TutR2_GeneticInfoProcessing

April 30, 2024

1 TutR2_Genetic Information Process Model

Here we create a simple model includes the simple genetic information processing(GIP):

[27]:
```
import jLM
from jLM.RegionBuilder import RegionBuilder
from jLM.RDME import Sim as RDMESim
from jLM.RDME import File as RDMEFile

import lm
from lm import IntMpdRdmeSolver


import numpy as np
```

2 1. Create the RDME simulation Object

[28]:
```
totalTime = 60             # total simulation time, in seconds
timeStep = 50e-6             # time step, in seconds
writeInterval = 20000         # the times steps write the info into␣
 ↪trajectories, units of timeStep, 20000 * 50e-6 = 1s
```

[29]:
```
from pyLM import LMLogger
LMLogger.setLMLogConsole()
#(logging.DEBUG)
```

[30]:
```
lattice_spacing = 8e-9 #m
N_edges = [64, 64, 64]
sim_center = [int(N_edges[0]/2),int(N_edges[1]/2),int(N_edges[2]/2)]
N_2_x=int(N_edges[0]/2)
N_2_y=int(N_edges[1]/2)
N_2_z=int(N_edges[2]/2)

filename = 'TutR2.GIP_result.lm'
```

[31]:
```
sim = RDMESim("T2_GIP",
                  filename,
                  N_edges,
                  lattice_spacing,
                  "extracellular")

sim.timestep = timeStep
sim.simulationTime=totalTime
sim.latticeWriteInterval=writeInterval
sim.speciesWriteInterval=writeInterval

sim.transitionRate(None, None, None, sim.diffusionZero)
```

3 2. Build up the Minimal Cell Spatial Geometry

We use the minimal bacteria cell JCVI-syn3A as the spatial cell geometry for our genetic information process system.

[32]:
```
radius_nm = 2.00e-7 #m minimal cell radius
cyto_radius = radius_nm/sim.latticeSpacing  #converted to lattice sites, # of␣
 ↪lattice sites from the center to the edge of the cell
```

[33]:
```
build = RegionBuilder(sim)

# create a sphere region as the cytoplasm
cytoplasm = build.ellipsoid(radius = cyto_radius, center = sim_center)
# create a spherical surface  as the shell region of the cell
cyto_dilation = build.dilate(cytoplasm, se = build.se26)
shell = cyto_dilation & ~cytoplasm

# create a spherical surface as the membrane
cyto_dilation = build.dilate(cyto_dilation, se = build.se26)
membrane = cyto_dilation & ~shell & ~cytoplasm
```

randomly place 500 ribosomes in cytoplasm:

[34]:
```
import T2_loading as loader

ribosomes = loader.getRibosomeSites(cytoplasm, N_edges)
```

Load the geometry of DNA from file

[35]:
```
# Load the DNA file generated from b-Tree Chromo
DNAfile = './supporting_data/x_chain_syn3a_rep00001.bin'# DNA bin file

DNAsites, DNA_pos = loader.getDNAsites(DNAfile, N_edges,lattice_spacing, N_2_x,␣
 ↪N_2_y, N_2_z)
```

```
# define cyto plasm and extra cellular region
cytoplasm = cytoplasm & ~DNAsites
extracellular = ~membrane & ~cytoplasm & ~ribosomes & ~DNAsites
```

[36]:
```
build.compose(
    (sim.region('extracellular'), extracellular),
    (sim.region('cytoplasm'), cytoplasm),
    (sim.region('DNA'),DNAsites),
    (sim.region('ribosomes'), ribosomes),
    (sim.region('shell'), shell),
    (sim.region('membrane'), membrane))
```

[37]:
```
ext=sim.region('extracellular')
cyt=sim.region('cytoplasm')
dna=sim.region('DNA')
ribo=sim.region('ribosomes')
she=sim.region('shell')
mem=sim.region('membrane')
```

[38]:
```
sim.displayGeometry()
```

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

4 3. Define all species

[39]:
```
with sim.construct():
    sim.species("gene", texRepr="gene", annotation="gene in gene info process")
    sim.species("mRNA", textRepr="mRNA", annotation="mRNA in gene info process")
    sim.species("mRNAr", textRepr="mRNA_{read}", annotation="mRNA after the␣
 ↪translation")
    sim.species("P", texRepr="Protein", annotation="Protein in gene info␣
 ↪process")
```

