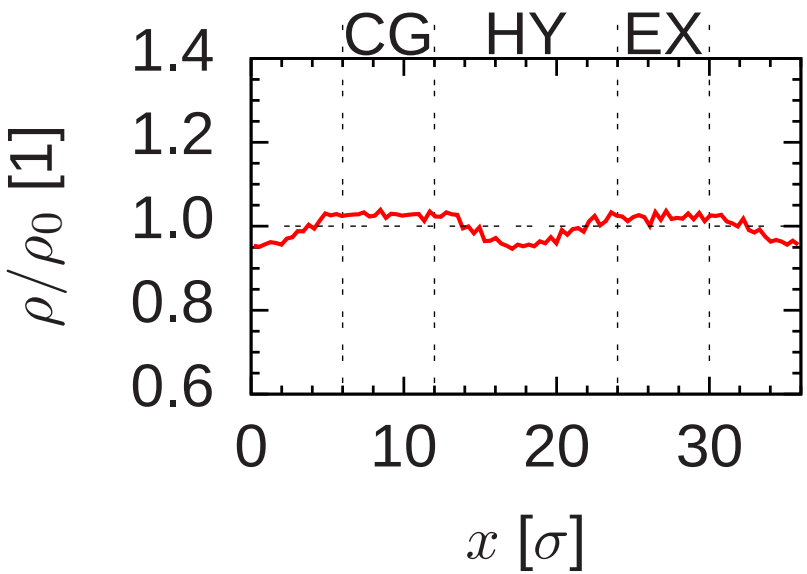


- Particles can freely diffuse through the hybrid region
- Profile is slightly asymmetric
- Coarse-grained dynamics is slightly faster

AdResS at a First Glance

Density Artifacts in the Hybrid Region

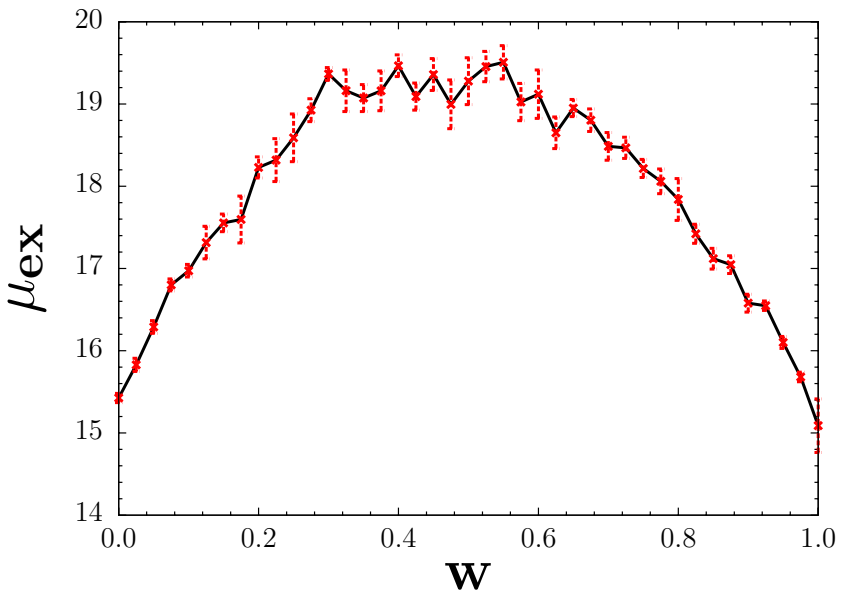
There is no free lunch!



- System is inhomogeneous in the hybrid region
- Linear interpolation is too simple
- Can be corrected, but is not necessary in all cases

Theory of the Thermodynamic Force

Idea



- Chemical potential in the hybrid region is different
- Add an external field[3]

$$\vec{f}_{\text{thermo}} = -\nabla(\mu_{AA} - \mu(w))$$

to the linear interpolation to repair the density inhomogeneity

- Correction is not always necessary
- Allows to couple systems of different pressures

[3] S. Poblete, M. Praprotnik, K. Kremer and L. Delle Site, JCP **132**, 114101 (2010)

Theory of the Thermodynamic Force

Pressure View

- Chemical potential is tedious to measure
- Assumption of constant weight
- To obtain a flat density profile one needs to compensate for the different pressures in the hybrid region[4]

$$\vec{f}_{\text{thermo}} = -\frac{1}{\rho_0}\nabla(p_{\text{AA}} - p(w))$$

- Local pressure depends on the local density

$$\vec{f}_{\text{thermo}} = -\frac{1}{\rho_0^2\kappa}\nabla(\rho(w))$$

- Easier, because $\rho(w)$ can be measured on the fly
- Iterative correction is possible

[4] S. Poblete, S. Fritsch, C. Junghans, G. Ciccotti, K. Kremer and L. Delle Site, PRL **108**, 170602 (2012)

Numerical Details

Overview I

The problem is the hybrid region!

Question

- How to reintroduce the atomistic details?
- How to initialize the atomistic velocities?
- How to introduced the correct bond distribution?
- How to map the molecular force interpolation to the atoms in the atomistic region?

Numerical Details

Overview II

Consumed Computer Times in MD

- 70% Force calculation
- 15% Communication
- 8% Neighbor search
- 5% Position update
- 2% IO

Position update is cheap $\rightarrow$ do NOT remove atomistic particles, but do not treat them force-wise and integrate them everywhere.

Double representation trick[5] ( everywhere)

[5] C. Junghans and S. Poblete, Comp. Phys. Comm. **181**, 1449 (2010).

Numerical Details

Virtual Sites

How to implement the double representation?

Virtual sites: Dummy particles, which are moved according to a geometrical rule rather than by Newton's equation of motion.

Force distribution

Force on an atom in an molecule with a virtual site:

$$\vec{F}_i^{\text{atom}} = -\frac{\partial(V + V^{\text{cg}})}{\partial \vec{r}_i} = \vec{F}_i^{\text{ex}} + \vec{F}^{\text{cg}} \frac{\partial \vec{r}^{\,\text{cg}}}{\partial \vec{r}_i} \overset{COM}{=} \vec{F}_i^{\text{ex}} + \frac{m_i}{\sum_{i \in \alpha} m_i} \vec{F}^{\text{cg}}$$

Can be easily added to the integrator!

Numerical Details

Integrator

Velocity Verlet Integrator (with AdResS and virtual sites)

1. $v(t + \Delta t/2) = v(t) + \Delta t/2\, f(t)/m$
2. $p(t + \Delta t) = p(t) + \Delta t\, v(t + \Delta t/2)$

2b. Update the positions, velocities and weighting functions $w(\vec{R})$ of the virtual sites

3. Calculate $f(t + \Delta t)$ from $p(t + \Delta t)$, $v(t + \Delta t/2)$ (and thermostat)

3b. Distribute the force of the virtual sites to the real particles

4. $v(t + \Delta t) = v(t + \Delta t/2) + \Delta t/2\, f(t + \Delta t)$

Virtual sites increase the amount of communication ($\mathcal{O}(N_{VS}^{2/3})$).

