GPU-powered Molecular Dynamics Simulations in Statistical Physics

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Perspectives of GPU Computing in Science

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Why molecular dynamics simulations?

- clean “experiments”, detailed view at nanoscale processes

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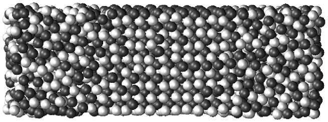
- make predictions (qualitative and quantitative)
    - materials research: surface tension, stress–strain relations
    - drug development: protein conformations, reaction pathways

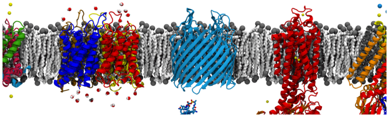
materials research



Kerrache, Horbach & Binder, EPL (Europhys. Lett.) 2008

liquid/crystal interfaces of $Al_{50}Ni_{50}$ alloy (EAM potentials)

cell biology



http://simbac.gatech.edu

membrane proteins embedded in a phospholipid bilayer

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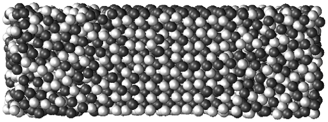
- clean "experiments", detailed view at nanoscale processes
- make predictions (qualitative and quantitative)
  - materials research: surface tension, stress–strain relations
  - drug development: protein conformations, reaction pathways
- test microscopic theories, e.g., in statistical physics
  rheology of polymer composites, glass transition dynamics, nucleation theory
- requires good models, coarse-grained descriptions

materials research



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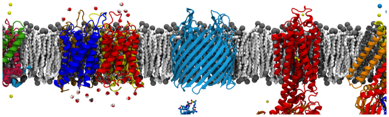

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Molecular dynamics simulations

- integration of Newton's equations of motion for N particles, N large

$$m_i \dot{\boldsymbol{r}}_i = \boldsymbol{p}_i \,, \qquad \dot{\boldsymbol{p}}_i = \underbrace{\boldsymbol{F}_i(\{\boldsymbol{r}_j\})\,,}_{\text{interaction}} \qquad i = 1, \dots, N$$

- conservation laws:
  - total momentum, total energy $H = \sum_i \boldsymbol{p}_i^2/2m_i + V(\{\boldsymbol{r}_j\}), \dots$
  - phase space volume (symplectic flows)

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  - phase space volume (symplectic flows)
- exact solution: $\{\boldsymbol{r}_i, \boldsymbol{p}_i\} \mapsto \mathrm{e}^{\mathrm{i}\mathcal{L}\tau}\{\boldsymbol{r}_i, \boldsymbol{p}_i\}, \qquad \mathcal{L} = \mathcal{L}_{\boldsymbol{r}} + \mathcal{L}_{\boldsymbol{p}}$

$$\mathrm{i}\mathcal{L}_{\boldsymbol{r}} = \sum_i (\boldsymbol{p}_i/m_i) \cdot \partial/\partial \boldsymbol{r}_i\,, \qquad \mathrm{i}\mathcal{L}_{\boldsymbol{p}} = -\sum_i \boldsymbol{F}_i(\{\boldsymbol{r}_j\}) \cdot \partial/\partial \boldsymbol{p}_i$$

→ velocity-Verlet algorithm: $\mathrm{e}^{\mathrm{i}\mathcal{L}\tau} = \mathrm{e}^{\mathrm{i}\mathcal{L}_{\boldsymbol{p}}\tau/2}\,\mathrm{e}^{\mathrm{i}\mathcal{L}_{\boldsymbol{r}}\tau}\,\mathrm{e}^{\mathrm{i}\mathcal{L}_{\boldsymbol{p}}\tau/2} + O\left(\tau^2\right)$

