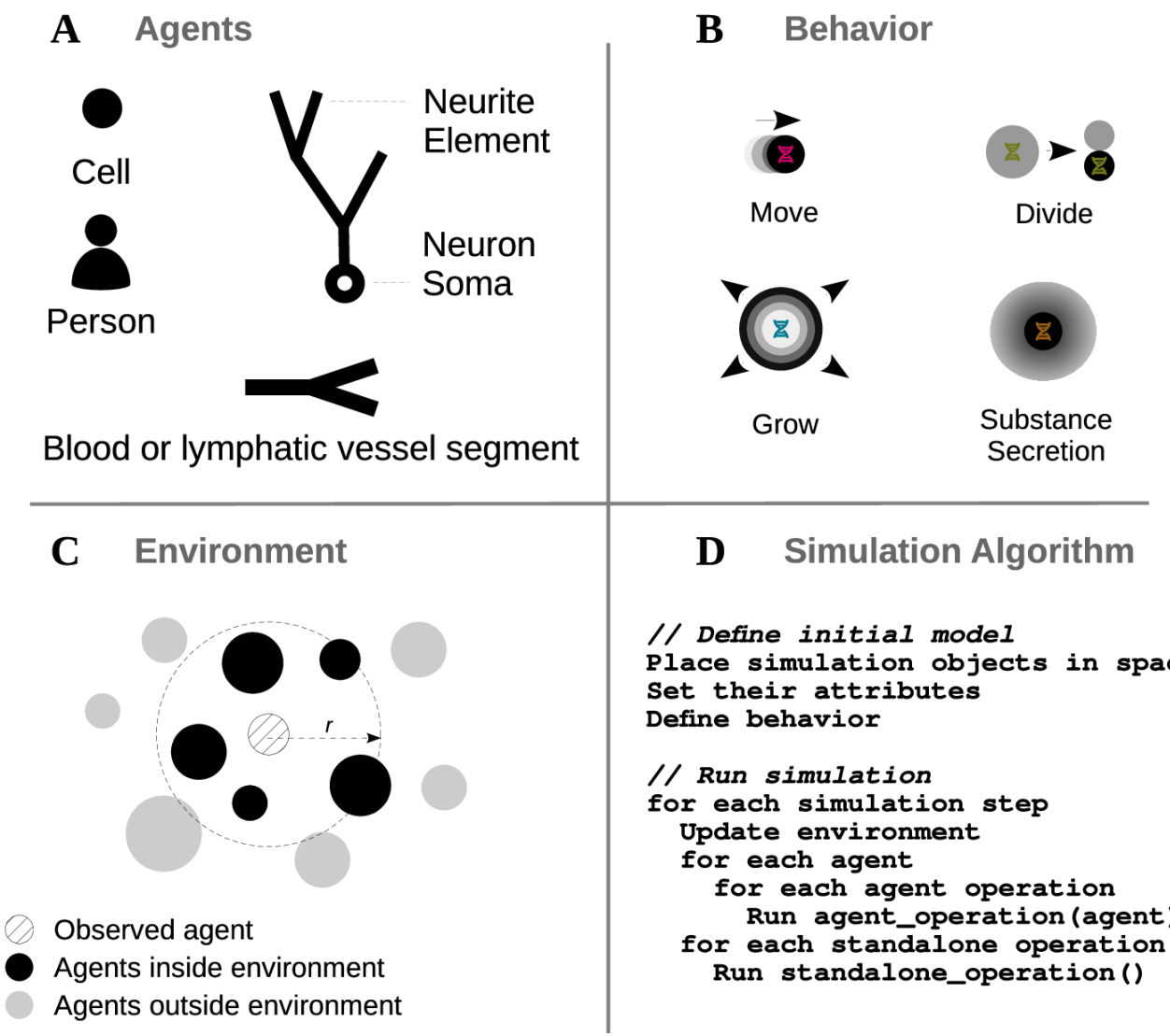
BioDynaMo: Current Status and Future Outlook