<IPython.core.display.HTML object>

[40]:
```
sp = sim.sp   # species object access
reg = sim.reg # region object access
rc = sim.rc   # rate constant object access
dc = sim.dc   # diffusion constant object access
```

[41]:
```
sim.transitionRate(None, None, None, sim.diffusionZero)
```

5 4. Define reactions and diffusions

After the mRNA transcribed from the gene represented as a particle in the Gene start site in the 3 dimensional lattice; we only allow mRNA to diffuse out of the `DNA` region to `cytoplasm` and we don't allow the particle to diffuse within the `DNA` region.

We also need to allow the mRNA to diffuse into the ribosome and out-of ribosome for the translation. Here, to prevent the mRNA getting trapped inside the `ribosomes`, and constantly translating, we form a new particle called $mRNA_{read}$.

$mRNA_{read}$ can be instantly convert back to m_{RNA} out side `ribosomes`.

[42]:
```
with sim.construct():
    sim.rateConst("trans", 0.019, order=1, annotation="transcription rate")
    sim.rateConst("transl", 0.0029, order=1, annotation="translation rate")
    sim.rateConst("degrad_m", 0.0023, order=1, annotation="mRNA degradation␣
 ↪rate")
    sim.rateConst("degrad_p", 7.7e-6, order=1, annotation="Protein degradation␣
 ↪rate")
    sim.rateConst("conversion", 1000000, order= 1, annotation="Conversion rate␣
 ↪from mRNA read state to ready state")
    # define all necessary reactions
    # transcription
    sim.reaction([sp.gene], [sp.gene, sp.mRNA], rc.trans, regions=[reg.DNA],␣
 ↪annotation="transcription")
    # mRNA degradation
    sim.reaction([sp.mRNA], [], rc.degrad_m, regions=[reg.shell],␣
 ↪annotation="mRNA degradation")
    sim.reaction([sp.mRNAr],[], rc.degrad_m, regions=[reg.shell],␣
 ↪annotation="mRNA read degradation")
    # translation
    sim.reaction([sp.mRNA], [sp.mRNAr, sp.P], rc.transl, regions=[reg.
 ↪ribosomes], annotation="translation")
    # protein degradation
    sim.reaction([sp.P], [], rc.degrad_p, regions=[reg.shell],␣
 ↪annotation="Protein degradation")

    # conversion from mRNA read state to ready state
    sim.reaction([sp.mRNAr], [sp.mRNA], rc.conversion, regions=[reg.shell, reg.
 ↪cytoplasm], annotation="Conversion from mRNA read state to ready state")
```

```
<IPython.core.display.HTML object>
```

now we need all the diffusion coefficients defined:

[43]:
```
with sim.construct():
    sim.transitionRate(None, None, None, sim.diffusionZero)
```

[44]:
```
with sim.construct():
    sim.diffusionConst('mrna',4.13e-14, texRepr=r'D_{mRNA}', annotation="mRNA␣
 ↪diffusion constant for JCVISYN3A_0001")
    sim.diffusionConst('protein', 0.1e-12, texRepr=r'Protein',␣
 ↪annotation="protein diffusion co.")
    # diffusion for mrna
    sim.transitionRate(sp.mRNA, reg.DNA, reg.cytoplasm, dc.mrna)
    sim.transitionRate(sp.mRNA, reg.cytoplasm, reg.ribosomes, dc.mrna)
    sim.transitionRate(sp.mRNA, reg.cytoplasm, reg.cytoplasm, dc.mrna)
    sim.transitionRate(sp.mRNA, reg.ribosomes, reg.ribosomes, dc.mrna)
    # diffusion for mrna_read, it is the read state after the mrna translation,
    # mrna_read formed in ribsomes, and conversion happen in cytoplasm and shell
    # so we must allow it to diffuse in cytoplasm and shell
    sim.transitionRate(sp.mRNAr, reg.ribosomes, reg.ribosomes, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.ribosomes, reg.cytoplasm, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.ribosomes, reg.shell, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.cytoplasm, reg.cytoplasm, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.cytoplasm, reg.shell, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.shell, reg.shell, dc.mrna)
    sim.transitionRate(sp.mRNAr, reg.shell, reg.cytoplasm, dc.mrna)

    # diffusion for protein
    sim.transitionRate(sp.P, reg.ribosomes, reg.ribosomes, dc.protein)
    sim.transitionRate(sp.P, reg.ribosomes, reg.cytoplasm, dc.protein)
    sim.transitionRate(sp.P, reg.ribosomes, reg.shell, dc.protein)
    sim.transitionRate(sp.P, reg.cytoplasm, reg.cytoplasm, dc.protein)
    sim.transitionRate(sp.P, reg.cytoplasm, reg.shell, dc.protein)
    sim.transitionRate(sp.P, reg.shell, reg.shell, dc.protein)
    sim.transitionRate(sp.P, reg.shell, reg.cytoplasm, dc.protein)
```

```
<IPython.core.display.HTML object>
```

