Optimized Monte Carlo Code

Hands on ParaGrandMC

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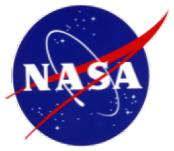


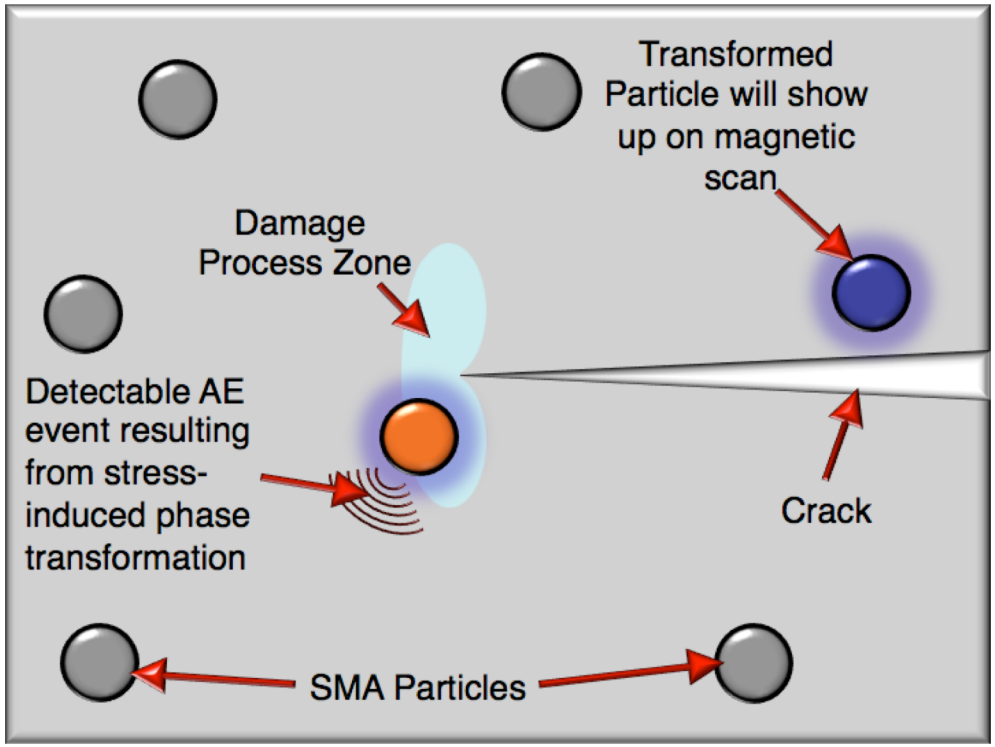
Outline

- Motivation for high-speed Monte Carlo
- Example studies with ParaGrandMC
- Parallelization strategy for Monte Carlo simulation method
- ParaGrandMC tutorial
- On hands exercises with ParaGrandMC

Motivation for High-Speed Monte Carlo

Sensory Alloy Concept

Creating a material with intrinsic sensory behavior*



- Improve early crack detection in metallic materials
- Improve vehicle reliabilty and safety
- Optimize structure and material performance (lower factor of safety)
- Decrease maintenance cost

Ferromagnetic Shape Memory Alloys (FSMA) as sensory material

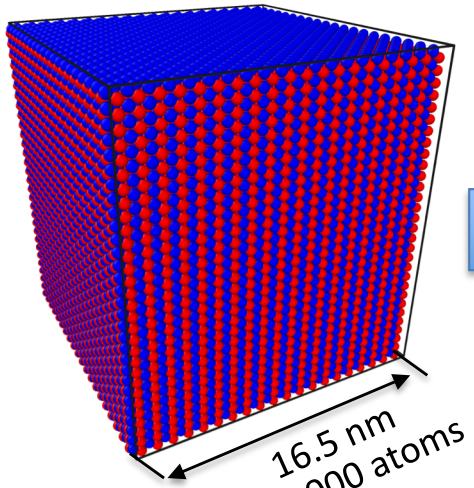
High strain in damage zone causes phase transformation
- **Acoustic emission (AE) that can be measured during flight**
- **Magnetic changes measurable using ground-based inspection equipment**

*Wallace, T.A., et. al, "Strain-Detecting Composite Materials". Patent Application Publication, Pub. No. US2010/0190026 A1, July 29, 2010.

System Preparation by MC Simulation

Thermodynamically equilibrated non-stoichiometric $Ni_{35}Al_{29}Co_{36}$

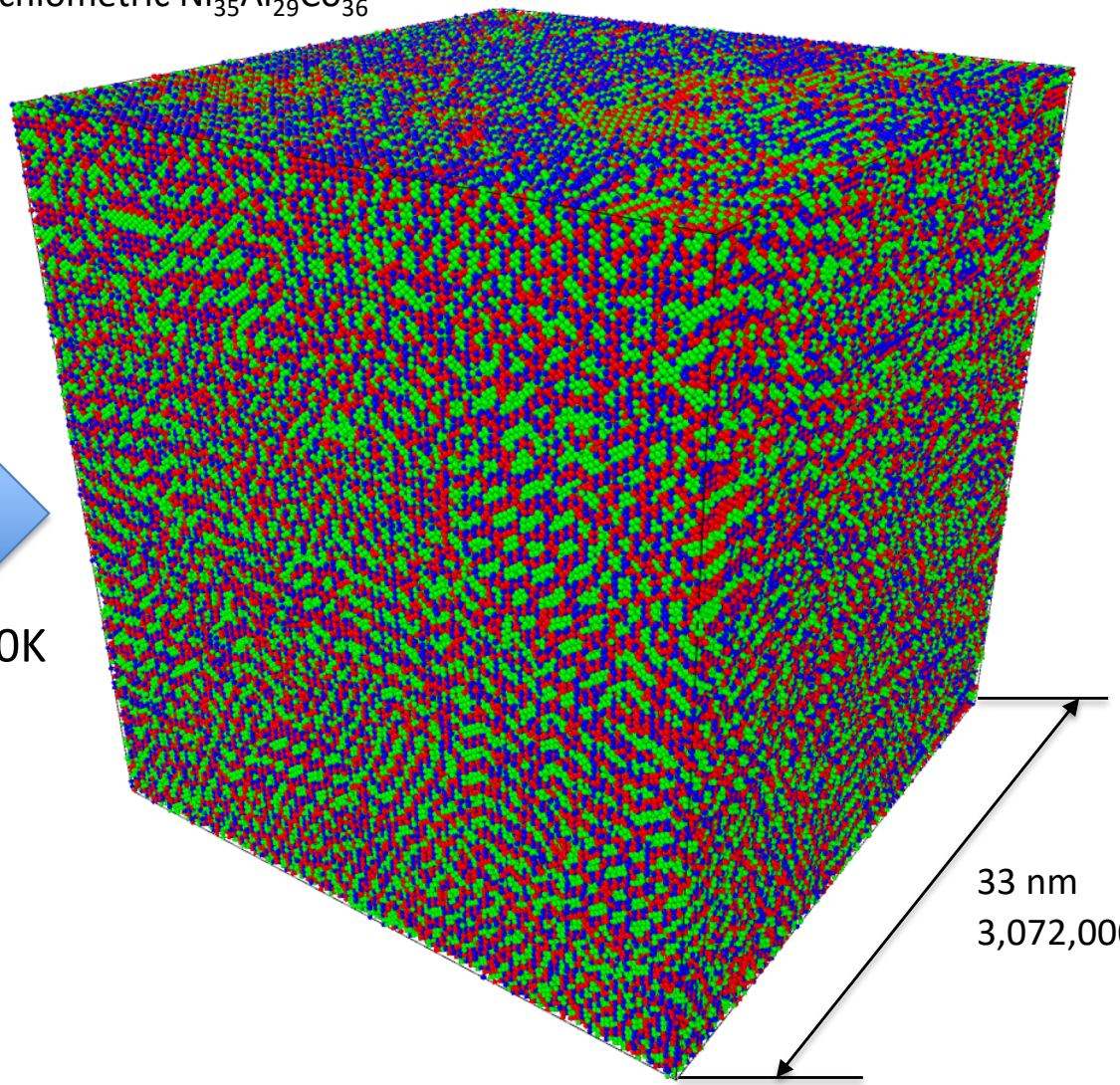
Initial system:
B2 NiAl



MC

+ Co

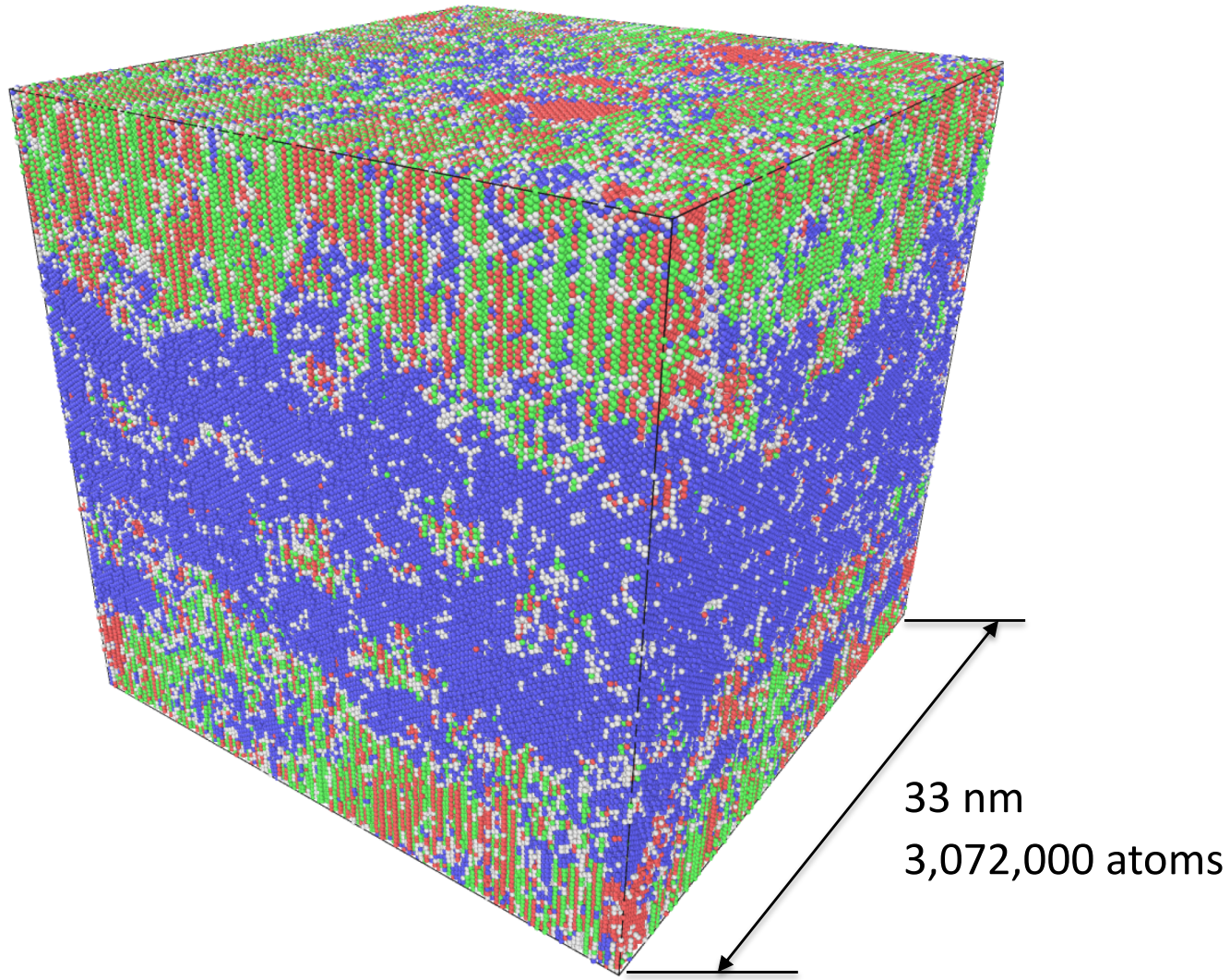
T = 700K



The simulations required the use of a substantial computational power and resources.

Martensitic Transformation by MC

Lowering temperature initiates martensitic transformation at $T < M_s$



Crystal Structure

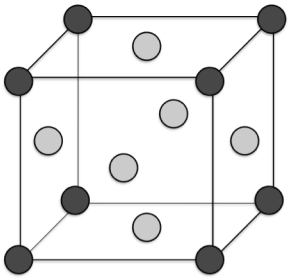
- BCC (austenite)
- HCP (twins)
- FCC (martensite)
- Undefined

The simulations required the use of a substantial computational power and resources.

Calculation of Interface Free Energy

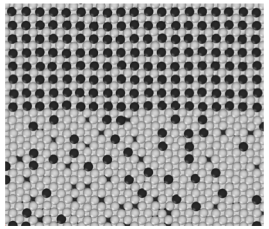
γ/γ' interface in the Ni-Al system by capillary fluctuation method

γ'-ordered

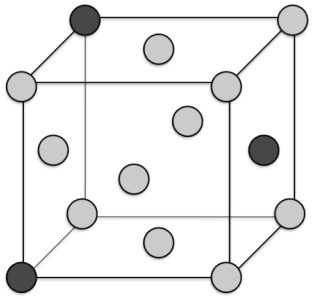


Base:
Al_1: 0 0 0
Ni_1: ½ ½ 0
Ni_2: ½ 0 ½
Ni_3: 0 ½ ½

- Ni
- Al

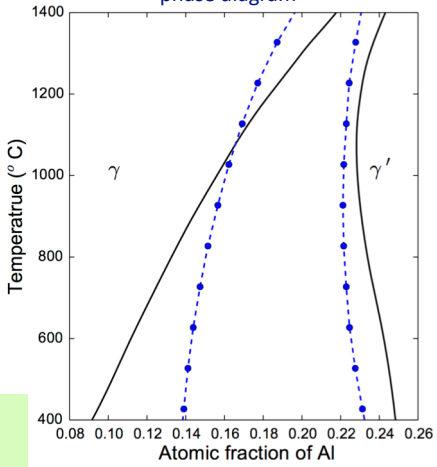


γ- disordered

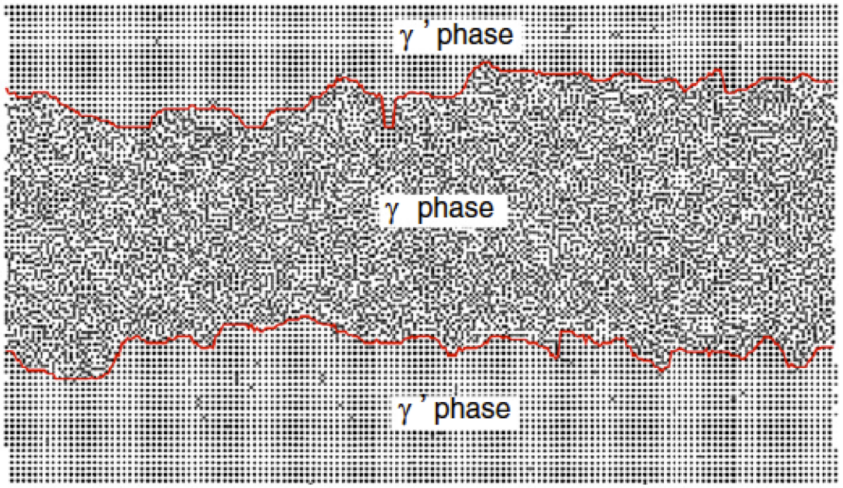


Occupational disorder: same lattice, random Ni-Al occupation.

