cameo Documentation

Release 0.1.0

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Contents

Warning: These pages are under construction. Feel free to look around ...

Cameo is a high-level python library developed to aid the strain design process in metabolic engineering projects. The library provides a modular framework of simulation methods, strain design methods, access to models, that targets developers that want custom analysis workflows.

Computationally heavy methods have been parallelized and can be run on a clusters using the IPython parallelization framework (see example and documentation for more details). The default fallback is python's multiprocessing library.

Furthermore, it exposes a high-level API to users that just want to compute promising strain designs.

```
from cameo.api import design
design(product='L-Serine')
```

You got curious? Head over to try.cameo.bio and give it a try.

CHAPTER 1

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1.1 Installation

1.1.1 Setting up a virtual environment first

We highly recommended installing cameo inside a virtual environment (virtualenv). virtualenvwrapper tremendously simplifies using virtualenv and can easily be installed using virtualenv-burrito. Once you installed virtualenv and virtualenvwrapper, run

```
$ mkvirtualenv cameo  # or whatever you'd like to call your virtual environment
$ workon cameo
```

and then continue with the installation instructions described below.

1.1.2 Non-python dependencies

cameo relies on optlang to solve optimization problems. Currently, optlang supports either glpk (open source) or cplex (academic licenses available), which are not python tools. At least one of them has to be installed before one can proceed with the cameo installation.

GLPK

Using cameo with glpk also requires swig to be installed (in order to generate python bindings). On ubuntu (or other similar linux platforms) we recommend using `apt-get`:

```
$ sudo apt-get install libglpk-dev glpk-utils swig
```

On macs we recommend using homebrew.

```
$ brew install swig
$ brew install glpk
```

CPLEX

The cplex contains a python directory (similar to `IBM/ILOG/CPLEX_Studio1251/cplex/python/x86-64_osx`). Inside this directory run

```
$ python setup.py install
```

to install the python bindings.

1.1.3 Normal installation

Warning: cameo is still under heavy development. We recommend installing the development version (see below) if you would like to stay up-to-date with the latest changes.

cameo can be installed using *pip*.

```
$ pip install cameo
```

1.1.4 Development setup

pip can also be used to install cameo directly from the github repository.

```
$ pip install -e git+https://github.com/biosustain/cameo.git@devel#egg=cameo
```

Alternatively, you can clone the repository (or your fork) and then run

```
$ python setup.py install
```

From withing the cameo directory.

```
from pandas import options
options.display.max_rows = 8
```

1.2 Getting started with

computer **a**ided **m**etabolic **e**ngineering and **o**ptimization

cameo reuses and extends model data structures defined by cobrapy (**CO**nstraints-**B**ased **R**econstruction and **A**nalysis tool for **Py**thon). So, in addition to following this quick start guide and other **cameo** tutorials, we encourage you to explore cobrapy's documentation as well.

1.2.1 Step 1: Load a model

Loading a model is easy. Just import the `load_model` function.

```
from cameo import load_model
```

For example, load the most current genome-scale metabolic reconstruction of *Escherichia coli*.

```
model = load_model("iJO1366")
```

Models, reactions, metabolites, etc., provide return HTML when evaluated in Jupyter notebooks and can thus be easily inspected.

```
model
```

1.2.2 Step 2: Simulate a model

The model can be simulated by executing `model.solve()`.

```
solution = model.solve()
```

A quick overview of the solution can be obtained in form of a pandas DataFrame (all solution objects in cameo provide access to data frames through a `data_frame` attribute).

```
solution
```

The data frame is accessible through `solution.data_frame`.

```
solution.data_frame
```

Data frames make it very easy to process results. For example, let's take a look at reactions with flux != 0

```
solution.data_frame.query('fluxes != 0')
```

1.2.3 Step 3: Exploring a model

Objects—models, reactions, metabolites, genes—can easily be explored in the Jupyter notebook, taking advantage of tab completion. For example, place your cursor after the period in `model.reactions.` and press the TAB key. A dialog will appear that allows you to navigate the list of reactions encoded in the model.

```
model.reactions. # place your cursor after the period and press the TAB key.
```

For example, you can access the E4PD (*Erythrose 4-phosphate dehydrogenase*) reaction in the model.

```
model.reactions.E4PD
```

