Maxim Lippeveld - 2022

SCIP: scalable cytometry image processing using Dask in a high performance computing environment

Software for distributed processing of bioimaging datasets

fwo Research Foundation Flanders Opening new horizons

DaMBi Data mining and Modelling for Biomedicine

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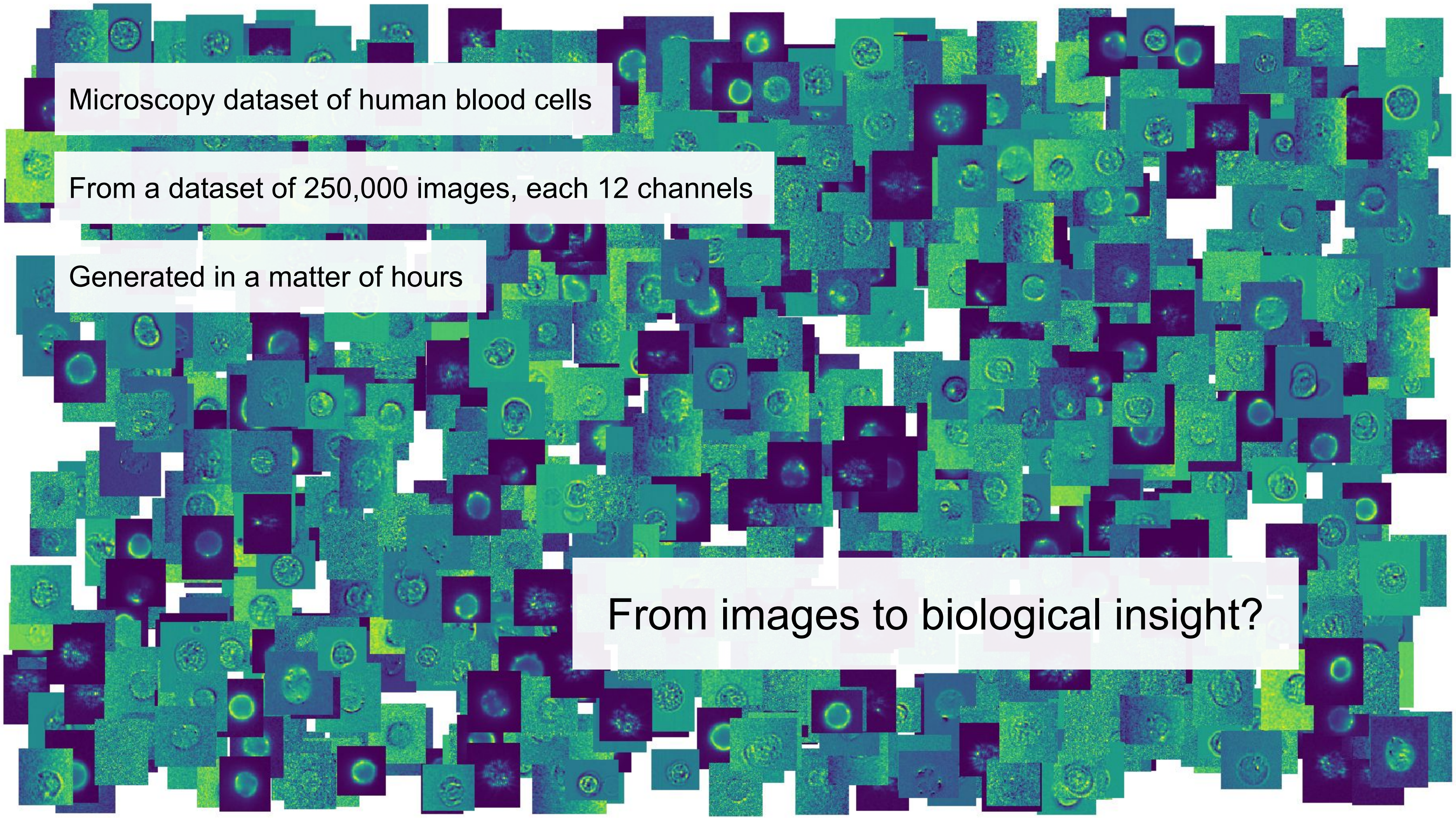