Experimental (—) vs simulated (•----•) γ/γ' phase diagram



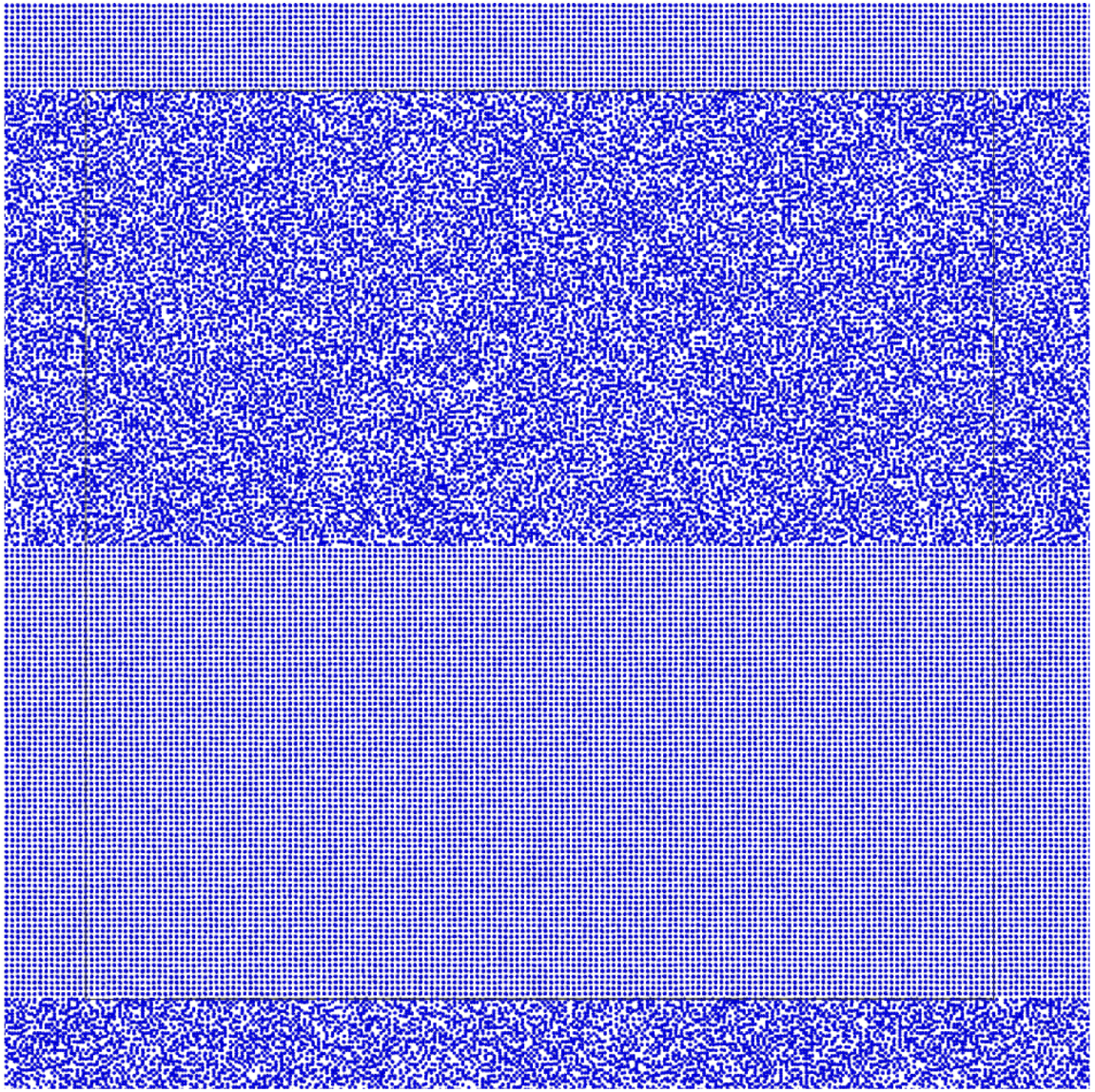
Modelling Simul. Mater. Sci. Eng. **22** (2014) 045001 Y Mishin



Using the equilibrium power spectrum of the interface boundary fluctuations to extract the interface free energy.

Figure 1. A typical snapshot of Monte Carlo simulations of γ and γ' phases at the temperature of 700 K. The simulation block is projected on the x–y plane showing only Al atoms. The red lines show the γ/γ' interfaces revealed by the visualization method applied in this work.

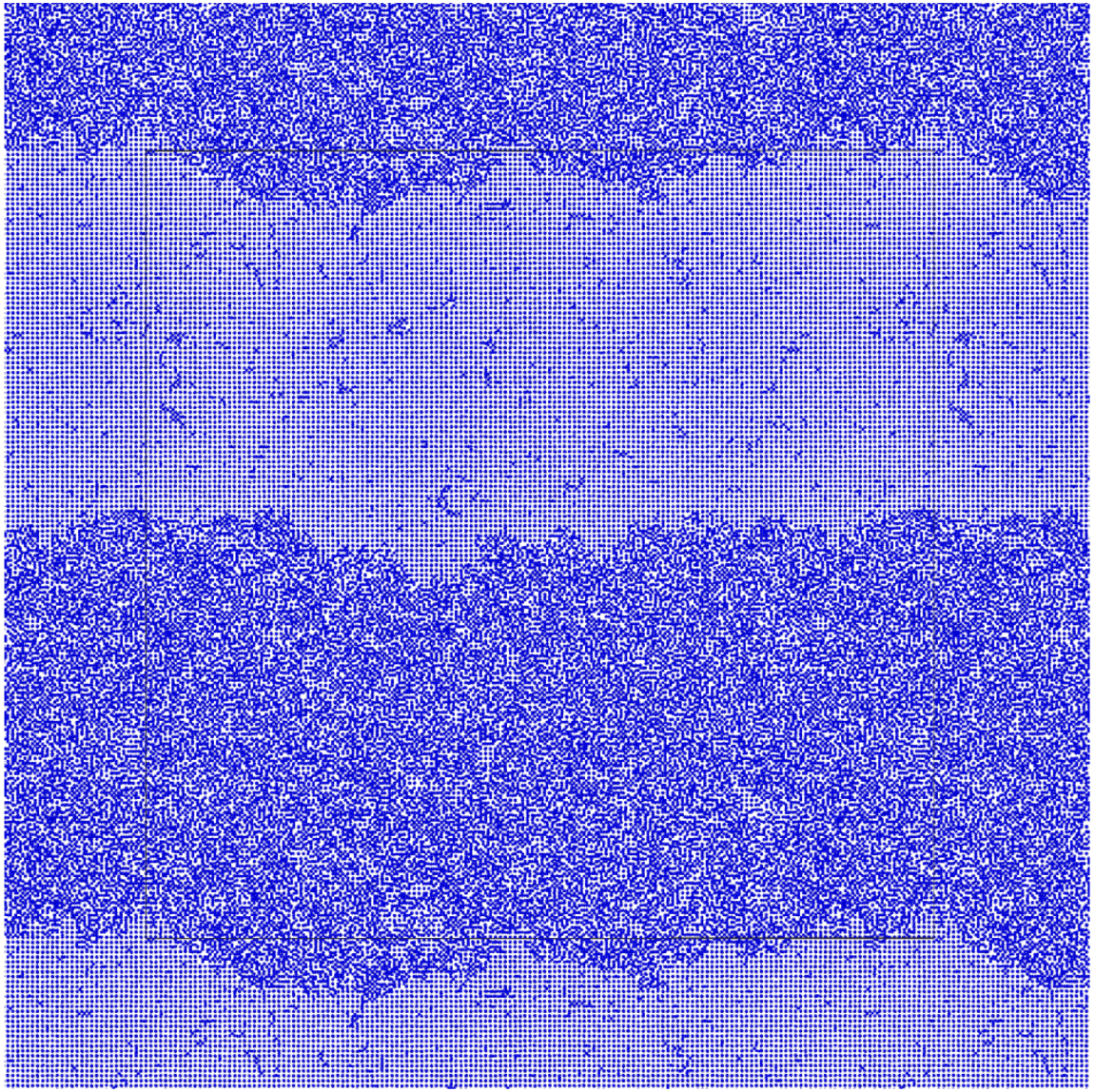
Calculation of Interface Free Energy



Initial system:

