LiquidLib: An MPI/OpenMP Parallelized Toolbox for Analyzing Molecular Dynamics Simulations with Applications to Neutron Scattering Experiments

http://z-laboratory.github.io/LiquidLib/

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Neutron scattering measures the variation/fluctuation in space and time.

double differential cross section

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l,l'}\overline{b_l b_{l'}}\int\left\langle e^{-i\mathbf{k}\cdot[\mathbf{r}_l(t)-\mathbf{r}_l(0)]}\right\rangle e^{-i\omega t}\mathrm{d}t$$

bound scattering length

$$\overline{b_l b_{l'}} = \bar{b}^2 + \delta_{ll'}(\overline{b^2} - \bar{b}^2) = b_{\mathrm{coh}}^2 + \delta_{ll'}b_{\mathrm{inc}}^2$$

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\left[b_{\mathrm{coh}}^2\sum_{l,l'}\int\left\langle e^{-i\mathbf{k}\cdot[\mathbf{r}_l(t)-\mathbf{r}_l(0)]}\right\rangle e^{-i\omega t}\mathrm{d}t + b_{\mathrm{inc}}^2\sum_{l}\int\left\langle e^{-i\mathbf{k}\cdot[\mathbf{r}_l(t)-\mathbf{r}_{l'}(0)]}\right\rangle e^{-i\omega t}\mathrm{d}t\right]$$

$$= \frac{k_f}{k_i}\frac{1}{\hbar}\left[b_{\mathrm{coh}}^2 S(k,E) + b_{\mathrm{inc}}^2 S_s(k,E)\right]$$

collective/coherent dynamic structure factor

$$S(k,E) = \frac{1}{2\pi}\int F(k,t)e^{-i\omega t}\mathrm{d}t$$

collective/coherent intermediate scattering function

$$F(k,t) = \sum_{l,l'}\left\langle e^{-i\mathbf{k}\cdot[\mathbf{r}_l(t)-\mathbf{r}_{l'}(0)]}\right\rangle$$

self/incoherent dynamic structure factor

$$S_s(k,E) = \frac{1}{2\pi}\int F_s(k,t)e^{-i\omega t}\mathrm{d}t$$

self/incoherent intermediate scattering function

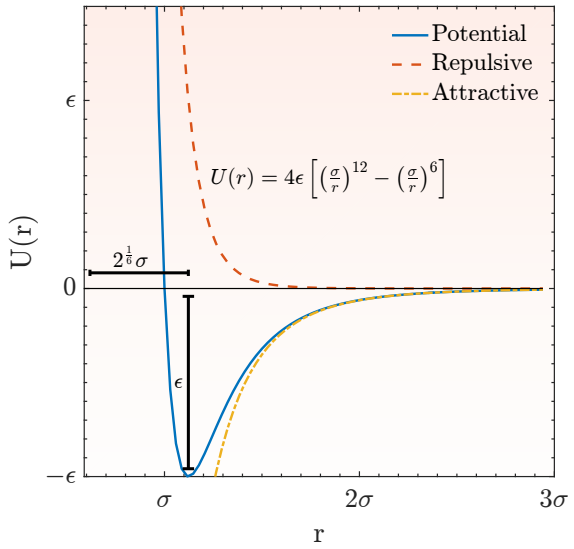
$$F_s(k,t) = \sum_{l}\left\langle e^{-i\mathbf{k}\cdot[\mathbf{r}_l(t)-\mathbf{r}_l(0)]}\right\rangle$$

$$\rho(\mathbf{k},t) = \sum_l e^{-i\mathbf{k}\cdot\mathbf{r}_l(0)}$$

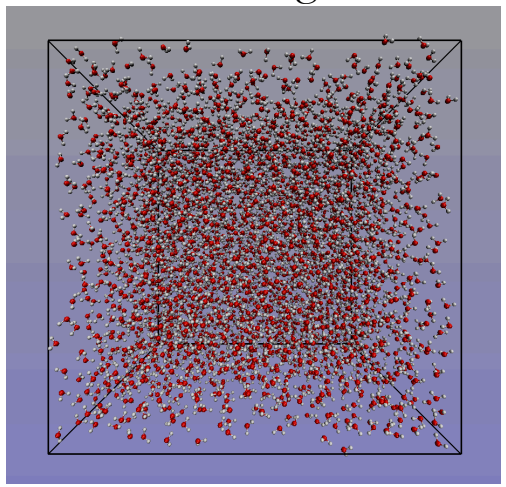
- Neutron scattering measures the variation/fluctuation in space and time, which is described by spatial-dependent density correlation functions.