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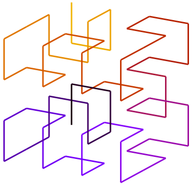
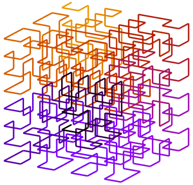
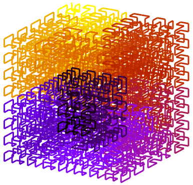
- parallelisation is trivial once the forces $\{\boldsymbol{F}_i\}$ are known:
  - thread $\#i$ → particle $\#i$ linear memory access, complexity $O(N)$
- interactions require communication naïvely: $O(N^2)$
  - Verlet neighbour lists for short-ranged pair forces → $M \cdot O(N)$
  - algorithmic primitives: radix sort and reduction → $O(N \log(N))$

Data locality: Hilbert's space-filling curve

- positions of neighbours have random locations in memory
  - fetch coordinates via read-only texture cache
  - limited cache size → memory locality

→ periodically re-order particle data in memory

J. A. Anderson *et al.*, J. Comp. Phys. **227** 5342 (2008)

- Hilbert's space-filling curve maps 3D space to 1D memory
  - Hilbert curve is recursively generated *on the GPU*
  - generate permutation using radix sort
  - rearrange particle data using texture reads and coalescable writes

Conservation laws: floating-point precision

- theory: conservation of total momentum and total energy
- reality: drift due to accumulation of round-off errors

P. H. Colberg and F. Höfling, Comput. Phys. Commun. **182**, 1120 (2011)

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- solution: use multi-precision floating-point arithmetics (double-single)
    - for the summation of forces (group opposite cells!)
    - in the velocity-Verlet algorithm
- but evaluate potentials in single precision
  saves 50% read/write access to global GPU memory
    - smooth truncation of potentials (C^2-continuous at the cutoff)

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➔ energy and momentum drifts essentially eliminated
momentum: less than 10^{-7} per 10^7 steps of $\delta t^* = 0.001$
energy: less than 10^{-5} per 10^8 steps for $\delta t^* = 0.001$, $h = 0.005$

- execution times increase by less than 10% (Nvidia Tesla K20X)

P. H. Colberg and F. Höfling, Comput. Phys. Commun. **182**, 1120 (2011)

Double-single floating-point precision

- poor double precision performance on Nvidia GTX and Maxwell
  no support for double precision prior to compute capability 1.3

→ double-single arithmetic based on native single precision instructions

  - DSFUN90 package provides double-single routines in Fortran

    D. H. Bailey (2005)

  - porting to CUDA straightforward, use C++ operator overloads
  - effective precision of 44 bits

- `dsfloat=(hi,lo)` $\leftrightarrow$ `float2` (lossless)

- wishlist: `double` $\leftrightarrow$ `float2=(float, rest)`

- store high and low floats in two different arrays
  → efficient access to positions in single precision (force computation)

Velocity-Verlet in double-single precision (CUDA & C++ templates)

```
template <int dimension, typename gpu_vector_type>
__global__ void integrate(
    float4* g_position, gpu_vector_type* g_image, float4* g_velocity, gpu_vector_type const* g_force
  , float timestep, fixed_vector<float, dimension> box_length
)
{
    unsigned int const thread = GTID;               // global thread ID
    unsigned int const nthread = GTDIM;             // total number of threads

     // load double-single precision values from global memory (2 float4)
     fixed_vector<dsfloat, dimension> r, v;
     unsigned int species; float mass;
     tie(r, species) <<= tie(g_position[thread], g_position[thread + nthread]);
     tie(v, mass)    <<= tie(g_velocity[thread], g_velocity[thread + nthread]);

    // load single precision values from global memory (1 float4)
    fixed_vector<float, dimension> f = g_force[thread];

     // actual computations with 2D/3D vectors in double-single precision
     v += f * (timestep / 2) / mass;
     r += v * timestep;
     fixed_vector<float, dimension> image = box_kernel::reduce_periodic(r, box_length);

    // write results to global memory
    tie(g_position[thread], g_position[thread + nthread]) <<= tie(r, species);
    tie(g_velocity[thread], g_velocity[thread + nthread]) <<= tie(v, mass);
    if (!(image == float_vector_type(0))) {
        g_image[thread] = image + static_cast<float_vector_type>(g_image[thread]);
    }
}
```