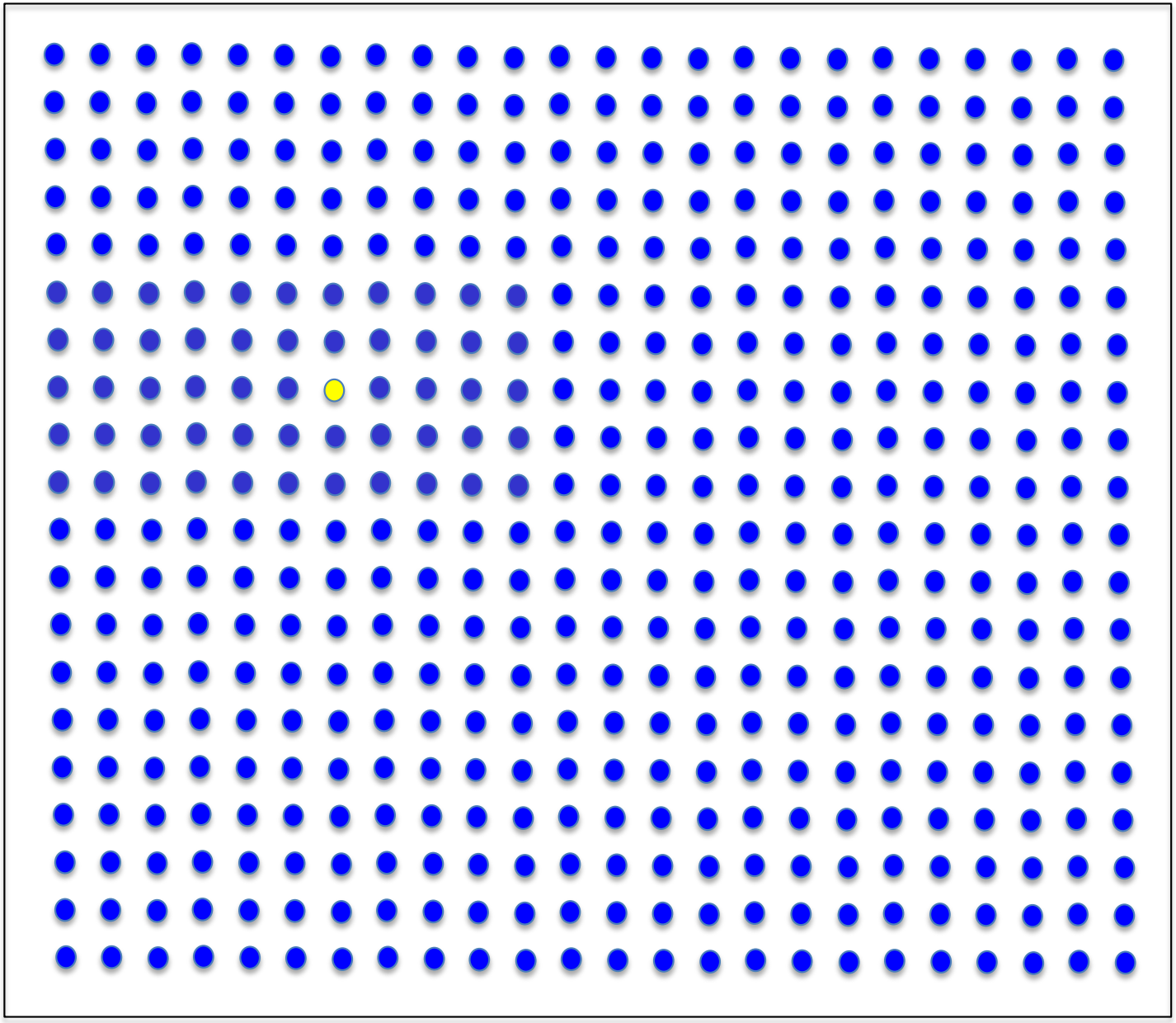
Perfectly flat interface:
512,000 atoms

Calculation of Interface Free Energy



Simulated for
> 1,000,000 MCS

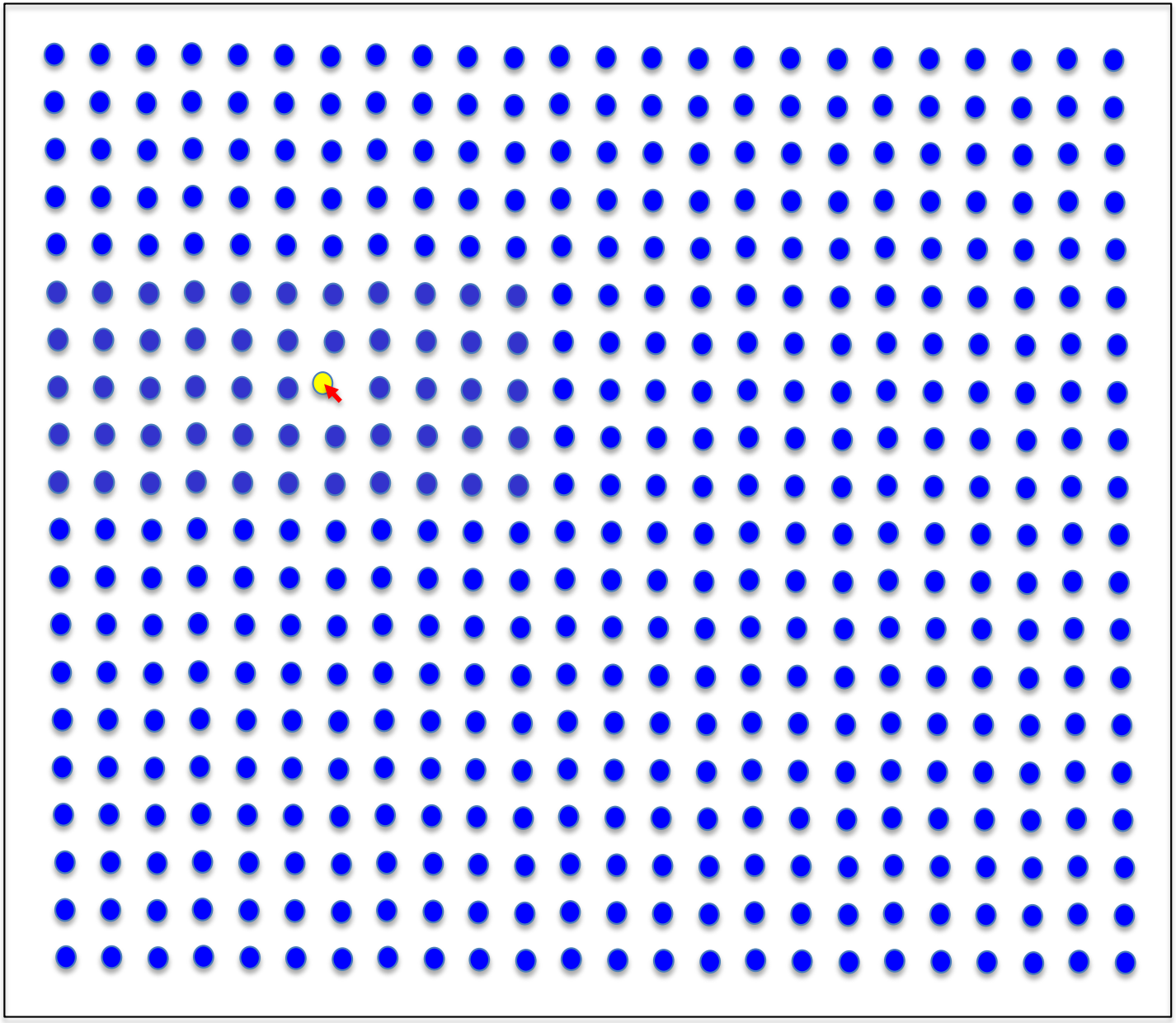
Monte-Carlo Algorithm



One MC move:

1. Pick a random atom
2. Execute a trial move
3. Calculate energy change, ΔE.
4. Accept with probability p=exp(-ΔE/kT)

Monte-Carlo Algorithm



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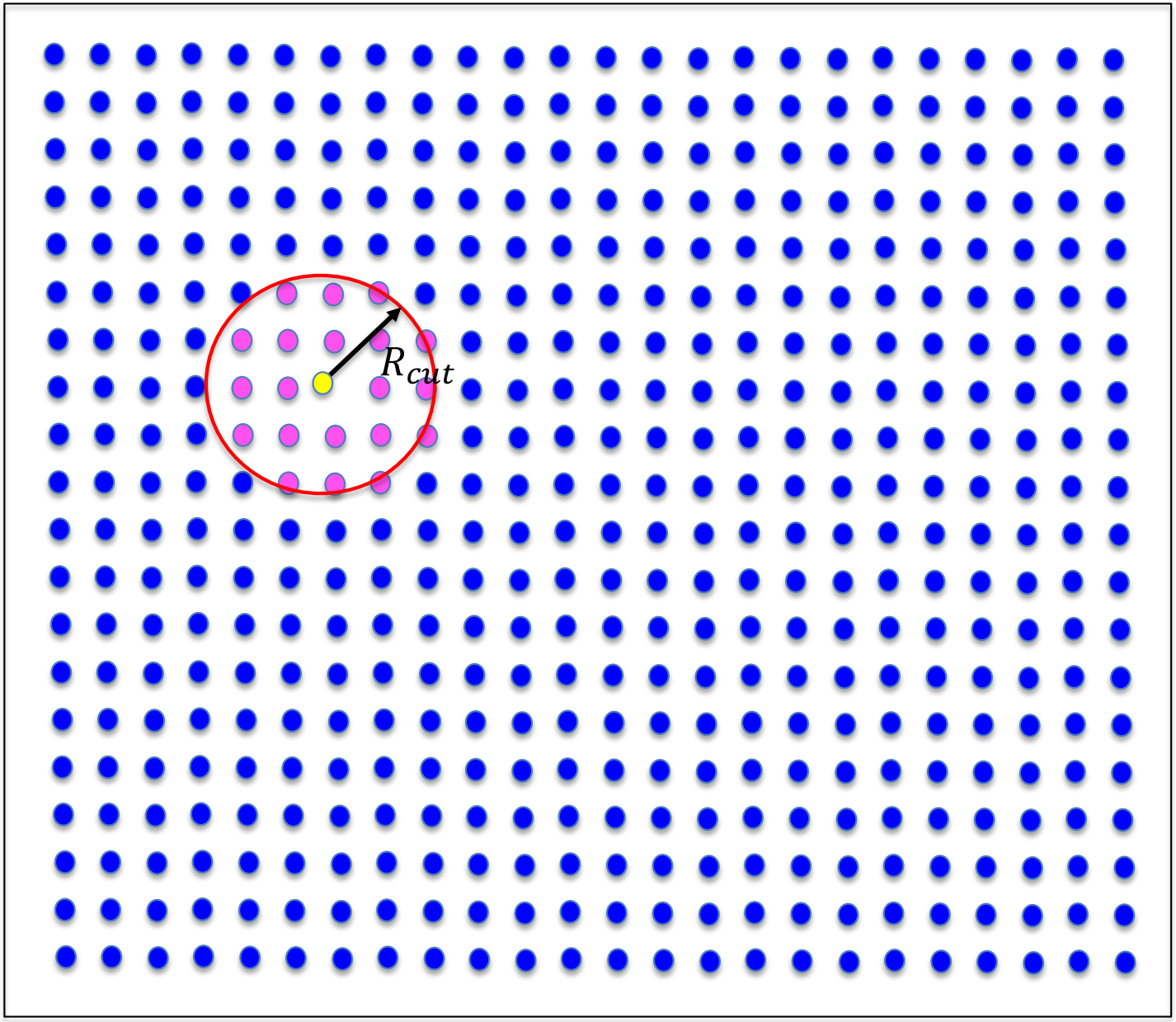

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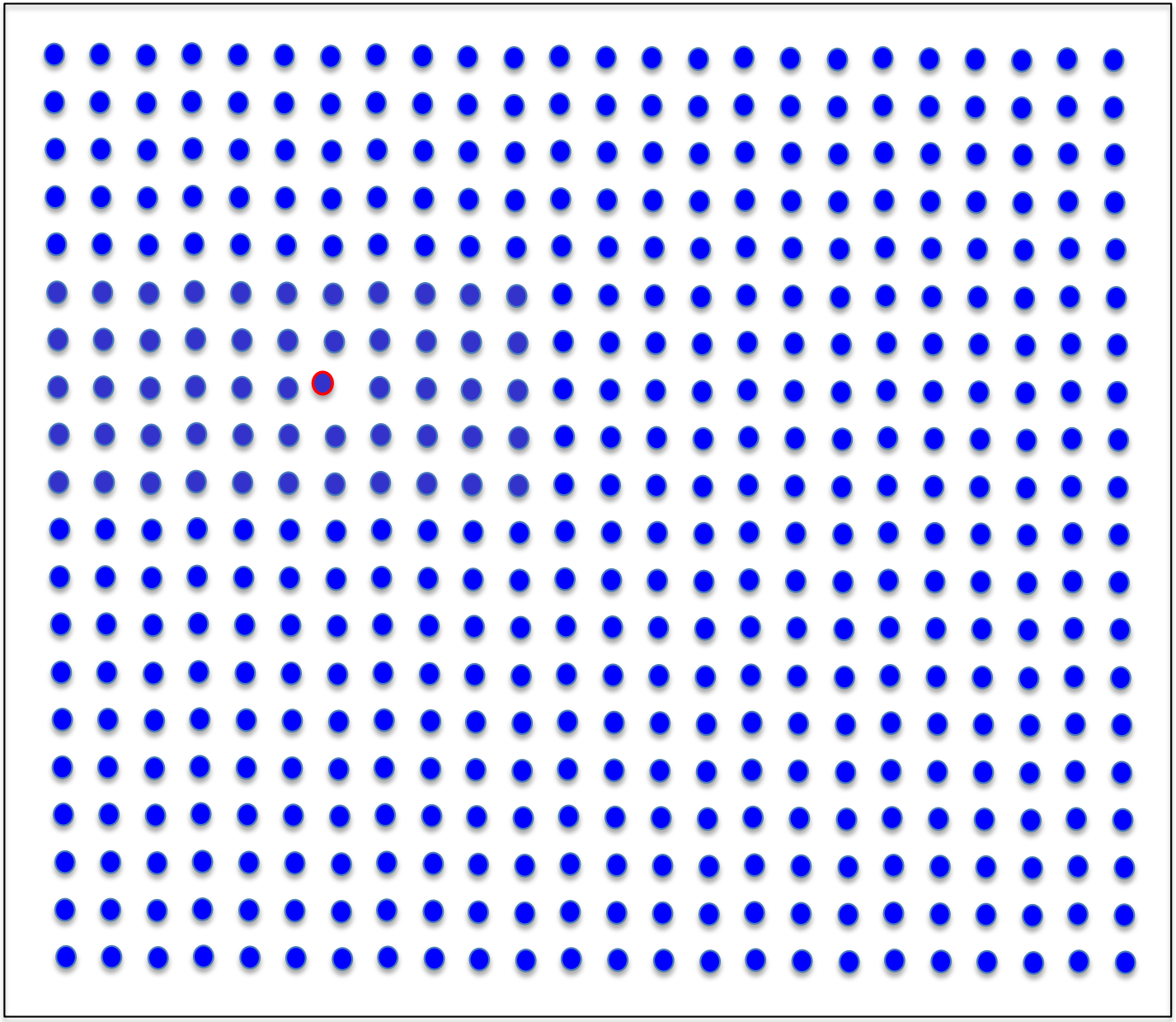
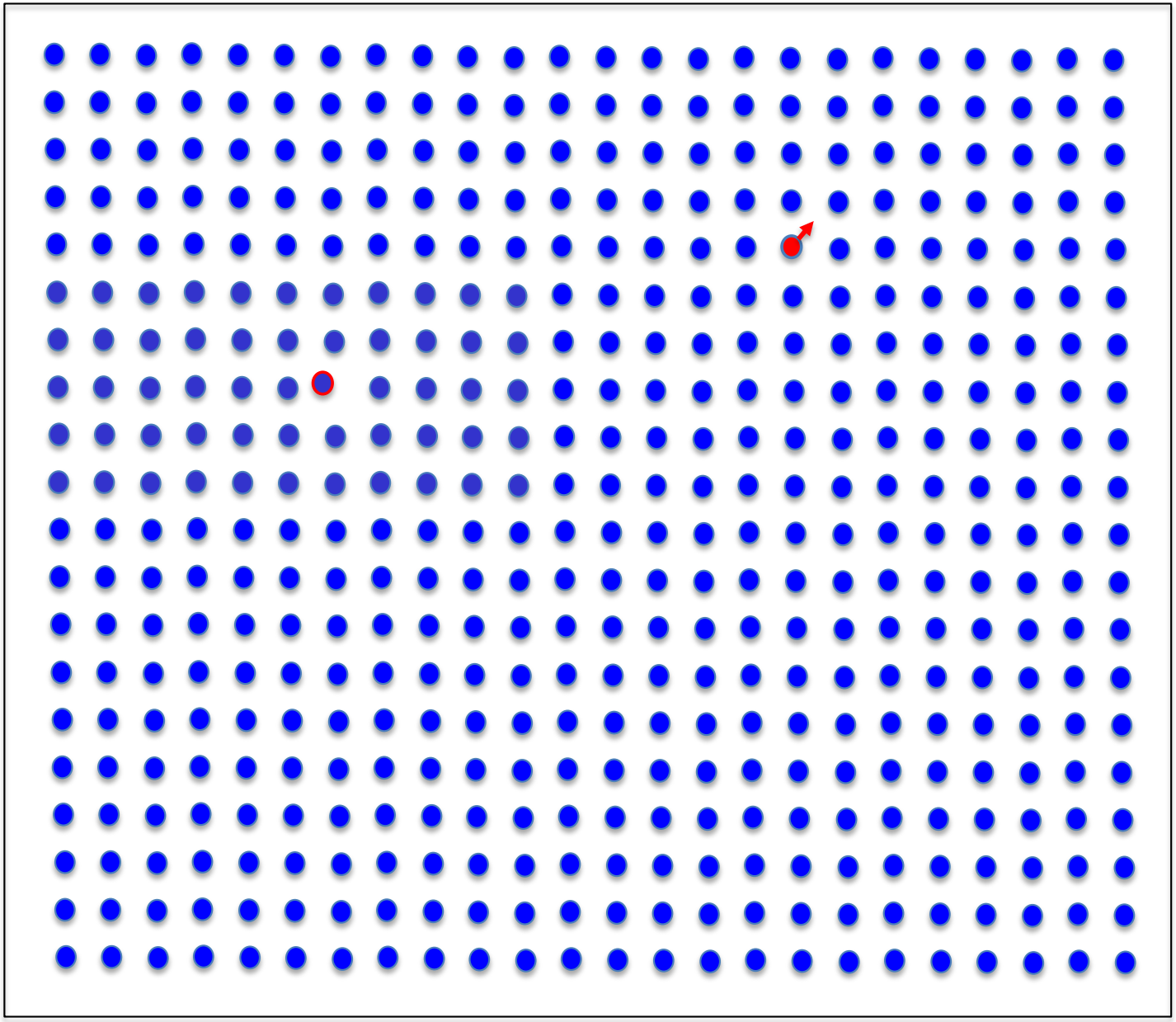


