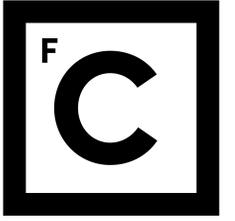# The impact of using single atomistic long-range cutoff schemes with the GROMOS 54A7 force field

Tomás F. D. Silva, Diogo Vila-Viçosa, Pedro B. P. S. Reis, Bruno L. Victor, Matthias Diem, Chris Oostenbrink, and Miguel Machuqueiro

MD simulations - Freedom (?) of choice

Simulation quality, accuracy and speed rely on 4 main levels:

1. **Hardware** - CPU, RAM and GPU;

2. **Software** - software package and versions ;

3. **Force fields** - different models/purposes (ex.: QM, AA, UA, CG) ;

4. **Settings and parameters** - parametrization and validation procedures.

MD simulations - Choosing software package

GROMACS
FAST. FLEXIBLE. FREE.

| Features	v3	v4.0	v4.6	v5	v2016	v2018
Release year	2004	2008	2013	2014	2016	2018
Group-based	✔	✔	✔	✔	✖	✖
Atomistic Verlet	✖	✖	✔	✔	✔	✔
Twin-range cutoff	✔	✔	✔	✔	✖	✖
Single cutoff	✔	✔	✔	✔	✔	✔
GPU support	✖	✖	✔	✔	✔	✔
CpHMD use	✔	✔	✔	✖*	✖	✖

3

MD simulations - Three questions

Why should we use GROMOS?

Why not PME instead of RF?

How did GROMACS development collide
with the use of GROMOS force fields?