Numerical Details

Thermostat

A thermostat is needed for a smooth transition.

Langevin Thermostat

Thermostat force acting on the atoms

$$\vec{f}_i^{\text{thermo}} = \vec{f}_i^{\text{D}} + \vec{f}_i^{\text{R}} = \xi_i \vec{v}_i + \sigma_i \vec{\eta}_i \ .$$

One can show that

$$\sum_{i \in \alpha} \vec{f}_i^{\text{thermo}} = \vec{F}_\alpha^{\text{D}} + \vec{F}_\alpha^{\text{R}}$$

is also a Langevin thermostat with a common fluctuation-dissipation theorem ($\sigma^2 = \mathrm{k_B} T \xi$) if the friction constants ξ_i have been scaled with the masses, $\xi_i = m_i \xi$.

DPD thermostat can also be used, but more theory is involved.

Numerical Details
Reinitialization

Possiblities for Velocity and Bond Reinitialization

- Initialization from Maxwell/bond distribution
- Freeze and unfreeze them
- Keep on integrating them

Reminder: We have hybrid molecules everywhere
Bonded interactions are cheap
$\rightarrow$ keep on integrating them is the easiest solution

Numerical Details
Cut-Offs

AdResS needs a molecule-based cut-off due to the force interpolation.

Molecular Cut-Offs

- Avoid that molecules interact half atomistic - half coarse-grained
- Avoid dipoles at the cut-off

Numerical Details

Speed-up

Simulation of a big system with small atomistic region: [6]

Ideal strong speed-up (const. systemsize)

$$
\begin{aligned}
s^{-1} &= \left(\frac{t_{\text{new}}}{t_{\text{old}}}\right) \\
&\overset{V_{\text{AA}} << V_{\text{CG}}}{=} \frac{t_{\text{not-forces}}}{t_{\text{total}}} + \frac{t_{\text{forces}}}{t_{\text{total}}} \frac{1}{(\text{atoms per molecule})^2} \\
&\overset{\text{Toluene}}{=} 0.26 + 0.74 \cdot \frac{1}{2 \times 12^2} \approx 3.6^{-1}
\end{aligned}
$$

[6] S. Fritsch, C. Junghans and K. Kremer, JCTC **8**, 398 (2012).

Basic Examples
Tetrahedral Liquid

Toy model for a liquid (methane-like). [7] 

Explicit (all-atom) Interactions

Non-bonded (even inside the molecules), LJ:

$$U_{LJ}^{ex}(r_{i\alpha j\beta}) = \begin{cases} 4\epsilon\left[(\sigma/r_{i\alpha j\beta})^{12} - (\sigma/r_{i\alpha j\beta})^{6} + \frac{1}{4}\right], & r_{i\alpha j\beta} \leq 2^{1/6}\sigma \\ 0, & r_{i\alpha j\beta} > 2^{1/6}\sigma \end{cases}$$

Bonded, FENE:

$$U_{FENE}^{ex}(r_{i\alpha j\alpha}) = \begin{cases} -\frac{1}{2}kR_0^2 \ln\left[1 - (r_{i\alpha j\beta}/R_0)^2\right], & r_{i\alpha j\beta} \leq R_0 \\ \infty & r_{i\alpha j\beta} > R_0 \end{cases}$$

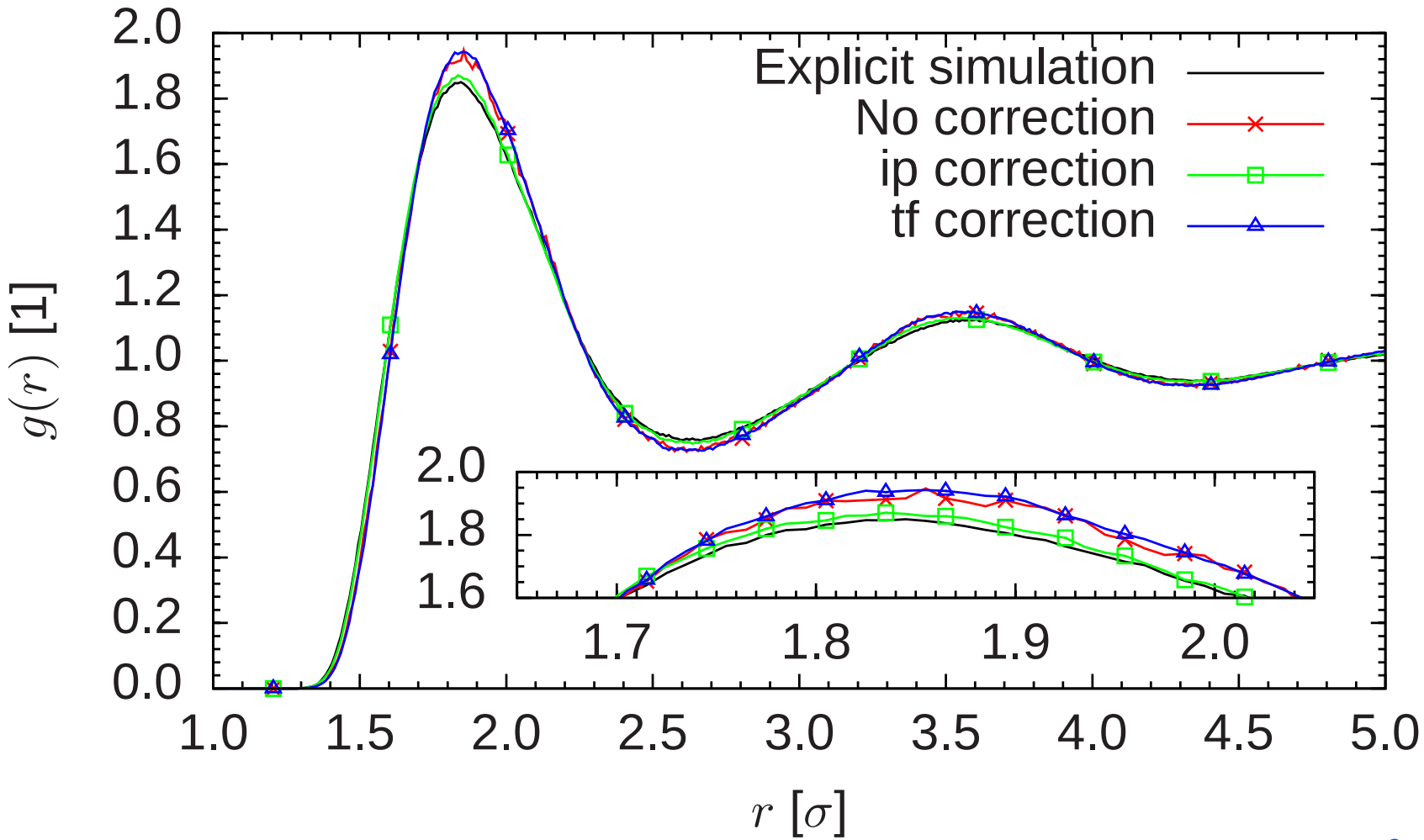
Coarse-grained Interactions

Isotropic one-site tabulated potential $U(r_{ij})$ by IBI

[7] C. Junghans and S. Poblete, Comp. Phys. Comm. **181**, 1449 (2010).