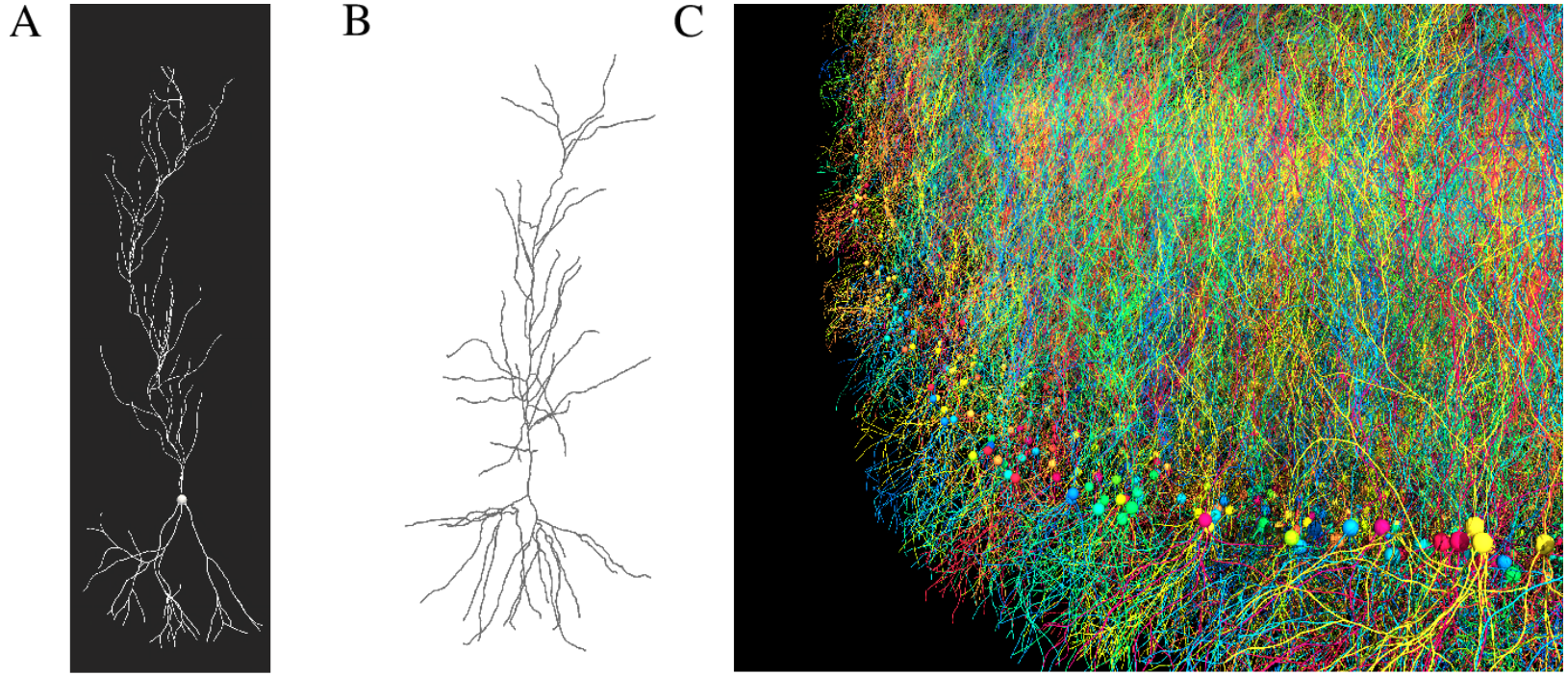
CERN openlab Technical Workshop
10.03.2021

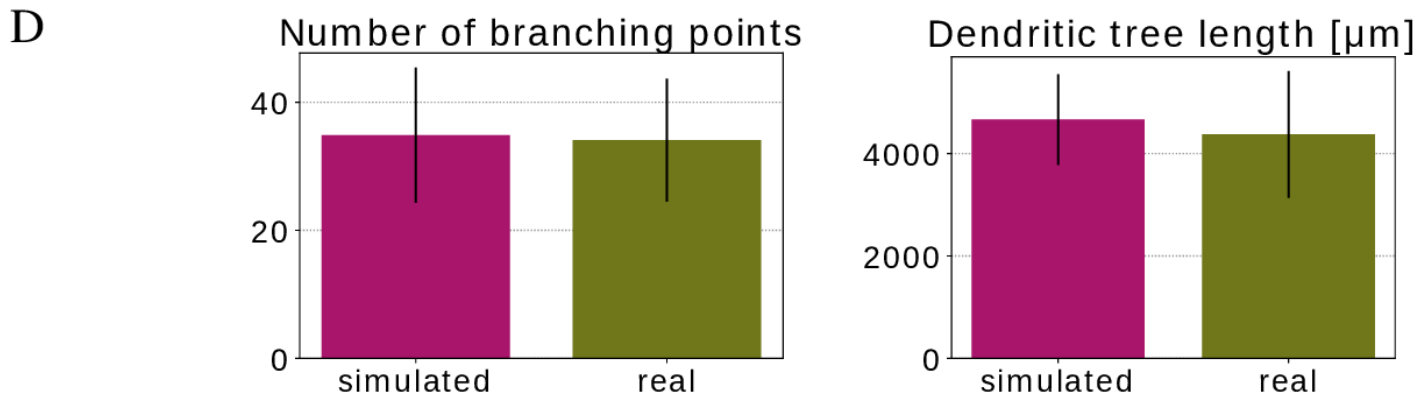
Lukas Breitwieser
on behalf of the BioDynaMo collaboration

