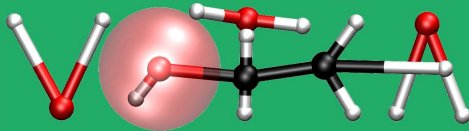




VOTCA

C. Junghans

Versatile Object-oriented Toolkit for Coarse-graining Applications



Victor Rühle, Christoph Junghans, Alexander Lukyanov,
Kurt Kremer and Denis Andrienko

Max Planck Institute for Polymer Research
Mainz

Nov 26, 2009

Introduction

Coarse-graining

VOTCA

C. Junghans

Introduction

Coarse-graining

Bottom-up CG

Iterative

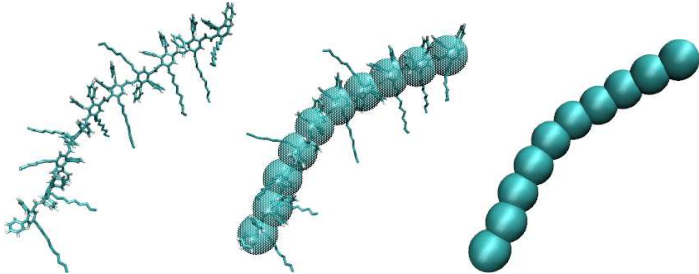
Methods

Examples

Conclusion

Why coarse-graining?

- Validate the physics of a low resolution model
- Throw away “unimportant” degrees of freedom
- Link time- and length-scales



Introduction

Bottom-up coarse-graining

VOTCA

C. Junghans

Introduction
Coarse-graining
Bottom-up CG
Iterative
Methods

Examples

Conclusion

Basic idea

Is there a force field for the coarse-grained model which reproduces a certain property of the reference system?

- Forces \rightarrow Force matching¹

$$\min |\vec{F}_I^{\text{CG}} - \sum_{i \in I} f_i^{\text{Ref}}|^2$$

- Two-body correlations (e.g. $g(r)$) \rightarrow iterative methods:

$$U_{n+1}^{\text{CG}} = U_n^{\text{CG}} + \Delta U(\text{nth CG Simulation})$$

- Pressure \rightarrow Pressure correction
- Diffusion \rightarrow Friction constant fitting

¹S. Izvekov and G. Voth, J. Chem. Phys. **123**, 134105 (2005).

Potential Update

- Iterative Boltzmann inversion²

$$\Delta U_n^{\text{CG}}(r) = k_B T \ln \frac{g_n^{\text{CG}}(r)}{g^{\text{Ref}}(r)}$$

- Inverse “Monte Carlo”³

$$\Delta U_n^{\text{CG}}(r) = \sum_{r'} A_n^{-1}(r, r') \left(g_n^{\text{CG}}(r') - g^{\text{Ref}}(r') \right),$$

where

$$A_n(r, r') \sim \langle g_n^{\text{CG}}(r) g_n^{\text{CG}}(r') \rangle - \langle g_n^{\text{CG}}(r) \rangle \langle g_n^{\text{CG}}(r') \rangle$$

²D. Reith et al., J. Comp. Chem. **24**, 1624-1636 (2003).

³A. Lyubartsev and A. Laaksonen, Phys. Rev. E **52**, 3730-3737 (1995).