6 5. Initial counts

We need one DNA particle in the starting site to represent gene. Since our gene is JCVISYN3A_0001, we put the gene particle in the first lattice cube of DNA_region.

Other species inital counts all set to be 0:

#gene = 1

#mRNA = 1

#mRNA_read = 0

#Protein = 0

[45]:
```
gene_pos = DNA_pos[0]
sim.placeNumber(sp=sp.gene,x=gene_pos[0], y=gene_pos[1], z=gene_pos[2], n=1)
```

```
# then we randomly put one mRNA in the cytoplasm
sim.distributeNumber(sp=sp.mRNA, reg=reg.cytoplasm, count=1)
```

[46]:
```
sim.showAllSpecies()
```

[46]:
```
<IPython.core.display.HTML object>
```

[47]:
```
sim
```

[47]:
```
<jLM.RDME.Sim at 0x7feddefc0518>
```

[48]:
```
sim.finalize()
```

7 6. Run the simulation

[49]:
```
sim.run(solver=IntMpdRdmeSolver(), cudaDevices=[0])
```

```
2024-04-30 12:09:20) Info: Using 32 processor(s) and 1 CUDA device(s) per
process.
2024-04-30 12:09:20) Info: Assigning 1.00 processor(s) and 1.00 CUDA device(s)
per replicate.
2024-04-30 12:09:20) Info: Data output thread running.
2024-04-30 12:09:29) Info: Time is 1.00000000000000
2024-04-30 12:09:29) Info: Lattice write time is 1.00000000000000, in steps is
20000
2024-04-30 12:09:29) Info: Next lattice write time is 40000
2024-04-30 12:09:39) Info: Time is 2.00000000000000
2024-04-30 12:09:39) Info: Lattice write time is 2.00000000000000, in steps is
40000
2024-04-30 12:09:39) Info: Next lattice write time is 60000
2024-04-30 12:09:49) Info: Time is 3.00000000000000
2024-04-30 12:09:49) Info: Lattice write time is 3.00000000000000, in steps is
60000
2024-04-30 12:09:49) Info: Next lattice write time is 80000
2024-04-30 12:09:59) Info: Time is 4.00000000000000
2024-04-30 12:09:59) Info: Lattice write time is 4.00000000000000, in steps is
80000
2024-04-30 12:09:59) Info: Next lattice write time is 100000
2024-04-30 12:10:09) Info: Time is 5.00000000000000
2024-04-30 12:10:09) Info: Lattice write time is 5.00000000000000, in steps is
100000
2024-04-30 12:10:09) Info: Next lattice write time is 120000
2024-04-30 12:10:19) Info: Time is 6.00000000000000
2024-04-30 12:10:19) Info: Lattice write time is 6.00000000000000, in steps is
120000
```

```
2024-04-30 12:10:19) Info: Next lattice write time is 140000
2024-04-30 12:10:20) Info: Average walltime per timestep: 0.49 ms. Progress:
6.0836s/60.0000s ( 10.1% done / 8.9 minutes walltime remaining)
2024-04-30 12:10:29) Info: Time is 7.00000000000000
2024-04-30 12:10:29) Info: Lattice write time is 7.00000000000000, in steps is
140000
2024-04-30 12:10:29) Info: Next lattice write time is 160000
2024-04-30 12:10:29) Info: Wrote 7 data sets (117440799 bytes) in the last 69.05
seconds (0.21 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:10:38) Info: Time is 8.00000000000000
2024-04-30 12:10:38) Info: Lattice write time is 8.00000000000000, in steps is
160000
2024-04-30 12:10:38) Info: Next lattice write time is 180000
2024-04-30 12:10:48) Info: Time is 9.00000000000000
2024-04-30 12:10:48) Info: Lattice write time is 9.00000000000000, in steps is
180000
2024-04-30 12:10:48) Info: Next lattice write time is 200000
2024-04-30 12:10:57) Info: Time is 10.00000000000000
2024-04-30 12:10:57) Info: Lattice write time is 10.00000000000000, in steps is
200000
2024-04-30 12:10:57) Info: Next lattice write time is 220000
2024-04-30 12:11:07) Info: Time is 11.00000000000000
2024-04-30 12:11:07) Info: Lattice write time is 11.00000000000000, in steps is
220000
2024-04-30 12:11:07) Info: Next lattice write time is 240000
2024-04-30 12:11:16) Info: Time is 12.00000000000000
2024-04-30 12:11:16) Info: Lattice write time is 12.00000000000000, in steps is
240000
2024-04-30 12:11:16) Info: Next lattice write time is 260000
2024-04-30 12:11:20) Info: Average walltime per timestep: 0.48 ms. Progress:
12.3768s/60.0000s ( 20.6% done / 7.6 minutes walltime remaining)
2024-04-30 12:11:25) Info: Time is 13.00000000000000