Molecular Dynamics (MD) Simulations

Potential & Force field



Initial Configuration

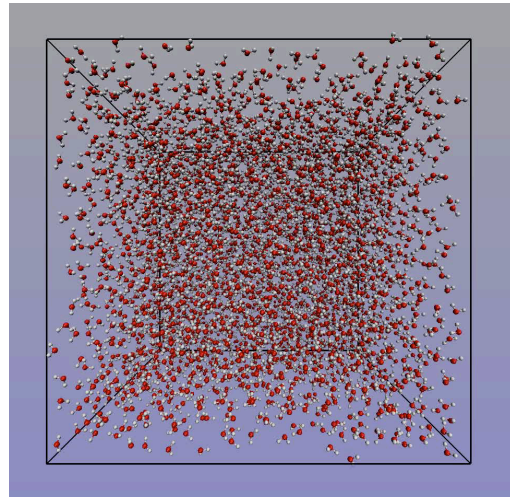


Integrate Newton's Equation of Motion

$$r(t + \Delta t) = r(t) + v(t)\Delta t$$
$$v(t + \Delta t) = v(t) + a(t)\Delta t$$
$$a(t) = F(t)/m$$

Packages:
LAMMPS, GROMACS
VASP, NAMD, etc.

Atomic trajectory over time



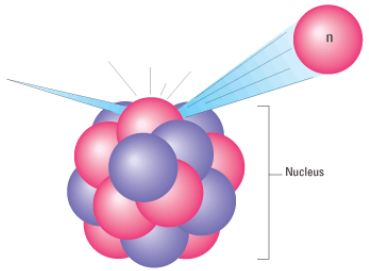
Time and Length Scales Probed by Molecular Dynamics and Neutron Scattering

	Molecular Dynamics	Neutron Scattering
Length Scale	Å – μm	10^{-4} – 50 $Å^{-1}$
Time Scale	fs – μs	sub μeV – eV

A perfect match!

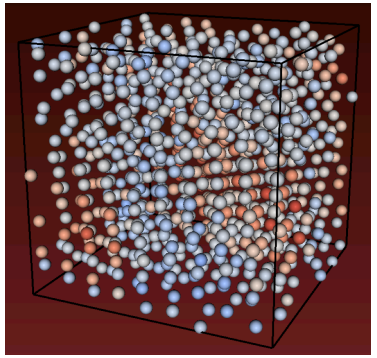
LiquidLib

Neutron Scattering Experiments



scattering lengths (Optional)

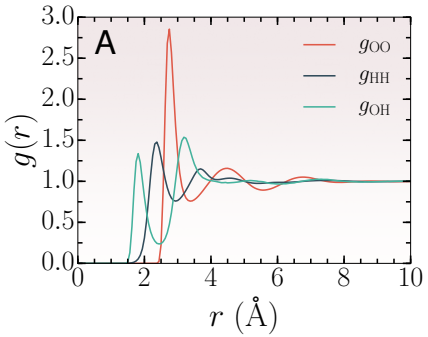
Molecular Dynamics Simulations



trajectory of atoms

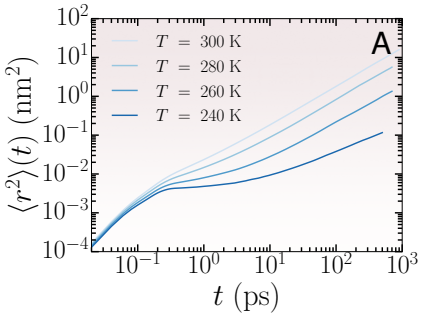
$$g(r) = \frac{1}{dV\,\rho N}\left\langle \sum_{l \neq l'} \delta(r - |\mathbf{r}_l - \mathbf{r}_{l'}|) \right\rangle$$

Structure of Materials



$$\langle r^2(t) \rangle = \frac{1}{N}\left\langle \sum_{l=1}^{N} |\mathbf{r}_l(t) - \mathbf{r}_l(0)|^2 \right\rangle$$

Dynamics of Materials



N. Walter, A. Jaiswal, Z. Cai, Y Z, *Comput. Phys. Commun.* 228 (2018) 209-218

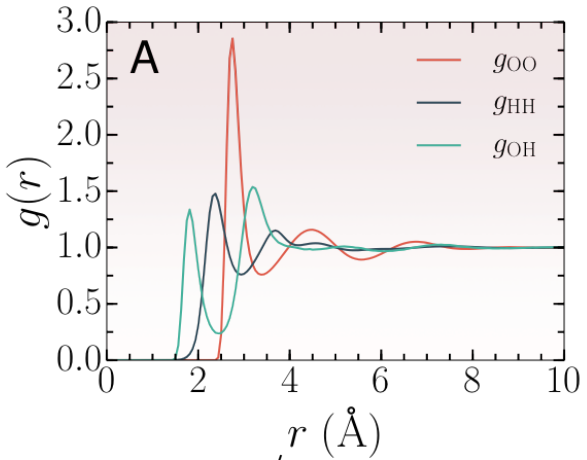
Quantities supported out of the box

- Pair Distribution Function
- Weighted and Unweighted Structure Factor
- Mean Squared Displacement
- Non-Gaussian Parameter
- Four-point Correlation Function
- Velocity Auto Correlation Function
- Self van Hove Correlation Function
- Collective van Hove Correlation Function
- Self Intermediate Scattering Function
- Collective Intermediate Scattering Function
- Bond Orientational Order Parameter
- Current Correlation Function
- Electric Current Correlation Function
- Trajectory Type Converter
- Molecular Calculations

And many more to come...