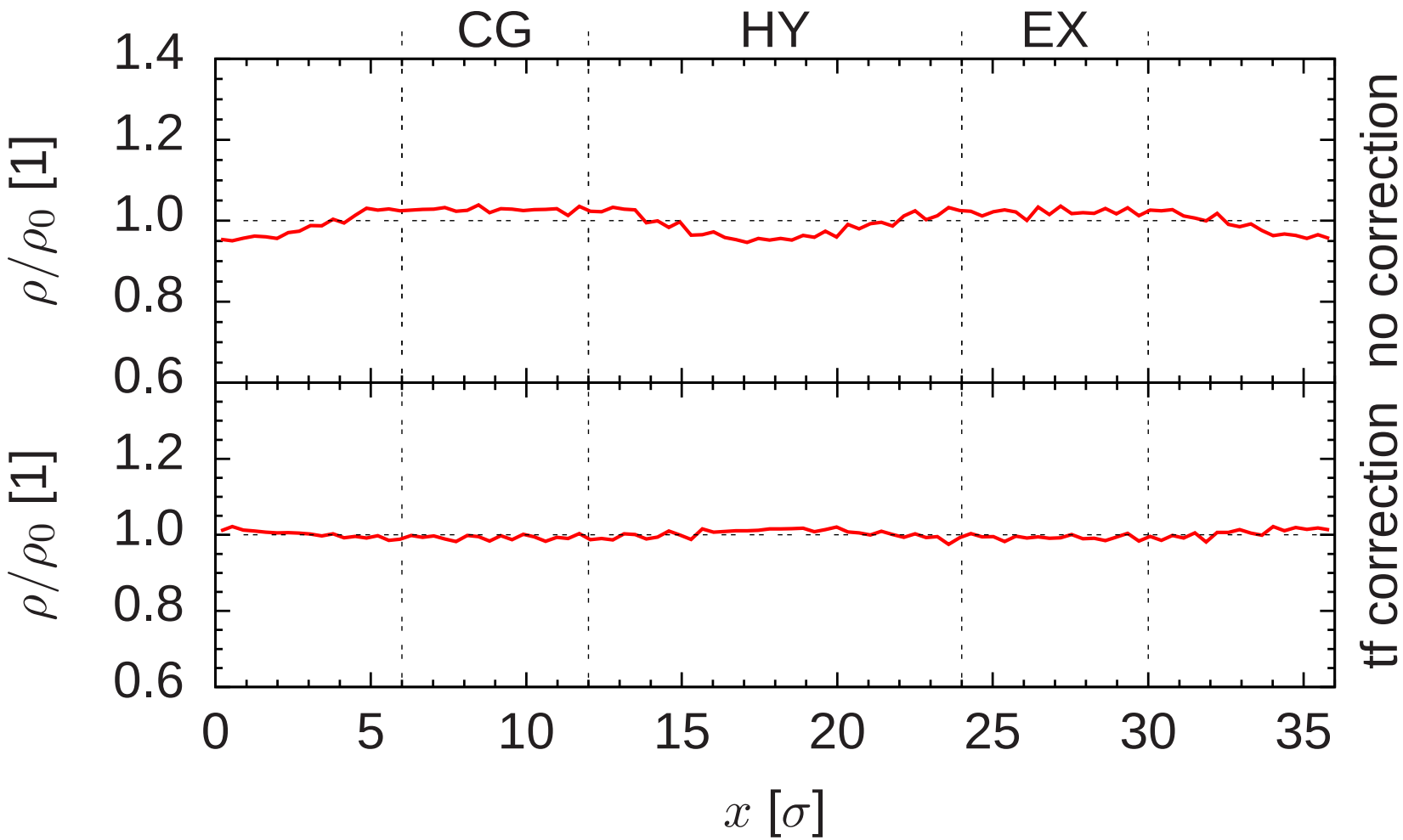
Basic Examples

Tetrahedral Liquid (Structure)

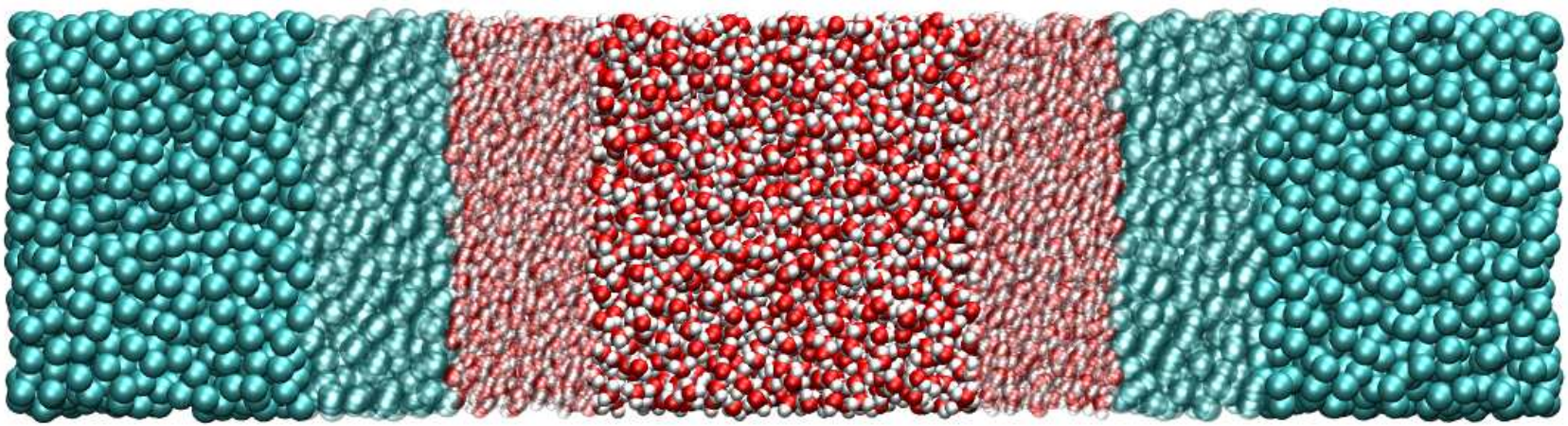


Basic Examples

Tetrahedral Liquid (Density profile)