One MC move:

1. Pick a random atom
2. Execute a trial move
3. Calculate energy change, ΔE.
4. Accept with probability $p=\exp(-\Delta E/kT)$

Monte-Carlo Algorithm

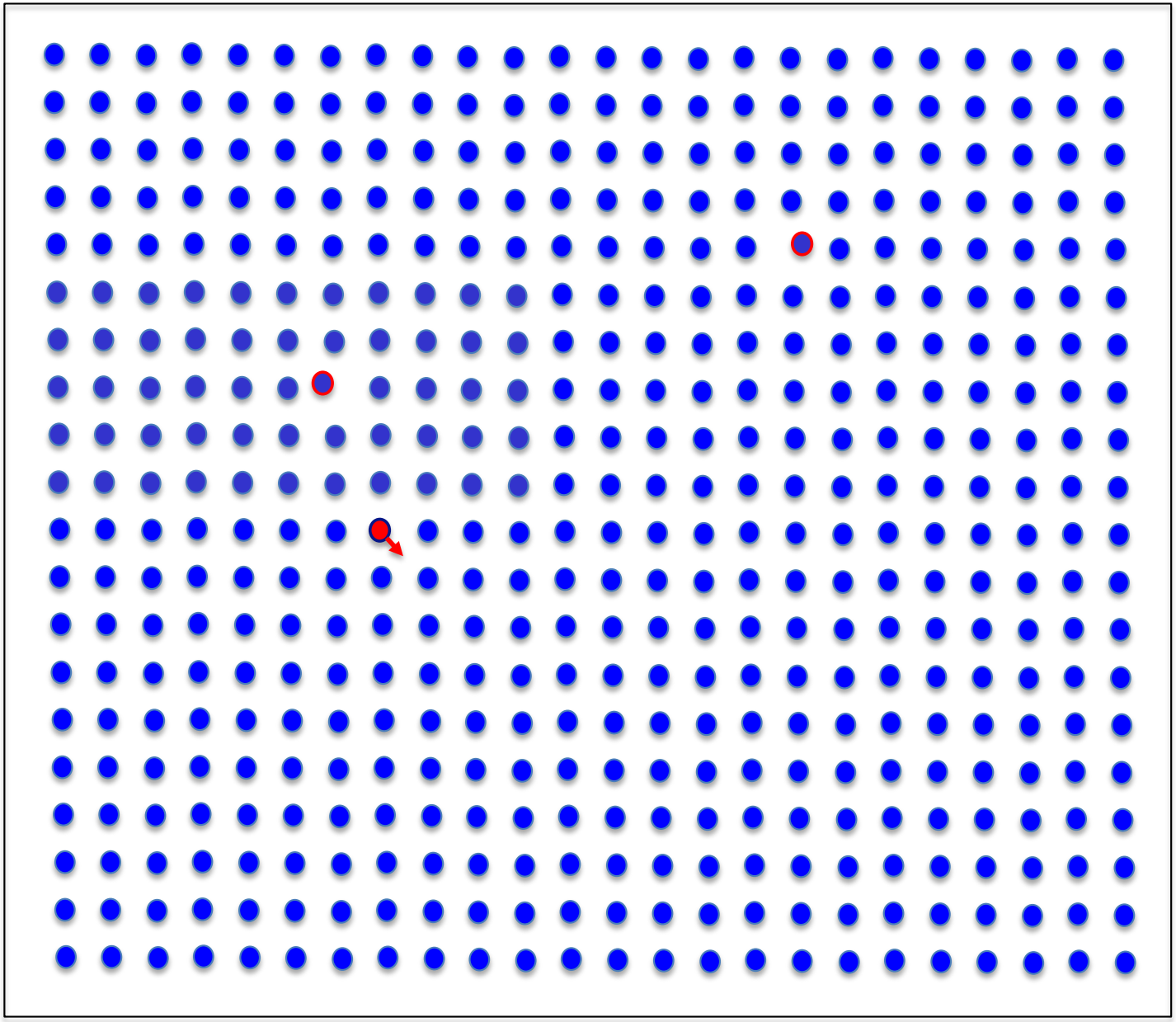


One MC move:

Repeat 1-4 multiple times:

1. Pick a random atom
2. Execute a trial move
3. Calculate energy change, ΔE.
4. Accept with probability p=exp(-ΔE/kT)

Monte-Carlo Algorithm



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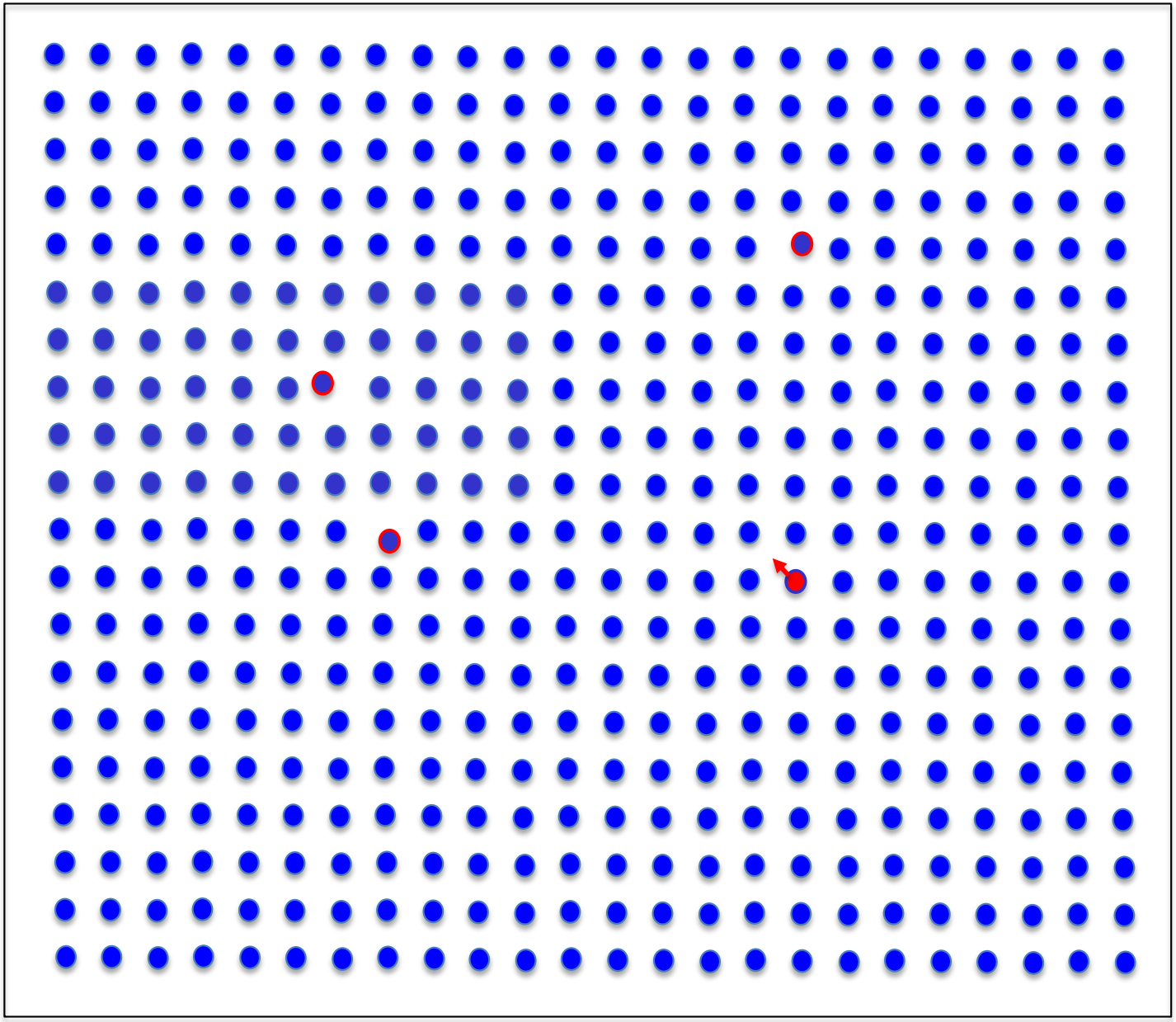
Monte-Carlo Algorithm



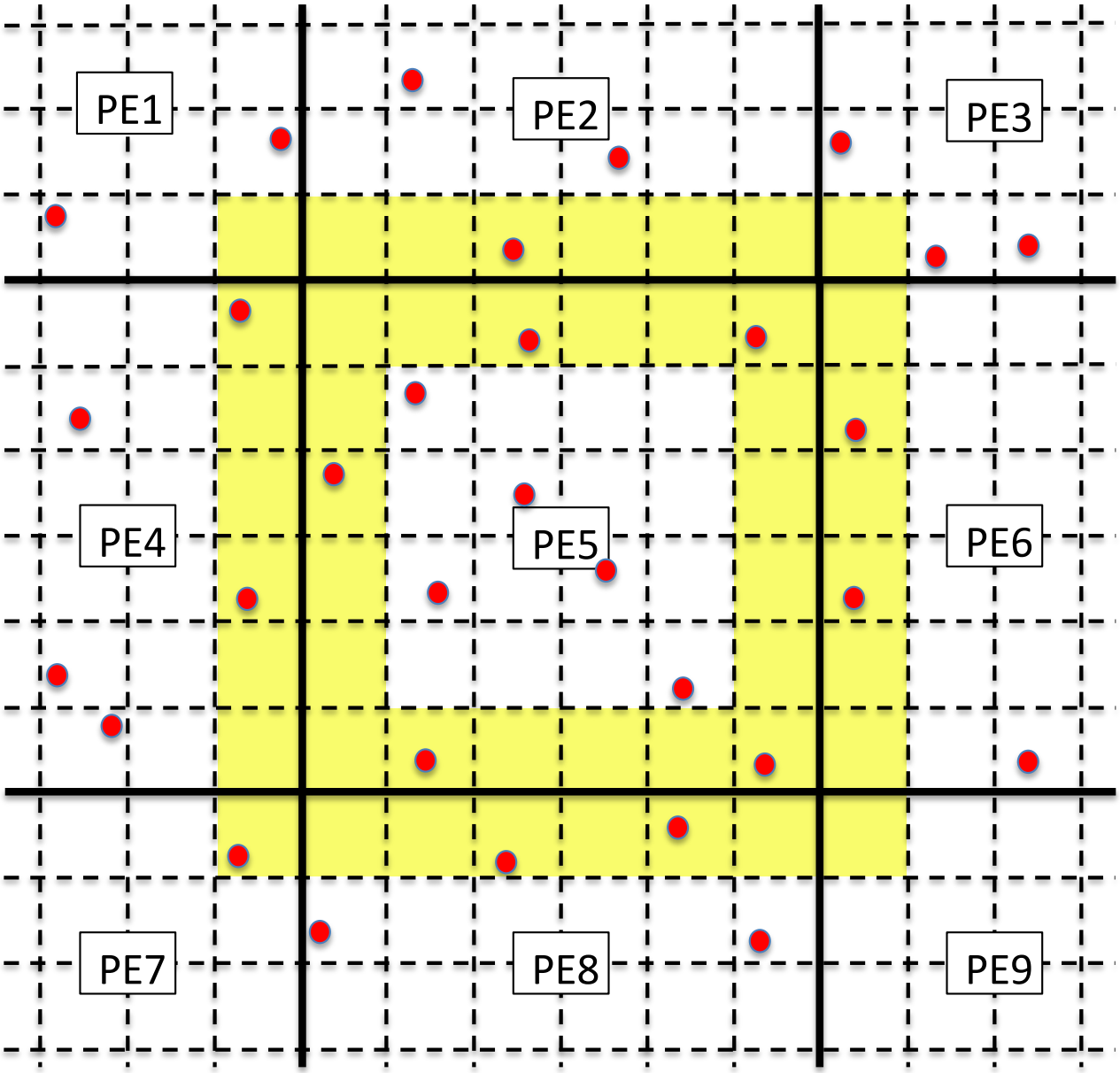
One MC move:

Repeat 1-4 multiple times:

1. Pick a random atom
2. Execute a trial move
3. Calculate energy change, ΔE.
4. Accept with probability $p=\exp(-\Delta E/kT)$

Sequential execution: the acceptance of each move depends on the previous ones.

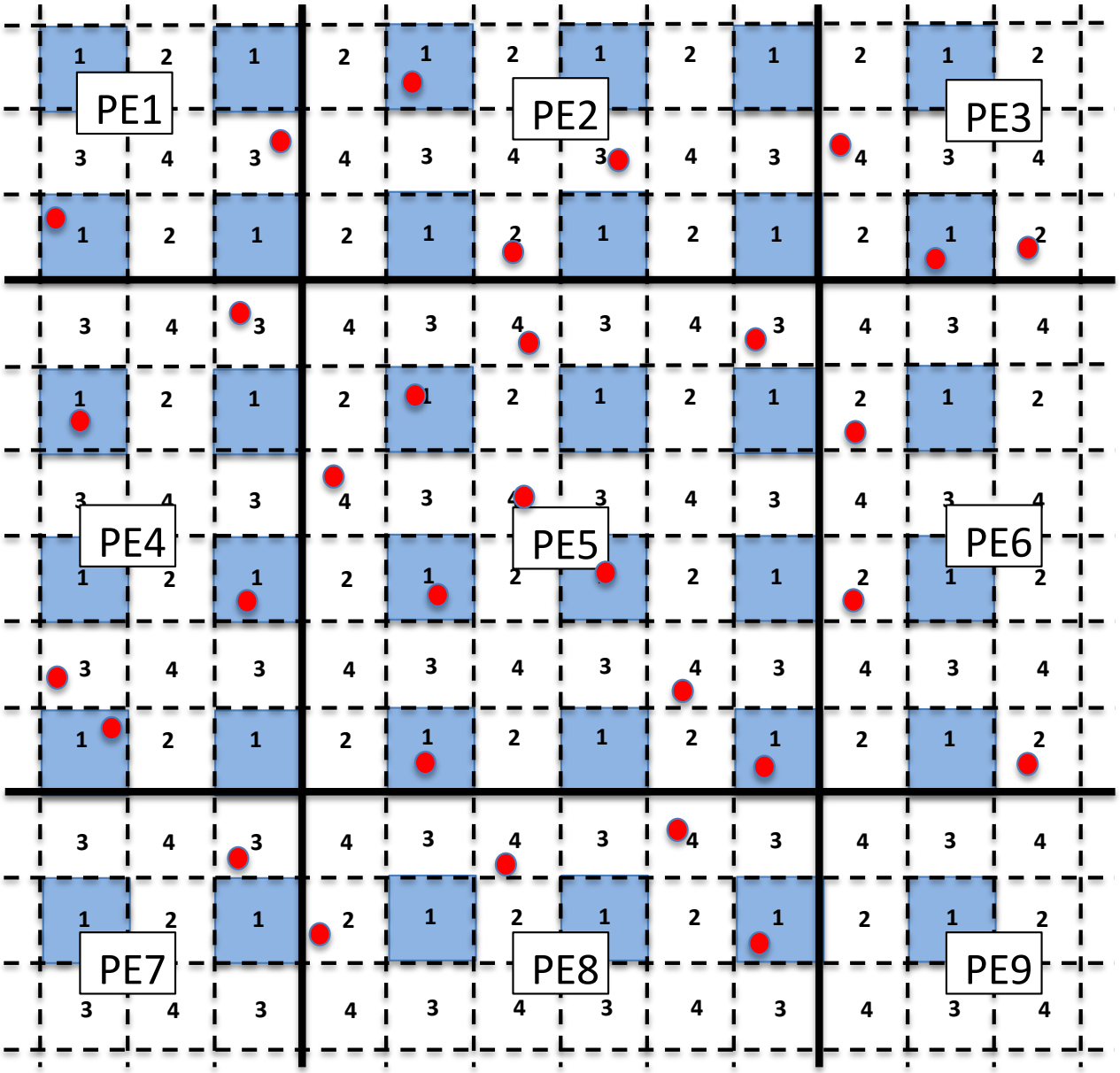
Parallel Monte-Carlo Algorithm



- Apply spatial decomposition with link-cell technique
- Multiple atoms are selected in random

Then… how to deal with the sequential moves?

