# TutR1.2 bimolecular polardistribute

April 30, 2024

# 1 Tutorial: RDME- Bimolecular Reaction Polar Distribution

The purpose of this tutorial is to get users familiar with the lm.jLM functions and show the diffusion phenomenon by comparing the results with the first tutorial TutR1.1\_bimolecular\_uni.

For comparison, all the parameter are the same, except how we place the particle A and B.

ps: For all the functions used here, you can check the jLM api docs for details.

#### 1.1 0.Environment Check

if you didn't install the environments in docker or any container, we suggest you do it through anaconda/miniconda.

basically, you need to install the dependencies

```
conda env create -f rdme_env.yml
```

Then import jLM package.

```
[1]: import jLM  # Set up the Jupyter environment from jLM.RDME import Sim as RDMESim  # Main simulation class from jLM.RegionBuilder import RegionBuilder # Deal with the spatial geometry from lm import IntMpdRdmeSolver  # lm::rdme::IntMpdRdmeSolver import numpy as np
```

<IPython.core.display.HTML object>

#### 2 1. Initialization

#### 2.1 1.1 RDME simulation object creation

First step is to create a object that contains all the essential information to start a simulation.

The class we use here is:

```
regionName,
dt=None)
```

- simulation\_name is what we call our system;
- filename: the name of the final output trajectory file.(hdf5 format)
- dimensions: the number of lattices in x,y,z dimension. in list [dimx,dimy,dimz], must be divisible by 32.
- latticeSpacing: the actual physical representation of the length of each subvolume cube, unit: meter.
- the Name of the entire sim region, default="external"
- dt: time steps for the RDME simulation, unit: second.

```
[2]: cellvol = 1.0e-15  # L=dm^3
simname = "Bimolecular_System_polar"
filename = "TutR1.2_bimolecular_polardis.lm"
Ldim = [64,64,64]  # Has to be multiples of 32
lattice_spacing = 32e-9  # in m
regionN = "extracellular"
dt = 25e-6  # in s
```

in case you forget, or want to redefine some key parameters in the simulation we define above, you can always call methods to adjust them.

for example, we can change the simulation time step by:

```
[4]: sim.timestep = 50e-6 # in s
```

next we need to define the total simulation time, the time interval to write results to our trajectory for lattice and species, normally we keep them the same.

Be careful, the unit for Interval is "time steps", and should be an integer.

The actual physical time for interval would be:

$$t = Interval * dt$$

since we define  $dt = 50 \times 10^{-6} s$ , the actual write interval would be:

$$2000 * 50 \times 10^{-6} = 0.1s$$

```
[5]: sim.simulationTime=30.0 # unit is seconds

sim.latticeWriteInterval= int(2000) # unit is timesteps, dt

sim.speciesWriteInterval= int(2000) # unit is timesteps, dt
```

## 2.2 1.2 Spatial Geometry Initialization

now, we need to add more spatial compartments to our system, for simplicity, our first toy system would only have three spatial regions: + extracellular + cytoplasm + plasm membrane

we want each of them mutually excluded, and if we combine them all together, it should be the entire lattice sites we create:

```
\texttt{lattice} = \texttt{extracellular} \cup \texttt{membrane} \cup \texttt{cytoplasm} and naturally \emptyset = \texttt{membrane} \cap \texttt{cytoplasm} \emptyset = \texttt{membrane} \cap \texttt{extracellular} \emptyset = \texttt{cytoplasm} \cap \texttt{extracellular}
```

In order to design the site lattice geometry, we create a RegionBuilder object, which reads the lattice dimensions from our simulation object sim.

```
[6]: build = RegionBuilder(sim)
```

we create a sphere to represent the cytoplasm with radius=25, center at [32,32,32]

```
[7]: radius = int(np.ceil((cellvol*3/4/np.pi)**(1/3)*0.1/lattice_spacing))
    print(radius)
    cytoplasm = build.ellipsoid(radius = radius, center = [32,32,32])
```

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Then we dilate the cytoplasm, and create a surface with the dilation method, and exclude the cytoplasm to represent our membrane

```
[8]: cytoplasm_dilation = build.dilate(cytoplasm, se = build.se26)
membrane = cytoplasm_dilation & ~cytoplasm
```

Finally, make sure our extracellular region excludes the cell.

```
[9]: # effectively, cytoplasm_dilation = cytoplasm and membrane
extracellular = ~cytoplasm_dilation
```

we need our simulation system to compose all the regions together.

```
[10]: cyt = sim.region('cytoplasm')
mem = sim.region('membrane')
ext = sim.region('extracellular')
```

wonderful, now we have all the geometric infomation, we can visualize it in two different ways: stacks and 3D

- [12]: sim.showRegionStack()
- [12]: <IPython.core.display.HTML object>
- [13]: sim.displayGeometry()
- [13]: <IPython.core.display.HTML object>

## 2.3 1.2 Species and diffusion Co. Initialization

For simplicity, we only want our bimolecular reaction take place in cytoplasm and only allow each species to diffuse in cytoplasm.

Our Template will be a reversible reaction as:

$$A + B \rightleftharpoons C$$

However, our software only accept one-way reaction, we need to separate it into two irreversible reactions:

$$A + B \xrightarrow{k_f} C$$

$$C \xrightarrow{k_r} A + B$$

initial condition:

#A = 1000

#B = 1000

#C = 0

• function references:

sim.species((str)name, [(str,latex)textPepr, (str)annotation])

Then you can call the following function to check the relevant info about your species:

- [15]: sim.showAllSpecies()
- [15]: <IPython.core.display.HTML object>
- [16]: sim.showSpecies('A')

[16]: <IPython.core.display.HTML object>

Now, you may notice all Diffusion rates are undefined, so we are going to **define all the diffusion** coefficients for each species.

```
[17]: sim.transitionRate(None, None, None, sim.diffusionZero) # initialization of the_{\sqcup} \hookrightarrow diffusion rates to 0
```

define a custom made diffusion coefficient.

```
[18]: sim.diffusionConst('diff1', 1e-14)
```

[18]: <jLM.Types.DiffusionConst at 0x7f1fd049c278>

set diffusion rate:

check the result:

```
[20]: sim.showAllSpecies()
```

[20]: <IPython.core.display.HTML object>

#### 2.4 1.3 Reactions Initialization

```
[21]: NA = 6.022e23  # molecules/mole
  # kf = sim.rateConst('kf', 1.07e5/(NA*cellvol), 2)
  kf = sim.rateConst('kf', 1.07e5, 2)
  # rate constant for the reaction A + B -> C, second order, /M/s
  kr = sim.rateConst('kr', 0.351 , 1)
  # rate constant for the reaction C -> A + B, first order, /s
```

Reactions can be added by the function: jLM.RDME.Sim.region('region\_name').addReaction Since we already define the name of the region we want to add reactions, there will be two ways you can add reactions:

```
[22]: sim.region('cytoplasm').addReaction([spA,spB], [spC], sim.rc.kf) cyt.addReaction([spC], [spA,spB], kr)
```

[22]: <jLM.Types.BuilderRegion at 0x7f1fd31230f0>

### 2.5 1.4 Add particles

Here, in order to see the effects of diffusion, we put 1000 species A at on side, and 1000 species at the other side. Instead of uniformly distribution.

```
[23]: # uniformly distribute the species in the cytoplasm
      # sim.distributeNumber(spA, cyt, 1000)
      # sim.distributeNumber(spB, cyt, 1000)
      # sim.distributeNumber(spC, cyt, 0)
      # sim.sp.A.placeNumberInto(cyt, 1000)
      cyto_cent = [32, 32, 32]
      cyto_left_cent = [32-int(radius/2),32,32]
      cyto_right_cent = [32+int(radius/2),32,32]
      total A = 1000
      total_B = 1000
      total_C = 0
      # write a BFS function to place the species in the cytoplasm start from
       ⇔cyto_left_cent
      def placeNumbersInCyto(sp, x, y, z, n):
          '''place certain amount of species in the cytoplasm, start from x, y, z
          neighbor_26 = [[0,0,1],[0,0,-1],[0,1,0],[0,-1,0],
                       [1,0,0],[-1,0,0],[0,1,1],[0,1,-1],
                       [0,-1,1], [0,-1,-1], [1,0,1], [1,0,-1],
                      [-1,0,1], [-1,0,-1], [1,1,0], [1,-1,0],
                      [-1,1,0], [-1,-1,0], [1,1,1], [1,1,-1],
                       [1,-1,1], [1,-1,-1], [-1,1,1], [-1,1,-1],
                       [-1,-1,1],[-1,-1,-1]
          q = []
          visited = []
          q.append([x,y,z])
          remaining = n
          while len(q) > 0:
              cur = q.pop(0)
              if remaining <= 0:</pre>
                  break
              visited.append(cur)
              if remaining / 16 >= 1:
                  sim.placeNumber(sp=sp, x=cur[0], y=cur[1], z=cur[2], n=16)
                  remaining -= 16
              else:
                  sim.placeNumber(sp=sp, x=cur[0], y=cur[1], z=cur[2], n=remaining)
                  remaining = 0
```

successfully placed 1000 speciesA in the cytoplasm. successfully placed 1000 speciesB in the cytoplasm.

```
[25]: sim.showAllSpecies()
```

[25]: <IPython.core.display.HTML object>

# 3 2 Check the system state

```
[26]: sim
```

[26]: <jLM.RDME.Sim at 0x7f1ff5f14f98>

now we confirmed it is what we want, we can now proceed to finalize the simulation we create.

```
[27]: sim.finalize()
```