GROMOS 54A7
Reaction Field

**Twin-Range
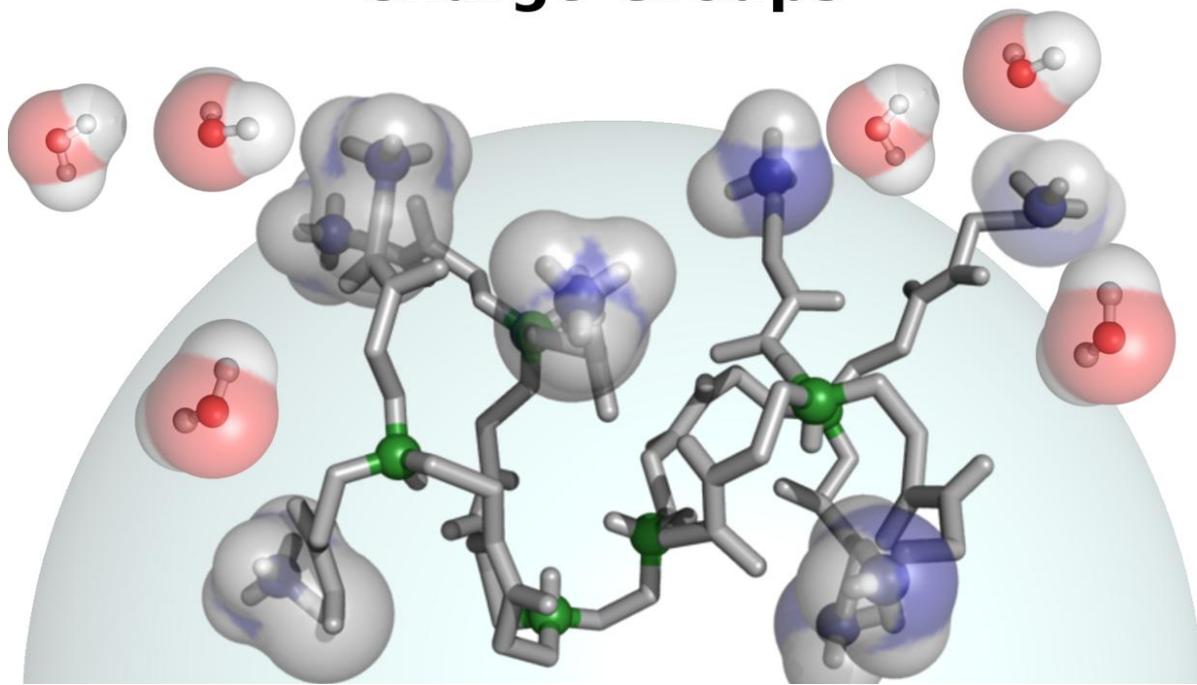Charge Groups**
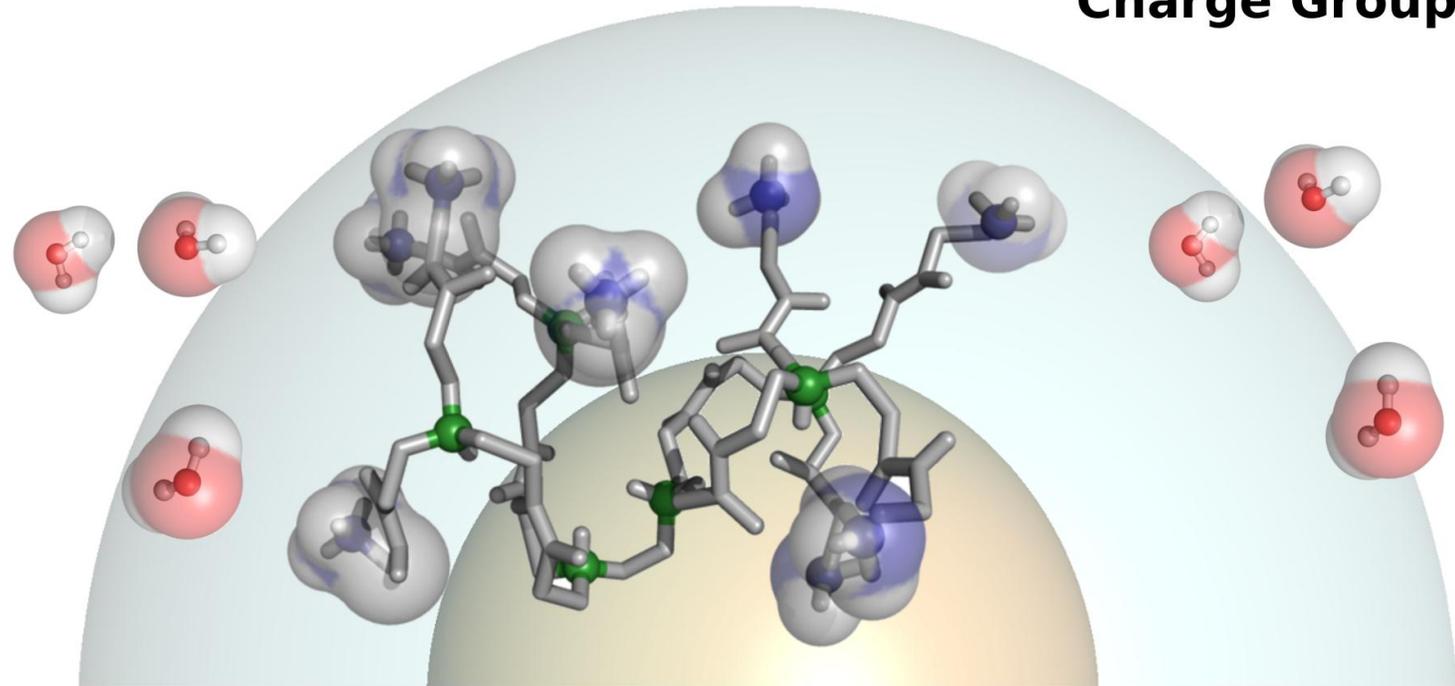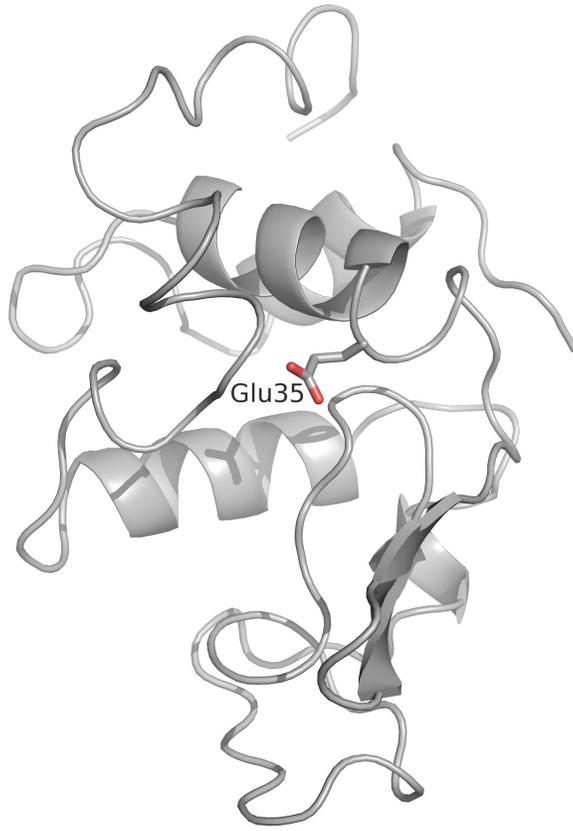
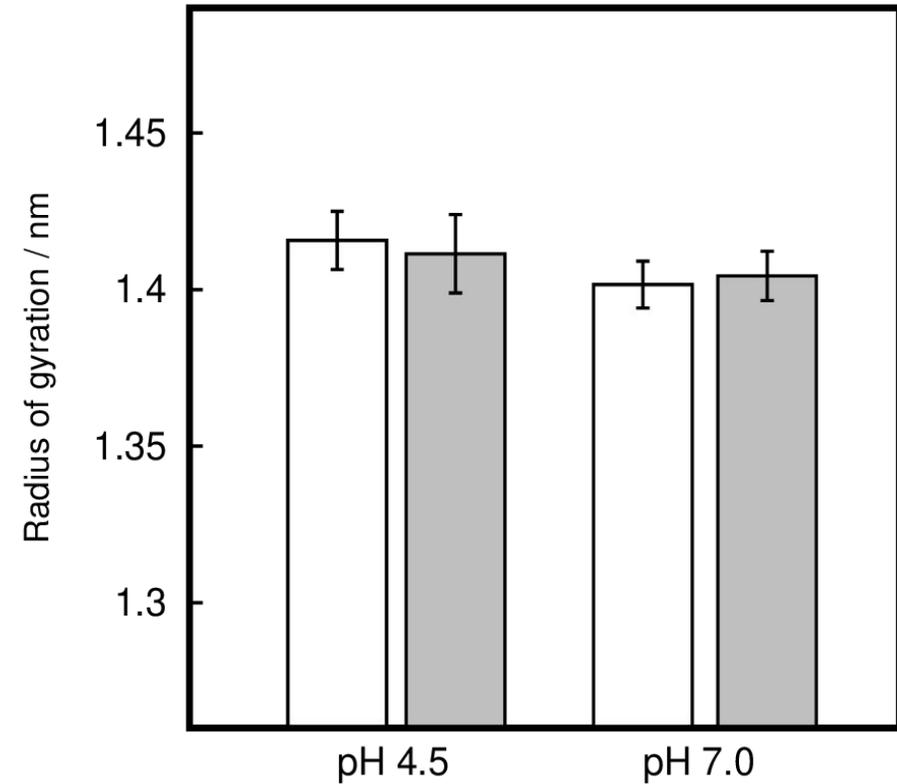# MD simulations - Changing conditions

