



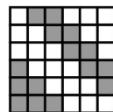
Molecular Modeling and Simulation for Industrial Applications:  
Physico-Chemical Properties and Processes

# ***ms2*: a molecular simulation tool for thermodynamic properties**

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H L R I S



IMEMO



Computational  
Molecular Engineering



## ***ms2*: underlying goals**

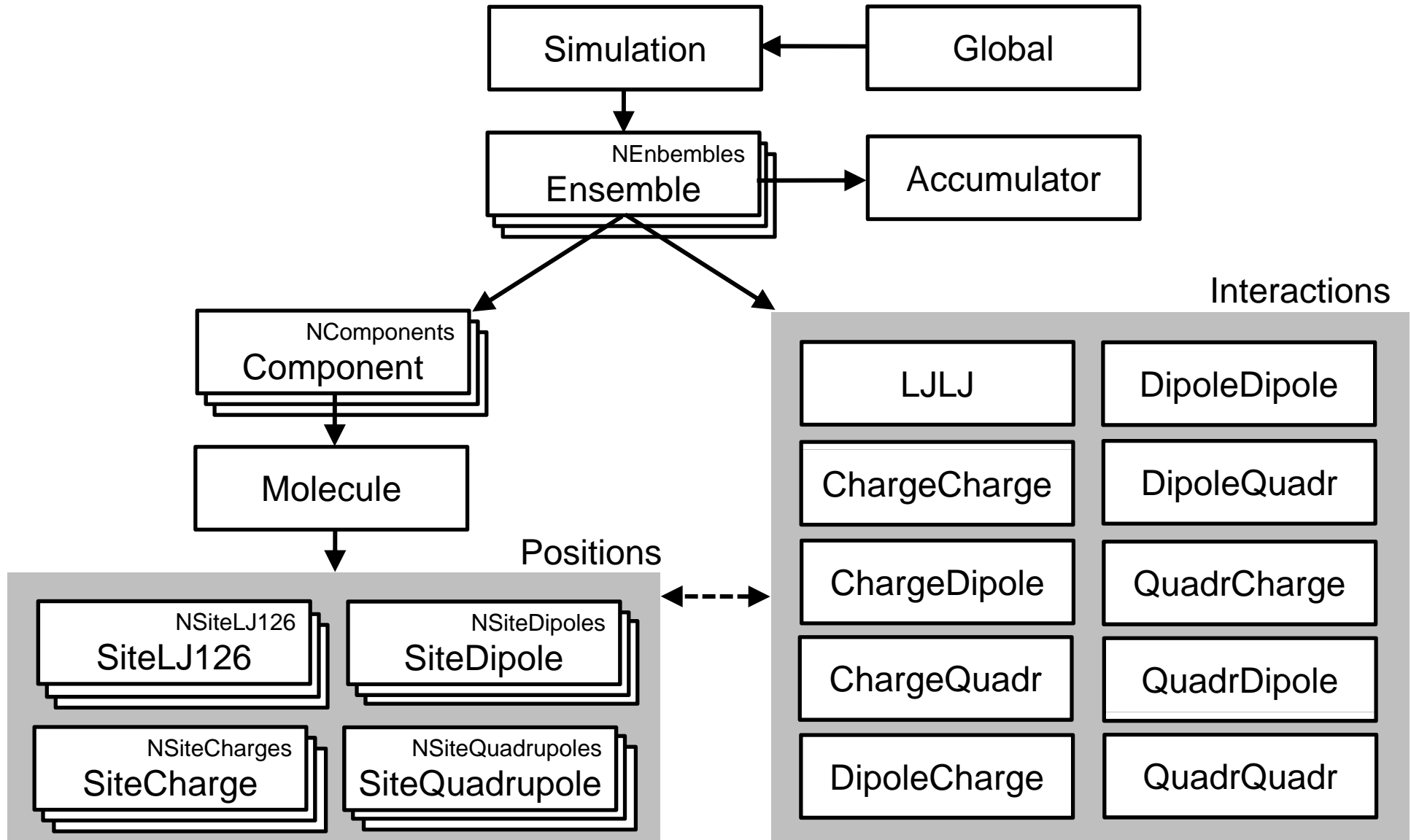
- Efficient simulation runs, short response times
- Taking advantage of future hardware speedup that can be expected to be  $10^3 - 10^4$  in the next 15 years
- Broad supported hardware basis
- Numerical robustness
- Broad application field
- Simple user handling
- GUI support for fast input and output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

