Molecular Modeling and Simulation for Industrial Applications:
Physico-Chemical Properties and Processes

*ms*2: a molecular simulation tool for thermodynamic properties

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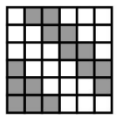


IMEMO

Computational
Molecular Engineering

ms2: underlying goals

- Efficient simulation runs, short response times
- Taking advantage of future hardware speedup
  that can be expected to be 10^3 – 10^4 in the next 15 years
- Broad supported hardware basis
- Numerical robustness
- Broad application field
- Simple user handling
- GUI support for fast input and output handling
- Developer friendly code

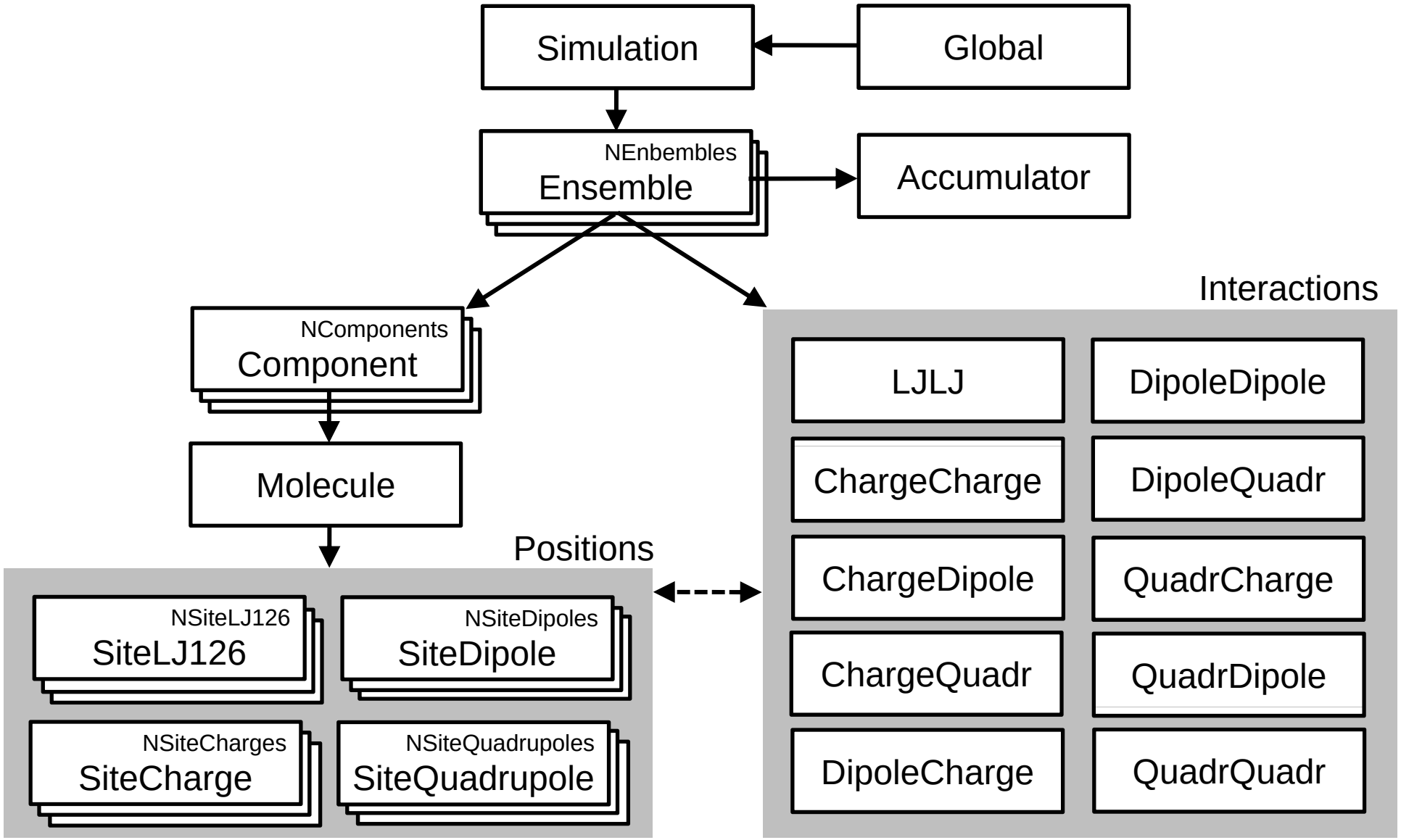
ms2: molecular simulation tool

- Molecular dynamics / Monte Carlo
- Arbitrary mixtures of rigid molecules
- Several ensembles
- Grand Equilibrium method for VLE calculations

