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# Repast for Python (Repast4Py) User Guide

Version 2.0 February 2023

## 1. Getting Started

Repast for Python (Repast4Py) is the newest member of the Repast Suite of free and open source agent-based modeling and simulation software. It builds on Repast HPC, and provides the ability to build large, distributed agent-based models (ABMs) that span multiple processing cores. Distributed ABMs enable the development of complex systems models that capture the scale and relevant details of many problems of societal importance. [1][2] Where Repast HPC is implemented in C++ and is more HPC expert focused, Repast4Py is a Python package and is designed to provide an easier on-ramp for researchers from diverse scientific communities to apply large-scale distributed ABM methods. Repast4Py is released under the BSD-3 open source license, and leverages Numba, NumPy, and PyTorch packages, and the Python C APItō create a scalable modeling system that can exploit the largest HPC resources and emerging computing architectures. See our paper on Repast4Py for additional information about the design and implementation. [3]

#### 1.1. Requirements

Repast4Py can run on Linux, macOS and Windows provided there is a working MPI implementationinstalled and mpi4py is supported. Repast4Py is developed and tested on Linux. We recommendthat Windows users use the Windows Subsystem for Linux (WSL). Installation instructions for WSL can be found here.

Under Linux, MPI can be installed using your OS's package manager. For example, under Ubuntu 20.04 (and thus WSL), the mpich MPI

#### Neighborhood Finder

implementation can be installed with:

```
$ sudo apt install mpich
```

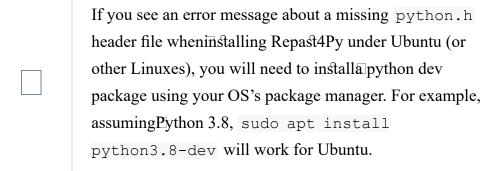
Installation instructions for MPI on macOS can be found here.

A typical campus cluster, or HPC resource will have MPI and mpi4py installed. Check the resource's documentation on available software for more details.

#### 1.2. Installation

Repast4Py can be downloaded and installed from PyPI using pip.Since Repast4Py includes native MPI C++ code that needs to be compiled,the C compiler CC environment variable must be setto the mpicxx (or mpic++) compiler wrapper provided by your MPI installation.

```
env CC=mpicxx pip install repast4py
```



#### 1.3. Documentation

- <u>User's Guide</u> (This document)
- API Docs
- Example Models

#### 1.4. Contact and Support

GitHub Issues

#### • GitHub Repository

In addition to filing issues on GitHub, support is also available via Stack Overflow. Please use the repast4py tag to ensure that we are notified of your question. Software announcements will be made on the repast-interest mailing list.

Jonathan Ozik is the Repast project lead. Please contact him through the <u>Argonne Staff Directory</u> if you have project-related questions.

## 2. Why Repast4Py?

Modern high-performance computing (HPC) capabilities have allowed for large-scale computational modeling and experimentation. HPC clusters and supercomputers — such as those hosted by universities, national laboratories, and cloud computing providers — can have thousands or more processor cores available, allowing for high concurrency. Even individual CPUs now typically contain multiple cores, which are capable of running concurrently. Distributed ABMs attempt to leverage this hardware by distributing an individual simulation over multiple processes running in parallel.

However, in order to take advantage of these increasingly ubiquitous parallel computing resources, a computational model must first be refashioned to run on multiple processors. Adapting a computational model that was built for a single processor to run on multiple processors can be a nontrivial endeavor, both conceptually and practically. Repast 4Py aims to ease the transition to distributed ABMs by hiding much of the complexity.

## 2.1. Distributed computing a natural fit for agentbased modeling

A typical agent-based simulation consists of a population of agents each of which performs some behavior each timestep or at some frequency. In practice, this is often implemented as a loop over the agent population in

which each agent executes its behavior. The time it takes to complete the loop depends on the number of agents and the complexity of the behavior. By distributing the agent population across multiple processes running in parallel, each process executes its own loop over only a subset of the population, allowing for larger agent populations and more complex behavior.

## 2.2. Repast4Py and the broader Repast family

While Repas4Py is meant to make the development of distributed ABMs easier, we encourage users new to the Repast Suite to look through the different versions of Repast to determine which toolkit is most appropriate for their needs. Of note, we recommend users new to agent-based modeling to first check out Repast Simphony to develop a better understanding of the concepts behind agent-based modeling and learn how to quickly build such models.

The following sections will provide some conceptual background for a Repast-style simulation, describe how such a simulation is distributed across multiple processes with Repast4Py, and end with providing a few basic tutorials.

## 3. Repast Simulation Overview

This overview section will provide some conceptual background for a Repast-style simulation well as describing how such a simulation is distributed across multiple processes.

#### 3.1. Contexts and Projections

Like the other members of the Repast ABM family, Repast4Py organizes a model in terms of *contexts* and *projections*. A context is a simple container with set semantics. Any type of object can be put into a context, with the simple caveat that only one instance of any given objectcan be contained by

the context. From a modeling perspective, the context represents a population of agents. The agents in a context are the population of a model. However, the context does not inherently provide any relationship or structure for that population. Projections take the population as defined in a contextand impose a structure on it. Actual projections are such things as a network structure that allows agents to form links (network type relations) with each other, a grid where each agent is located in amatrix-type space, or a continuous space where an agent's location is expressible as a non-discrete coordinate. Projections have a many-to-one relationship with contexts. Each context can have an arbitrary number of projections associated with it. When writing a model, you will create a context, populate it with agents, and attach projections to that context.

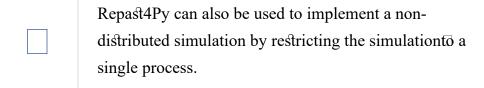
#### 3.2. Scheduling Events

A Repast simulation moves forward by repeatedly determining the next event to execute and then executing that event. Events in Repast simulations are driven by a discrete-event scheduler. These events are scheduled to occur at aparticular tick. Ticks do not necessarily represent clock-time but rather the priority of an associated event. In this way, ticks determine the order in which events occur with respect to each other. For example, if event A is scheduled at tick 3 and event B at tick 6, event A will occur before event B. Assuming nothing is scheduled at the intervening ticks, A will be immediately followed by B. There is no inherent notion of B occurring after a duration of 3 ticks. Of course, ticks can and are often given some temporal significance through the model implementation. A traffic simulation, for example, may move the traffic forward the equivalent of 30 seconds for each tick. Events can also be scheduled dynamically such that the execution of an event may schedule further events at that same or at some future tick. When writing a model, you willcreate a Schedule object and schedule events using that object. The events are essentially Python Callables (methods or functions) scheduled for execution at some particular tick or tick frequency.

#### 3.3. Distributed Simulation

Repast4Py was designed from the ground up as a distributed simulation framework. In practice, this meansthat the simulation is spread over multiple

computer processes none of which have access to each other's memory, and communicate via message passing using the Message Passing Interface (MPI) and its Python implementation MPI for Python (Impi4py).



Repast4Py distributes a simulation by providing *shared* implementations of the components described above. By shared, we want to emphasize the partitioned and distributed nature of the simulation. The global simulation shared among a pool of processes, each of which is responsible for some portion of it, and stiched into a global whole through the use of non-local, or *ghost*, agents and buffered projections.

An MPI application identifies its processes by a rank id. For example, if the application is run with 4 processes, therewill be 4 ranks: 0 - 3. The code in an MPI application is run concurrently on each rank. Anythinginstantiated in that code resides in that processes' memory and is *local* to that process. Other processes do nothave access to the variables, objects, etc. created on another process. A simple "hello world" typeMPI4Py script illustrates this.

```
# hello_world.py
from mpi4py import MPI

size = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()

print('Hello, World! I am process {} of {}'.format(rank, size))
```

- 1 Gets the world size, that is, the total number of process ranks.
- 2 Gets the rank of the process the code is running on.
- 3 Prints out the size and current rank.

Running this with 4 process ranks ( mpirun -n 4 python hello\_world.py ) will produce something like following output where can see how each of the 4 ranks runs the script independently on its own process

rank.

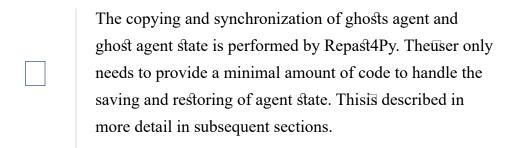
```
Hello, World! I am process 2 of 4
Hello, World! I am process 1 of 4
Hello, World! I am process 0 of 4
Hello, World! I am process 3 of 4
```

The output may be more mixed together than the above example as each processwrites it output concurrently.

In a more ABM flavored example, assuming 4 ranks, the following code creates 10 agents on each rank, for a total of 40 agents.

These agents are said to be *local* to the ranks on which they are created. In order to stitch these individual ranksinto a global whole, Repast4Py uses the concept of a non-local, *ghost* agent: a copy of an agent from another rank that local agents can interact with. Repast4Py provides the functionality to create these ghosts and keep theirstate synchronized from the ghosts' local ranks to the ranks on which they are ghosted. Ghosts are also used to create projections, such as a network or grid that span across process ranks.

Figure 1 illustrates how ghosts are used in a network projection. The top part of the figure shows that agent A1 is local to process 1 and hasa directed netework link to agent B2, which is local to process 2. Presumably, some aspect of the agent's behavior is conditional on the network link, for example checking some attribute of its network neighbors and responding accordingly. Given that B2 is on a different process there is no way for A1 toquery B2. However, the bottom part of the figure shows how ghost agents are used to tie the network together. B2 iscopied to process 1 where a local link is created between it and A1. A1 can now query the state of B2. Similarly, a ghost of A1 is copied to process 2 where B2 can now interact with it.



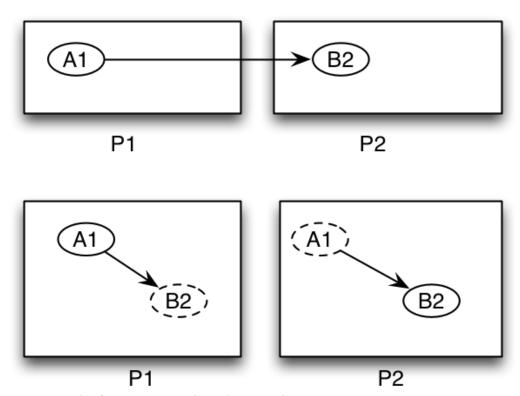


Figure 1. Ghost Agents in a Shared Network

Do not update the state of non-local ghost agents. They only exist to be *seen* by local agents and objects. Any state changes to any agent must be performed on the agent's local process. The SharedContext component makes a clear distinction between the two types of agents, allowing you to work with only the local agents.

Spatial projections such as a grid or continuous space are stitched together through the use of *buffers* and ghosts agents.

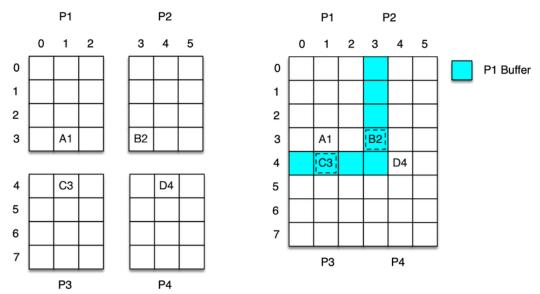
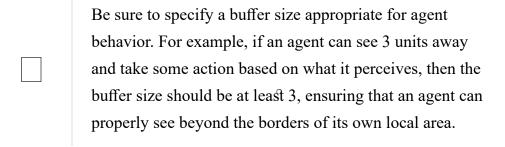


Figure 2. Ghost Agents in a Buffered Area

This is illustrated in Figure 2, where the full 6x8 grid is distributed across 4 process ranks. Each rank is responsible forits own 3x4 quarter of the global grid (left hand side of Figure 2).On the right hand side, we see how the quarters are stitched together. Each subsection of the grid contains a buffer that is a copy of the contents of the adjacent subsections. The blue part of the image is the area for process 1's grid subsection. There, we canse the ghost agents C3 and B2 copied from processes 3 and 2 respectively. In this way, agent A1 can see and interact with agents C3 and B2.