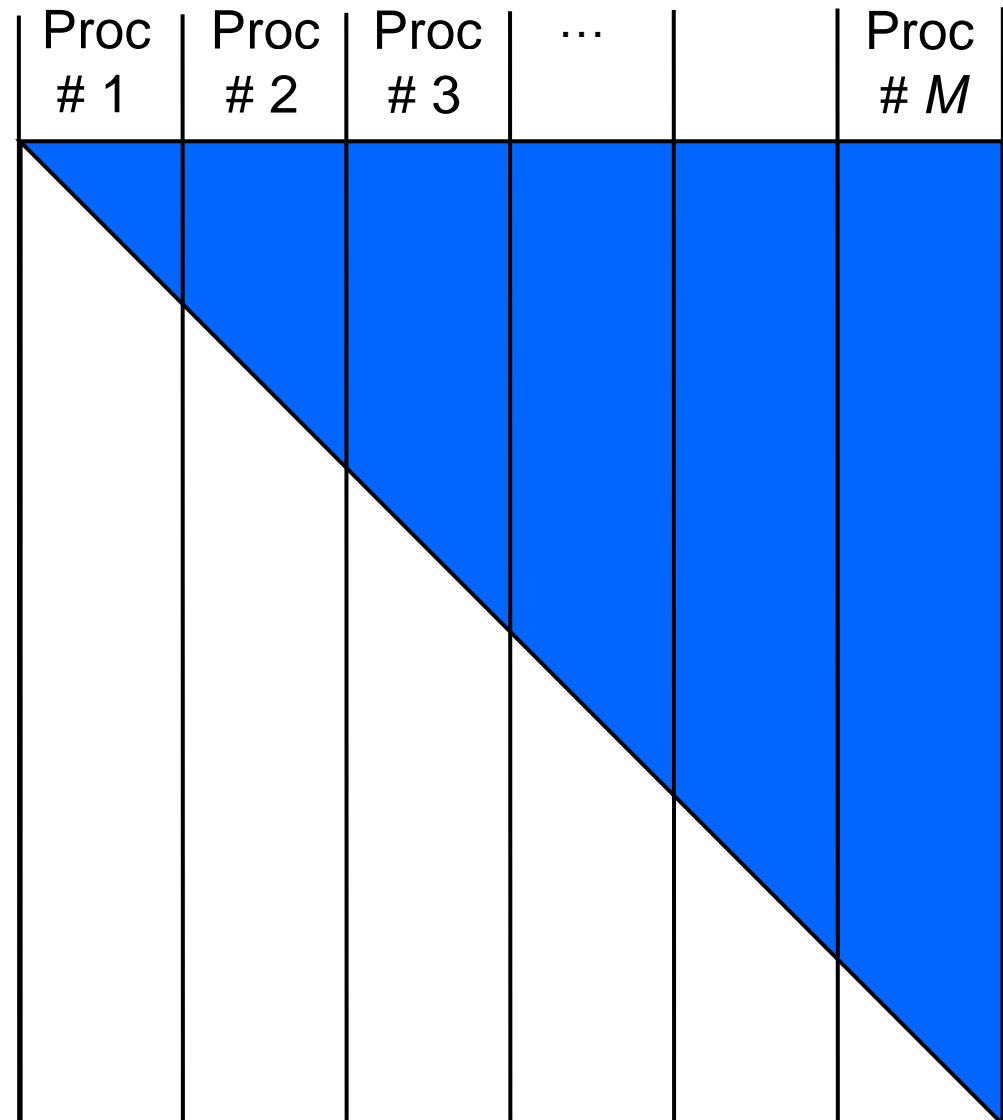
Evaluation of energies,  
forces and torques