Be aware though that due variable naming restrictions in Python dot notation access to reactions (and other objects) might not work in some cases.

```
model.reactions.12DGR120tipp
```

```
  File "<ipython-input-11-fa7ea4193315>", line 1
    model.reactions.12DGR120tipp
                    ^
SyntaxError: invalid syntax
```

In these cases you need to use the `model.reactions.get_by_id`.

```
model.reactions.get_by_id('12DGR120tipp')
```

Metabolites are accessible through `model.metabolites`. For example, D-glucose in the cytosolic compartment.

```
model.metabolites.glc_dsh_D_c
```

```
<Metabolite glc_dsh_D_c at 0x112a22f98>
```

A list of the genes encoded in the model can be accessed via `model.genes`.

```
model.genes
```

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```

A few additional attributes have been added that are not available in a cobrapy model. For example, exchange reactions that allow certain metabolites to enter or leave the model can be accessed through `model.exchanges`.

```
model.exchanges
```

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```

Or, the current medium can be accessed through `model.medium`.

```
model.medium
```

It is also possible to get a list of essential reactions ...

```
model.essential_reactions()
```

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... and essential genes.

```
model.essential_genes()
```

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```

```
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<Gene b2026 at 0x114b37278>,
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<Gene b1662 at 0x114b5b400>,
```

```
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 <Gene b1693 at 0x1148f7d30>,
 <Gene b2746 at 0x114a63d30>,
 <Gene b2687 at 0x114b5bd30>,
 <Gene b0826 at 0x114a8bd68>,
 <Gene b2515 at 0x114a63da0>,
 <Gene b0072 at 0x114a0fe10>,
 <Gene b0071 at 0x114a0fe48>,
 <Gene b3433 at 0x11485fef0>,
 <Gene b0074 at 0x114a0ffd0>]
```

```
from cameo import webmodels
```

```
models = webmodels.index_models()
```

```
models
```

```
from pandas import options
options.display.max_rows = 8
from cameo import load_model
model = load_model("iJO1366")
```

1.3 Simulating models with

computer **a**ided **m**etabolic **e**ngineering and **o**ptimization

cameo uses and extends the model data structures defined by cobrapy, our favorite **CO**nstraints-**B**ased **R**econstruction and **A**nalysis tool for **Py**thon. **cameo** is thus 100% compatible with **cobrapy**. For efficiency reasons, however, **cameo** implements its own simulation methods that take advantage of a more advanced solver interface.

1.3.1 Primer: Constraint-Based Modeling

Constraint-based modeling is a powerful modeling framework for analyzing metabolism on the genome scale (McCloskey et al., 2013). For a model that encompasses n reactions that involve m metabolites, $\mathbf{S}$ is a matrix of dimension $m \times n$ that encodes the stoichiometry of the metabolic reaction system; it is usually referred to as stoichiometric matrix. Assuming that the system is in a steady state—the concentration of metabolites are constant—the system of flux-balances can be formulated as

$$\mathbf{S}\mathbf{v} = 0\,, \tag{1.1}$$

where $\mathbf{v}$ is the vector of flux rates. With the addition of a biologically meaningful objective, flux capacity constraints, information about the reversibility of reactions under physiological conditions, an optimization problem can be formulated that can easily be solved using linear programming.

, e.g., maximimization of biomass production,Given the maximization of growth rate as one potential biological objective $v_{biomass}$, i.e., the flux of an artificial reaction that consumes biomass components in empirically determined proportions, and assuming that the cell is evolutionary optimized to achieve that objective, and incorporating knowledge about reaction reversibility, uptake and secretion rates, and maximum flux capacities in the form of lower and uppers bounds ($\mathbf{v}_{lb}$ and $\mathbf{v}_{ub}$) on the flux variables $\mathbf{v}$, one can formulate and solve an optimization problem to identify an optimal set of flux rates using flux balance analysis (FBA):

$$\begin{aligned} Max \;\; & Z_{obj} = \mathbf{c}^T\mathbf{v} && (1.2)\\ \text{s.t.} \;\; & \mathbf{S}\mathbf{v} = 0 && (1.3)\\ & \mathbf{v}_{lb} \leq \mathbf{v} \leq \mathbf{v}_{ub} && (1.4) \end{aligned}$$

1.3.2 Flux Balance Analysis

In **cameo**, flux balance analysis can be performed with the function `fba`.

```
from cameo import fba
fba_result = fba(model)
```

Basically, `fba` calls `model.solve()` and wraps the optimization solution in a `FluxDistributionResult` object. The maximum objective values (corresponding to a maximum growth rate) can obtained throug `result.objective_value`.

```
fba_result.objective_value
```

```
0.9823718127269799
```

