Gauß-Allianz e.V.

Status conference “Competence in High Performance Computing”

Capturing the divergence of length and time scales at the critical point by molecular dynamics simulation

Schwetzingen, June 22, 2010

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ThEt

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VERFAHRENSTECHNIK
TU KAISERSLAUTERN

Corresponding states and molecular modeling

Pitzer, *J. Chem. Phys.* **7**: 583 (1939).

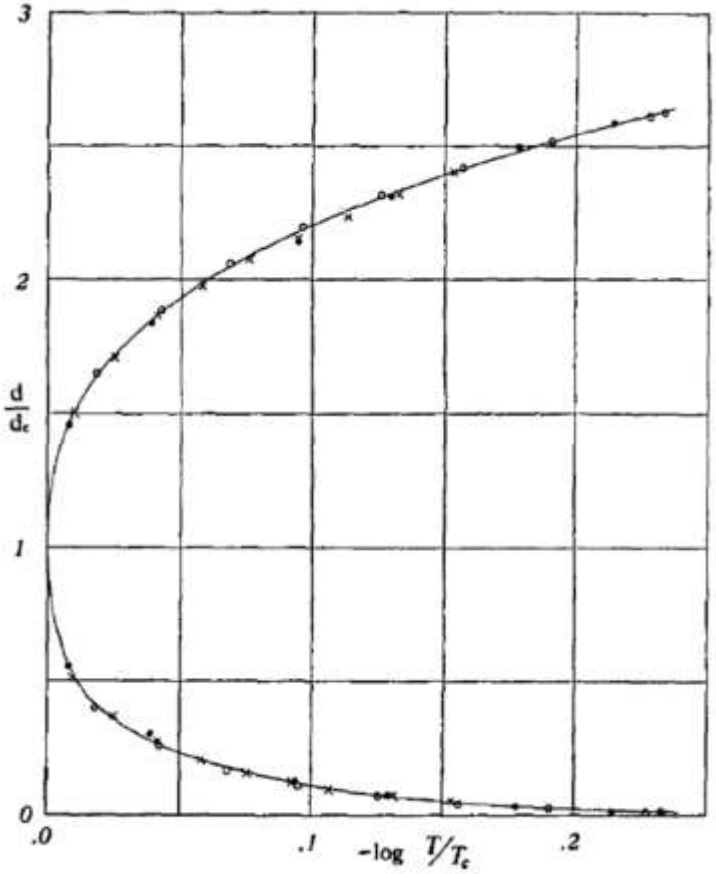
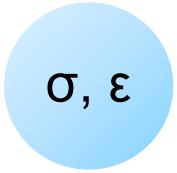


FIG. 3. Reduced density data: ● argon, 0 methane, x xenon.

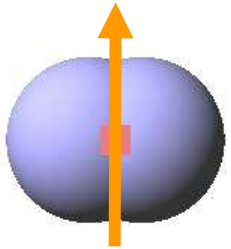
Simple molecular models

Lennard-Jones



noble gases
methane

2CLJD / 2CLJQ



78 real fluids
97.4% of their mixtures

Parametrization

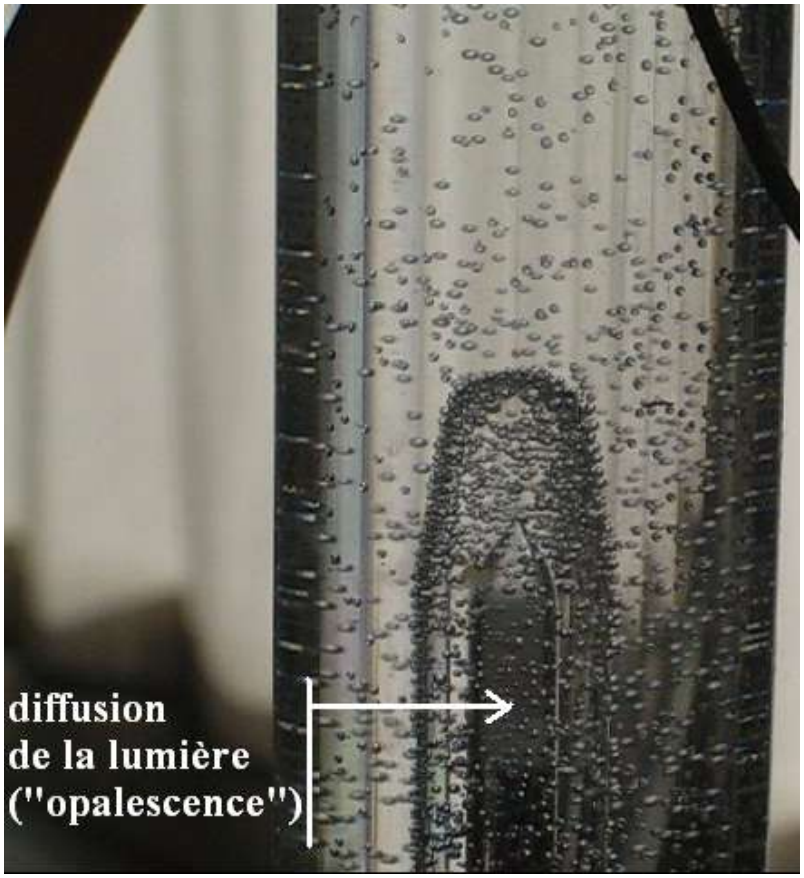
Fit to large number of VLE data

or

T_c and ρ_c

T_c, p_c, ρ_c, and $p_s(0.7\ T_c)$

Determination of the critical point



fr.wikipedia.org

In the critical limit,

- the correlation length ξ,
- the relaxation time τ,
- local density fluctuations (e.g. β_T),
- local energy fluctuations (e.g. c_v),

… diverge while for VLE data, the precision decreases.