$$\sim N(N-1) / 2$$

Densely populated  
in small systems, where

$$r_c \sim \text{system size}$$

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

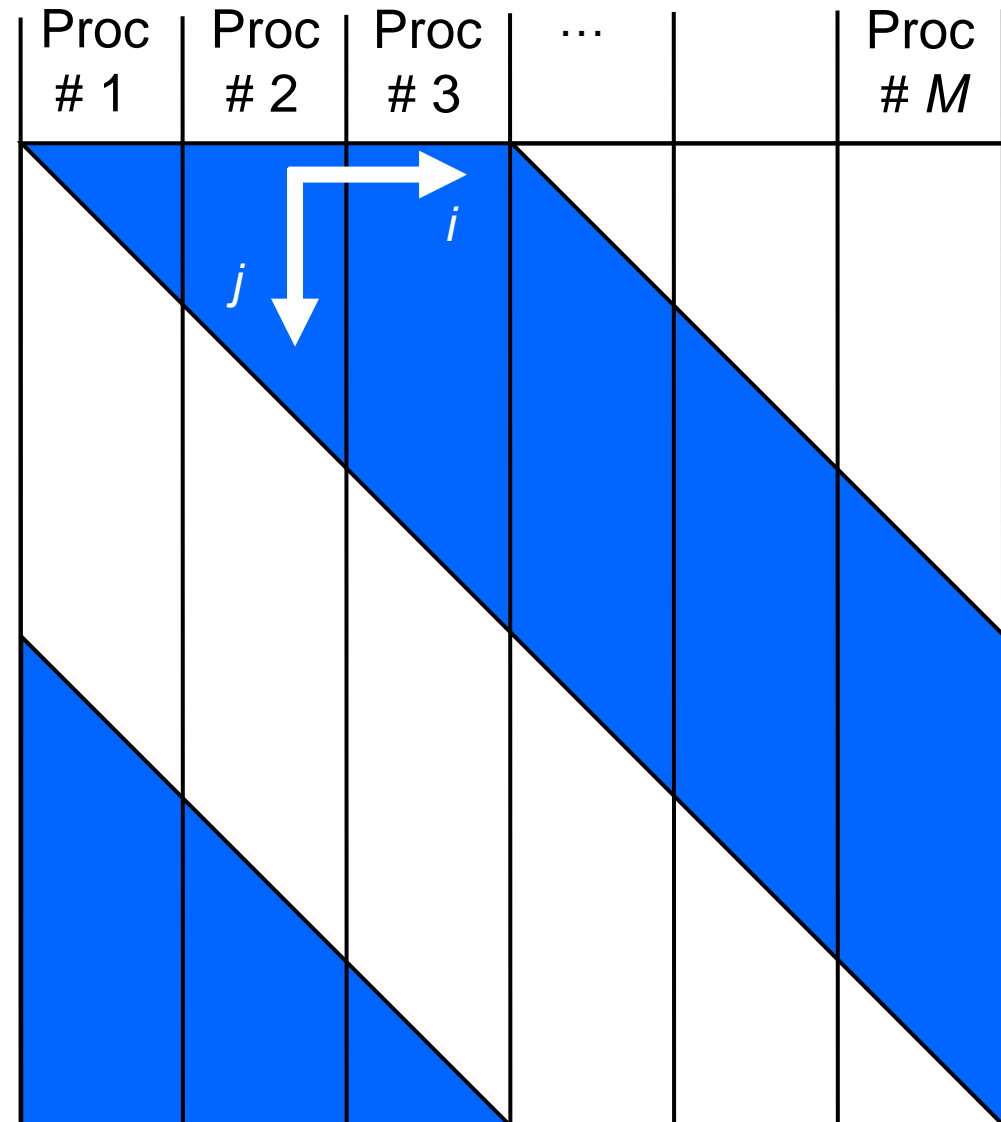


## Molecular dynamics vector-parallelization (II)

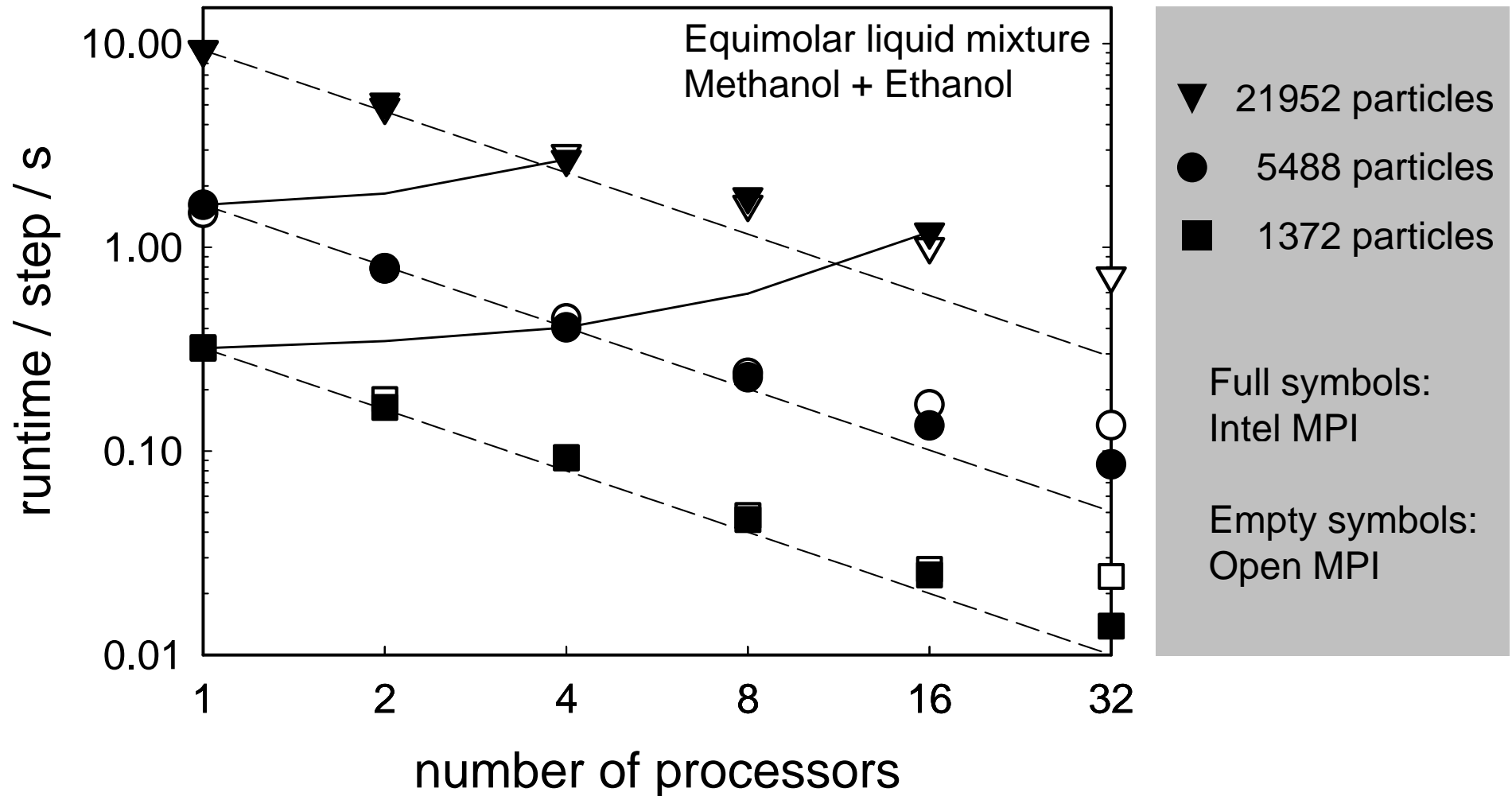
