Split Molecular Dynamics

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***Goal*: Learn MPI communicator concept using *in situ* data analysis of molecular dynamics simulation**

MPI_Comm_split()

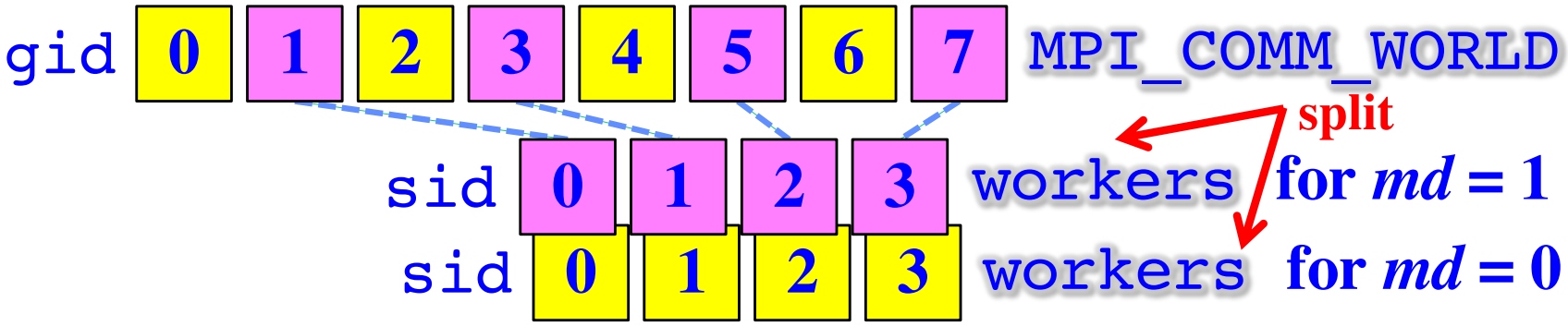
```
MPI_Comm mothercomm, daughtercomm;
int color, key;
MPI_Comm_split(mothercomm, color, key, &daughtercomm);
```

- **`MPI_Comm_split()` subdivides a communicator, `mothercomm`, into a set of daughter communicators, where processes of the same `color` belong to the same daughter communicator. Processes within each `color` are ranked according to `key`, or if `key` is the same, according to the rank in `mothercomm`. It returns a pointer to a daughter communicator, `daughtercomm`, to which the process belongs.**
- **`MPI_Comm_split()` is a simpler, higher-level function to construct communicators, instead of using `MPI_Comm_create()` combined with `MPI_Group_excl()` or `MPI_Group_incl()`.**

MD & Analysis Communicators

- **Split MPI_COMM_WORLD into two communicators; one performs molecular dynamics (MD) simulation, whereas the other analyzes simulation data on the fly in background.**

```
int gid,sid,md;
MPI_Comm workers;
MPI_Comm_rank(MPI_COMM_WORLD,&gid);  //Global rank
md = gid%2;  // = 1 (MD workers) or 0 (analysis workers)
MPI_Comm_split(MPI_COMM_WORLD,md,0,&workers);
MPI_Comm_rank(workers,&sid);  // Rank in workers
```