Agent-based Simulation



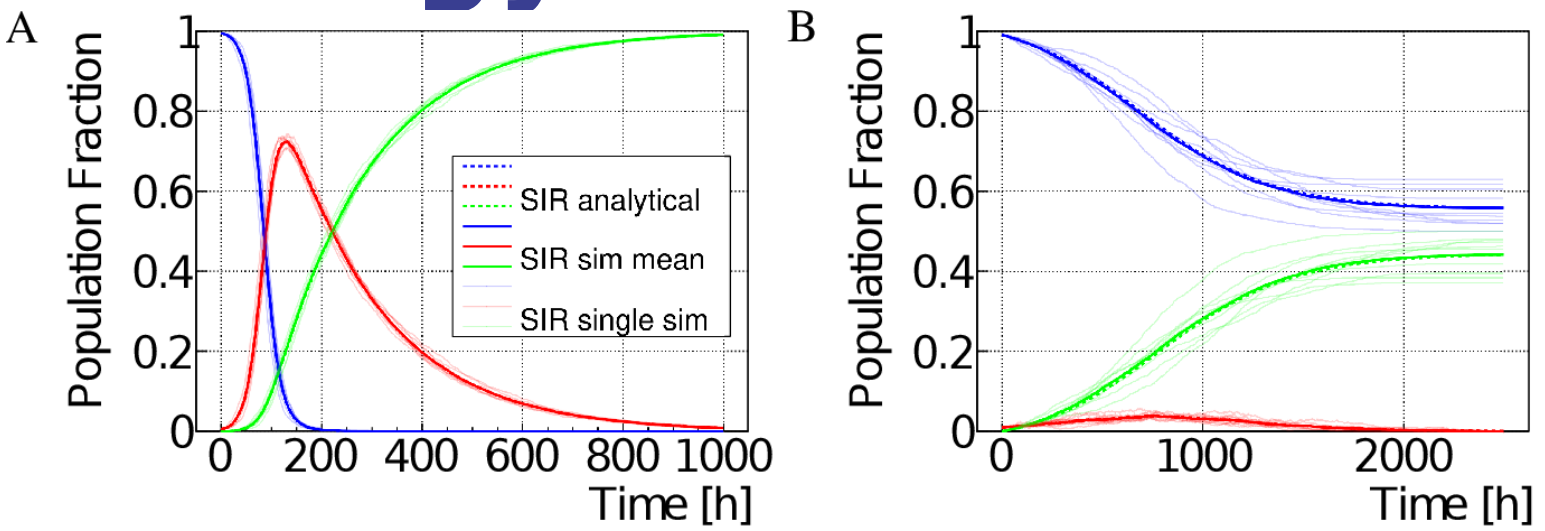
Neuroscience Use Case

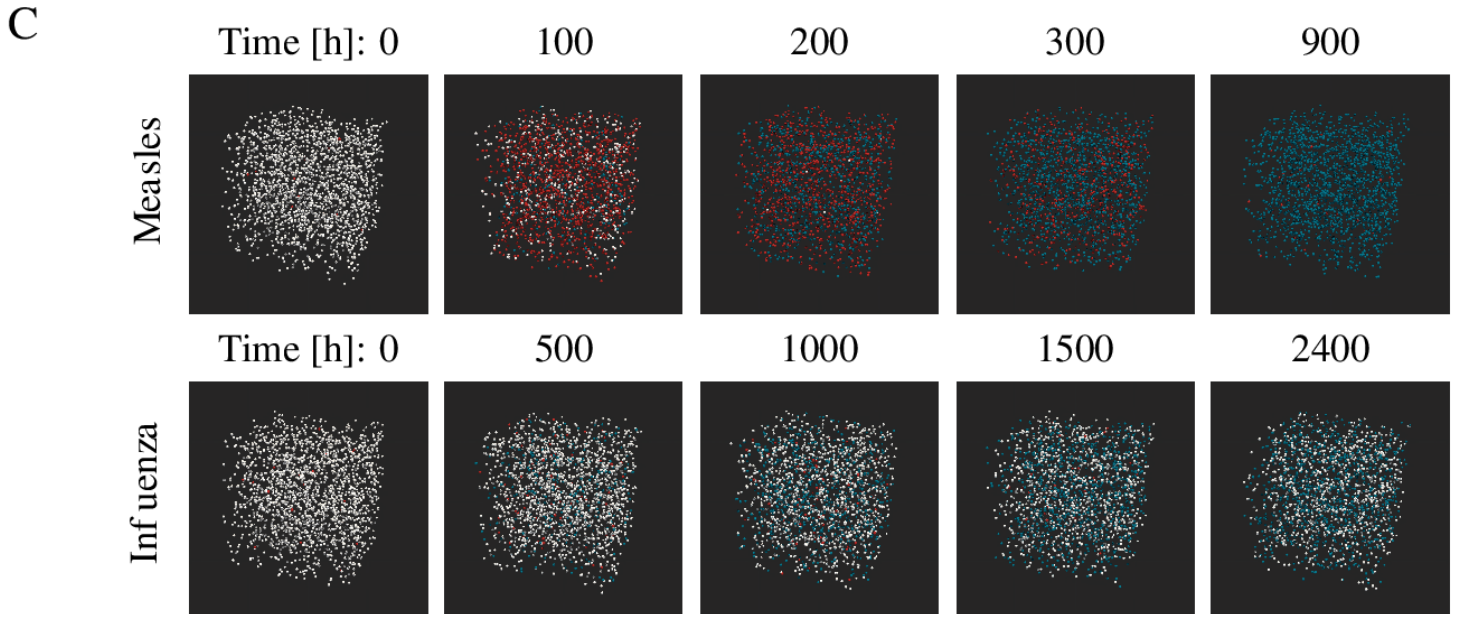




Further Information : Breitwieser et al. 2021

