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# **nufeb**<sub>*tools*</sub>*Documentation*

***Release unknown***

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## 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)
```



docs/\_static/images/total\_biomass\_vs\_time.png

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()
```



docs/\_static/images/colonies.png

**LICENSE**

The MIT License (MIT)

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## 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



## 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 Tessellation 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  $\sqrt{D_{\text{sucrose}}/\mu_{\text{cyano}}}$

Z2: Relative neighbor distance 2 divided by  $\sqrt{D_{\text{sucrose}}/\mu_{\text{ecw}}}$

Z1\_2: Relative neighbor distance 1 divided by  $\sqrt{D_{\text{sucrose}}/\mu_{\text{ecw}}}$

Z2\_1: Relative neighbor distance 2 divided by  $\sqrt{D_{\text{sucrose}}/\mu_{\text{cyano}}}$

LogNearest 1:  $\log(\text{Nearest 1})$

LogNearest 2:  $\log(\text{Nearest 2})$

LogNearest:  $\log(\text{Nearest Neighbor})$

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

			moth	hyp	prev	col	mo	ito	Nea	Nea	Nea	C	IC	IC	IC	Rel	Rel	Rel	Z1	Z2	Z1	Z2	Log	Neg	Neg	Nv	Inv	Log	Log	Colony
								Area	Rata	est	est	est	Neigh			a-	a-	a-					ear	Neg	Neg	Nv	Inv	Log	Log	Area
								tio	biom	2	2	bor				Neigh	Neigh	Neigh					1	2	1	2		Inv	Inv	2
0	17	1	1.37	266	607	1.05	0.05	0.05	0.05	0.06	0.06	0.06				1	2					11.31	11.31	11.31	11.31	11.31	11.31	11.31	11.31	11.31
1	9	1	3.19	969	286	0.06	0.06	0.06	0.06	0.06	0.06	0.06										11.60	11.60	11.60	11.60	11.60	11.60	11.60	11.60	11.60
2	18	1	0.0	56	423	0.05	0.06	0.06	0.06	0.06	0.06	0.06										10.97	10.97	10.97	10.97	10.97	10.97	10.97	10.97	10.97
3	11	1	9.40	505	255	0.05	0.06	0.06	0.06	0.06	0.06	0.06										10.63	10.63	10.63	10.63	10.63	10.63	10.63	10.63	10.63
4	8	1	1.08	44	445	0.05	0.06	0.06	0.06	0.06	0.06	0.06										11.01	11.01	11.01	11.01	11.01	11.01	11.01	11.01	11.01

## 4.3 Plotting

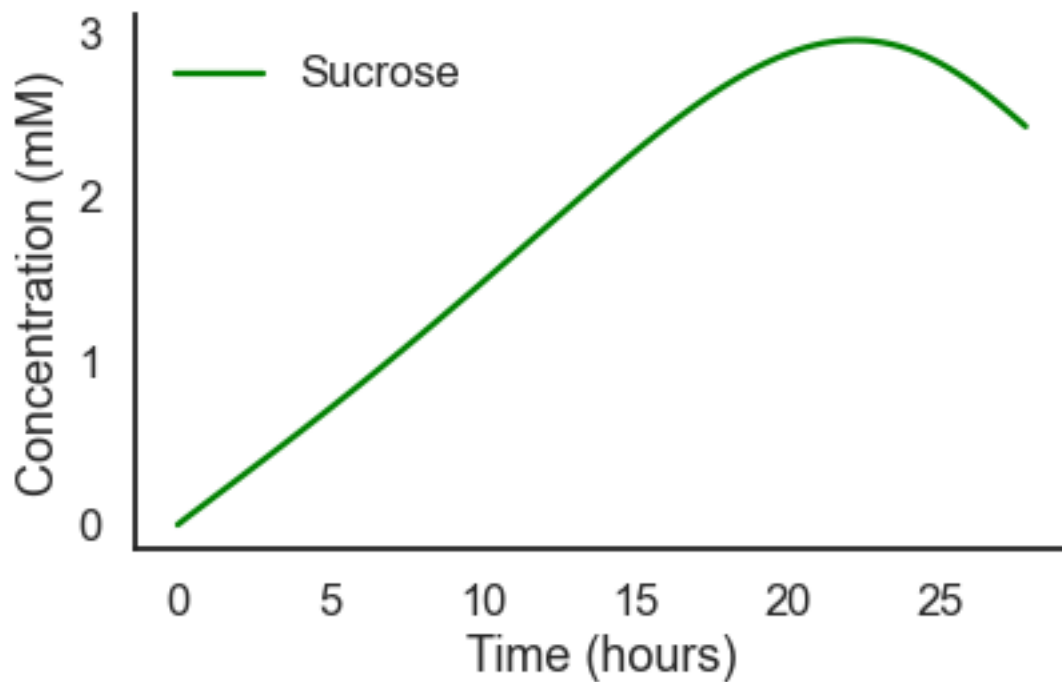
### 4.3.1 Average Nutrient Concentration