Basic Examples
Water



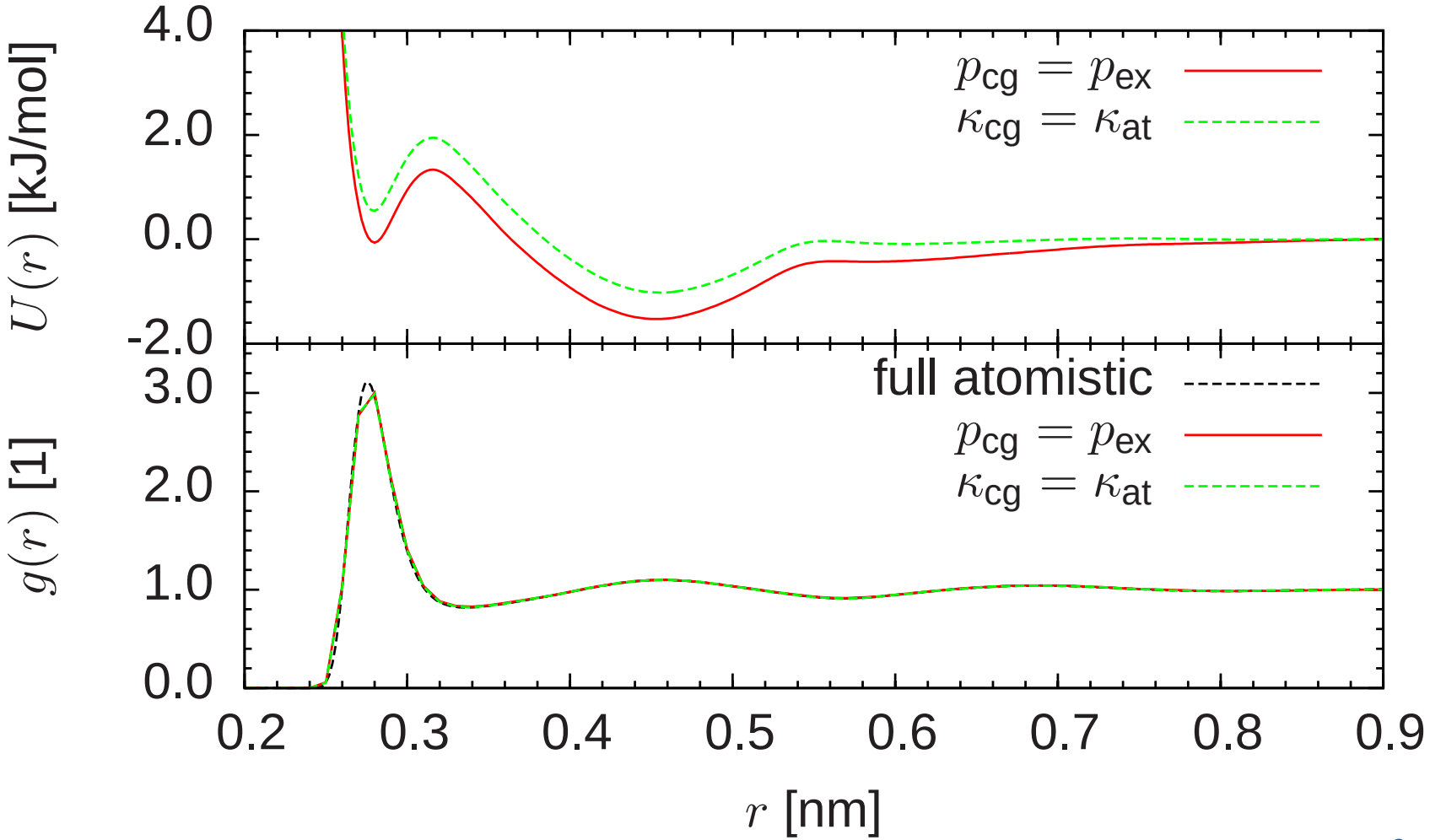
- A realistic, but simple system
- Electrostatics by Reaction Field
- One bead coarse-grained model

Can we couple a not pressure-corrected model, too? [8]

[8] S. Poblete, S. Fritsch, C. Junghans, G. Ciccotti, K. Kremer and L. Delle Site, PRL **108**, 170602 (2012)