#### 4 3. Run the Simulation

```
2024-04-30 11:30:53) Info: Next lattice write time is 4000
2024-04-30 11:30:53) Warning: 11 uses of the particle overflow list in the last
1000 timesteps, performance may be degraded.
2024-04-30 11:30:54) Info: Time is 0.20000000000000
2024-04-30 11:30:54) Info: Lattice write time is 0.2000000000000, in steps is
4000
2024-04-30 11:30:54) Info: Next lattice write time is 6000
2024-04-30 11:30:55) Info: Time is 0.30000000000000
2024-04-30 11:30:55) Info: Lattice write time is 0.3000000000000, in steps is
6000
2024-04-30 11:30:55) Info: Next lattice write time is 8000
2024-04-30 11:30:56) Info: Time is 0.40000000000000
2024-04-30 11:30:56) Info: Lattice write time is 0.4000000000000, in steps is
8000
2024-04-30 11:30:56) Info: Next lattice write time is 10000
2024-04-30 11:30:57) Info: Time is 0.50000000000000
2024-04-30 11:30:57) Info: Lattice write time is 0.5000000000000, in steps is
10000
2024-04-30 11:30:57) Info: Next lattice write time is 12000
2024-04-30 11:30:58) Info: Time is 0.60000000000000
2024-04-30 11:30:58) Info: Lattice write time is 0.6000000000000, in steps is
12000
2024-04-30 11:30:58) Info: Next lattice write time is 14000
2024-04-30 11:30:59) Info: Time is 0.7000000000000
2024-04-30 11:30:59) Info: Lattice write time is 0.7000000000000, in steps is
14000
2024-04-30 11:30:59) Info: Next lattice write time is 16000
2024-04-30 11:31:00) Info: Time is 0.80000000000000
2024-04-30 11:31:00) Info: Lattice write time is 0.8000000000000, in steps is
16000
2024-04-30 11:31:00) Info: Next lattice write time is 18000
2024-04-30 11:31:01) Info: Time is 0.90000000000000
2024-04-30 11:31:01) Info: Lattice write time is 0.9000000000000, in steps is
18000
2024-04-30 11:31:01) Info: Next lattice write time is 20000
2024-04-30 11:31:02) Info: Time is 1.00000000000000
2024-04-30 11:31:02) Info: Lattice write time is 1.0000000000000, in steps is
20000
2024-04-30 11:31:02) Info: Next lattice write time is 22000
2024-04-30 11:31:03) Info: Time is 1.10000000000000
2024-04-30 11:31:03) Info: Lattice write time is 1.1000000000000, in steps is
22000
2024-04-30 11:31:03) Info: Next lattice write time is 24000
2024-04-30 11:31:04) Info: Time is 1.20000000000000
2024-04-30 11:31:04) Info: Lattice write time is 1.2000000000000, in steps is
2024-04-30 11:31:04) Info: Next lattice write time is 26000
2024-04-30 11:31:05) Info: Time is 1.30000000000000
```

```
2024-04-30 11:31:05) Info: Lattice write time is 1.3000000000000, in steps is
26000
2024-04-30 11:31:05) Info: Next lattice write time is 28000
2024-04-30 11:31:06) Info: Time is 1.40000000000000
2024-04-30 11:31:06) Info: Lattice write time is 1.4000000000000, in steps is
28000
2024-04-30 11:31:06) Info: Next lattice write time is 30000
2024-04-30 11:31:07) Info: Time is 1.50000000000000
2024-04-30 11:31:07) Info: Lattice write time is 1.5000000000000, in steps is
30000
2024-04-30 11:31:07) Info: Next lattice write time is 32000
2024-04-30 11:31:08) Info: Time is 1.60000000000000
2024-04-30 11:31:08) Info: Lattice write time is 1.6000000000000, in steps is
32000
2024-04-30 11:31:08) Info: Next lattice write time is 34000
2024-04-30 11:31:09) Info: Time is 1.70000000000000
2024-04-30 11:31:09) Info: Lattice write time is 1.7000000000000, in steps is
34000
2024-04-30 11:31:09) Info: Next lattice write time is 36000
2024-04-30 11:31:10) Info: Time is 1.80000000000000
2024-04-30 11:31:10) Info: Lattice write time is 1.8000000000000, in steps is
36000
2024-04-30 11:31:10) Info: Next lattice write time is 38000
2024-04-30 11:31:11) Info: Time is 1.90000000000000
2024-04-30 11:31:11) Info: Lattice write time is 1.9000000000000, in steps is
38000
2024-04-30 11:31:11) Info: Next lattice write time is 40000
2024-04-30 11:31:12) Info: Time is 2.00000000000000
2024-04-30 11:31:12) Info: Lattice write time is 2.0000000000000, in steps is
40000
2024-04-30 11:31:12) Info: Next lattice write time is 42000
2024-04-30 11:31:13) Info: Time is 2.1000000000000
2024-04-30 11:31:13) Info: Lattice write time is 2.1000000000000, in steps is
42000
2024-04-30 11:31:13) Info: Next lattice write time is 44000
2024-04-30 11:31:14) Info: Time is 2.20000000000000
2024-04-30 11:31:14) Info: Lattice write time is 2.2000000000000, in steps is
44000
2024-04-30 11:31:14) Info: Next lattice write time is 46000
2024-04-30 11:31:15) Info: Time is 2.30000000000000
2024-04-30 11:31:15) Info: Lattice write time is 2.3000000000000, in steps is
46000
2024-04-30 11:31:15) Info: Next lattice write time is 48000
2024-04-30 11:31:16) Info: Time is 2.40000000000000
2024-04-30 11:31:16) Info: Lattice write time is 2.4000000000000, in steps is
2024-04-30 11:31:16) Info: Next lattice write time is 50000
2024-04-30 11:31:17) Info: Time is 2.50000000000000
```

```
2024-04-30 11:31:17) Info: Lattice write time is 2.5000000000000, in steps is
50000
2024-04-30 11:31:17) Info: Next lattice write time is 52000
2024-04-30 11:31:18) Info: Time is 2.60000000000000
2024-04-30 11:31:18) Info: Lattice write time is 2.6000000000000, in steps is
52000
2024-04-30 11:31:18) Info: Next lattice write time is 54000
2024-04-30 11:31:19) Info: Time is 2.70000000000000
2024-04-30 11:31:19) Info: Lattice write time is 2.7000000000000, in steps is
54000
2024-04-30 11:31:19) Info: Next lattice write time is 56000
2024-04-30 11:31:20) Info: Time is 2.80000000000000
2024-04-30 11:31:20) Info: Lattice write time is 2.8000000000000, in steps is
56000
2024-04-30 11:31:20) Info: Next lattice write time is 58000
2024-04-30 11:31:21) Info: Time is 2.90000000000000
2024-04-30 11:31:21) Info: Lattice write time is 2.9000000000000, in steps is
58000
2024-04-30 11:31:21) Info: Next lattice write time is 60000
2024-04-30 11:31:22) Info: Time is 3.00000000000000
2024-04-30 11:31:22) Info: Lattice write time is 3.0000000000000, in steps is
60000
2024-04-30 11:31:22) Info: Next lattice write time is 62000
2024-04-30 11:31:23) Info: Time is 3.1000000000000
2024-04-30 11:31:23) Info: Lattice write time is 3.1000000000000, in steps is
62000
2024-04-30 11:31:23) Info: Next lattice write time is 64000
2024-04-30 11:31:24) Info: Time is 3.20000000000000
2024-04-30 11:31:24) Info: Lattice write time is 3.2000000000000, in steps is
64000
2024-04-30 11:31:24) Info: Next lattice write time is 66000
2024-04-30 11:31:25) Info: Time is 3.30000000000000
2024-04-30 11:31:25) Info: Lattice write time is 3.3000000000000, in steps is
66000
2024-04-30 11:31:25) Info: Next lattice write time is 68000
2024-04-30 11:31:26) Info: Time is 3.40000000000000
2024-04-30 11:31:26) Info: Lattice write time is 3.4000000000000, in steps is
68000
2024-04-30 11:31:26) Info: Next lattice write time is 70000
2024-04-30 11:31:27) Info: Time is 3.50000000000000
2024-04-30 11:31:27) Info: Lattice write time is 3.5000000000000, in steps is
70000
2024-04-30 11:31:27) Info: Next lattice write time is 72000
2024-04-30 11:31:28) Info: Time is 3.60000000000000
2024-04-30 11:31:28) Info: Lattice write time is 3.600000000000, in steps is
2024-04-30 11:31:28) Info: Next lattice write time is 74000
2024-04-30 11:31:29) Info: Time is 3.70000000000000
```

```
2024-04-30 11:31:29) Info: Lattice write time is 3.7000000000000, in steps is
74000
2024-04-30 11:31:29) Info: Next lattice write time is 76000
2024-04-30 11:31:30) Info: Time is 3.80000000000000
2024-04-30 11:31:30) Info: Lattice write time is 3.8000000000000, in steps is
76000
2024-04-30 11:31:30) Info: Next lattice write time is 78000
2024-04-30 11:31:31) Info: Time is 3.90000000000000
2024-04-30 11:31:31) Info: Lattice write time is 3.9000000000000, in steps is
78000
2024-04-30 11:31:31) Info: Next lattice write time is 80000
2024-04-30 11:31:32) Info: Time is 4.00000000000000
2024-04-30 11:31:32) Info: Lattice write time is 4.0000000000000, in steps is
80000
2024-04-30 11:31:32) Info: Next lattice write time is 82000
2024-04-30 11:31:33) Info: Time is 4.10000000000000
2024-04-30 11:31:33) Info: Lattice write time is 4.1000000000000, in steps is
82000
2024-04-30 11:31:33) Info: Next lattice write time is 84000
2024-04-30 11:31:34) Info: Time is 4.20000000000000
2024-04-30 11:31:34) Info: Lattice write time is 4.2000000000000, in steps is
84000
2024-04-30 11:31:34) Info: Next lattice write time is 86000
2024-04-30 11:31:35) Info: Time is 4.30000000000000
2024-04-30 11:31:35) Info: Lattice write time is 4.3000000000000, in steps is
86000
2024-04-30 11:31:35) Info: Next lattice write time is 88000
2024-04-30 11:31:36) Info: Time is 4.40000000000000
2024-04-30 11:31:36) Info: Lattice write time is 4.4000000000000, in steps is
88000
2024-04-30 11:31:36) Info: Next lattice write time is 90000
2024-04-30 11:31:37) Info: Time is 4.50000000000000
2024-04-30 11:31:37) Info: Lattice write time is 4.5000000000000, in steps is
90000
2024-04-30 11:31:37) Info: Next lattice write time is 92000
2024-04-30 11:31:37) Info: Time is 4.60000000000000
2024-04-30 11:31:37) Info: Lattice write time is 4.6000000000000, in steps is
92000
2024-04-30 11:31:37) Info: Next lattice write time is 94000
2024-04-30 11:31:38) Info: Time is 4.70000000000000
2024-04-30 11:31:38) Info: Lattice write time is 4.7000000000000, in steps is
94000
2024-04-30 11:31:38) Info: Next lattice write time is 96000
2024-04-30 11:31:39) Info: Time is 4.80000000000000
2024-04-30 11:31:39) Info: Lattice write time is 4.800000000000, in steps is
2024-04-30 11:31:39) Info: Next lattice write time is 98000
2024-04-30 11:31:40) Info: Time is 4.90000000000000
```

```
2024-04-30 11:31:40) Info: Lattice write time is 4.9000000000000, in steps is
98000
2024-04-30 11:31:40) Info: Next lattice write time is 100000
2024-04-30 11:31:41) Info: Time is 5.00000000000000
2024-04-30 11:31:41) Info: Lattice write time is 5.0000000000000, in steps is
100000
2024-04-30 11:31:41) Info: Next lattice write time is 102000
2024-04-30 11:31:42) Info: Time is 5.10000000000000
2024-04-30 11:31:42) Info: Lattice write time is 5.1000000000000, in steps is
102000
2024-04-30 11:31:42) Info: Next lattice write time is 104000
2024-04-30 11:31:43) Info: Time is 5.20000000000000
2024-04-30 11:31:43) Info: Lattice write time is 5.2000000000000, in steps is
104000
2024-04-30 11:31:43) Info: Next lattice write time is 106000
2024-04-30 11:31:44) Info: Time is 5.30000000000000
2024-04-30 11:31:44) Info: Lattice write time is 5.300000000000, in steps is
106000
2024-04-30 11:31:44) Info: Next lattice write time is 108000
2024-04-30 11:31:45) Info: Time is 5.40000000000000
2024-04-30 11:31:45) Info: Lattice write time is 5.4000000000000, in steps is
108000
2024-04-30 11:31:45) Info: Next lattice write time is 110000
2024-04-30 11:31:46) Info: Time is 5.50000000000000
2024-04-30 11:31:46) Info: Lattice write time is 5.5000000000000, in steps is
110000
2024-04-30 11:31:46) Info: Next lattice write time is 112000
2024-04-30 11:31:47) Info: Time is 5.60000000000000
2024-04-30 11:31:47) Info: Lattice write time is 5.6000000000000, in steps is
112000
2024-04-30 11:31:47) Info: Next lattice write time is 114000
2024-04-30 11:31:48) Info: Time is 5.70000000000000
2024-04-30 11:31:48) Info: Lattice write time is 5.7000000000000, in steps is
114000
2024-04-30 11:31:48) Info: Next lattice write time is 116000