- Many static properties (thermal, caloric, entropic)
- Transport properties (Green-Kubo)

- Consistent FORTRAN90 code
- Reasonably object oriented
- Distributed memory parallelization by MPI
- All relevant loops vectorized
- Interface to 2,5D (OpenGL) and 3D Virtual Reality visualization

ms2: modular code structure



Molecular dynamics vector-parallelization (I)

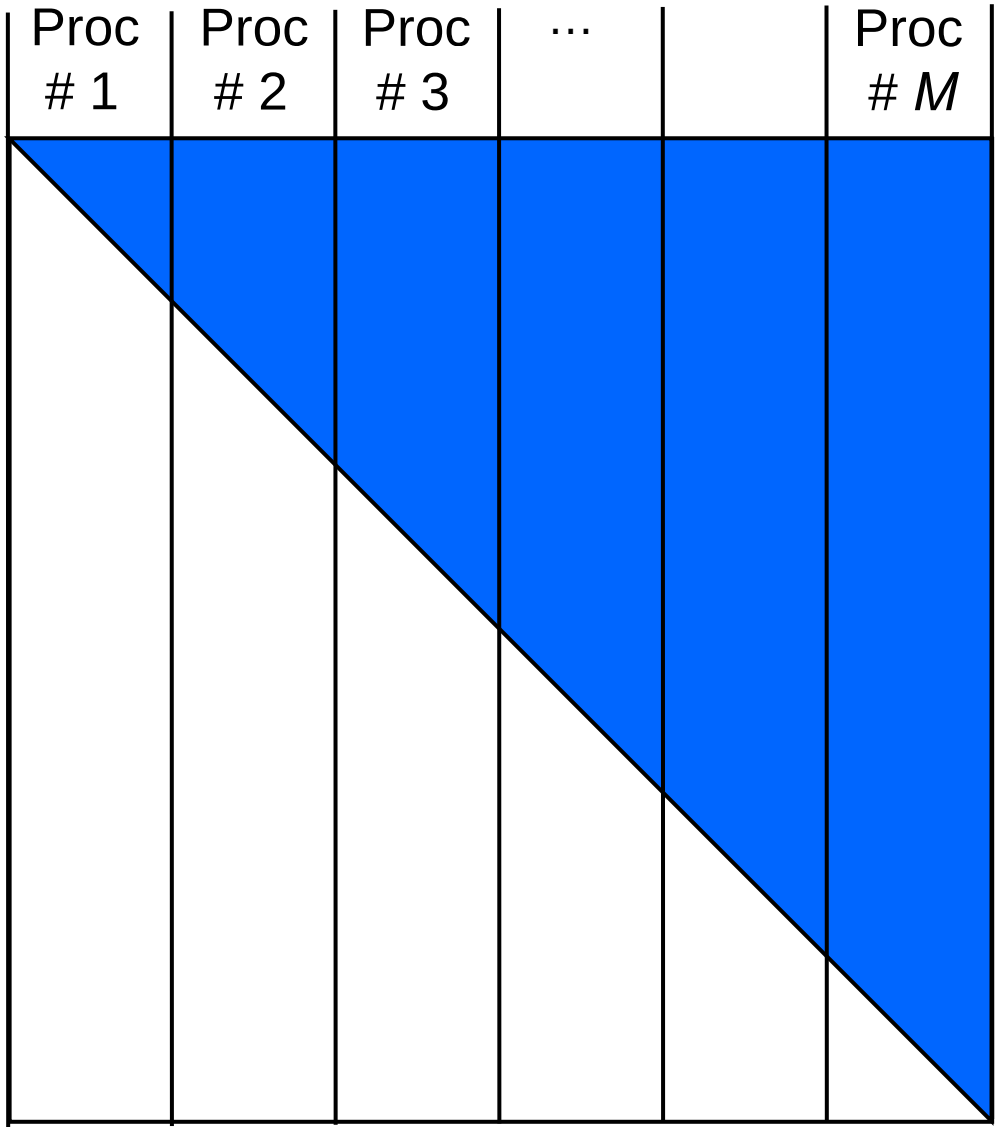
Evaluation of energies, forces and torques