Run as mpirun –n 2× *nproc*

# of processes needed for MD (specified in pmd.h)

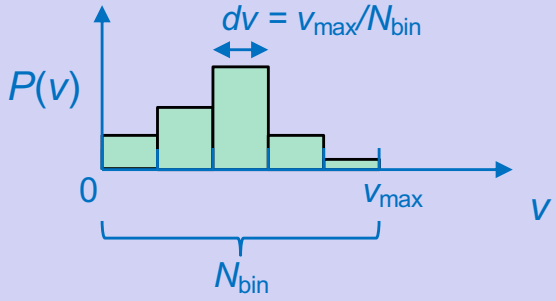
Analysis: Velocity Probability Density

P(*v*): Probability density function of atom velocity *v*

```
#define VMAX 5.0   // Maximum velocity value to construct a velocity histogram
#define NBIN 100   // # of bins in the histogram

void calc_pv() {
  double lpv[NBIN],pv[NBIN],dv,v;
  int i;

  dv = VMAX/NBIN;   // Bin size
  for (i=0; i<NBIN; i++) lpv[i] = 0.0; // Reset local histogram
  for (i=0; i<n; i++) {
    v = sqrt(pow(rv[i][0],2)+pow(rv[i][1],2)+pow(rv[i][2],2));
    lpv[v/dv < NBIN ? (int)(v/dv) : NBIN-1] += 1.0; // Increment histogram
  }
  MPI_Allreduce(lpv,pv,NBIN,MPI_DOUBLE,MPI_SUM,workers);
  MPI_Allreduce(&n,&nglob,1,MPI_INT,MPI_SUM,workers);
  for (i=0; i<NBIN; i++) pv[i] /= (dv*nglob); // Normalization
  if (sid == 0) {
    for (i=0; i<NBIN; i++) fprintf(fpv,"%le %le\n",i*dv,pv[i]);
    fprintf(fpv,"\n");
  }
}
```



$$v = |\vec{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}$$

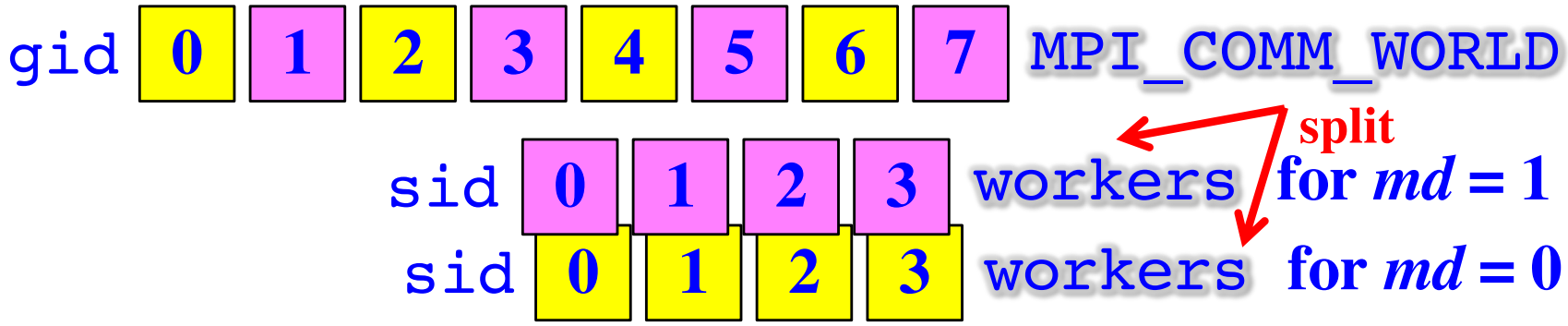
$$\int dv\, p(v) \cong dv \sum_{i=0}^{N_{\mathrm{bin}}-1} p(v_i) = 1$$

Main Program: Initialization

```
init_params();
if (md) {
  set_topology();
  init_conf();
  atom_copy();
  compute_accel();
}
else
  if (sid == 0) fpv = fopen("pv.dat","w");
```

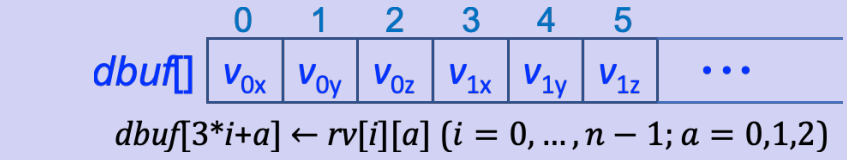
Define `FILE *fpv;`

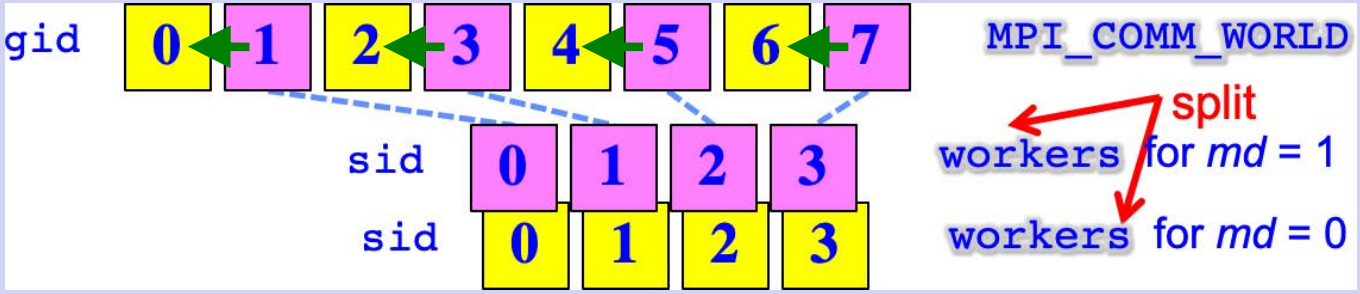
- **All processes read input parameters, `init_params()`. The `nproc` processes of MD workers (`md == 1`) perform MD initialization tasks, whereas only rank 0 among the other `nproc` analysis workers (`md == 0`) opens a file to output the calculated velocity probability density function.**