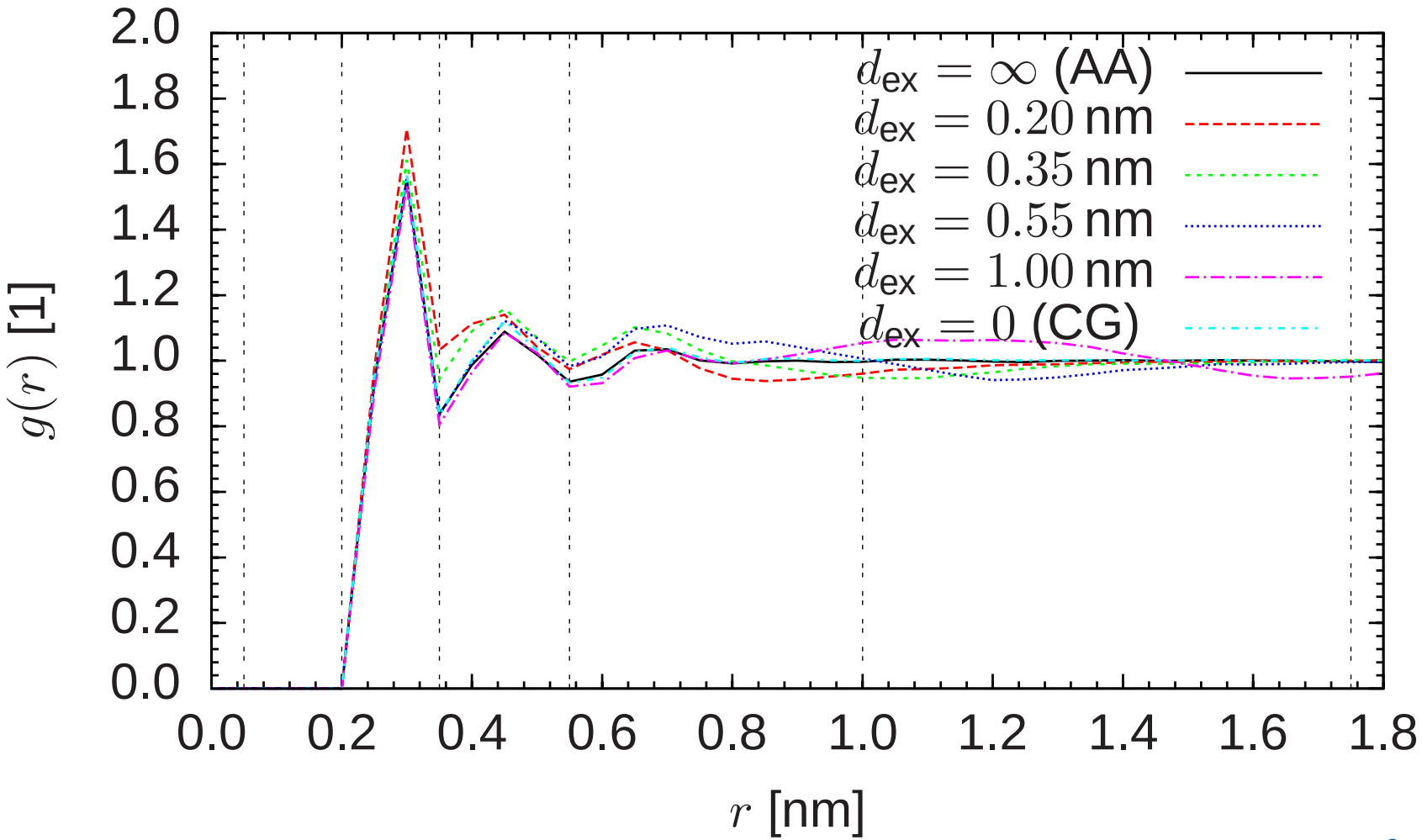
Basic Examples

Water (Coarse-grained Model)



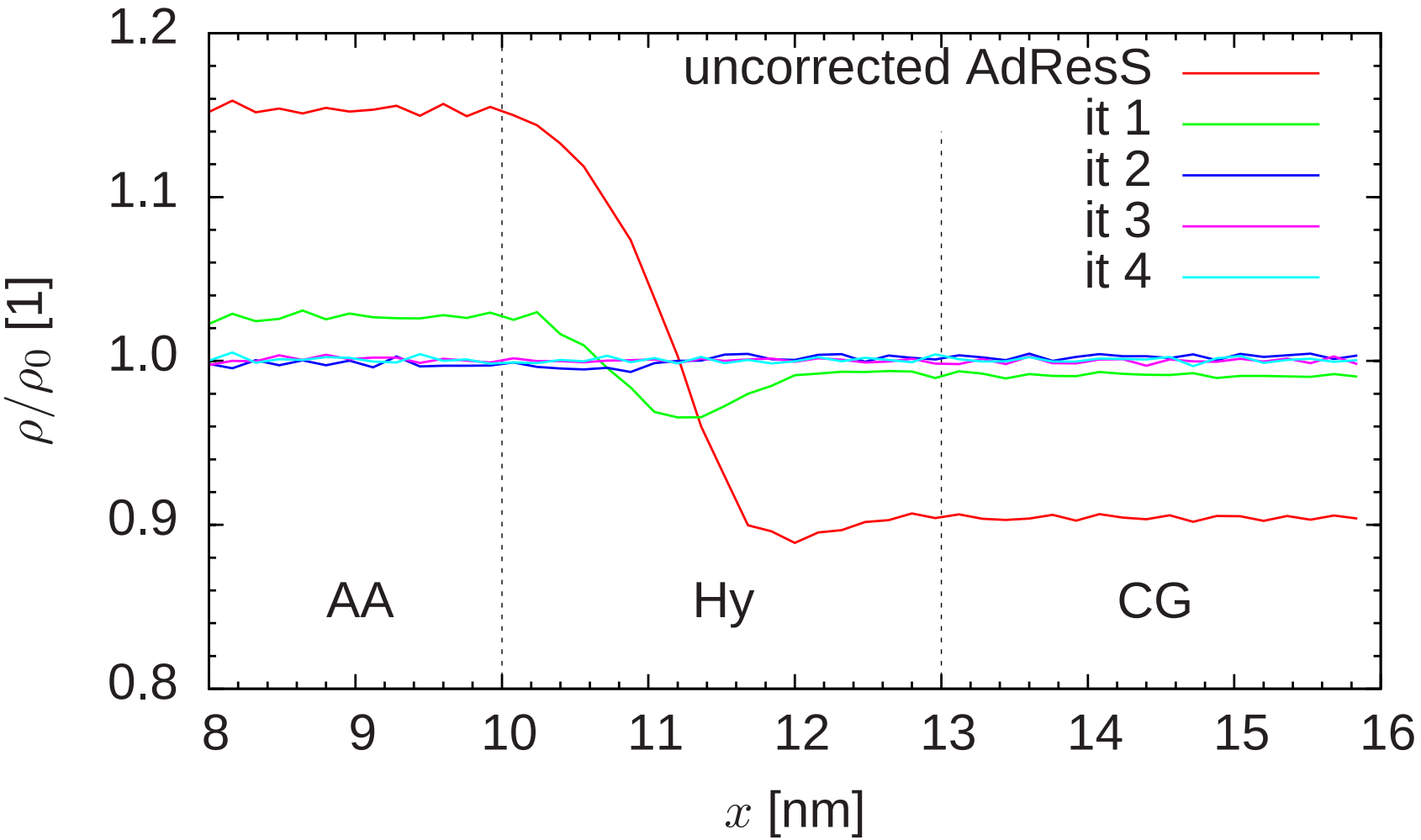
Basic Examples

Water (Perturbation without Thermodynamic Force)