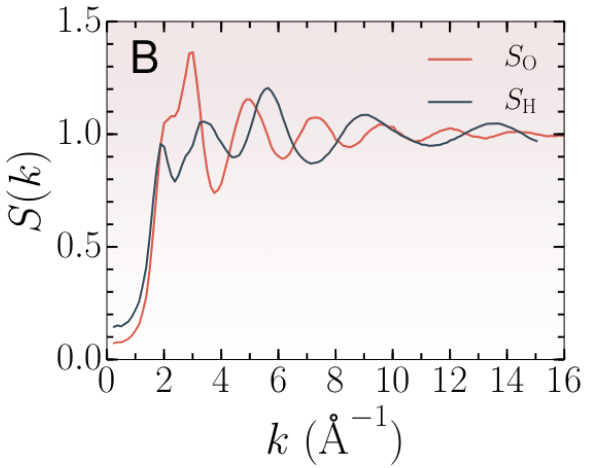
Static Structure Quantities

Partial Pair Distribution Function



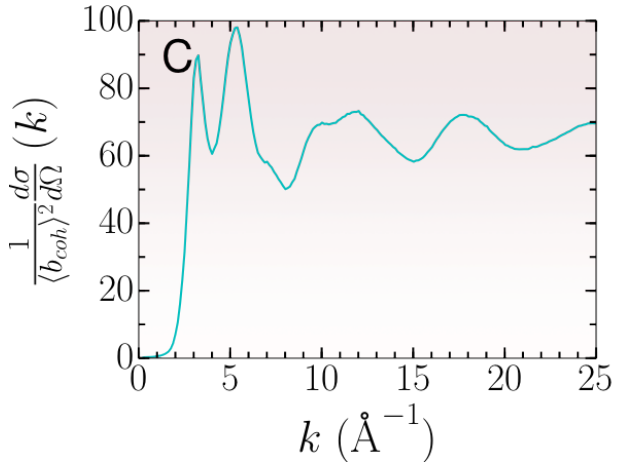
$$g(r) = \frac{1}{4\pi r^2 dr}\frac{1}{\rho N \langle b_{coh}\rangle^2}\left\langle \sum_{l\neq l'} b_l b_{l'} \delta(r - |\mathbf{r}_l - \mathbf{r}_{l'}|)\right\rangle$$

Partial Structure Factor



$$S(k) = \frac{1}{N}\left\langle \sum_{l,l'=1}^{N} \exp\{-i\mathbf{k}\cdot[\mathbf{r}_l - \mathbf{r}_{l'}]\}\right\rangle$$

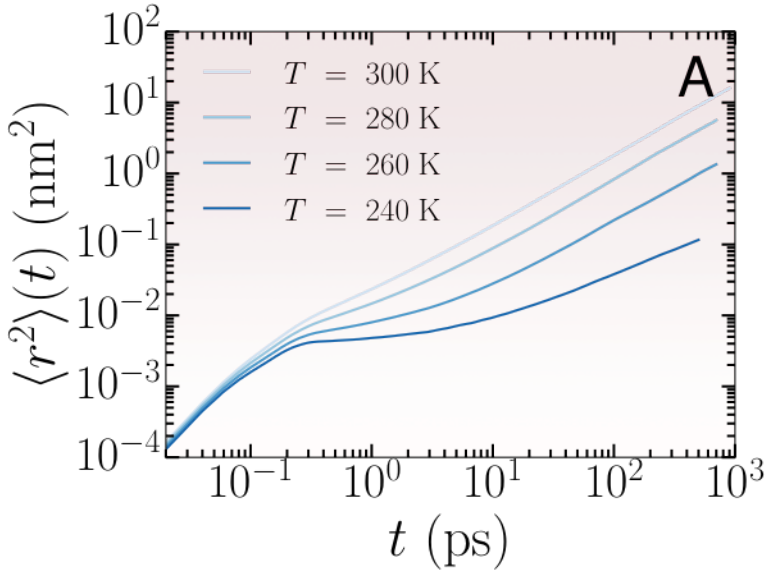
Total Structure Factor



$$\frac{1}{\langle b_{coo}\rangle^2}\frac{d\sigma}{d\Omega}(k) = \frac{1}{N\langle b_{coh}\rangle^2}\left\langle \sum_{l,l'=1}^{N} b_l b_{l'} \exp\{-i\mathbf{k}\cdot[\mathbf{r}_l - \mathbf{r}_{l'}]\}\right\rangle$$