Break-down of the algorithm

Binary mixture of 256,000 Lennard-Jones particles

HALMD ● HAL’s MD package
Highly Accelerated Large-scale Molecular Dynamics

task	time [ms]	#calls	share	complexity
MD integration step	4.1	10,000	99%	
dump system state (GPU $\rightarrow$ disk)	410	1	1%	
compute short-ranged forces	2.9	10,000	68%	$M \cdot O(N)$
velocity-Verlet integration	.41	10,000	10%	$O(N)$

(Nvidia Tesla K20Xm, $r_c = 2.5\sigma, r_{\text{skin}} = 0.5\sigma, \delta t^* = 0.001, \rho^* = 1.2$)

Break-down of the algorithm

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- use generic algorithms for complex tasks, express them in terms of
  - radix sort and reduction operations $O(N \log(N))$
  - simple operations $O(N)$

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velocity-Verlet integration	.41	10,000	10%	$O(N)$
generate neighbour lists	21	163	8%	$O(N \log(N))$
re-order particle data	15	163	6%	$O(N \log(N))$
generate cell lists	6.1	163	2%	$O(N \log(N))$
neighbour list criterion	.08	10,000	2%	$O(N \log(N))$

(Nvidia Tesla K20Xm, $r_c = 2.5\sigma, r_{\text{skin}} = 0.5\sigma, \delta t^* = 0.001, \rho^* = 1.2$)

What to do with the vast amount of data generated?

- avoid disk I/O → data locality!
- exploit parallel computing also for the data analysis

→ online evaluation of relevant quantities
thermodynamic variables, spatial profiles, time correlation functions, coarse-grained variables, . . .

- decide *before* the simulation what is relevant
the information needed is determined by the questions asked

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H5MD!

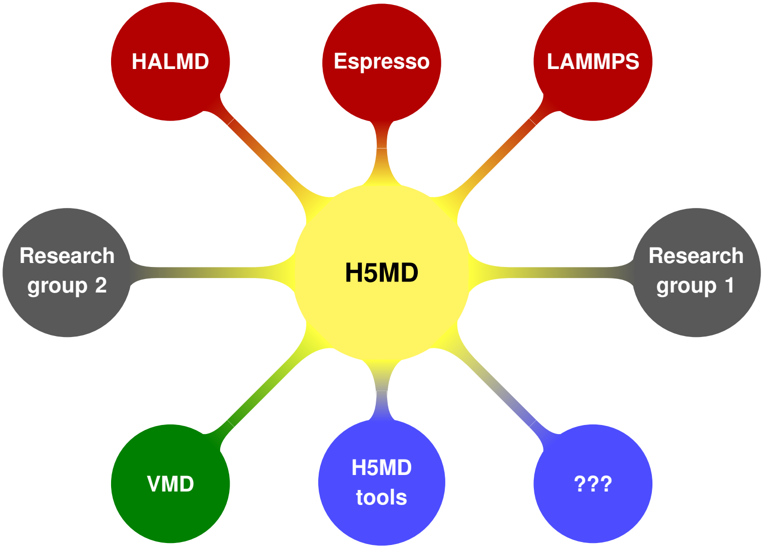
- HDF5 for Molecular Data: `http://nongnu.org/h5md`

P. de Buyl, P. H. Colberg, and F. Höfling, Comput. Phys. Commun. **185**, 1546 (2014)

- efficient, structured, and portable storage of heterogeneous data
- binary format, data compression, fast and parallel I/O
- based on the HDF5 library
bindings for C, C++, Fortran, Python; support by Matlab, Mathematica, . . .