$\sim N\,(N\text{-}1) / 2$

Densly populated in small systems, where

$r_c \sim$ system size

Intuitive distribution of the computational effort on M processors would be extremely unbalanced

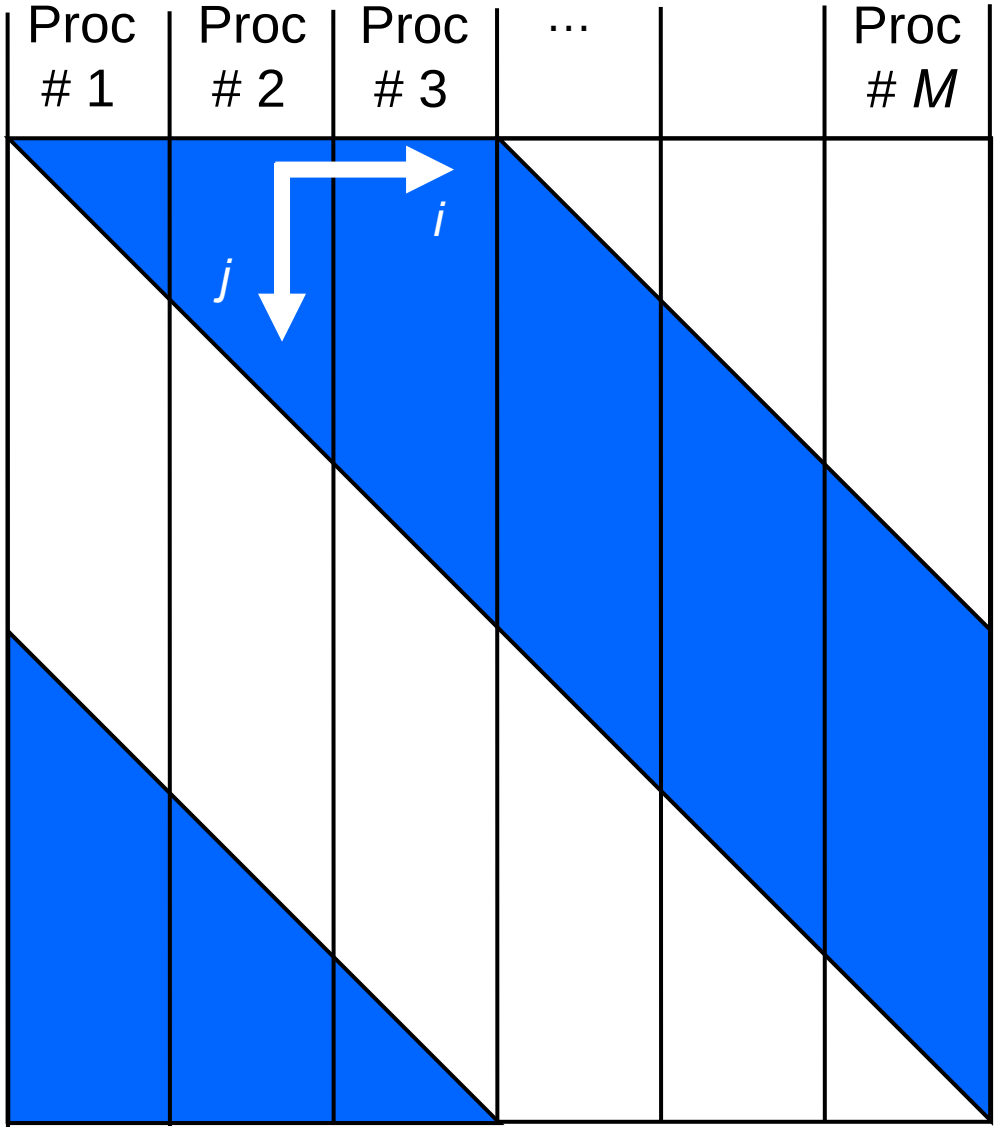


Molecular dynamics vector-parallelization (II)