Experiment: Critical opalescence.

Innovative HPC Methods for Molecular Simulation

Bundesministerium für Bildung und Forschung

memo

Technische Universität Kaiserslautern

Fraunhofer ITWM

HLRS

Technische Universität München

Universität Paderborn

BASF The Chemical Company

Bayer

Evonik Industries

IBM

ls1 mardyn

ms2 (www.ms-2.de)

future challenges!

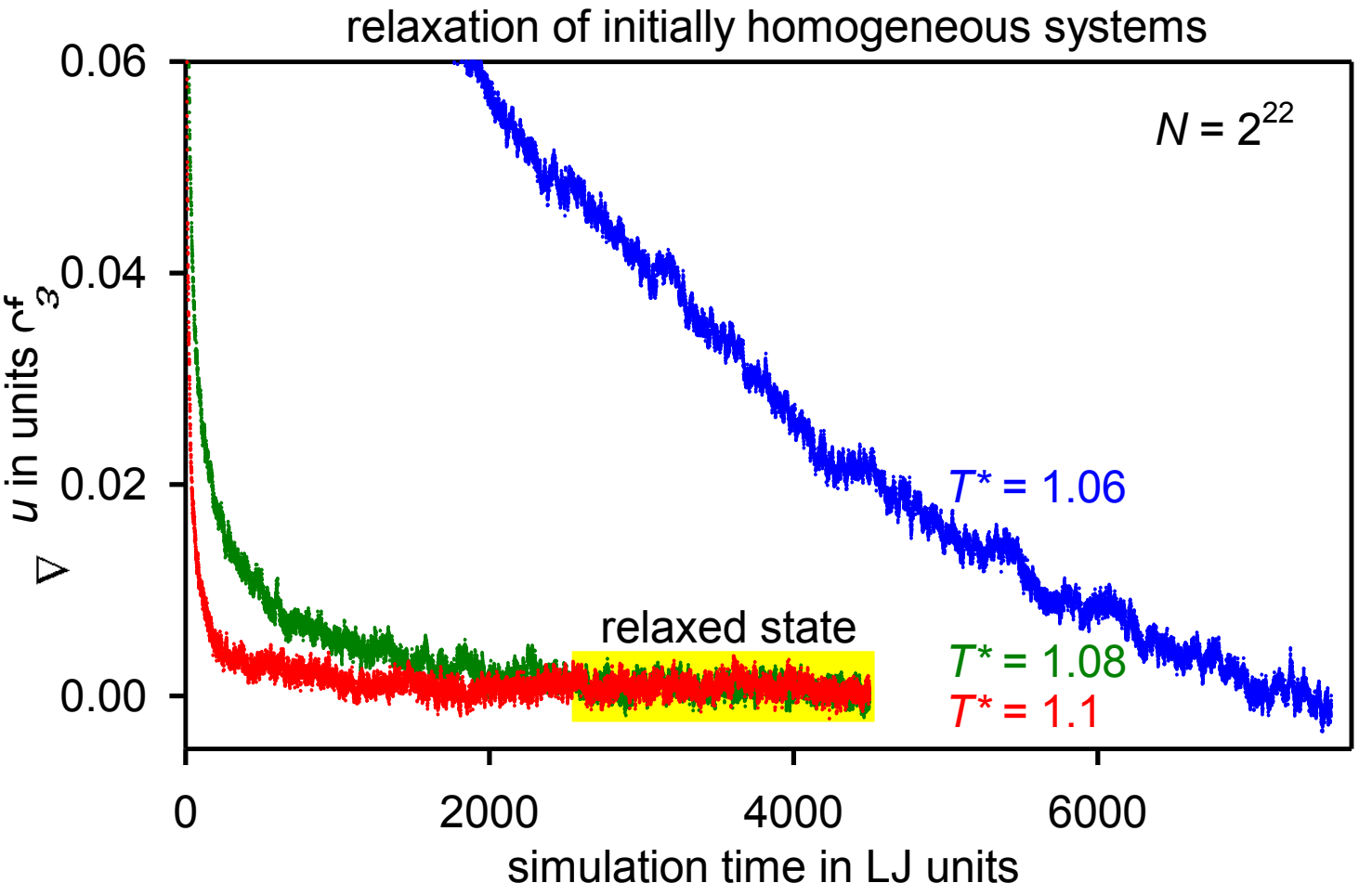
adsorption

ionic liquids

critical behaviour

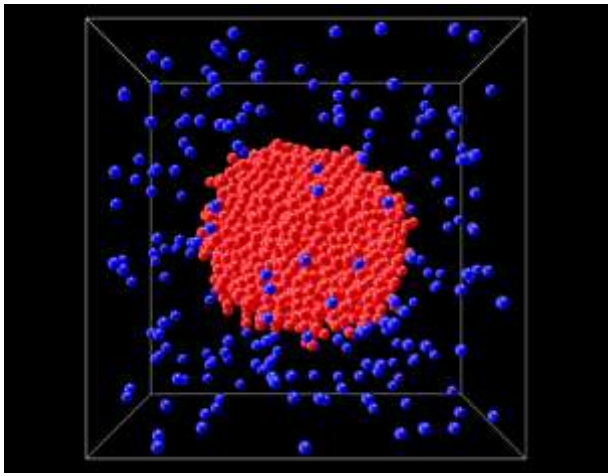
toxic/explosive fluids

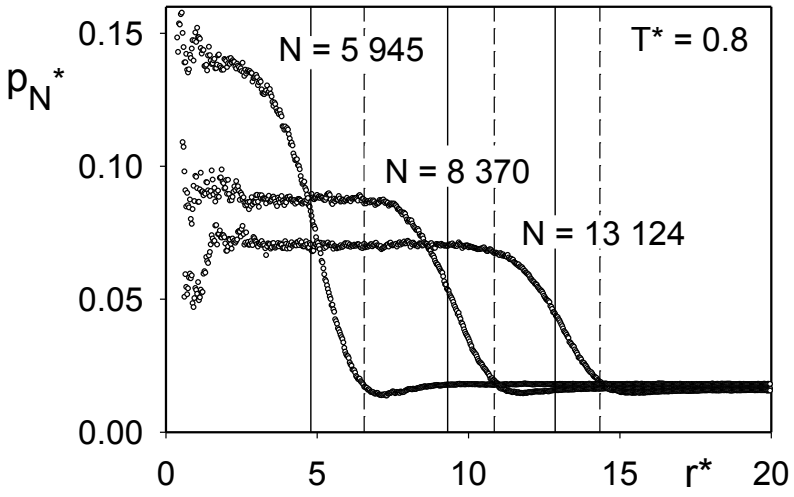
Direct approach: Isochoric heat capacity

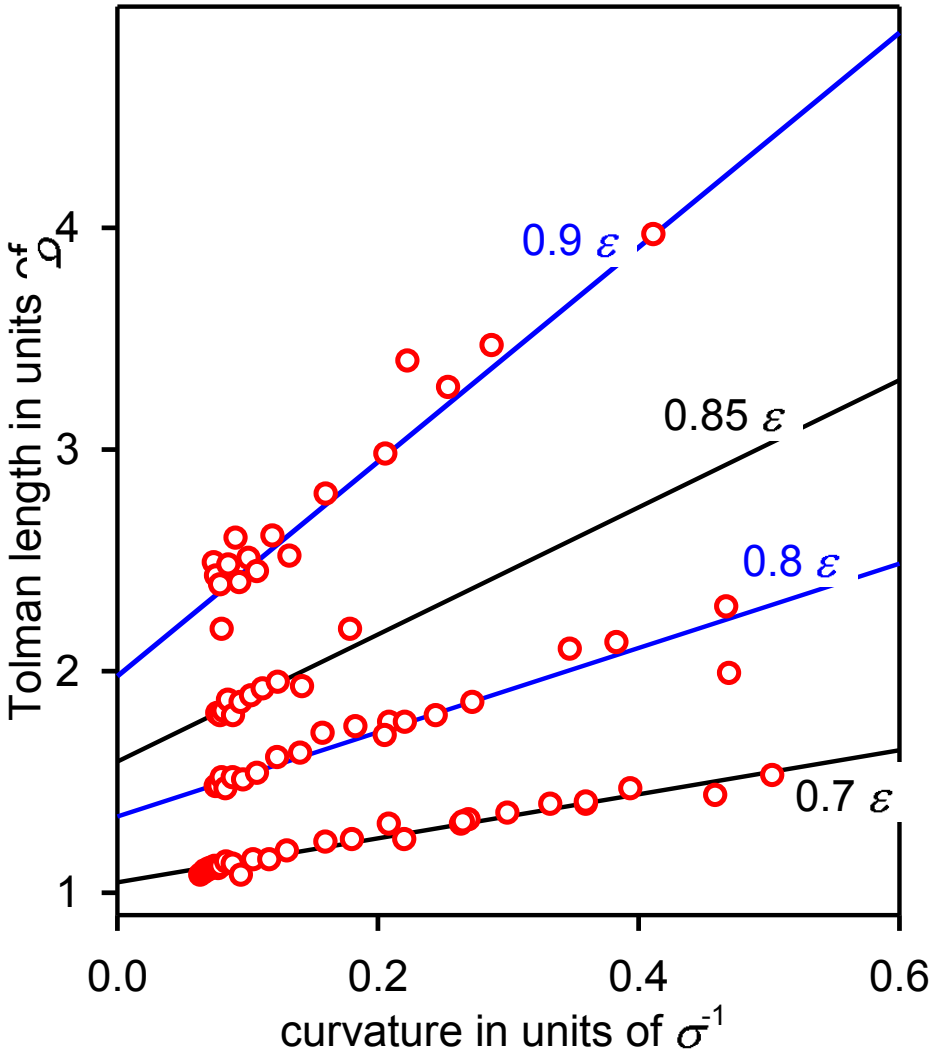


(truncated-shifted LJ potential; the time unit roughly corresponds to 2 ps)