Basic Examples

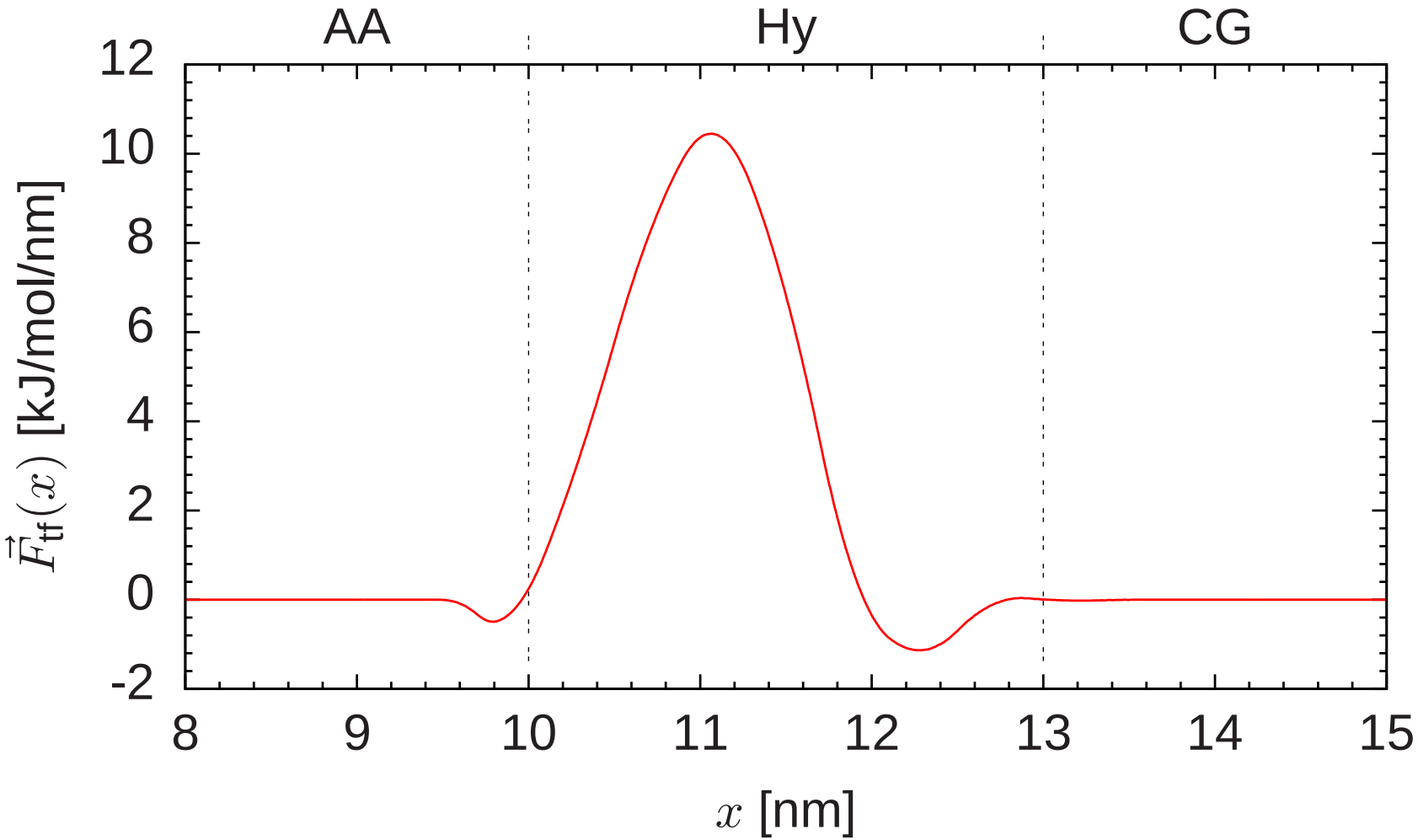
Water (Density profile)



One can even bring non-pressure corrected model in equilibrium

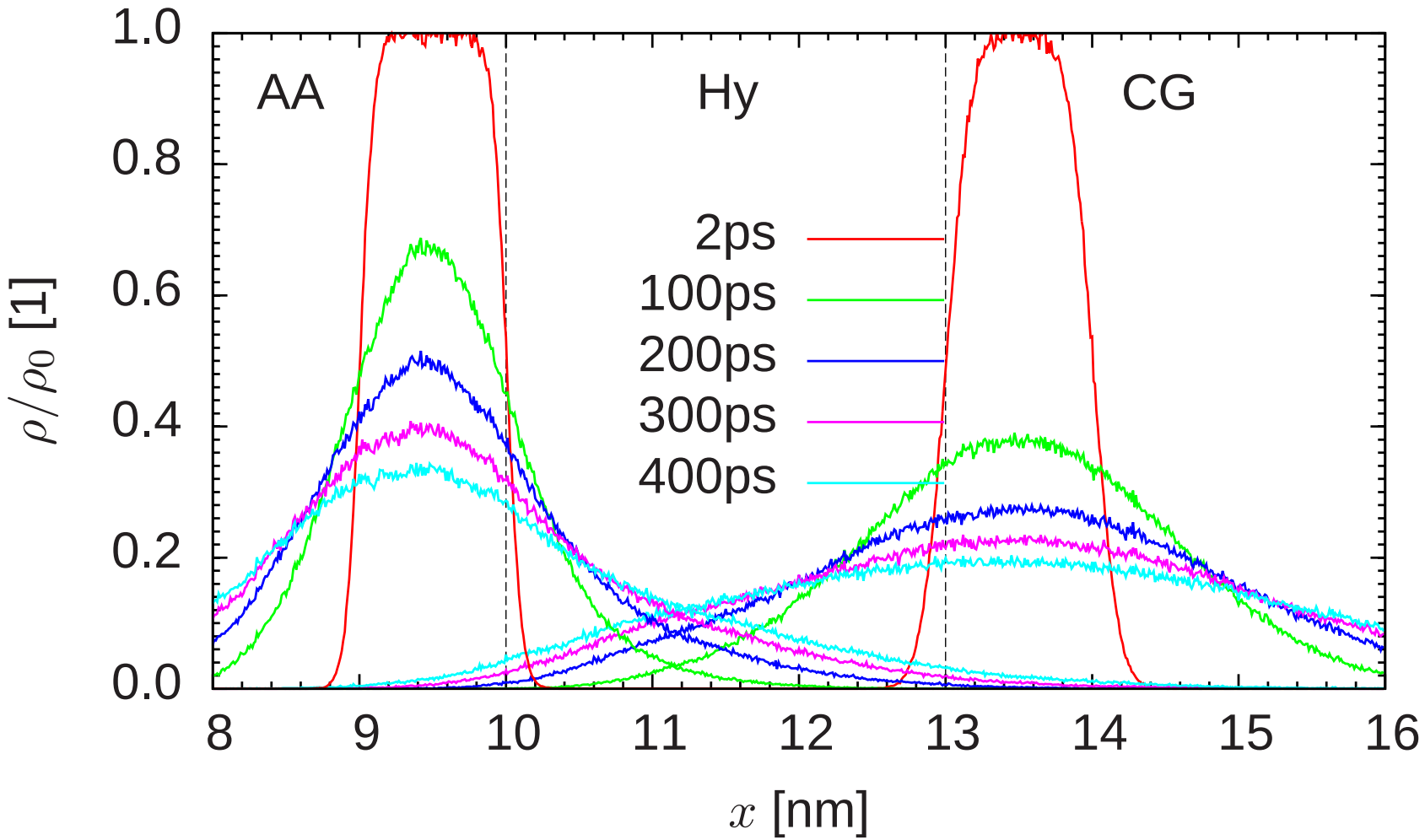
Basic Examples

Water (Thermodynamic Force)