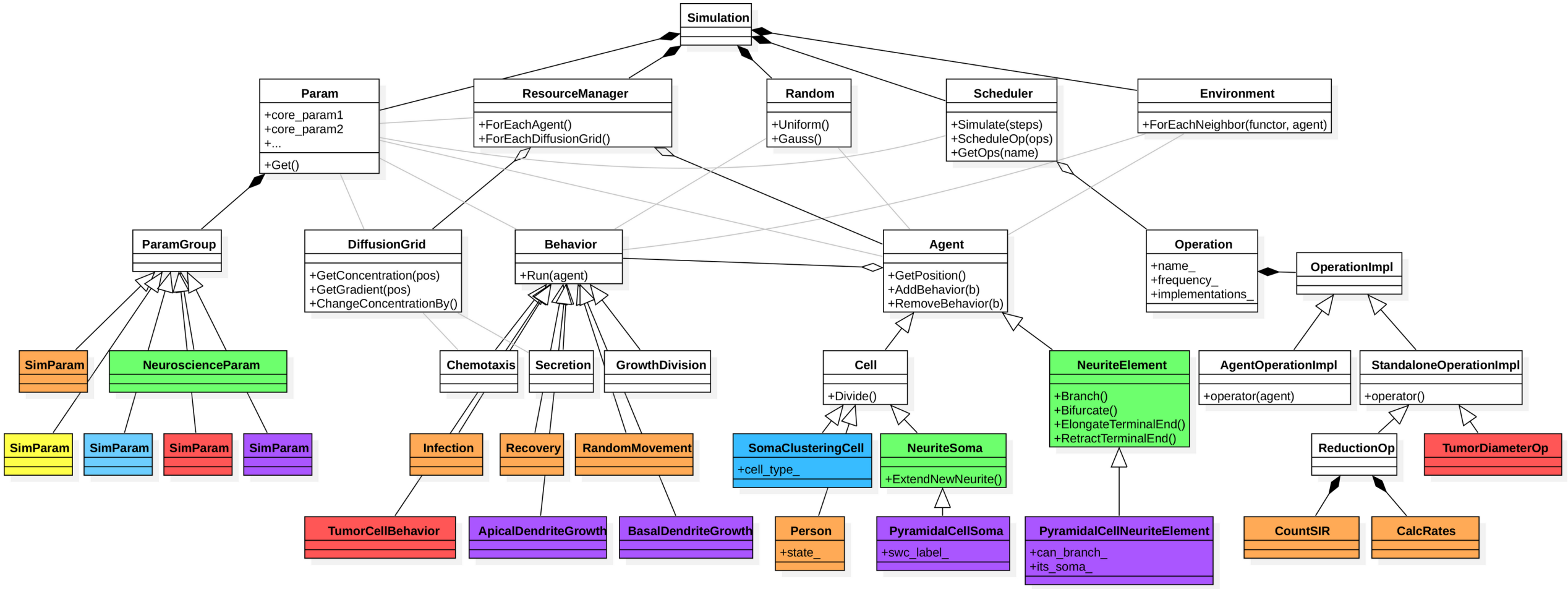
Epidemiology Use Case





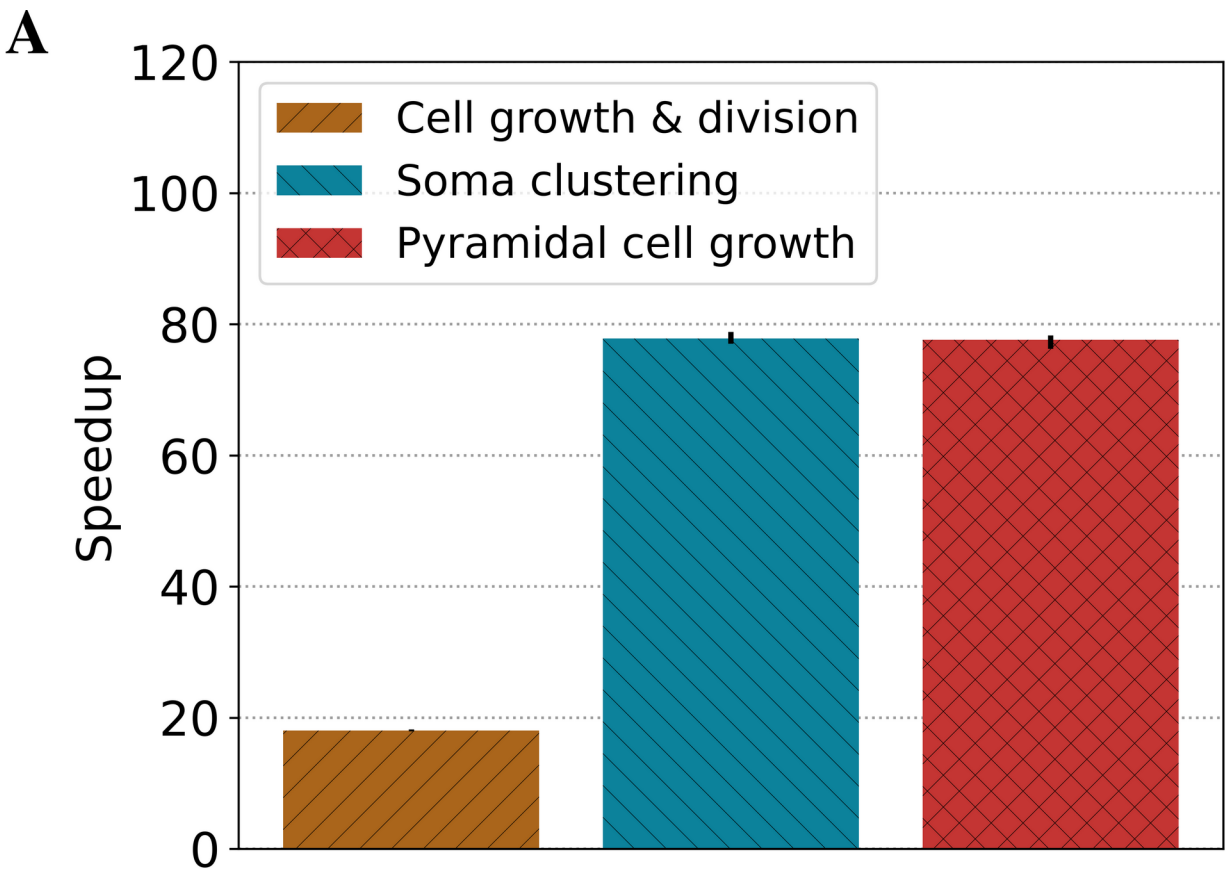
Further Information : Breitwieser et al. 2021