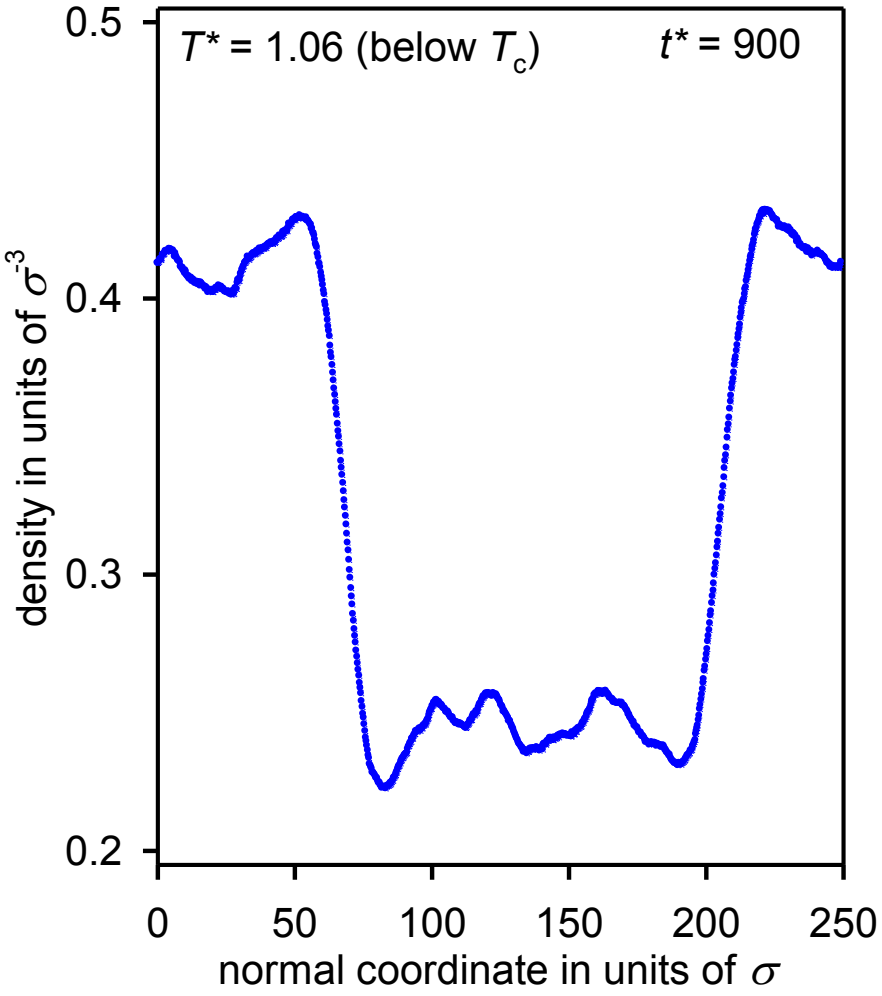
Indirect approach: Phase coexistence below T_c