Results - Twin-range cutoff vs single cutoff
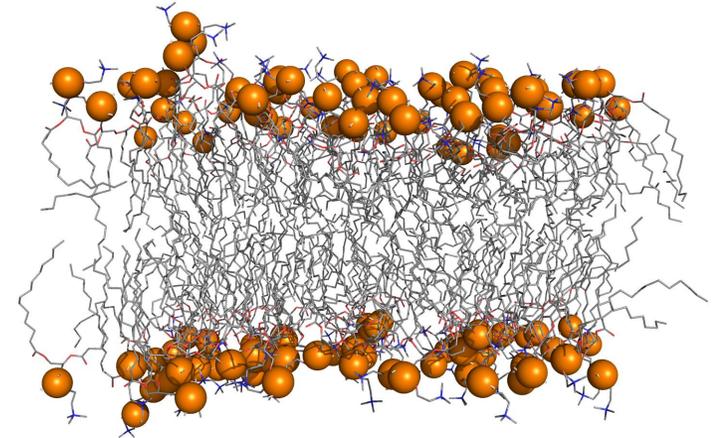
HEWL

CpHMD: GROMACS 4.0.7 with GRF

1 Silva, T. F. D., Vila-Viçosa, D., Reis, P. B. P. S., Victor, B. L., Diem, M., Oostenbrink, C., and Machuqueiro, M. (2018) "The impact of using single atomistic long range cutoff schemes with the GROMOS 54A7 force field", J. Chem. Theory Comput., 14, 5823-5833
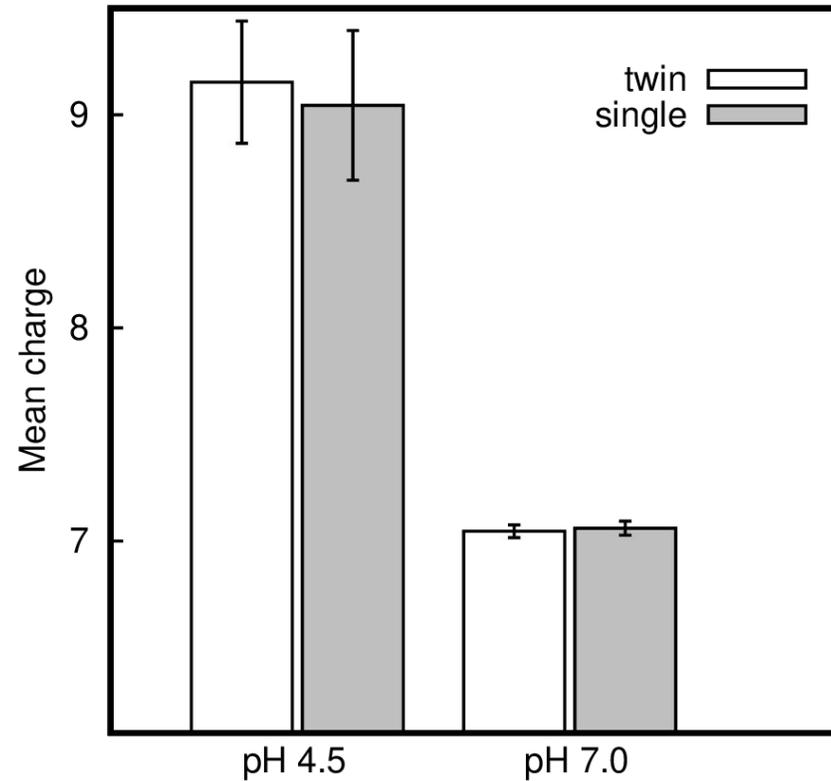
Results - Twin-range cutoff vs single cutoff