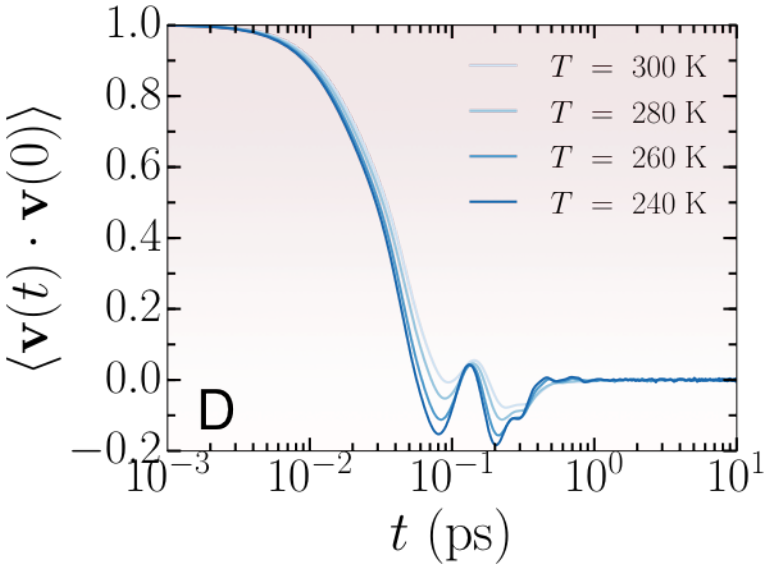
Diffusive Quantities

Mean Squared Displacement



$$\langle r^2(t) \rangle = \frac{1}{N} \left\langle \sum_{l=1}^{N} |\mathbf{r}_l(t) - \mathbf{r}_l(0)|^2 \right\rangle$$

Velocity Auto Correlation



$$C_{vv}(t) = \frac{1}{\langle b_{inc}^2 \rangle} \langle b_i \mathbf{v}_i(0) \cdot b_i \mathbf{v}_i(t) \rangle$$

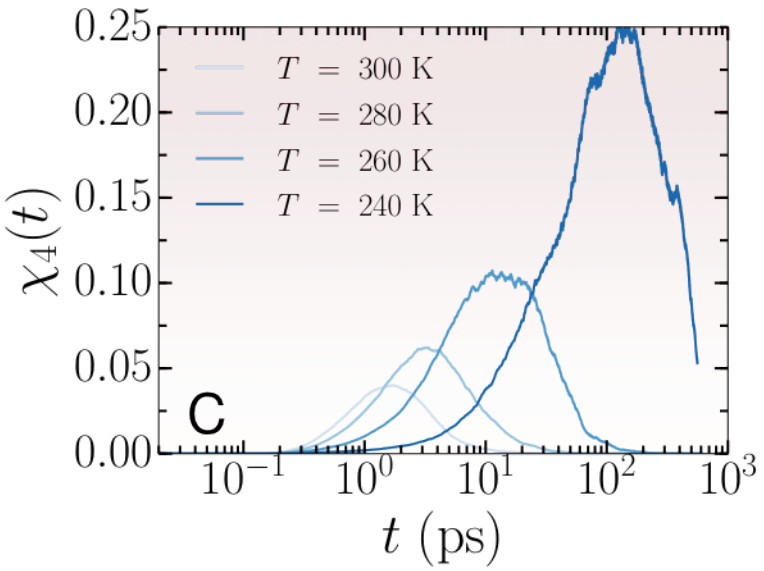
Diffusion Coefficient Computed as

$$\lim_{t \to \infty} \langle r^2(t) \rangle = 2dDt$$

$$D = \frac{1}{3} \int_0^\infty C_{vv}(t) dt$$

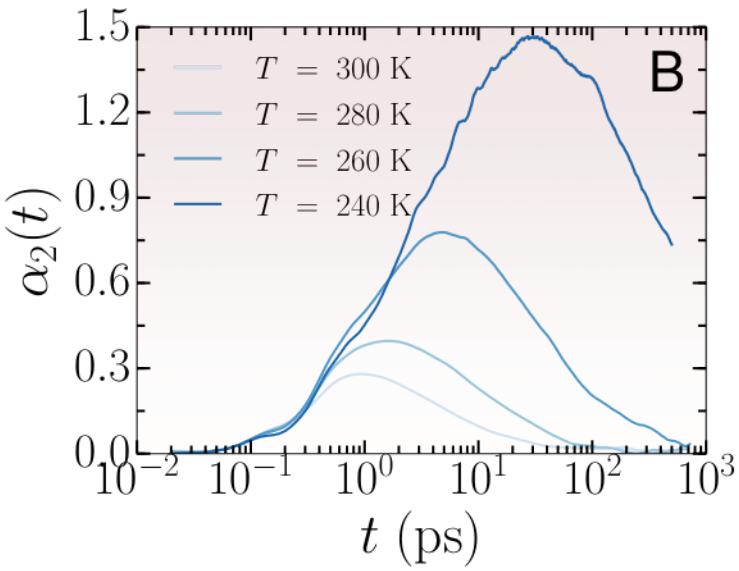
Dynamic Heterogeneity Quantities

Four Point Correlation Function



$$\chi_4(t) = \frac{V}{T} \int G_4(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, t) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4$$