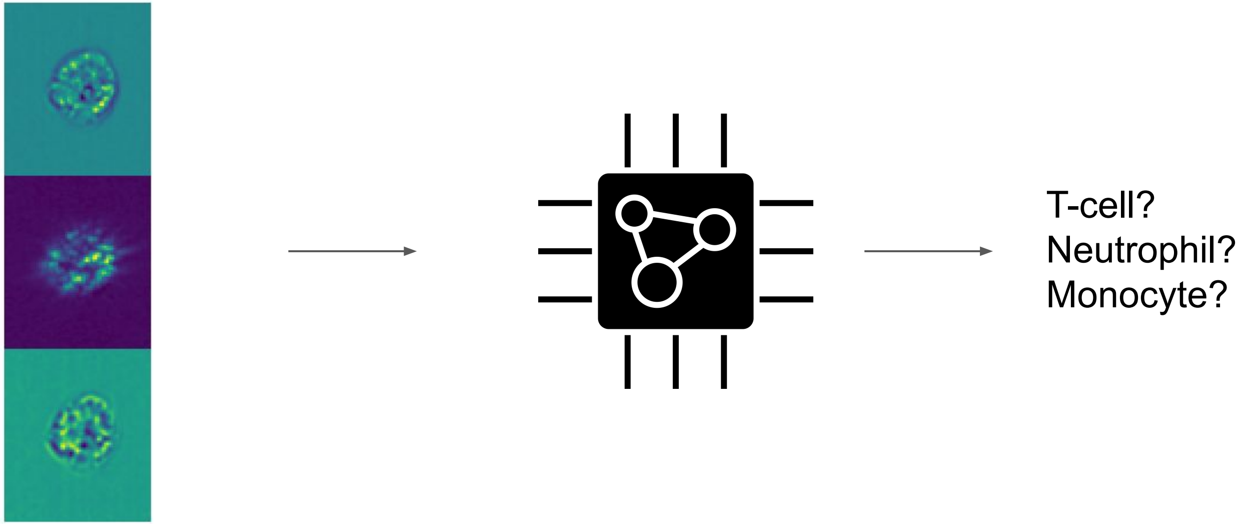
Microscopy dataset of human blood cells

From a dataset of 250,000 images, each 12 channels

Generated in a matter of hours

From images to biological insight?

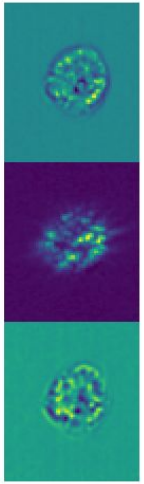
Predict cell types from microscopy images of cells



T-cell?
Neutrophil?
Monocyte?

Many steps are required to extract biological insight from raw microscopy data

Raw input data › Transformation › Pre-processing › Quality control › Insight



Segmentation

Masking

Filtering

Feature extraction

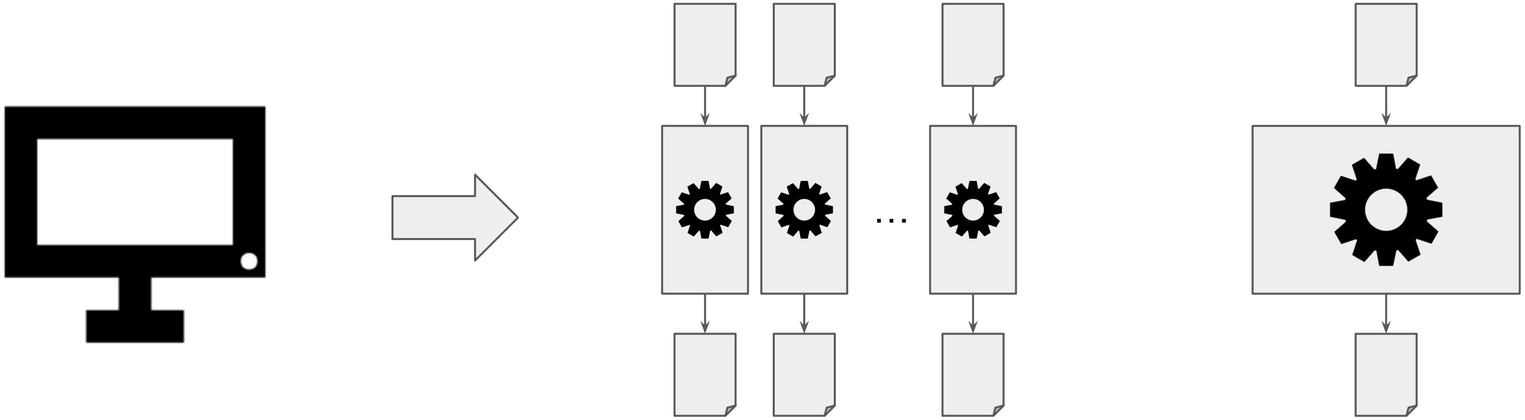
T-cell?
Neutrophil?
Monocyte?