Agents can, of course, move around grids and continuous spaces. When an agent moves beyond the borders of its local subsection then it is moved from that rank to the rank of the new subsection to which it has moved. For example, if in Figure 2, agent D4 moves from grid coordinate 4,4 to 4,2 then it will be moved during Repast4Py's synchronization phase to process 2 where it becomes localto that process. Cross-process movement and synchronization will be discussed more in the next sections.

## 4. Cross-Process Code Requirements

We've seen in the <u>Distributed Simulation</u> section how ghost agents(non-local copies) are used to stitch a simulation together across processes and that when agents move out of their local grid or continuous space subsection they are moved to the process responsible for the destination besection. While much of this is handled internally by Repast 4Py, this section describes in more detail the code the user needs to provide in order for moving and copying to work correctly. We will use examples from the Zombies and Rumor demonstration models. See the <u>Repast 4Py Examples</u> page to download the source code for these models and for more information on getting started with the examples.

#### 4.1. Agent ID

For moving and copying agents across processes to work each agent must have a unique id. This id has three components:

- 1. An integer that uniquely identifies the agent on the rank on which it was created
- 2. An integer that identifies its type
- 3. The integer rank on which the agent was created

Combining the first component with the last allows us to uniquely identify an agent across the multi-process imulation while the second allows us to create agents of the appropriate type when they are copied between ranks.

In order to ensure that all agents in Repast4Py have an agent id, all agents must inherit from the <a href="repast4py.core.Agent">repast4py.core.Agent</a> class which requires these components in its constructor. For example, in the Zombies demonstration model, the Human agents are subclasses of the <a href="repast4py.core.Agent">repast4py.core.Agent</a>.

```
class Human (repast4py.core.Agent): 1

"""The Human Agent
```

```
4
        Args:
5
       a id: a integer that uniquely identifies this
6
    Human on its
7
                starting rank
8
           rank: the starting MPI rank of this Human.
9
        mmm
10
11
       ID = 0
12
13
        def init (self, a id: int, rank: int):
            super(). init (id=a id, type=Human.ID,
    rank=rank) 2
```

- 1 Human inherits from repast4py.core.Agent
- 2 Calling the repast4py.core.Agent constructor with the agent id components.

The components as well as the full unique id are accessible asattributes of the repast4py.core.Agent class.

- id: the id component from the agent's unique id
- type: the type component from the agent's unique id
- rank: the rank component from the agent's unique id
- uid: the unique id tuple (id, type, rank)

All agents must subclass repast4py.core.Agent.

See the API documenation for repast4py.core.Agent for more details of the Agent class.

### 4.2. Saving and Restoring Agents

Moving or copying an agent between processes consists of saving the agent state, moving / copying that stateto another process, and then restoring the agent state as an agent on the destination process. For this to work, each agent is required to implement a save method that returns a tuple containing the full agent state. The first element of thisfull state tuple is the agent's unique id, itself a tuple (accessed via the uid attribute), and the secondis the dynamic state of that agent. For example, in the Zombie demonstration model the state of each Human is represented by two variables:

- 1. infected: a boolean that indicates whether or not the Human is infected
- 2. infected\_duration: an integer tracking how long the agent has been infected

The save method creates a tuple consisting of these two variables and the unique id tuple.

```
def save(self) -> Tuple:
    """Saves the state of this Human as a tuple.

Used to move this Human from one MPI rank to
another.

Returns:
    The saved state of this Human.
    """
    return (self.uid, self.infected,
self.infected_duration)
```

The agent state in the tuple returned from save can also consist of other tuples, listsand so on, in addition to primitive values, as long as the unique id tuple is the first element.

All agents must implement a save method.

You must also provide a restore function that takes the tuple produced by the save method andreturns an agent either created from or updated with that state. The function is used during synchronization create the agents on the destination ranks. In the Zombies demonstration model, the restore\_agent function, when given agent state, returns Human and Zombie agents. It uses a caching schemeto avoid re-instantiating agents that have previously been created on a rank, and updates the state of those previously created agents. This can be a useful performance improvement at the expense of using more memory.

```
agent cache = {}
 2
    def restore agent(agent data: Tuple): 2
 4
        """Creates an agent from the specified agent data.
 5
 6
        This is used to re-create agents when they have moved
 7
    from one MPI rank
 8
         to another. The tuple returned by the agent's save()
9
    method is moved
10
        between ranks and create agent is called for each
11
     tuple in order
12
        to create the agent on that rank. Here we also use
13
        a cache to store any agents already created on this
14
15
        and only update their state rather than recreating
16
     them from scratch.
17
18
        Args:
19
            agent data: the data from which to create the
20
     agent. This is the tuple
21
                        returned from the agent's save()
22
     method where the first
23
                       element is the agent id tuple, and
24
     any remaining
25
                        arguments encapsulate agent state.
         11 11 11
27
        uid = agent data[0]
29
         # in uid element 0 is id, 1 is type, 2 is rank
        if uid[1] == Human.ID:
     4
32
             if uid in agent cache:
     5
34
                h = agent cache[uid]
            else:
                h = Human(uid[0], uid[2])
                 agent cache[uid] = h
38
39
             # restore the agent state from the agent data
```

```
tuple
41
             h.infected = agent data[1]
     6
             h.infected duration = agent data[2]
             return h
        else:
     Ø
             # note that the zombie has no internal state
             # so there's nothing to restore other than
             # the Zombie itself
             if uid in agent cache:
                return agent cache[uid]
             else:
                 z = Zombie(uid[0], uid[2])
                agent cache[uid] = z
                 return z
```

- 1 Cache for previously instantiated agents. Key is an agent's unique id (uid) tuple and value is the agent.
- agent\_data is a tuple of the format produced by the save method. For Humans this is (uid, infected, infected\_duration). For Zombies, this is just (uid).
- 3 The first element of the agent\_data tuple is the uid tuple. The uid tuple is (id, type, starting rank).
- 4 Checks if the agent is a Human or Zombie, using the type component of the uid.
- 5 Checks if the agent is already cached, if so then get it (line 23), otherwise create a new Human agent (line 25).
- 6 Updates the cached / created Human with the passed in agent state.
- agent\_data is for a Zombie so search cache and if necessary create a new one.

Lastly, in a distributed network, agents are not typically moved between processesbut rather the ghost agents remain on a process once the network is created. Repast4Py tracksthese ghost agents and does not recreate the agents every synchronization step via a restore method, instead a state update is sent to the appropriate ghost agents. In that case, an agent's update method is called to handle the state update. The Rumor demonstration model has an example of this.

```
class RumorAgent(core.Agent):

...

def update(self, data: bool):

"""Updates the state of this agent when it is a

ghost

agent on some rank other than its local one.

Args:

data: the new agent state (received_rumor)

"""

self.received_rumor = data
```

Updates ghost agent state from saved agent state. Here the data argument is only the dynamic state element of the tuple returned from the agent's save method, namely, the self.received\_rumor bool from (self.uid, self.received rumor).

#### 4.3. Synchronization

As mentioned in the <u>Distributed Simulation</u> section, each process in a Repast4Py application runs in a separate memory space from all the other processes. Consequently, we need to synchronize the model state across processes by moving agents, filling projection buffers with ghosts, and updating ghosted states, as necessary. Synchronization is performed by calling the <u>SharedContext.synchronize</u> method and passing it your restore function. The <u>synchronization</u> method will use the agent <u>save</u> method(s) and your restore function to synchronize the state of the simulation across its processes.

## Tutorial 1 - A Simple Random WalkModel

This tutorial will guide you through coding a simple model, focusing on components and concepts common to every model. The simulation itself consists of a number of agents moving at random around a two-dimensional

grid and logging the aggregate and agent-levelcolocation counts. Each timestep the following occurs:

- 1. All the agents (*walkers*) choose a random direction and move one unit in that direction.
- 2. All the agents count the number of other agents they *meet* at their current location by determining the number of colocated agents at their grid locations.
- 3. The sum, minimum, and maximum number of agents met are calculated across all process ranks, and these values are logged as the total, minimum, and maximum meet values.

In addition, every 10 timesteps:

1. The individual agent *meet* counts are logged across all the process ranks.

See the <u>Repast4Py Examples</u> page to download the source code for this modeland for more information on getting started with the examples.

The code consists of the following components:

- 1. A Walker class that implements the agent state and behavior.
- 2. A Model class responsible for initialization and managing the simulation.
- 3. A restore\_walker function used to create an individual Walker when that Walker has moved (i.e., walked) to another process.
- 4. A run function that creates and starts the simulation.
- 5. An if name == "main" block that allows the simulation to be run from the command line.

This is the canonical way to organize a Repast4Py simulation: agents implemented as classes, a *model*-type class to initialize and manage the simulation, a function to handle restoring agents as they move between processes,

and some additional code to run the simulation from the command line. Of course, in a more complex simulation the responsibilities and behavior of the agent and model classes can befactored out into additional classes, functions, and modules as necessary, but the overall organization remains the same.

#### 5.1. The Walker Agent

The Walker class implements our Walker agent, encapsulating its:

- State: a count of all the other walkers that it has colocated with, and the walker's current location
- Behavior: moving randomly around a 2D dimensional grid and counting the number of colocations

As required for all Repast4Py agent implementations, the Walker class subclasses <u>repast4py.core.Agent</u>, passing it the components of the unique agent id tuple.

```
from repast4py.space import DiscretePoint
2
    from repast4py import core
    import numpy as np
    class Walker(core.Agent):
6
7
        TYPE = 0
8
        OFFSETS = np.array([-1, 1])
                                       3
9
        def init (self, local id: int, rank: int, pt:
10
11
    DiscretePoint):
            super(). init (id=local id, type=Walker.TYPE,
13
                  4
    rank=rank)
            self.pt = pt
            self.meet count = 0
```

- 1 Walker subclasses repast4py.core.Agent.Subclassing Agent is a requirement for all Repast4Py agent implementations.
- 2 TYPE is a class variable that defines an agent type id for our walker agent. This is a required part of the unique agent id tuple (see 4).

- 3 OFFSETS is a numpy array used in the agent behavior implementation to select the direction to move in. See the discussion of the walk method below.
- 4 repast4py.core.Agent constructor takes 3 arguments: an integer id that uniquely identifes an agent on the process where it was created, a non-negative integer identifying the type of the agent, and the rank on which the agent is created. Taken together, these three uniquely identify the agent across all ranks in the simulation.

The agent's behavior is implemented in the walk and the count\_colocations methods. In the walk method, the agent randomly chooses an offset from its current location (self.pt), adds those offsets to its current location to create a new location, and then moves to that new location on the grid. The moved-to-location becomes the agent's new current location.

#### 5.1.1. Walking the Walker

```
1
    from repast4py import random
2
    from repast4py.space import DiscretePoint
4
    OFFSETS = np.array([-1, 1])
5
6
    def walk(self, grid: SharedGrid):
7
        # choose two elements from the OFFSET array
8
         # to select the direction to walk in the
9
         # x and y dimensions
        xy dirs = random.default rng.choice(Walker.OFFSETS,
11
    size=2)
        self.pt = grid.move(self, DiscretePoint(self.pt.x +
    xy dirs[0],
                             self.pt.y + xy dirs[1], 0)) 4
```

- 1 repast4py.random contains an instance of a numpy.random.Generator as the module level variable default\_rng, as well as a function for intializing this variable. See the numpy random.Generator api reference for more details.
- 2 All the walker agents move on the same grid. An instance of this grid, a repast4py.space.SharedGrid object is passed in.
- 3 The <u>numpy.random.Generator.choice</u> randomly chooses size number of elements from a numpy array. In this case randomly selecting

- either -1 or 1 from OFFSETS. The two chosen values correspond to the direction to move along the x and y dimensions, respectively.
- A SharedGrid.move moves an agent to a location in the grid and returns the destination location. Grid locations are represented by a repast4py.space.DiscretePoint and an instance of that with updated new x and y coordinates is passed to the move method.

Repast4Py provides a default random number generator in repast4py.random.default\_rng. Thisrandom number generator is initialized when the module is imported, with the current time as the seed. The seed can also be set by specifying a random.seed model input parameter and using Repast4Py's model input parameters utility code. (See Running the Simulation for more details.) random.default\_rng is an instance of numpy.random.Generator. See the numpy random.Generator api reference for more information on the available distributions and sampling functions.