The H5MD universe

simulation software visualisation software analysis tools people



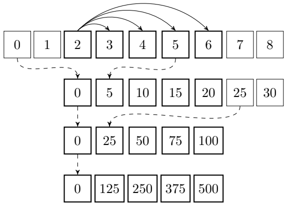
Evaluation of time correlation functions

- slow complex dynamics extends over many decades in time
- evaluate time correlation functions *in situ* on the GPU

$$C_{AB}(t) = \langle A(t)^* B(0) \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T A(t+\tau)^* B(\tau)\, \mathrm{d}\tau$$

→ multiple-τ correlator ("blocking scheme"):

- time interval Δt increases geometrically with block level → logarithmic time grid
- calculate correlations only within the same block → modest memory usage



$$C_{AB}(m\Delta t) \approx \frac{1}{M'} \sum_{j=0}^{M'} A^*_{m+j} B_j$$

$$M' = T/\Delta t - m, \; A_k = A(k\Delta t), \; \ldots$$

- compute particle averages using parallel reduction algorithms

HALMD ● HAL's MD package

Highly Accelerated Large-scale Molecular Dynamics

- **acceleration:** specifically designed to run on GPU processors
  1 GPU comparable to **3–4 Ivy Bridge nodes** à 20 cores
  [HALMD @ "Kepler" K20Xm *vs.* LAMMPS @ supercomputer *Hydra* of the Max Planck Society]
- **applications:** the statistical physics of inhomogeneous fluids
  glass transition, liquid–vapour interfaces, demixing of binary fluids,
  confined fluids, porous media, 2D/3D systems, . . .
- **precision:** excellent numerical long-time stability
  conservation laws → double-single floating-point arithmetics, C^2-smooth potentials
- **efficient:** online evaluation of dynamic correlations minimises disk I/O
- output as structured, compressed, and portable H5MD files

P. de Buyl, P. H. Colberg, and F. Höfling, Comput. Phys. Commun. **185**, 1546 (2014)

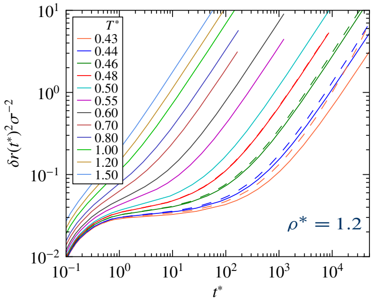
- **modular** & generic design → user scripts define complex tasks
- **educational** tool for M.Sc. students, lab courses → LGPL license

http://halmd.org

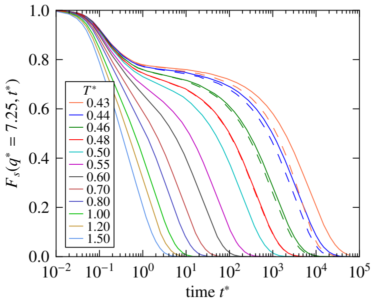
P. H. Colberg and F. Höfling, Comput. Phys. Commun. **182**, 1120 (2011)

Glassy dynamics of a supercooled liquid

- binary mixture of 50,000 LJ spheres
  “Kob–Andersen”, $r_c = 2.5\sigma$, $\rho^* = 1.2$
  production runs of 10^7 NVE steps finished within 8 hours on a Tesla T10 GPU
- slow dynamics upon cooling (or compression)
- single precision: quantitatively and qualitatively wrong results



mean-square displacement

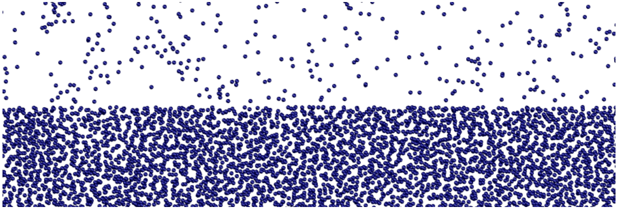


self-intermediate scattering function

Colberg & Höfling, Comput. Phys. Commun. (2011)

Application: structure of liquid–vapour interfaces

- planar interface between coexisting liquid and vapour phases

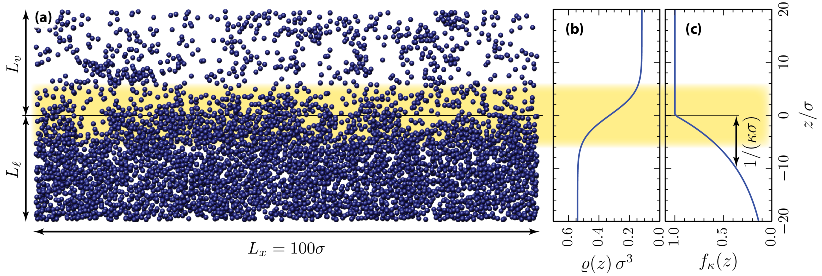


Lennard-Jones fluid: cross section of 3D simulation at $T^* = 1.0 \approx 0.82 T_c^*$