G1-PAMAM
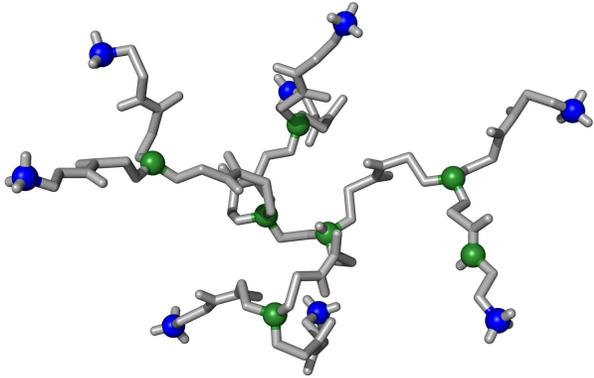
DMPC

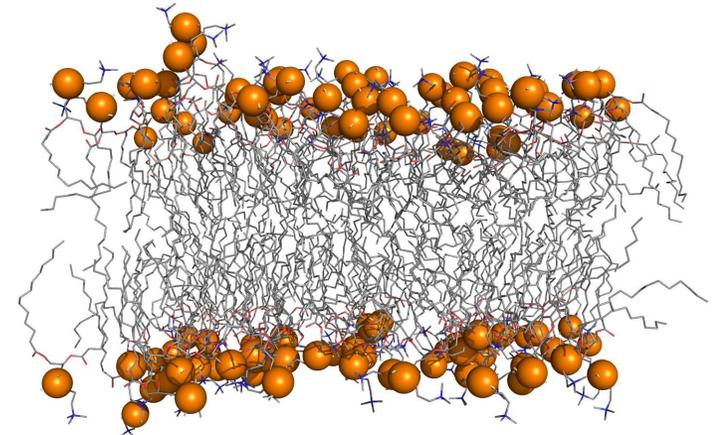**GROMACS 4.0.7**
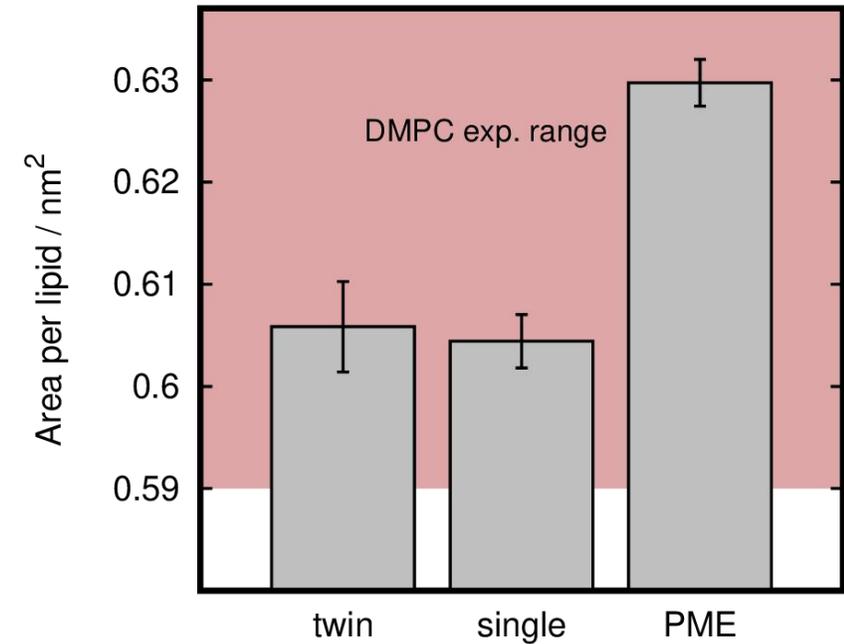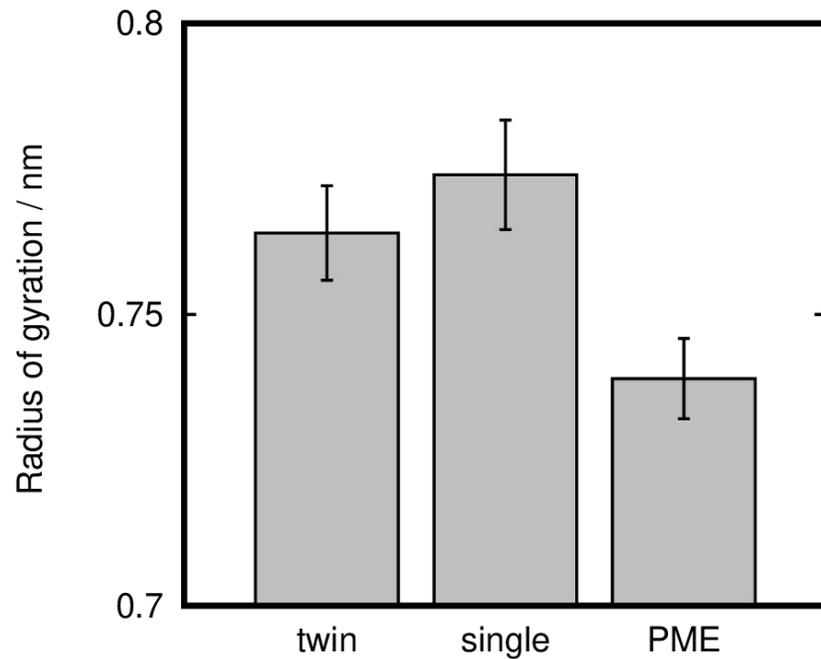
Results - Charge groups vs Verlet atomistic