#### 5.1.2. Logging the Walker

The count\_colocations method gets the number of other agents at the current location, and updates both the agent's individual running total of other agents met, as well as a MeetLog dataclassin stance that is used to log the total number of meets and the minimum and maximum.

```
1
    @dataclass
2
     class MeetLog:
        total meets: int = 0
4
         min meets: int = 0
5
         max meets: int = 0
6
7
     . . .
8
9
     def count colocations (self, grid: SharedGrid, meet log:
10
    MeetLog):
11
         # subtract self
                                                          1
12
         num here = grid.get num agents(self.pt) - 1
13
         meet log.total meets += num here
14
         if num here < meet log.min meets:</pre>
15
             meet log.min meets = num here
```

```
if num_here > meet_log.max_meets:
    meet_log.max_meets = num_here
    self.meet_count += num_here
```

1 SharedGrid.get\_num\_agents returns the number of agents at a specified location.

```
To learn more about built-in agent and grid functionality, see the API documentation for <a href="mailto:repast4py.core.Agent">repast4py.core.Agent</a> and <a href="mailto:repast4py.space.SharedGrid">repast4py.space.SharedGrid</a>.
```

As we will see below, the Model class will schedule the execution of these two functions on every agent at every timestep. In this way, each agent executes its behavior each timestep.

#### 5.1.3. Serializing the Walker

When a Walker walks beyond the bounds of the local grid managed by its currentprocess rank, or when populating the buffer area of the local grid sections, Repast4Py needs to serialize the Walker state to a tuple, which is then usedto recreate that Walker on a different process. The Walker save method performs this serialization, saving the agent's unique id, its current meet count, and location.

```
1  def save(self) -> Tuple:
2    """Saves the state of this Walker as a Tuple.
3
4    Returns:
5     The saved state of this Walker.
6    """
7    return (self.uid, self.meet_count, self.pt.coordinates)
```

1 Returns the Walker state as a tuple. The first element of this tuple

MUST be the agent's unique id (self.uid). self.pt is an instance
of a DiscretePoint whose coordinates method returns the
point's coordinates as a numpy array.

Every agent must implement a save method that returns



the state of the agent as a tuple. The first element of this tuple MUST be the agent's unique id (self.uid). The remaining elements should encapsulate any dynamic agent state.

#### 5.2. The Model Class

The Model class encapsulates the simulation and is responsible for initialization. It schedules events, creates agents and the grid the agents inhabit, and manages logging. In addition, the scheduled events that drive the simulation forward are methods of the Model class.

In the Model constructor, we create the simulation schedule, the context that holdsour agents, the grid on which they move, the agents themselves, and the loggers thatwe use to log various simulation statistics to files. We begin with the constructorsignature, and the schedule runner creation.

#### 5.2.1. Scheduling Events

The SharedScheduledRunner class encapsulates a dynamic schedule of executable events shared andsynchronized across processes. Events are added to the schedule for execution at a particular *tick*. The first valid tick is 0. Events will be executed in tick order, earliest before latest. When multiple events are scheduled for the same tick, the events' priorities will be used to determine the order of execution within that tick. If during the execution of a tick, an event is scheduled before the executing tick (i.e., scheduled to occur in the past) then that event is ignored. The schedule is synchronized across process ranks by determining the global cross-process minimum next scheduled event time and executing events for that time. In this way, no schedule runs ahead of any other. In practice an event is a Python function or method.

```
def __init__(self, comm: MPI.Intracomm, params: Dict):

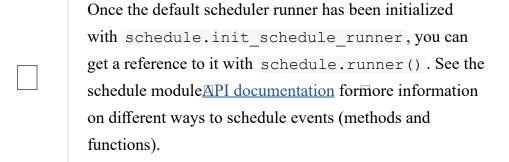
# create the schedule
self.runner = schedule.init_schedule_runner(comm)

self.runner.schedule_repeating_event(1, 1, self.step)

self.runner.schedule_repeating_event(1, 1, self.step)
```

```
self.runner.schedule_repeating_event(1.1, 10,
self.log_agents)
self.runner.schedule_stop(params['stop.at'])
# once initialized the schedule runner can be accessed
with schedule.runner
schedule.runner().schedule_end_event(self.at_end)
```

- 1 The Model constructor takes an MPI communicator and a dictionary of model input parameters as arguments.
- 2 Before any events can be scheduled, the schedule runner must be initialized.
- 3 Schedules Model.step on this instance of the model to execute starting at tick 1 and then every tick thereafter. Repeating events are scheduled with schedule.repeating\_event. The first argument is the start tick, and the second is the frequency for repeating.
- 4 schedule\_stop schedules the tick at which the simulation should stop. At this tick, events will no longer be popped off the schedule and executed.
- schedule\_end\_event can be used to schedule methods that perform some sort of *clean up* type operation when the simulation ends, closing a log file, for example. This is called at the time specified in the call to schedule stop.



A simulation stopping time must be set with schedule\_stop. Without a stopping timethe simulation will continue to run, seeming to hang if there are no events to execute, or continuing to execute any scheduled events without stopping. The stopping time does not need to be set during initialization, but can be set during a

By default events are scheduled with a random priority type, meaning that events scheduled for the same tick will be executed in random order. Other priority types are available though:

- PriorityType.FIRST events will execute before those with other PriorityTypes.All events with a FIRST priority type will execute in the order in which they are scheduledwith respect to other FIRST priority type events.
- PriorityType.RANDOM events will execute in a random order, after the FIRST priority type events, and before the LAST priority type events. If there are BY\_PRIORITY events scheduled for the same tick as RANDOM events, the RANDOM events will be shuffled atrandom into the ordered BY\_PRIORITY events.
- PriorityType.BY\_PRIORITY events will execute in the order specified by an additional priority parameter (lower values are higher priority), and after any FIRST priority events and before any LAST priority events. If there are RANDOM priority events scheduled for the same tick as BY\_PRIORITY events, those will be shuffled at random into the ordered BY PRIORITY events.
- PriorityType.LAST events will execute after those with other priority types.All events with a LAST priority type will execute in the order in which they are scheduledwith respect to other LAST priority type events.

An event's PriorityType and optional priority can specified via the scheduling methods (e.g., schedule\_repeating\_event). See the schedule moduleAPI documentation formore information on different ways to schedule events (methods and functions).

#### 5.2.2. Creating the Context and Grid

Once the schedule has been initialized and events have been added, the context, which holds the population of agents, and the grid projection on which the agents move are created (contexts and projections are described in

#### Contexts and Projections).

```
from repast4py import context as ctx
2
4
    # create the context to hold the agents and manage cross
5
    process
6
    # synchronization
7
    self.context = ctx.SharedContext(comm)
8
    # create a bounding box equal to the size of the entire
9
    global world grid
    box = space.BoundingBox(0, params['world.width'], 0,
11
    params['world.height'], 0, 0)
    # create a SharedGrid of 'box' size with sticky borders
13
    that allows multiple agents
14
    # in each grid location.
    self.grid = space.SharedGrid(name='grid', bounds=box,
    borders=space.BorderType.Sticky,
     occupancy=space.OccupancyType.Multiple,
                                     buffer size=2, comm=comm)
    self.context.add projection(self.grid)
```

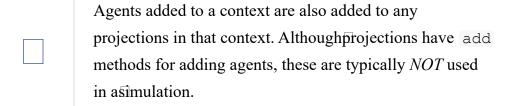
- 1 Creates the <u>SharedContext</u> for this simulation. The SharedContext contains the population of agents and manages synchronization of the projections across ranks.
- A BoundingBox is used to initialize the size of Repast4Py's cartesian spaces. Its arguments are the minimum x coordinate, the extent of the x dimension, and then the same for the y and z dimensions. Here we create a 2D box (the z extent is 0) starting at (0,0) and extending for params ['world.width] in the x dimension and params ['world.height'] in the y dimension.
- 3 space. SharedGrid takes a name, its bounds, its border, and occupancy types, as well as a buffer size, and a communicator as arguments. See the SharedGrid API documentation for a description of these arguments. The concept of a buffer was described in the Distributed Simulation section.
- 4 Once a <u>projection</u> has been created it must be added to the context so that it can be properly synchronized across processes.

#### 5.2.3. Creating the Agents

When creating the agents, we create the number of Walker agents specified in the walker.count input parameter, assigning each a random location.

```
1
    rank = comm.Get rank()
2
    for i in range(params['walker.count']):
3
        # get a random x,y location in the grid
4
        pt = self.grid.get random local pt(rng)
5
        # create and add the walker to the context
6
        walker = Walker(i, rank, pt)
7
        self.context.add(walker)
8
        self.grid.move(walker, pt)
```

- 1 Gets random location within the grid's local bounds. Each rank is responsible for some subsection of the total global grid and get\_random\_local\_pt gets a random location within those local bounds.
- 2 Creates the Walker, passing it an id, its starting rank, and its current location. See <u>Section 5.1</u>, "The Walker Agent" for more.
- 3 Adds the new Walker to the context. Once created, an agent must be added to the context in order to be properly synchronized and iterated through as part of the agent population.
- 4 Move the walker to its starting location.



#### 5.2.4. Initializing Logging

Logging refers to gathering simulation output data and writing it to a file. There are two types of logging supported by Repast4Py.

1. Tabular logging in which the user supplies row values to be logged, and Repast4Pyconcatenates these rows across processes and writes them to a file. This is usefulfor logging events and individual agent attributes. See the repast4py.logging.TabularLogger API for more information.

2. Reduce-type logging where the user supplies the aggregate values to be loggedin the form of a Python dataclasses.dataclass and Repast4Py performs a cross-processfeduce-type (e.g., summation) operation on those values. To use thistype of logging, you create a logger, which is responsible for logging the dataclass field(s) and performing the reduction operation on the field(s). These loggers are then added to logging.ReducingDataSet.Calling logging.ReducingDataSet.log(tick) will log thecurrent value of the dataclass field(s) in the loggers and perform the cross-process reduction. See the logging module API documentation for more information.

The Walker Model uses both of these logging types. The first is used to log the individual *meet\_count* of each agent, and the second to log that total number of meets, as well as the minimum and maximum number.

```
@dataclass
2
    class MeetLog:
        total meets: int = 0
4
        min meets: int = 0
5
        max meets: int = 0
6
7
8
     self.agent logger = logging.TabularLogger(comm,
9
    params['agent log file'],
                                                ['tick',
11
     'agent id', 'agent uid rank',
12
                                                'meet count'])
13
     2
14
     self.meet log = MeetLog()
15
     loggers = logging.create loggers(self.meet log,
16
     op=MPI.SUM,
17
                                      names={'total meets':
18
     'total'}, rank=rank)
19
     loggers += logging.create loggers(self.meet log,
    op=MPI.MIN,
                                       names={'min meets':
     'min'}, rank=rank)
     loggers += logging.create loggers(self.meet log,
     op=MPI.MAX,
                                       names={'max meets':
     'max'}, rank=rank)
    self.data set = logging.ReducingDataSet(loggers,
    MPI.COMM WORLD,
                                 Ø
    params['meet log file'])
```

- 1 MeetLog is the dataclass used by the aggregate reduce logging. As we saw in Section 5.1.2, "Logging the Walker" each agent updates the shared MeetLog instance as appropriate in its count\_colocations method.
- The TabularLogger class is used for tabular-style logging. The constructor arguments are the communicator over which to concatenate all the table's rows and the column header values.

  self.agent\_logger is then used to log the individual agent meet counts.
- 3 Creates the MeetLog object that contains the aggregate colocation statistics that we want to log.
- 4 Creates a logger that uses self.meet\_log as the source of the data to log, performing a cross process summation (op=MPI.SUM) of that data to log, and logs the value of the total field in self.meet\_log. The names argument specifies the fields to log as a dictionary where the key is the dataclass field to log, and the value is the column header text for that value.
- 5 Creates a logger for the self.meet\_log.min field, minimizing the value across processes. The created logger is added to the list of loggers created in 4.
- 6 Creates a logger for the self.meet\_log.max field, maximizing the value across processes. The created logger is added to the list of loggers created in 4.
- 7 Creates a logging.ReducingDataSet from the list of loggers.

  params['meet log file] is the name of the file to log to.