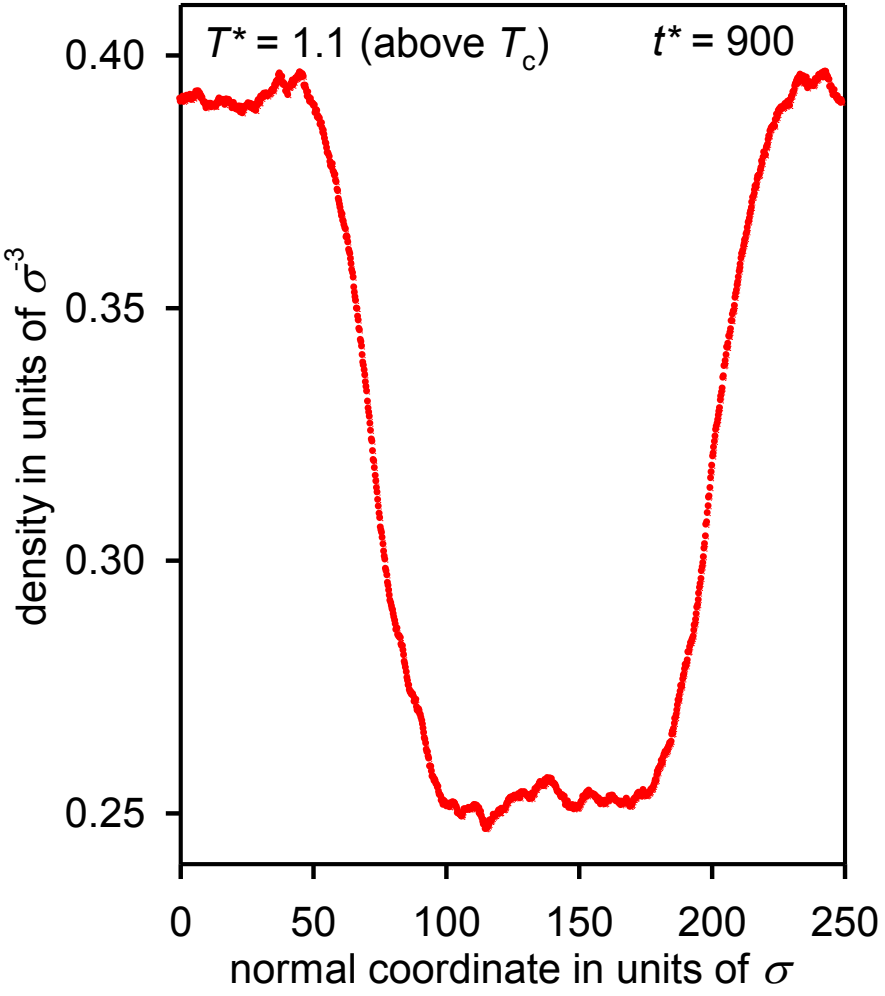




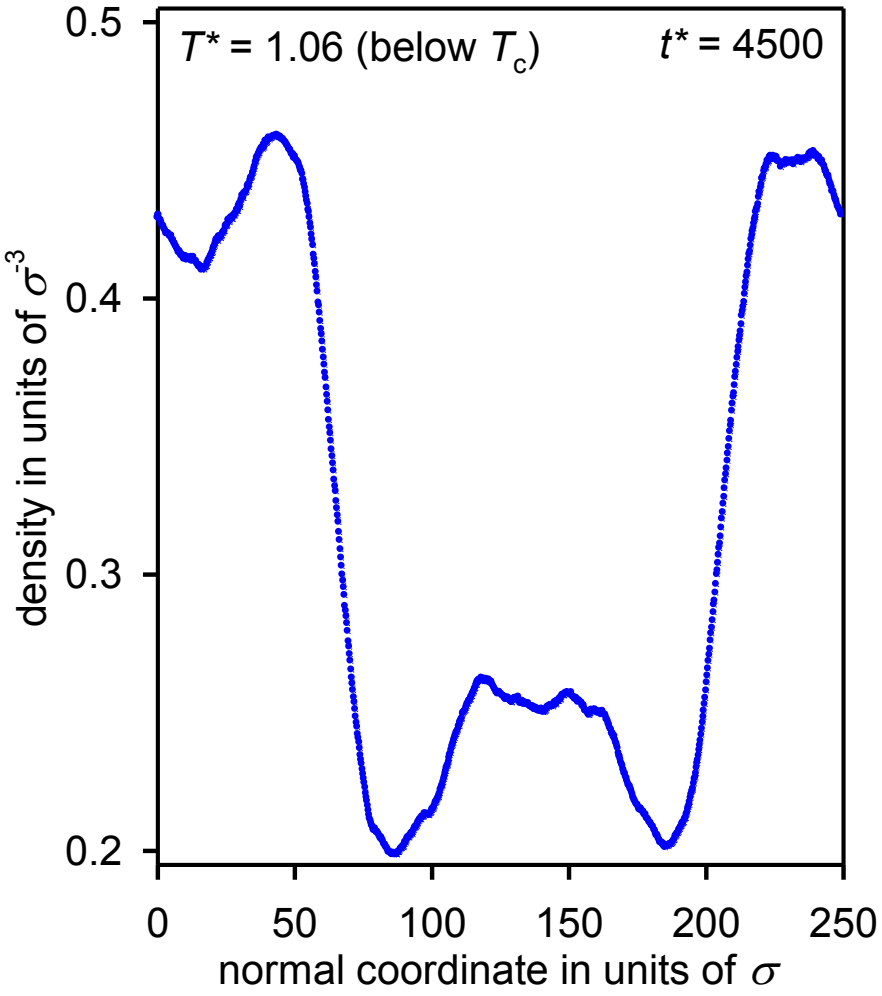


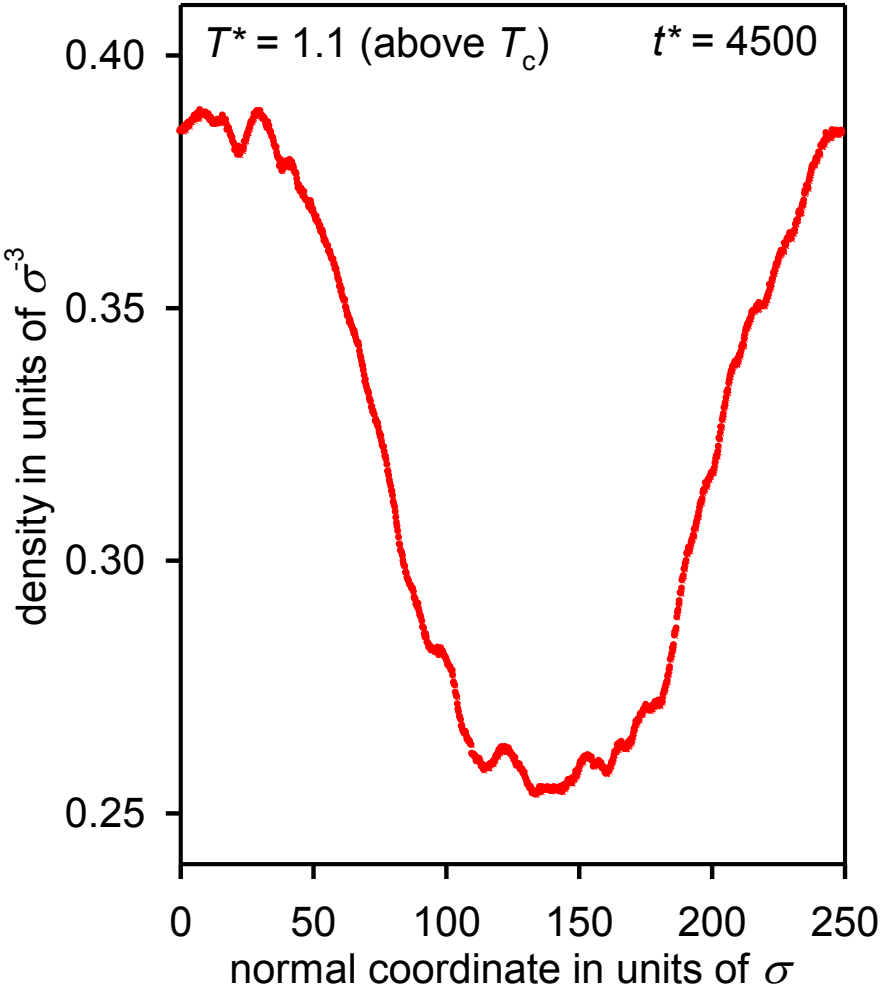
Interfacial relaxation time





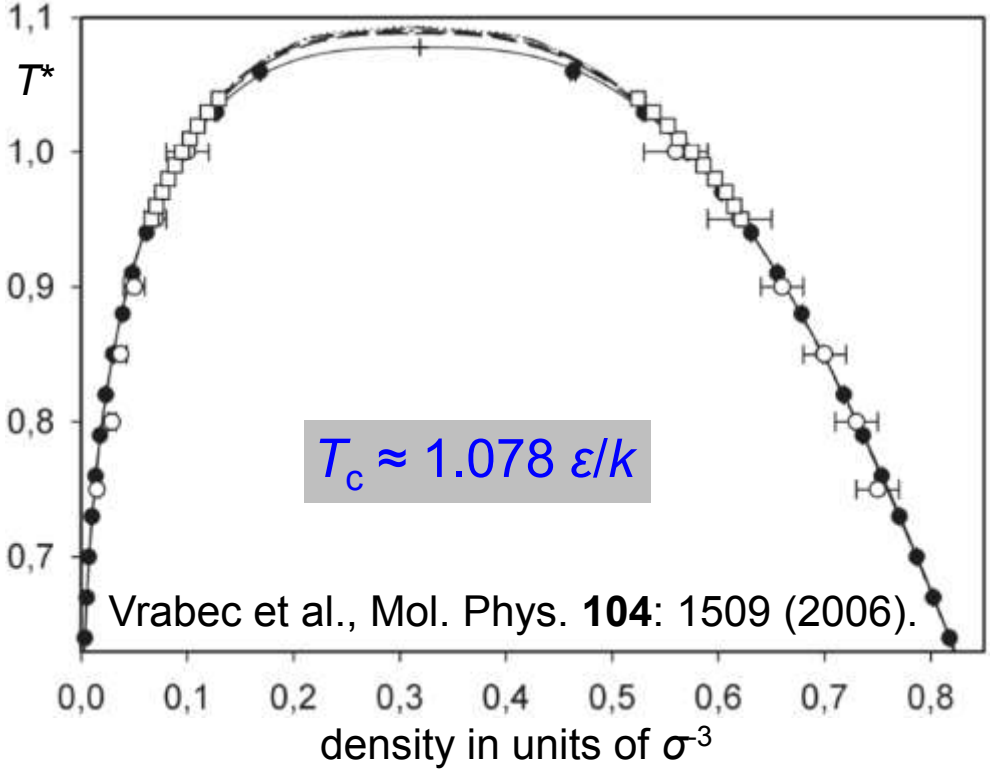