`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)
```

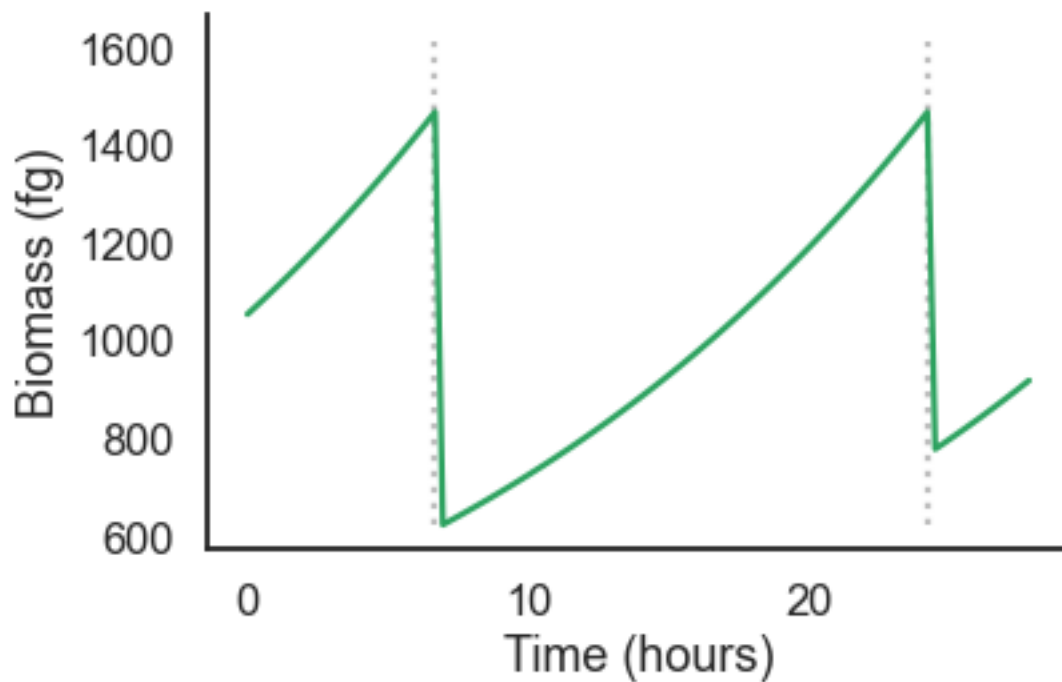
### 4.3.2 Single Cell Growth

`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`

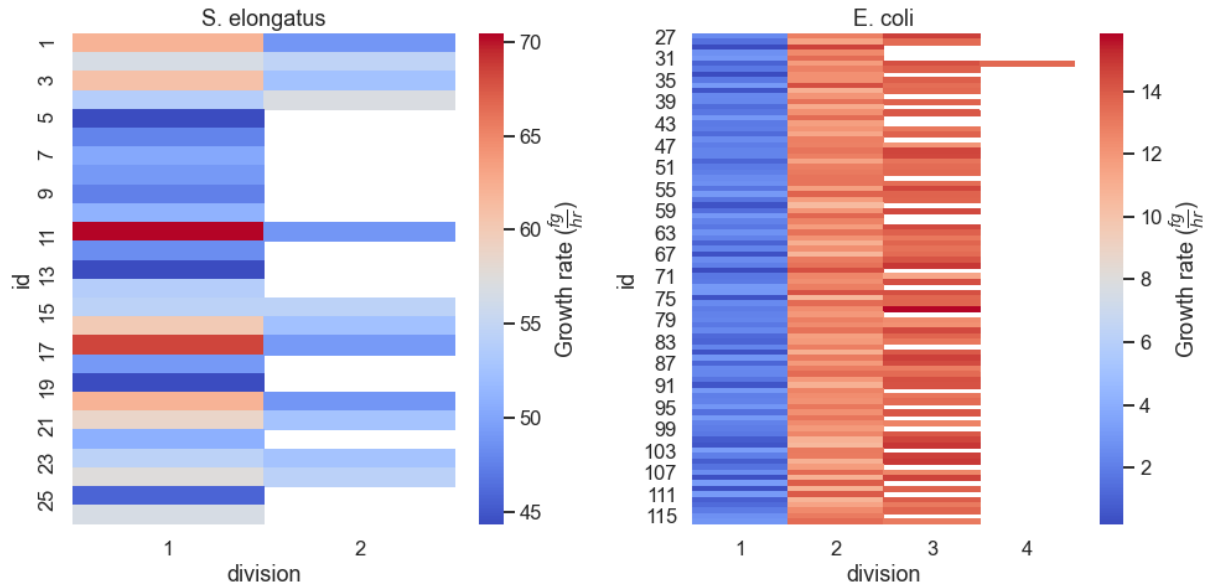