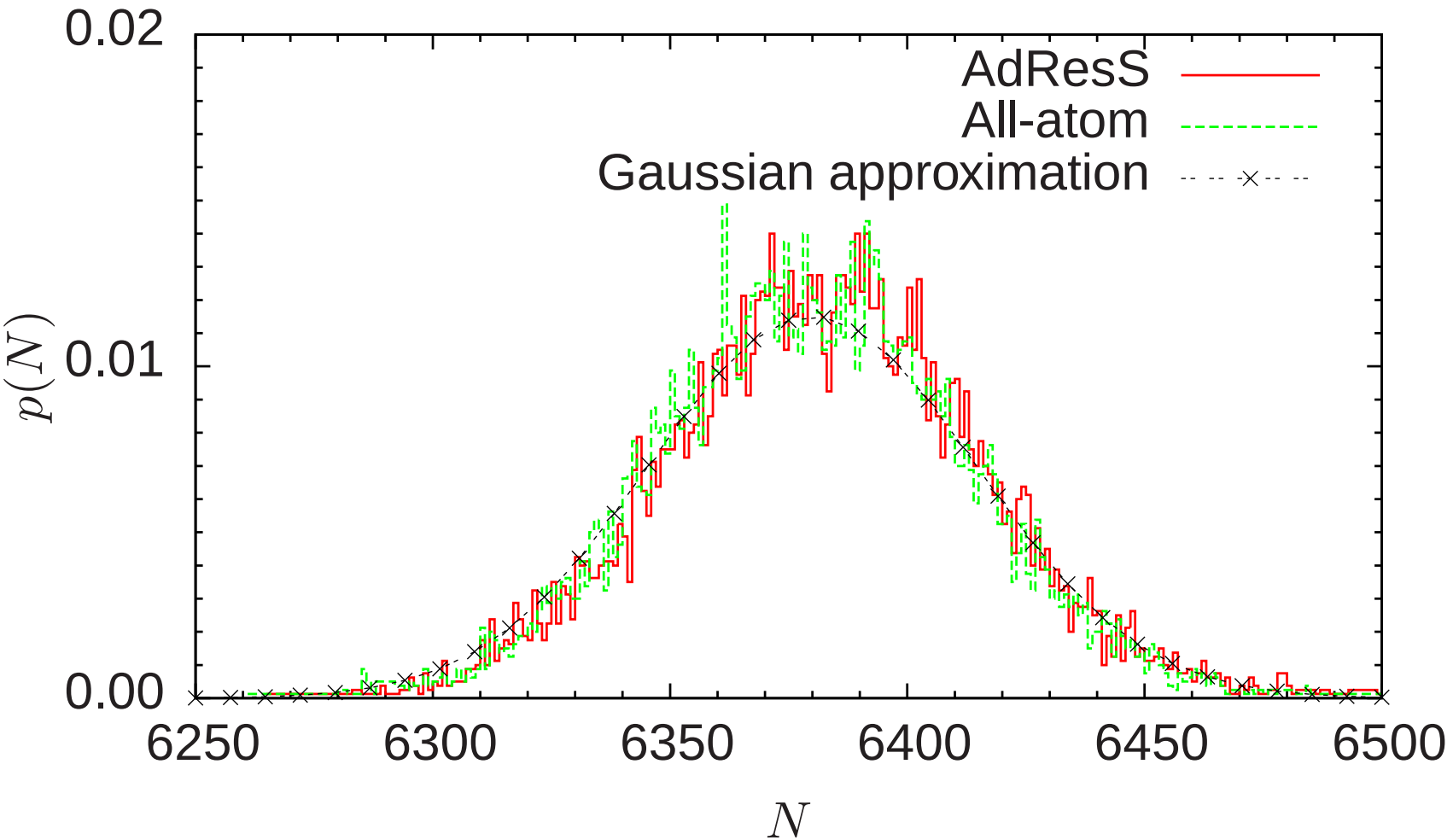
Basic Examples

Water (Diffusion Profile)



Basic Examples

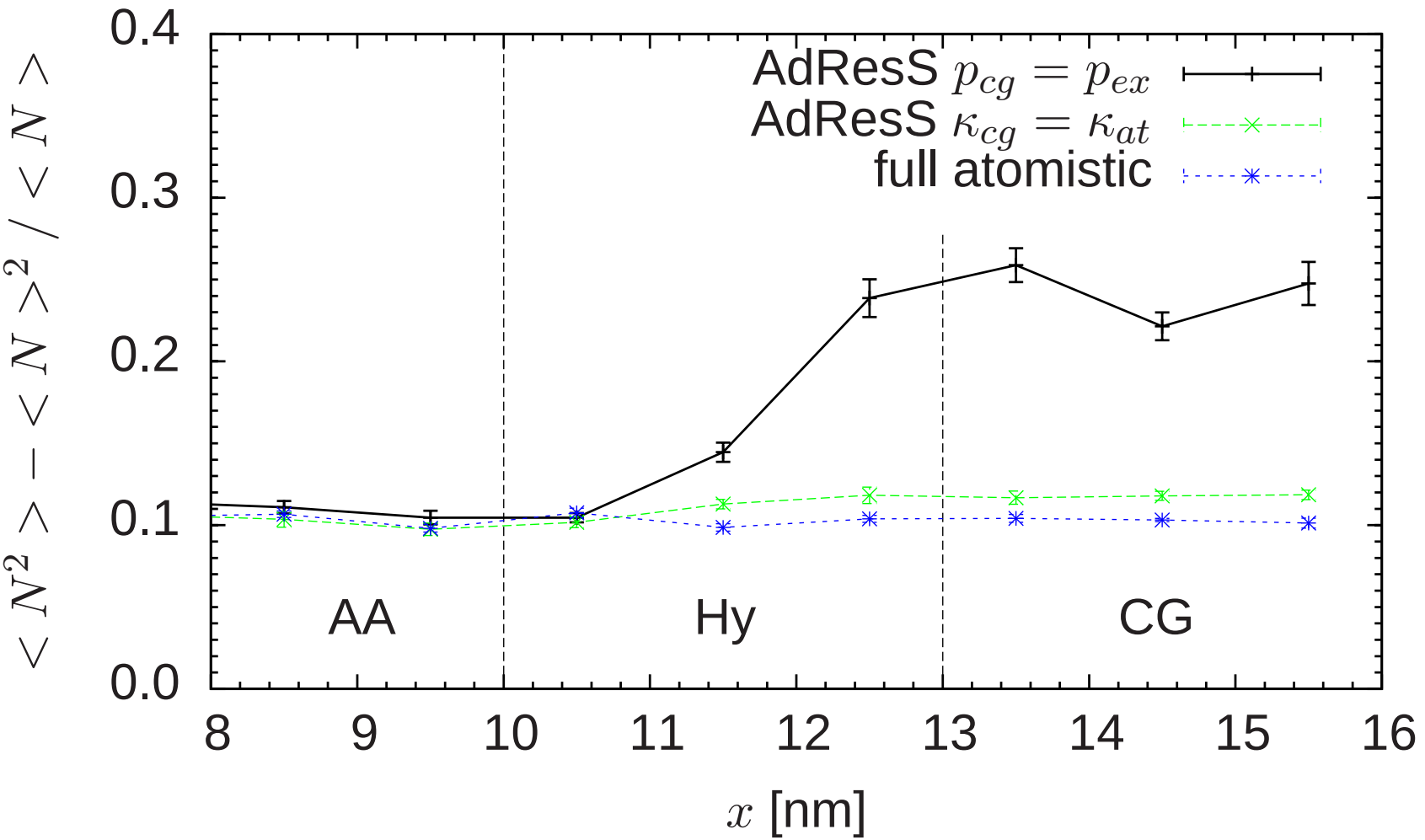
Water (Particle Fluctuations in AA zone)