Force decomposition

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

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



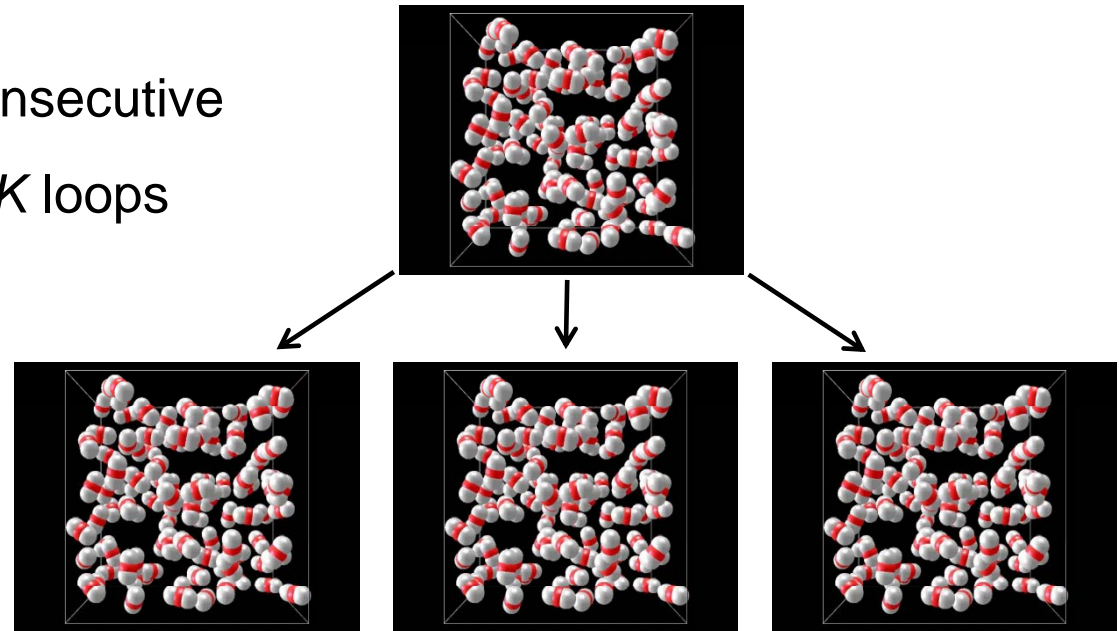
# Molecular dynamics efficiency



## 