nufeb$_{t}ools Documentation$

Release unknown

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NOTES

CHAPTER

ONE

NUFEB_TOOLS

1.1 Description

Python-based tools and utilities for NUFEB simulations

1.2 Getting Started

Install via pip:

```
pip install nufeb-tools
```

Generate NUFEB simulations from the CLI:

```
nufeb-seed
```

Remove old runs:

```
nufeb-clean
```

Get data from a simulation for analysis

```
from nufeb_tools import utils
x = utils.get_data(test=True)
```

Plot the overall growth

```
from nufeb_tools import plot
import matplotlib.pyplot as plt
f, ax = plt.subplots()
plot.overall_growth(x.biomass,ax=ax)
```

Plot colonies based on initial seed cells

```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
x = utils.get_data(directory=r'E:\sucrose\runs\Run_50_50_1.00e+00_1_2022-01-11_48525')
f,ax = plt.subplots()
plot.colony(x,25900,colors,ax=ax)
plt.show()
```

CHAPTER

TWO

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CHAPTER

THREE

ATOM GENERATION

3.1 Generate Atoms

nufeb_tools.generate_atom.**clean**()
Remove old NUFEB runs

nufeb_tools.generate_atom.**main**(*args*)
Wrapper function to generate new NUFEB simulation conditions

Parameters **args** (*List[str]*) – command line parameters as list of strings

nufeb_tools.generate_atom.**parse_args**(*args*)
Parse command line parameters

Parameters **args** (*List[str]*) – command line parameters as list of strings (for example ["--help"]).

Returns command line parameters namespace

Return type argparse.Namespace

nufeb_tools.generate_atom.**run**()
Calls main() passing the CLI arguments extracted from sys.argv

This function can be used as entry point to create console scripts with setuptools.

nufeb_tools.generate_atom.**setup_logging**(*loglevel*)
Setup basic logging

Parameters **loglevel** (*int*) – minimum loglevel for emitting messages

3.2 Generate Atoms (development version)

This is a script to seed NUFEB simulations

class nufeb_tools.generate_atom_dev.**Cell**(*Species*, *Group*, *idx*, *args*, *Info={'cyano': {'Decay': 0, 'Density': 370, 'Diameter': 1e-06, 'GrowthRate': 1.67e-05, 'Inertia': {'ixx': 0, 'ixy': 0, 'ixz': 0, 'iyy': 0, 'iyz': 0, 'izz': 9.2e-23}, 'K_s': {'co2': 0.000138, 'light': 0.00035, 'o2': 0.0002, 'suc': 0.01}, 'Maintenance': 0, 'Yield': 0.55, 'max_length': 5e-06, 'min_length': 1e-06}, 'ecw': {'Decay': 2e-05, 'Density': 236, 'Diameter': 7.3e-07, 'GrowthRate': 0.00027, 'Inertia': {'ixx': 0, 'ixy': 0, 'ixz': 0, 'iyy': 0, 'iyz': 0, 'izz': 9.2e-23}, 'K_s': {'co2': 0.05, 'light': 0, 'o2': 0.001, 'suc': 3.6}, 'Maintenance': 9.5e-07, 'Yield': 0.43, 'max_length': 2.72e-06, 'min_length': 1.94e-06}}*)

Bacteria object class

Atom()
Function to return atom (cell) positions to render atom.in file

Bacillus()
Function to return rod shape (bacillus) parameters to render atom.in file

Check()
Return cell position, orientation, and size

Report()
Return cell position, orientation, and size

rotate(*z_dim=False*)
Randomly generate cell orientation displacements based on input angle

class nufeb_tools.generate_atom_dev.**Culture**(*args*)
Create a collection of cells with defined positions, lengths, and orientations

Check()
Check initial positions of each cell and move one of them if there is a collision

class nufeb_tools.generate_atom_dev.**Nutrient**(*c*, *d*, *mw*, *state*, *bc*)
Nutrient class to define the chemicals present in the simulation volume, their concentrations, and their properties

nufeb_tools.generate_atom_dev.**main**(*args*)
Wrapper function to generate new NUFEB simulation conditions

Parameters **args** (*List[str]*) – command line parameters as list of strings

nufeb_tools.generate_atom_dev.**parse_args**(*args*)
Parse command line parameters

Parameters **args** (*List[str]*) – command line parameters as list of strings (for example `["--help"]`).