G1-PAMAM
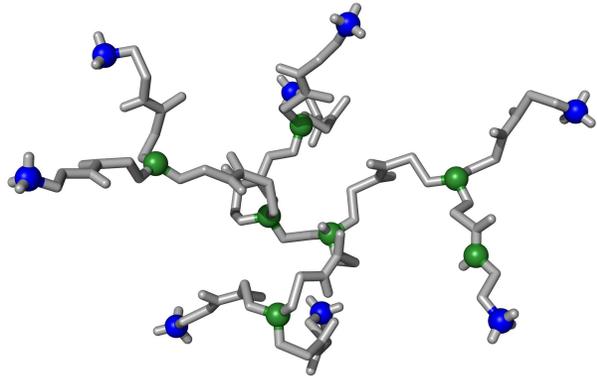
DMPC

1	Group-based Twin-range Charge groups
2	Group-based Single cutoff Charge groups
3	Group-based Single cutoff Atomistic
4	Verlet Single Cutoff Atomistic
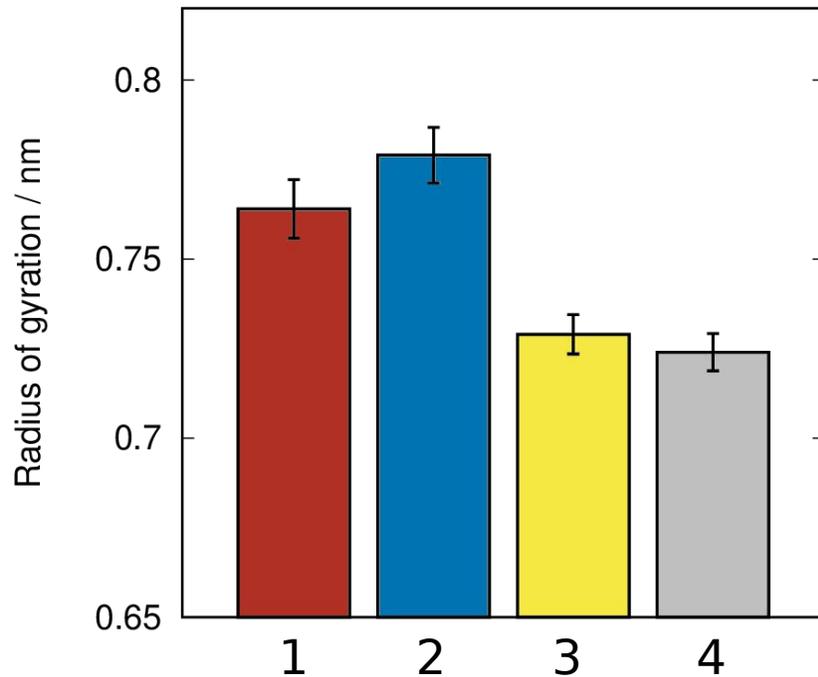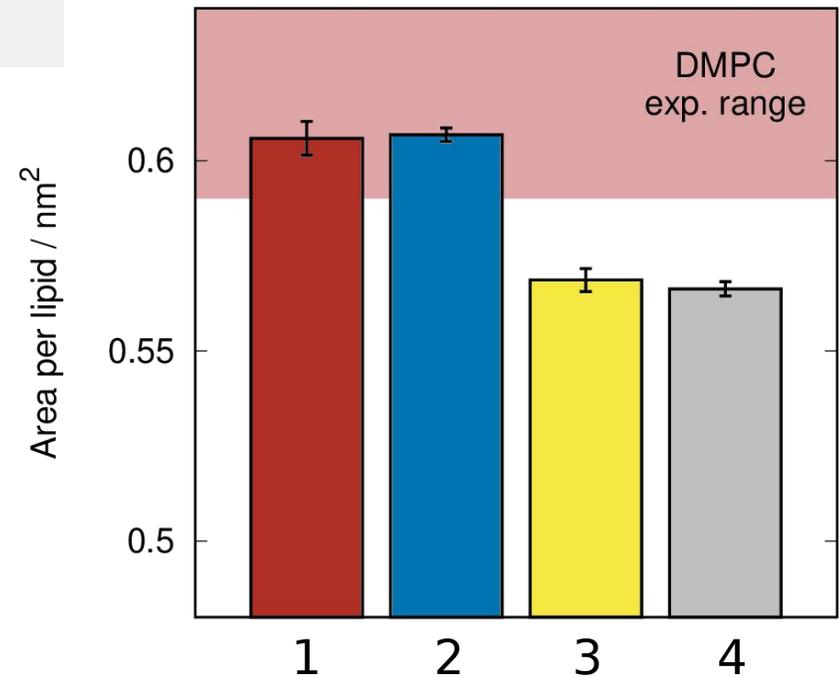
Results- Charge groups vs Verlet atomistic