Interfacial relaxation time

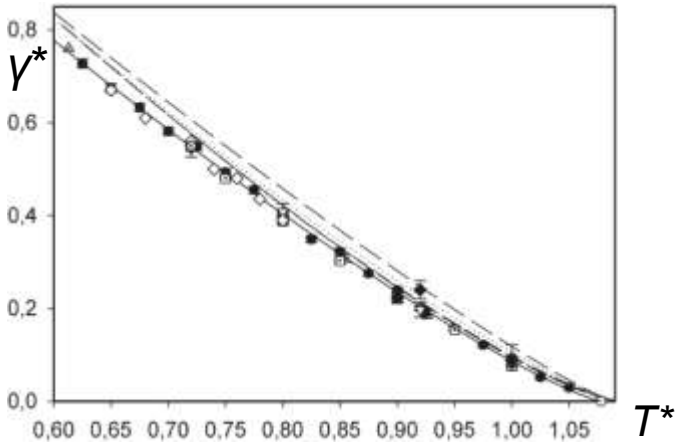


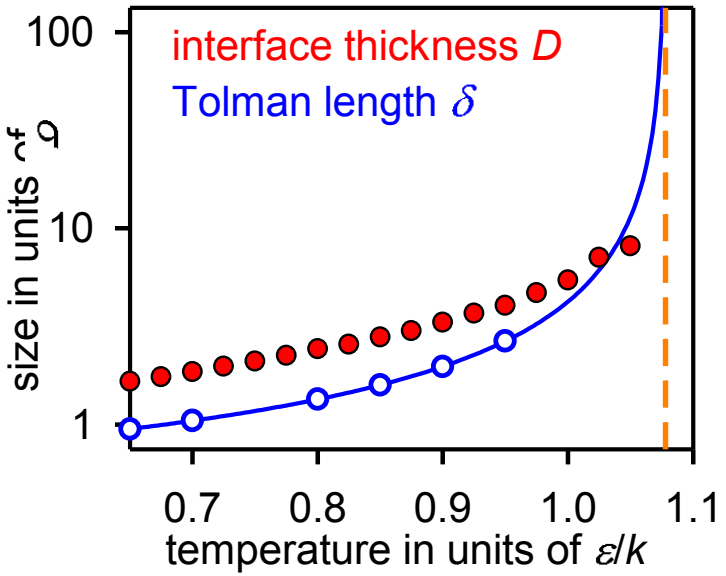


Critical temperature by extrapolation