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

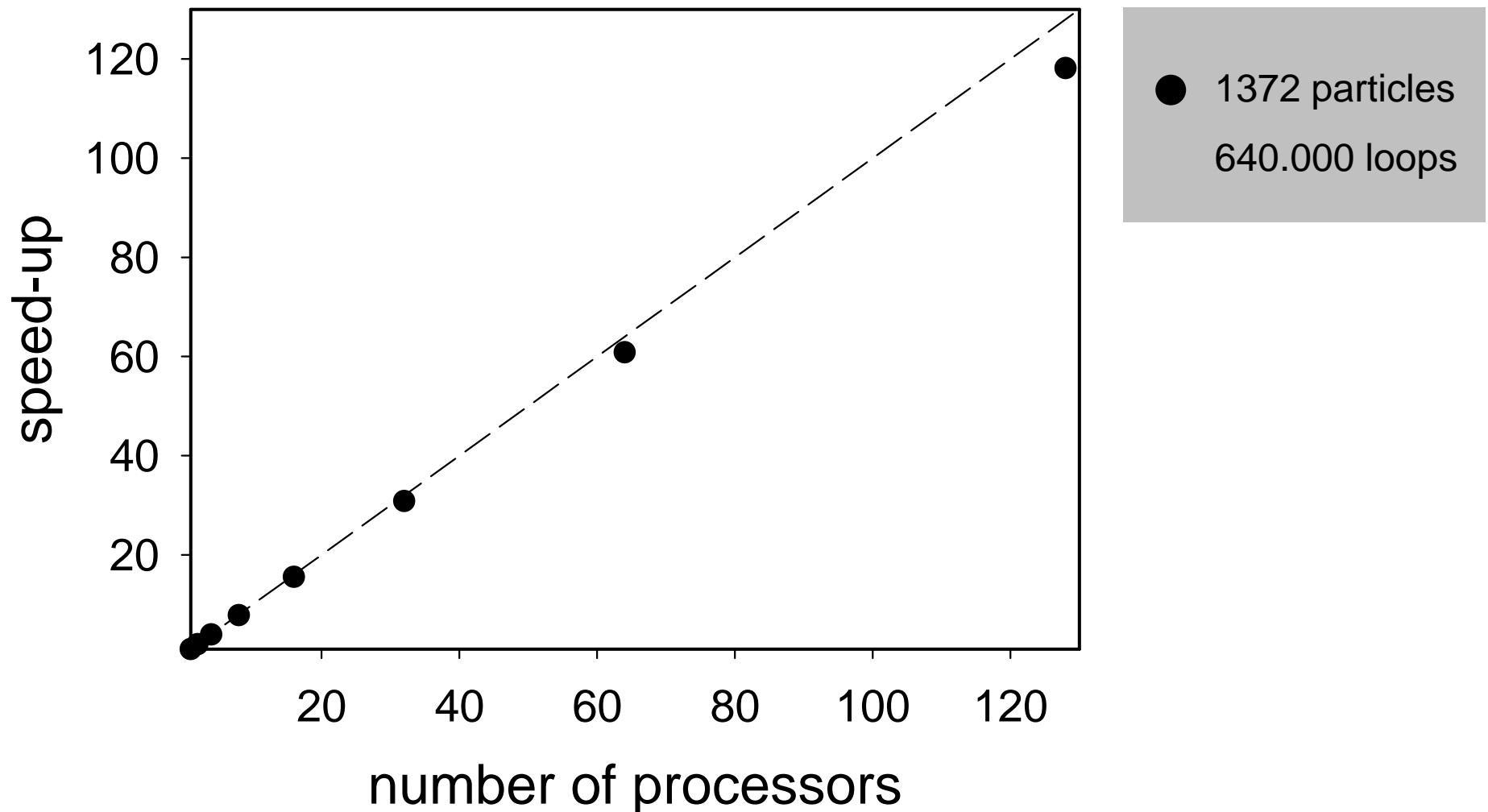


- Efficient, as hardly any communication is necessary
- For displaced particles, only “new energy “ calculated , “old energy” gathered from interaction energy array