After the logging is initialized, we log the starting tick 0 state of the simulation.

```
# count the initial colocations at time 0 and log
for walker in self.context.agents():
    walker.count_colocations(self.grid, self.meet_log)

1 self.data_set.log(0)
self.meet_log.max_meets = self.meet_log.min_meets = self.meet_log.total_meets = 0
self.log_agents()
```

- 1 Updates self.meet\_log with each agents colocation data by calling count\_colocations on each agent. See Section 5.1.2, "Logging the Walker" for the details.
- 2 Logs the current values of the self.meet\_log by calling log on the self.data\_set ReducingDataSet. The log method takes a floating point argument that specifies the tick at which the data was logged (in this case tick 0).
- 3 Resets the self.meet\_log values back to 0 given that we want to log the data per tick, rather than a running total.
- 4 Logs the individual agent meet counts. See the method definition below.

The log\_agents method logs each agent's meet\_count using the self.agent logger TabularLogger.

- **1** Gets the current tick value
- 2 Iterates over all the local agents in the context.

  SharedContext.agents() returns an iterator over the local agent population.
- 3 For each Walker, log the current tick, the Walker's id, its unique id rank, and its meet\_count using the log\_row method. Each call to log row becomes a row in the tabular output.
- 4 Writes the currently logged rows to a file. It is not strictly necessary to call write every time rows are logged as the rows will accumulate until write is eventually called.

#### 5.2.5. Scheduled Methods

In <u>Section 3.2</u>, "<u>Scheduling Events</u>" we saw how to schedule events that repeat and that executewhen the simulation ends. In this model, the events to be scheduled are methods of the <u>Modell</u> class. The methods are called

according to how they are scheduled, driving the simulation forward. The first of these, the step method, is scheduled to execute starting at tick 1 and then every tick thereafter.

```
# scheduled with: self.runner.schedule repeating event(1,
2
     1, self.step)
    def step(self):
                                                  1
4
        for walker in self.context.agents():
5
             walker.walk(self.grid)
 6
7
         self.context.synchronize(restore walker)
8
9
         for walker in self.context.agents():
             walker.count colocations(self.grid,
11
     self.meet log)
13
        tick = self.runner.schedule.tick
14
         self.data set.log(tick)
         # clear the meet log counts for the next tick
         self.meet log.max meets = self.meet log.min meets =
    self.meet log.total meets = 0
```

- 1 Calls walk on each Walker agent. self.context.agents returns an iterator over all the agents in the model. See Section 5.1.1, "Walking the Walker" for more information on the walk method, and the SharedContext API documenation for more information on the agents method.
- 2 Synchronizes the state of the simulation across processes using the restore\_walker function to restore any Walkers that have moved processes. See Section 5.3, "Restoring Walkers" for more information.
- 3 Updates self.meet\_log with each agent's colocation data by calling count\_colocations on each Walker. See Section 5.1.2, "Logging the Walker" for the details.
- 4 Logs the current values of the self.meet\_log by calling log on the self.data\_set ReducingDataSet. As we saw earlier, the log method takes a floating point argument that specifies the tick at which the data was logged. In this case, we use the current tick value.
- 5 Resets the self.meet\_log values back to 0 because we want to log the data per tick, rather than a running total.

Call synchronize on your SharedContext



whenever you need to synchronize the state of the simulation across processes. For example, when agents moving on agrid or space may have crossed into a subsection of the global grid that ismanaged by a different process or when the buffer areas need to be updated.

#### The second repeating event

```
(self.runner.schedule_repeating_event(1.1, 10, self.log_agents)) is scheduled to call Model.log_agents starting at tick 1.1, and then every 10 ticks thereafter. See the discussion of log_agents in Section 5.2.4, "Initializing Logging" for more information.
```

#### The final event

(self.runner.schedule\_end\_event(self.at\_end)) is scheduled to call Model.at\_end when the simulation ends. This method closes the two logs, insuring that any remaining unwritten data is written to their respective files.

```
1    def at_end(self):
2        self.data_set.close()
3        self.agent_logger.close()
```



Do not forget to call close on your logging class instances when the simulation ends.

#### 5.3. Restoring Walkers

The restore\_walker function is used to create an individual Walker when that Walker has moved (i.e., walked) to another process. This function is passed to the synchronize method (i.e., self.context.synchronize(restore\_walker)) and is called in the synchronization mechanism. The restore\_walker function the reverse of the Walker.save method discussed in Section 5.1.3, "Serializing the Walker", unpacking the tuple returned by that to create a Walker agent.

```
walker cache = {}
2
                                                 2
     def restore walker(walker data: Tuple):
4
5
        Args:
6
             walker data: tuple containing the data returned
7
    by Walker.save.
8
9
         # uid is a 3 element tuple: 0 is id, 1 is type, 2 is
     rank
11
        uid = walker data[0]
        pt array = walker data[2]
13
        pt = DiscretePoint(pt array[0], pt array[1], 0)
     4
14
15
16
         if uid in walker cache:
17
             walker = walker cache[uid]
18
         else:
             walker = Walker(uid[0], uid[2], pt)
             walker cache[uid] = walker
21
                                                7
         walker.meet count = walker data[1]
         walker.pt = pt
         return walker
```

- 1 We use a caching strategy when restoring Walkers. This dictionary is the cache of previously created walkers. The dictionary keys are the Walker unique ids, and the values are the Walker instances.
- 2 The walker\_data tuple is the same tuple as created by the Walker.save method.
- 3 The first element of the tuple is the Walker's unique id.
- 4 Creates a DiscretePoint from point coordinate array. This is the current location of the Walker being restored.
- **5** Checks if the Walker unique id is in the cache. If it is, then retrieve that Walker.
- 6 If the unique id is not in the cache, then create a Walker.
- 1 Updates the Walker state with the meet count and point data.

## 5.4. Running the Simulation

The simulation is run from the command line:

mpirun -n 4 python examples/rndwalk/rndwalk.py

```
examples/rndwalk/random walk.yaml
```

Here we are running the simulation with 4 process ranks and the model input parameters are in the examples/rndwalk/random\_walk.yaml file.

```
random.seed: 42
stop.at: 50
walker.count: 1000
world.width: 2000
world.height: 2000
meet_log_file: 'output/meet_log.csv'
agent_log_file: 'output/agent_log.csv'
```

#### 5.4.1. Parsing Input Parameters

An if name == 'main' code block is used to parse the input parameters and fun the simulation. The repast4py.parameters module contains utility functions for parsing both command line and model input parameter files, including a default parser for command line arguments.

```
if __name__ == "__main__":
    parser = parameters.create_args_parser()
    args = parser.parse_args()
    params = parameters.init_params(args.parameters_file,
    args.parameters)
    run(params)
```

- 1 Creates the default command line argument parser.
- 2 Parses the command line into its arguments using that default parser
- 3 Creates the model input parameters dictionary from those arguments using parameters.init\_params.

The default command line parser created with

parameters.create\_args\_parser acceptsapath to a yaml format parameters input file, and a json format dictionary stringthat will override parameters in the parameters file.

```
$ python examples/rndwalk/rndwalk.py -h
usage: rndwalk.py [-h] parameters_file [parameters]
```

```
positional arguments:
   parameters_file parameters file (yaml format)
   parameters json parameters string

optional arguments:
   -h, --help show this help message and exit
```

parameters.init\_params takes the parameters file and the json string and creates a dictionaryof model input parameters whose keys are the parameter names and values are the parameter values. This dictionary is returned by the function and is available via the module itself as parameters.params. For example,

```
from repast4py import parameters

num_agents = parameters.params['num.agents']

from repast4py import parameters

num_agents = parameters.parameters.

parameters.

param
```

If the parameters file or the json input contains a parameter named random.seed, the default random number generator (i.e., repast4py.random.default\_rng) is initialized with that seed. See the repast4py.parameters API documentation for more information.

Lastly we have a simple run function that creates the Model class and calls its start method, which starts the simulation by starting schedule execution. This run function is called in the if name == 'main' code block.

```
def run(params: Dict):
    model = Model(MPI.COMM_WORLD, params)
    model.start()

class Model:

def start(self):
    self.runner.execute()
```

1 Start the simulation by executing the schedule which calls the scheduled methods at the appropriate times and frequency.

The code in the run function could be moved to the if

name == 'main' code block, but it is often useful to
have an entry type function that initializes and starts a
simulation.

## 6. Tutorial 2 - The Rumor Network Model

#### 6.1. Overview

The Rumor model is a simple network model that illustrates Repast4Py's networkagent-based model features. The simulation models the spread of a rumor through a networked population. During initialization some number of agents (network nodes) are marked as rumor spreaders. At each iteration of the simulation, a random draw is made to determine if the neighbors of any rumor-spreading nodes have received the rumor. This draw is performed once for each neighbor. After all of the neighbors that can receive the rumor have been processed, the collection of rumor spreaders is updated to include those nodes that received the rumor.

This text assumes you have already read the *Repast4Py Users Guide* up through <u>Tutorial 1</u>.

See the <u>Repast4Py Examples</u> page to download the source code for this modeland for more information on getting started with the examples.

#### 6.2. The Network

The Rumor model network is initialized from the

examples/rumor/network.txt file included with the example model. This file assigns each network node, corresponding to each model agent, to a process rank. Repast4Py creates a

repast4py.network.SharedNetwork from this file, instantiating the agents on the correct ranks and creating the edges betweenthe agents appropriately. When an edge is between agents on different process ranks

Repast4Py will create a *ghost* agent whose state mirrors that of the agent on the other process, and then create an edge using this ghost. For example, if an edge exists between A and B and A is on rank 1 and B on rank 2, then Repast4Py will:

- 1. Create a ghost of B on rank 1
- 2. Create a ghost of A on rank 2
- 3. Create an edge between A and the ghost B on rank 1
- 4. Create an edge between B and the ghost A on rank 2

For more information about ghost agents and how their state is maintained see the <u>Distributed Simulation</u> and <u>Cross-Process Code Requirements</u> sections.

The network.txt file was created using

rumor.generate\_network\_file to distribute aconnected Watts and Strogatz graph generated by the <a href="network">network</a> Python package across 4 process ranks. <a href="rumor.generate\_network\_file@tes Repast4Py">rumor.generate\_network\_file@tes Repast4Py</a>'s capability to take a <a href="network">network</a> Graph object and distribute it across a specified number of process ranks and write this distributed network to a file. A model can then create a SharedNetwork instance from this file.

```
import networkx as nx
 2
     from repast4py.network import write network, read network
 4
    def generate network file(fname: str, n ranks: int,
 5
     n agents: int):
 6
        """Generates a network file using
 7
     Repast4Py.network.write network.
 8
 9
        Args:
10
            fname: the name of the file to write to
11
            n ranks: the number of process ranks to
12
     distribute the file over
13
            n agents: the number of agents (node) in the
14
     network
15
16
        g = nx.connected watts strogatz graph(n agents, 2,
17
     0.25)
        try:
             import nxmetis
             write network(g, 'rumor network', fname, n ranks,
```

```
partition_method='metis')
    except ImportError:
        write_network(g, 'rumor_network', fname, n_ranks)
3
```

- 1 Creates a connected Watts and Strogatz graph using <u>networkx</u>. See the networkx <u>API Docs</u> for more details.
- 2 If the nxmetis package is available, distribute the graph using the metis partition method, and write it out to fname.
- 3 If nxmetis is not available, distribute the graph using the default random partition method, and write it out to fname.

See the API documentation for <a href="repast4py.network.write\_network">repast4py.network.write\_network</a> for more information.

## 6.3. The Rumor Model Implementation

The Rumor Model implementation follows the typical Repast4Py structure and consists of the following parts.