2024-04-30 11:31:49) Info: Time is 5.80000000000000
2024-04-30 11:31:49) Info: Lattice write time is 5.8000000000000, in steps is
116000
2024-04-30 11:31:49) Info: Next lattice write time is 118000
2024-04-30 11:31:50) Info: Time is 5.90000000000000
2024-04-30 11:31:50) Info: Lattice write time is 5.9000000000000, in steps is
118000
2024-04-30 11:31:50) Info: Next lattice write time is 120000
2024-04-30 11:31:51) Info: Time is 6.000000000000000
2024-04-30 11:31:51) Info: Lattice write time is 6.000000000000, in steps is
2024-04-30 11:31:51) Info: Next lattice write time is 122000
2024-04-30 11:31:52) Info: Average walltime per timestep: 0.49 ms. Progress:
```

```
6.0614s/30.0000s (20.2% done / 3.9 minutes walltime remaining)
2024-04-30 11:31:52) Info: Time is 6.10000000000000
2024-04-30 11:31:52) Info: Lattice write time is 6.1000000000000, in steps is
2024-04-30 11:31:52) Info: Next lattice write time is 124000
2024-04-30 11:31:52) Info: Wrote 61 data sets (1023412677 bytes) in the last
60.48 seconds (1.87 seconds writing). 0 datasets queued. Flushing.
2024-04-30 11:31:53) Info: Time is 6.20000000000000
2024-04-30 11:31:53) Info: Lattice write time is 6.2000000000000, in steps is
124000
2024-04-30 11:31:53) Info: Next lattice write time is 126000
2024-04-30 11:31:54) Info: Time is 6.30000000000000
2024-04-30 11:31:54) Info: Lattice write time is 6.3000000000000, in steps is
126000
2024-04-30 11:31:54) Info: Next lattice write time is 128000
2024-04-30 11:31:55) Info: Time is 6.40000000000000
2024-04-30 11:31:55) Info: Lattice write time is 6.4000000000000, in steps is
128000
2024-04-30 11:31:55) Info: Next lattice write time is 130000
2024-04-30 11:31:56) Info: Time is 6.50000000000000
2024-04-30 11:31:56) Info: Lattice write time is 6.5000000000000, in steps is
130000
2024-04-30 11:31:56) Info: Next lattice write time is 132000
2024-04-30 11:31:57) Info: Time is 6.60000000000000
2024-04-30 11:31:57) Info: Lattice write time is 6.6000000000000, in steps is
132000
2024-04-30 11:31:57) Info: Next lattice write time is 134000
2024-04-30 11:31:58) Info: Time is 6.70000000000000
2024-04-30 11:31:58) Info: Lattice write time is 6.7000000000000, in steps is
134000
2024-04-30 11:31:58) Info: Next lattice write time is 136000
2024-04-30 11:31:58) Info: Time is 6.80000000000000
2024-04-30 11:31:58) Info: Lattice write time is 6.8000000000000, in steps is
136000
2024-04-30 11:31:58) Info: Next lattice write time is 138000
2024-04-30 11:31:59) Info: Time is 6.90000000000000
2024-04-30 11:31:59) Info: Lattice write time is 6.9000000000000, in steps is
138000
2024-04-30 11:31:59) Info: Next lattice write time is 140000
2024-04-30 11:32:00) Info: Time is 7.00000000000000
2024-04-30 11:32:00) Info: Lattice write time is 7.0000000000000, in steps is
140000
2024-04-30 11:32:00) Info: Next lattice write time is 142000
2024-04-30 11:32:01) Info: Time is 7.10000000000000
2024-04-30 11:32:01) Info: Lattice write time is 7.1000000000000, in steps is
2024-04-30 11:32:01) Info: Next lattice write time is 144000
2024-04-30 11:32:02) Info: Time is 7.2000000000000
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2024-04-30 11:32:02) Info: Lattice write time is 7.2000000000000, in steps is
144000
2024-04-30 11:32:02) Info: Next lattice write time is 146000
2024-04-30 11:32:03) Info: Time is 7.30000000000000
2024-04-30 11:32:03) Info: Lattice write time is 7.3000000000000, in steps is
146000
2024-04-30 11:32:03) Info: Next lattice write time is 148000
2024-04-30 11:32:04) Info: Time is 7.4000000000000
2024-04-30 11:32:04) Info: Lattice write time is 7.4000000000000, in steps is
148000
2024-04-30 11:32:04) Info: Next lattice write time is 150000
2024-04-30 11:32:05) Info: Time is 7.50000000000000
2024-04-30 11:32:05) Info: Lattice write time is 7.5000000000000, in steps is
150000
2024-04-30 11:32:05) Info: Next lattice write time is 152000
2024-04-30 11:32:06) Info: Time is 7.60000000000000
2024-04-30 11:32:06) Info: Lattice write time is 7.6000000000000, in steps is
152000
2024-04-30 11:32:06) Info: Next lattice write time is 154000
2024-04-30 11:32:07) Info: Time is 7.70000000000000
2024-04-30 11:32:07) Info: Lattice write time is 7.7000000000000, in steps is
154000
2024-04-30 11:32:07) Info: Next lattice write time is 156000
2024-04-30 11:32:08) Info: Time is 7.80000000000000
2024-04-30 11:32:08) Info: Lattice write time is 7.8000000000000, in steps is
156000
2024-04-30 11:32:08) Info: Next lattice write time is 158000
2024-04-30 11:32:09) Info: Time is 7.90000000000000
2024-04-30 11:32:09) Info: Lattice write time is 7.9000000000000, in steps is
158000
2024-04-30 11:32:09) Info: Next lattice write time is 160000
2024-04-30 11:32:10) Info: Time is 8.00000000000000
2024-04-30 11:32:10) Info: Lattice write time is 8.0000000000000, in steps is
160000
2024-04-30 11:32:10) Info: Next lattice write time is 162000
2024-04-30 11:32:11) Info: Time is 8.10000000000000
2024-04-30 11:32:11) Info: Lattice write time is 8.1000000000000, in steps is
162000
2024-04-30 11:32:11) Info: Next lattice write time is 164000
2024-04-30 11:32:11) Info: Time is 8.20000000000000
2024-04-30 11:32:11) Info: Lattice write time is 8.2000000000000, in steps is
164000
2024-04-30 11:32:11) Info: Next lattice write time is 166000
2024-04-30 11:32:12) Info: Time is 8.30000000000000
2024-04-30 11:32:12) Info: Lattice write time is 8.300000000000, in steps is
2024-04-30 11:32:12) Info: Next lattice write time is 168000
2024-04-30 11:32:13) Info: Time is 8.40000000000000
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2024-04-30 11:32:13) Info: Lattice write time is 8.4000000000000, in steps is
168000
2024-04-30 11:32:13) Info: Next lattice write time is 170000
2024-04-30 11:32:14) Info: Time is 8.50000000000000
2024-04-30 11:32:14) Info: Lattice write time is 8.5000000000000, in steps is
170000
2024-04-30 11:32:14) Info: Next lattice write time is 172000
2024-04-30 11:32:15) Info: Time is 8.60000000000000
2024-04-30 11:32:15) Info: Lattice write time is 8.6000000000000, in steps is
172000
2024-04-30 11:32:15) Info: Next lattice write time is 174000
2024-04-30 11:32:16) Info: Time is 8.70000000000000
2024-04-30 11:32:16) Info: Lattice write time is 8.7000000000000, in steps is
174000
2024-04-30 11:32:16) Info: Next lattice write time is 176000
2024-04-30 11:32:17) Info: Time is 8.80000000000000
2024-04-30 11:32:17) Info: Lattice write time is 8.8000000000000, in steps is
176000
2024-04-30 11:32:17) Info: Next lattice write time is 178000
2024-04-30 11:32:18) Info: Time is 8.90000000000000
2024-04-30 11:32:18) Info: Lattice write time is 8.9000000000000, in steps is
178000
2024-04-30 11:32:18) Info: Next lattice write time is 180000
2024-04-30 11:32:19) Info: Time is 9.00000000000000
2024-04-30 11:32:19) Info: Lattice write time is 9.0000000000000, in steps is
180000
2024-04-30 11:32:19) Info: Next lattice write time is 182000
2024-04-30 11:32:20) Info: Time is 9.10000000000000
2024-04-30 11:32:20) Info: Lattice write time is 9.1000000000000, in steps is
182000
2024-04-30 11:32:20) Info: Next lattice write time is 184000
2024-04-30 11:32:21) Info: Time is 9.20000000000000
2024-04-30 11:32:21) Info: Lattice write time is 9.2000000000000, in steps is
184000
2024-04-30 11:32:21) Info: Next lattice write time is 186000
2024-04-30 11:32:22) Info: Time is 9.30000000000000
2024-04-30 11:32:22) Info: Lattice write time is 9.3000000000000, in steps is
186000
2024-04-30 11:32:22) Info: Next lattice write time is 188000
2024-04-30 11:32:23) Info: Time is 9.40000000000000
2024-04-30 11:32:23) Info: Lattice write time is 9.4000000000000, in steps is
188000
2024-04-30 11:32:23) Info: Next lattice write time is 190000
2024-04-30 11:32:24) Info: Time is 9.50000000000000
2024-04-30 11:32:24) Info: Lattice write time is 9.5000000000000, in steps is
2024-04-30 11:32:24) Info: Next lattice write time is 192000
2024-04-30 11:32:25) Info: Time is 9.60000000000000
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2024-04-30 11:32:25) Info: Lattice write time is 9.6000000000000, in steps is
192000
2024-04-30 11:32:25) Info: Next lattice write time is 194000
2024-04-30 11:32:26) Info: Time is 9.70000000000000
2024-04-30 11:32:26) Info: Lattice write time is 9.7000000000000, in steps is
194000
2024-04-30 11:32:26) Info: Next lattice write time is 196000
2024-04-30 11:32:27) Info: Time is 9.80000000000000
2024-04-30 11:32:27) Info: Lattice write time is 9.8000000000000, in steps is
196000
2024-04-30 11:32:27) Info: Next lattice write time is 198000
2024-04-30 11:32:27) Info: Time is 9.90000000000000
2024-04-30 11:32:27) Info: Lattice write time is 9.9000000000000, in steps is
198000
2024-04-30 11:32:27) Info: Next lattice write time is 200000
2024-04-30 11:32:28) Info: Lattice write time is 10.000000000000, in steps is
200000
2024-04-30 11:32:28) Info: Next lattice write time is 202000
2024-04-30 11:32:29) Info: Time is 10.1000000000000
2024-04-30 11:32:29) Info: Lattice write time is 10.1000000000000, in steps is
202000
2024-04-30 11:32:29) Info: Next lattice write time is 204000
2024-04-30 11:32:30) Info: Time is 10.2000000000000
2024-04-30 11:32:30) Info: Lattice write time is 10.2000000000000, in steps is
204000
2024-04-30 11:32:30) Info: Next lattice write time is 206000
2024-04-30 11:32:31) Info: Time is 10.30000000000000
2024-04-30 11:32:31) Info: Lattice write time is 10.3000000000000, in steps is
206000
2024-04-30 11:32:31) Info: Next lattice write time is 208000
2024-04-30 11:32:32) Info: Time is 10.40000000000000
2024-04-30 11:32:32) Info: Lattice write time is 10.4000000000000, in steps is
208000
2024-04-30 11:32:32) Info: Next lattice write time is 210000
2024-04-30 11:32:33) Info: Time is 10.50000000000000
2024-04-30 11:32:33) Info: Lattice write time is 10.5000000000000, in steps is
210000
2024-04-30 11:32:33) Info: Next lattice write time is 212000
2024-04-30 11:32:34) Info: Time is 10.60000000000000
2024-04-30 11:32:34) Info: Lattice write time is 10.6000000000000, in steps is
212000
2024-04-30 11:32:34) Info: Next lattice write time is 214000
2024-04-30 11:32:35) Info: Time is 10.70000000000000
2024-04-30 11:32:35) Info: Lattice write time is 10.700000000000, in steps is
2024-04-30 11:32:35) Info: Next lattice write time is 216000
2024-04-30 11:32:36) Info: Time is 10.80000000000000
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2024-04-30 11:32:36) Info: Lattice write time is 10.8000000000000, in steps is
216000
2024-04-30 11:32:36) Info: Next lattice write time is 218000
2024-04-30 11:32:37) Info: Time is 10.90000000000000
2024-04-30 11:32:37) Info: Lattice write time is 10.9000000000000, in steps is
218000
2024-04-30 11:32:37) Info: Next lattice write time is 220000
2024-04-30 11:32:38) Info: Time is 11.00000000000000
2024-04-30 11:32:38) Info: Lattice write time is 11.0000000000000, in steps is
220000
2024-04-30 11:32:38) Info: Next lattice write time is 222000
2024-04-30 11:32:39) Info: Time is 11.10000000000000
2024-04-30 11:32:39) Info: Lattice write time is 11.1000000000000, in steps is
222000
2024-04-30 11:32:39) Info: Next lattice write time is 224000
2024-04-30 11:32:40) Info: Time is 11.20000000000000
