MooViE:
Multi-objective optimization Visualization Engine

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Multi-objective Experimental Design for ^{13}C Metabolic Flux Analysis

In ^{13}C Metabolic Flux Analysis microorganisms are fed with a ^{13}C-labeled substrate. The labeling incorporation within the cell is then used to infer the internal metabolic reaction rates, called fluxes. Different substrates are available that influence how well the fluxes can be determined. Finding an optimal substrate mixture is a multi-objective problem, because there are several ways to define the quality of a substrate and cost consideration play also a role. Since these objectives are conflicting, no single optimal solution but a set of compromises exists, in which it is not possible to improve one objective without changing other objectives to the worse. These design are called Pareto optimal.

Evaluating Multi-objective Experimental Design Data

The high dimensionality and density of the design solutions raise the need for a suitable visualization technique that allows in-depth inspection of the data. That is:

- accessing conflicts in the objectives
- connecting the mixture design to the objectives
- supporting the selection process

Since the available approaches (e.g. scatter plots, parallel coordinates, dimension reduction) fail here, a new approach is created.

A novel visualization scheme: **MooViE**

MooViE, our new approach for visualization of high-volume multi-objective data is:

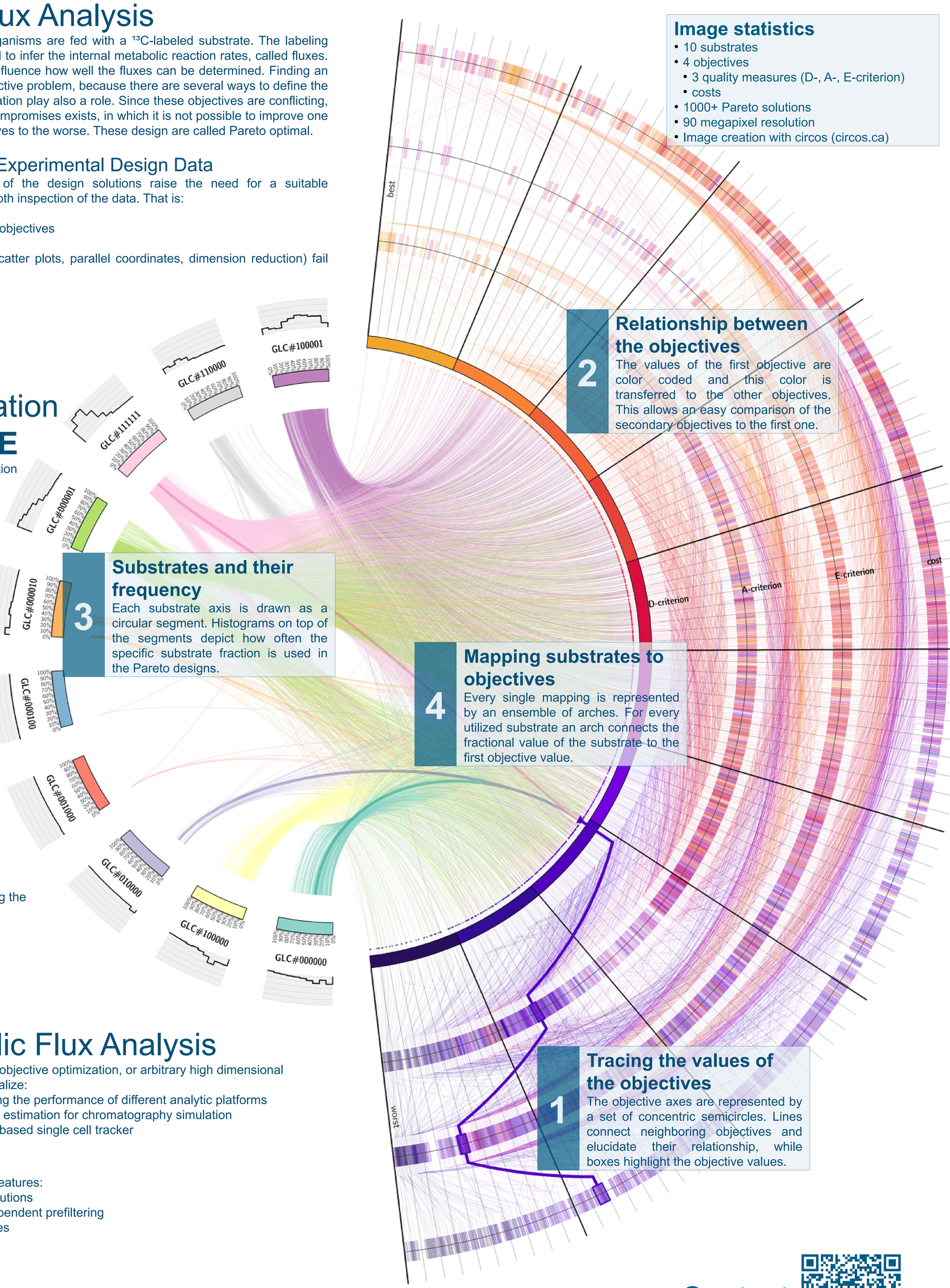
Intuitive
Two dimensional graphics that uses established visualization elements

Information rich
Visualization of relationship between the objectives, mapping of substrates to objectives and substrate frequency

Visually appealing
Aesthetically pleasing circular layout with carefully selected colors

Versatile
Dedicated techniques for sparse datasets and the case of two objectives

Fast
Lightweight C++11 codebase utilizing the cairo (cairographics.org) library



Beyond Metabolic Flux Analysis

MooViE can handle data from any multi-objective optimization, or arbitrary high dimensional mapping. We have used MooViE to visualize:

- a large-scale MO-ED study, comparing the performance of different analytic platforms
- results of a multi-objective parameter estimation for chromatography simulation
- a parameter study for a Monte Carlo based single cell tracker

Interactive features

MooViE will be extended by interactive features:

- selecting and highlighting specific solutions
- choosing data subsets by context dependent prefiltering
- reordering and rescaling the objectives

Software

https://github.com/modsim/MooViE

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