Pre-processing software needs to scale with rapidly evolving imaging technology

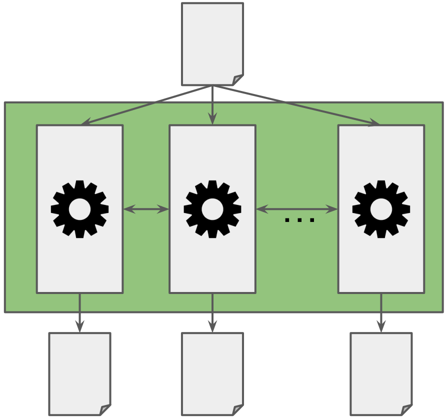
CellProfiler™
cell image analysis software

Local workstation execution with graphical interface

Scale with **split-apply-combine** strategy or **vertically**



Scalability has to be inherent to the pre-processing software



Focused on local workstation execution with GUI

Scale with split-apply-combine strategy or vertically

✓ Extensibility, interoperability, open-source

✚ Beyond split-apply-combine strategy

✚ Proper support for distributed computing

Scalable Cytometry Image Processing is a scalable, open-source preprocessing tool

Executes all parts of preprocessing pipeline

Embedded in the Python data science ecosystem

Implemented on top of Dask, a framework for scalable computing with Python

https://github.com/ScalableCytometryImageProcessing/SCIP

DASK

SCIP's design allows
more complex datasets
to be pre-processed with
more complex algorithms

SCIP: scalable cytometry image processing

Scalability beyond split-apply-combine

Operations across large-scale datasets

Classifying human cells with SCIP output

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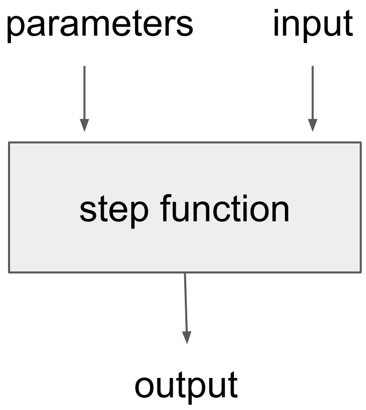
Modular pipeline steps make SCIP scalable and flexible



Steps are implemented with pure functions

- Output depends only on input and parameters
- Produce no side effects

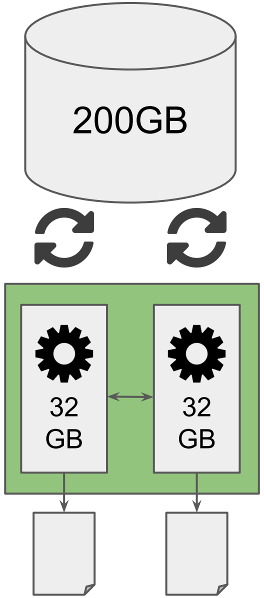
Allows for steps to be

- interchangeable,
- chained together easily and
- executed independently.