Examples

Water

VOTCA

C. Junghans

Introduction

Examples

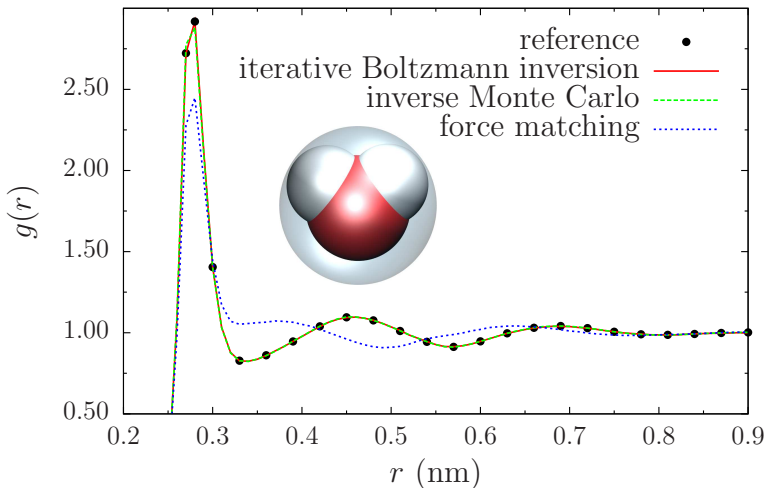
Water

Propane

Hexane

Conclusion

Radial distribution functions



Examples

Water

VOTCA

C. Junghans

Introduction

Examples

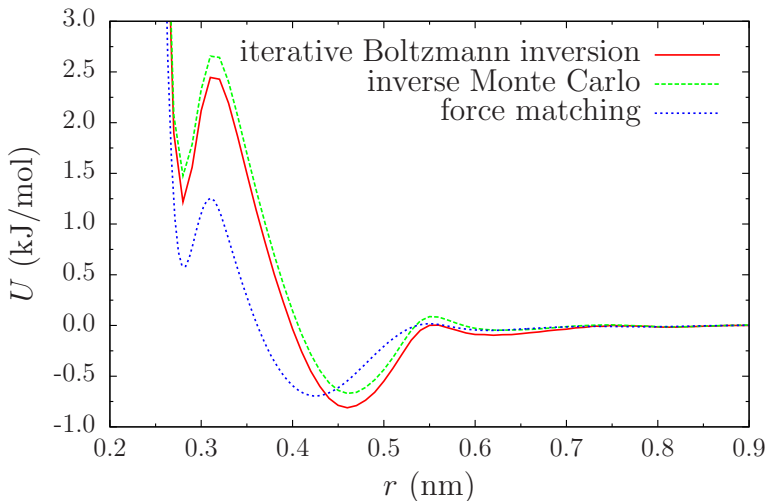
Water

Propane

Hexane

Conclusion

Coarse-grained potentials



Examples

Water

VOTCA

C. Junghans

Introduction

Examples

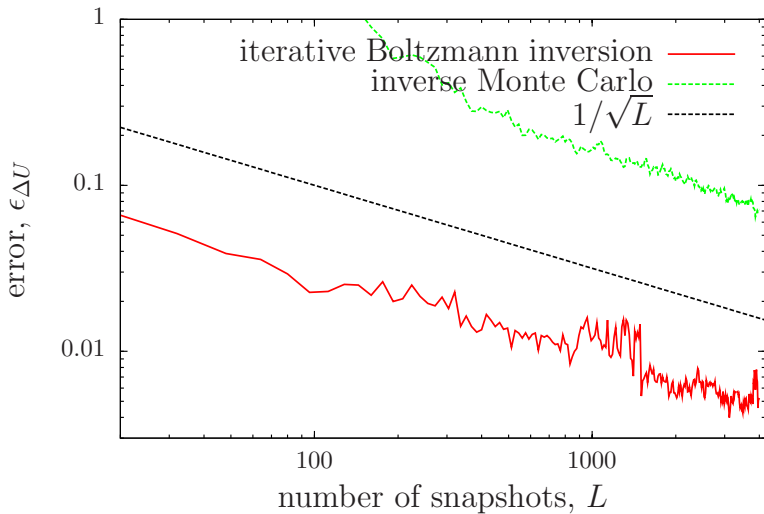
Water

Propane

Hexane

Conclusion

Average error of the potential update



Examples

Water

VOTCA

C. Junghans

Introduction

Examples

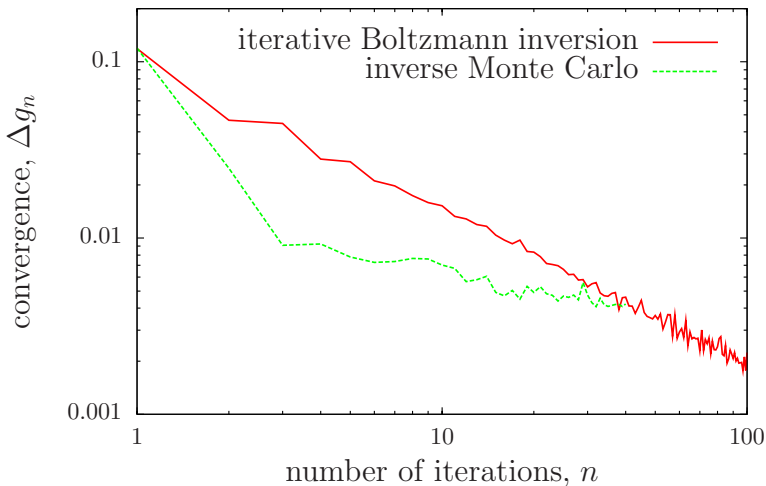
Water

Propane

Hexane

Conclusion

Deviation of reference and current $g(r)$



Examples

Liquid Propane

VOTCA

C. Junghans

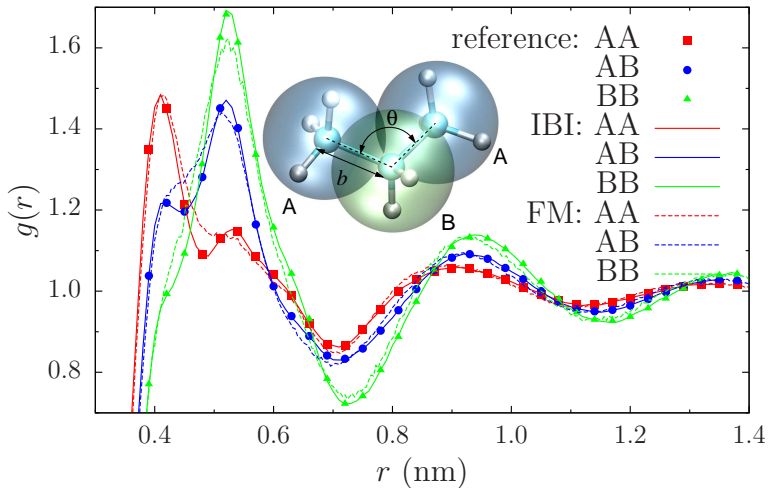
Introduction

Examples