- 1. A RumorAgent class that implements the agent state and behavior
- 2. A Model class responsible for initialization and managing the simulation
- 3. A create\_rumor\_agent function used to create the Rumor agents when creating thenetwork from a saved file
- 4. A restore\_agent function used to create an individual

  RumorAgent when that RumorAgent has been ghosted (i.e., created as a ghost agent) on another process rank
- 5. A run function that creates and starts the simulation
- 6. An if name == "main" block that allows the simulation to be run from the command line

#### 6.3.1. The Rumor Agent

The Rumor model's agent is a simple class with a single received rumor boolean attribute that specifies whether or not the agent

has received the rumor. It also has the canonical save and update methods used to move and copy the agent between processes and to update the state of aghost agent from its originating process rank.

```
class RumorAgent(core.Agent):
                                      1
 2
         def init (self, nid: int, agent type: int, rank:
 4
     int, received rumor=False):
 5
             super(). init (nid, agent type, rank)
             self.received rumor = received rumor
 6
 7
 8
         def save(self):
 9
            """Saves the state of this agent as a tuple.
10
11
             A non-ghost agent will save its state using this
12
             method, and any ghost agents of this agent will
13
             be updated with that data (self.received rumor).
14
15
            Returns:
16
                 The agent's state
17
18
             return (self.uid, self.received rumor)
19
20
         def update(self, data: bool):
21
             """Updates the state of this agent when it is a
22
     ghost
             agent on a rank other than its local one.
24
             Args:
                 data: the new agent state (received rumor)
             11 11 11
27
             if not self.received rumor and data:
29
                # only update if the received rumor state
                 # has changed from false to true
                 model.rumor spreaders.append(self)
                 self.received rumor = data
```

- 1 RumorAgent extends repast4py.core.agent as is required by all Repast4Py agents
- 2 Calls the core. Agent constructor, passing the node id, agent\_type, and originating rank. Together these will create a globally unique id for this agent.
- 3 The received\_rumor boolean specifies whether the agent has received the rumor and is able to spread it.
- The required save method for saving the agent's state as a tuple. This state can be used to update ghosts of this agent on other ranks.

5 The required update method for updating ghosts from saved agent state. Here, we only update if the received\_rumor state has changed from False to True. If so, then add this agent to the Model's list of rumor spreading agents (Section 6.3.2.2, "Seeding the Rumors").

#### 6.3.2. The Model Class

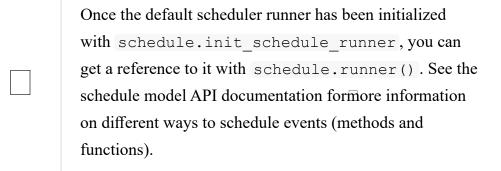
As in <u>Tutorial 1</u>, the Model class encapsulates the simulation. It is responsible for initialization, scheduling events, creating agents and their network, and managing logging. It also defines the scheduled events that drive the simulation forward.

In the Model constructor, we create the simulation schedule, the network, seed the network with the rumors, and initialize the loggers that we use to log the rumor counts to a file.

```
1
    from repast4py import core, random, schedule, logging,
2
    parameters
   class Model:
4
5
6
        def init (self, comm, params):
7
            self.runner = schedule.init schedule runner(comm)
    0
8
9
            self.runner.schedule repeating event(1, 1,
    self.step)
            self.runner.schedule stop(params['stop.at'])
    3
            self.runner.schedule end event(self.at end)
    4
            . . .
```

- 1 Before any events can be scheduled, the schedule runner must be initialized.
- 2 Schedules Model.step to execute starting at tick 1 and then every tick thereafter. Repeating events are scheduled with schedule.repeating\_event. The first argument is the start tick, and the second is the frequency for repeating.
- 3 schedule\_stop schedules the tick at which the simulation should stop. At this tick, events will no longer be popped off the schedule and executed.

schedule\_end\_event can be used to schedule methods that perform some sort of *clean up* type operation when the simulation ends, closing a log file, for example. This is called at the tick specified in schedule stop.



A simulation stopping time must be set with schedule\_stop. Without a stopping timethe simulation will continue to run, seeming to hang if there are no events to execute, or continuing to execute any scheduled events without stopping. The stopping time does not need to be set during initialization, but can be set during a simulation run when astopping condition is reached.

### Creating the Network

As described in <u>Section 6.2</u>, "<u>The Network</u>" the Rumor model network is initialized from a file. The <u>repast4py.network.read\_network</u> function reads this file and creates a Shared Network instance from the network description in the file.

```
fpath = params['network_file']
self.context = ctx.SharedContext(comm)
read_network(fpath, self.context, create_rumor_agent,
restore_agent)
self.net = self.context.get_projection('rumor_network')
```

- 1 Gets the path to the file describing the network from the parameters dictionary
- 2 Creates a context to hold the agents and the network projection
- 3 Creates the network from the named file, using the

- create\_rumor\_agent, and restore\_agent functions to create the agents and their necessary ghosts (Section 6.3.3, "Creating and Restoring RumorAgents"). The created network is added to the specified context as part of this call.
- 4 Gets a reference to the named network from the context. The network input file specifies the network name on its first line. This is the network created in <3> and is an instance of an <u>UndirectedSharedNetwork</u>.

### Seeding the Rumors

We seed the network with some initial rumor spreaders by selecting a parameterized number of agents and setting their received\_rumor attribute to True. These agents are added to the Model's list of rumor spreaders.

```
def __init__(self, comm, params):
    ...
self.rumor_spreaders = []
self.rank = comm.Get_rank()
self._seed_rumor(params['initial_rumor_count'], comm)
```

The \_seed\_rumor method uses MPI's Scatter function to sendeach rank the number of agents to initialize as rumor spreaders. An MPI4Py scatter call takes a collection or array of values created onone rank (the root rank) and sends the \_ith\_ element of that collection or array to rank i. So for example, rank 0 gets the zeroth element, rank 1 gets the first, and so on. In \_seed\_rumor, we use a numpy array of ints as the array to scatter and the \_ith\_ element of the array is the number of rumors preaders to initialize on

```
1
    def seed rumor(self, init rumor count: int, comm):
2
        world size = comm.Get size()
         # np array of world size, the value of i'th element
4
    of the array
5
        # is the number of rumors to seed on rank i.
        rumor counts = np.zeros(world size, np.int32)
7
        if (self.rank == 0):
8
             for in range(init rumor count):
9
                 idx = random.default rng.integers(0,
10
     high=world size)
11
                 rumor counts[idx] += 1
12
```

rank i.

```
rumor_count = np.empty(1, dtype=np.int32)
comm.Scatter(rumor_counts, rumor_count, root=0)

for agent in
self.context.agents(count=rumor_count[0], shuffle=True):
    agent.received_rumor = True
    self.rumor_spreaders.append(agent)
```

- 1 Get the total number of ranks over which the simulation is distributed
- 2 Initialize a numpy array of world\_size with zeros. rumor\_counts will hold the number of initial rumor spreaders for each rank.
- 3 If this Model's rank is 0, then randomly select an index into the rumor\_counts array, and increment the value at that index by one. Do this for a number of times equal to the initial number of rumors to seed.
- 4 Create an empty array of size 1 to receive the number of rumors from the Scatter call.
- 5 Scatter the values in rumor\_counts from root rank 0 into the rumor\_count array on all the ranks. rumor\_count now holds the number of initial rumor spreaders assigned to the current rank.
- 6 Using the SharedContext.agents method, get an iterator over a number of agents equal to the single value in rumor\_count at random (shuffle=True). Set each one of those agent's received\_rumor attribute to True, and add each one to the Model's rumor\_spreaders list.

Using MPI4Py's Scatter in this way is a useful method for randomly dividing up a total initialization value among ranks. In the Rumor Model, we tell each rank to initialize a number of rumor spreaders, and the sum of all these values is the total number of initial rumor spreaders specified by the input parameter.

# Logging

As we saw in <u>Tutorial 1</u>, there are two types of logging supported by Repast4Py, tabular and reduce-type logging (see the repast4py.logging module <u>API documentation</u> for more

information).

The Rumor model uses the second of these log types. The dataclass that we log records the total number of rumor spreaders and the number of new rumor spreaders added during attick.

```
1  | @dataclass
2  | class RumorCounts:
3  | total_rumor_spreaders: int
4  | new_rumor_spreaders: int
```

```
def init (self, comm, params):
2
       . . .
3
                                                     a
4
       rumored count = len(self.rumor spreaders)
5
       self.counts = RumorCounts(rumored count,
6
  rumored count)
       loggers = logging.create loggers(self.counts,
8
    op=MPI.SUM, rank=self.rank)
                                   3
       self.data set = logging.ReducingDataSet(loggers,
   MPI.COMM WORLD,
    params['counts file'])
       self.data set.log(0)
```

- 1 Get the current number of rumor spreaders immediately after rumor seeding
- 2 Create the RumorCount instance, setting the total\_rumor\_spreaders and new\_rumor\_spreaders to the current number of rumor spreaders
- 3 Create a list of loggers that use self.counts as the source of the data to log, and that perform a cross process rank summation of that data. The names argument is not specified, so the RumorCounts field names will be used as column headers.
- 4 Create a logging.ReducingDataSet from the loggers where params['counts file'] is the name of the file to log to.
- Log the initial (i.e., tick 0) values from self.counts.

#### Scheduled Methods

The Model's step method is scheduled to execute starting at tick 1 and

then every tick thereafter. It is in the step method that the rumor spreading is implemented. The implementation is a nested loop that iterates through all the network neighbors of each rumor spreader. If the network neighbor has not yet received a rumor, is local to the current rank, and the draw against the probability of a rumor spreading is successful, then we set the neighbor's received rumor attribute to True, and ultimately add it to the Model's list of rumor spreaders.

Each repast4py.network.SharedNetwork instance contains a reference to a networkx.Graph instance named graph. Use graph for any network queries that do not change thestructure of the network. For example, graph.neighbors(n) will return the network neighborsof agent n. See the networkx API documentation for more info.

```
1
     def step(self):
                                      0
2
         new rumor spreaders = []
        rng = random.default rng
4
         for agent in self.rumor spreaders:
5
             for ngh in self.net.graph.neighbors(agent):
 6
                 if not ngh.received rumor and ngh.local rank
7
     == self.rank \
8
                    and rng.uniform() <= self.rumor prob:</pre>
9
                     ngh.received rumor = True
                     new rumor spreaders.append(ngh)
11
12
                                                         3
         self.rumor spreaders += new rumor spreaders
13
         self.counts.new rumor spreaders =
14
     len(new rumor spreaders)
15
        self.counts.total rumor spreaders +=
     self.counts.new rumor spreaders 5
                                                          6
         self.data set.log(self.runner.schedule.tick)
                                                     7
         self.context.synchronize(restore agent)
```

- 1 Create a list to hold any new rumor spreaders, i.e., agents whose received rumor attribute is set to True during this iteration
- 2 For each rumor spreader, iterate through all of its network neighbors. If the network neighbor has not yet received a rumor, is local to the current rank, and the draw against the probability of a rumor spreading is successful, then set the neighbor's received rumor attribute to True,

and add it to the list of new rumor spreaders.

- 3 Add the new rumor spreaders to the list of current rumor spreaders
- 4 Set the new number of rumor spreaders on the self.counts log
- 5 Set the total number of rumor spreaders on the self.counts log
- 6 Log the self.count values for the current tick
- 7 Synchronize the model state across all ranks. This will update all the ghost agent states, calling RumorAgent.update on the ghost agents.

The list of rumor spreaders (rumor\_spreaders) can contain ghost agents. As we saw in The Rumor Agent, RumorAgent.update is called to update the state of ghost agents. If the update changes the received\_rumor attribute to True, then that ghost agent is added to the Model's list of rumor spreaders.

Never update the state of a ghost agent. A ghost agent is a mirror of an agent localto some other process. The ghost agent's state will be updated from that local source agent during the synchronize call overwriting any changes. The Rumor Model checks if the local rankof a rumor spreader's network neighbor is the current rank (ngh.local\_rank == self.rank)before updating the neighbor's state in order to avoid updating ghost state.

#### The final event

(self.runner.schedule\_end\_event(self.at\_end)) is scheduled to call Model.at\_end when the simulation ends. This method closes the logging data set, ensuring that any remaining unwritten data is written out.

```
1    def at_end(self):
2    self.data_set.close()
```

Do not forget to call close on your logging class instances when the simulation ends.

### 6.3.3. Creating and Restoring RumorAgents

RumorAgents are created during the read\_network call in the Model constructor.

```
1     read_network(fpath, self.context, create_rumor_agent,
     restore_agent)
```

There, as part of creating the network, the nodes (i.e., agents)of that network are also created. Each rank creates the nodes that are assigned toil using the passed in create rumor agent function.

```
def create_rumor_agent(nid, agent_type, rank, **kwargs):
    return RumorAgent(nid, agent_type, rank)
```

The nid, agent\_type, and rank arguments are read from the network input file and passed to this function. See the repast4py.network.read\_network API documentation for more info.