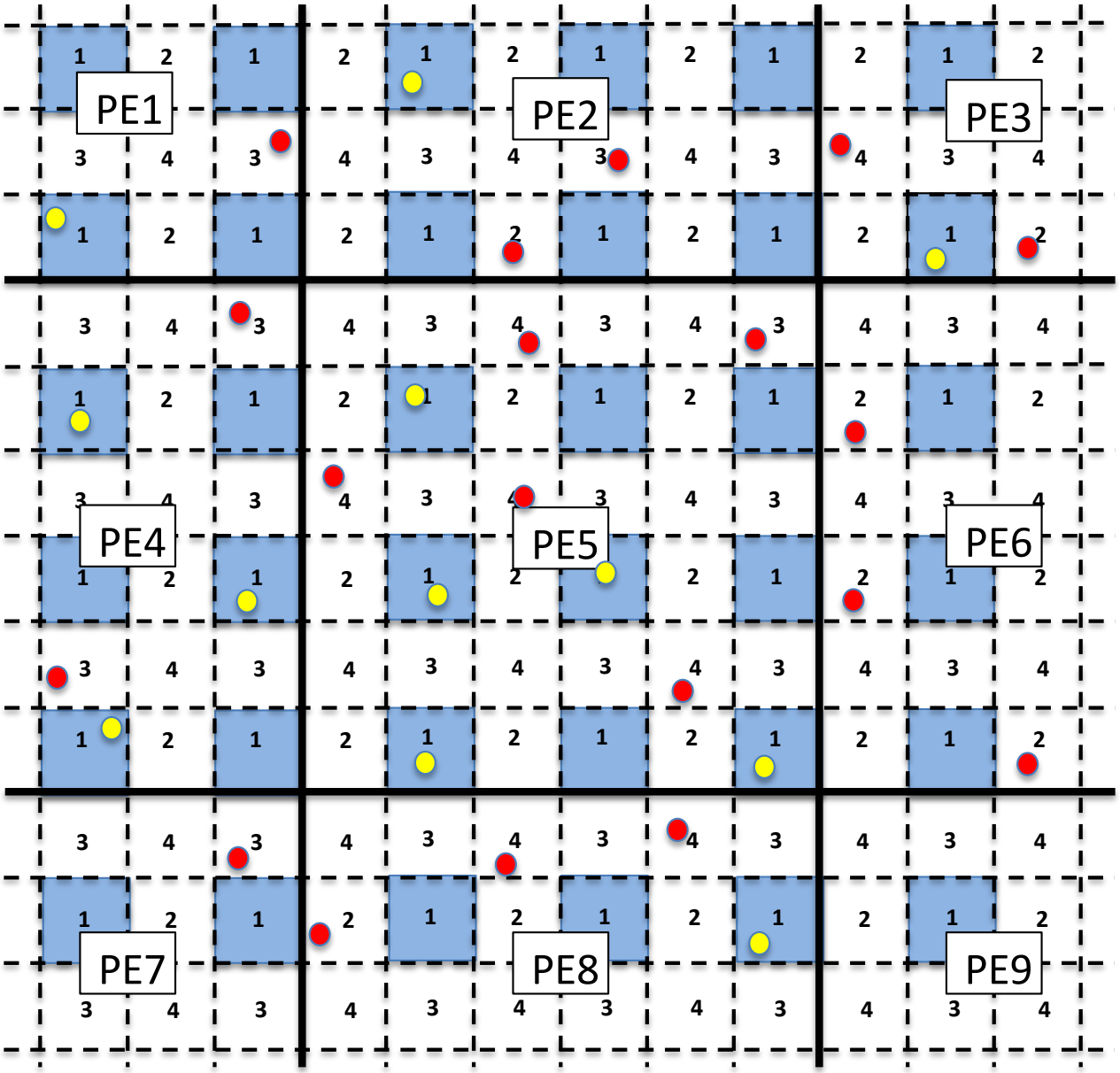
Parallel Monte-Carlo Algorithm



- Apply spatial decomposition with link-cell technique
- Multiple atoms are selected in random
- Group link-cells into sets of four in a checker board manner.

S. Plimpton et al., SANDIA report: SAND2009-6226, October (2009)

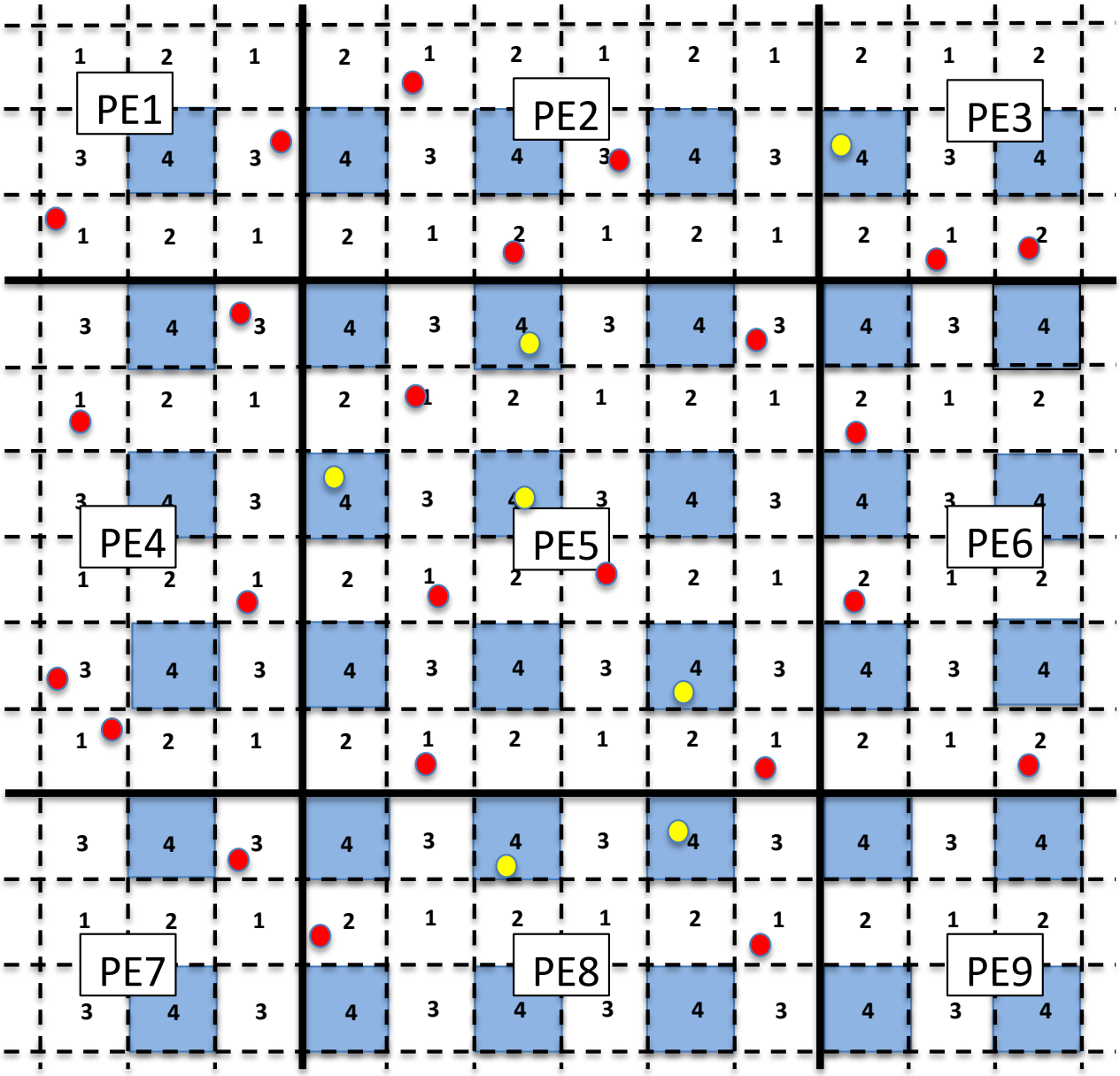
Parallel Monte-Carlo Algorithm



- Apply spatial decomposition with link-cell technique
- Multiple atoms are selected in random
- Group link-cells into sets of four in a checker board manner.
- Execute moves on atoms from the same set only.

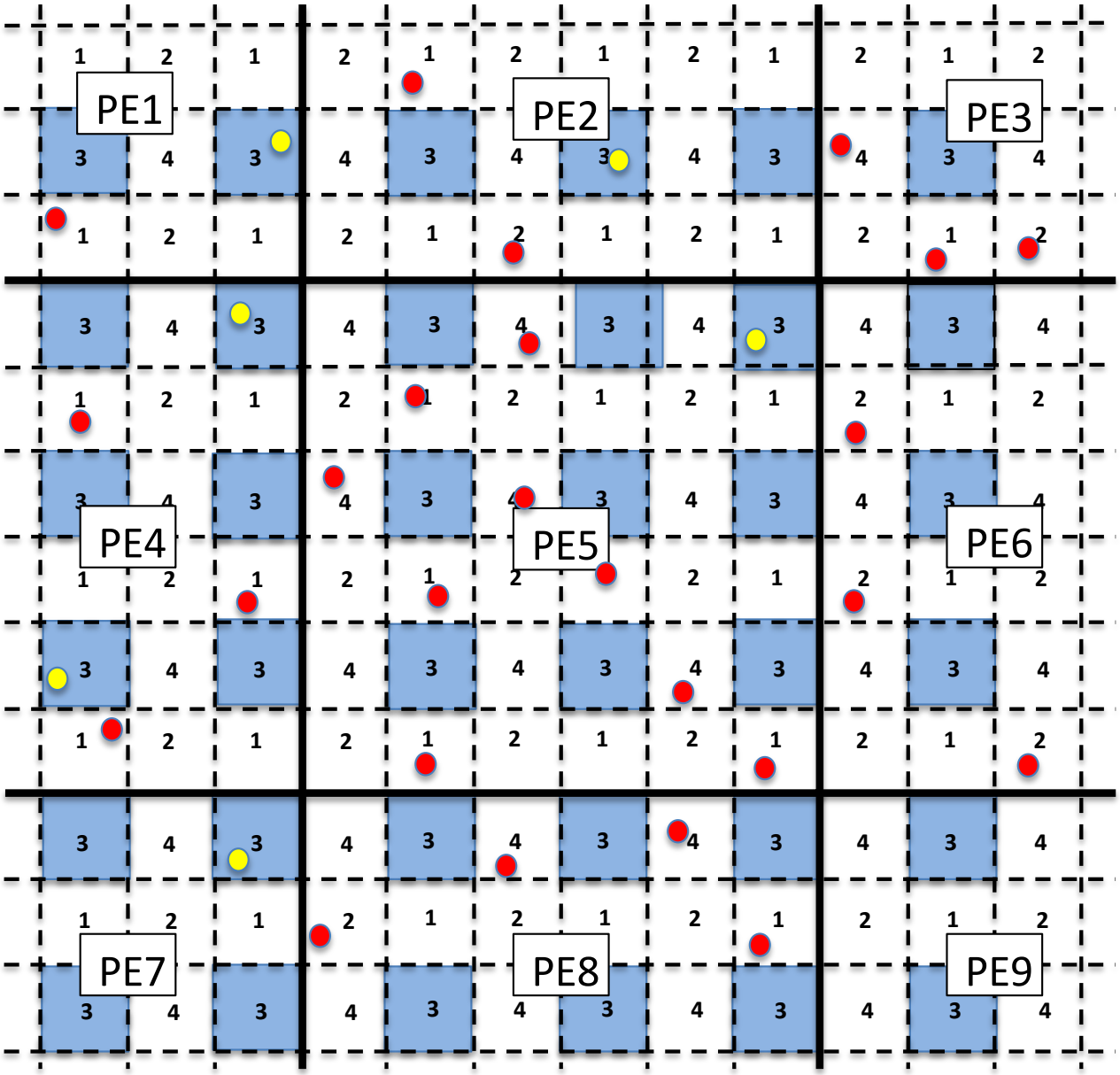
This ensures that the trial atoms are far enough from each other, so that their moves are independent and can be executed simultaneously.