Water
Propane
Hexane

Conclusion

Radial distribution functions



Examples

Liquid Propane

VOTCA

C. Junghans

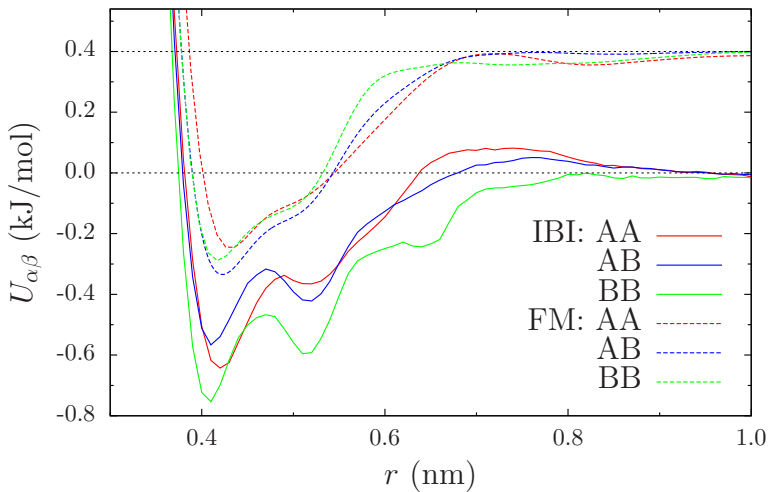
Introduction

Examples

Water
Propane
Hexane

Conclusion

Coarse-grained potentials





Examples

Liquid Propane

VOTCA

C. Junghans

Introduction

Examples

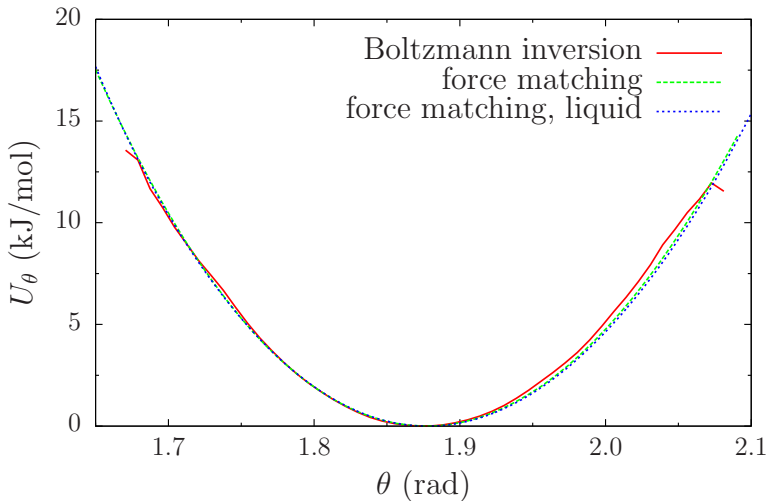
Water

Propane

Hexane

Conclusion

Angle potentials



Examples

Liquid Hexane - Single molecule in vacuum

VOTCA

C. Junghans

Introduction

Examples

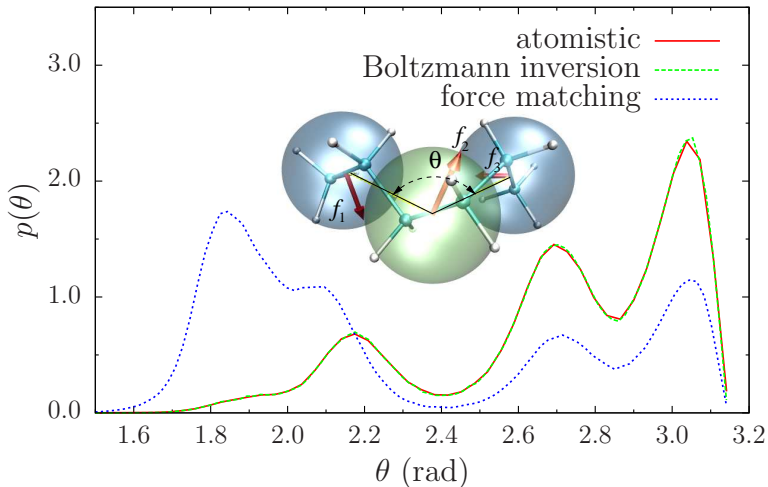
Water

Propane

Hexane

Conclusion

Probability density





Conclusion

VOTCA

C. Junghans

Introduction

Examples

Conclusion

Package

Be careful⁴:

- CG models never reproduce all features
- Completeness of the CG force field (basis sets)
- Correlations in parameters