Makes extensibility easier

API can be easily used in other programs

Out-of-core processing of large-scale datasets with lazy execution



Microscopy images can be very large, larger than memory

Spread reading from disk over entire execution

⇒ Defer loading pixels to when they are needed

Control over where steps can be executed is important for advanced pipelines

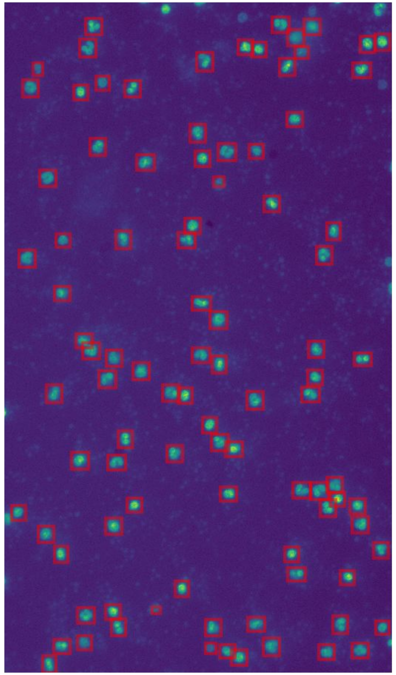


Image segmentation accelerated on the GPU

Texture features computed on powerful CPUs

For example, Gray-level co-occurrence matrices

Such steps have to be executed on specialized nodes

⇒ Granular execution control

Dask is a framework for scaling up workflows with Python

DASK

Enables all requirements to implement scalable bioimage pre-processing

Scales from laptops to clusters

Integrates seamlessly with other data science packages

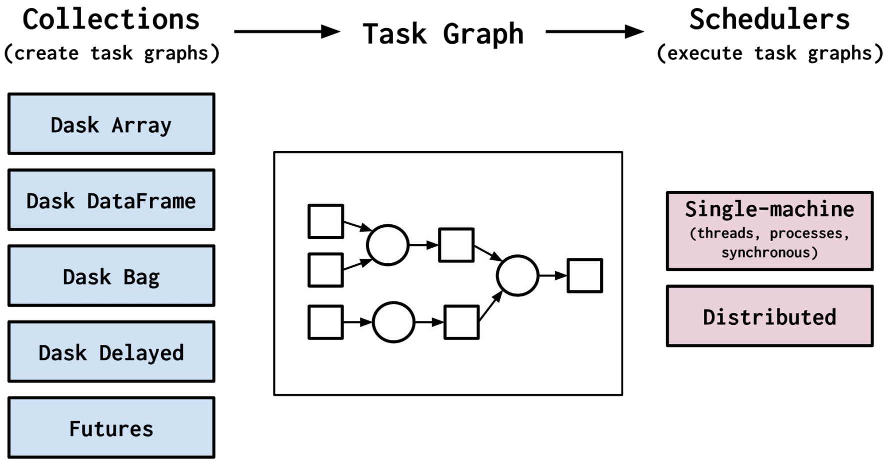
Easy to understand, but powerful

Dask DataFrame, Array and Bag are used throughout SCIP execution

DataFrame: features
Array: microscopy image planes
Bag: intermediate single-cell data

Provide map, fold, filter and aggregation functions

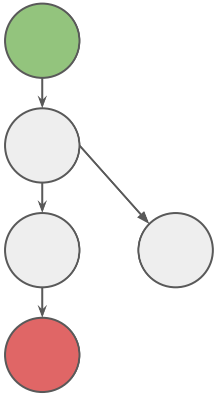
Make distribution logic transparent to the user



https://docs.dask.org/en/stable/

Task graphs are easily constructed using Dask collections

```
images = Bag([im1.tiff, im2.tiff,…])
images = images.map(load_from_disk)
masked = images.map(mask)
features = images.map(extract)
```



```
df = features.compute()
```

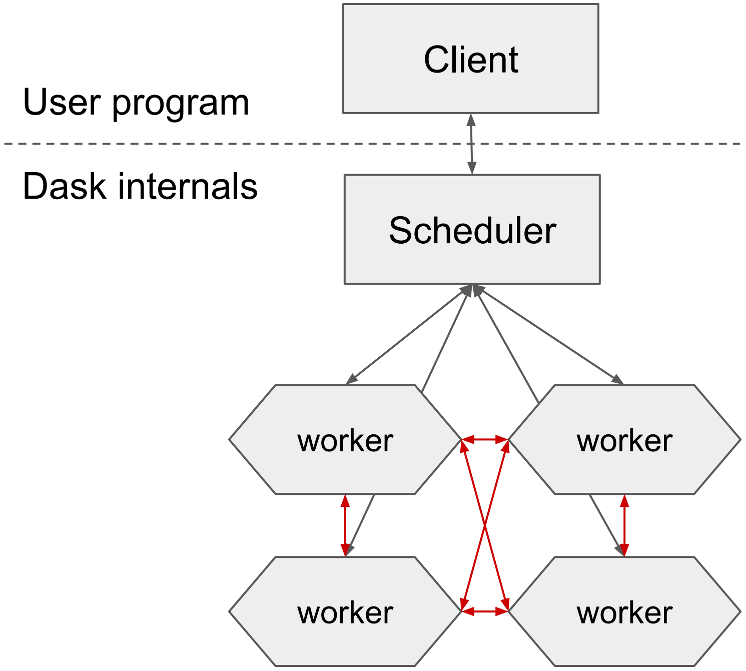
→ Scheduler analyzes task graph and executes