Binodal line for the truncated-shifted LJ fluid



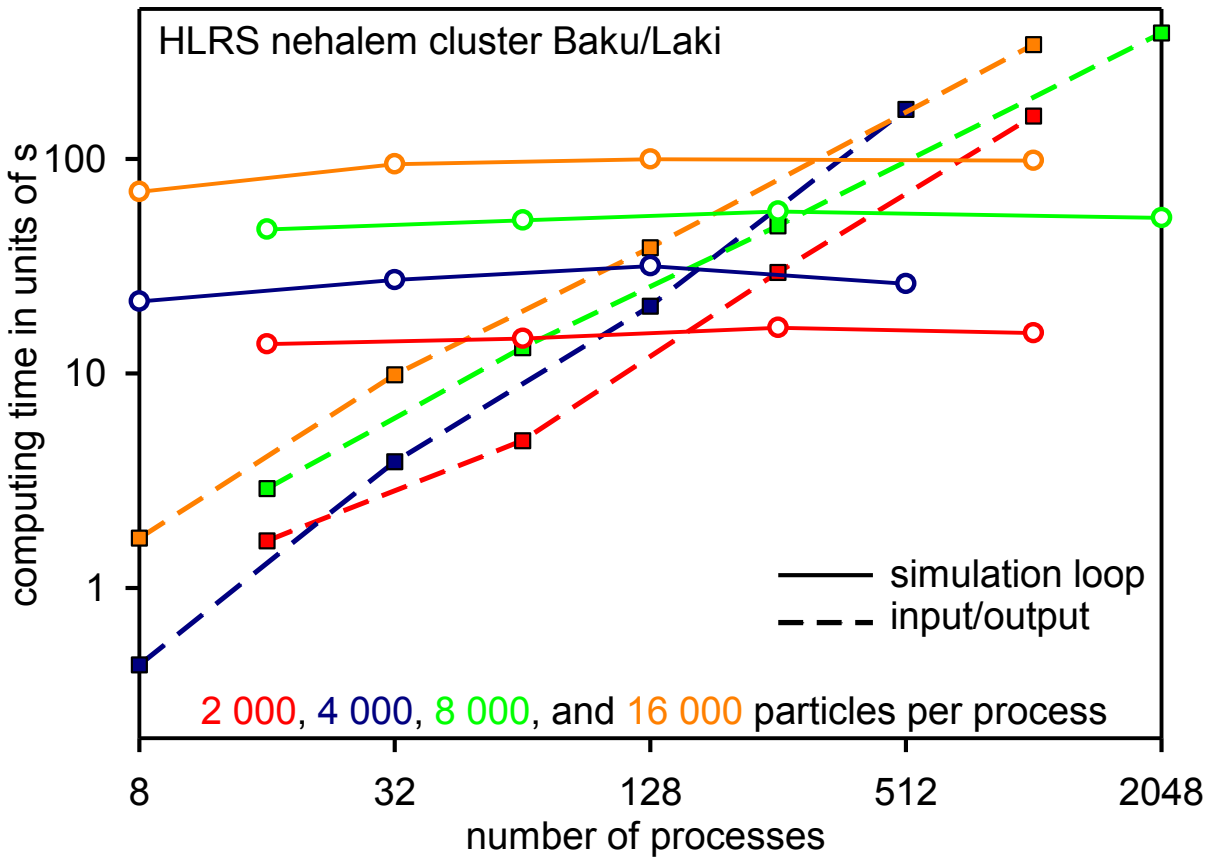




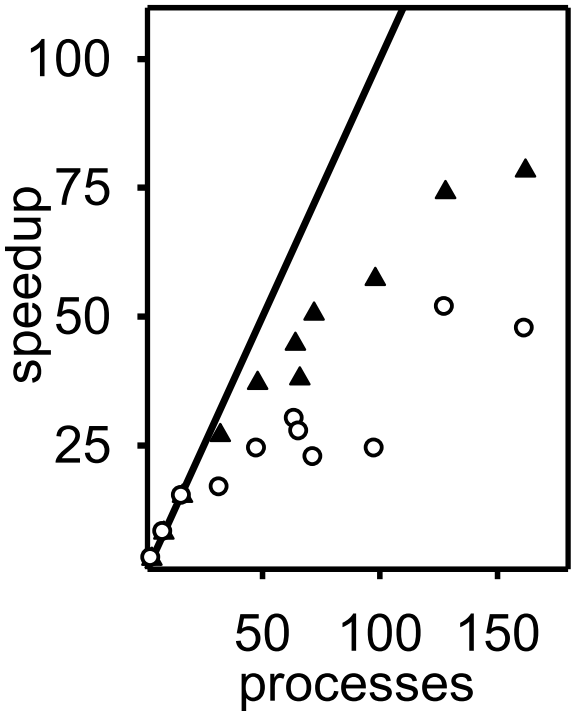
Guggenheim approach
Assumption: critical exponent $\beta = 1/3$