`nufeb_tools.plot.growth_rate_time(df, period=3)`

Plot a heatmap of the single cell growth rates over time

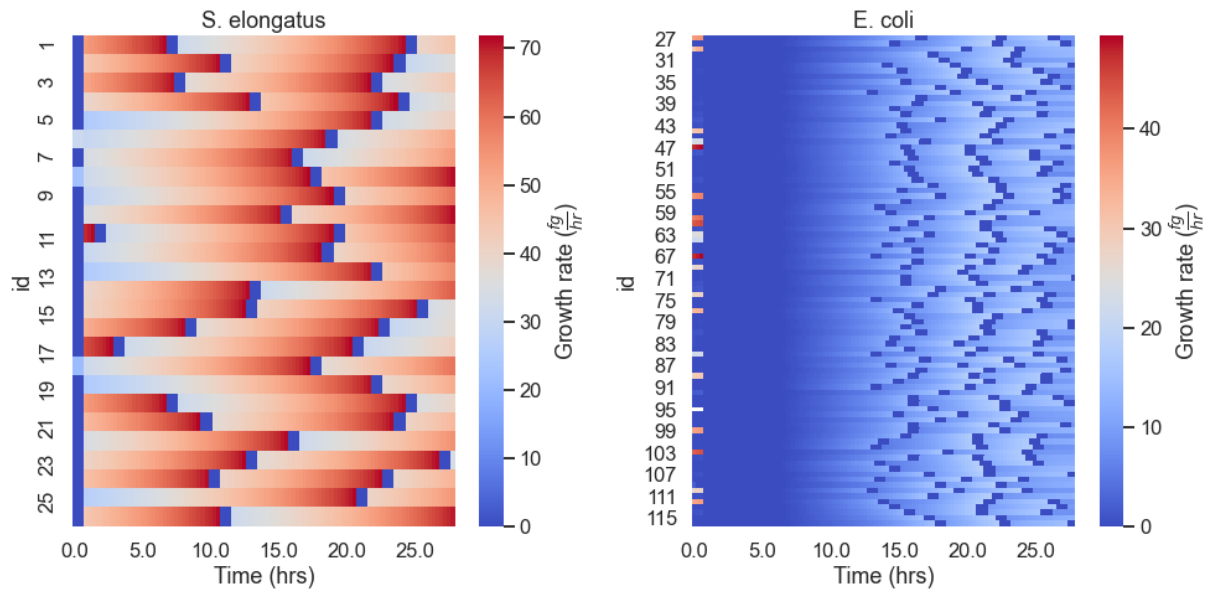
#### Parameters

- **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)
```