Dask executes tasks using distributed workers orchestrated by scheduler

1. Set up cluster (local or distributed)
2. Connect client to cluster
3. Lazily define tasks in a task graph
4. Compute

Smart task scheduling uses computational resources as efficiently as possible

Fault tolerance makes SCIP more robust to hardware failure

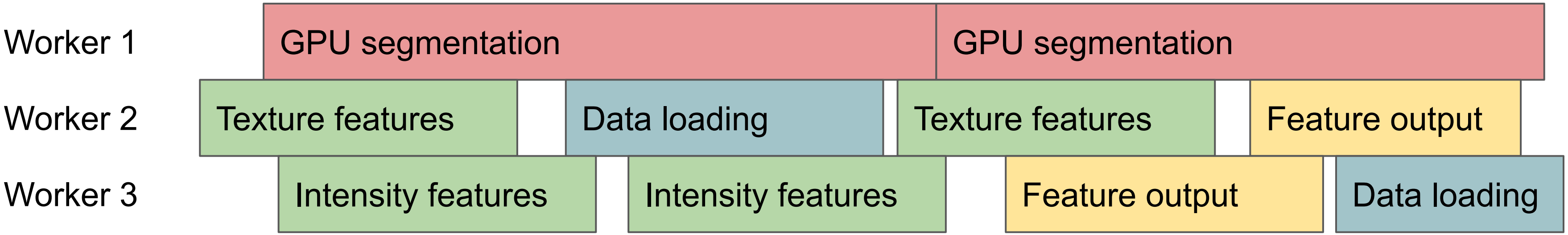


Resource annotations allow steps to be computed on specialized hardware

Use heterogeneous resources as efficiently as possible

Scheduler sends tasks to appropriate workers

Other tasks continue on other nodes



Worker 1 GPU segmentation GPU segmentation

Worker 2 Texture features Data loading Texture features Feature output

Worker 3 Intensity features Intensity features Feature output Data loading

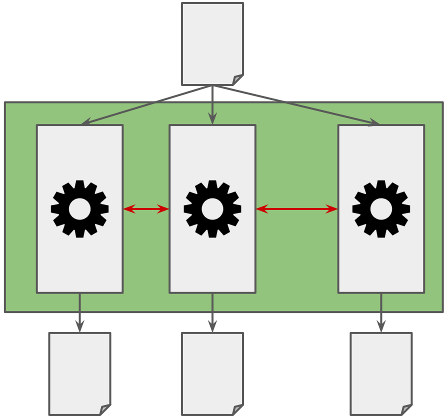
SCIP: scalable cytometry image processing

Scalability beyond split-apply-combine

Operations across large-scale datasets

Classifying human cells with SCIP output

Image filtering prior to feature extraction requires reduction across dataset

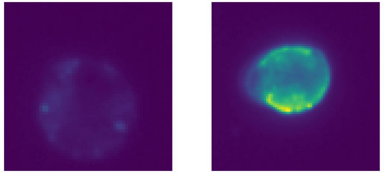


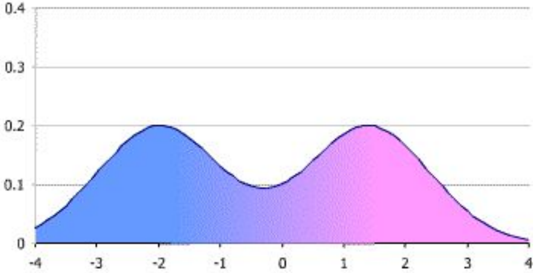
Many cells are imaged, not all of interest