Scaling of the ls1 mardyn program

homogeneous truncated-shifted LJ system

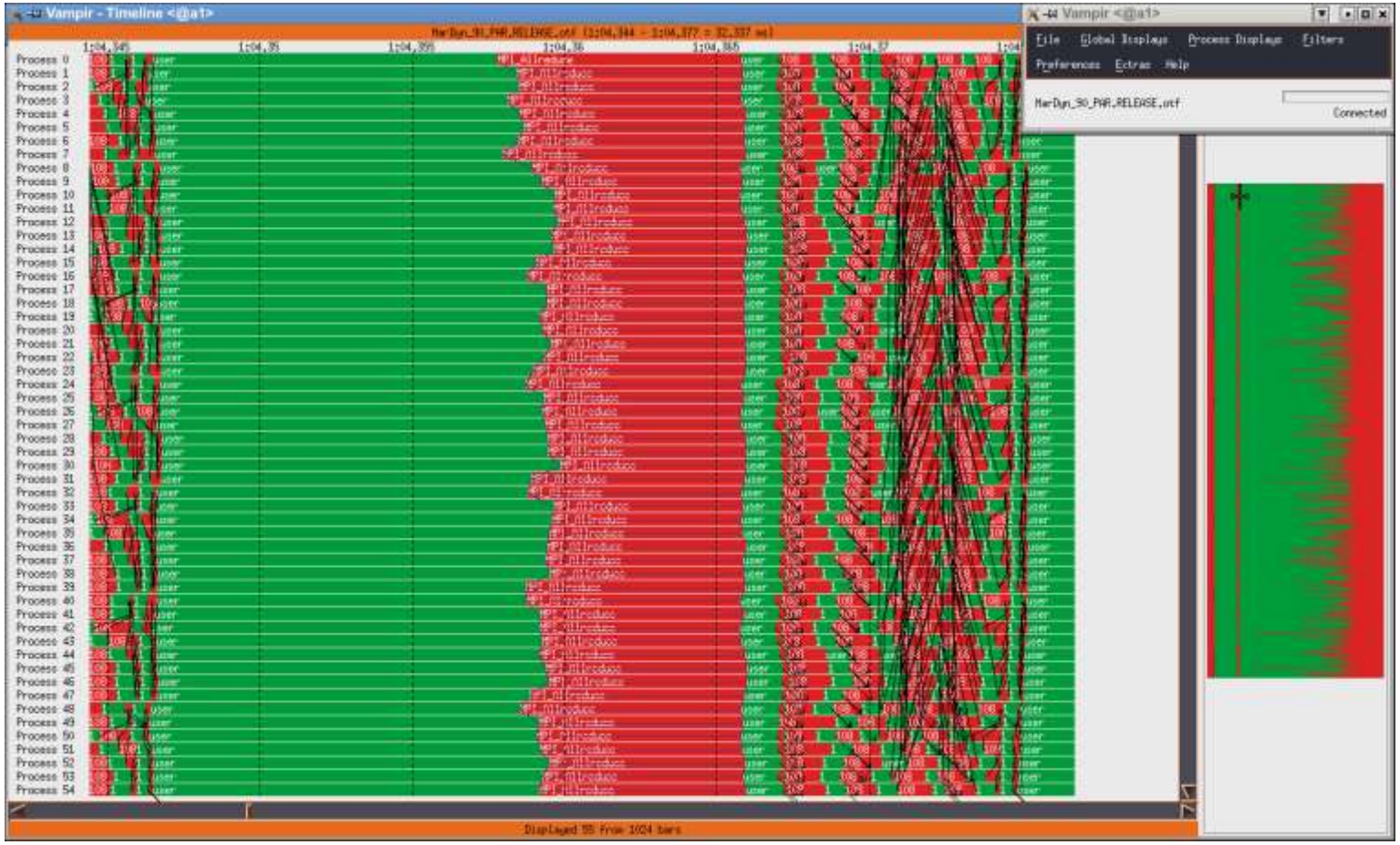


methane + graphite



○ uniform subdomains
▲ static load balancing

Communication and load balance



OpenMPI, gcc-4.1.2, HLRS nehalem cluster Baku/Laki.

Conclusion

Approaches to analyzing critical behaviour by molecular simulation:

- Divergence of fluctuation related quantities
- Disappearance of the vapour-liquid coexistence

… require relatively large systems and a long simulation time.

- Extrapolation of VLE properties

… data become less reliable near T_c.

- Extrapolation of interface properties

… in the vicinity of T_c, relatively large V and Δt are required as well.

competence in high performance computing → capturing critical behaviour