Charge Group
Reaction Field
Rc = 1.4 nm

Verlet Atomistic
Reaction Field
Rc = 1.4 nm

DMPC - Area per Lipid

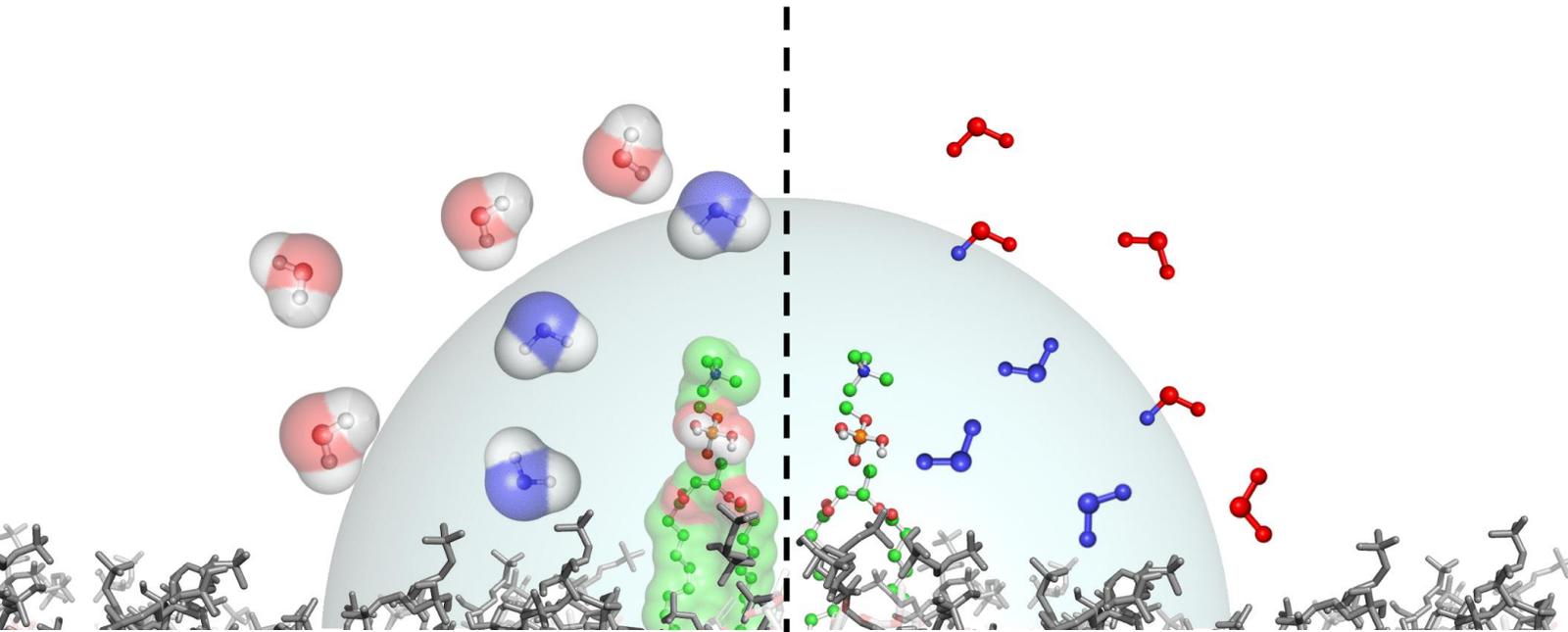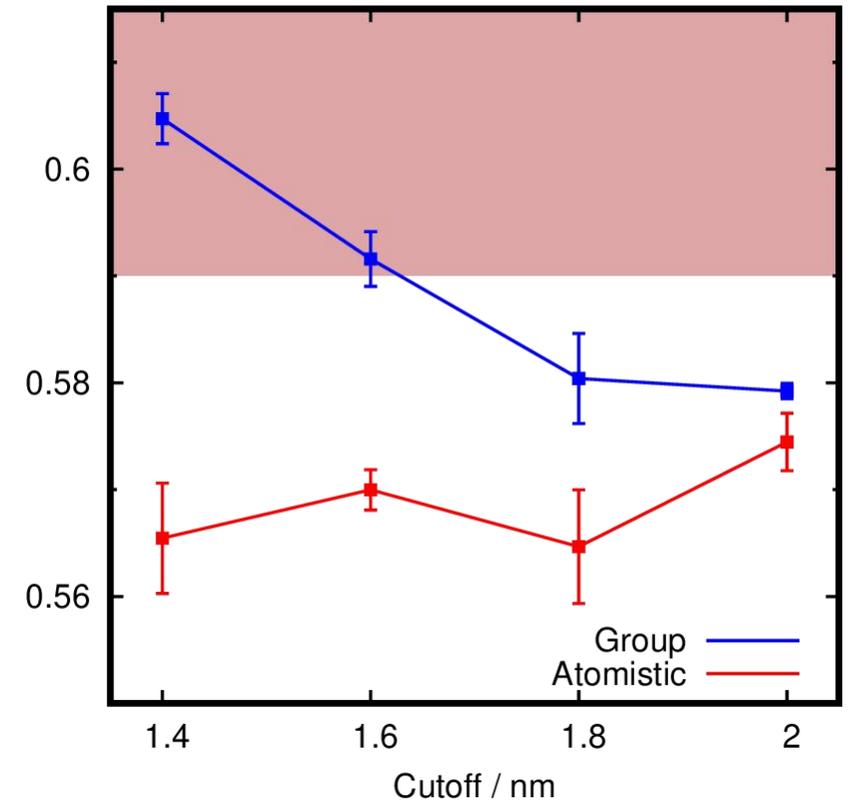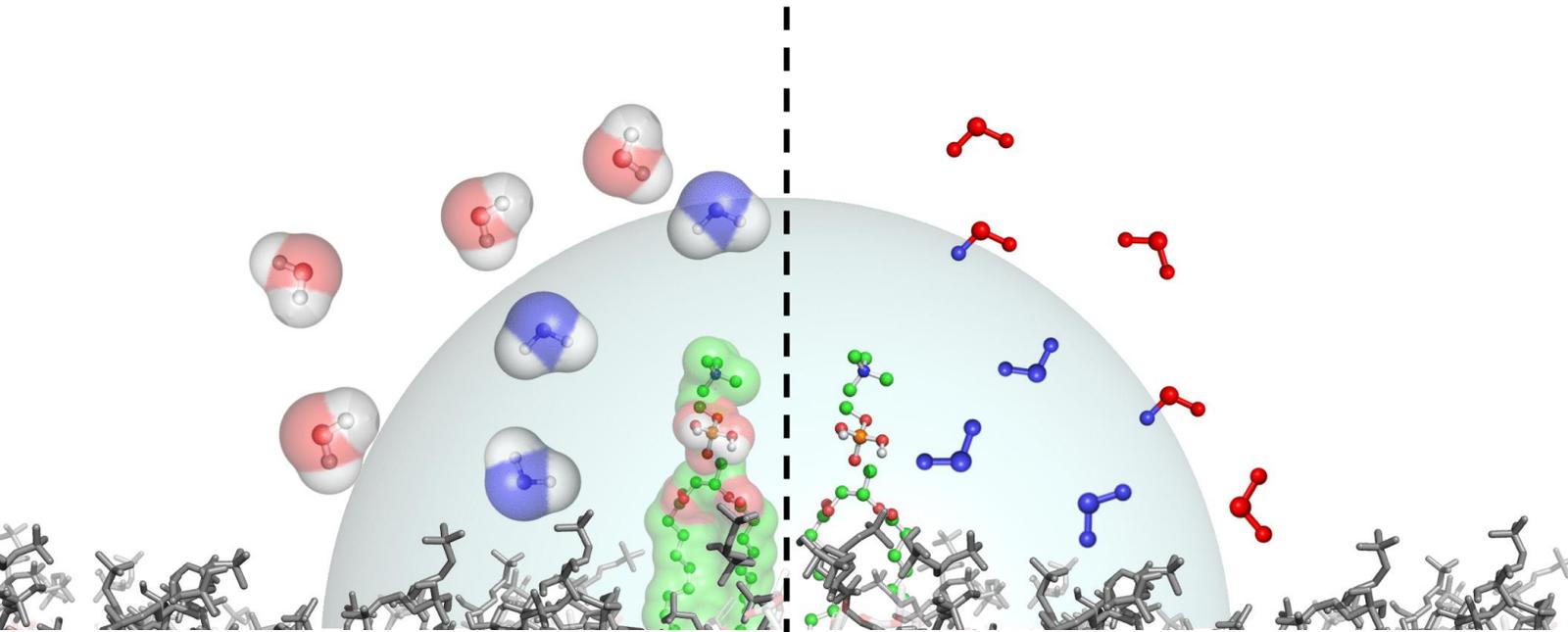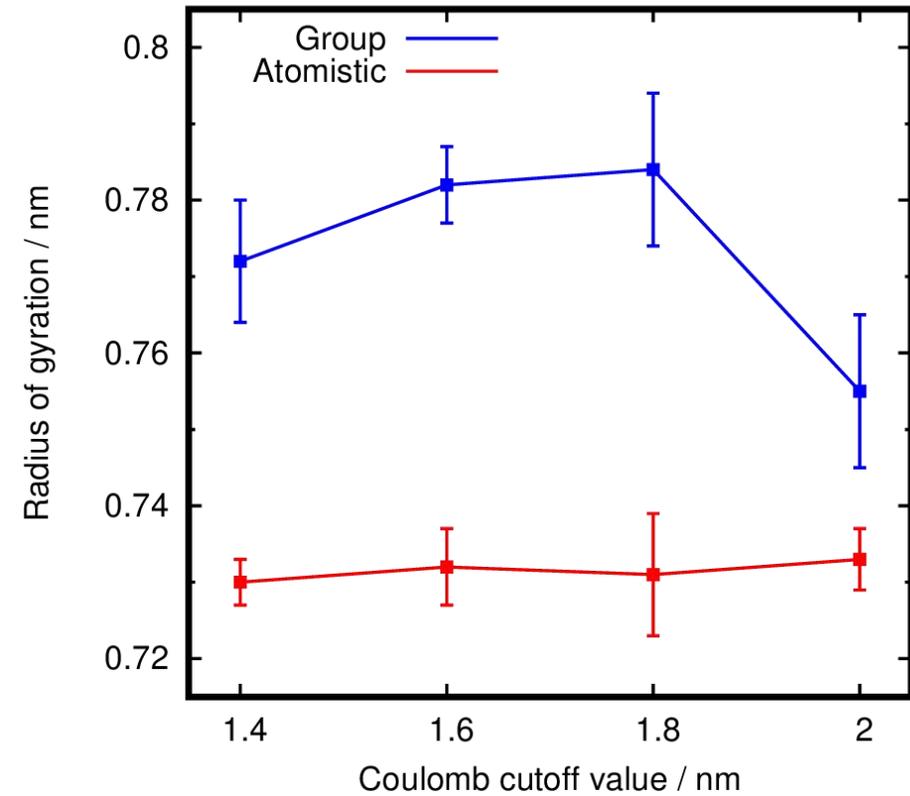# **Results-** Charge groups vs Verlet atomistic