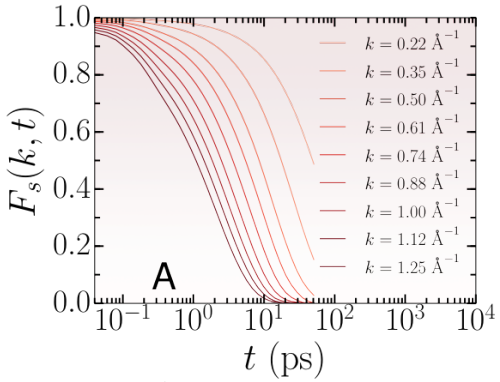
Non-Gaussian Parameter



$$\alpha_2(t) = \frac{3\left\langle \sum_{l=1}^{N} [\mathbf{r}_l(t) - \mathbf{r}_l(0)]^4 \right\rangle}{5\left\langle \sum_{l=1}^{N} [\mathbf{r}_l(t) - \mathbf{r}_l(0)]^2 \right\rangle^2} - 1$$

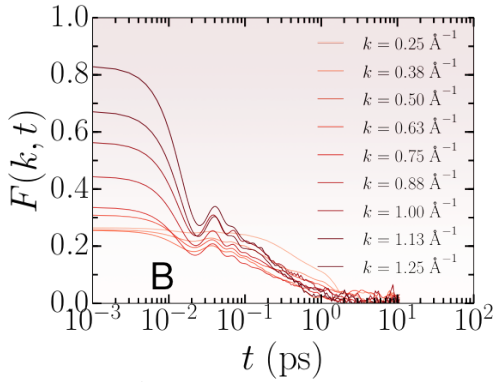
Scattering Quantities

Self Intermediate Scattering Function



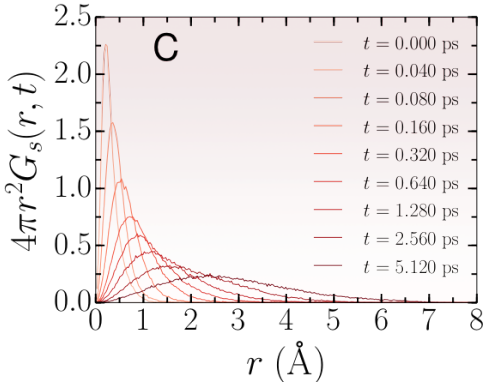
$$F_s(k,t) = \frac{1}{N\langle b_{inc}^2\rangle}\left\langle \sum_{l=1}^{N} b_l^2 \exp\{-i\mathbf{k}\cdot[\mathbf{r}_l(t) - \mathbf{r}_l(0)]\}\right\rangle$$

Collective Intermediate Scattering Function



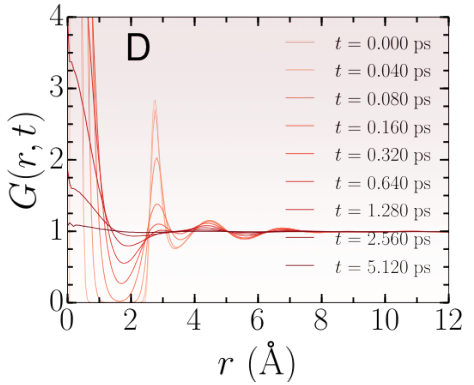
$$F(k,t) = \frac{1}{N\langle b_{coh}\rangle^2}\left\langle \sum_{l=1}^{N}\sum_{l'=1}^{N} b_l b_{l'} \exp\{-i\mathbf{k}\cdot[\mathbf{r}_l(t) - \mathbf{r}_{l'}(0)]\}\right\rangle$$

Self van Hove Correlation Function



$$G_s(r,t) = \frac{1}{4\pi r^2 dr}\frac{1}{N\langle b_{inc}^2\rangle}\left\langle \sum_{l=1}^{N} b_l^2 \delta(\mathbf{r} + \mathbf{r}_l(0) - \mathbf{r}_l(t))\right\rangle$$

Collective van Hove Correlation Function



$$G(r,t) = \frac{1}{4\pi r^2 dr N\langle b_{coh}\rangle^2}\left\langle \sum_{l=1}^{N}\sum_{l'=1}^{N} b_l b_{l'} \delta(\mathbf{r} + \mathbf{r}_l(0) - \mathbf{r}_{l'}(t))\right\rangle$$