1.3.3 Parsimonious Flux Balance Analysis

Parsimonious flux balance analysis (Lewis et al., 2010), a variant of FBA, performs FBA in in a first step to determine the maximum objective value Z_{obj}, fixes it in form of an additional model constraint ($\mathbf{c}^T\mathbf{v} \geq Z_{obj}$), and then minimizes

in a second optimization the L_1 norm of $\mathbf{v}$. The assumption behind the pFBA is that cells try to minimize flux magnitude as well in order to keep the costs of protein low.

$$
\begin{aligned}
Max \quad & |\mathbf{v}| && (1.5)\\
\text{s.t.} \quad & \mathbf{S}\mathbf{v} = 0 && (1.6)\\
& \mathbf{c}^T\mathbf{v} \geq Z_{obj} && (1.7)\\
& \mathbf{v}_{lb} \leq \mathbf{v} \leq \mathbf{v}_{ub} && (1.8)
\end{aligned}
$$

In **cameo**, pFBA can be performed with the function `pfba`.

```
from cameo import pfba
pfba_result = pfba(model)
```

The `objective_function` value is $|\mathbf{v}|$ ...

```
pfba_result.objective_value
```

```
699.0222751839377
```

... whis is significantly smaller than flux vector of the original FBA solution.

```
abs(fba_result.data_frame.flux).sum()
```

```
764.91487969777245
```

1.3.4 Setp 2: Simulate knockouts phenotypes

Although PFBA and FBA can be used to simulate the effect of knockouts, other methods have been proven more valuable for that task: MOMA and ROOM. In *cameo* we implement a linear version of MOMA.

Simulating knockouts:

- Manipulate the bounds of the reaction (or use the shorthand method knock_out)

```
model.reactions.PGI
```

```
model.reactions.PGI.knock_out()
model.reactions.PGI
```

- Simulate using different methods:

```
%time
fba_knockout_result = simulation.fba(model)
fba_knockout_result[model.objective]
```

```
CPU times: user 2 µs, sys: 0 ns, total: 2 µs
Wall time: 5.01 µs
```

```
0.905983
```

```
pfba_knockout_result = simulation.pfba(model)
pfba_knockout_result[model.objective]
```

```
0.905983
```

MOMA and ROOM relly on a reference (wild-type) flux distribution and we can use the one previously computed.

Parsimonious FBA references seem to produce better results using this methods

```
lmoma_result["2 * EX_glc_lp_e_rp_"]
```

```
-18.7358
```

```
%time
lmoma_result = simulation.lmoma(model, reference=pfba_result.fluxes)
lmoma_result[model.objective]
```

```
CPU times: user 2 µs, sys: 1 µs, total: 3 µs
Wall time: 5.01 µs
```

```
0.791393
```

```
%time
room_result = simulation.room(model, reference=pfba_result.fluxes)
room_result[model.objective]
```

```
CPU times: user 2 µs, sys: 1 µs, total: 3 µs
Wall time: 5.01 µs
```

```
0.887440
```

```
room_result
```

```
<cameo.core.result.FluxDistributionResult at 0x10aa75b50>
```

1.4 Analyzing models with

computer **a**ided **m**etabolic **e**ngineering and **o**ptimization

cameo uses and extends the model data structures defined by cobrapy, our favorite **CO**nstraints-**B**ased **R**econstruction and **A**nalysis tool for **Py**thon. **cameo** is thus 100% compatible with **cobrapy**. For efficiency reasons though **cameo** implements its own analysis methods that take advantage of a more advanced solver interface.

```
from cameo import load_model
model = load_model("iJO1366")
```

1.4.1 Flux Variability Analysis

Flux variability analysis (FVA) enables the computation of lower and upper bounds of reaction fluxes.

```
from cameo import flux_variability_analysis
```

```
flux_variability_analysis(model, reactions=[model.reactions.PGI, model.reactions.EX_glc_lp_e_rp_])
```

One very useful application of FVA is determining if alternative optimal solution exist.

```
flux_variability_analysis(model, reactions=[model.reactions.PGI, model.reactions.EX_glc_lp_e_rp_],
                          fraction_of_optimum=1.)
```