As described in <u>Section 6.2</u>, "The <u>Network</u>", when an edge links two nodes on different ranks, Repast4Py will create ghost agents as necessary and reate an edge between the ghosts and the local agents. The <u>restore\_agent</u> function is used to create the ghost on the rank it is ghosted to, using the state from the source agent's <u>save</u> method.

```
def restore_agent(agent_data):
    uid = agent_data[0]
    return RumorAgent(uid[0], uid[1], uid[2],
    agent_data[1])
```

1 agent data is the tuple produced by an agent's save method.

### 6.3.4. Running the Simulation

The simulation is run from the command line. For example, from within the examples/rumor directory:

```
mpirun -n 4 python rumor.py rumor model.yaml
```

Here we are running the simulation with 4 process ranks and the model input parameters are in the rumor model.yaml file.

```
network_file: network.txt
initial_rumor_count: 5
stop.at: 100
rumor_probability: 0.1
counts_file: output/rumor_counts.csv
```

The Rumor Model uses the standard if name == 'main' code block to parse the input parameters and run the simulation.

```
if __name__ == "__main__":
    parser = parameters.create_args_parser()
args = parser.parse_args()
params = parameters.init_params(args.parameters_file,
args.parameters)
run(params)
```

- 1 Create the default command line argument parser
- 2 Parse the command line into its arguments using that default parser
- 3 Create the model input parameters dictionary from those arguments using parameters.init params

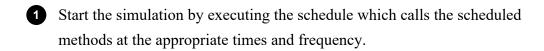
See <u>Parsing Input Parameters</u> in Tutorial 1 for more details.

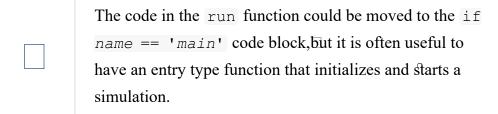
Lastly we have a simple run function that creates the Model class and calls its start method which starts the simulation by starting schedule execution. This run function is called the if name == 'main' code block.

```
def run(params: Dict):
    model = Model(MPI.COMM_WORLD, params)
    model.start()

class Model:

def start(self):
    self.runner.execute()
```





# 7. Tutorial 3 - The Zombies Model

In <u>Tutorial 1</u>, we developed a simple model in which agents walk at random around a 2-dimensional Cartesian grid. The Zombies Model builds on this simple movement implementation, adding an additional agent type and using a Continuous Space.

This text assumes you have already read the *Repast4Py Users Guide* up through <u>Tutorial 1</u>.

In the Zombies model, human agents are pursued by zombie agents, and once caught become zombies themselves. Each timestep, the following occurs:

#### 1. All the Zombies:

- a. Query their immediate neighborhood to determine the adjacent grid location with the most number of Humans
- b. Move towards that location, assuming any Humans are found
- c. Infect the Humans at that location, also assuming any Humans are found

#### 2. All the Humans:

- a. Become a Zombie, after being infected for 10 timesteps, else
- b. Query their immediate neighborhood to determine the adjacent grid

location with the fewest number of Zombies

c. Move to that location at twice the speed of a Zombie.

See the <u>Repast4Py Examples</u> page to download the source code for this modeland for more information on getting started with the examples.

The code consists of the following components:

- Two agent classes: a <u>Zombie class</u> that implements the behavior of the zombie agents, and a <u>Human class</u> that implements the state and behavior of the human agents.
- A restore function that creates both Zombie and Human agents when they are moved from one MPI rank to another.
- A <u>Model class</u> responsible for initializing and managing the simulation and simulation components, including:
  - the model's context
  - Continuous Space and Discrete Grid projections,
  - Scheduled Events, and
  - Logging
- A <u>GridNghFinder</u> class for quickly computing neighboring grid locations usingnumpy and the the <u>Numba</u> Python package to accelerate the computation
- The standard run function that creates and starts the simulation.
- The standard if name == "main" block in which input parameters are parsed and allows the simulation to be run from the command line.

The Model class instance model is a global variable defined as an attribute of the zombies module itself.

Consequently, it is available to all the code in zombies.py as just[model, that is, you will see it referenced as model rather than self.model or as a function argument. The Model class contains references to the discrete grid and continuous spaceprojections as

well as the grid neighborhood finder. These are used by the agents in the implementation of their behavior. By making model a global variable, our agents can conveniently access these required components.

# 7.1. The Agent Classes

The Zombies model implements two agent classes: a Zombie and a Human. The zombie's behavioris to pursue humans across a two dimensional Cartesian space and infect them. The human's behavioris to flee from zombies. Humans contain a boolean (infected) field indicating whether or not they are infected, and an integer (infected\_duration) field tracking the duration of the infection. When thatvalue reaches 10, that human is replaced with a zombie. The methods that implement infection, andthe transition from human to zombie are described in the Zombie step method, the the Human step method, and the Model class scheduled step method.

Both agents inhabit two two-dimensional projections: a SharedGrid and a SharedCSpace. The first of these is a matrix type grid where the agent locations are expressible as discrete integer coordinates. The second is a continuous space where the agent locations are expressible as continuous floating point coordinates. The grid is used to implement agentvision. Humans and zombies can see the zombies and humans in the grid locations that neighbor their own, and act accordingly. The continuous space is used for movement, and until the Walker agents in Tutorial 1 which move a single grid unit at a time, the human and zombie agents move in fractions of a grid unit, 0125 for zombies, and 0.5 grid units for humans. In this way, the humans are twice as fast as the zombies. When a human or zombie moves in the continuous space, a method in the Model class updates its location in the grid space. These spatial aspects are described indetail in the Implementing Spatial Projections subsection.

# 7.1.1. The Zombie Agent

We implement our Zombie agent using the Zombie class. As required for all Repast4Py agent implementations, the Zombie class extends

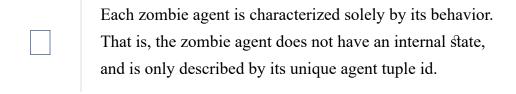
repast4py.core.Agent, passing it the components of the unique agent id tuple.

```
1
    from repast4py import core
2
4
5
    class Zombie (core.Agent): 1
6
        TYPE = 1 2
7
8
9
        def init (self, a id, rank):
            super(). init (id=a id, type=Zombie.TYPE,
11
    rank=rank) 3
12
```

- 1 Zombie subclasses repast4py.core.Agent.Subclassing Agent is a requirement for all Repast4Py agent implementations.
- 2 TYPE is a class variable that defines the agent type id for the Zombie agents. This is a required part of the unique agent id tuple.
- In order to uniquely identify the agent across all ranks in the simulation, the <a href="repast4py.core.Agent">repast4py.core.Agent</a> constructor takes the following three arguments: an integer id that uniquely identifies an agent on the process where it was created, a non-negative integer identifying the type of the agent, and the rank on which the agent is created.

# The Zombie step() Method

The zombie agent behavior is implemented in its step method. Here, the zombie queries its immediate neighborhood to find the location with the most humans. Assuming some humans are found, the zombie will then move towards that grid location. If multiple grid locations have the maximum number of humans, including when the maximum is 0, the zombie will choose one of those locations at random.



The 8 member neighborhood of grid cells surrounding an agent's 2D grid location is called its Moore neighborhood. Given a grid location, its 8 neighbors and the current location are computed using the <a href="https://grdNghFinder">GrdNghFinder</a>.

```
1
     from repast4py import core, space, schedule, logging,
2
     random
     from repast4py.space import ContinuousPoint as cpt
     from repast4py.space import DiscretePoint as dpt
 4
 5
 6
7
     class Zombie(core.Agent):
8
9
         def step(self):
                                   1
10
             grid = model.grid
11
             pt = grid.get location(self)
             nghs = model.ngh finder.find(pt.x, pt.y)
13
14
             at = dpt(0, 0)
15
             maximum = [[], -(sys.maxsize - 1)]
16
             for ngh in nghs:
                                  (6)
17
                 at. reset from array(ngh)
                                                7
18
                 count = 0
                 for obj in grid.get_agents(at):
                                                      8
                     if obj.uid[1] == Human.ID:
                         count += 1
                 if count > maximum[1]:
                                            9
23
                     maximum[0] = [ngh]
24
                     maximum[1] = count
                                                10
                 elif count == maximum[1]:
                     maximum[0].append(ngh)
27
             max ngh = maximum[0]
29
                                                            Œ
     [random.default rng.integers(0, len(maximum[0]))]
                                                            12
             if not np.all(max ngh == pt.coordinates):
                 direction = (max ngh - pt.coordinates[0:3])
             13
     0.25
34
                 cpt = model.space.get location(self)
                 model.move(self, cpt.x + direction[0], cpt.y
                        Œ
     + direction[1])
                                              16
38
             pt = grid.get location(self)
             for obj in grid.get agents(pt):
                 if obj.uid[1] == Human.ID:
                     obj.infect()
                     break
```

1 The Model contains both the grid and continuous space in its grid and

- space fields. The model variable contains the instance of the Model class.
- 2 Get the location of this zombie. This location is a Discrete Point.
- 3 Use the Model's instance of a GridNghFinder to get the Moore neighborhood coordinates of the zombie's current location.
- 4 Create a temporary <u>DiscretePoint</u> for use in the loop over the Moore neighborhood coordinates.
- Initialize a list maximum that will be used to store the current maximum number of human agents and the location(s) containing that maximum number. The first element of the list stores the location(s), and the second the current maximum. We set the initial maximum number of humans as -(sys.maxsize 1), the smallest negative integer. Consequently, if there are 0 neighboring humans then that becomes the new maximum, and the maximum list always contains at least one location.
- 6 Iterate through all the neighboring locations to find the location(s) with the maximum number of humans. For each neighbor location, we count the number of humans at that location, and if the total count is equal to or greater than the current maximum, update or reset the maximum list appropriately.
- Reset the the at DiscretePoint to the current neighbor coordinates.

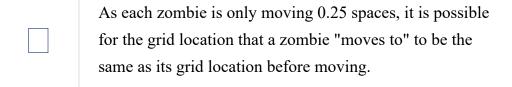
  This will be used in the get\_agents call to come, which takes a

  DiscretePoint argument and this converts the ngh numpy array to a

  DiscretePoint.
- 8 Get all the agents at the current neighbor location, and iterate through those agents to count the number of humans. Humans are those agents where the type component of their unique id tuple is equal to Human. ID.
- 9 If the count is greater than the current maximum count, reset the maximum list to the current location, and maximum count.
- 10 If the count is equal to the current maximum count, then append the current location to the maximum list.
- Select one of the *maximum neighbor locations* at random using Repast4Py's default random number generator. See the API documentation for more details.
- 12 Check if the maximum neighbor location is the zombie's current location,

- using the is\_equal function. If not, move the zombie toward the selected location.
- Calculate the direction to move by subtracting the zombie's current location from its desired location. The zombie is only able to move a distance of 0.25 spaces per step (i.e., its speed is 0.25 spaces/tick), and so we multiply the direction vector by 0.25.
- Get the zombie's current location in the continuous space. As with the grid, the Model class instance model contains the continuous space over which the agents move.
- Move the zombie using the Model's move () method to the location computed by adding the current location to the direction vector.

  Model.move() is described in the Implementing Spatial Projections subsection.
- Get the zombie's current location in grid space and infect any humans found at that location. Infection is described in the <u>next section</u>.



# Saving the Zombie agent state

To move our zombie agent between processes, we must save its state. Because the zombie agent does not have an internal state, our save method returns only the zombie agent's unique id tuple.

```
class Zombie(core.Agent):

def save(self):
    return (self.uid,)
```

# 7.1.2. The Human Agent

The human agent state is composed of two variables:

• Whether or not the human is infected, and

• The duration of the infection

Additionally, the human has the following behavior:

- Querying the current neighborhood for the fewest number of zombies
- Moving towards the location with the fewest number of zombies
- Becoming a zombie after 10 time steps, once infected.

We implement our human agents using the Human class, subclassing repast4py.core.Agent, passing it the components of the unique agent id tuple. The constructor also initializes the infected boolean to False and the duration of infection to 0.

```
1
    from repast4py import core
2
                                1
    class Human (core.Agent):
4
                    2
5
       TYPE = 0
6
7
        def init (self, a id, rank):
            super(). init (id=a id, type=Human.TYPE,
8
9
    rank=rank)
10
            self.infected = False
            self.infected duration = 0
```

- 1 Human subclasses repast4py.core.Agent.Subclassing Agent is a requirement for all Repast4Py agent implementations.
- 2 TYPE is a class variable that defines the agent type id the Human agent. This is a required part of the unique agent id tuple.