Modular Software Architecture

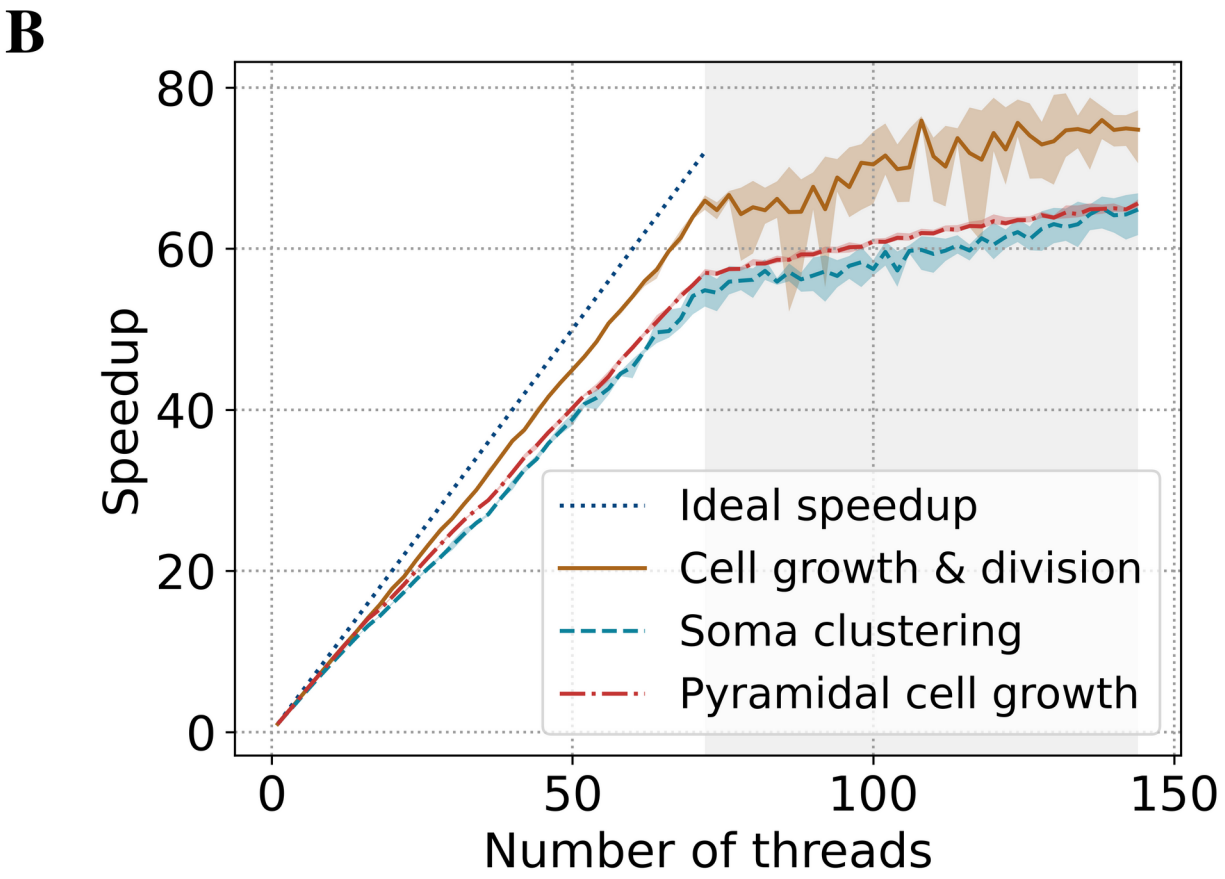


High-Performance Simulation Engine 1/2

Comparison between BioDynaMo and Cortex3D



Strong scaling analyis of BioDynaMo

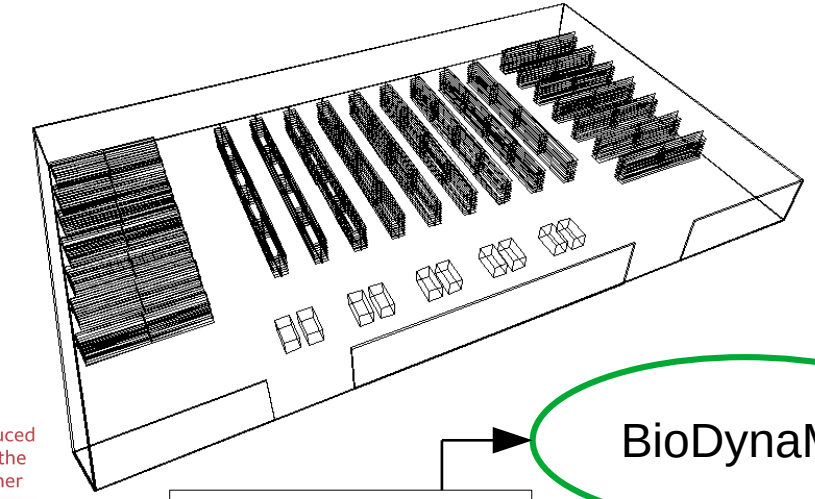


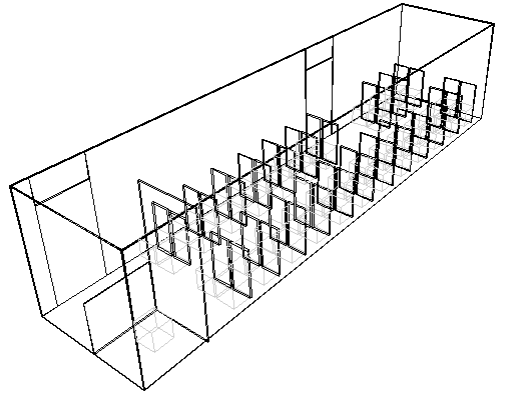
High-Performance Simulation Engine 2/2

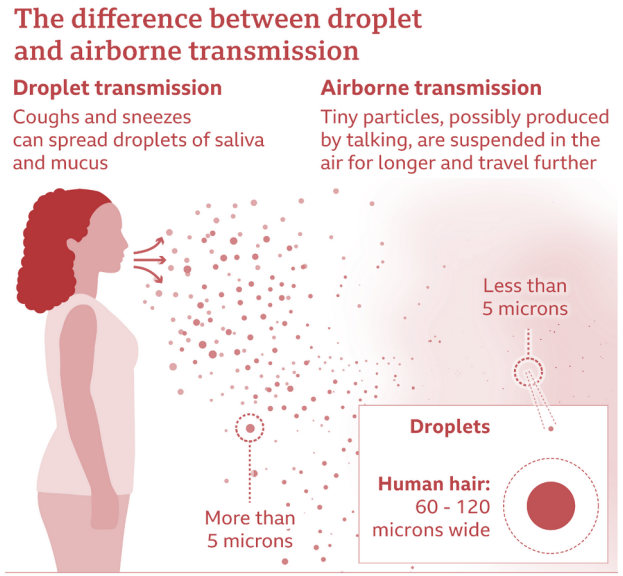
Simulation	Agents	Diffusion volumes	Iterations	System (Table 4)	Physical CPUs	Runtime	Memory
Neuroscience use case							
Single (Figure 3A in the main manuscript)	1 494	250	500	A	1	0.16 s	375 MB
				D	1	0.13 s	471 MB
Large-scale (Figure 3C in the main manuscript)	9 041 632	65 536	500	A	72	45 s	6 GB
				D	2	10 min 53 s	5.3 GB
Very-large-scale	1 018 280 997	5 606 442	500	B	72	1 h 37 min	507 GB
Oncology use case (Figure 4 in the main manuscript)							
2000 initial cells	4 169	0	312	A	1	1.24 s	378 MB
				D	1	0.98 s	475 MB
4000 initial cells	5 241	0	312	A	1	2.09 s	380 MB
				D	1	1.62 s	477 MB
8000 initial cells	8 225	0	288	A	1	4.16 s	381 MB
				D	1	3.39 s	477 MB
Large-scale	10 123 903	0	288	A	72	2 min 20 s	9.02 GB
				D	2	53 min 31 s	5.94 MB
Very-large-scale	1 012 302 977	0	288	B	72	6 h 49 min	639 GB
Epidemiology use case (Figure 5C in the main manuscript)							
Measles	2 010	0	1000	A	1	0.59 s	372 MB
Seasonal Influenza	2 020	0	2500	A	1	1.59 s	373 MB
Large-scale (measles)	10 050 000	0	1000	A	72	1 min 25 s	6.02 GB
				D	2	54 min 22 s	3.61 GB
Very-large-scale (measles)	1 005 000 000	0	1000	B	72	3 h 54 min	326 GB