2024-04-30 11:32:40) Info: Lattice write time is 11.200000000000, in steps is
2024-04-30 11:32:40) Info: Next lattice write time is 226000
2024-04-30 11:32:41) Info: Time is 11.30000000000000
2024-04-30 11:32:41) Info: Lattice write time is 11.3000000000000, in steps is
226000
2024-04-30 11:32:41) Info: Next lattice write time is 228000
2024-04-30 11:32:42) Info: Time is 11.40000000000000
2024-04-30 11:32:42) Info: Lattice write time is 11.400000000000, in steps is
228000
2024-04-30 11:32:42) Info: Next lattice write time is 230000
2024-04-30 11:32:43) Info: Time is 11.50000000000000
2024-04-30 11:32:43) Info: Lattice write time is 11.500000000000, in steps is
230000
2024-04-30 11:32:43) Info: Next lattice write time is 232000
2024-04-30 11:32:44) Info: Time is 11.60000000000000
2024-04-30 11:32:44) Info: Lattice write time is 11.6000000000000, in steps is
232000
2024-04-30 11:32:44) Info: Next lattice write time is 234000
2024-04-30 11:32:45) Info: Time is 11.70000000000000
2024-04-30 11:32:45) Info: Lattice write time is 11.7000000000000, in steps is
234000
2024-04-30 11:32:45) Info: Next lattice write time is 236000
2024-04-30 11:32:46) Info: Time is 11.80000000000000
2024-04-30 11:32:46) Info: Lattice write time is 11.8000000000000, in steps is
236000
2024-04-30 11:32:46) Info: Next lattice write time is 238000
2024-04-30 11:32:47) Info: Time is 11.90000000000000
2024-04-30 11:32:47) Info: Lattice write time is 11.900000000000, in steps is
2024-04-30 11:32:47) Info: Next lattice write time is 240000
2024-04-30 11:32:48) Info: Time is 12.00000000000000
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2024-04-30 11:32:48) Info: Lattice write time is 12.0000000000000, in steps is
240000
2024-04-30 11:32:48) Info: Next lattice write time is 242000
2024-04-30 11:32:49) Info: Time is 12.1000000000000
2024-04-30 11:32:49) Info: Lattice write time is 12.1000000000000, in steps is
242000
2024-04-30 11:32:49) Info: Next lattice write time is 244000
2024-04-30 11:32:50) Info: Time is 12.2000000000000
2024-04-30 11:32:50) Info: Lattice write time is 12.2000000000000, in steps is
244000
2024-04-30 11:32:50) Info: Next lattice write time is 246000
2024-04-30 11:32:51) Info: Time is 12.30000000000000
2024-04-30 11:32:51) Info: Lattice write time is 12.3000000000000, in steps is
246000
2024-04-30 11:32:51) Info: Next lattice write time is 248000
2024-04-30 11:32:52) Info: Average walltime per timestep: 0.47 ms. Progress:
12.3981s/30.0000s ( 41.3% done / 2.8 minutes walltime remaining)
2024-04-30 11:32:52) Info: Time is 12.4000000000000
2024-04-30 11:32:52) Info: Lattice write time is 12.400000000000, in steps is
248000
2024-04-30 11:32:52) Info: Next lattice write time is 250000
2024-04-30 11:32:53) Info: Time is 12.50000000000000
2024-04-30 11:32:53) Info: Lattice write time is 12.5000000000000, in steps is
250000
2024-04-30 11:32:53) Info: Next lattice write time is 252000
2024-04-30 11:32:53) Info: Wrote 64 data sets (1073744448 bytes) in the last
60.66 seconds (1.96 seconds writing). 0 datasets queued. Flushing.
2024-04-30 11:32:54) Info: Time is 12.60000000000000
2024-04-30 11:32:54) Info: Lattice write time is 12.600000000000, in steps is
252000
2024-04-30 11:32:54) Info: Next lattice write time is 254000
2024-04-30 11:32:55) Info: Time is 12.70000000000000
2024-04-30 11:32:55) Info: Lattice write time is 12.7000000000000, in steps is
254000
2024-04-30 11:32:55) Info: Next lattice write time is 256000
2024-04-30 11:32:55) Info: Time is 12.80000000000000
2024-04-30 11:32:55) Info: Lattice write time is 12.8000000000000, in steps is
256000
2024-04-30 11:32:55) Info: Next lattice write time is 258000
2024-04-30 11:32:56) Info: Time is 12.9000000000000
2024-04-30 11:32:56) Info: Lattice write time is 12.900000000000, in steps is
258000
2024-04-30 11:32:56) Info: Next lattice write time is 260000
2024-04-30 11:32:57) Info: Time is 13.00000000000000
2024-04-30 11:32:57) Info: Lattice write time is 13.000000000000, in steps is
2024-04-30 11:32:57) Info: Next lattice write time is 262000
2024-04-30 11:32:58) Info: Time is 13.1000000000000
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2024-04-30 11:32:58) Info: Lattice write time is 13.1000000000000, in steps is
262000
2024-04-30 11:32:58) Info: Next lattice write time is 264000
2024-04-30 11:32:59) Info: Time is 13.20000000000000
2024-04-30 11:32:59) Info: Lattice write time is 13.2000000000000, in steps is
264000
2024-04-30 11:32:59) Info: Next lattice write time is 266000
2024-04-30 11:33:00) Info: Time is 13.30000000000000
2024-04-30 11:33:00) Info: Lattice write time is 13.3000000000000, in steps is
266000
2024-04-30 11:33:00) Info: Next lattice write time is 268000
2024-04-30 11:33:01) Info: Time is 13.40000000000000
2024-04-30 11:33:01) Info: Lattice write time is 13.4000000000000, in steps is
268000
2024-04-30 11:33:01) Info: Next lattice write time is 270000
2024-04-30 11:33:02) Info: Time is 13.50000000000000
2024-04-30 11:33:02) Info: Lattice write time is 13.5000000000000, in steps is
270000
2024-04-30 11:33:02) Info: Next lattice write time is 272000
2024-04-30 11:33:03) Info: Time is 13.60000000000000
2024-04-30 11:33:03) Info: Lattice write time is 13.6000000000000, in steps is
272000
2024-04-30 11:33:03) Info: Next lattice write time is 274000
2024-04-30 11:33:04) Info: Time is 13.7000000000000
2024-04-30 11:33:04) Info: Lattice write time is 13.700000000000, in steps is
274000
2024-04-30 11:33:04) Info: Next lattice write time is 276000
2024-04-30 11:33:05) Info: Time is 13.80000000000000
2024-04-30 11:33:05) Info: Lattice write time is 13.8000000000000, in steps is
276000
2024-04-30 11:33:05) Info: Next lattice write time is 278000
2024-04-30 11:33:06) Info: Time is 13.9000000000000
2024-04-30 11:33:06) Info: Lattice write time is 13.900000000000, in steps is
278000
2024-04-30 11:33:06) Info: Next lattice write time is 280000
2024-04-30 11:33:07) Info: Time is 14.00000000000000
2024-04-30 11:33:07) Info: Lattice write time is 14.0000000000000, in steps is
280000
2024-04-30 11:33:07) Info: Next lattice write time is 282000
2024-04-30 11:33:08) Info: Time is 14.10000000000000
2024-04-30 11:33:08) Info: Lattice write time is 14.1000000000000, in steps is
282000
2024-04-30 11:33:08) Info: Next lattice write time is 284000
2024-04-30 11:33:09) Info: Time is 14.20000000000000
2024-04-30 11:33:09) Info: Lattice write time is 14.200000000000, in steps is
2024-04-30 11:33:09) Info: Next lattice write time is 286000
2024-04-30 11:33:10) Info: Time is 14.30000000000000
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2024-04-30 11:33:10) Info: Lattice write time is 14.3000000000000, in steps is
286000
2024-04-30 11:33:10) Info: Next lattice write time is 288000
2024-04-30 11:33:11) Info: Time is 14.40000000000000
2024-04-30 11:33:11) Info: Lattice write time is 14.4000000000000, in steps is
288000
2024-04-30 11:33:11) Info: Next lattice write time is 290000
2024-04-30 11:33:11) Info: Time is 14.50000000000000
2024-04-30 11:33:11) Info: Lattice write time is 14.5000000000000, in steps is
290000
2024-04-30 11:33:11) Info: Next lattice write time is 292000
2024-04-30 11:33:12) Info: Time is 14.60000000000000
2024-04-30 11:33:12) Info: Lattice write time is 14.6000000000000, in steps is
292000
2024-04-30 11:33:12) Info: Next lattice write time is 294000
2024-04-30 11:33:13) Info: Time is 14.70000000000000
2024-04-30 11:33:13) Info: Lattice write time is 14.7000000000000, in steps is
2024-04-30 11:33:13) Info: Next lattice write time is 296000
2024-04-30 11:33:14) Info: Time is 14.80000000000000
2024-04-30 11:33:14) Info: Lattice write time is 14.8000000000000, in steps is
296000
2024-04-30 11:33:14) Info: Next lattice write time is 298000
2024-04-30 11:33:15) Info: Time is 14.9000000000000
2024-04-30 11:33:15) Info: Lattice write time is 14.900000000000, in steps is
298000
2024-04-30 11:33:15) Info: Next lattice write time is 300000
2024-04-30 11:33:16) Info: Time is 15.00000000000000
2024-04-30 11:33:16) Info: Lattice write time is 15.0000000000000, in steps is
300000
2024-04-30 11:33:16) Info: Next lattice write time is 302000
2024-04-30 11:33:17) Info: Time is 15.10000000000000
2024-04-30 11:33:17) Info: Lattice write time is 15.1000000000000, in steps is
302000
2024-04-30 11:33:17) Info: Next lattice write time is 304000
2024-04-30 11:33:18) Info: Time is 15.20000000000000
2024-04-30 11:33:18) Info: Lattice write time is 15.2000000000000, in steps is
304000
2024-04-30 11:33:18) Info: Next lattice write time is 306000
2024-04-30 11:33:19) Info: Time is 15.30000000000000
2024-04-30 11:33:19) Info: Lattice write time is 15.3000000000000, in steps is
306000
2024-04-30 11:33:19) Info: Next lattice write time is 308000
2024-04-30 11:33:20) Info: Time is 15.40000000000000
2024-04-30 11:33:20) Info: Lattice write time is 15.400000000000, in steps is
2024-04-30 11:33:20) Info: Next lattice write time is 310000
2024-04-30 11:33:21) Info: Time is 15.50000000000000
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2024-04-30 11:33:21) Info: Lattice write time is 15.5000000000000, in steps is
310000
2024-04-30 11:33:21) Info: Next lattice write time is 312000
2024-04-30 11:33:22) Info: Time is 15.60000000000000
2024-04-30 11:33:22) Info: Lattice write time is 15.6000000000000, in steps is
312000
2024-04-30 11:33:22) Info: Next lattice write time is 314000
2024-04-30 11:33:23) Info: Time is 15.70000000000000
2024-04-30 11:33:23) Info: Lattice write time is 15.7000000000000, in steps is
314000
2024-04-30 11:33:23) Info: Next lattice write time is 316000
2024-04-30 11:33:24) Info: Time is 15.80000000000000
2024-04-30 11:33:24) Info: Lattice write time is 15.8000000000000, in steps is
316000
2024-04-30 11:33:24) Info: Next lattice write time is 318000
2024-04-30 11:33:25) Info: Time is 15.90000000000000
2024-04-30 11:33:25) Info: Lattice write time is 15.9000000000000, in steps is
2024-04-30 11:33:25) Info: Next lattice write time is 320000
2024-04-30 11:33:26) Info: Time is 16.00000000000000
2024-04-30 11:33:26) Info: Lattice write time is 16.0000000000000, in steps is
320000
2024-04-30 11:33:26) Info: Next lattice write time is 322000
2024-04-30 11:33:26) Info: Time is 16.10000000000000
2024-04-30 11:33:26) Info: Lattice write time is 16.100000000000, in steps is
322000
2024-04-30 11:33:26) Info: Next lattice write time is 324000
2024-04-30 11:33:27) Info: Time is 16.20000000000000
2024-04-30 11:33:27) Info: Lattice write time is 16.2000000000000, in steps is
324000
2024-04-30 11:33:27) Info: Next lattice write time is 326000
2024-04-30 11:33:28) Info: Time is 16.30000000000000
2024-04-30 11:33:28) Info: Lattice write time is 16.3000000000000, in steps is
326000
2024-04-30 11:33:28) Info: Next lattice write time is 328000
2024-04-30 11:33:29) Info: Time is 16.40000000000000
2024-04-30 11:33:29) Info: Lattice write time is 16.4000000000000, in steps is
328000
2024-04-30 11:33:29) Info: Next lattice write time is 330000
2024-04-30 11:33:30) Info: Time is 16.50000000000000
2024-04-30 11:33:30) Info: Lattice write time is 16.5000000000000, in steps is
330000
2024-04-30 11:33:30) Info: Next lattice write time is 332000