Charge Group
Reaction Field
Rc = 1.4 nm

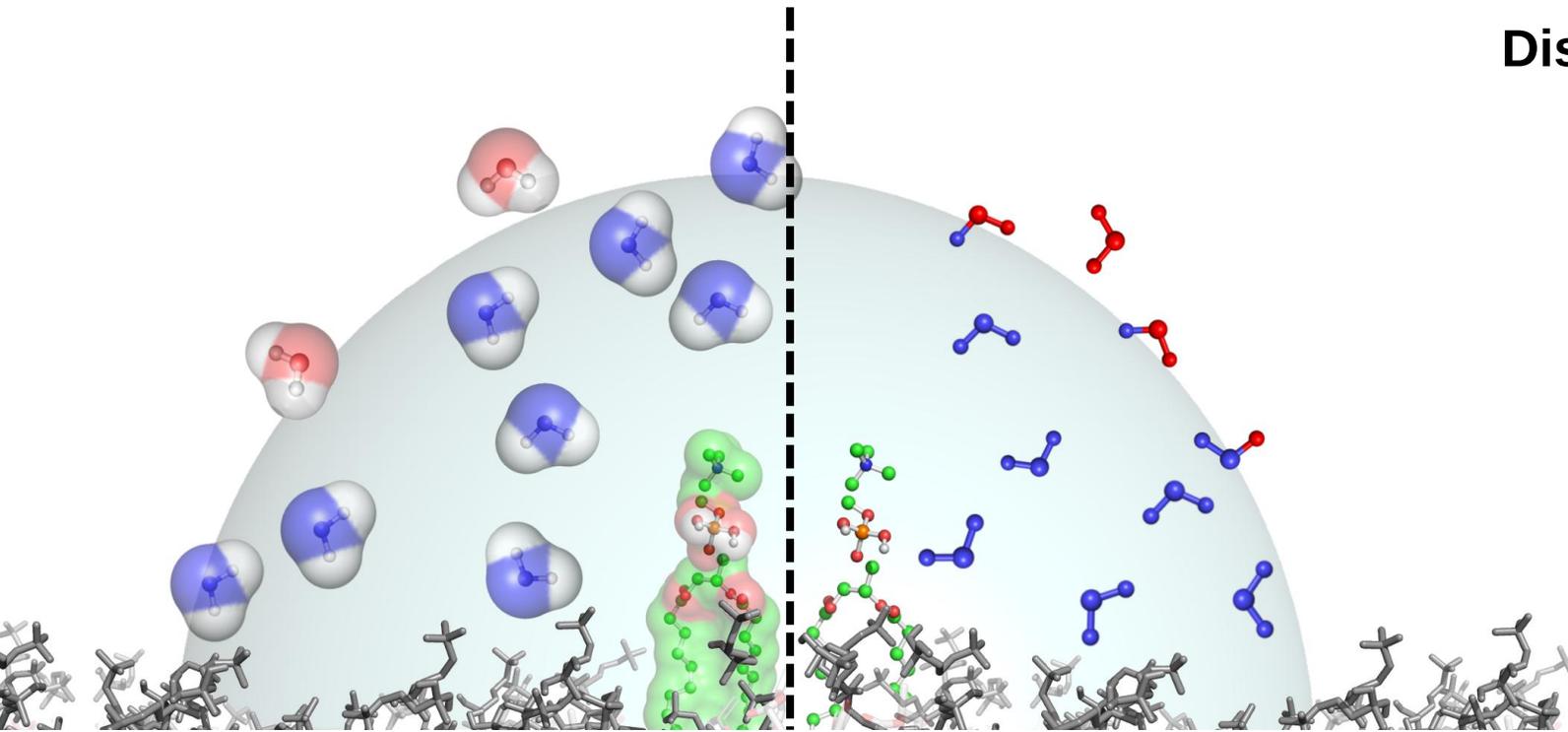**Verlet Atomistic**
Reaction Field
Rc = 1.4 nm