For example, dead cells

Solution: filtering prior to feature extraction

Discard cells with low signal





⇒ Requires reduction across dataset

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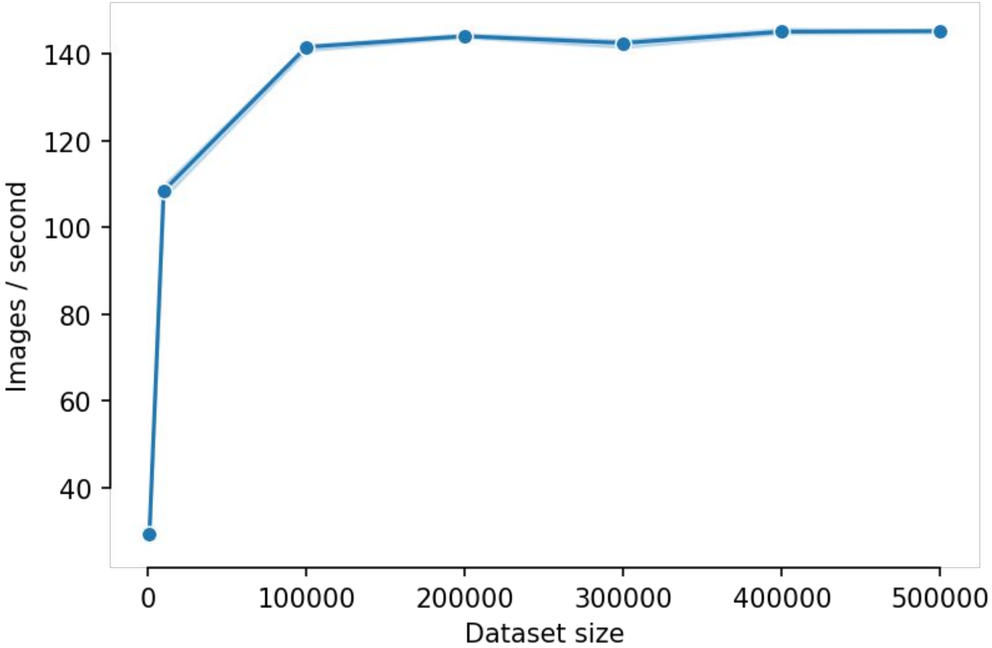
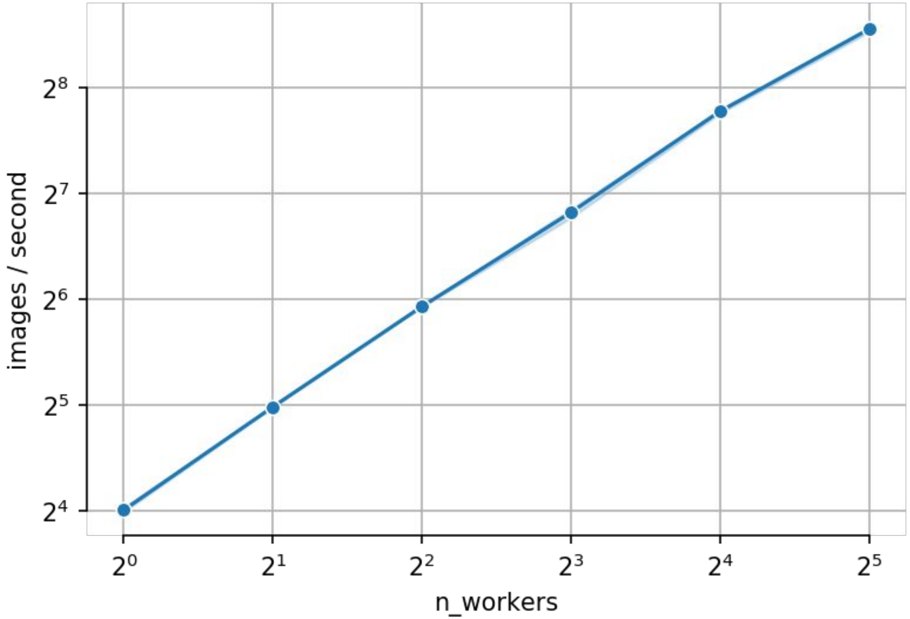
Overhead on runtime
minimal from 100 000 images or more