Returns command line parameters namespace

Return type argparse.Namespace

nufeb_tools.generate_atom_dev.**run**()
Calls `main()` passing the CLI arguments extracted from `sys.argv`

This function can be used as entry point to create console scripts with setuptools.

nufeb_tools.generate_atom_dev.**setup_logging**(*loglevel*)
Setup basic logging

Parameters **loglevel** (*int*) – minimum loglevel for emitting messages

CHAPTER

FOUR

NUFEB SIMULATION ANALYSIS

4.1 Get Simulation Data

class nufeb_tools.utils.**get_data**(*directory=None*, *id=None*, *test=None*, *timestep=10*)

Bases: object

Collect results for analysis.

NUFEB simulation data class to collect results for analysis

test
Set *test* = *True* to get example data from the Github repository

Type bool

directory
Path to the directory containing NUFEB simulation data.

Type str

timestep
Length of simulation timestep in seconds

Type int

SucRatio
Relative cyanobacterial sucrose secretion level, 0-100

Type int

timepoints
List of timepoints in the simulation

Type List(str)

dims
Size of the simulation boundaries in micrometers

Type List(str)

numsteps
Number of timepoints

Type int

biomass
Pandas Dataframe containing the biomass vs time data from biomass.csv

Type pandas.DataFrame

ntypes
Pandas Dataframe containing the cell number vs time data from ntypes.csv

Type pandas.DataFrame

avg_con
Pandas Dataframe containing the average nutrient concentrations vs time data from avg_concentration.csv

Type pandas.DataFrame

positions
Pandas Dataframe containing the single cell biomass over time of all cell ids present at the timepoint

Type pandas.DataFrame

get_local_data()
Collect NUFEB simulation data from a local directory.

convert_units_avg_con()
Convert the object attribute avg_con, which contains the average nutrient concentration, units to hours and mM.

convert_units_biomass()
Convert the object attribute biomass units to hours and femtograms.

calc_biomass()

collect_positions(*h5*)
Extract the x, y, z position of each cell during the simulation.

Parameters **timepoint** (*int*) – The simulation timestep to get the position data from.

Returns Dataframe containing Timestep, ID, type, radius, x, y, z columns

Return type pandas.DataFrame

get_neighbor_distance(*id*, *timepoint*)
Get the nearest neighbor cell distances

Parameters

- **id** (*int*) – The ID of the reference cell
- **timepoint** (*int*) – The timepoint to check the neighbor distances from

Returns Dataframe containing ID, type, Distance

Return type pandas.DataFrame

get_neighbors(*timestep*)
Get the nearest neighbor cell distances

Parameters **timestep** (*int*) – The timepoint to check the neighbor distances from

Returns Pandas dataframe containing pairwise neighbor distances

Return type pd.DataFrame

get_mothers__old()
Assign mother cells based on initial cells in the simulation.

Returns Dataframe containing ID, type, position, radius, and mother_cell

Return type pandas.DataFrame

get_mothers()
Assign mother cells based on initial cells in the simulation.

Returns Dataframe containing Timestep, ID, type, position, radius, biomass, total biomass, and mother_cell

Return type pandas.DataFrame

count_colony_area(*timestep*)
Count the 2d area in pixel dimensions of each colony at a given timestep.

Parameters **timestep** (*int*) – Timestep to count

get_colony_areas()
Count colony areas for all timesteps

get_nutrient_grid(*h5*)

get_local_con(*timestep*, *cellID*)
Get the local nutrient concentration of a cell

Parameters

- **timestep** (*int*) – The timestep at which to check the concentration
- **cellID** (*int*) – The cell identification number

Returns The concentration of the specified nutrient within the cell's grid

Return type Nutrient Concentration (float)

get_fitness(*timestep*, *cellID*)
Get the fitness of an individual cell based on the relative Monod growth rate at a given timestep

Parameters

- **timestep** (*int*) – The timestep at which to check the concentration
- **cellID** (*int*) – The cell identification number

Returns The Monod growth rate (1/s)

Return type float

collect_fitness()

4.2 Spatial Analysis

nufeb_tools.spatial.**fitness_metrics**(*obj*)
Function to calculate colony-level fitness metrics.