Main Program: Main MD Loop

```
for (stepCount=1; stepCount<=StepLimit; stepCount++) {
  if (md) single_step();
  if (stepCount%StepAvg == 0) {
    if (md) {
      Send # of atoms, n, to rank gid-1 in MPI_COMM_WORLD
      Send velocities of n atoms to rank gid-1 in MPI_COMM_WORLD
      eval_props();
    }
    else {
      Receive # of atoms, n, from rank gid+1 in MPI_COMM_WORLD
      Receive velocities of n atoms from rank gid+1 in MPI_COMM_WORLD
      calc_pv();
    }
  }
}
```





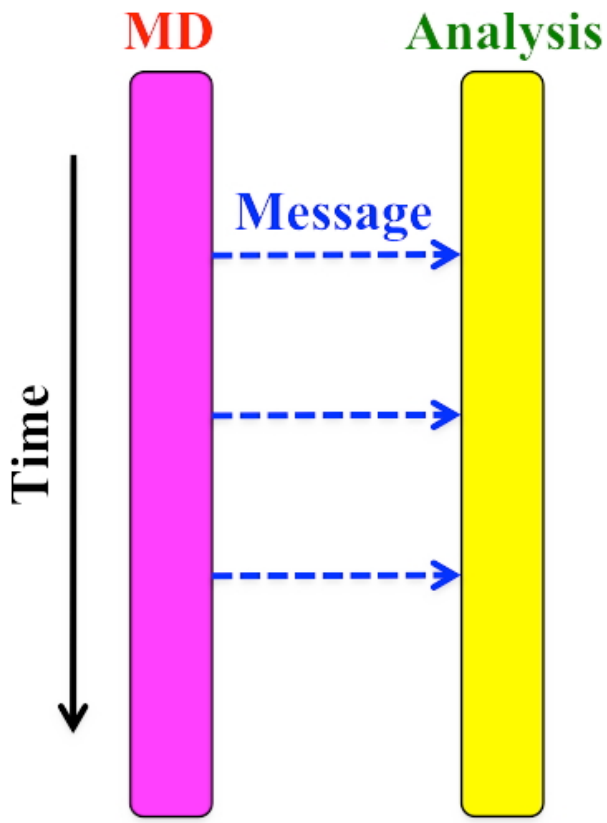
- **MD workers perform MD simulation. Every `stepAvg` steps, MD workers send their atom velocities to corresponding analysis workers (*i.e.*, those with the same ranks in respective daughter communicators). Upon receiving the velocities, analysis workers calculate the velocity probability density function.**