1.4.2 Phenotpic Phase Plane

```
model.reactions.EX_o2_lp_e_rp_.lower_bound = -10
result = analysis.phenotypic_phase_plane(model,
                                         variables=[model.reactions.BiomassEcoli],
                                         objective=model.reactions.EX_succ_lp_e_rp_,
                                         points=10)
```

```
result.plot(height=400)
```

```
result.data_frame
```

1.5 Differential flux variability analysis

```
from cameo import load_model
from cameo.flux_analysis.analysis import phenotypic_phase_plane
from cameo.strain_design.deterministic import DifferentialFVA
```

```
:0 [1;31mFutureWarning[0m: IPython widgets are experimental and may change in the future.
```

1.5.1 E. coli model and succinate production

Load the E. coli core model.

```
model = load_model('iJO1366')
```

The production envelope looks like this.

```
production_envelope = phenotypic_phase_plane(model,
                                             variables=[model.reactions.Ec_biomass_iJO1366_core_53p95
                                             objective=model.reactions.EX_succ_lp_e_rp_)
production_envelope.plot(height=300)
```

Set up a model that represents a reference state (in this case a model with a constrained growth rate).

```
reference_model = model.copy()
biomass_rxn = reference_model.reactions.Ec_biomass_iJO1366_core_53p95M
biomass_rxn.lower_bound = 0.3
target = reference_model.reactions.EX_succ_lp_e_rp_
target.lower_bound = 2
```

Set up the differential flux variability analysis strain design method.

```
diffFVA = DifferentialFVA(design_space_model=model,
                          reference_model=reference_model,
                          objective=target,
                          variables=[biomass_rxn],
                          normalize_ranges_by=biomass_rxn,
                          points=10)
```

Run differential flux variability analysis (only on the surface of the production envelope)

```
result = diffFVA.run(surface_only=True)
result.plot(height=300)
```

```
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```

```
result.display_on_map("iJO1366.Central metabolism")
```

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

1.6 E. coli core model

```
import cameo
from cameo import models
from cameo.strain_design.heuristic import GeneKnockoutOptimization, ReactionKnockoutOptimization
from cameo.strain_design.heuristic.objective_functions import biomass_product_coupled_yield, product_
from cameo.flux_analysis.simulation import fba
from cameo.parallel import SequentialView
import inspyred
```

```
model = models.bigg.e_coli_core
```

```
objective1 = biomass_product_coupled_yield(
    model.reactions.Biomass_Ecoli_core_w_GAM,
    model.reactions.EX_ac_e,
    model.reactions.EX_glc_e)

objective2 = number_of_knockouts()
objective = [objective1, objective2]
```

```
ko = GeneKnockoutOptimization(model=model,
                                    simulation_method=fba,
                                    objective_function=objective,
                                    heuristic_method=inspyred.ec.emo.NSGA2,
                                    seed=1234)
```

```
results = ko.run(max_evaluations=3000, popuplation_size=100, view=SequentialView())
```

```
Starting optimization at Fri, 17 Jul 2015 13:53:04
```

```
Using saved session configuration for http://localhost:5006/
To override, pass 'load_from_config=False' to Session
```

```
/Users/niko/.virtualenvs/cameo_py3/lib/python3.4/site-packages/bokeh/session.py:319 [1;31mUserWarning
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```
Finished after 00:00:16
```

```
results
```

1.7 iJO1366 model

```
model = models.bigg.iJO1366
```

```
of1 = product_yield(model.reactions.Ec_biomass_iJO1366_core_53p95M,
                    model.reactions.EX_glc_e)
of2 = number_of_knockouts()
of3 = biomass_product_coupled_yield(model.reactions.Ec_biomass_iJO1366_core_53p95M,
                                    model.reactions.EX_ac_e,
                                    model.reactions.EX_glc_e)
```

```
ko = GeneKnockoutOptimization(model=model, objective_function=[of1, of2, of3],
                                  simulation_method=fba, heuristic_method=inspyred.ec.emo.NSGA2)
```

```
ko.run(max_evaluations=5000, n=10, mutation_rate=0.3, population_size=100)
```

```
Starting optimization at Fri, 17 Jul 2015 13:54:18
```

```
Using saved session configuration for http://localhost:5006/
To override, pass 'load_from_config=False' to Session
```

```
/Users/niko/.virtualenvs/cameo_py3/lib/python3.4/site-packages/bokeh/session.py:319 [1;31mUserWarning
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```
Finished after 00:07:08
```

```
from IPython.display import display
import re
```

```
from cameo import models
from cameo.strain_design import pathway_prediction
```