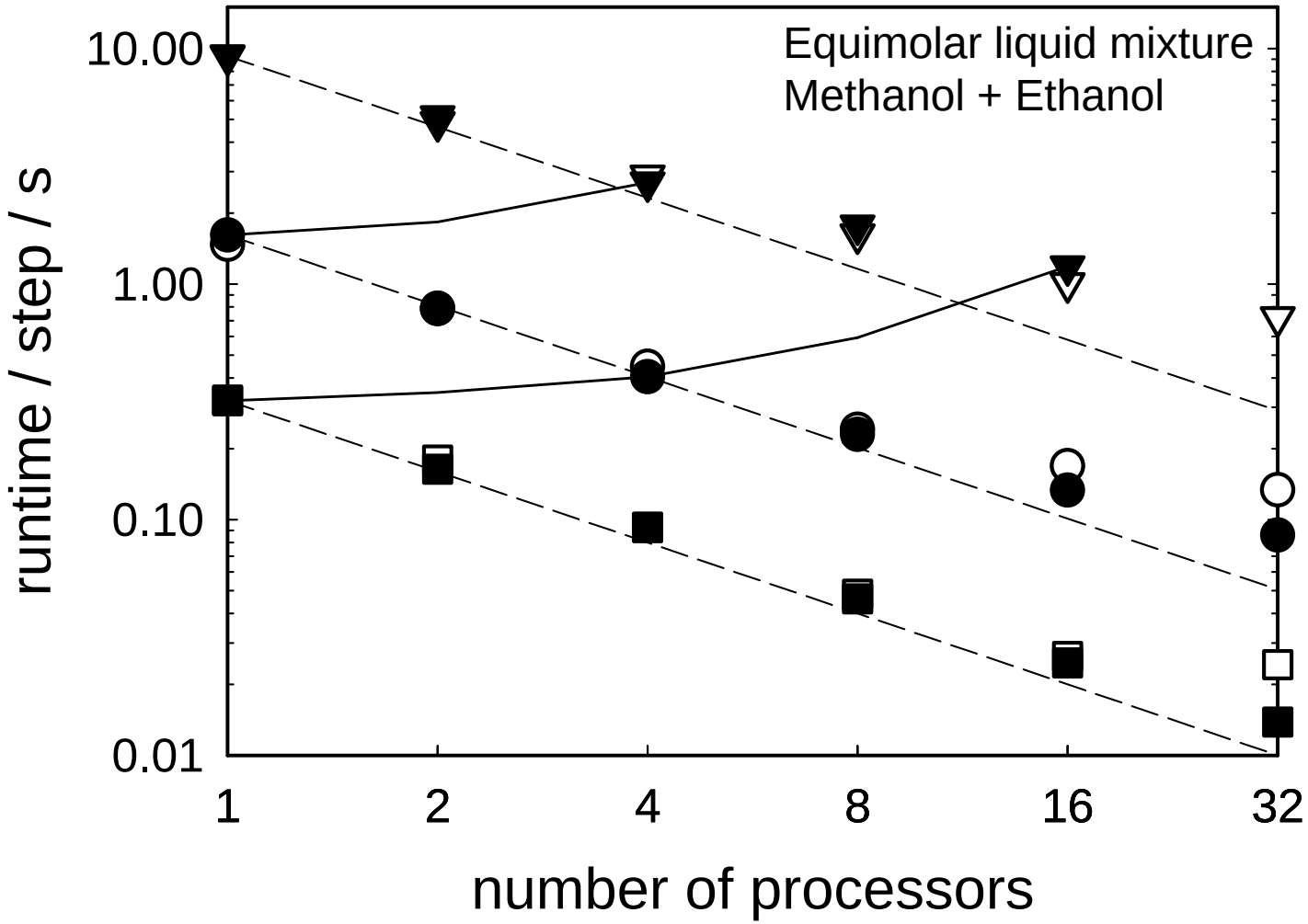
Force decomposition

Proc *m*: do some *i*
do *increment* = *N*/2, *N*
jj = *i* + *increment*
j = mod (*jj*, *N*)
calculate $i \leftrightarrow j$
end do