Mother cell: Cell ID which seeded the colony

Type: Cell type - cyanobacteria are type 1 and E. coli are type 2

Voronoi area: Area of species-specific Voronoi Tesselation at the beginning of the simulation

IPTG: Sucrose induction level

total biomass: Biomass of each colony at the end of the simulation (fg)

Nearest 1: Distance to nearest cyanobacteria colony

Nearest 2: Distance to nearest E. coli colony

Nearest Neighbor: Distance to nearest colony

IC1: Average distance to nearest cyanobacteria colony

IC2: Average distance to nearest E. coli colony

IC: Average distance to nearest colony

Relative Neighbor Dist 1: Distance to nearest cyanobacteria colony divided by IC1

Relative Neighbor Dist 2: Distance to nearest E. coli colony divided by IC2

Relative Neighbor Dist: Distance to nearest colony divided by IC

Z1: Relative neighbor distance 1 divided by sqrt(D_sucrose/mu_cyano)

Z2: Relative neighbor distance 2 divided by sqrt(D_sucrose/mu_ecw)

Z1_2: Relative neighbor distance 1 divided by sqrt(D_sucrose/mu_ecw)

Z2_1: Relative neighbor distance 2 divided by sqrt(D_sucrose/mu_cyano)

LogNearest 1: log(Nearest 1)

LogNearest 2: log(Nearest 2)

LogNearest: log(Nearest Neighbor)

Inv1: Inverse sum of neighbor distance 1

Inv2: Inverse sum of neighbor distance 2

Log Inv1: Log squared inverse sum of neighbor distance 1

Log Inv2: Log squared inverse sum of neighbor distance 2

Colony Area: 2D area of colony at the end of the simulation

Parameters **obj** (*nufeb_tools.utils.get_data*) – Data object collected with nufeb_tools.utils.get_data

Returns Dataframe containing colony number (mother cell ID), cell type, total biomass, colony area, Voronoi area, nearest neighbor, mean neighbor distance, etc.

Return type pandas.DataFrame

```
from nufeb_tools import utils, spatial
x = utils.get_data(directory = None,test=True)
metrics = spatial(x)
metrics.head()
```

Table 1: Metrics

	mother	type	Area	Ratio	total biomass	Nearest 1	Nearest 2	Nearest Neighbor	IC1	IC2	IC	Relative Neighbor Dist 1	Relative Neighbor Dist 2	Relative Neighbor Dist	Z1	Z2	Z1_l	Z2_l	Log Nearest 1	Log Nearest 2	Log Nearest	Inv1	Inv2	Log Inv1	Log Inv2	Colony Area
0	17	1	1.37[illegible] 10	[illegible]	[illegible]	[illegible] 05	[illegible] 05	[illegible] 05	[illegible] 06	[illegible] 06	[illegible] 06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible] 11.3[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
1	9	1	3.19[illegible] 09	[illegible]	[illegible]	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible] 11.6[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	18	1	0.0	56	4237[illegible]	[illegible] 05	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible] 10.9[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
3	11	1	9.40[illegible] 09	[illegible]	[illegible]	[illegible] 05	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible] 10.6[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
4	8	1	1.08[illegible] 09	[illegible]	[illegible]	[illegible] 05	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible] 06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible] 11.0[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