PAMAM - Radius of Gyration

Conclusion

Charge Group
Reaction Field

Verlet Atomistic
Reaction Field

Advantages:

- GROMOS compatibility;
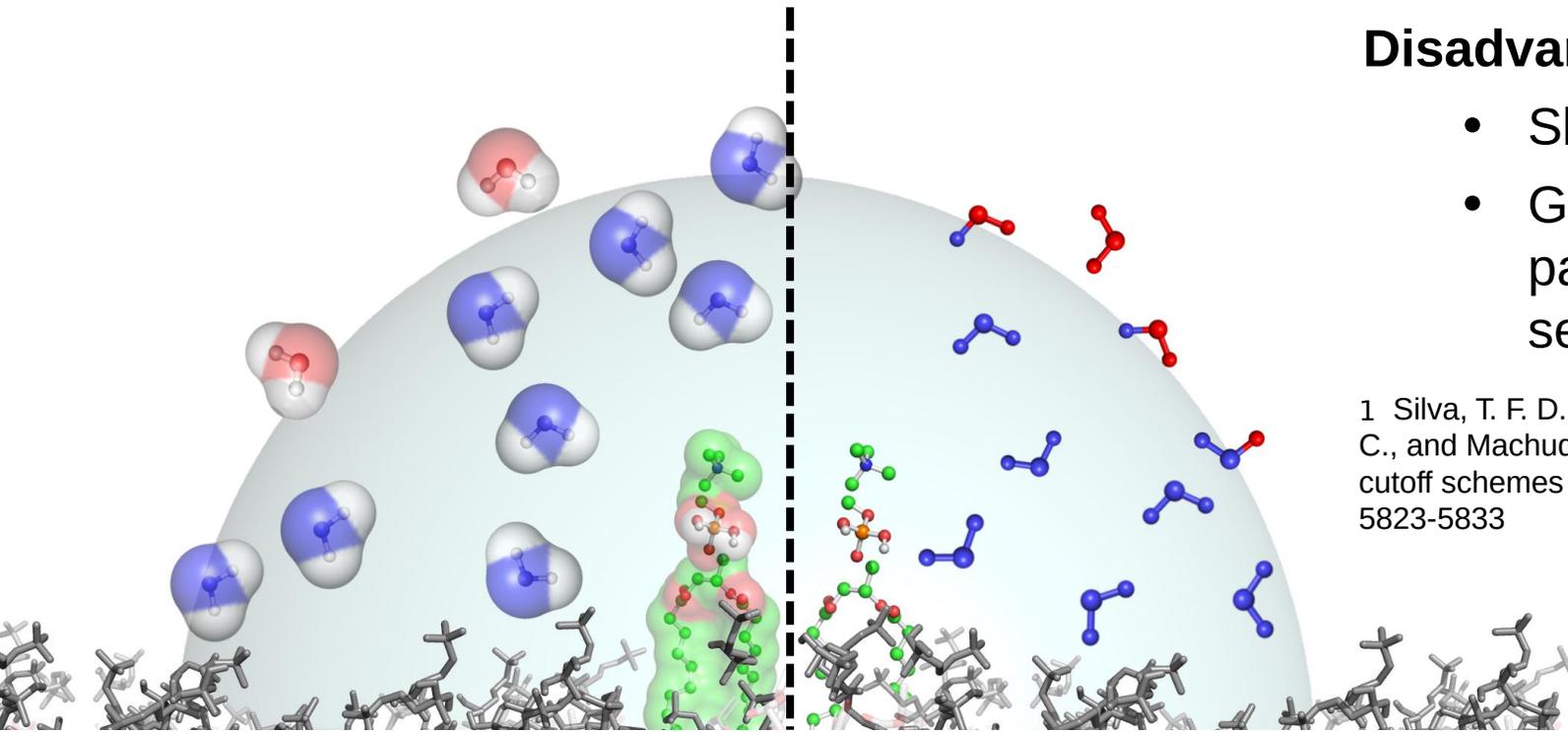- Increased speed (and faster with twin range scheme).

Disadvantages:

- Possible instabilities coupled with twin range;
- Lack of support for new packages of GROMACS;
- No convergence when using larger single cutoffs.

Conclusion

Charge Group
Reaction Field

Verlet Atomistic
Reaction Field

Advantages:

- Speed can be improved;
- Future use of newer software packages and features (i.e. GPU).

Disadvantages:

- Slower than charge groups;
- GROMOS force field wasn't parametrized for these settings.

✔

1 Silva, T. F. D., Vila-Viçosa, D., Reis, P. B. P. S., Victor, B. L., Diem, M., Oostenbrink, C., and Machuqueiro, M. (2018) "The impact of using single atomistic long range cutoff schemes with the GROMOS 54A7 force field", J. Chem. Theory Comput., 14, 5823-5833

Acknowledgments

Miguel Machuqueiro

Diogo Vila Viçosa

Bruno Victor

Pedro Reis

- **Collaboration**:

  Prof. Chris Oostenbrink (BOKU, Vienna)

  Matthias Diem (BOKU, Vienna)

- **MMS Group**

- **ITC Group**:

  Prof. Maria José Calhorda

  Paulo Costa

  Rafael Nunes