Performance with Parallelization

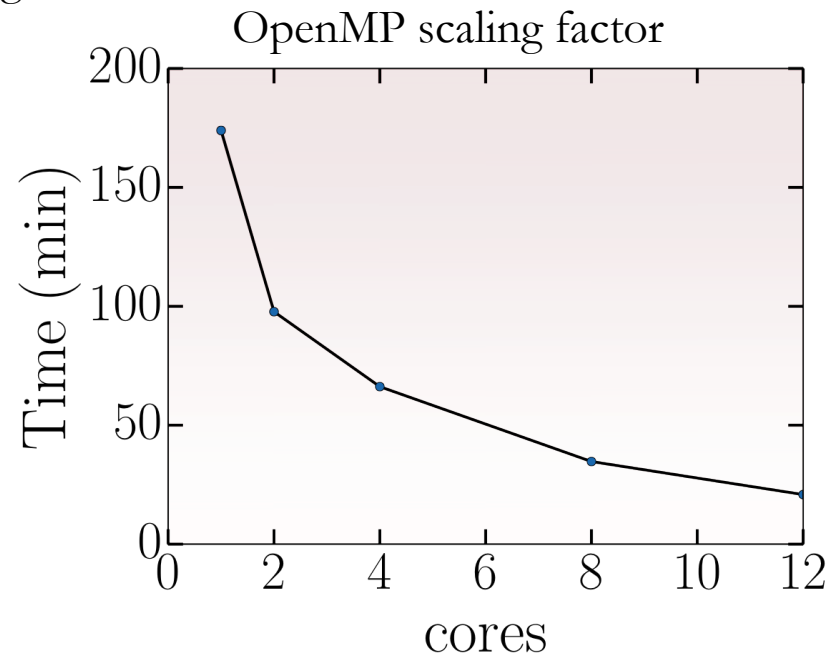
Computations can take hours and longer depending on the quantity and size of simulation

Collective correlation quantities have a complexity $\mathcal{O}(N^2)$
Self correlation quantities have a complexity $\mathcal{O}(N)$

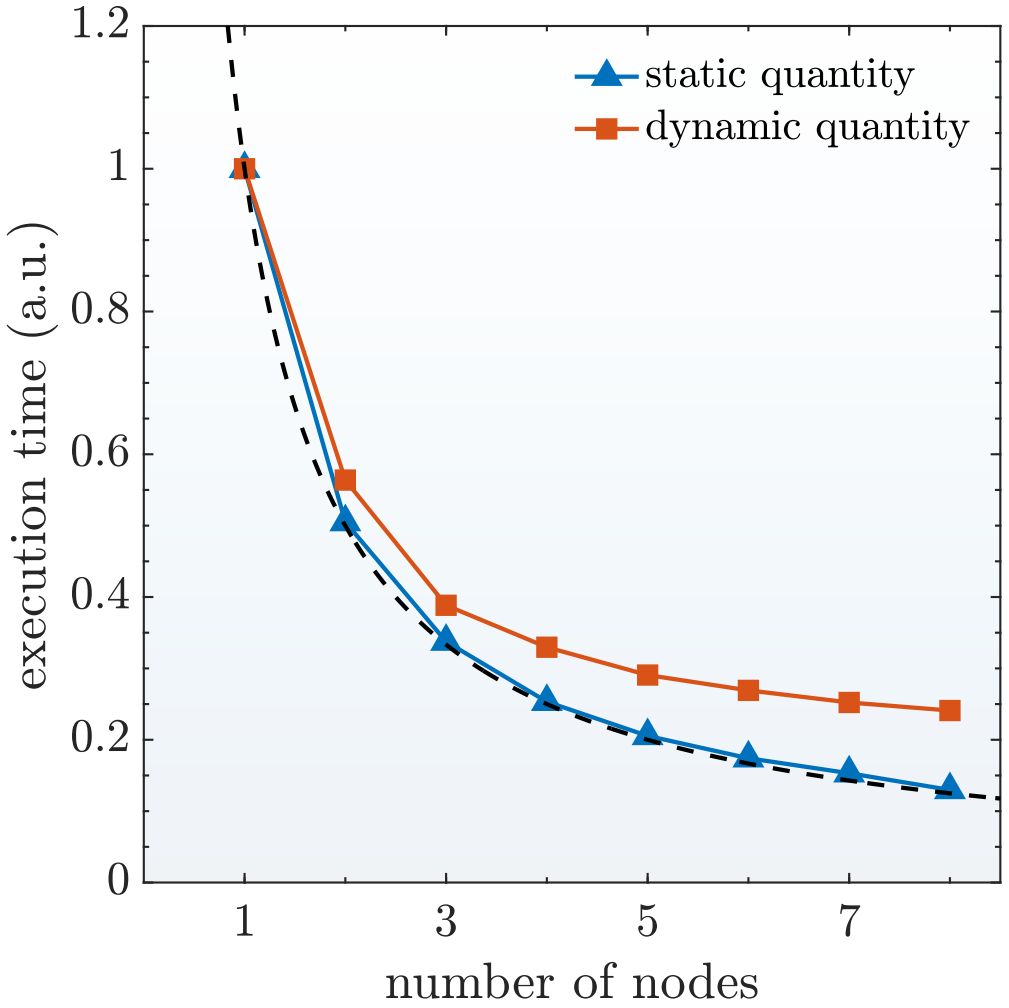
In serial, LiquidLib is at least 4 times faster than comparable packages