4.3 Plotting

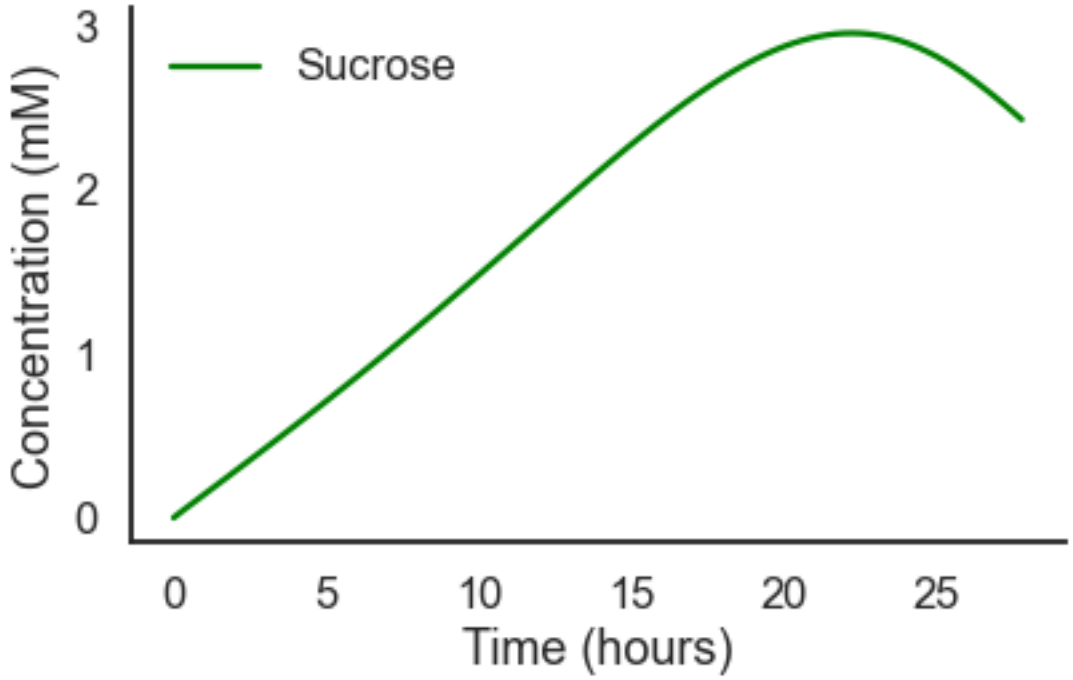
4.3.1 Average Nutrient Concentration

`nufeb_tools.plot.average_nutrients` (*df*, *nutrient*, *ax=None*, *legend=None*, ***kwargs*)

This is a function to plot the nutrient concentration over time

Parameters

- **df** (*pandas.DataFrame*) – Pandas Dataframe containing nutrient data
- **nutrient** (*str*) – Name of the nutrient to plot, e.g., `'Sucrose'`
- **ax** – Axis on which to make the plot
- **legend** (*bool*) – Include legend in the plot
- ****kwargs** – Additional arguments to pass to plt.plot




```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
import seaborn as sns
x = utils.get_data(directory = None,test=True)
f, ax = plt.subplots()
sns.set_context('talk')
sns.set_style('white')
plot.average_nutrients(x.avg_con,'Sucrose',color='Green',legend=True)
```

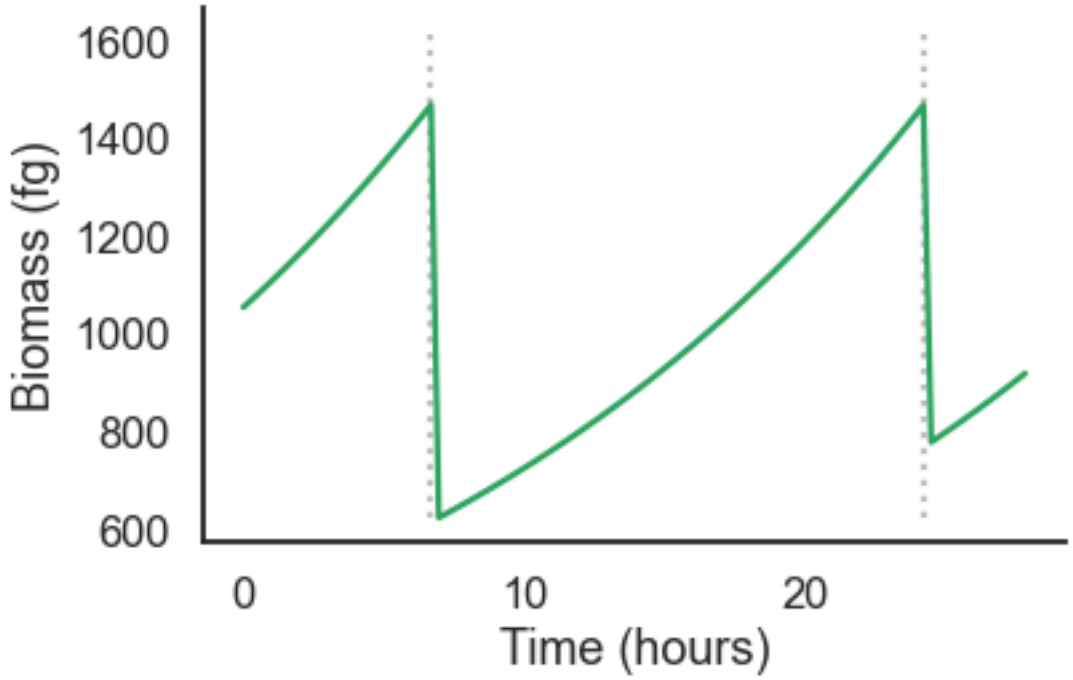
4.3.2 Single Cell Growth

nufeb_tools.plot.**biomass_time**(*df*, *id=None*, *ax=None*, *legend=None*, ***kwargs*)