Ongoing Projects

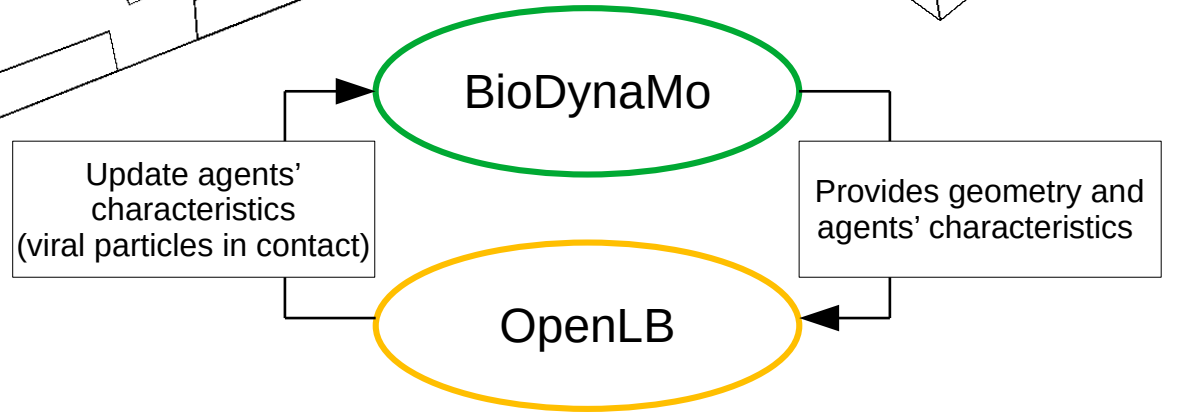
Modelling COVID-19 Spreading in Closed Environments

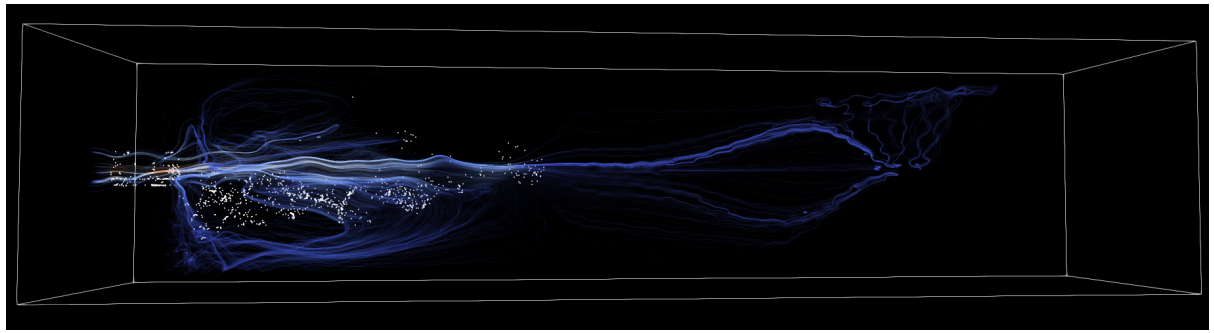






Source : WHO





OpenLB

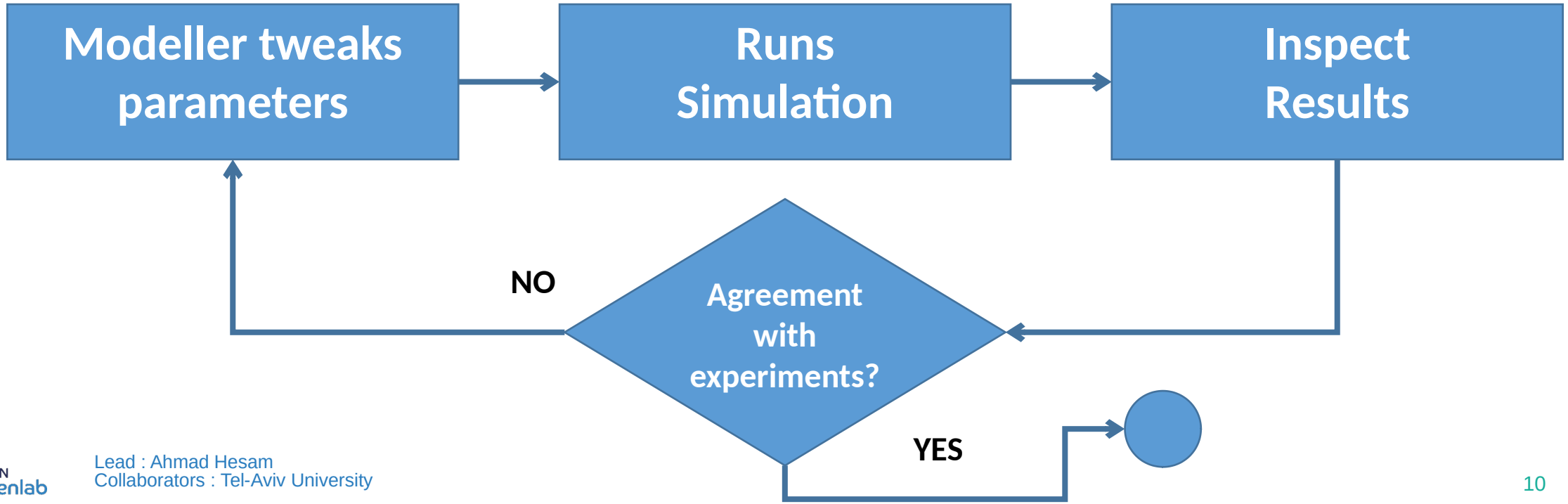
CERN openlab

Lead : Jean De Montigny
Collaborators : University of Geneva, University of Cyprus, University of Surrey

Data-Driven Model Optimization

Common issue: how to tune model-parameters to match experimental / analytical data?