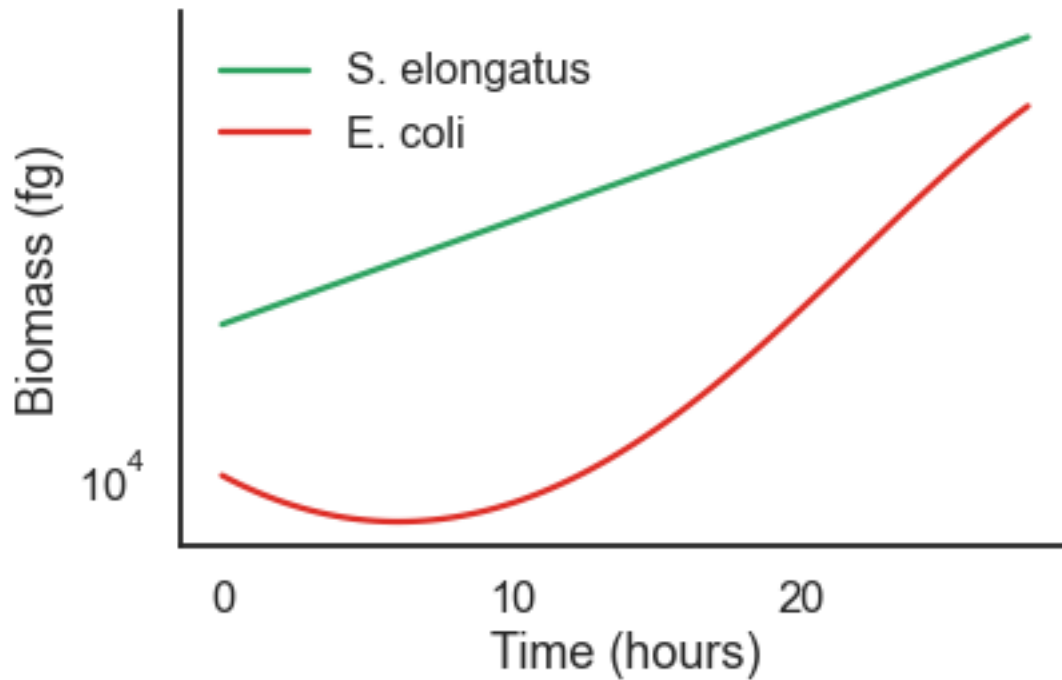
### 4.3.4 Overall Cell Growth

`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()
```

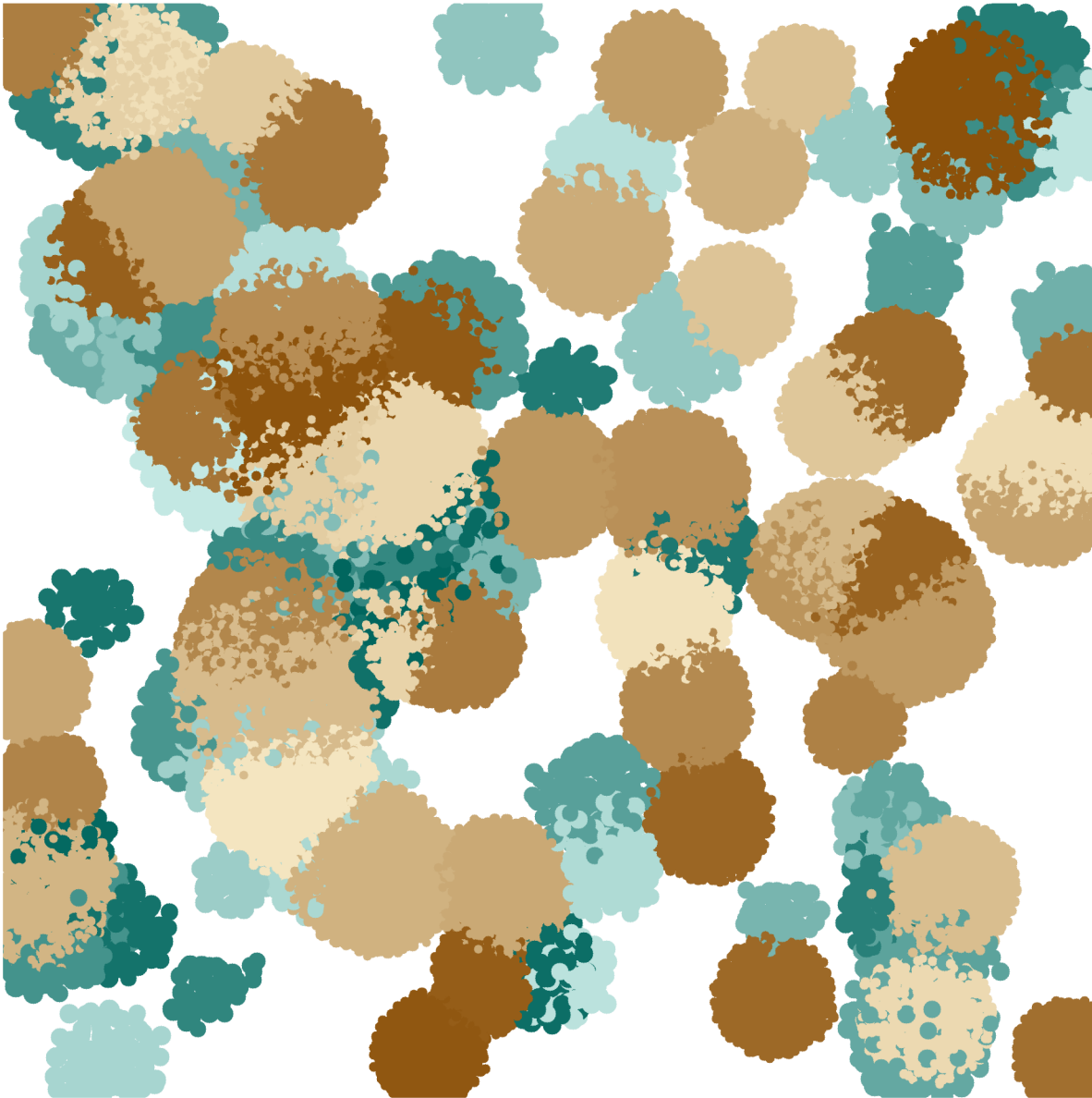
### 4.3.5 Whole Colony Plotting

```