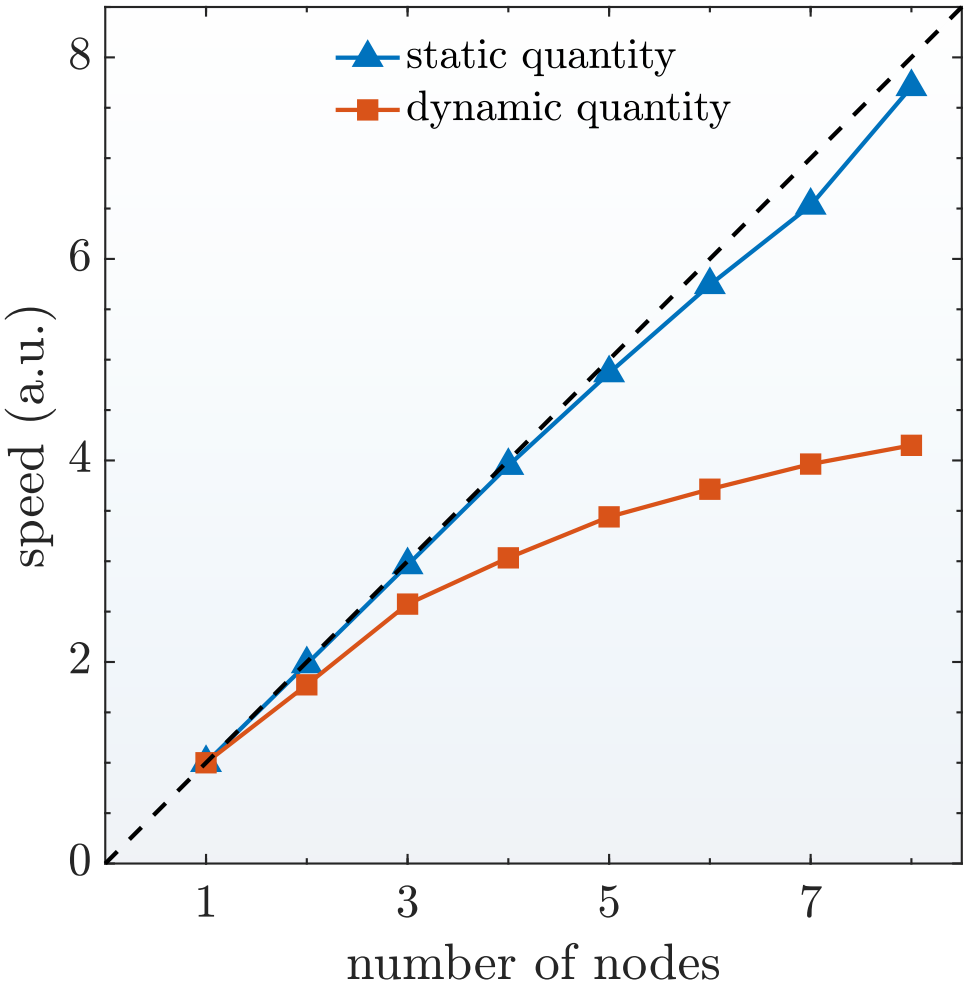
Added options to compensate for memory limited computations at the cost of speed.

MPI/OpenMP parallelization.