Grand-canonical behaviour

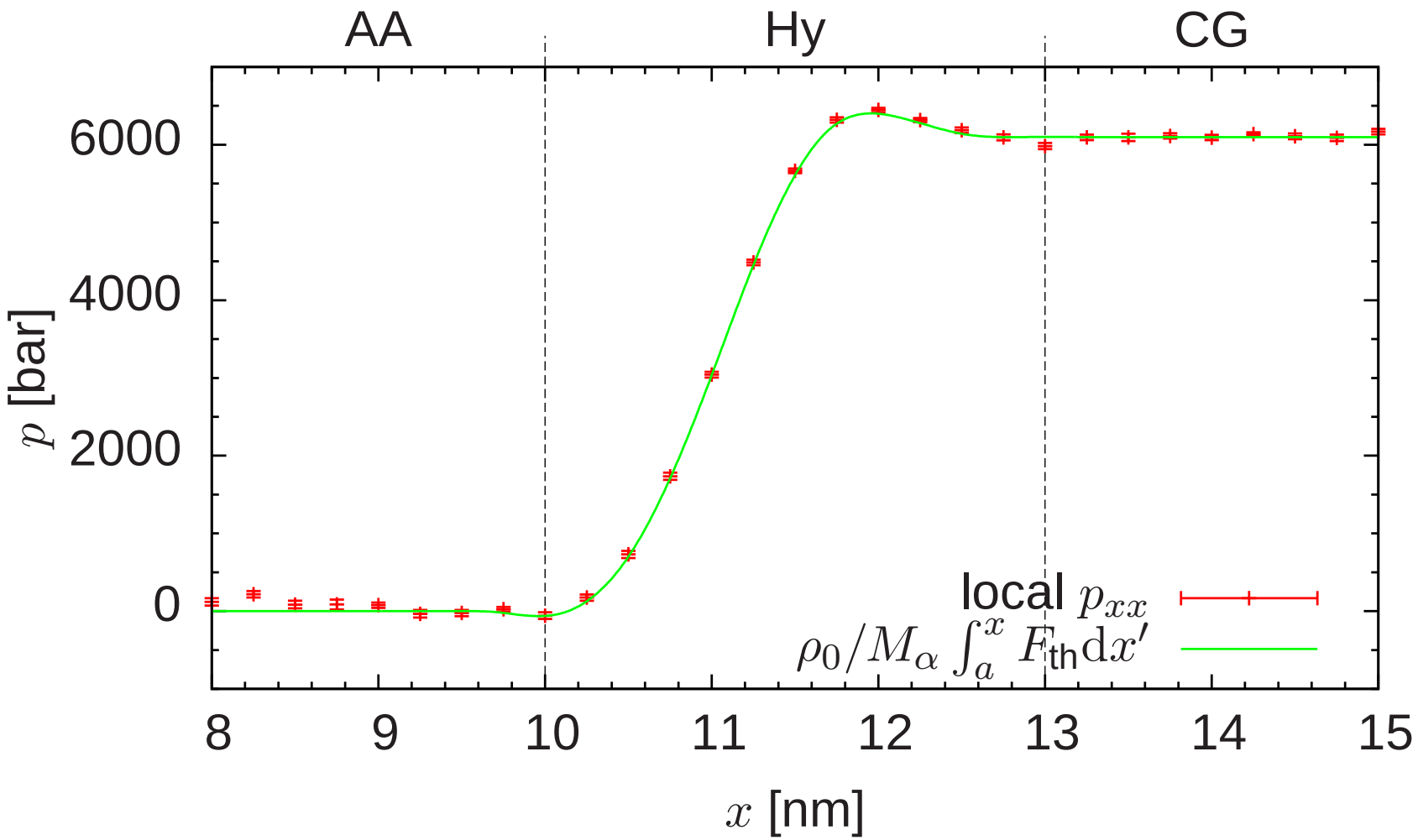
Basic Examples

Water (Particle Fluctuations)



Basic Examples

Water (Thermodynamic Force)



Thermodynamic force compensates the pressure difference.

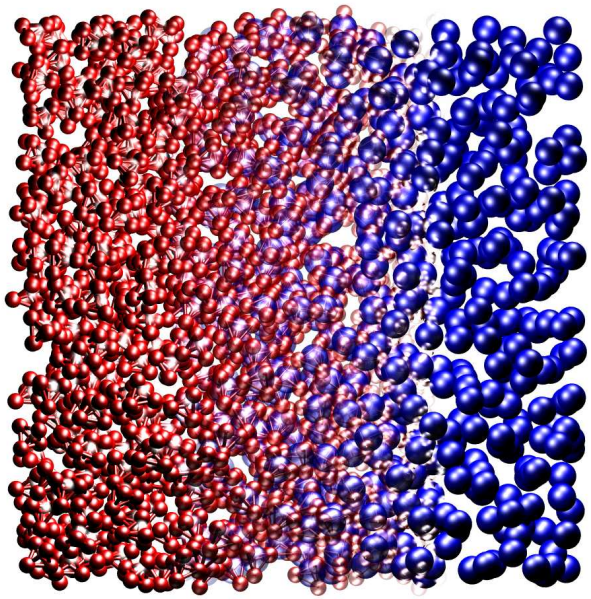
Outlook

AdResS:

- Useful analysis tool
- Speed-up simulations
- Molecules exchange between the two resolutions

Things to work on:

- Electrostatics
- Adaptive implementation $\rightarrow$ESPResSo $++$ ✓



The End

Thank you for your attention !

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