- **Balanced effort**
- **Vectorizable**



Molecular dynamics efficiency



▼ 21952 particles
● 5488 particles
■ 1372 particles

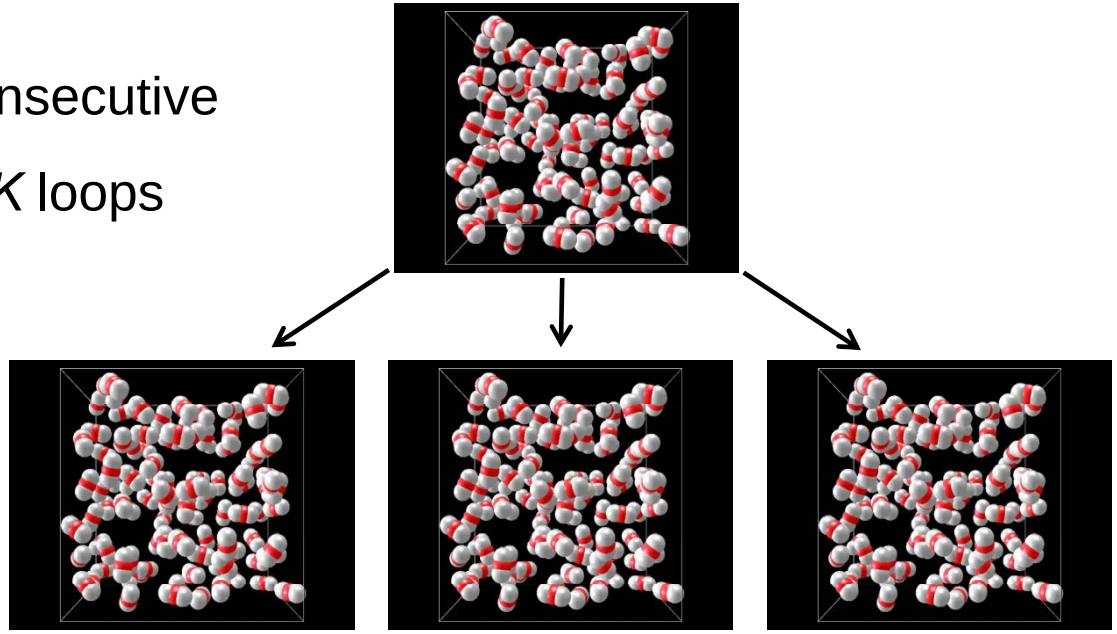
Full symbols:
Intel MPI

Empty symbols:
Open MPI

Monte Carlo embarrassing parallelization

Instead of performing one consecutive probabilistic simulation over *K* loops

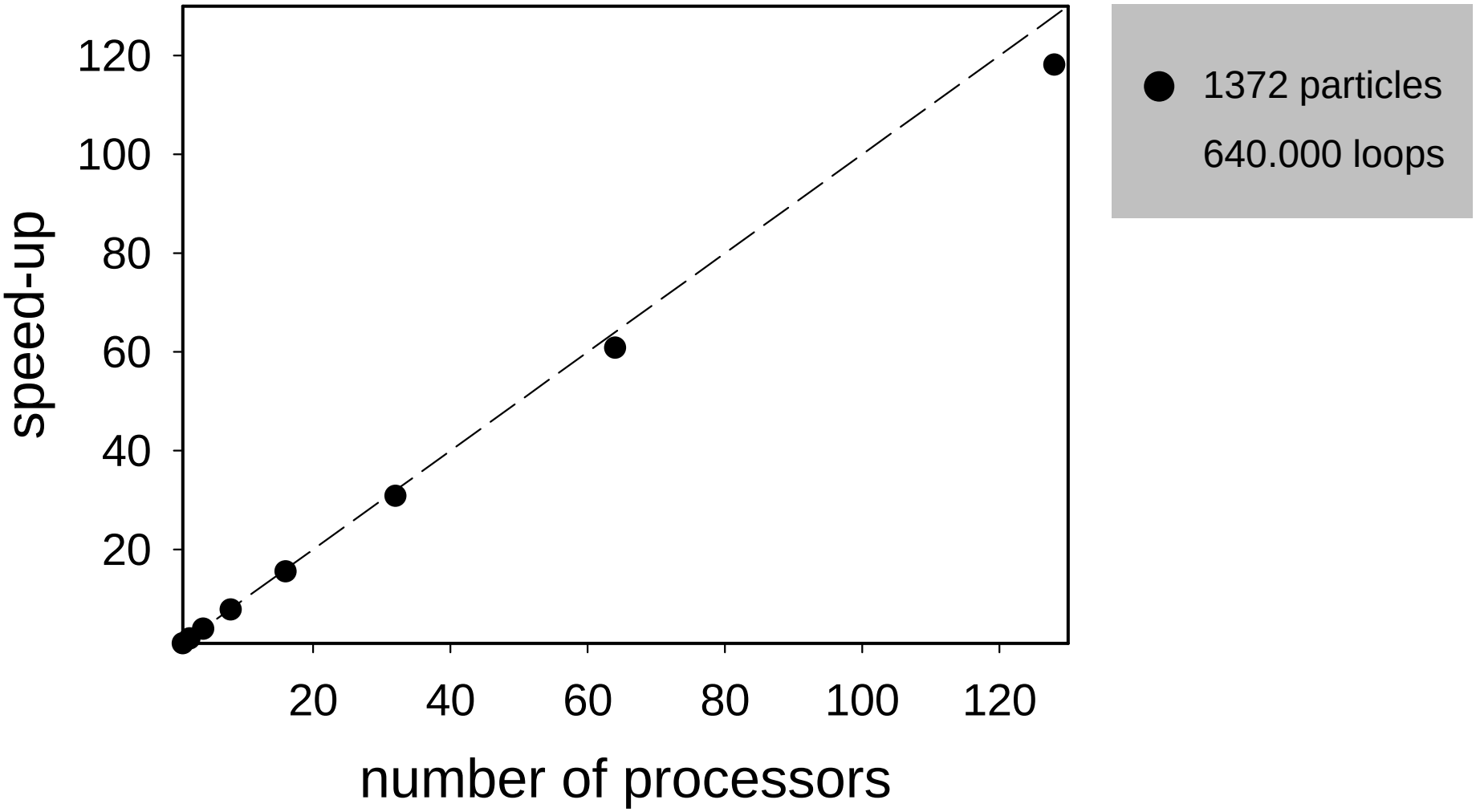
M ensembles (on *M* processors) can be performed over *K* / *M* loops