2024-04-30 11:33:31) Info: Time is 16.600000000000000
2024-04-30 11:33:31) Info: Lattice write time is 16.600000000000, in steps is
2024-04-30 11:33:31) Info: Next lattice write time is 334000
2024-04-30 11:33:32) Info: Time is 16.70000000000000
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2024-04-30 11:33:32) Info: Lattice write time is 16.7000000000000, in steps is
334000
2024-04-30 11:33:32) Info: Next lattice write time is 336000
2024-04-30 11:33:33) Info: Time is 16.80000000000000
2024-04-30 11:33:33) Info: Lattice write time is 16.8000000000000, in steps is
336000
2024-04-30 11:33:33) Info: Next lattice write time is 338000
2024-04-30 11:33:34) Info: Time is 16.90000000000000
2024-04-30 11:33:34) Info: Lattice write time is 16.9000000000000, in steps is
338000
2024-04-30 11:33:34) Info: Next lattice write time is 340000
2024-04-30 11:33:35) Info: Time is 17.00000000000000
2024-04-30 11:33:35) Info: Lattice write time is 17.0000000000000, in steps is
340000
2024-04-30 11:33:35) Info: Next lattice write time is 342000
2024-04-30 11:33:36) Info: Time is 17.10000000000000
2024-04-30 11:33:36) Info: Lattice write time is 17.1000000000000, in steps is
342000
2024-04-30 11:33:36) Info: Next lattice write time is 344000
2024-04-30 11:33:37) Info: Time is 17.2000000000000
2024-04-30 11:33:37) Info: Lattice write time is 17.2000000000000, in steps is
344000
2024-04-30 11:33:37) Info: Next lattice write time is 346000
2024-04-30 11:33:38) Info: Time is 17.3000000000000
2024-04-30 11:33:38) Info: Lattice write time is 17.3000000000000, in steps is
346000
2024-04-30 11:33:38) Info: Next lattice write time is 348000
2024-04-30 11:33:39) Info: Time is 17.4000000000000
2024-04-30 11:33:39) Info: Lattice write time is 17.4000000000000, in steps is
348000
2024-04-30 11:33:39) Info: Next lattice write time is 350000
2024-04-30 11:33:40) Info: Time is 17.50000000000000
2024-04-30 11:33:40) Info: Lattice write time is 17.5000000000000, in steps is
350000
2024-04-30 11:33:40) Info: Next lattice write time is 352000
2024-04-30 11:33:41) Info: Time is 17.60000000000000
2024-04-30 11:33:41) Info: Lattice write time is 17.6000000000000, in steps is
352000
2024-04-30 11:33:41) Info: Next lattice write time is 354000
2024-04-30 11:33:42) Info: Time is 17.70000000000000
2024-04-30 11:33:42) Info: Lattice write time is 17.7000000000000, in steps is
354000
2024-04-30 11:33:42) Info: Next lattice write time is 356000
2024-04-30 11:33:43) Info: Time is 17.80000000000000
2024-04-30 11:33:43) Info: Lattice write time is 17.800000000000, in steps is
2024-04-30 11:33:43) Info: Next lattice write time is 358000
2024-04-30 11:33:44) Info: Time is 17.90000000000000
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2024-04-30 11:33:44) Info: Lattice write time is 17.9000000000000, in steps is
358000
2024-04-30 11:33:44) Info: Next lattice write time is 360000
2024-04-30 11:33:45) Info: Time is 18.00000000000000
2024-04-30 11:33:45) Info: Lattice write time is 18.0000000000000, in steps is
360000
2024-04-30 11:33:45) Info: Next lattice write time is 362000
2024-04-30 11:33:46) Info: Time is 18.10000000000000
2024-04-30 11:33:46) Info: Lattice write time is 18.1000000000000, in steps is
362000
2024-04-30 11:33:46) Info: Next lattice write time is 364000
2024-04-30 11:33:47) Info: Time is 18.20000000000000
2024-04-30 11:33:47) Info: Lattice write time is 18.2000000000000, in steps is
364000
2024-04-30 11:33:47) Info: Next lattice write time is 366000
2024-04-30 11:33:48) Info: Time is 18.30000000000000
2024-04-30 11:33:48) Info: Lattice write time is 18.300000000000, in steps is
2024-04-30 11:33:48) Info: Next lattice write time is 368000
2024-04-30 11:33:49) Info: Time is 18.4000000000000
2024-04-30 11:33:49) Info: Lattice write time is 18.4000000000000, in steps is
368000
2024-04-30 11:33:49) Info: Next lattice write time is 370000
2024-04-30 11:33:50) Info: Time is 18.50000000000000
2024-04-30 11:33:50) Info: Lattice write time is 18.5000000000000, in steps is
370000
2024-04-30 11:33:50) Info: Next lattice write time is 372000
2024-04-30 11:33:51) Info: Time is 18.60000000000000
2024-04-30 11:33:51) Info: Lattice write time is 18.6000000000000, in steps is
372000
2024-04-30 11:33:51) Info: Next lattice write time is 374000
2024-04-30 11:33:52) Info: Average walltime per timestep: 0.48 ms. Progress:
18.6879s/30.0000s (62.3% done / 1.8 minutes walltime remaining)
2024-04-30 11:33:52) Info: Time is 18.70000000000000
2024-04-30 11:33:52) Info: Lattice write time is 18.7000000000000, in steps is
374000
2024-04-30 11:33:52) Info: Next lattice write time is 376000
2024-04-30 11:33:53) Info: Time is 18.80000000000000
2024-04-30 11:33:53) Info: Lattice write time is 18.8000000000000, in steps is
2024-04-30 11:33:53) Info: Next lattice write time is 378000
2024-04-30 11:33:53) Info: Wrote 63 data sets (1056967191 bytes) in the last
60.10 seconds (1.93 seconds writing). 0 datasets queued. Flushing.
2024-04-30 11:33:54) Info: Time is 18.90000000000000
2024-04-30 11:33:54) Info: Lattice write time is 18.900000000000, in steps is
2024-04-30 11:33:54) Info: Next lattice write time is 380000
2024-04-30 11:33:55) Info: Time is 19.00000000000000
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2024-04-30 11:33:55) Info: Lattice write time is 19.000000000000, in steps is
380000
2024-04-30 11:33:55) Info: Next lattice write time is 382000
2024-04-30 11:33:56) Info: Time is 19.10000000000000
2024-04-30 11:33:56) Info: Lattice write time is 19.1000000000000, in steps is
382000
2024-04-30 11:33:56) Info: Next lattice write time is 384000
2024-04-30 11:33:57) Info: Time is 19.20000000000000
2024-04-30 11:33:57) Info: Lattice write time is 19.2000000000000, in steps is
384000
2024-04-30 11:33:57) Info: Next lattice write time is 386000
2024-04-30 11:33:58) Info: Time is 19.30000000000000
2024-04-30 11:33:58) Info: Lattice write time is 19.3000000000000, in steps is
386000
2024-04-30 11:33:58) Info: Next lattice write time is 388000
2024-04-30 11:33:59) Info: Time is 19.40000000000000
2024-04-30 11:33:59) Info: Lattice write time is 19.4000000000000, in steps is
388000
2024-04-30 11:33:59) Info: Next lattice write time is 390000
2024-04-30 11:34:00) Info: Time is 19.5000000000000
2024-04-30 11:34:00) Info: Lattice write time is 19.5000000000000, in steps is
390000
2024-04-30 11:34:00) Info: Next lattice write time is 392000
2024-04-30 11:34:01) Info: Time is 19.60000000000000
2024-04-30 11:34:01) Info: Lattice write time is 19.600000000000, in steps is
392000
2024-04-30 11:34:01) Info: Next lattice write time is 394000
2024-04-30 11:34:02) Info: Time is 19.7000000000000
2024-04-30 11:34:02) Info: Lattice write time is 19.7000000000000, in steps is
394000
2024-04-30 11:34:02) Info: Next lattice write time is 396000
2024-04-30 11:34:03) Info: Time is 19.80000000000000
2024-04-30 11:34:03) Info: Lattice write time is 19.8000000000000, in steps is
396000
2024-04-30 11:34:03) Info: Next lattice write time is 398000
2024-04-30 11:34:04) Info: Time is 19.90000000000000
2024-04-30 11:34:04) Info: Lattice write time is 19.9000000000000, in steps is
398000
2024-04-30 11:34:04) Info: Next lattice write time is 400000
2024-04-30 11:34:05) Info: Time is 20.00000000000000
2024-04-30 11:34:05) Info: Lattice write time is 20.0000000000000, in steps is
400000
2024-04-30 11:34:05) Info: Next lattice write time is 402000
2024-04-30 11:34:06) Info: Time is 20.10000000000000
2024-04-30 11:34:06) Info: Lattice write time is 20.100000000000, in steps is
2024-04-30 11:34:06) Info: Next lattice write time is 404000
2024-04-30 11:34:07) Info: Time is 20.20000000000000
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2024-04-30 11:34:07) Info: Lattice write time is 20.2000000000000, in steps is
404000
2024-04-30 11:34:07) Info: Next lattice write time is 406000
2024-04-30 11:34:08) Info: Time is 20.30000000000000
2024-04-30 11:34:08) Info: Lattice write time is 20.3000000000000, in steps is
406000
2024-04-30 11:34:08) Info: Next lattice write time is 408000
2024-04-30 11:34:09) Info: Time is 20.4000000000000
2024-04-30 11:34:09) Info: Lattice write time is 20.4000000000000, in steps is
408000
2024-04-30 11:34:09) Info: Next lattice write time is 410000
2024-04-30 11:34:10) Info: Time is 20.50000000000000
2024-04-30 11:34:10) Info: Lattice write time is 20.5000000000000, in steps is
410000
2024-04-30 11:34:10) Info: Next lattice write time is 412000
2024-04-30 11:34:11) Info: Time is 20.60000000000000
2024-04-30 11:34:11) Info: Lattice write time is 20.6000000000000, in steps is
412000
2024-04-30 11:34:11) Info: Next lattice write time is 414000
2024-04-30 11:34:12) Info: Time is 20.70000000000000
2024-04-30 11:34:12) Info: Lattice write time is 20.7000000000000, in steps is
414000
2024-04-30 11:34:12) Info: Next lattice write time is 416000
2024-04-30 11:34:13) Info: Time is 20.8000000000000
2024-04-30 11:34:13) Info: Lattice write time is 20.8000000000000, in steps is
416000
2024-04-30 11:34:13) Info: Next lattice write time is 418000
2024-04-30 11:34:14) Info: Time is 20.90000000000000
2024-04-30 11:34:14) Info: Lattice write time is 20.900000000000, in steps is
418000
2024-04-30 11:34:14) Info: Next lattice write time is 420000
2024-04-30 11:34:15) Info: Time is 21.00000000000000
2024-04-30 11:34:15) Info: Lattice write time is 21.0000000000000, in steps is
420000
2024-04-30 11:34:15) Info: Next lattice write time is 422000
2024-04-30 11:34:16) Info: Time is 21.10000000000000
2024-04-30 11:34:16) Info: Lattice write time is 21.1000000000000, in steps is
422000
2024-04-30 11:34:16) Info: Next lattice write time is 424000
2024-04-30 11:34:17) Info: Time is 21.20000000000000
2024-04-30 11:34:17) Info: Lattice write time is 21.2000000000000, in steps is
424000
2024-04-30 11:34:17) Info: Next lattice write time is 426000
2024-04-30 11:34:18) Info: Time is 21.30000000000000
2024-04-30 11:34:18) Info: Lattice write time is 21.300000000000, in steps is
2024-04-30 11:34:18) Info: Next lattice write time is 428000
2024-04-30 11:34:19) Info: Time is 21.40000000000000
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2024-04-30 11:34:19) Info: Lattice write time is 21.4000000000000, in steps is
428000
2024-04-30 11:34:19) Info: Next lattice write time is 430000
2024-04-30 11:34:20) Info: Time is 21.50000000000000
2024-04-30 11:34:20) Info: Lattice write time is 21.5000000000000, in steps is
430000
2024-04-30 11:34:20) Info: Next lattice write time is 432000
2024-04-30 11:34:21) Info: Time is 21.60000000000000
2024-04-30 11:34:21) Info: Lattice write time is 21.6000000000000, in steps is
432000
2024-04-30 11:34:21) Info: Next lattice write time is 434000
2024-04-30 11:34:22) Info: Time is 21.70000000000000
2024-04-30 11:34:22) Info: Lattice write time is 21.7000000000000, in steps is
434000
2024-04-30 11:34:22) Info: Next lattice write time is 436000
2024-04-30 11:34:23) Info: Time is 21.80000000000000
2024-04-30 11:34:23) Info: Lattice write time is 21.8000000000000, in steps is
2024-04-30 11:34:23) Info: Next lattice write time is 438000
2024-04-30 11:34:24) Info: Time is 21.9000000000000
2024-04-30 11:34:24) Info: Lattice write time is 21.9000000000000, in steps is