2024-04-30 12:11:25) Info: Lattice write time is 13.00000000000000, in steps is
260000
2024-04-30 12:11:25) Info: Next lattice write time is 280000
2024-04-30 12:11:35) Info: Time is 14.00000000000000
2024-04-30 12:11:35) Info: Lattice write time is 14.00000000000000, in steps is
280000
2024-04-30 12:11:35) Info: Next lattice write time is 300000
2024-04-30 12:11:35) Info: Wrote 7 data sets (117440799 bytes) in the last 66.18
seconds (0.21 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:11:44) Info: Time is 15.00000000000000
2024-04-30 12:11:44) Info: Lattice write time is 15.00000000000000, in steps is
300000
2024-04-30 12:11:44) Info: Next lattice write time is 320000
2024-04-30 12:11:54) Info: Time is 16.00000000000000
2024-04-30 12:11:54) Info: Lattice write time is 16.00000000000000, in steps is
320000
```

```
2024-04-30 12:11:54) Info: Next lattice write time is 340000
2024-04-30 12:12:03) Info: Time is 17.00000000000000
2024-04-30 12:12:03) Info: Lattice write time is 17.00000000000000, in steps is
340000
2024-04-30 12:12:03) Info: Next lattice write time is 360000
2024-04-30 12:12:12) Info: Time is 18.00000000000000
2024-04-30 12:12:12) Info: Lattice write time is 18.00000000000000, in steps is
360000
2024-04-30 12:12:12) Info: Next lattice write time is 380000
2024-04-30 12:12:20) Info: Average walltime per timestep: 0.47 ms. Progress:
18.7608s/60.0000s ( 31.3% done / 6.5 minutes walltime remaining)
2024-04-30 12:12:22) Info: Time is 19.00000000000000
2024-04-30 12:12:22) Info: Lattice write time is 19.00000000000000, in steps is
380000
2024-04-30 12:12:22) Info: Next lattice write time is 400000
2024-04-30 12:12:31) Info: Time is 20.00000000000000
2024-04-30 12:12:31) Info: Lattice write time is 20.00000000000000, in steps is
400000
2024-04-30 12:12:31) Info: Next lattice write time is 420000
2024-04-30 12:12:41) Info: Time is 21.00000000000000
2024-04-30 12:12:41) Info: Lattice write time is 21.00000000000000, in steps is
420000
2024-04-30 12:12:41) Info: Next lattice write time is 440000
2024-04-30 12:12:41) Info: Wrote 7 data sets (117440799 bytes) in the last 65.98
seconds (0.23 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:12:50) Info: Time is 22.00000000000000
2024-04-30 12:12:50) Info: Lattice write time is 22.00000000000000, in steps is
440000
2024-04-30 12:12:50) Info: Next lattice write time is 460000
2024-04-30 12:13:00) Info: Time is 23.00000000000000
2024-04-30 12:13:00) Info: Lattice write time is 23.00000000000000, in steps is
460000
2024-04-30 12:13:00) Info: Next lattice write time is 480000
2024-04-30 12:13:09) Info: Time is 24.00000000000000
2024-04-30 12:13:09) Info: Lattice write time is 24.00000000000000, in steps is
480000
2024-04-30 12:13:09) Info: Next lattice write time is 500000
2024-04-30 12:13:18) Info: Time is 25.00000000000000
2024-04-30 12:13:18) Info: Lattice write time is 25.00000000000000, in steps is
500000
2024-04-30 12:13:18) Info: Next lattice write time is 520000
2024-04-30 12:13:20) Info: Average walltime per timestep: 0.47 ms. Progress:
25.1427s/60.0000s ( 41.9% done / 5.5 minutes walltime remaining)
2024-04-30 12:13:28) Info: Time is 26.00000000000000
2024-04-30 12:13:28) Info: Lattice write time is 26.00000000000000, in steps is
520000
2024-04-30 12:13:28) Info: Next lattice write time is 540000
2024-04-30 12:13:37) Info: Time is 27.00000000000000
```

```
2024-04-30 12:13:37) Info: Lattice write time is 27.00000000000000, in steps is
540000
2024-04-30 12:13:37) Info: Next lattice write time is 560000
2024-04-30 12:13:47) Info: Time is 28.00000000000000
2024-04-30 12:13:47) Info: Lattice write time is 28.00000000000000, in steps is
560000
2024-04-30 12:13:47) Info: Next lattice write time is 580000
2024-04-30 12:13:47) Info: Wrote 7 data sets (117440799 bytes) in the last 65.82
seconds (0.21 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:13:56) Info: Time is 29.00000000000000