```
model = models.bigg.iMM904
```

```
predictor = pathway_prediction.PathwayPredictor(model=model, compartment_regexp=re.compile(".*_c$"))
```

```
pathways = predictor.run(product="vanillin", max_predictions=5)
```

```
from cameo import phenotypic_phase_plane
from cameo.util import TimeMachine
from cameo.visualization.plotting import Grid
```

```
with Grid(nrows=3) as grid:
    for i, pathway in enumerate(pathways):
        with TimeMachine() as tm:
            pathway.plug_model(model, tm=tm)
            ppp = phenotypic_phase_plane(model, variables=[model.reactions.biomass_SC5_notrace], obje
            ppp.plot(grid=grid, width=450, height=350, title="Pathway %i" % (i+1), axis_font_size="12
```

1.8 Parallelization

Most methods in cameo can be parallelized using views.

1.9 cameo vs. cobrapy

1.9.1 Importing a model

cobrapy (load a model in SBML format):

```
from cobra.io import read_sbml_model
model = read_sbml_model('path/to/model.xml')
```

cameo (load models from different formats):

```
from cameo import load_model
# read SBML model
model = load_model('path/to/model.xml')
# ... or read a pickled model
model = load_model('path/to/model.pickle')
# ... or just import a model by ID from http://darwin.di.uminho.pt/models
iAF1260 = load_model('iAF1260')
```

1.9.2 Solving models

cobrapy:

```
solution = model.optimize()
if solution.status == 'optimal':
    # proceed
```

```
try:
    solution = model.solve()
except cameo.exceptions.SolverError:
    print "A non-optimal solution was returned by the solver"
else:
    # proceed
```

It is important to note that cameo models maintain *optimize* to maintain compatibility with cobrapy but we discourage its use.

1.10 How to ...

- ... run differential flux-variability analysis
- ... perform a heuristic gene knockout optimization (single-objective)
- ... perform a heuristic gene knockout optimization (multi-objective)

1.11 API

1.11.1 cameo package

Subpackages

cameo.api package

Submodules

cameo.api.designer module

cameo.api.hosts module

cameo.api.products module

Module contents

cameo.core package

Submodules

cameo.core.reaction module

cameo.core.result module

cameo.core.solution module

cameo.core.solver_based_model module

Module contents

cameo.data package

Submodules

cameo.data.metanetx module

Module contents

cameo.flux_analysis package

Submodules

cameo.flux_analysis.analysis module

cameo.flux_analysis.distance module

cameo.flux_analysis.simulation module

Module contents

cameo.models package

Submodules

cameo.models.universal module

cameo.models.webmodels module

Module contents

cameo.network_analysis package

Submodules

cameo.network_analysis.networkx_based module

cameo.network_analysis.util module

Module contents

cameo.strain_design package

Subpackages

cameo.strain_design.deterministic package

Submodules

cameo.strain_design.deterministic.flux_variability_based module

Module contents

cameo.strain_design.heuristic package

Subpackages

cameo.strain_design.heuristic.multiprocess package

Submodules

cameo.strain_design.heuristic.multiprocess.migrators module

cameo.strain_design.heuristic.multiprocess.observers module

cameo.strain_design.heuristic.multiprocess.optimization module

cameo.strain_design.heuristic.multiprocess.plotters module

Module contents

Submodules

cameo.strain_design.heuristic.archivers module

cameo.strain_design.heuristic.decoders module

cameo.strain_design.heuristic.generators module

cameo.strain_design.heuristic.genomes module

cameo.strain_design.heuristic.metrics module

cameo.strain_design.heuristic.objective_functions module

cameo.strain_design.heuristic.observers module

cameo.strain_design.heuristic.optimization module

cameo.strain_design.heuristic.plotters module

cameo.strain_design.heuristic.stats module

cameo.strain_design.heuristic.variators module

Module contents

cameo.strain_design.pathway_prediction package

Submodules

cameo.strain_design.pathway_prediction.util module

Module contents

Module contents

cameo.ui package

Module contents

cameo.visualization package

Submodules

cameo.visualization.escher_ext module

cameo.visualization.plotting module

cameo.visualization.visualization module

Module contents

Submodules

cameo.config module

cameo.exceptions module

cameo.io module

cameo.parallel module

cameo.stuff module

cameo.util module

Module contents

CHAPTER 2

Indices and tables

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- modindex
- search