438000
2024-04-30 11:34:24) Info: Next lattice write time is 440000
2024-04-30 11:34:25) Info: Time is 22.0000000000000
2024-04-30 11:34:25) Info: Lattice write time is 22.0000000000000, in steps is
440000
2024-04-30 11:34:25) Info: Next lattice write time is 442000
2024-04-30 11:34:26) Info: Time is 22.1000000000000
2024-04-30 11:34:26) Info: Lattice write time is 22.1000000000000, in steps is
442000
2024-04-30 11:34:26) Info: Next lattice write time is 444000
2024-04-30 11:34:27) Info: Time is 22.2000000000000
2024-04-30 11:34:27) Info: Lattice write time is 22.2000000000000, in steps is
444000
2024-04-30 11:34:27) Info: Next lattice write time is 446000
2024-04-30 11:34:28) Info: Time is 22.3000000000000
2024-04-30 11:34:28) Info: Lattice write time is 22.3000000000000, in steps is
446000
2024-04-30 11:34:28) Info: Next lattice write time is 448000
2024-04-30 11:34:29) Info: Time is 22.4000000000000
2024-04-30 11:34:29) Info: Lattice write time is 22.4000000000000, in steps is
448000
2024-04-30 11:34:29) Info: Next lattice write time is 450000
2024-04-30 11:34:30) Info: Time is 22.50000000000000
2024-04-30 11:34:30) Info: Lattice write time is 22.500000000000, in steps is
2024-04-30 11:34:30) Info: Next lattice write time is 452000
2024-04-30 11:34:31) Info: Time is 22.60000000000000
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2024-04-30 11:34:31) Info: Lattice write time is 22.6000000000000, in steps is
452000
2024-04-30 11:34:31) Info: Next lattice write time is 454000
2024-04-30 11:34:32) Info: Time is 22.7000000000000
2024-04-30 11:34:32) Info: Lattice write time is 22.7000000000000, in steps is
454000
2024-04-30 11:34:32) Info: Next lattice write time is 456000
2024-04-30 11:34:33) Info: Time is 22.8000000000000
2024-04-30 11:34:33) Info: Lattice write time is 22.8000000000000, in steps is
456000
2024-04-30 11:34:33) Info: Next lattice write time is 458000
2024-04-30 11:34:34) Info: Time is 22.90000000000000
2024-04-30 11:34:34) Info: Lattice write time is 22.9000000000000, in steps is
458000
2024-04-30 11:34:34) Info: Next lattice write time is 460000
2024-04-30 11:34:35) Info: Time is 23.00000000000000
2024-04-30 11:34:35) Info: Lattice write time is 23.0000000000000, in steps is
2024-04-30 11:34:35) Info: Next lattice write time is 462000
2024-04-30 11:34:36) Info: Time is 23.1000000000000
2024-04-30 11:34:36) Info: Lattice write time is 23.1000000000000, in steps is
462000
2024-04-30 11:34:36) Info: Next lattice write time is 464000
2024-04-30 11:34:37) Info: Time is 23.2000000000000
2024-04-30 11:34:37) Info: Lattice write time is 23.2000000000000, in steps is
464000
2024-04-30 11:34:37) Info: Next lattice write time is 466000
2024-04-30 11:34:38) Info: Time is 23.30000000000000
2024-04-30 11:34:38) Info: Lattice write time is 23.3000000000000, in steps is
466000
2024-04-30 11:34:38) Info: Next lattice write time is 468000
2024-04-30 11:34:39) Info: Time is 23.40000000000000
2024-04-30 11:34:39) Info: Lattice write time is 23.4000000000000, in steps is
468000
2024-04-30 11:34:39) Info: Next lattice write time is 470000
2024-04-30 11:34:40) Info: Time is 23.50000000000000
2024-04-30 11:34:40) Info: Lattice write time is 23.5000000000000, in steps is
470000
2024-04-30 11:34:40) Info: Next lattice write time is 472000
2024-04-30 11:34:41) Info: Time is 23.60000000000000
2024-04-30 11:34:41) Info: Lattice write time is 23.6000000000000, in steps is
472000
2024-04-30 11:34:41) Info: Next lattice write time is 474000
2024-04-30 11:34:42) Info: Time is 23.70000000000000
2024-04-30 11:34:42) Info: Lattice write time is 23.700000000000, in steps is
2024-04-30 11:34:42) Info: Next lattice write time is 476000
2024-04-30 11:34:43) Info: Time is 23.80000000000000
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2024-04-30 11:34:43) Info: Lattice write time is 23.8000000000000, in steps is
476000
2024-04-30 11:34:43) Info: Next lattice write time is 478000
2024-04-30 11:34:44) Info: Time is 23.90000000000000
2024-04-30 11:34:44) Info: Lattice write time is 23.9000000000000, in steps is
478000
2024-04-30 11:34:44) Info: Next lattice write time is 480000
2024-04-30 11:34:45) Info: Time is 24.00000000000000
2024-04-30 11:34:45) Info: Lattice write time is 24.0000000000000, in steps is
480000
2024-04-30 11:34:45) Info: Next lattice write time is 482000
2024-04-30 11:34:46) Info: Time is 24.10000000000000
2024-04-30 11:34:46) Info: Lattice write time is 24.1000000000000, in steps is
482000
2024-04-30 11:34:46) Info: Next lattice write time is 484000
2024-04-30 11:34:47) Info: Time is 24.20000000000000
2024-04-30 11:34:47) Info: Lattice write time is 24.2000000000000, in steps is
484000
2024-04-30 11:34:47) Info: Next lattice write time is 486000
2024-04-30 11:34:48) Info: Time is 24.3000000000000
2024-04-30 11:34:48) Info: Lattice write time is 24.3000000000000, in steps is
486000
2024-04-30 11:34:48) Info: Next lattice write time is 488000
2024-04-30 11:34:49) Info: Time is 24.4000000000000
2024-04-30 11:34:49) Info: Lattice write time is 24.4000000000000, in steps is
488000
2024-04-30 11:34:49) Info: Next lattice write time is 490000
2024-04-30 11:34:50) Info: Time is 24.50000000000000
2024-04-30 11:34:50) Info: Lattice write time is 24.5000000000000, in steps is
490000
2024-04-30 11:34:50) Info: Next lattice write time is 492000
2024-04-30 11:34:51) Info: Time is 24.60000000000000
2024-04-30 11:34:51) Info: Lattice write time is 24.6000000000000, in steps is
492000
2024-04-30 11:34:51) Info: Next lattice write time is 494000
2024-04-30 11:34:52) Info: Average walltime per timestep: 0.50 ms. Progress:
24.6989s/30.0000s (82.3% done / 53 seconds walltime remaining)
2024-04-30 11:34:52) Info: Time is 24.70000000000000
2024-04-30 11:34:52) Info: Lattice write time is 24.7000000000000, in steps is
494000
2024-04-30 11:34:52) Info: Next lattice write time is 496000
2024-04-30 11:34:53) Info: Time is 24.80000000000000
2024-04-30 11:34:53) Info: Lattice write time is 24.800000000000, in steps is
496000
2024-04-30 11:34:53) Info: Next lattice write time is 498000
2024-04-30 11:34:54) Info: Time is 24.90000000000000
2024-04-30 11:34:54) Info: Lattice write time is 24.90000000000000, in steps is
498000
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2024-04-30 11:34:54) Info: Next lattice write time is 500000
2024-04-30 11:34:54) Info: Wrote 61 data sets (1023412677 bytes) in the last
60.91 seconds (1.90 seconds writing). 0 datasets queued. Flushing.
2024-04-30 11:34:55) Info: Time is 25.00000000000000
2024-04-30 11:34:55) Info: Lattice write time is 25.0000000000000, in steps is
500000
2024-04-30 11:34:55) Info: Next lattice write time is 502000
2024-04-30 11:34:56) Info: Time is 25.1000000000000
2024-04-30 11:34:56) Info: Lattice write time is 25.1000000000000, in steps is
502000
2024-04-30 11:34:56) Info: Next lattice write time is 504000
2024-04-30 11:34:57) Info: Time is 25.20000000000000
2024-04-30 11:34:57) Info: Lattice write time is 25.200000000000, in steps is
504000
2024-04-30 11:34:57) Info: Next lattice write time is 506000
2024-04-30 11:34:58) Info: Time is 25.30000000000000
2024-04-30 11:34:58) Info: Lattice write time is 25.300000000000, in steps is
506000
2024-04-30 11:34:58) Info: Next lattice write time is 508000
2024-04-30 11:34:59) Info: Time is 25.4000000000000
2024-04-30 11:34:59) Info: Lattice write time is 25.4000000000000, in steps is
508000
2024-04-30 11:34:59) Info: Next lattice write time is 510000
2024-04-30 11:35:00) Info: Time is 25.50000000000000
2024-04-30 11:35:00) Info: Lattice write time is 25.5000000000000, in steps is
510000
2024-04-30 11:35:00) Info: Next lattice write time is 512000
2024-04-30 11:35:01) Info: Time is 25.60000000000000
2024-04-30 11:35:01) Info: Lattice write time is 25.6000000000000, in steps is
512000
2024-04-30 11:35:01) Info: Next lattice write time is 514000
2024-04-30 11:35:02) Info: Time is 25.7000000000000
2024-04-30 11:35:02) Info: Lattice write time is 25.7000000000000, in steps is
514000
2024-04-30 11:35:02) Info: Next lattice write time is 516000
2024-04-30 11:35:03) Info: Time is 25.80000000000000
2024-04-30 11:35:03) Info: Lattice write time is 25.8000000000000, in steps is
516000
2024-04-30 11:35:03) Info: Next lattice write time is 518000
2024-04-30 11:35:04) Info: Time is 25.90000000000000
2024-04-30 11:35:04) Info: Lattice write time is 25.900000000000, in steps is
518000
2024-04-30 11:35:04) Info: Next lattice write time is 520000
2024-04-30 11:35:05) Info: Time is 26.00000000000000
2024-04-30 11:35:05) Info: Lattice write time is 26.000000000000, in steps is
2024-04-30 11:35:05) Info: Next lattice write time is 522000
2024-04-30 11:35:06) Info: Time is 26.10000000000000
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2024-04-30 11:35:06) Info: Lattice write time is 26.1000000000000, in steps is
522000
2024-04-30 11:35:06) Info: Next lattice write time is 524000
2024-04-30 11:35:07) Info: Time is 26.20000000000000
2024-04-30 11:35:07) Info: Lattice write time is 26.2000000000000, in steps is
524000
2024-04-30 11:35:07) Info: Next lattice write time is 526000
2024-04-30 11:35:08) Info: Time is 26.30000000000000
2024-04-30 11:35:08) Info: Lattice write time is 26.3000000000000, in steps is
526000
2024-04-30 11:35:08) Info: Next lattice write time is 528000
2024-04-30 11:35:09) Info: Time is 26.40000000000000
2024-04-30 11:35:09) Info: Lattice write time is 26.4000000000000, in steps is
528000
2024-04-30 11:35:09) Info: Next lattice write time is 530000
2024-04-30 11:35:10) Info: Time is 26.50000000000000
2024-04-30 11:35:10) Info: Lattice write time is 26.5000000000000, in steps is
530000
2024-04-30 11:35:10) Info: Next lattice write time is 532000
2024-04-30 11:35:11) Info: Time is 26.60000000000000
2024-04-30 11:35:11) Info: Lattice write time is 26.6000000000000, in steps is
532000
2024-04-30 11:35:11) Info: Next lattice write time is 534000
2024-04-30 11:35:12) Info: Time is 26.70000000000000
2024-04-30 11:35:12) Info: Lattice write time is 26.7000000000000, in steps is
534000
2024-04-30 11:35:12) Info: Next lattice write time is 536000
2024-04-30 11:35:13) Info: Time is 26.80000000000000
2024-04-30 11:35:13) Info: Lattice write time is 26.8000000000000, in steps is
536000
2024-04-30 11:35:13) Info: Next lattice write time is 538000
2024-04-30 11:35:14) Info: Time is 26.90000000000000
2024-04-30 11:35:14) Info: Lattice write time is 26.900000000000, in steps is
538000
2024-04-30 11:35:14) Info: Next lattice write time is 540000
2024-04-30 11:35:15) Info: Time is 27.00000000000000
2024-04-30 11:35:15) Info: Lattice write time is 27.0000000000000, in steps is
540000
2024-04-30 11:35:15) Info: Next lattice write time is 542000
2024-04-30 11:35:16) Info: Time is 27.10000000000000
2024-04-30 11:35:16) Info: Lattice write time is 27.1000000000000, in steps is
542000
2024-04-30 11:35:16) Info: Next lattice write time is 544000
2024-04-30 11:35:17) Info: Time is 27.20000000000000
2024-04-30 11:35:17) Info: Lattice write time is 27.200000000000, in steps is
2024-04-30 11:35:17) Info: Next lattice write time is 546000
2024-04-30 11:35:18) Info: Time is 27.3000000000000
```