2024-04-30 12:13:56) Info: Lattice write time is 29.00000000000000, in steps is
580000
2024-04-30 12:13:56) Info: Next lattice write time is 600000
2024-04-30 12:14:06) Info: Time is 30.00000000000000
2024-04-30 12:14:06) Info: Lattice write time is 30.00000000000000, in steps is
600000
2024-04-30 12:14:06) Info: Next lattice write time is 620000
2024-04-30 12:14:15) Info: Time is 31.00000000000000
2024-04-30 12:14:15) Info: Lattice write time is 31.00000000000000, in steps is
620000
2024-04-30 12:14:15) Info: Next lattice write time is 640000
2024-04-30 12:14:20) Info: Average walltime per timestep: 0.48 ms. Progress:
31.4200s/60.0000s ( 52.4% done / 4.6 minutes walltime remaining)
2024-04-30 12:14:25) Info: Time is 32.00000000000000
2024-04-30 12:14:25) Info: Lattice write time is 32.00000000000000, in steps is
640000
2024-04-30 12:14:25) Info: Next lattice write time is 660000
2024-04-30 12:14:35) Info: Time is 33.00000000000000
2024-04-30 12:14:35) Info: Lattice write time is 33.00000000000000, in steps is
660000
2024-04-30 12:14:35) Info: Next lattice write time is 680000
2024-04-30 12:15:13) Info: Time is 34.00000000000000
2024-04-30 12:15:13) Info: Lattice write time is 34.00000000000000, in steps is
680000
2024-04-30 12:15:13) Info: Next lattice write time is 700000
2024-04-30 12:15:13) Info: Wrote 6 data sets (100663542 bytes) in the last 86.45
seconds (0.18 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:15:20) Info: Average walltime per timestep: 1.11 ms. Progress:
34.1215s/60.0000s ( 56.9% done / 9.6 minutes walltime remaining)
2024-04-30 12:16:07) Info: Time is 35.00000000000000
2024-04-30 12:16:07) Info: Lattice write time is 35.00000000000000, in steps is
700000
2024-04-30 12:16:07) Info: Next lattice write time is 720000
2024-04-30 12:16:20) Info: Average walltime per timestep: 2.72 ms. Progress:
35.2255s/60.0000s ( 58.7% done / 22 minutes walltime remaining)
2024-04-30 12:17:02) Info: Time is 36.00000000000000
2024-04-30 12:17:02) Info: Lattice write time is 36.00000000000000, in steps is
720000
```

```
2024-04-30 12:17:02) Info: Next lattice write time is 740000
2024-04-30 12:17:02) Info: Wrote 2 data sets (33554514 bytes) in the last 108.74
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:17:20) Info: Average walltime per timestep: 2.72 ms. Progress:
36.3282s/60.0000s ( 60.5% done / 21 minutes walltime remaining)
2024-04-30 12:17:56) Info: Time is 37.00000000000000
2024-04-30 12:17:56) Info: Lattice write time is 37.00000000000000, in steps is
740000
2024-04-30 12:17:56) Info: Next lattice write time is 760000
2024-04-30 12:18:20) Info: Average walltime per timestep: 2.73 ms. Progress:
37.4258s/60.0000s ( 62.4% done / 21 minutes walltime remaining)
2024-04-30 12:18:51) Info: Time is 38.00000000000000
2024-04-30 12:18:51) Info: Lattice write time is 38.00000000000000, in steps is
760000
2024-04-30 12:18:51) Info: Next lattice write time is 780000
2024-04-30 12:18:51) Info: Wrote 2 data sets (33554514 bytes) in the last 109.20
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:19:20) Info: Average walltime per timestep: 2.76 ms. Progress:
38.5133s/60.0000s ( 64.2% done / 20 minutes walltime remaining)
2024-04-30 12:19:47) Info: Time is 39.00000000000000
2024-04-30 12:19:47) Info: Lattice write time is 39.00000000000000, in steps is
780000
2024-04-30 12:19:47) Info: Next lattice write time is 800000
2024-04-30 12:20:20) Info: Average walltime per timestep: 2.30 ms. Progress:
39.8204s/60.0000s ( 66.4% done / 15 minutes walltime remaining)
2024-04-30 12:20:29) Info: Time is 40.00000000000000
2024-04-30 12:20:29) Info: Lattice write time is 40.00000000000000, in steps is
800000
2024-04-30 12:20:29) Info: Next lattice write time is 820000
2024-04-30 12:20:29) Info: Wrote 2 data sets (33554514 bytes) in the last 98.41
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:21:20) Info: Average walltime per timestep: 2.70 ms. Progress:
40.9335s/60.0000s ( 68.2% done / 17 minutes walltime remaining)
2024-04-30 12:21:23) Info: Time is 41.00000000000000
2024-04-30 12:21:23) Info: Lattice write time is 41.00000000000000, in steps is
820000
2024-04-30 12:21:23) Info: Next lattice write time is 840000
2024-04-30 12:22:18) Info: Time is 42.00000000000000
2024-04-30 12:22:18) Info: Lattice write time is 42.00000000000000, in steps is
840000
2024-04-30 12:22:18) Info: Next lattice write time is 860000
2024-04-30 12:22:18) Info: Wrote 2 data sets (33554514 bytes) in the last 108.52
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:22:20) Info: Average walltime per timestep: 2.73 ms. Progress:
42.0320s/60.0000s ( 70.1% done / 16 minutes walltime remaining)
2024-04-30 12:23:13) Info: Time is 43.00000000000000
2024-04-30 12:23:13) Info: Lattice write time is 43.00000000000000, in steps is
860000
```

```
2024-04-30 12:23:13) Info: Next lattice write time is 880000
2024-04-30 12:23:20) Info: Average walltime per timestep: 2.75 ms. Progress:
43.1211s/60.0000s ( 71.9% done / 15 minutes walltime remaining)
2024-04-30 12:24:08) Info: Time is 44.00000000000000
2024-04-30 12:24:08) Info: Lattice write time is 44.00000000000000, in steps is
880000
2024-04-30 12:24:08) Info: Next lattice write time is 900000
2024-04-30 12:24:08) Info: Wrote 2 data sets (33554514 bytes) in the last 110.00
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:24:20) Info: Average walltime per timestep: 2.74 ms. Progress:
44.2157s/60.0000s ( 73.7% done / 14 minutes walltime remaining)
2024-04-30 12:25:03) Info: Time is 45.00000000000000
2024-04-30 12:25:03) Info: Lattice write time is 45.00000000000000, in steps is
900000
2024-04-30 12:25:03) Info: Next lattice write time is 920000
2024-04-30 12:25:20) Info: Average walltime per timestep: 2.74 ms. Progress:
45.3120s/60.0000s ( 75.5% done / 13 minutes walltime remaining)
2024-04-30 12:25:44) Info: Time is 46.00000000000000
2024-04-30 12:25:44) Info: Lattice write time is 46.00000000000000, in steps is
920000
2024-04-30 12:25:44) Info: Next lattice write time is 940000
2024-04-30 12:25:44) Info: Wrote 2 data sets (33554514 bytes) in the last 96.25
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:26:20) Info: Average walltime per timestep: 2.22 ms. Progress:
46.6623s/60.0000s ( 77.8% done / 9.9 minutes walltime remaining)
2024-04-30 12:26:38) Info: Time is 47.00000000000000
2024-04-30 12:26:38) Info: Lattice write time is 47.00000000000000, in steps is
940000
2024-04-30 12:26:38) Info: Next lattice write time is 960000
2024-04-30 12:27:20) Info: Average walltime per timestep: 2.70 ms. Progress:
47.7740s/60.0000s ( 79.6% done / 11 minutes walltime remaining)
2024-04-30 12:27:32) Info: Time is 48.00000000000000
2024-04-30 12:27:32) Info: Lattice write time is 48.00000000000000, in steps is
960000
2024-04-30 12:27:32) Info: Next lattice write time is 980000
2024-04-30 12:27:32) Info: Wrote 2 data sets (33554514 bytes) in the last 107.51
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:28:20) Info: Average walltime per timestep: 2.73 ms. Progress:
48.8749s/60.0000s ( 81.5% done / 10 minutes walltime remaining)
2024-04-30 12:28:27) Info: Time is 49.00000000000000
2024-04-30 12:28:27) Info: Lattice write time is 49.00000000000000, in steps is
980000
2024-04-30 12:28:27) Info: Next lattice write time is 1000000
2024-04-30 12:29:20) Info: Average walltime per timestep: 2.81 ms. Progress:
49.9437s/60.0000s ( 83.2% done / 9.4 minutes walltime remaining)
2024-04-30 12:29:23) Info: Time is 50.00000000000000
2024-04-30 12:29:23) Info: Lattice write time is 50.00000000000000, in steps is
1000000
```

```
2024-04-30 12:29:23) Info: Next lattice write time is 1020000
2024-04-30 12:29:23) Info: Wrote 2 data sets (33554514 bytes) in the last 111.15
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:30:19) Info: Time is 51.00000000000000