Main Program: Finalization

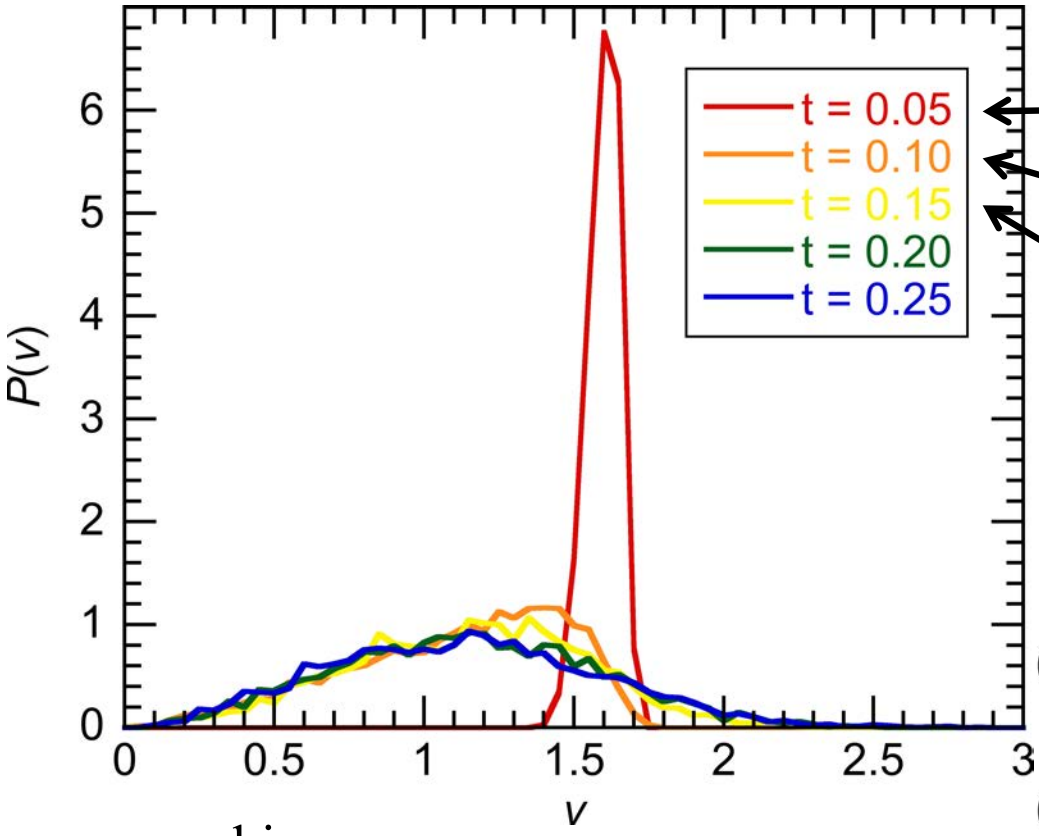
```
if (md && sid == 0)
  printf("CPU & COMT = %le %le\n",cpu,comt);
if (!md && sid == 0)
  fclose(fpv);
```

- **Rank 0 of MD workers reports the computing & communication times, whereas rank 0 of analysis workers closes the probability density output file.**

- **Finally: Change all MPI_COMM_WORLD's in the original MD functions to workers ~ it's only a matter in the small MD world!**