Parallel Monte-Carlo Algorithm



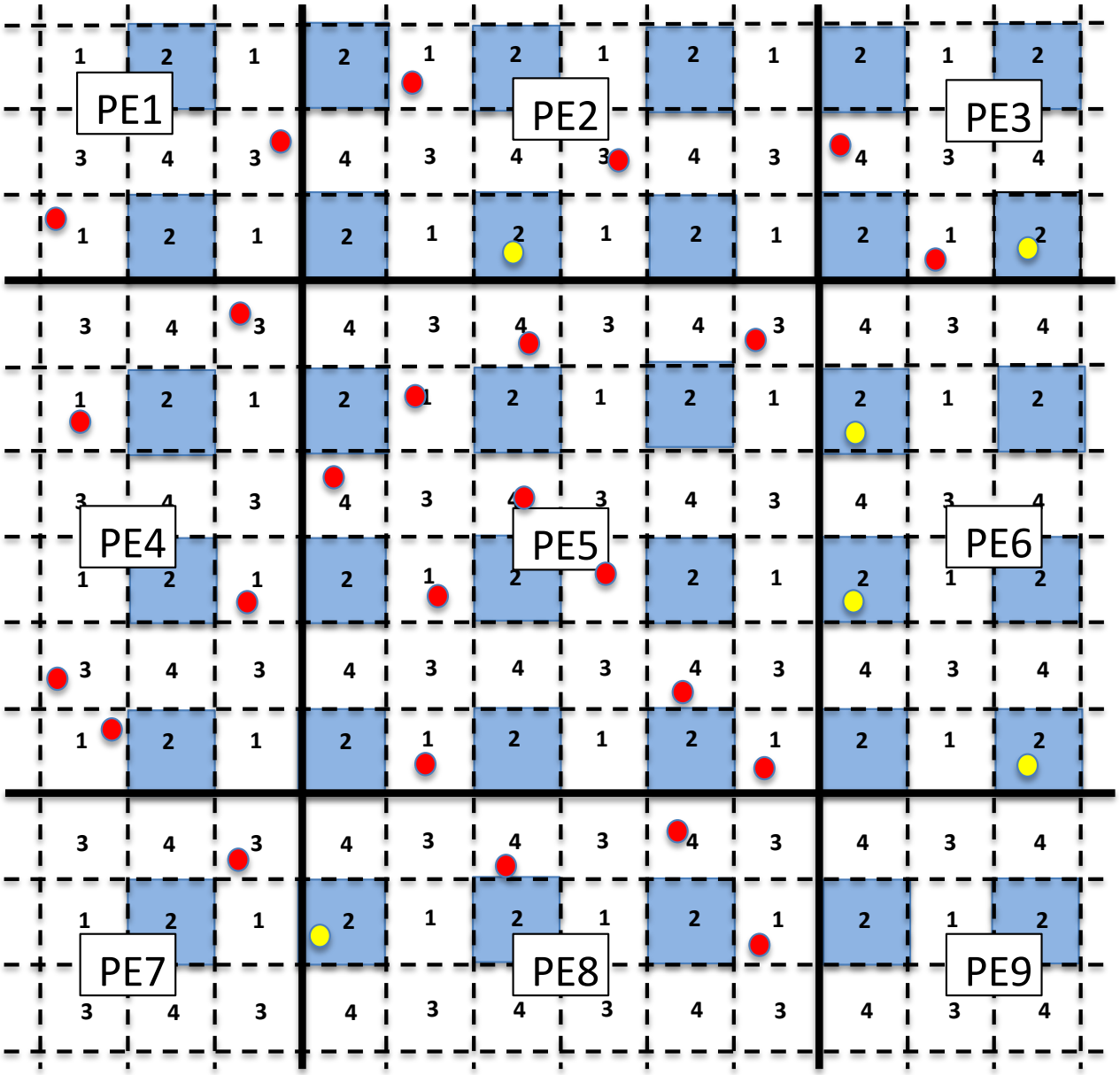
Switch between sets (1,.. 4) in a random fashion, until all chosen atoms are tried.

Parallel Monte-Carlo Algorithm



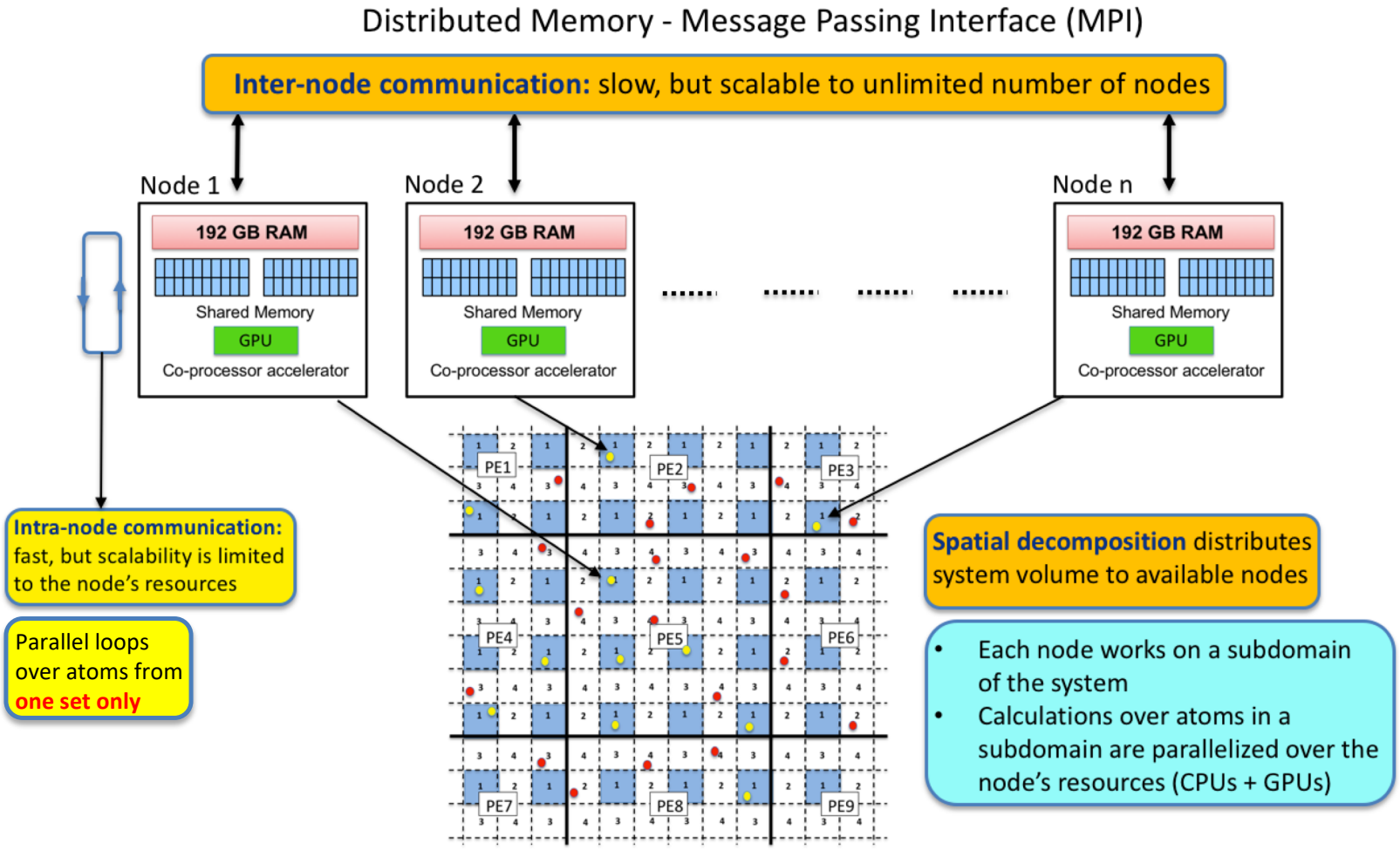
Switch between sets (1,.. 4) in a random fashion, until all chosen atoms are tried.

Parallel Monte-Carlo Algorithm



Switch between sets (1,.. 4) in a random fashion, until all chosen atoms are tried.

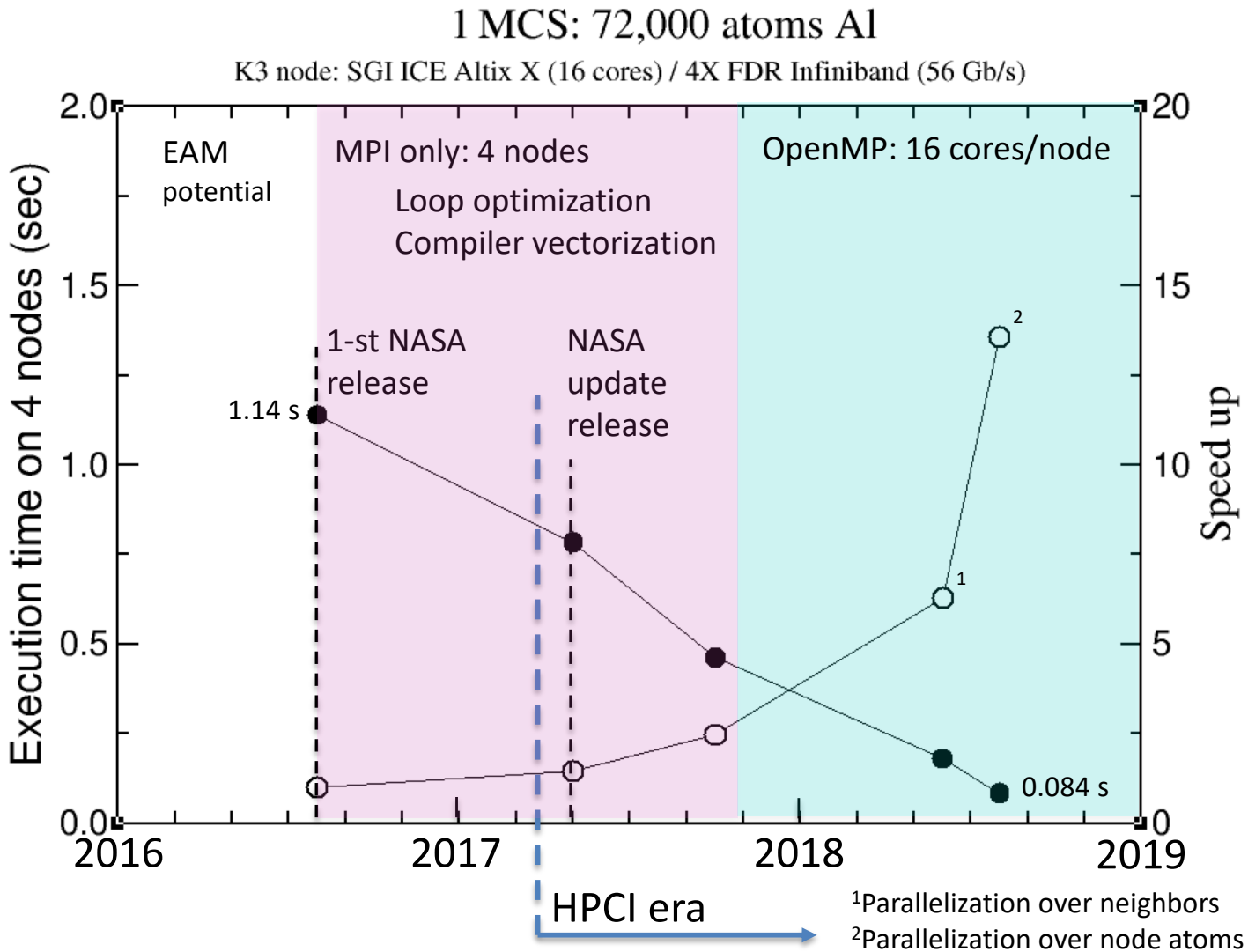
Parallelization Strategy in MC
(Similar to MD, but less efficient)



Parallelization in MC:

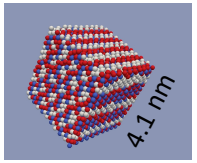
- Benefits from the spatial decomposition and the link-cell technique.
- Less efficient than MD with respect to multithread intra-node parallelization.