MPI Parallelization Scaling Factor

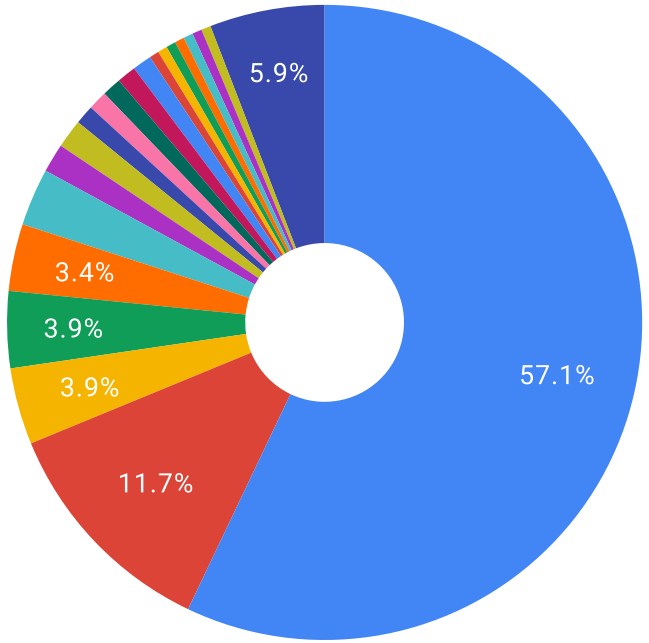




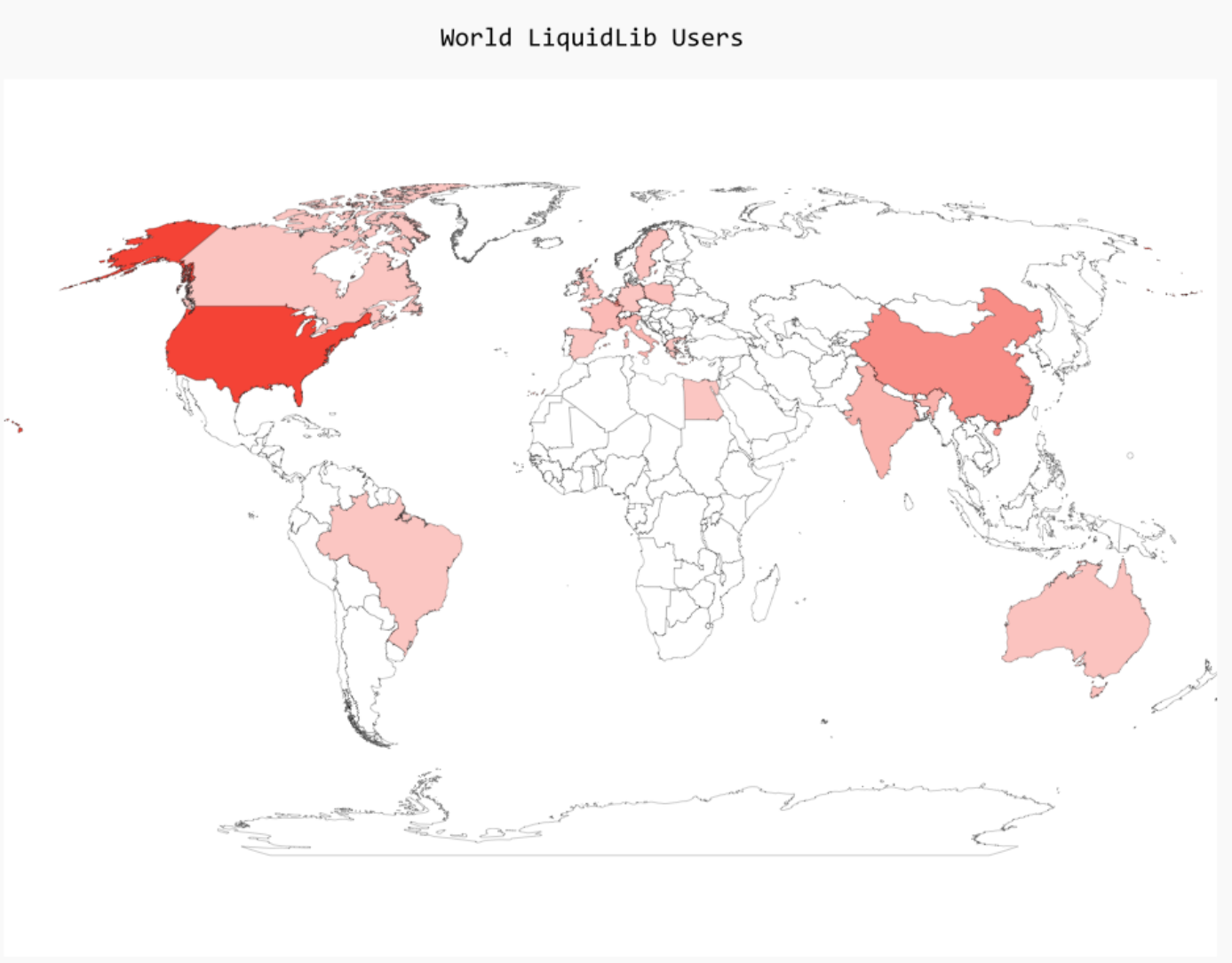
export OMP_NUM_THREADS=16 && mpiexec -n 4 --map-by node computeMeanSquareDisplacement -i r2_t.in

LiquidLib

LiquidLib User Demographics



USA China India United Kingdom Italy France Germany Poland
Sweden Australia Egypt Canada Spain Greece Luxembourg Brazil
Japan Russia Columbia Romania Unknown



Key Features of LiquidLib

- A single, high performance, and extendable package to compute statistical quantities from classical and *ab initio* molecular dynamics (MD) trajectories
- Written in C++, highly extendable, new quantities can be added easily
- Support MPI/OpenMP parallelization
- Support for CUDA & HIP is on the way
- Support N-dimensional calculations
- Allows for species selection for partial quantity computation
- All quantities can be weighted by the neutron scattering lengths to allow for direct comparison to neutron scattering data
- Emphasis on quantities relevant to liquids and liquid-like matter
- Both GUI and CLI support

http://z-laboratory.github.io/LiquidLib/

Developers of LiquidLib

Nathan Walter

Zhikun Cai

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Previous Developers

Yanqin Zhai

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Prof. Y Z

Hossam Farag

Shao-Chun Lee

Current Developers

LiquidLib

http://z-laboratory.github.io/LiquidLib/

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