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2024-04-30 11:35:18) Info: Lattice write time is 27.3000000000000, in steps is
546000
2024-04-30 11:35:18) Info: Next lattice write time is 548000
2024-04-30 11:35:19) Info: Time is 27.40000000000000
2024-04-30 11:35:19) Info: Lattice write time is 27.4000000000000, in steps is
548000
2024-04-30 11:35:19) Info: Next lattice write time is 550000
2024-04-30 11:35:20) Info: Time is 27.50000000000000
2024-04-30 11:35:20) Info: Lattice write time is 27.5000000000000, in steps is
550000
2024-04-30 11:35:20) Info: Next lattice write time is 552000
2024-04-30 11:35:21) Info: Time is 27.60000000000000
2024-04-30 11:35:21) Info: Lattice write time is 27.6000000000000, in steps is
552000
2024-04-30 11:35:21) Info: Next lattice write time is 554000
2024-04-30 11:35:22) Info: Time is 27.70000000000000
2024-04-30 11:35:22) Info: Lattice write time is 27.7000000000000, in steps is
554000
2024-04-30 11:35:22) Info: Next lattice write time is 556000
2024-04-30 11:35:23) Info: Time is 27.8000000000000
2024-04-30 11:35:23) Info: Lattice write time is 27.8000000000000, in steps is
556000
2024-04-30 11:35:23) Info: Next lattice write time is 558000
2024-04-30 11:35:24) Info: Time is 27.9000000000000
2024-04-30 11:35:24) Info: Lattice write time is 27.900000000000, in steps is
558000
2024-04-30 11:35:24) Info: Next lattice write time is 560000
2024-04-30 11:35:25) Info: Time is 28.00000000000000
2024-04-30 11:35:25) Info: Lattice write time is 28.0000000000000, in steps is
560000
2024-04-30 11:35:25) Info: Next lattice write time is 562000
2024-04-30 11:35:26) Info: Time is 28.1000000000000
2024-04-30 11:35:26) Info: Lattice write time is 28.1000000000000, in steps is
562000
2024-04-30 11:35:26) Info: Next lattice write time is 564000
2024-04-30 11:35:27) Info: Time is 28.20000000000000
2024-04-30 11:35:27) Info: Lattice write time is 28.2000000000000, in steps is
564000
2024-04-30 11:35:27) Info: Next lattice write time is 566000
2024-04-30 11:35:28) Info: Time is 28.30000000000000
2024-04-30 11:35:28) Info: Lattice write time is 28.3000000000000, in steps is
566000
2024-04-30 11:35:28) Info: Next lattice write time is 568000
2024-04-30 11:35:29) Info: Time is 28.40000000000000
2024-04-30 11:35:29) Info: Lattice write time is 28.400000000000, in steps is
2024-04-30 11:35:29) Info: Next lattice write time is 570000
2024-04-30 11:35:30) Info: Time is 28.50000000000000
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2024-04-30 11:35:30) Info: Lattice write time is 28.5000000000000, in steps is
570000
2024-04-30 11:35:30) Info: Next lattice write time is 572000
2024-04-30 11:35:31) Info: Time is 28.60000000000000
2024-04-30 11:35:31) Info: Lattice write time is 28.6000000000000, in steps is
572000
2024-04-30 11:35:31) Info: Next lattice write time is 574000
2024-04-30 11:35:32) Info: Time is 28.7000000000000
2024-04-30 11:35:32) Info: Lattice write time is 28.7000000000000, in steps is
574000
2024-04-30 11:35:32) Info: Next lattice write time is 576000
2024-04-30 11:35:33) Info: Time is 28.80000000000000
2024-04-30 11:35:33) Info: Lattice write time is 28.8000000000000, in steps is
576000
2024-04-30 11:35:33) Info: Next lattice write time is 578000
2024-04-30 11:35:34) Info: Time is 28.90000000000000
2024-04-30 11:35:34) Info: Lattice write time is 28.900000000000, in steps is
578000
2024-04-30 11:35:34) Info: Next lattice write time is 580000
2024-04-30 11:35:35) Info: Time is 29.00000000000000
2024-04-30 11:35:35) Info: Lattice write time is 29.0000000000000, in steps is
580000
2024-04-30 11:35:35) Info: Next lattice write time is 582000
2024-04-30 11:35:36) Info: Time is 29.1000000000000
2024-04-30 11:35:36) Info: Lattice write time is 29.1000000000000, in steps is
582000
2024-04-30 11:35:36) Info: Next lattice write time is 584000
2024-04-30 11:35:37) Info: Time is 29.20000000000000
2024-04-30 11:35:37) Info: Lattice write time is 29.2000000000000, in steps is
584000
2024-04-30 11:35:37) Info: Next lattice write time is 586000
2024-04-30 11:35:38) Info: Time is 29.30000000000000
2024-04-30 11:35:38) Info: Lattice write time is 29.3000000000000, in steps is
586000
2024-04-30 11:35:38) Info: Next lattice write time is 588000
2024-04-30 11:35:39) Info: Time is 29.40000000000000
2024-04-30 11:35:39) Info: Lattice write time is 29.4000000000000, in steps is
588000
2024-04-30 11:35:39) Info: Next lattice write time is 590000
2024-04-30 11:35:40) Info: Time is 29.50000000000000
2024-04-30 11:35:40) Info: Lattice write time is 29.5000000000000, in steps is
590000
2024-04-30 11:35:40) Info: Next lattice write time is 592000
2024-04-30 11:35:41) Info: Time is 29.60000000000000
2024-04-30 11:35:41) Info: Lattice write time is 29.600000000000, in steps is
2024-04-30 11:35:41) Info: Next lattice write time is 594000
2024-04-30 11:35:42) Info: Time is 29.70000000000000
```

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2024-04-30 11:35:42) Info: Lattice write time is 29.7000000000000, in steps is
594000
2024-04-30 11:35:42) Info: Next lattice write time is 596000
2024-04-30 11:35:43) Info: Time is 29.80000000000000
2024-04-30 11:35:43) Info: Lattice write time is 29.8000000000000, in steps is
596000
2024-04-30 11:35:43) Info: Next lattice write time is 598000
2024-04-30 11:35:44) Info: Time is 29.90000000000000
2024-04-30 11:35:44) Info: Lattice write time is 29.9000000000000, in steps is
598000
2024-04-30 11:35:44) Info: Next lattice write time is 600000
2024-04-30 11:35:45) Info: Time is 30.00000000000000
2024-04-30 11:35:45) Info: Lattice write time is 30.0000000000000, in steps is
600000
2024-04-30 11:35:45) Info: Next lattice write time is 602000
2024-04-30 11:35:45) Info: Data output thread finished.
2024-04-30 11:35:45) Info: Simulation file closed.
```