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

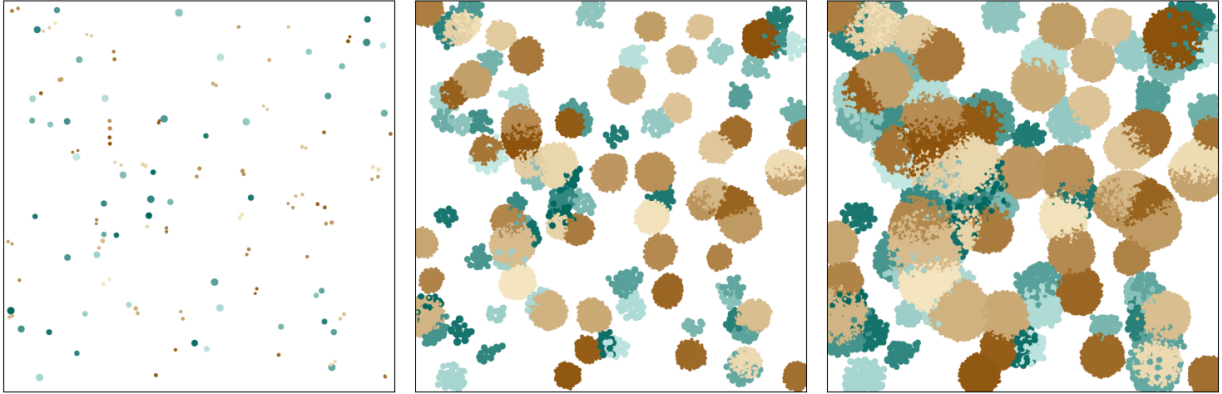
#### Parameters

- **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()
```



## NOTEBOOKS

Examples go here



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