This is a function to plot the cell biomass over time

Parameters

- **df** (*pandas.DataFrame*) – Pandas Dataframe containing biomass data
- **ax** – Axis on which to make the plot
- **legend** (*bool*) – Include legend in the plot
- ****kwargs** – Additional arguments to pass to plt.plot




```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
import seaborn as sns
f, ax = plt.subplots()
sns.set_context('talk')
sns.set_style('white')
x = utils.get_data(directory = None,test=True)
plot.biomass_time(x.positions)
f.tight_layout()
```

4.3.3 Single Cell Growth Rate

nufeb_tools.plot.**growth_rate_div**(*df*, ***kwargs*)

Plot a heatmap of the single cell growth rates relative to each division

Parameters

- **df** (*pandas.DataFrame*) – Pandas Dataframe containing biomass data
- ****kwargs** – Additional arguments to pass to plt.plot

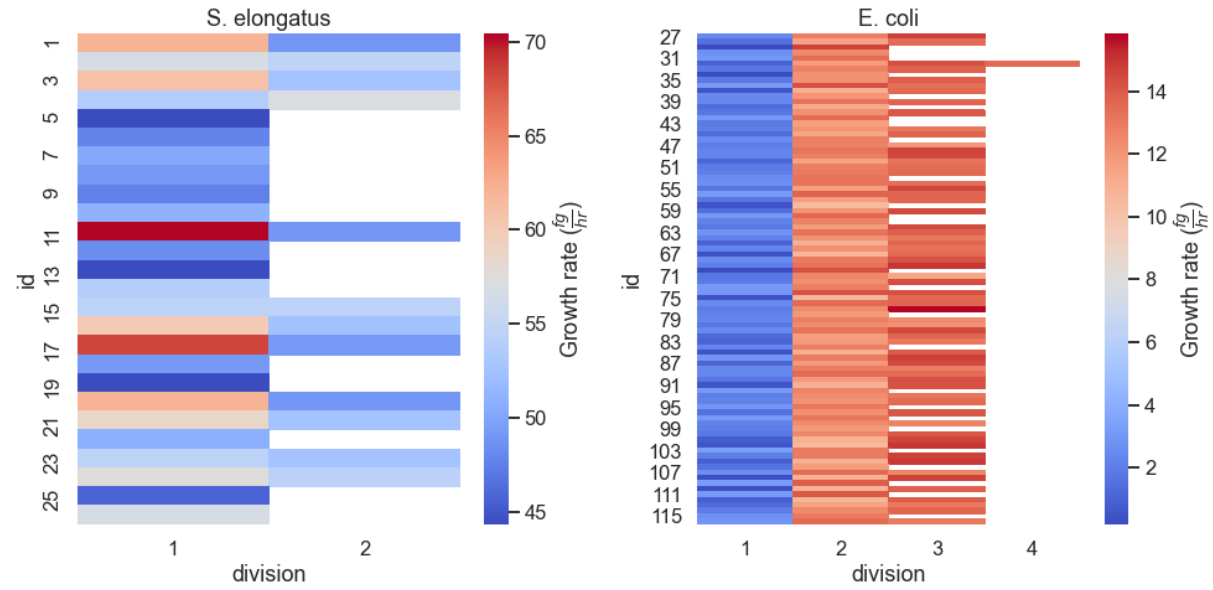
nufeb_tools.plot.**growth_rate_time**(*df*, *period=3*)