Application: structure of liquid–vapour interfaces

- planar interface between coexisting liquid and vapour phases
- broadened by thermal fluctuations → mean profile $\rho(z)$

→ determined by temperature T and interparticle attraction
coexisting densities ρ_v, ρ_ℓ and interface width ζ



Lennard-Jones fluid: cross section of 3D simulation at $T^* = 1.15 \approx 0.94 T_c^*$

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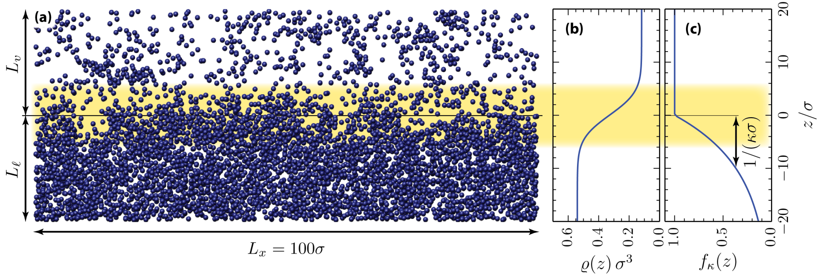
- "surface roughness" → bulk-like fluctuations & capillary waves
- CWs are controlled by mesoscopic surface tension $\gamma(q)$



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Grazing-incidence small-angle X-ray scattering (GISAXS)

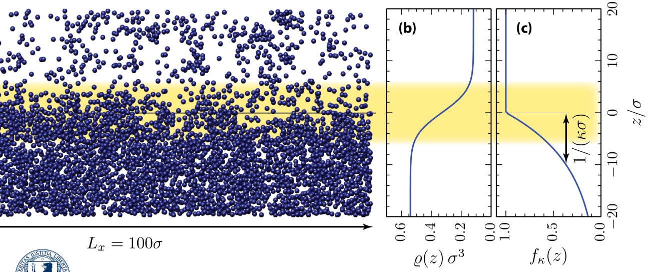
- liquid side: evanescent wave with penetration depth $1/\kappa(\alpha_i, \alpha_f)$
- scattering cross section proportional to [Dietrich & Haase, Phys. Rep. (1995)]

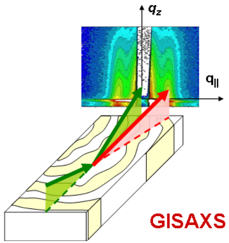
$$I_{\text{tot}}(\boldsymbol{q};\kappa) = \iint_{-L_\ell}^{L_v} \mathrm{d}z\,\mathrm{d}z'\; f_\kappa(z)^*\; f_\kappa(z')\; \boxed{G(\boldsymbol{q}, z, z')}$$

$$\int \mathrm{d}^2 R\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}} \left[\langle\hat\rho(\mathbf{0}, z)\hat\rho(\boldsymbol{R}, z')\rangle - \rho(z)\rho(z')\right]$$

- weighting factor $f_\kappa(z) = \mathrm{e}^{-\kappa|z|}$ for $z < 0$
- sufficiently deep penetration required $(1/\kappa \gg \zeta)$