- CG force fields are made for a part of the phase space only
- Dynamics in multicomponent system

⁴J. Chem. Theo. Comp. doi: 10.1021/ct900369w (2009)

Conclusion

Package

VOTCA

C. Junghans

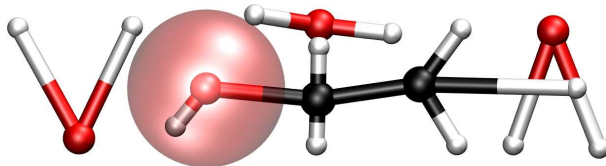
Introduction

Examples

Conclusion
Package

Linus Torvalds:

Talk is cheap, show me the code.



Versatile **O**bject-oriented **T**oolkit for **C**oarse-graining **A**pplications

Modular C++ kernel

Scripting for iterative workflow

Simple integration of other simulation packages

Iterative Boltzmann inversion

Inverse Monte Carlo

Force matching

- It's free
- All examples are in the tutorial
- Release: Dec 1st

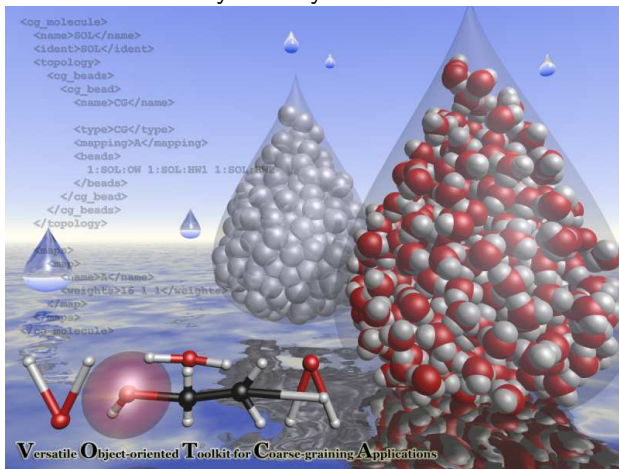
Visit us at www.votca.org

The End

VOTCA

C. Junghans

Thank you for your attention !



Visit us at www.votca.org