Plot a heatmap of the single cell growth rates over time

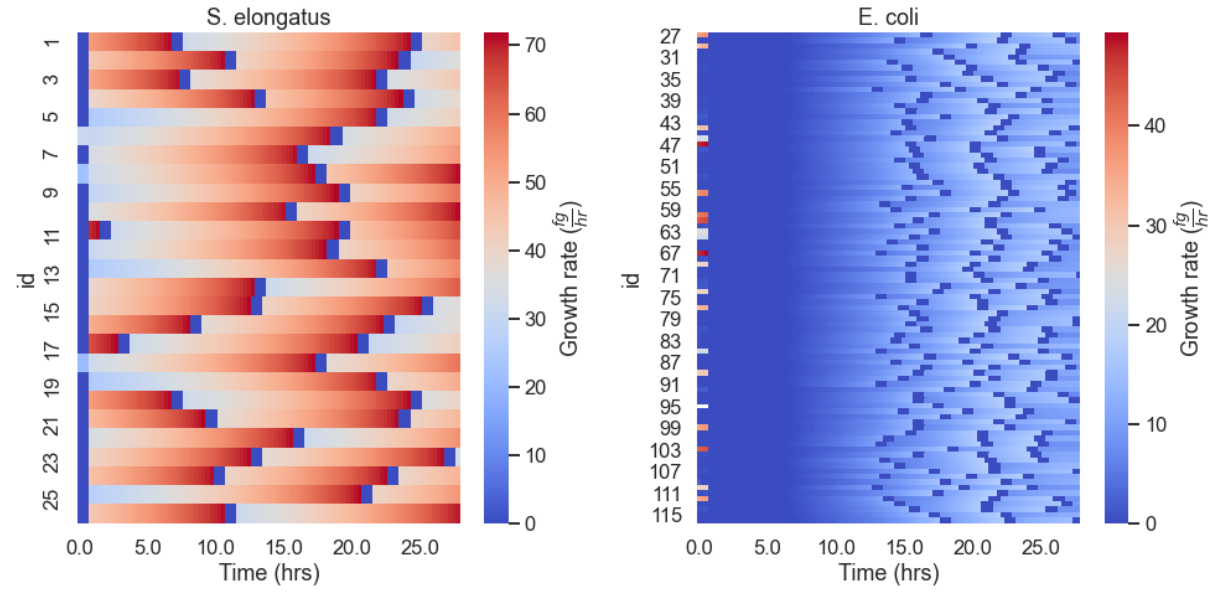
Parameters

- **df** (*pandas.DataFrame*) – Pandas Dataframe containing biomass data
- **period** (*int*) – Number of timesteps to average growth rate calculation over
- ****kwargs** – Additional arguments to pass to plt.plot

Returns matplotlib.figure.Figure




```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
x = utils.get_data(directory = None,test=True)
plot.growth_rate_div(x.positions)
```




```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
x = utils.get_data(directory = None,test=True)
plot.growth_rate_time(x.positions)
```