  but: sizeable background from bulk on top of interface signal

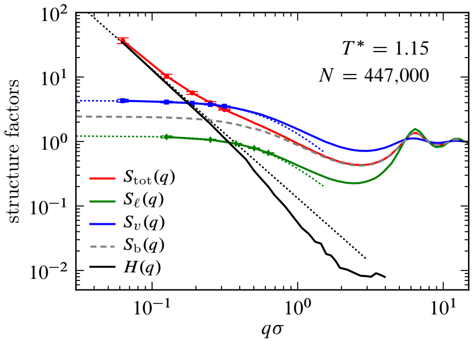


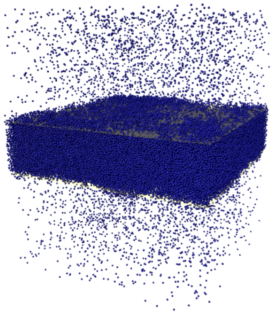


Simulation results: interface structure factor

- synthetic scattering data $S_{\text{tot}}(q)$, similar to GISAXS $\sim 1/\gamma_0 q^2$
- determine properties of liquid and vapour bulk separately $\rightarrow S_b(q)$

$\rightarrow$ interface structure factor $\widetilde{H}(q) = S_{\text{tot}}(q) - S_{\text{b}}(q)$





447,000 Lennard-Jones particles, cutoff $r_c = 3.5\sigma$, $T^* = 1.15 \approx 0.94T_c^*$
box size $L_x = L_y = 100\sigma$, $L_z = 200\sigma$, liquid slab $w = 50\sigma$
30 runs over 10^7 steps for $S_{\text{tot}}(q) \rightarrow$ 840 GPU hours (Tesla K20Xm)

Höfling and Dietrich, EPL (Europhys. Lett.) **109**, 46002 (2015)

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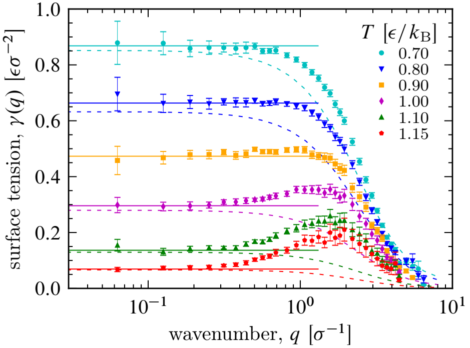

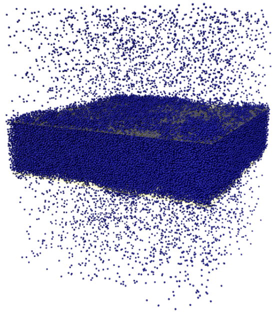

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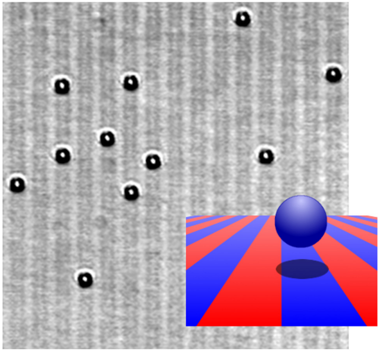
Höfling and Dietrich, EPL (Europhys. Lett.) **109**, 46002 (2015)

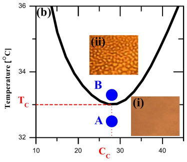
Colloids in a critical water–oil solvent

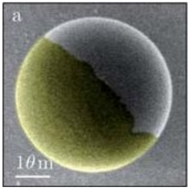


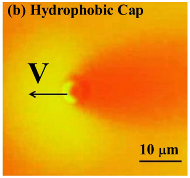
Courtesy of M. Tröndle

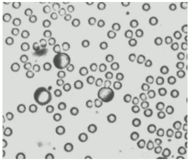
Tröndle, Bechinger, Dietrich *et al.*, Mol. Phys. **109**, 1169 (2011)