## Monte Carlo speed-up – without equilibration



## Comparison with other simulation programs

For VLE calculations (Monte Carlo only):

Single processor run

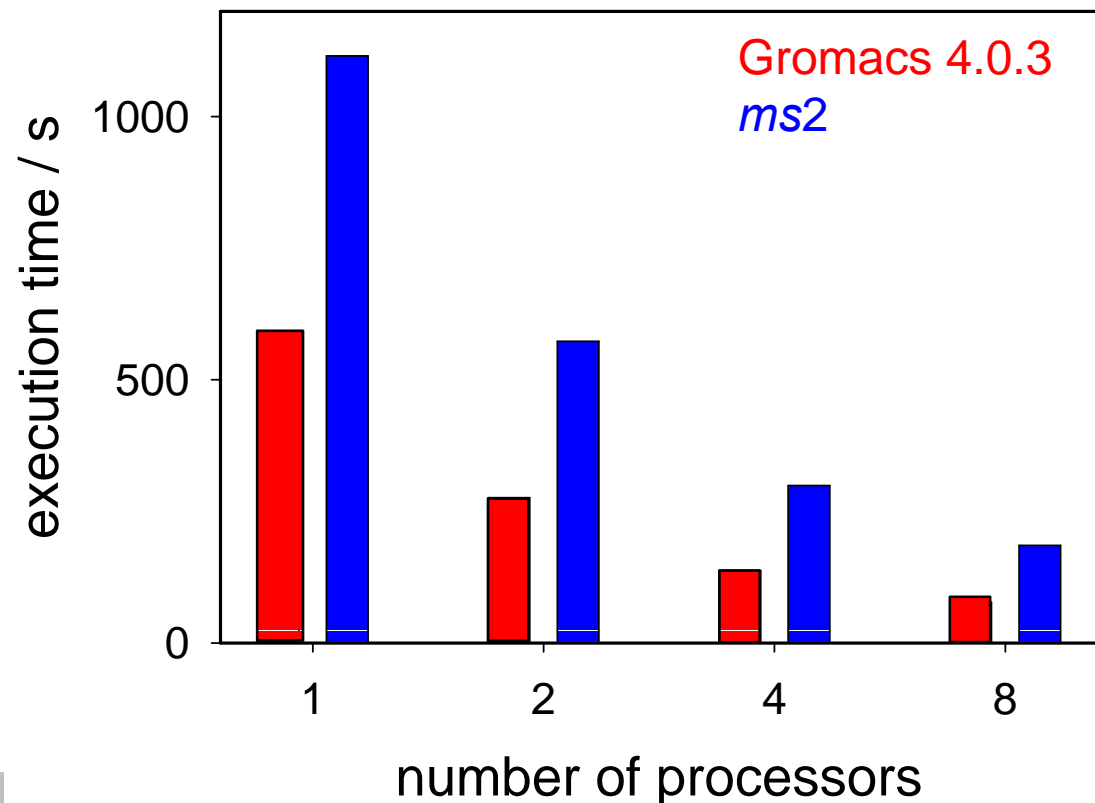
Towhee 6.2.7 vs. *ms2*, execution time

**4.9 vs. 1**

For molecular dynamics only:

Gromacs 4.0.3 vs. *ms2*

execution time  
 roughly **1 vs. 2**

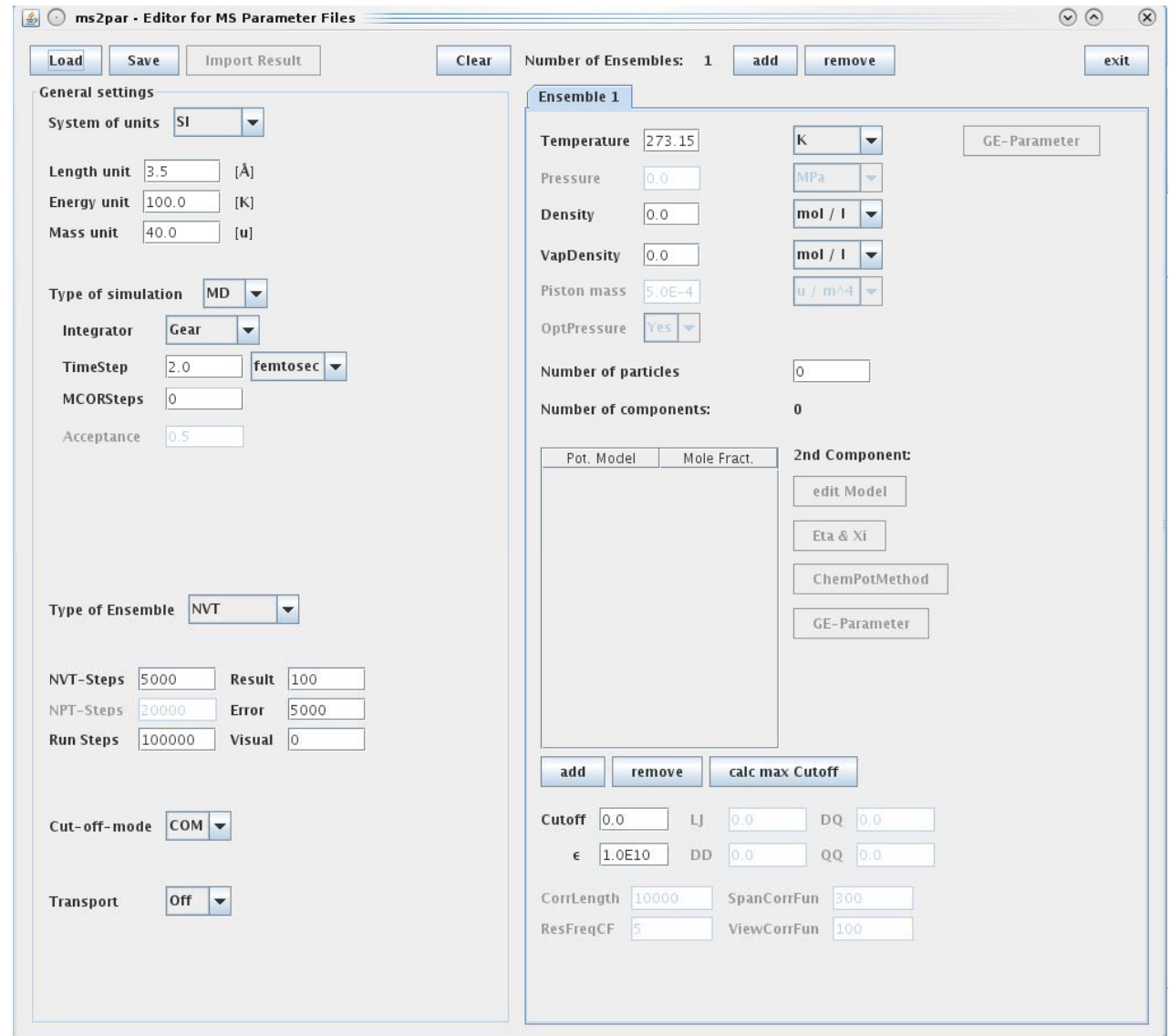


# ms2par: Input file tool

Java based GUI

Creates/modifies  
one ASCII input file

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



The screenshot shows the 'ms2par - Editor for MS Parameter Files' window. It features a top toolbar with 'Load', 'Save', 'Import Result', 'Clear', 'add', 'remove', and 'exit' buttons. The main interface is divided into several sections:

- General settings:** Includes dropdowns for 'System of units' (SI), 'Type of simulation' (MD), and 'Type of Ensemble' (NVT). It also has input fields for 'Length unit' (3.5 Å), 'Energy unit' (100.0 K), 'Mass unit' (40.0 u), 'Integrator' (Gear), 'TimeStep' (2.0 femtosec), 'MCORSteps' (0), 'Acceptance' (0.5), 'NVT-Steps' (5000), 'NPT-Steps' (20000), 'Run Steps' (100000), 'Result' (100), 'Error' (5000), 'Visual' (0), 'Cut-off-mode' (COM), and 'Transport' (Off).
- Ensemble 1:** Contains input fields for 'Temperature' (273.15 K), 'Pressure' (0.0 MPa), 'Density' (0.0 mol/l), 'VapDensity' (0.0 mol/l), 'Piston mass' (5.0E-4 u/m^4), and 'OptPressure' (Yes). It also has 'Number of particles' (0) and 'Number of components' (0).
- 2nd Component:** Includes a table with columns 'Pot. Model' and 'Mole Fract.', and buttons for 'edit Model', 'Eta & Xi', 'ChemPotMethod', and 'GE-Parameter'.
- Bottom section:** Features buttons for 'add', 'remove', and 'calc max Cutoff', along with input fields for 'Cutoff' (0.0), 'LJ' (0.0), 'DQ' (0.0), 'epsilon' (1.0E10), 'DD' (0.0), 'QQ' (0.0), 'CorrLength' (10000), 'SpanCorrFun' (300), 'ResFreqCF' (5), and 'ViewCorrFun' (100).