#### **Human Behavior**

Each human has three underlying behaviors:

- 1. Moving towards the area with the fewest zombies
- 2. Becoming infected by a zombie

The <u>step()</u> method for the human agent implements (1), and the <u>infect()</u> method implements (2).

### The Human step() Method

Much of the human step method is similar to that of the zombie. The humanalso queries its Moore neighborhood, and moves in the direction of its selected location. However, the human is searching for the location with the fewest number of zombies, and moves to that location. In addition, the human also increments its infected duration in the step method and becomes a zombie if infected for 10 time steps.

Given the similarities with the Zombie step() method only the relevant differences will be highlighted below.

```
1
     class Human (core.Agent):
2
5
         def step(self):
6
             space pt = model.space.get location(self)
7
             alive = True
8
             if self.infected:
                                     (2)
9
                 self.infected duration += 1
10
                 alive = self.infected duration < 10</pre>
11
12
             if alive:
                 grid = model.grid
14
                 pt = grid.get location(self)
15
                 nghs = model.ngh finder.find(pt.x, pt.y)
16
                                                  3
17
                 minimum = [[], sys.maxsize]
18
                 at = dpt(0, 0, 0)
19
                 for ngh in nghs:
                      at. reset from array(ngh)
21
                      count = 0
                      for obj in grid.get agents(at):
23
                          if obj.uid[1] == Zombie.TYPE:
24
                              count += 1
25
                      if count < minimum[1]:</pre>
                          minimum[0] = [ngh]
27
                          minimum[1] = count
                      elif count == minimum[1]:
29
                          minimum[0].append(ngh)
31
                 min ngh = minimum[0]
     [random.default rng.integers(0, len(minimum[0]))]
34
                 if not is equal(min ngh, pt.coordinates):
                      direction = (min ngh - pt.coordinates) *
     0.5
                      model.move(self,
```

```
space_pt.x + direction[0],
space_pt.y + direction[1])

return (not alive, space_pt)

...
```

- 1 Initialize an alive variable that specifies whether or not this human is still alive (not a zombie).
- 2 If the human is infected, increment its infection duration. If the infection duration is 10 or more, then set alive to False, indicating that this human should become a zombie.
- Initialize a list minimum that will be used to store the current minimum number of zombie agents and the location(s) containing that minimum number. The first element of the list stores the location(s), and the second the current minimum. We set the initial minimum number of humans as sys.maxsize, the largest integer, so that anything below that counts as the new minimum value.
- 4 Checks if the zombie count is less than the current minimum value, updating appropriately if so.
- Moves this human using the same mechanism as the zombie, but twice as far, 0.5 vs 0.25.
- 6 Return a tuple of alive and the human's current location in the continuous space. This is returned to the Model class calling code, which will replace the human with a zombie if the human is no longer alive.

### The infect() method

We saw that zombies infect humans by calling the human's infect() method. This methodsimply changes the infected state from False to True.

```
class Human(core.Agent):
    def infect(self):
    self.infected = True
```

# Saving the Human Agent State

To move the human agent between processes, we must save its state. Unlike our zombie agent, saving the human state entails saving its infected and infected\_duration states in addition to its unique agent id tuple. The save method for the human agent was described in detail in Section 4.2, "Saving and Restoring Agents".

### 7.1.3. Restoring the Agents

The restore\_agent function is used to create an individual zombie or human when that agent has moved to another process. This function is passed to the synchronize method (i.e.,

self.context.synchronize (restore\_agent) ) and is called in the synchronization mechanism. This function has also alreadybeen described in detail in <u>Section 4.2</u>, "<u>Saving and Restoring Agents</u>".

### 7.2. The Model class

As was demonstrated in the earlier tutorials, the Model class encapsulates the simulation and is responsible for initialization, scheduling events, creating agents and their grid/space environment, and managing logging. In addition, the scheduled events that drive the simulation forward are methods of the Model class.

# 7.2.1. Scheduling Events and Creating the Context

For the Zombies model, the scheduling of events and the creation of the context are similar to the implementations in the <u>Random Walker Model</u>. Here both are implemented in the <u>Model</u> constructor.

```
1 |
    from repast4py import core, space, schedule, logging,
2
     random
     from repast4py import context as ctx
4
     from repast4py.parameters import create args parser,
5
     init params
6
7
     . . .
8
9
     class Model:
11
         def init (self, comm, params):
12
             self.comm = comm
             self.context = ctx.SharedContext(comm)
```

```
self.rank = self.comm.Get_rank()

self.runner = schedule.init_schedule_runner(comm)

self.runner.schedule_repeating_event(1, 1,
self.step)
self.runner.schedule_stop(params['stop.at'])
self.runner.schedule_end_event(self.at_end)

self.runner.schedule_end_event(self.at_end)

...
...
```

- 1 Create a context to hold the agents and the network projection
- 2 Initialize schedule runner
- 3 Schedule the repeating event of Model.step, beginning at tick 1 and repeating every tick thereafter
- 4 Schedule the tick at which the simulation should stop, and events will no longer be executed
- 5 Schedule a simulation end event to occur after events have stopped

### 7.2.2. Implementing Spatial Projections

After initializing the schedule, adding events, and creating the context to hold the population of agents, the Model constructor creates the two spatial projections, the <u>SharedGrid</u> and the <u>SharedCSpace</u>.

Before we create our projections, we first must define a BoundingBox equal to the desired size of our space:

```
15
     occupancy=OccupancyType.Multiple,
16
                                           buffer size=2,
17
     comm=comm)
             self.context.add projection(self.grid)
                                                        3
18
19
             self.space = space.SharedCSpace('space',
     bounds=box, borders=BorderType.Sticky,
     occupancy=OccupancyType.Multiple,
                                              buffer size=2,
     comm=comm,
     tree threshold=100)
                                                         5
             self.context.add projection(self.space)
```

- 1 Create a BoundingBox to initialize the size of the Cartesian spaces. Its arguments are the minimum x coordinate, the extent of the x dimension, and then the same for the y and z dimensions. Here we create a 2D box (the z extent is 0) starting at (0,0) and extending for params ['world.width'] in the x dimension and params ['world.height'] in the y dimension.
- 2 Create the grid projection. repast4py.space.SharedGrid takes a name, its bounds, its border, and occupancy types, as well as a buffer size, and a MPI communicator as arguments. See the SharedGrid API documentation for a description of these arguments. The concept of a buffer was described in the Distributed Simulation section.
- 3 Add the grid to the context so that it can be properly synchronized across processes
- 4 Create the space projection. repast4py.space.SharedCSpace takes a name, its bounds, its border, and occupancy types, as well as a buffer size, a MPI communicator, and a tree threshold as arguments. See the SharedCSpace API documentation for a description of these arguments.
- 5 Add the space to the context so that it can be properly synchronized across processes

We use two spatial projections in our Zombies model: a discrete grid projection, and a continuous space projection. Even though the space and grid projections are distinct from each other, they are initialized with the same bounding box. Thus, they are the same size, which allows us to translate between the two projections such that the grid is overlaid on the

continuous space. As you have seen, the grid is used for neighborhood queries, and the continuous space for movement.

Within the Model class, a move method is defined and called during the movements ections of the agents' step methods (<u>Zombie.step()</u> and <u>Human.step()</u>). This move method performs the translation and movement on both the grid and continuous space.

```
1
     from repast4py.space import ContinuousPoint as cpt
2
     from repast4py.space import DiscretePoint as dpt
4
5
    class Model:
6
7
         . . .
8
9
        def move(self, agent, x, y): 1
10
             self.space.move(agent, cpt(x, y))
             self.grid.move(agent, dpt(int(math.floor(x)),
     int(math.floor(y))))
12
13
```

- 1 Pass the move method the x and y coordinates in the space projection that the agent argument is moving to.
- Move the agent to the specified point in the continuous space, creating a new ContinuousPoint from the x and y coordinates. See the move API documentation for more details.
- Move the agent to the corresponding location in the grid space. The grid takes a DiscretePoint as its location argument. To create one, we take the floor of the x and y coordinates, convert those to ints, and create a DiscretePoint from those ints. See the move API documentation for more details.

# 7.2.3. Creating the Agents

The population of agents is created within the Model class. The model input parameters human.count and zombie.count specify the total number of humans and zombies to create. These total amounts are distributed evenly among each process rank, with any remainder accounted for by assigning one agent to each rank, starting with 0, until the total amount has been

distributed.

Once the number of agents to create on each rank has been computed, that number of agents is created, assigning each a random location in the grid and continuous space.

```
1
    class Model:
2
         def init (self, comm, params):
4
             self.rank = self.comm.Get rank()
6
             world size = comm.Get size()
8
                                                           3
             total human count = params['human.count']
9
             pp human count = int(total human count /
10
     world size)
             if self.rank < total human count % world size:</pre>
     5
12
13
                 pp human count += 1
14
15
             local bounds = self.space.get local bounds()
     6
17
             for i in range(pp human count):
18
                 h = Human(i, self.rank)
19
                 self.context.add(h)
21
     random.default rng.uniform(local bounds.xmin,
22
     local bounds.xmin
23
                                                 +
24
     local bounds.xextent)
25
                 y =
     random.default rng.uniform(local bounds.ymin,
     local bounds.ymin
     local bounds.yextent)
                 self.move(h, x, y)
```

- 1 Get the rank that is executing this code, the current process rank
- 2 Get the number of process ranks over which the simulation is distributed
- 3 Get the total number of Humans to create from the input parameters dictionary
- 4 Compute the number of Human agents per processor

- Increment the number of agents to create on this rank, if this rank's id is less than the number of remaining agents to create. This will assign each rank, starting with 0, an additional agent in order to reach the total when the total number of agents cannot be evenly divided among all the process ranks.
- Get the local bounds of the continuous space. Each rank is responsible for some part of the total area defined by the space's bounding box. For example, assuming 4 process ranks, each rank would be responsible for some quadrant of the space. get\_local\_bounds returns the area that the calling rank is responsible for as a BoundingBox.
- 7 Iterate through the number of humans to be assigned to each rank
- 8 Create a human agent
- 9 Add the new human agent to the context
- 10 Choose a random x and y location within the current local bounds using repast4py's default random number generator. See the API documentation for more details.
- Move the new human agent to that location, using Model.move.

The code for creating the zombie agents is nearly identical, except that the the zombie.count input parameter is used as the total number of agents to create, and a zombie agent is created rather than a human.

```
1
     class Model:
2
         def init (self, comm, params):
4
5
             . . .
 6
             total zombie count = params['zombie.count']
8
             pp zombie count = int(total zombie count /
9
     world size)
             if self.rank < total zombie count % world size:</pre>
11
                 pp zombie count += 1
12
13
             for i in range (pp zombie count):
14
                 zo = Zombie(i, self.rank)
15
                 self.context.add(zo)
16
17
     random.default rng.uniform(local bounds.xmin,
18
     local bounds.xmin + local bounds.xextent)
19
     random.default rng.uniform(local bounds.ymin,
```

1 Set the next integer id for newly created zombies to the number of zombies created on this rank. When a human becomes a zombie, this zombie\_id is used as the id of that new zombie, and then incremented for the next time a human becomes a zombie.

### 7.2.4. Logging

As we saw in <u>Tutorial 1</u>, there are two types of logging supported by Repast4Py, tabular and reduce-type logging (see the repast4py.logging module <u>API documentation</u> for more information).

The Zombies model uses the second of these log types. The dataclass that we log records the total number of humans and zombies each tick.

### **Initializing Logging**

```
1
    @dataclass
    class Counts:
       humans: int = 0
4
        zombies: int = 0
5
7
    class Model:
8
9
        def init (self, comm, params):
11
             self.counts = Counts()
12
            loggers = logging.create loggers(self.counts,
13
     op=MPI.SUM, rank=self.rank)
                                    2
            self.data set = logging.ReducingDataSet(loggers,
    self.comm, params['counts file'])
```

- 1 Create the Counts instance that we use to record the number of humans and zombies on each rank
- 2 Create a list of loggers that use self.counts as the source of the data to log, and that perform a cross process rank summation of that data. The names argument is not specified, so the Counts field names will be

used as column headers.