critical Casimir effect





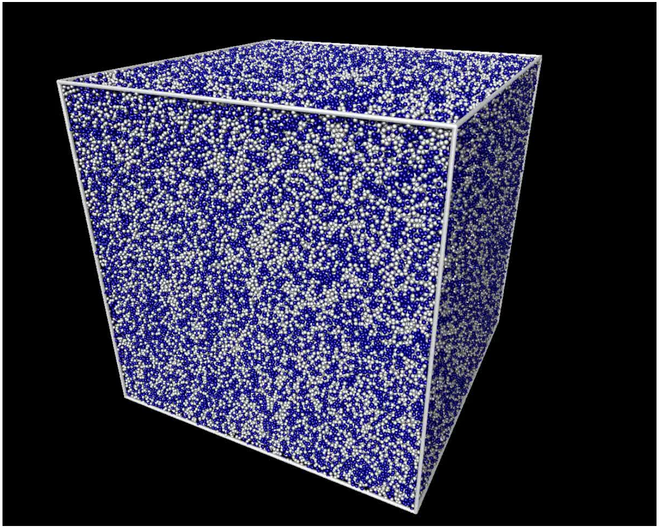


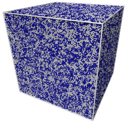


Bechinger *et al.*, Soft Matter **7**, 8810 (2011); J. Phys.: Condens. Matter **24**, 284129 (2012)

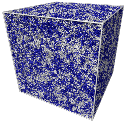
self-propelled Janus particle

Spinodal decomposition of a binary mixture

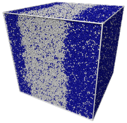




$T > T_c$



$T = T_c$



$T < T_c$

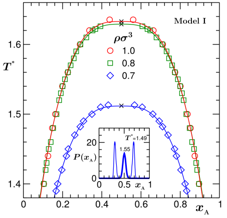
700k particles, 10^8 NVE steps, temperature quench to $T = .93T_c$ (5 days on a GTX980)

Continuous demixing transition of a binary liquid

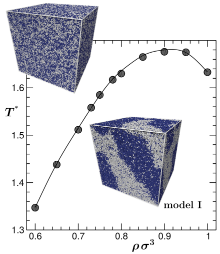
S. Roy, S. Dietrich & F.H., J. Chem. Phys. **145**, 134505 (2016)

- critical phenomenon: universality class of model H'
  - conserved scalar order parameter: local composition fluctuation
  - couples to local number density and transverse momentum
- fluctuations of the local composition:
  divergence of both correlation length and relaxation time
  $\xi \sim |T - T_c|^{-\nu}$, $\nu \approx 0.630$ and $\tau_R \sim \xi^z$, $z \approx 3.06$

→ critical slowing down, interdiffusion ceases at T_c



coexistence curves
(ρ = const)



λ-line $T_c(\rho)$
(x_A = const)

Structure: Ising universality class

- static structure factor $S_{cc}(|\boldsymbol{k}|) = N^{-1}\langle \delta c_{\boldsymbol{k}}^{*}\, \delta c_{\boldsymbol{k}} \rangle$

→ correlation length ξ and "susceptibility" χ

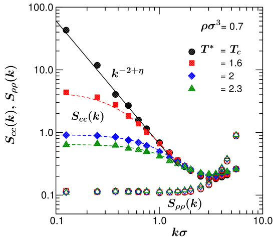
from extended Ornstein–Zernike form: $S_{cc}(k \ll \sigma) \simeq \rho k_{\mathrm{B}} T \chi / [1 + (k\xi)^2]^{1-\eta/2}$

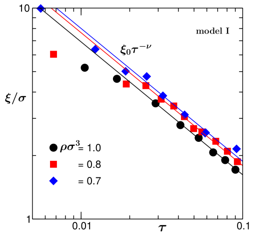
- critical scaling of Ising universality class

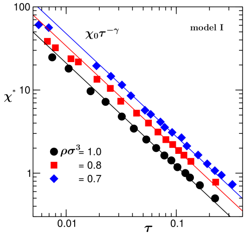
$$S_{cc}(k) = k^{-2+\eta} s(k\xi), \quad \xi \simeq \xi_0 \tau^{-\nu}, \; \chi \simeq \chi_0 \tau^{-\gamma}$$

$$d = 3: \quad \nu \approx 0.630, \quad \eta \approx 0.036, \quad \gamma = \nu(2-\eta)$$

- amplitudes ξ_0, χ_0 depend on the specific system (e.g., fluid density ρ)