2024-04-30 12:30:19) Info: Lattice write time is 51.00000000000000, in steps is
1020000
2024-04-30 12:30:19) Info: Next lattice write time is 1040000
2024-04-30 12:30:20) Info: Average walltime per timestep: 2.80 ms. Progress:
51.0133s/60.0000s ( 85% done / 8.4 minutes walltime remaining)
2024-04-30 12:31:10) Info: Time is 52.00000000000000
2024-04-30 12:31:10) Info: Lattice write time is 52.00000000000000, in steps is
1040000
2024-04-30 12:31:10) Info: Next lattice write time is 1060000
2024-04-30 12:31:10) Info: Wrote 2 data sets (33554514 bytes) in the last 107.44
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:31:20) Info: Average walltime per timestep: 2.25 ms. Progress:
52.3459s/60.0000s ( 87.2% done / 5.7 minutes walltime remaining)
2024-04-30 12:31:55) Info: Time is 53.00000000000000
2024-04-30 12:31:55) Info: Lattice write time is 53.00000000000000, in steps is
1060000
2024-04-30 12:31:55) Info: Next lattice write time is 1080000
2024-04-30 12:32:20) Info: Average walltime per timestep: 2.70 ms. Progress:
53.4562s/60.0000s ( 89.1% done / 5.9 minutes walltime remaining)
2024-04-30 12:32:49) Info: Time is 54.00000000000000
2024-04-30 12:32:49) Info: Lattice write time is 54.00000000000000, in steps is
1080000
2024-04-30 12:32:49) Info: Next lattice write time is 1100000
2024-04-30 12:32:49) Info: Wrote 2 data sets (33554514 bytes) in the last 98.96
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:33:20) Info: Average walltime per timestep: 2.72 ms. Progress:
54.5577s/60.0000s ( 90.9% done / 4.9 minutes walltime remaining)
2024-04-30 12:33:43) Info: Time is 55.00000000000000
2024-04-30 12:33:43) Info: Lattice write time is 55.00000000000000, in steps is
1100000
2024-04-30 12:33:43) Info: Next lattice write time is 1120000
2024-04-30 12:34:20) Info: Average walltime per timestep: 2.67 ms. Progress:
55.6798s/60.0000s ( 92.8% done / 3.9 minutes walltime remaining)
2024-04-30 12:34:37) Info: Time is 56.00000000000000
2024-04-30 12:34:37) Info: Lattice write time is 56.00000000000000, in steps is
1120000
2024-04-30 12:34:37) Info: Next lattice write time is 1140000
2024-04-30 12:34:37) Info: Wrote 2 data sets (33554514 bytes) in the last 107.58
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:35:20) Info: Average walltime per timestep: 2.64 ms. Progress:
56.8181s/60.0000s ( 94.7% done / 2.8 minutes walltime remaining)
2024-04-30 12:35:29) Info: Time is 57.00000000000000
2024-04-30 12:35:29) Info: Lattice write time is 57.00000000000000, in steps is
1140000
```

```
2024-04-30 12:35:29) Info: Next lattice write time is 1160000
2024-04-30 12:36:20) Info: Average walltime per timestep: 2.60 ms. Progress:
57.9708s/60.0000s ( 96.6% done / 1.8 minutes walltime remaining)
2024-04-30 12:36:21) Info: Time is 58.00000000000000
2024-04-30 12:36:21) Info: Lattice write time is 58.00000000000000, in steps is
1160000
2024-04-30 12:36:21) Info: Next lattice write time is 1180000
2024-04-30 12:36:21) Info: Wrote 2 data sets (33554514 bytes) in the last 104.40
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:37:00) Info: Time is 59.00000000000000
2024-04-30 12:37:00) Info: Lattice write time is 59.00000000000000, in steps is
1180000
2024-04-30 12:37:00) Info: Next lattice write time is 1200000
2024-04-30 12:37:20) Info: Average walltime per timestep: 2.15 ms. Progress:
59.3691s/60.0000s ( 98.9% done / 27 seconds walltime remaining)
2024-04-30 12:37:53) Info: Time is 60.00000000000000
2024-04-30 12:37:53) Info: Lattice write time is 60.00000000000000, in steps is
1200000
2024-04-30 12:37:53) Info: Next lattice write time is 1220000
2024-04-30 12:37:53) Info: Wrote 2 data sets (33554514 bytes) in the last 91.75
seconds (0.06 seconds writing). 0 datasets queued. Flushing.
2024-04-30 12:37:53) Info: Data output thread finished.
2024-04-30 12:37:53) Info: Simulation file closed.
```