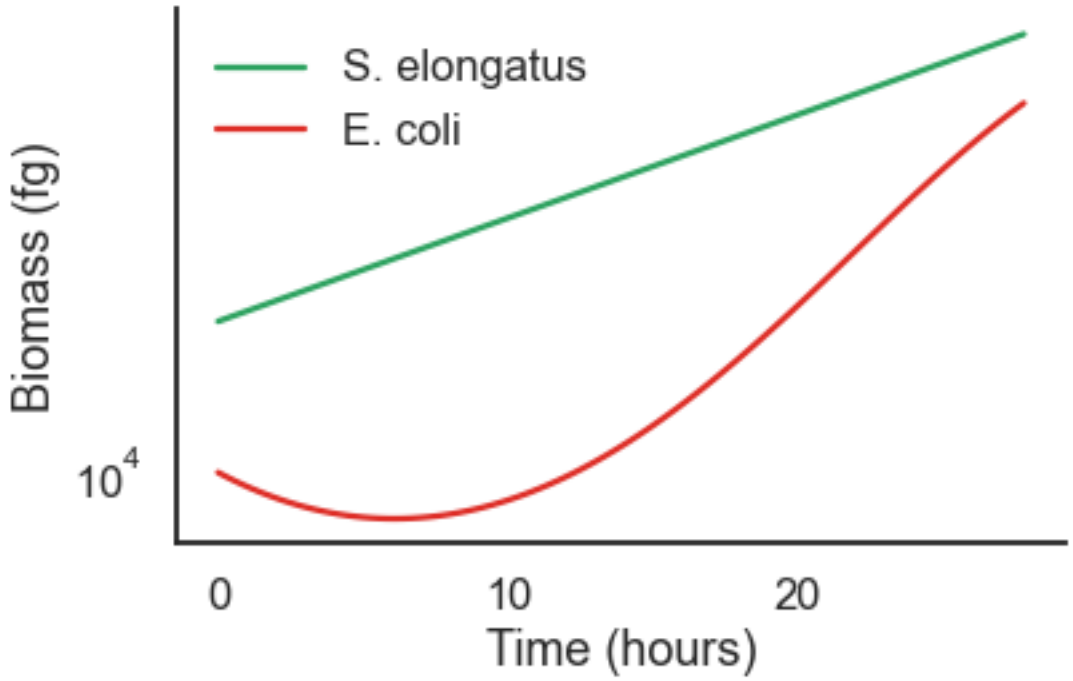
4.3.4 Overall Cell Growth

nufeb_tools.plot.**overall_growth**(*df*, *ax=None*, ***kwargs*)

This is a function to generate growth curve plots

Parameters

- **df** (*pandas.DataFrame*) – Pandas Dataframe containing biomass data over time
- **ax** (*plt.ax*) – Axis to plot data on
- ****kwargs** –




```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
import seaborn as sns
sns.set_style('white')
sns.set_context('talk')
f, ax = plt.subplots()
x = utils.get_data(directory = None,test=True)
plot.overall_growth(x.biomass,ax=ax)
f.tight_layout()
```