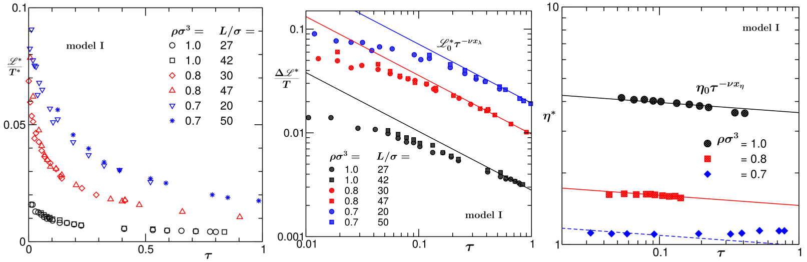






Critical singularities of transport coefficients (model H')

- interdiffusion vanishes: $D_{\mathrm{AB}} \sim \xi^{-x_D}$ $\quad x_D \approx 1.068$
  - use Onsager coefficient $\mathscr{L} = \chi D_{\mathrm{AB}}$ instead
  - critical enhancement: $\Delta\mathscr{L}(T) = \mathscr{L}(T) - \mathscr{L}_b k_{\mathrm{B}} T \simeq \mathscr{L}_0 k_{\mathrm{B}} T \tau^{-\nu x_\lambda}$ $\quad \nu x_\lambda \approx 0.567$
- shear viscosity diverges slowly: $\bar{\eta} \simeq \eta_0 \tau^{-\nu x_\eta}$ $\quad \nu x_\eta \approx 0.043$
- transport coefficients are calculated from time correlation functions



87,500 particles ($L = 50\sigma$), 20 runs over 10^7 steps → 6 h on 20 Tesla K20Xm for each T, ρ

Universal ratios of critical amplitudes

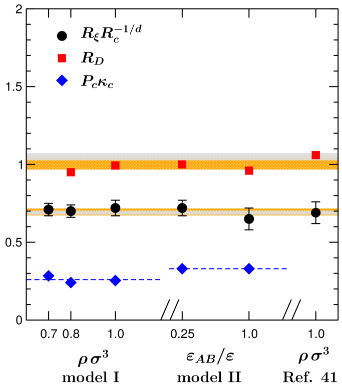
- some ratios of (non-universal) critical amplitudes are universal
  example: correlation length $\xi \simeq \xi_0^{\pm}|\tau|^{-\nu} \rightarrow \xi_0^+/\xi_0^- \approx 2.02$
- "static" amplitude ratio:
  involves only structural properties

$$R_\xi^+ R_c^{-1/d} = \xi_0^+ \left(\frac{\varphi_0^2}{k_\mathrm{B} T \chi_0^+}\right)^{1/d} \approx 0.69$$

- "dynamic" amplitude ratio:
  involves also transport coefficients

$$R_D = \frac{6\pi \eta_0^+ \xi_0^+ \mathcal{L}_0^+}{\chi_0^+} \approx 1.0$$

- also: $P_c \kappa_c \approx$ const (?!)



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University of Toronto, Canada

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Katholieke Universiteit Leuven, Belgium

supercomputer *Hydra*

Max Planck Computing and Data Facility Garching, Germany
700 Kepler GPUs (K20Xm), recent upgrade: 200 Maxwell GPUs (GTX980)

Summary

- **HAL's MD package:** specifically designed for use with GPUs
- floating-point precision crucial for numerical long-time stability

  Colberg & Höfling, Comput. Phys. Commun. (2011)
- online evaluation of time correlation functions avoids disk I/O
- **H5MD:** HDF5 for Molecular Data `http://nongnu.org/h5md`

  de Buyl, Colberg & Höfling, Comput. Phys. Commun. (2014)
- applications: inhomogeneous fluids at the molecular scale
  glass transition, liquid–vapour interfaces, demixing of binary fluids,
  confined fluids, porous media, 2D/3D systems, . . .

  Höfling & Dietrich, EPL (2015)
  Roy, Dietrich & Höfling, J. Chem. Phys. (2016)

→ scope for multi-GPU simulations (in the near future)

Come to Berlin for a free tutorial on HAL's MD package!

HALMD ● HAL's MD package
Highly Accelerated Large-scale Molecular Dynamics

`http://halmd.org`