Images per second approximately doubles when number of workers doubles

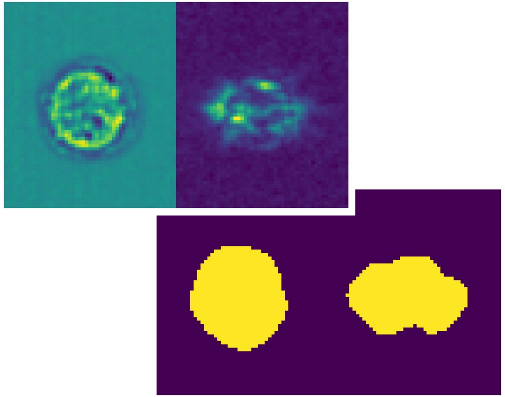


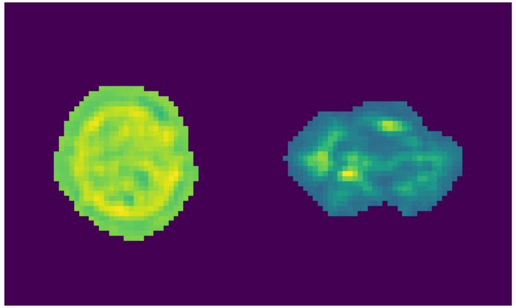
Processing a cytometry dataset of human immune system cells for classification