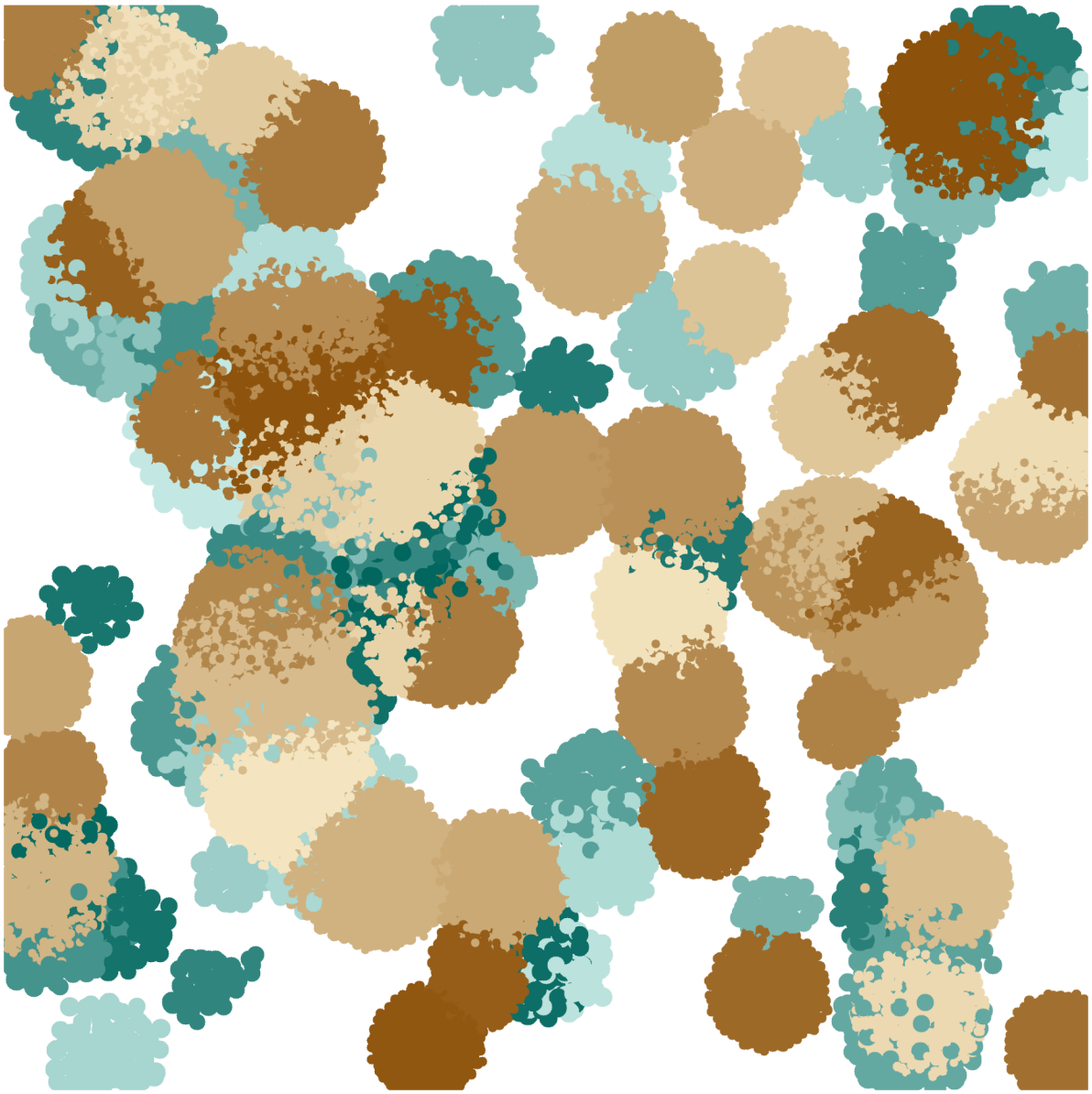
4.3.5 Whole Colony Plotting

nufeb_tools.plot.**colony**(*obj*, *time*, *colors=None*, *colony=None*, *ax=None*, *by=None*, *img=array([], dtype=float64)*, *fitness=None*, *overlay=None*, ***kwargs*)

Plot bacterial colonies at a specific timepoint

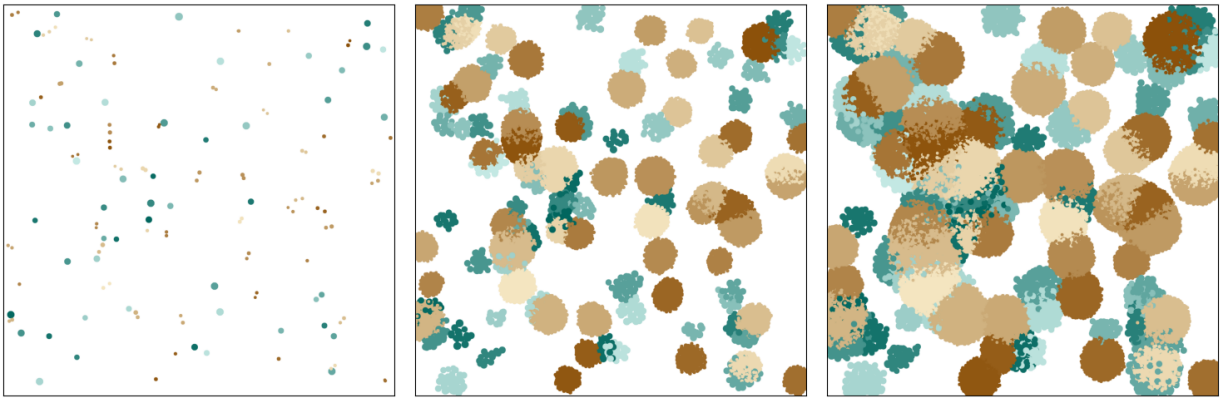
Parameters

- **obj** (*nufeb_tools.utils.get_data*) – Object containing cell locations
- **time** (*int*) – Simulation timestep to plot
- **colors** (*dict, optional*) – Dictionary of colors to plot each colony. Defaults to random.
- **colony** (*int, optional*) – Plot a specific colony. Defaults to None.
- **ax** (*matplotlib.pyplot.axes, optional*) – Axis to plot on. Defaults to None.
- **by** (*str, optional*) – Plot by species. Defaults to None.
- **img** (*np.array, optional*) – Image array to overlay colonies onto.
- **fitness** (*pandas.DataFrame,optional*) – Takes a dataframe containing spatial metrics data as an input or if bool, will calculate the metrics internally. Defaults to None.
- **overlay** (*bool, optional*) – If True, plot a specific colony on top of the others.



```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
x = utils.get_data(directory=r'E:\sucrose\runs\Run_50_50_1.00e+00_1_2022-01-11_48525')
f,ax = plt.subplots()
plot.colony(x,35000,colors,ax=ax)
plt.show()
```

Plot colonies over time by species:



```
from nufeb_tools import utils, plot
import matplotlib.pyplot as plt
x = utils.get_data(directory=r'E:\sucrose\runs\Run_50_50_1.00e+00_1_2022-01-11_48525')
f, axes = plt.subplots(ncols=3,figsize=(15,5))
for ax, time in zip(axes,[100,20000,25900]):
    plot.plot_colony(x,time,by='Species',ax=ax)
plt.show()
```

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FIVE

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Examples go here

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