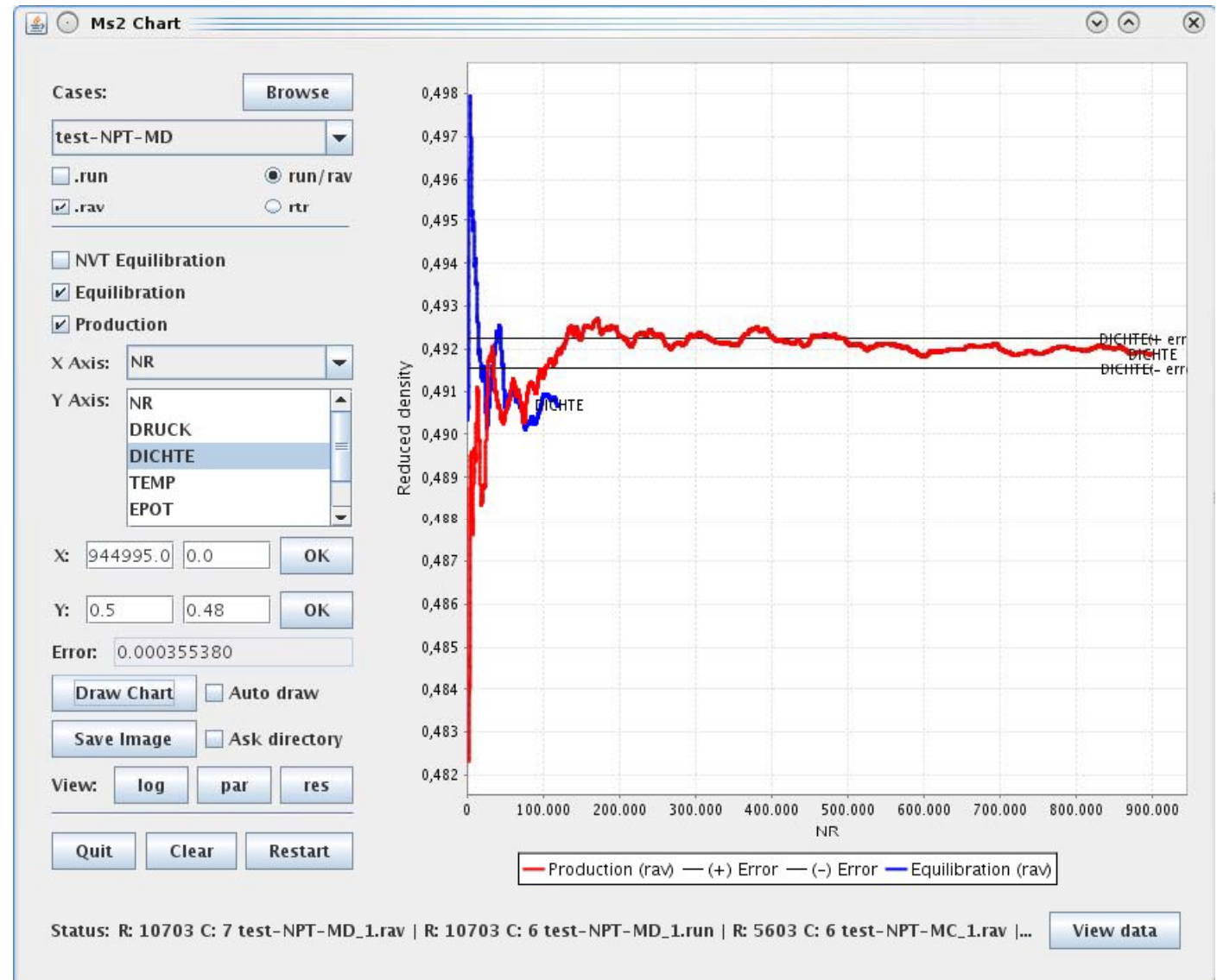
# ms2chart: Output analysis tool

Java based GUI

Fast output  
analysis

Intended for large  
number of  
simulation runs

Green-Kubo  
autocorrelation  
functions supported





# *ms2*molecules: Visualization tool



## Conclusion and Outlook

- An efficient molecular simulation tool for thermodynamic properties
- *ms2* can be downloaded from [www.ms-2.de](http://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)?