- Efficient, as hardly any communication is necessary

- For displaced particles, only “new energy “ calculated , “old energy” gathered from interaction energy array

Monte Carlo speed-up – without equilibriation



Comparison with other simulation programs

For VLE calculations (Monte Carlo only):

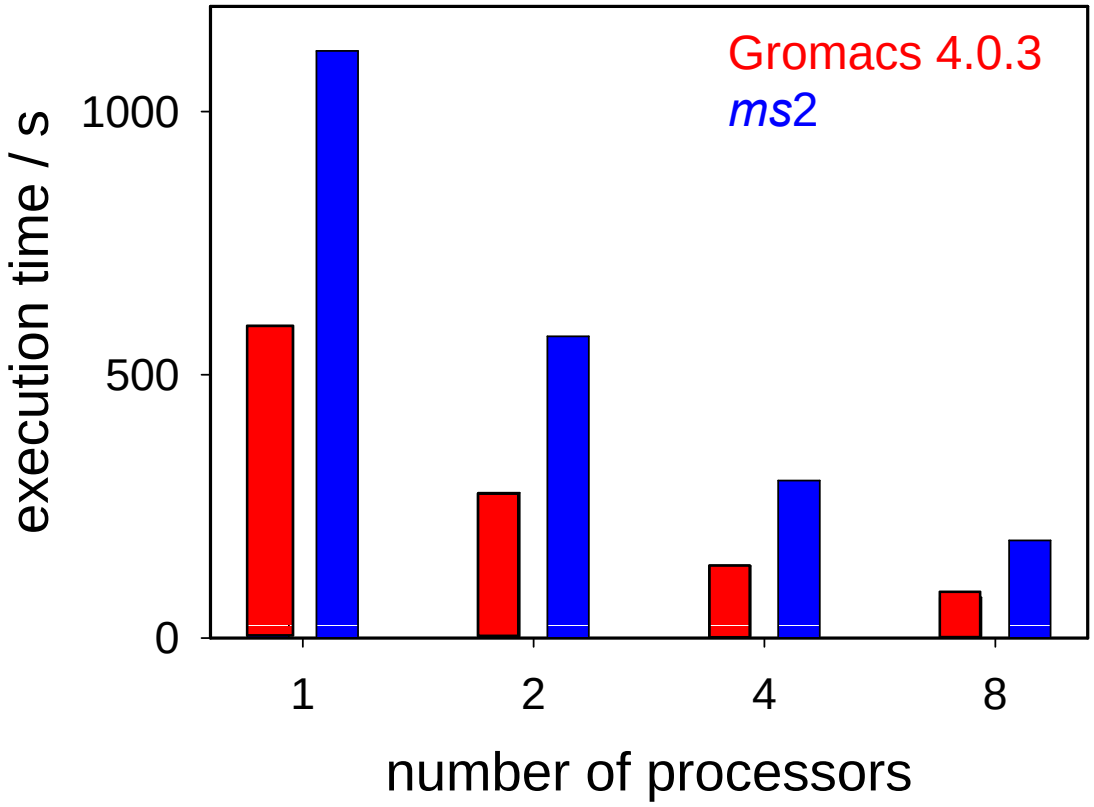
Single processor run

Towhee 6.2.7 vs. *ms*2, execution time **4.9 vs. 1**

For molecular dynamics only:

Gromacs 4.0.3 vs. *ms*2

execution time
roughly **1 vs. 2**

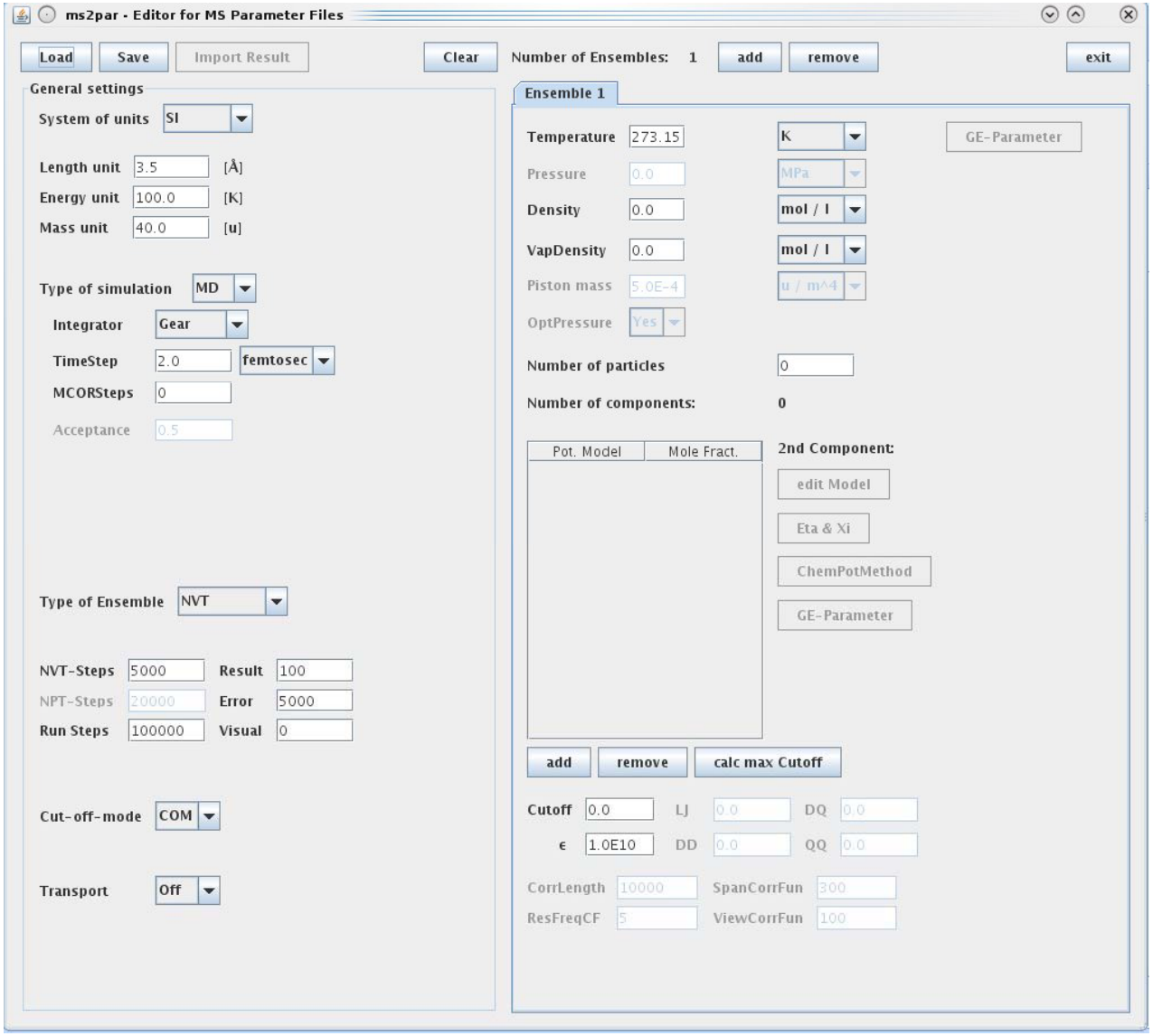


*ms*2par: Input file tool

Java based GUI

Creates/modifies one ASCII input file

For execution, only one additional potential model file per component is needed



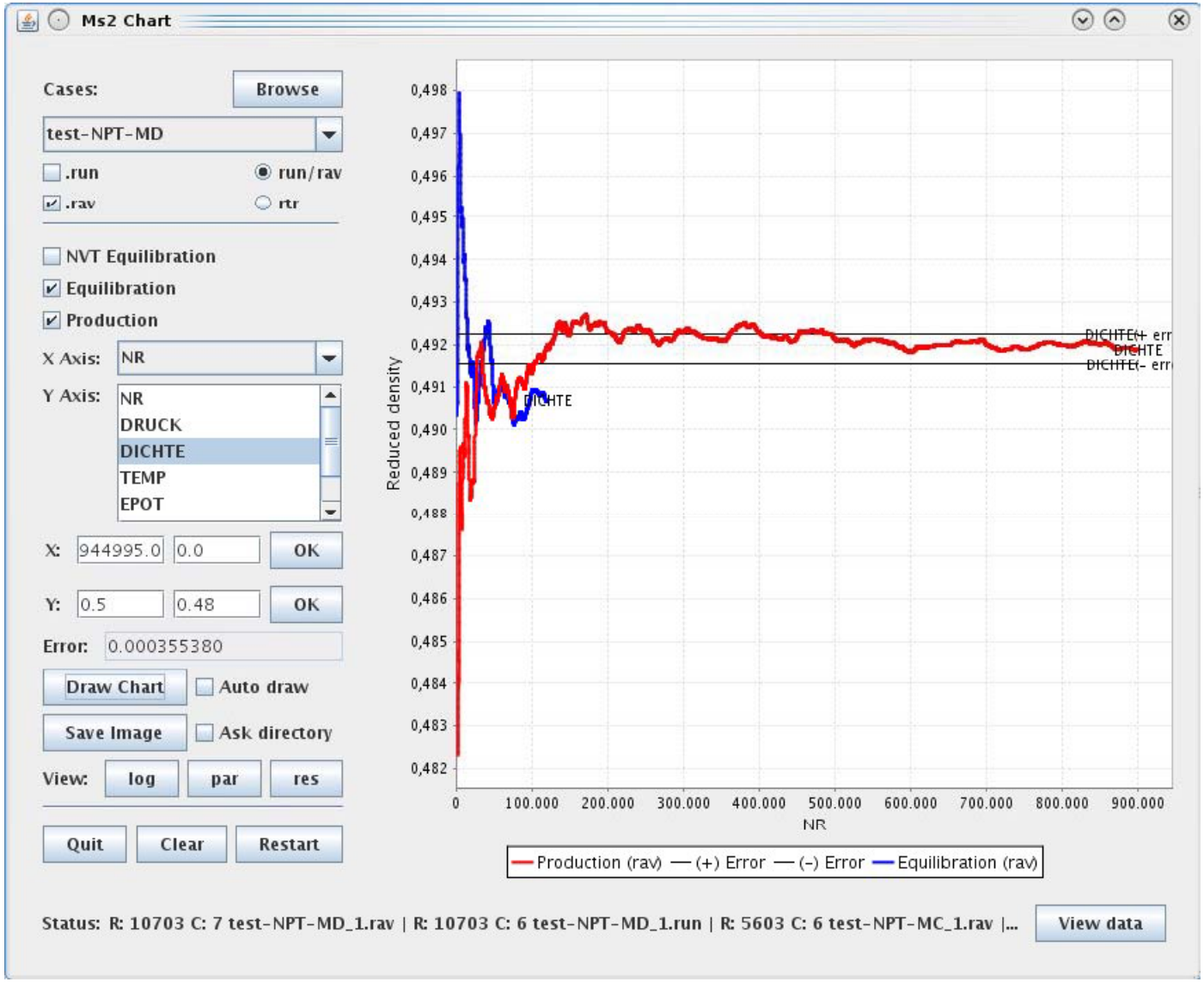
*ms*2chart: Output analysis tool

Java based GUI

Fast output analysis

Intended for large number of simulation runs

Green-Kubo autocorrelation functions supported



*ms*2molecules: Visualization tool

Conclusion and Outlook

- An efficient molecular simulation tool for thermodynamic properties
- *ms*2 can be downloaded from **www.ms-2.de**

- Integer arithmetics
- Pair correlation functions
- Internal degrees of freedom
- Ewald summation for charged particles
- Hybrid MPI/OpenMP parallelization
- Execution on Graphics Processing Units (GPUs)?