3 Create a logging.ReducingDataSet from the list of loggers.
params['counts\_file'] is the name of the file to log to.

### The log counts Method

At each tick the log\_counts method is called by Model.step() to record the number of humans and zombies at that tick.

```
1
    class Model:
2
3
        def log counts(self, tick):
4
            # Get the current number of zombies and humans and
5
   log
6
            num agents = self.context.size([Human.TYPE,
7
    Zombie.TYPE])
8
            self.counts.humans = num agents[Human.TYPE]
                                                            2
            self.counts.zombies = num agents[Zombie.TYPE]
    3
                                       4
            self.data set.log(tick)
```

- 1 Get the number of agents of the specified types currently in the context.

  context.size takes a list of agent type ids and returns a dictionary where the type ids are the keys and the values are the number of agents of that type.
- 2 Set the self.counts.humans to the number of humans
- 3 Set the self.counts.zombies to the number of zombies
- 4 Log the values for the specified tick. This will sum the values in self.counts across all the ranks and log the results.

### 7.2.5. Scheduled Methods

The events for this model are methods defined within the Model class.

### Step

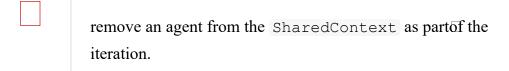
The first of our scheduled events is the step method, which is scheduled to execute starting at tick 1 and for every tick thereafter:

```
1 class Model:
2
3 ...
```

```
5
         def step(self):
                                                   0
 6
             tick = self.runner.schedule.tick
 7
             self.log counts(tick)
             self.context.synchronize(restore agent)
8
9
                                                             4
             for z in self.context.agents(Zombie.TYPE):
                 z.step()
             dead humans = []
14
             for h in self.context.agents(Human.TYPE):
15
                 dead, pt = h.step()
16
                 if dead:
17
                     dead humans.append((h, pt))
18
19
             for h, pt in dead humans: 8
                 model.remove agent(h)
                 model.add zombie(pt)
```

- 1 Get the current tick value from the schedule runner
- 2 Log the current number of humans and zombies by calling the log counts method.
- 3 Synchronize the state of the simulation across processes using the restore\_agent function to restore any agents (Zombies and Humans) that have moved processes. See Section 4.2, "Saving and Restoring Agents" for more details.
- 4 Iterate over all the Zombie agents in the model, calling step on each one.
- 5 Create an empty list for collecting the dead humans and their current location. This is used later in step to replace the humans with zombies.
- one. Human step returns a boolean that indicates whether or not the Human has died (and thus should become a Zombie), and the current location of that human.
- 7 If the human has died, then append it and its current location to the dead humans list.
- 8 Iterate over the dead human data, removing the human from the model, and replacing it with a zombie at its former location.

The iterator returned from SharedContext.agents is not modifiable duringiferation, that is, it is not possible to



Given that it is not possible to remove an agent as part of iteration, we need to collect the humans to remove in a list. After the iteration has completed, we can iterate over that list, and remove the agents using

Model.remove agent.

```
class Model:

def remove_agent(self, agent):
    self.context.remove(agent)
```

1 Remove the agent from the context.

Humans are converted into zombies in the add\_zombie() method, which adds a new zombie agent at the final location of the newly removed human.

```
class Model:

def add_zombie(self, pt):
    z = Zombie(self.zombie_id, self.rank)

self.zombie_id += 1
self.context.add(z)
self.move(z, pt.x, pt.y)
```

- 1 The final location of the human agent that just died is passed into the add zombie method
- 2 Create a new zombie agent, using the zombie\_id field instantiated in the constructor
- 3 Increment the zombie id to create the id for the next created zombie
- 4 Add the newly created zombie to the Model's context
- 5 Move the zombie to the location of the dead human the zombie is replacing

#### At End

Model.at end runs when the simulation reaches its final tick and ends.

This method closes the data\_set log, ensuring that any remaining unwritten data is written to the output file.

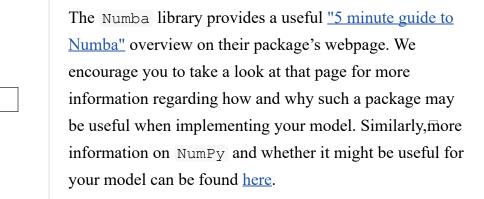
```
class Model:

def at_end(self):
    self.data_set.close()
```

# 7.3. The Grid Neighborhood Finder

Every agent at every tick must search their neighborhood of grid locations to determine which grid location has the most humans or the fewest zombies. Because this neighborhood of grid locations is dependent on each agent's current location, the neighborhood must be computed *every* tick for *every* agent. If, for example, the simulation is run for 50 ticks and 8400 agents, the neighborhood finding code is run over 400,000 times. Consequently, neighborhood finding is a good candidate for optimization, and a good exampleof how such an optimization can be implemented using 3rd party Python libraries.

The GridNghFinder is a class that can quickly compute these neighboring grid locationsusing the NumPy and Numba Python packages. NumPy is a fundamental Python package forscientific computing, providing support for multi-dimensional arrays and matrices, along withfast, optimized mathematical functions that operate on those arrays. Numba is a *just-in-time* compiler for Python. It can compile certain kinds of Python functions and classes into optimizednative machine code that bypasses the slower Python interpreter. It is particularly useful for code that is numerically oriented and uses NumPy arrays.



We implement our GridNghFinder as a class. Neighborhood finding in the GridNghFinder works by taking a location and adding an array of offsets to that location to create a new array consisting of the neighboring coordinates. For example, if we want to get the left and right coordinate values along the x-axisfor an x coordinate of 4, we can add the array [-1, 1] to 4 resulting in the array [3, 5]. The GridNghFinder performs this operation using 9 element offset arrays in both the x and ydimensions. 9 elements yields the Moore neighborhood coordinates as well as the original center location. The GridNghFinder also performs some additional checksto make sure that the coordinates are not outside of the bounds of the grid. The arrays in this case are NumPy arrays, and given the numericnature of the operation, Numba can compile it into native code.

In order to utilize Numba for our GridNghFinder class, we must first declare the native data types of the fields used in our class.

```
from numba import int32

spec = [
    ('mo', int32[:]),
    ('no', int32[:]),
    ('xmin', int32),
    ('ymin', int32),
    ('ymax', int32),
    ('ymax', int32),
    ('xmax', int32)
]
```

- 1 Create a Numba class specification. The specification is a list of tuples, where each tuple consists of a field name, and the native type of that field. The names correspond to the field names in the class for which this is the specification.
- 2 Create a tuple for the mo field with a NumPy array of 32-bit integers as its type.
- 3 Create a tuple for the xmin field with a 32-bit integer type.

See the Numba <u>API documentation</u> for @jitclass for more details on compiling classes with Numba.

The GridNghFinder constructor initializes the offset arrays and global grid bounds.

```
from numba.experimental import jitclass
                                                1
2
     @jitclass(spec)
     class GridNghFinder:
4
5
        def init (self, xmin, ymin, xmax, ymax):
6
7
            self.mo = np.array([-1, 0, 1, -1, 0, 1, -1, 0,
8
    1], dtype=np.int32)
                            4
9
            self.no = np.array([1, 1, 1, 0, 0, 0, -1, -1,
     -1], dtype=np.int32)
                                 5
            self.xmin = xmin
12
            self.ymin = ymin
            self.xmax = xmax
            self.ymax = ymax
```

- 1 Import the numba.jitclass decorator
- 2 Decorate GridNghFinder with jitclass passing our spec that defines the field types
- 3 Pass the global grid bounds to the constructor as x and y maximum and minimum values
- 4 Create the mo and no offset arrays containing the specified 32-bit integers
- 5 Set the minimum and maximum possible x and y values from the passed in global grid bounds

The neighborhood coordinate computation is performed in the find method.

```
1
         def find(self, x, y):
2
             xs = self.mo + x
             ys = self.no + y
4
             xd = (xs \ge self.xmin) & (xs \le self.xmax)
6
             xs = xs[xd]
             ys = ys[xd]
8
9
                                                               7
             yd = (ys >= self.ymin) & (ys <= self.ymax)</pre>
10
             xs = xs[yd]
11
             ys = ys[yd]
12
             return np.stack((xs, ys, np.zeros(len(ys),
```

```
dtype=np.int32)), axis=-1) 8
```

- 1 The find method takes a 2D location specified as x and y coordinates. This location is the location we want the neighboring coordinates of.
- 2 Add the x offset array to the x coordinate, resulting in a new array xs that contains the neighboring x-axis coordinates.
- 3 Add the y offset array to the y coordinate, resulting in a new array ys that contains the neighboring y-axis coordinates.
- 4 Compute the array indices in the xs array whose values are within the global x-axis bounds.
- 5 Keep only those values from xs, assigning that array to xs
- 6 Do the same for the ys array. If an x value is out of bounds, we discard its corresponding y value.
- 7 Compute the array indices in the ys array whose values are within the global y-axis bounds. Then reset xs and ys to contain only the values at those indices.
- 8 Combine the xs and ys indices with each other and a z-axis coordinate array of all zeros to create an array of arrays where the inner arrays are 3D points consisting of x, y, and z coordinates. This 3 element array format is necessary to reset the repast4py.space.DiscretePoint at variable that is used in both the Zombie step, method and the Human step method.

# 7.4. Running the Simulation

The simulation is run from the command line. For example, from within the examples/zombies directory:

```
mpirun -n 4 python zombies.py zombie model.yaml
```

Here we are running the simulation with 4 process ranks and the model input parameters are in the zombie model.yaml file.

```
random.seed: 42
stop.at: 50.0
human.count: 8000
zombie.count: 400
```

```
world.width: 200
world.height: 200
run.number: 1
counts_file: './output/agent_counts.csv'
```

The Zombie Model uses the standard if name == 'main' code block to parse the input parameters and run the simulation.

```
if __name__ == "__main__":
    parser = parameters.create_args_parser()
args = parser.parse_args()
params = parameters.init_params(args.parameters_file,
args.parameters)
run(params)
```

- 1 Create the default command line argument parser
- 2 Parse the command line into its arguments using that default parser
- 3 Create the model input parameters dictionary from those arguments using parameters.init params
- 4 Call the run function to run the simulation.

See <u>Parsing Input Parameters</u> in Tutorial 1 for more details.

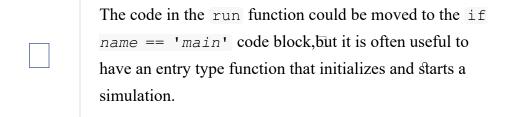
The run function creates the Model class and calls its run method, which then begins the simulation by initiating schedule execution. This run function is called in the if name == 'main' code block.

```
1
    from mpi4py import MPI
2
    def run (params: Dict):
4
        global model
        model = Model(MPI.COMM WORLD, params)
6
        model.run()
8
    class Model:
9
        def run(self):
                                      3
11
            self.runner.execute()
```

- 1 Use the global keyword to indicate that model refers to the module level model variable and not a local variable
- 2 Create the model instance, passing the Model constructor the MPI world

communicator and the input parameters dictionary

3 Start the simulation by executing the schedule which calls the scheduled methods at the appropriate times and frequency



- 1. Ozik, J., Wozniak, J. M., Collier, N., Macal, C. M., & Binois, M. (2021). A population data-driven workflow for COVID-19 modeling and learning. The International Journal of High Performance Computing Applications, 35(5), 483–499. https://doi.org/10.1177/10943420211035164
- Ozik, J., Collier, N. T., Wozniak, J. M., Macal, C. M., & An, G. (2018). Extreme-Scale Dynamic Exploration of a Distributed Agent-Based Model With the EMEWS Framework. IEEE Transactions on Computational Social Systems, 5(3), 884–895. <a href="https://doi.org/10.1109/TCSS.2018.2859189">https://doi.org/10.1109/TCSS.2018.2859189</a>
- 3. Collier, N. T., Ozik, J., & Tatara, E. R. (2020). Experiences in Developing a Distributed Agent-based Modeling Toolkit with Python. 2020 IEEE/ACM 9th Workshop on Python for High-Performance and Scientific Computing (PyHPC), 1–12. https://doi.org/10.1109/PyHPC51966.2020.00006

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