Results



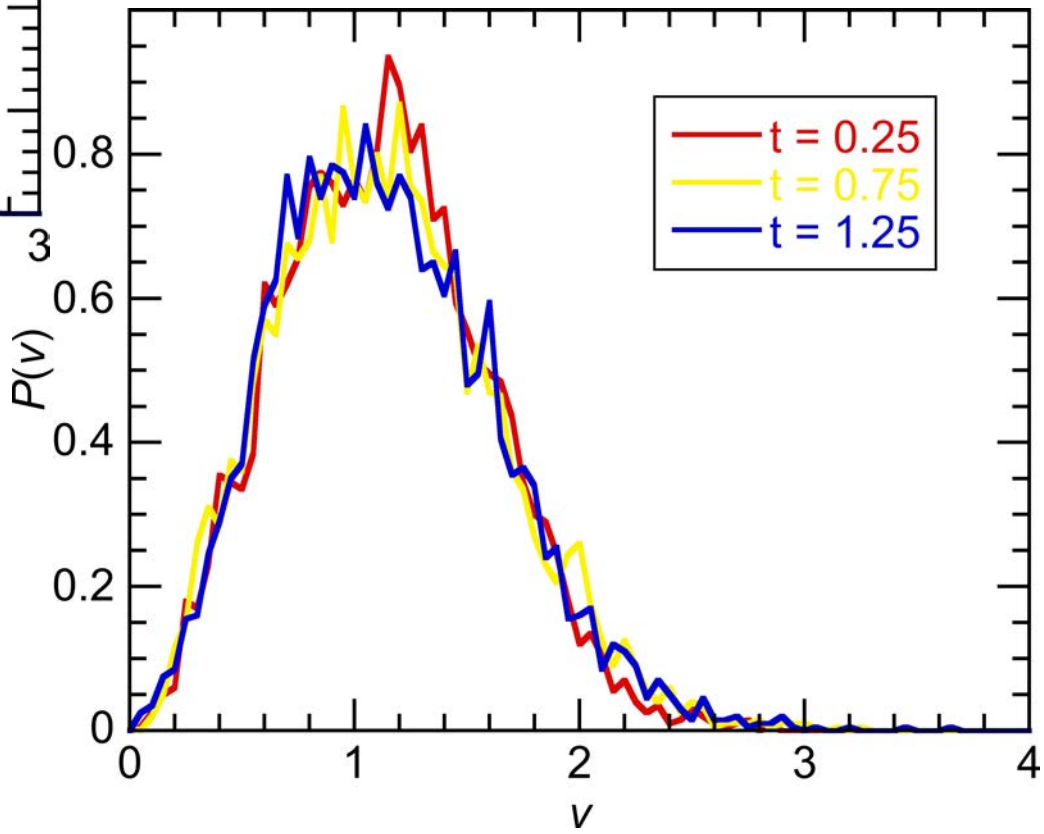
step 10

step 20

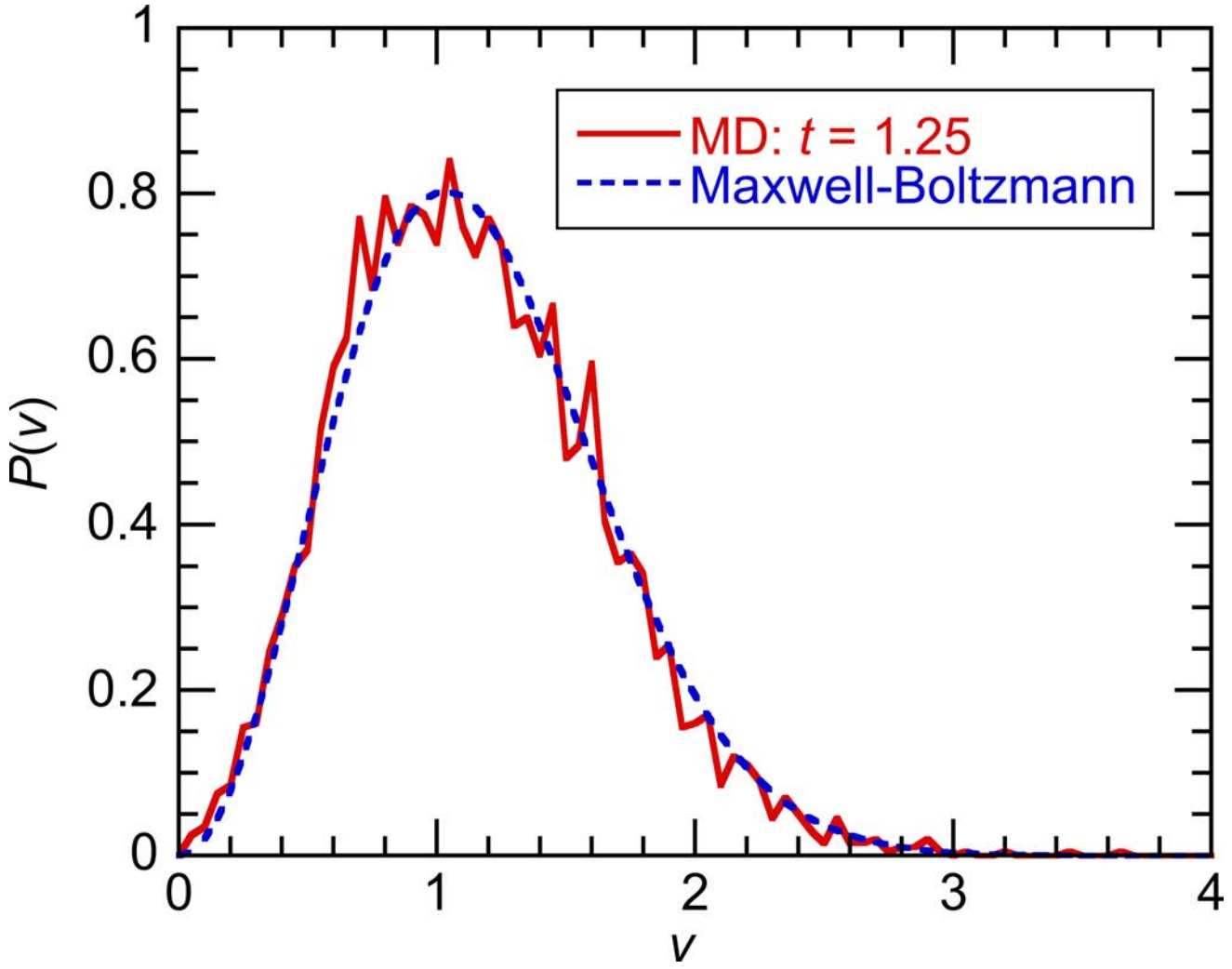
step 30

pmd.in

```
5 5 5 // InitUcell[0|1|2]
0.8   // Density
1.0   // InitTemp
0.005 // DeltaT
30    // StepLimit
10    // StepAvg
```