[49]:
```
<jLM.RDME.File at 0x7feddf0a19b0>
```

8 7. Analysis

[50]:
```
import matplotlib.pyplot as plt
import seaborn as sns
from jLM.RDME import File as RDMEFile
```

[51]:
```
traj = RDMEFile(filename,replicate=1)
ts, genes = traj.getNumberTrajectory(species="gene")
ts, mRNAs = traj.getNumberTrajectory(species="mRNA")
ts, mRNArs = traj.getNumberTrajectory(species="mRNAr")
ts, proteins = traj.getNumberTrajectory(species="P")
```

[54]:
```
# now visuzlize the trajectories with seaborn and plt
sns.set(style="whitegrid")
# Create a color palette

colors = sns.color_palette("husl", 3)
plt.figure(figsize=(10,6))
plt.plot(ts, genes, label='gene',color=palette[0])
plt.plot(ts, mRNAs + mRNArs, label='mRNA',color=palette[1])
```

```
plt.plot(ts, proteins, label='protein',color=palette[2])

plt.title('Trajectories of Genetic information process')
plt.yticks(np.arange(0, 2.1, step=1))
plt.xlabel('Time (s)')
plt.ylabel('Counts')
plt.legend()
plt.savefig('./images/TutR2_GIP.png')
plt.show()
```