Development of ParaGrandMC Code



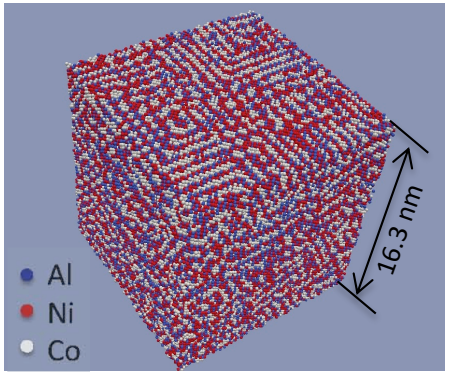
Serial MC

NiCoAl alloy system

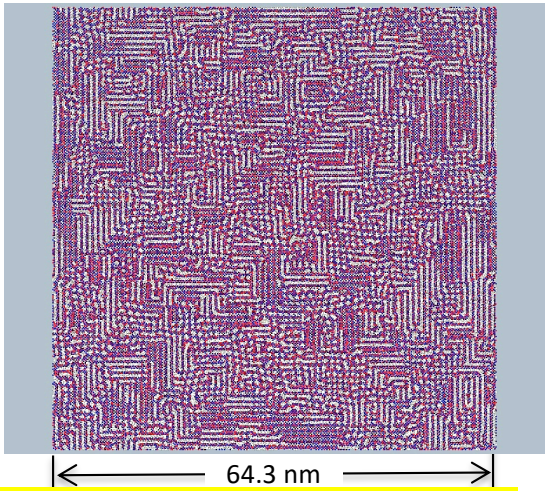


6,000 atoms

ParaGrandMC



384,000 atoms

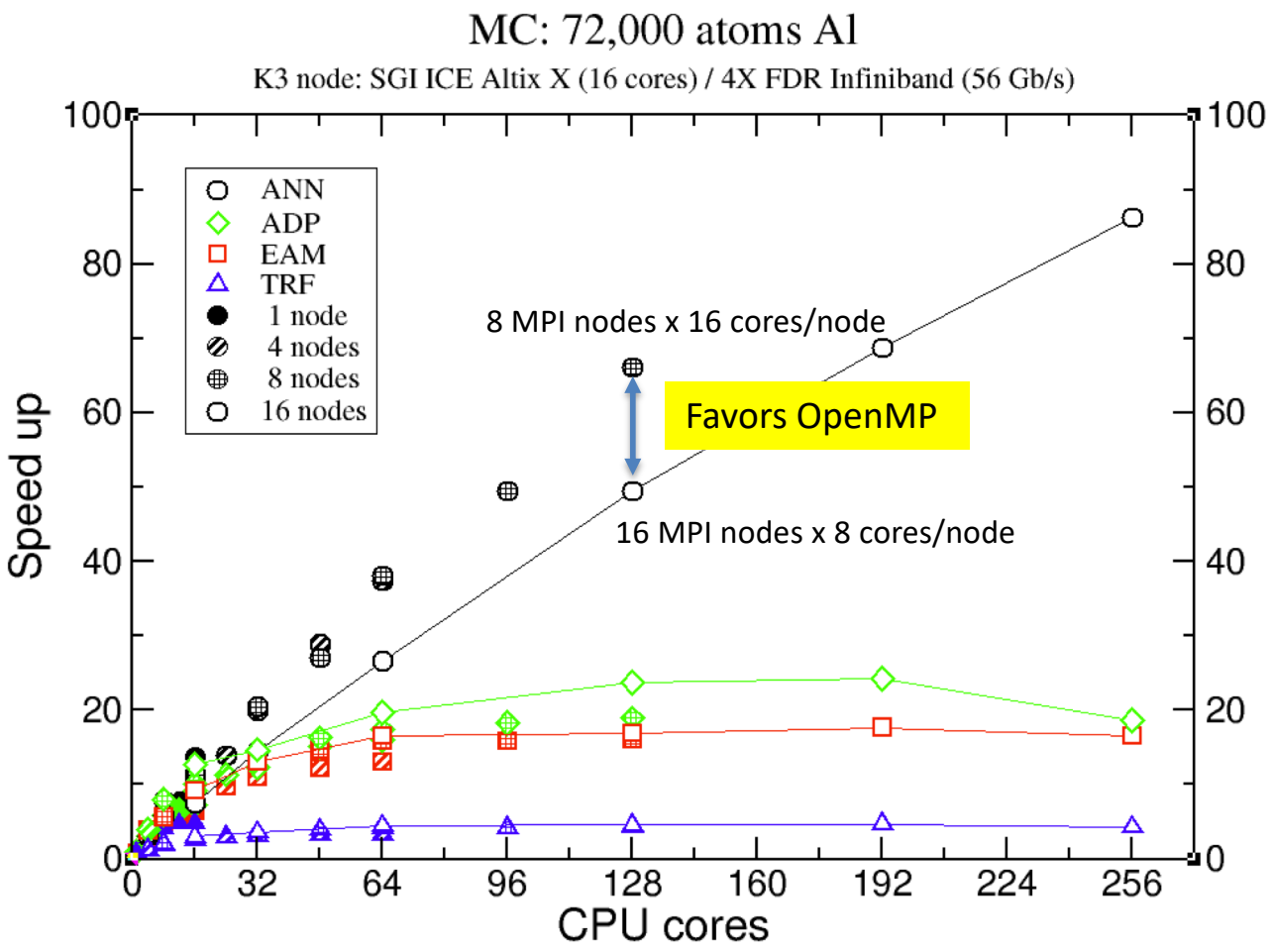


The code is in active development process – MPI+OpenMP+… (CUDA in the near future).

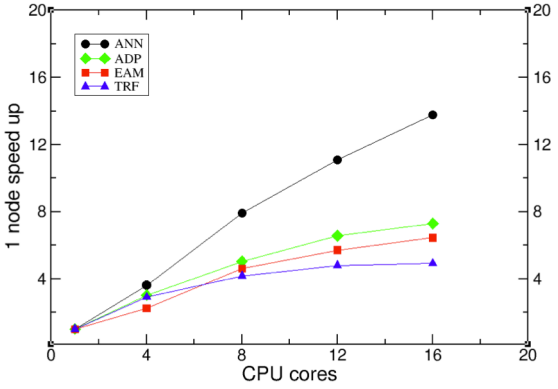
Speed Up Tests

Scalability comparison for different potential types

Distributed (MPI) + shared memory (OpenMP) parallelization on 16 MPI nodes with 1-16 cores/node



Scalability on a single node



ANN – Artificial Neural Network
Machine Learning potential

TRF – Tersoff Potential
3-body potential (molecular crystals)

ADP – Angular Dependent Potential
many-body anisotropic potential (rare earth metals)

EAM – Embedded Atom Method
many-body isotropic potential (metal alloys)

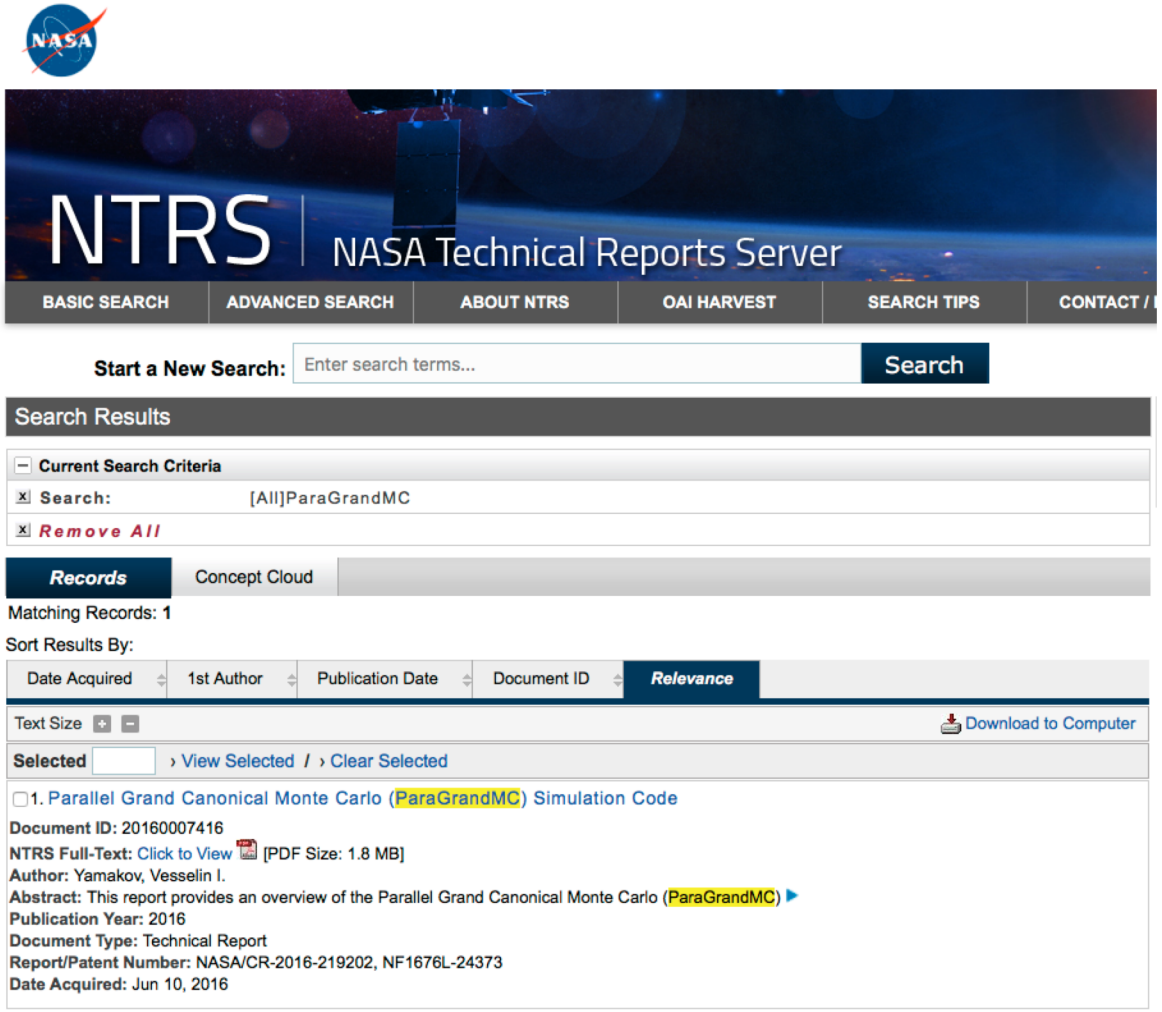
Speed up is limited for the functional potentials, but it is substantial for the ANN potential.

ParaGrandMC Tutorial

ParaGrandMC Tutorial: NASA/CR–2016-219202

http://www.sti.nasa.gov

Type “ParaGrandMC” in the search field.



Simulation Regimes and Ensembles

Algorithm: Generate a random trial move and accept with a probability, P:

$$P = \begin{cases} 1 & , \Delta\Phi \leq 0 \\ exp(-\Delta\Phi / k_B T), & \Delta\Phi > 0 \end{cases}$$

$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

Ensembles:

1. Canonical Monte Carlo:
   - constant volume (NVT): $V = const$

$N = const$

N- total number of particles

Displacement moves:

$\Delta\Phi = \Delta E$

Simulation Regimes and Ensembles

Algorithm: Generate a random trial move and accept with a probability, P:

$$P = \begin{cases} 1 & ,\Delta\Phi \leq 0 \\ exp(-\Delta\Phi/k_B T), & \Delta\Phi > 0 \end{cases}$$

$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

Ensembles:

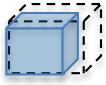
1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT): $P = const$

N- total number of particles

$$\Delta\Phi = \Delta E - Nk_B T ln(V'/V)$$

Displacement moves:

+ volume change (strain):



Simulation Regimes and Ensembles

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$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

Ensembles:

1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT):
2. Semi-Grand Canonical MC: $\mu_\alpha = const$:
   - constant volume (μVT):

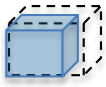
N- total number of particles

$$\Delta\Phi = \Delta E + \Delta\mu_{\alpha\beta} + \frac{3}{2}k_B T ln(m_\alpha/m_\beta)$$

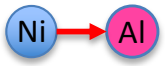
$$\sum_\alpha N_\alpha(\mu_\alpha) = const = N \qquad \Delta\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$$

Displacement moves:

+ volume change (strain):



+ element change:



Simulation Regimes and Ensembles

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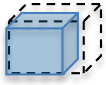
$T = const$ - temperature

Ensembles:

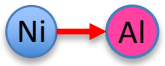
1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT):
2. Semi-Grand Canonical MC: $\mu_\alpha = const$:
   - constant volume (μVT): $P = const$
   - constant pressure (stress) (μPT):

Displacement moves:

+ volume change (strain):



+ element change:



N- total number of particles

$$\Delta\Phi = \Delta E + \Delta\mu_{\alpha\beta} + \frac{3}{2}k_B T ln(m_\alpha/m_\beta) - N k_B T ln(V'/V)$$

$$\sum_\alpha N_\alpha(\mu_\alpha) = const = N \qquad \Delta\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$$

Simulation Regimes and Ensembles

Algorithm: Generate a random trial move and accept with a probability, *P*:

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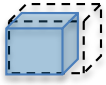
$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

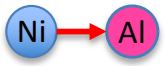
Ensembles:

Displacement moves:

+ volume change (strain):



+ element change:



1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT):
2. Semi-Grand Canonical MC: $\mu_\alpha = const$:
   - constant volume (μVT): $P = const$
   - constant pressure (stress) (μPT):
   - Feedback SGMC (cVT or cPT):

N- total number of particles

$$\Delta\Phi = \Delta E + \Delta\mu_{\alpha\beta} + \frac{3}{2}k_B T ln(m_\alpha/m_\beta) - N k_B T ln(V'/V)$$

$$\sum_\alpha N_\alpha(\mu_\alpha) = const = N \qquad \Delta\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$$

Concentration of element α, $c_\alpha \to c_\alpha^0 = const$

$$\mu_\alpha^{(n)} = \begin{cases} \mu_\alpha^{(n-1)} - a_\alpha \left(\frac{c_\alpha^{(n-1)} + c_\alpha^{(n-2)}}{2} - c_\alpha^0 \right), & for\ n \ge 2 \\ \mu_\alpha^{(0)}, & for\ n < 2 \end{cases}$$

Simulation Regimes and Ensembles

Algorithm: Generate a random trial move and accept with a probability, *P*:

$$P = \begin{cases} 1 & ,\Delta\Phi \le 0 \\ exp(-\Delta\Phi/k_B T), & \Delta\Phi > 0 \end{cases}$$

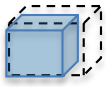
$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

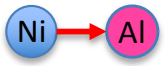
Ensembles:

Displacement moves:

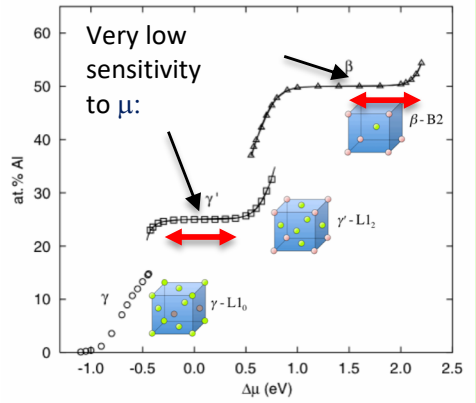
+ volume change (strain):



+ element change:



1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT):
2. Semi-Grand Canonical MC: $\mu_\alpha = const$:
   - constant volume (μVT): $P = const$
   - constant pressure (stress) (μPT):
   - Feedback SGMC (cVT or cPT):
   - Variance-constrained SGMC:



B. Sadigh et al., Phys Rev B 85 (2012) 184203-1-11.

N- total number of particles

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$$\mu_\alpha^{(n)} = \begin{cases} \mu_\alpha^{(n-1)} - 2b_\alpha \frac{c_\alpha^{(n-1)} - c_\alpha^{(n-2)}}{2}, & for\ n \ge 2 \\ \mu_\alpha^{(0)}, & for\ n < 2 \end{cases}$$

Simulation Regimes and Ensembles

Algorithm: Generate a random trial move and accept with a probability, *P*:

$$P = \begin{cases} 1 & ,\Delta\Phi \le 0 \\ exp(-\Delta\Phi/k_B T), & \Delta\Phi > 0 \end{cases}$$

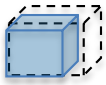
$\Delta\Phi$ - thermodynamic potential

$T = const$ - temperature

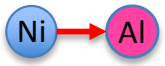
Ensembles:

Displacement moves:

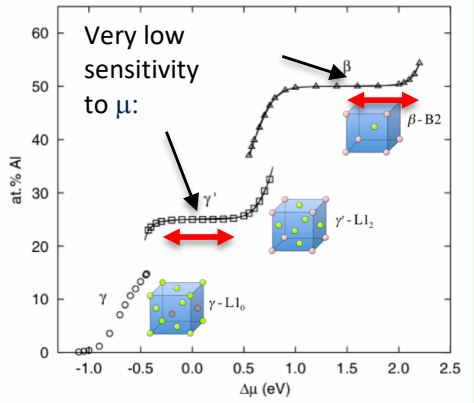
+ volume change (strain):



+ element change:



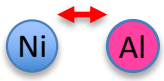
1. Canonical Monte Carlo: $N = const$
   - constant volume (NVT): $V = const$
   - constant pressure (stress) (NPT):
2. Semi-Grand Canonical MC: $\mu_\alpha = const$:
   - constant volume (μVT): $P = const$
   - constant pressure (stress) (μPT):
   - Feedback SGMC (cVT or cPT):



- Variance-constrained SGMC:

B. Sadigh et al., Phys Rev B 85 (2012) 184203-1-11.

3. Canonical MC with swap moves



N- total number of particles

$$\Delta\Phi = \Delta E + \Delta\mu_{\alpha\beta} + \frac{3}{2}k_B T ln(m_\alpha/m_\beta) - N k_B T ln(V'/V)$$

$$\sum_\alpha N_\alpha(\mu_\alpha) = const = N \qquad \Delta\mu_{\alpha\beta} = \mu_\alpha - \mu_\beta$$

Concentration of element α, $c_\alpha \to c_\alpha^0 = const$

$$\mu_\alpha^{(n)} = \begin{cases} \mu_\alpha^{(n-1)} - a_\alpha \left(\frac{c_\alpha^{(n-1)} + c_\alpha^{(n-2)}}{2} - c_\alpha^0 \right), & for\ n \ge 2 \\ \mu_\alpha^{(0)}, & for\ n < 2 \end{cases}$$

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Simulation Regimes and Ensembles

Molecular Dynamics regime to supplement MC simulations

1. Micro Canonical MD:
   - constant energy at fixed volume (NVE)

     5-th order Gear predictor-corrector integrator

2. Canonical MD:
   - constant temperature and volume (NVT)
   - constant temperature and pressure (stress) (NPT)

     Nose-Hoover thermostat + Parrinello-Rahman barostat

Allows seamless switch between MC and MD simulations

Input Files

Structure File: structure.plt, or structure.lam – LAMMPS format

Example for plt – format (used in some old codes, e.g. “sold”)

--- structure.plt ---

```
# -0.1792446164E+02 -0.1788684653E+02 -0.1782515785E+02  ! -h11/2 -h22/2 -h33/2 initial
#  0.1792446164E+02  0.1788684653E+02  0.1782515785E+02  !  h11/2  h22/2  h33/2 initial
# -0.1792446164E+02 -0.1788684653E+02 -0.1782515785E+02  ! -h11/2 -h22/2 -h33/2 current
#  0.1792446164E+02  0.1788684653E+02  0.1782515785E+02  !  h11/2  h22/2  h33/2 current
#       2    4000    4000    4000                       ! n/a  N_atoms, N_buf, N_free
#    0.67248840E+01       1       1       1             ! n/a
#      -1      -1      -1                               ! n/a
#       0       0                                       ! n/a
# -0.4430826192E+01     922.6                           ! Pot.energy/atom, T of the system
224 -0.1789335455E+02  0.1597144817E+01  0.1494689416E+01  2  2  ! id X Y Z type constraint
226 -0.1619578319E+02  0.1830532545E+01  0.3288215770E+01  1  0  ! .
230 -0.1617572658E+02  0.1722213549E+01  0.7033719156E+01  1  0  ! .
     .
3682  0.1612777159E+02 -0.8918761584E+01 -0.1782246887E+02  1  0
1                                                          ! 0: no velocities; 1: with velocities
224  0.1405660198E+01  0.0000000000E+00  0.1132724982E+01 ! id  v_x  v_y  v_z (Å/ps)
226  0.9420957345E+01 -0.2580232213E+01  0.1855807313E+01
230 -0.1426233611E+01  0.4245608319E+01  0.1019702603E+01
     .
3682 -0.1731818246E+01  0.2910471448E+01 -0.7523290612E+00
1.0 1.0                                                    ! default numbers for end of file.
```

$$x_i = h_{11}s_{xi} + h_{12}s_{yi} + h_{13}s_{zi}$$
$$y_i = h_{22}s_{yi} + h_{23}s_{zi}$$
$$z_i = h_{33}s_{zi}$$

$h_{12}, h_{13}, h_{23} = 0$ in .plt format.
Use LAMMPS (.lam) file format

Input Files

Potential File: pot.dat (Inherited from "sold")

Examples:

NiAl EAM potential from NIST repository: www.ctcms.nist.gov/potentials/

--- pot.dat ---

```
2 - number of chemical species in the system
'Ni'  58.71     ! chemical symbol and atomic mass
'Al'  26.982
0 - regular EAM alloy potential
'./NiAl-2004/pni.dat'     ! pair Ni-Ni potential
'./NiAl-2004/pnial.dat'   ! pair Ni-Al potential
'./NiAl-2004/pal.dat'     ! pair Al-Al potential
'./NiAl-2004/fni.dat'     ! Ni electron density
'./NiAl-2004/fal.dat'     ! Al electron density
'./NiAl-2004/F_ni.dat'    ! Ni embedded function
'./NiAl-2004/F_al.dat'    ! Al embedded function
```

NiAl EAM potential in LAMMPS format:

```
2 lammps - number of chemical species in the system
'Ni'  58.71     ! chemical symbol and atomic mass
'Al'  26.982
0 - regular EAM alloy potential
'./NiAl-2004/NiAl2004.eam.alloy'  ! path and file name
```

Currently supported potential formats:

0: EAM alloy potential
1: ADP – Angular Dependent Pot.
2: MEAM (in progress)
3: Tersoff – (conventional: Tersoff_1 in LAMMPS)
4: Tersoff-modified:
see T.Kumagai et al., Comp. MAt. Sci (2007) 456
5: EAM/fs – Finnis-Sinclair EAM
6: BOP – Bond Order Potential (Y. Mishin format)
100: ANN – Straight Arfitificial Neural Netwrok
106: ANN-BOP – Physically guided ANN (see James talk)
.. – more to come

Input Files

Command File: pgmc.com

A script text file with commands and parameters to control the simulation

Example:

```
--- pgmc.com ---
ini:  2 600.0 0.05 0.0005     ! Initialization with <MC_rank> <temp> <dr> <dh/h>
3                             ! Number of elements
Al                            ! First element (as defined in the pot.dat file)
Co                            ! Second element
Ni                            ! Third element
'Filename'                    ! Output filename (up to 64 symbols)
input: plt                    ! Input structure file format (plt, or lam for LAMMPS input)
output: lam                   ! Output structure file format (LAMMPS format in this case)
time: 10000                   ! Start time (MCS or MDS)
# MC specific parameters follow:  ! Comment line, not executed
comp: 0.29 0.36 0.35          ! Chemical composition (sum = 1.0)
mue:   0.0  -0.43  0.28       ! Chemical potentials for each element (one must be 0)
alpha: 0.0  0.01  0.01        ! Multiplier coefficients to each mue (ensemble types 3-6)
mc: 1 1000 10 300.0 2 3 0     ! MC run with parameters

# MD specific parameters follow:
md_step: 2.0                  ! MD time step (fs); default value 1.0
diss:  1.0                    ! Heat dissipation coefficient for the Nose-Hoover thermostat
wmass: 16.0                   ! Effective wall mass for Parrinello-Rahmann const. stress
wdamp: 25.0                   ! Effective wall damping for Parrinello-Rahmann const. stress
md: 1 1000 10 300.0 1 3 0     ! MD run with parameters

end:                          ! end of the simulation (no commands are executed after that)
```

All commands are given in Appendix A of the Users Manual

Output Files

Structure File: filename.#########.plt,
or filename. #########.lam – LAMMPS format

Format: same as the input structure file (can be used directly as an input file).
######### - 8 digits number indicating the number of MCS (or fs in MD regime)
e.g. NiAl_model.00123456.lam

Stress File (optional): filename.#########.stress

Example:

atom id, atom type, σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{xz}, σ_{yz}, E_p								
236	1	..	..	..	..	..	..	..

σ_{ij} - stress components in GPa
E_p - potential energy in eV.

Output Files

Data File: filename.########.dat

Reported data is specified by command “measure:” in the pgmc.com file

Example:

--- pgmc.com ---

```
..
'Ni85Al15_N4k'                  ! Output filename
..
measure: hii Ti                 ! Measured parameters
mc:  1  30 10  300.0  3  3  0   ! nruns nsteps rep_step T ens irig, isv
md:  1  30  10  300.0  0  1  0  ! nruns nsteps rep_step T ens irig, isv
end:
```

Output:

--- Ni85Al15_N4k.00000000.dat ---

Run step	Time(MCS/fs)	Ek	Ep	Etot	T(K)	h(1,1)	h(2,2)	h(3,3)	T(Al)	T(Ni)
0	0.00	0.02851095	−4.53168118	−4.50317023	220.57	3.5287	3.5333	3.5296	138.14	664.87
10	10.00	0.03877800	−4.54034854	−4.50157054	300.00	3.5283	3.5346	3.5302	300.00	300.00
20	20.00	0.03877800	−4.55407302	−4.51529502	300.00	3.5299	3.5344	3.5322	300.00	300.00
30	30.00	0.03877800	−4.57035424	−4.53157625	300.00	3.5310	3.5349	3.5351	300.00	300.00
10	40.00	0.04200614	−4.57356222	−4.53155608	324.97	3.5310	3.5349	3.5351	322.48	307.39
20	50.00	0.04640474	−4.57796082	−4.53155608	359.00	3.5310	3.5349	3.5351	351.25	323.41
30	60.00	0.04683165	−4.57838769	−4.53155604	362.31	3.5310	3.5349	3.5351	345.83	341.65

Suitable for plotting

Output Files

Visualization File: filename.########.imd

IMD type format used by OVITO (Open Visualization Tool) program

Visualized data is specified by command “ovito:” in the pgmc.com file

Example:

--- pgmc.com ---

..

'Al112_edge_disl' ! Output filename

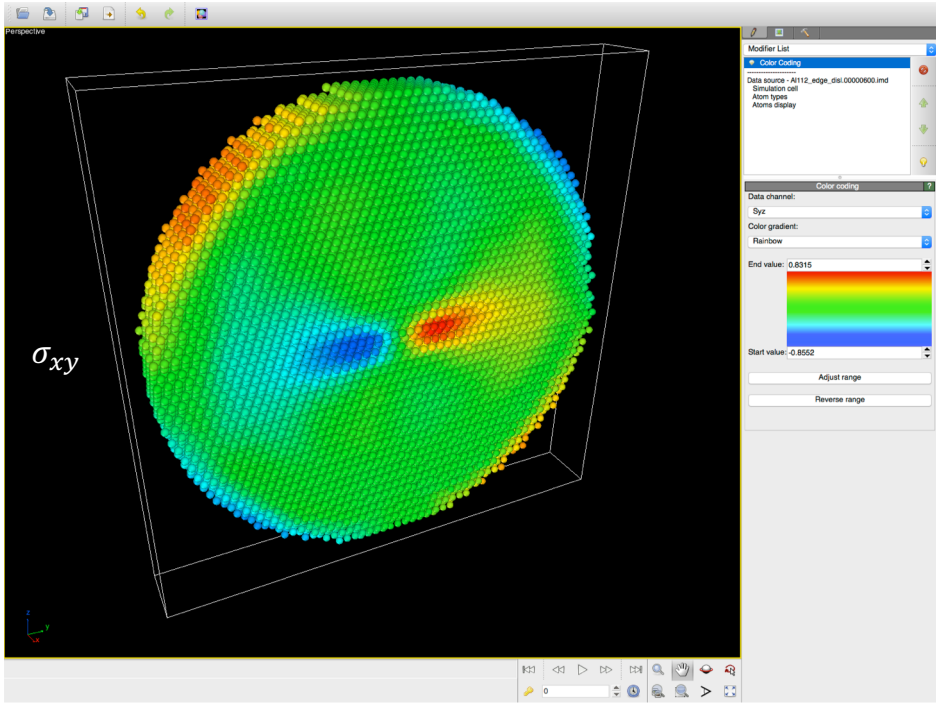
..

ovito: Ep Ek Et Q A T V Sij ! Measured parameters

mc: 1 600 10 500.0 1 1 0 ! nruns nsteps rep_step T ens irig, isv

…

end:



Output:

--- Al112_edge_disl.00000600.imd ---

```
#F A 1 1 1 3 1 1 1 1 1 1 3 6
#C id type mass x y z Ep Ek Etot Q A T Vx Vy Vz Sxx Syy Szz Sxy Sxz Syz
#X    19.51660502     0.00000000     0.00000000
#Y     0.00000000   158.84738334     0.00000000
#Z     0.00000000     0.00000000   155.29445372
#E
     10301  0   58.693     6.5989   102.9720    79.4144   -4.039140  0.064630   -3.974510  0.0000E+00   -3.974510    500.00     0.503280     0.480994    -0.142808   13.8431   13.5073   14.3725
     10302  2   58.933    16.2047   103.1280    79.4282   -4.044127  0.064630   -3.979497  0.0000E+00   -3.979497    500.00    -0.498082     0.153606     0.339893   13.8193   13.5865   14.4717
     10307  2   58.933    11.5452   103.9185    79.6769   -4.066903  0.064630   -4.002273  0.0000E+00   -4.002273    500.00     0.447890    -0.505020    -0.158023   13.8955   14.0961   14.4413
     10308  0   58.693     1.2080   103.8326    79.8288   -4.019377  0.064630   -3.954747  0.0000E+00   -3.954747    500.00    -0.564205     0.416927    -0.615488   13.8055   13.0264   14.2115
…
```

Conclusions

What is beneficial in PGMC?

- **Massively parallel MC/MD code for large systems (~ 10^6-10^7 atoms)**
- **Implements regimes not always found in other MC codes**

  (Semi-Grand Canonical with Feed-Back or Variation Constrained algorithms)
- **Supports ANN and Physically Inspired NN potentials – the newest generation of machine learning potentials**
- **Under active development to utilize the most advanced HPC hardware**
- **It is free upon request (subject to NASA requirements)**

  https://software.nasa.gov/search/software/ParagrandMC