Maxwell-Boltzmann Distribution

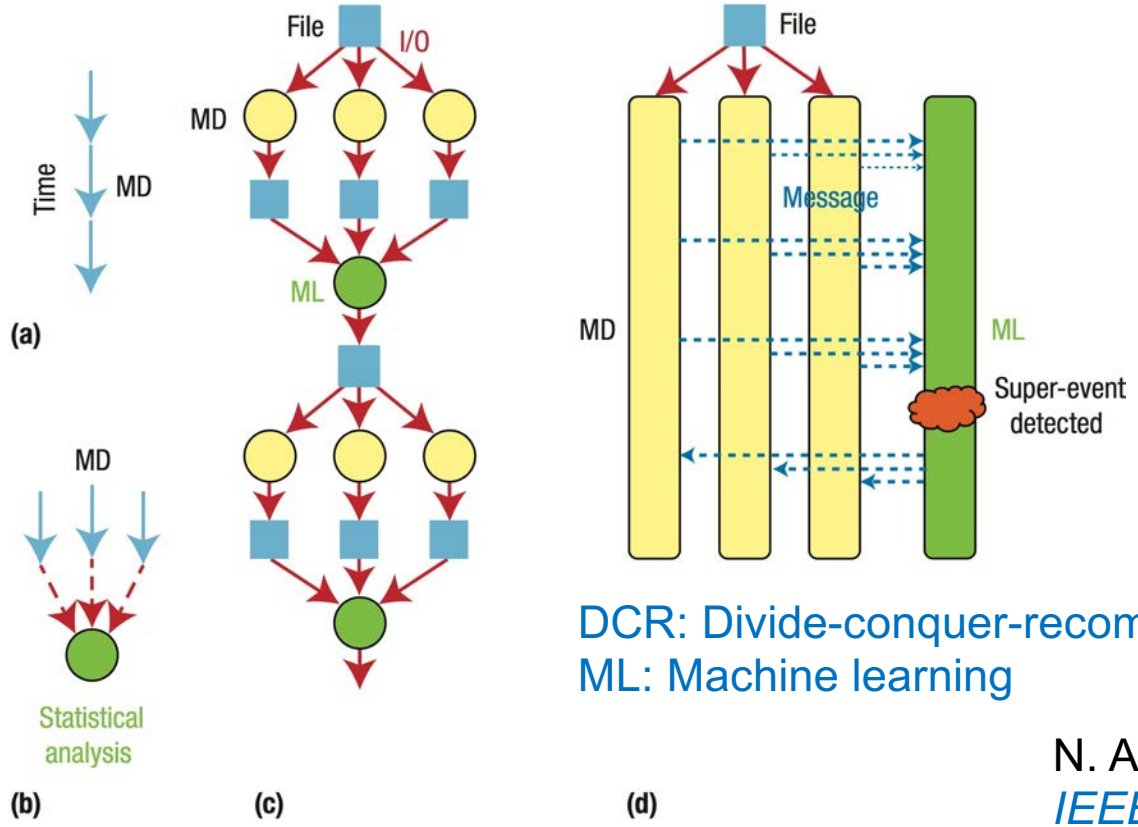


$$P_{\text{Maxwell–Boltzmann}}(v) = \frac{4}{\sqrt{\pi}}\left(\frac{m}{2k_{\text{B}}T}\right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2k_{\text{B}}T}\right)$$

K. Shimamura *et al.*, *Appl. Phys. Lett.* **107**, 231903 ('15)

In Situ Data Analysis

Use communicators to add data analytics & extra logic to parallel simulations



DCR: Divide-conquer-recombine
ML: Machine learning

N. A. Romero *et al.*,
IEEE Computer **48(11)**, 33 ('15)

FIGURE 2. DCR in time. (a) Molecular dynamics (MD) simulations have sequential time dependence. (b) Parallel replica dynamics (PRD) predicts long-time behavior through statistical analysis of multiple parallel MD trajectories. (c) Conventional file-based and (d) new in situ PRD simulations. ML represents machine-learning tasks.

See also T. Do *et al.*, A lightweight method for evaluating *in situ* workflow efficiency, *J. Comput. Sci.* **4**8, 101259 ('21)