250,000 images of blood cells

12-channel image capturing different cell characteristics

Runtime: 101 min using 16 workers





eccentricity	area	intensity	contrast
0.4	200	30000	0.8

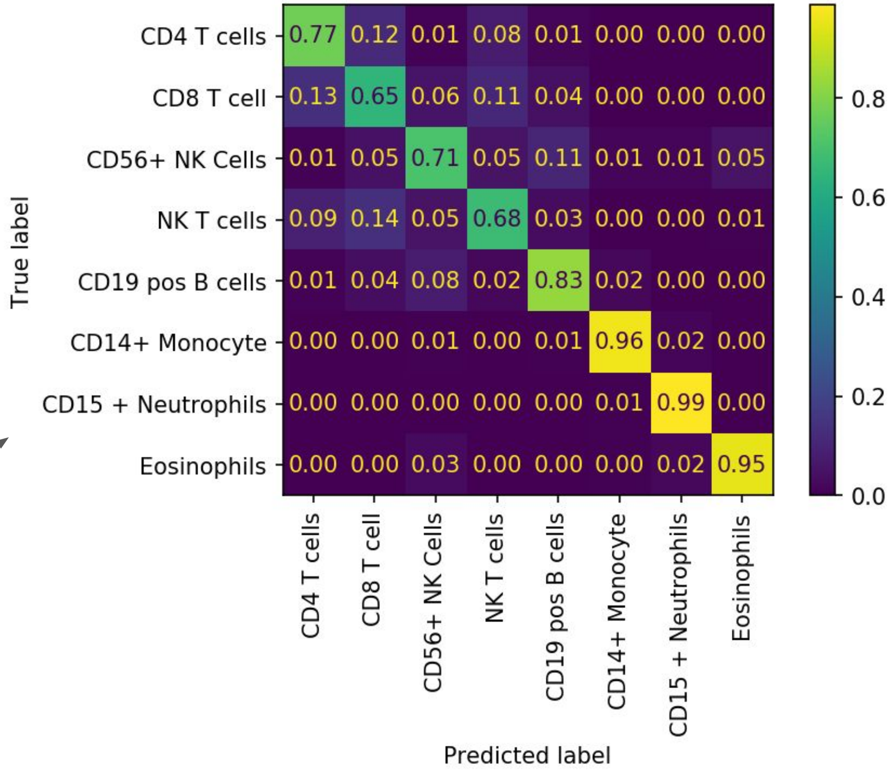
209 features / channel

SCIP features are used to predict cell type with machine learning

Using extreme gradient boosting

Balanced accuracy of 0.81 on test set

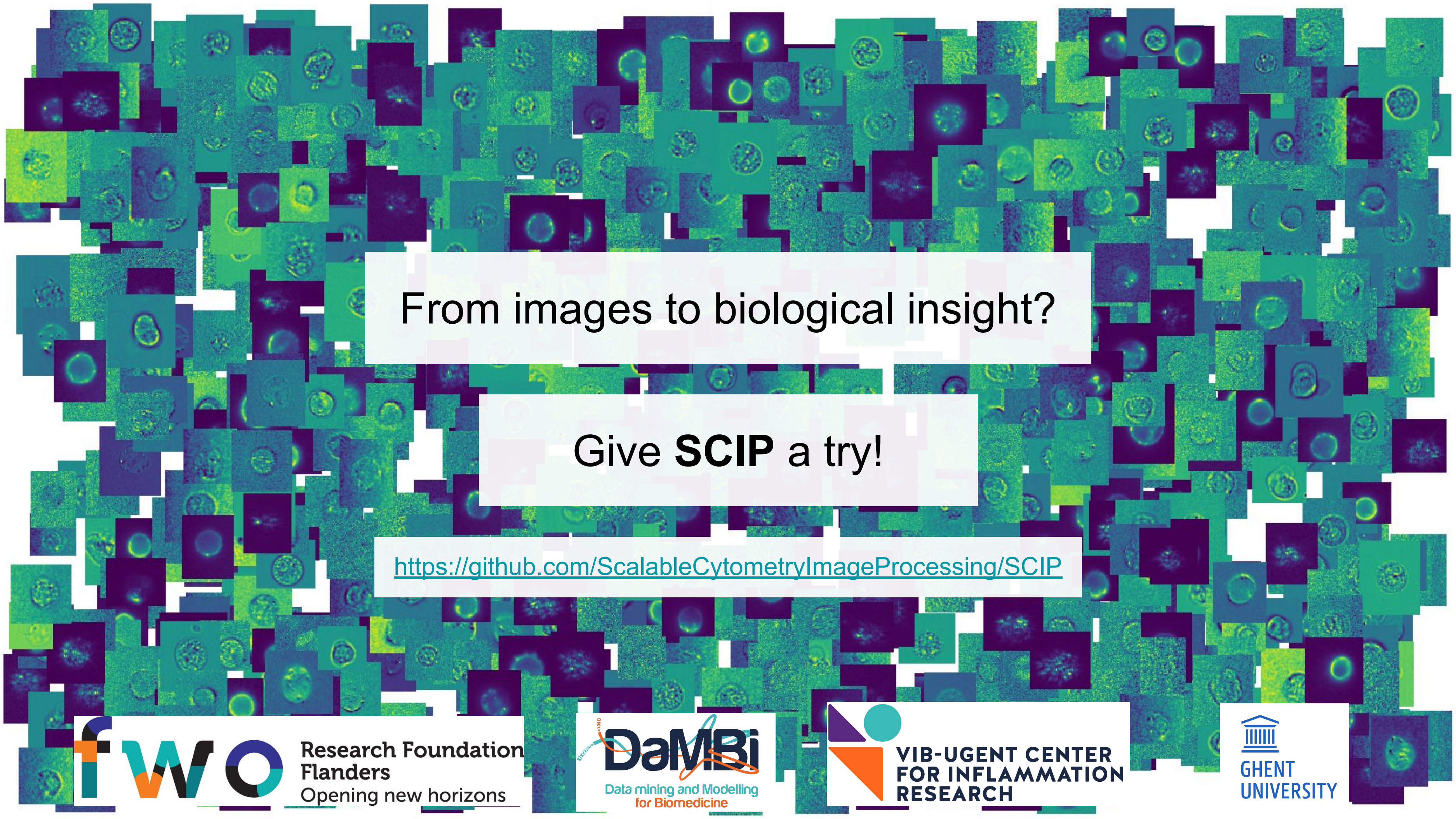
eccentricity	area	intensity	contrast
0.4	200	30000	0.8



True label \ Predicted label	CD4 T cells	CD8 T cell	CD56+ NK Cells	NK T cells	CD19 pos B cells	CD14+ Monocyte	CD15 + Neutrophils	Eosinophils
CD4 T cells	0.77	0.12	0.01	0.08	0.01	0.00	0.00	0.00
CD8 T cell	0.13	0.65	0.06	0.11	0.04	0.00	0.00	0.00
CD56+ NK Cells	0.01	0.05	0.71	0.05	0.11	0.01	0.01	0.05
NK T cells	0.09	0.14	0.05	0.68	0.03	0.00	0.00	0.01
CD19 pos B cells	0.01	0.04	0.08	0.02	0.83	0.02	0.00	0.00
CD14+ Monocyte	0.00	0.00	0.01	0.00	0.01	0.96	0.02	0.00
CD15 + Neutrophils	0.00	0.00	0.00	0.00	0.00	0.01	0.99	0.00
Eosinophils	0.00	0.00	0.03	0.00	0.00	0.00	0.02	0.95

Conclusion

- Tool for pre-processing large-scale bioimaging datasets
- Robust and inherently scalable
- Handles heterogeneous computational resources
- Enables implementation of dataset-wide computations
- Transform imaging data into machine learning-ready input



From images to biological insight?

Give **SCIP** a try!

https://github.com/ScalableCytometryImageProcessing/SCIP

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