[28]: <jLM.RDME.File at 0x7f1fd0496a90>

# 5 4. Analysis

The trajectory will be saved as h5 format, we need the python package h5py to access it, or you can download the HDFView to see it in a GUI.

```
[29]: import matplotlib.pyplot as plt import seaborn as sns from jLM.RDME import File as RDMEFile
```

```
[30]: # traj_file = h5py.File('T1_bimolecular.lm ', 'r')
traj = RDMEFile(filename)
ts, As = traj.getNumberTrajectory(species="A")
ts, Bs = traj.getNumberTrajectory(species="B")
ts, Cs = traj.getNumberTrajectory(species="C")
```

```
[31]: # now visuzlize the trajectories with seaborn and plt
sns.set(style="whitegrid")
# Create a color palette
palette = sns.color_palette()
plt.figure(figsize=(10,6))
plt.plot(ts, As, label='A',marker='o', linestyle='-',color=palette[0])
plt.plot(ts, Bs, label='B',marker='x', linestyle='--',color=palette[1])
plt.plot(ts, Cs, label='C',color=palette[2])

plt.title('Trajectories of Biomolecular System with polar distribution')
plt.xlabel('Time (s)')
plt.ylabel('Counts')
```

```
plt.legend()
plt.savefig('./images/TutR1.2_bimolecular_polardis.png')
plt.show()
```