Current approach:



Data-Driven Model Optimization

- Use experimental data for optimizing model parameters
- Compute error between experimental and simulated data
- Iteratively choose new simulation parameters to minimize error
- Explore parameter space rapidly on HPC cluster

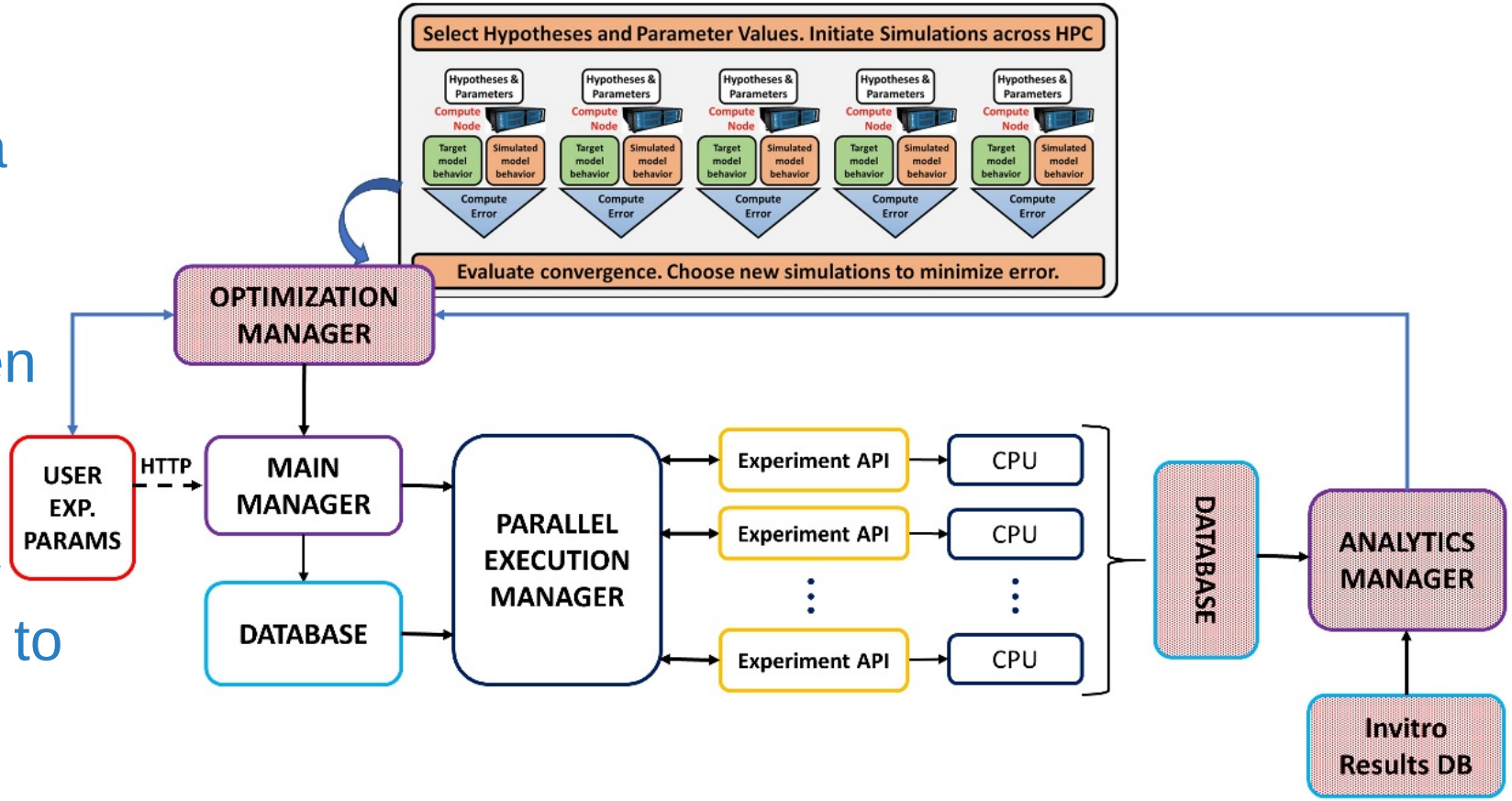


Figure : Avner Priel, Andrea Perissinotto (Tel-Aviv University)

Further Ongoing Projects Using BioDynaMo

- Distributed runtime to support simulations on multiple servers
- Retinal mosaic development
- Cryopreservation
- Multiscale (organ-to-cell) cancer modelling
- Radiation-induced tissue damage
- Simulations in the socio-economic field

Summary

BioDynaMo enables scientists to :

- develop models in various computational biology fields in a modular fashion
- obtain results rapidly with the high-performance execution engine
- scale up the model to billions of agents on a single server, and
- produce results that are in agreement with validated experimental data

Questions?

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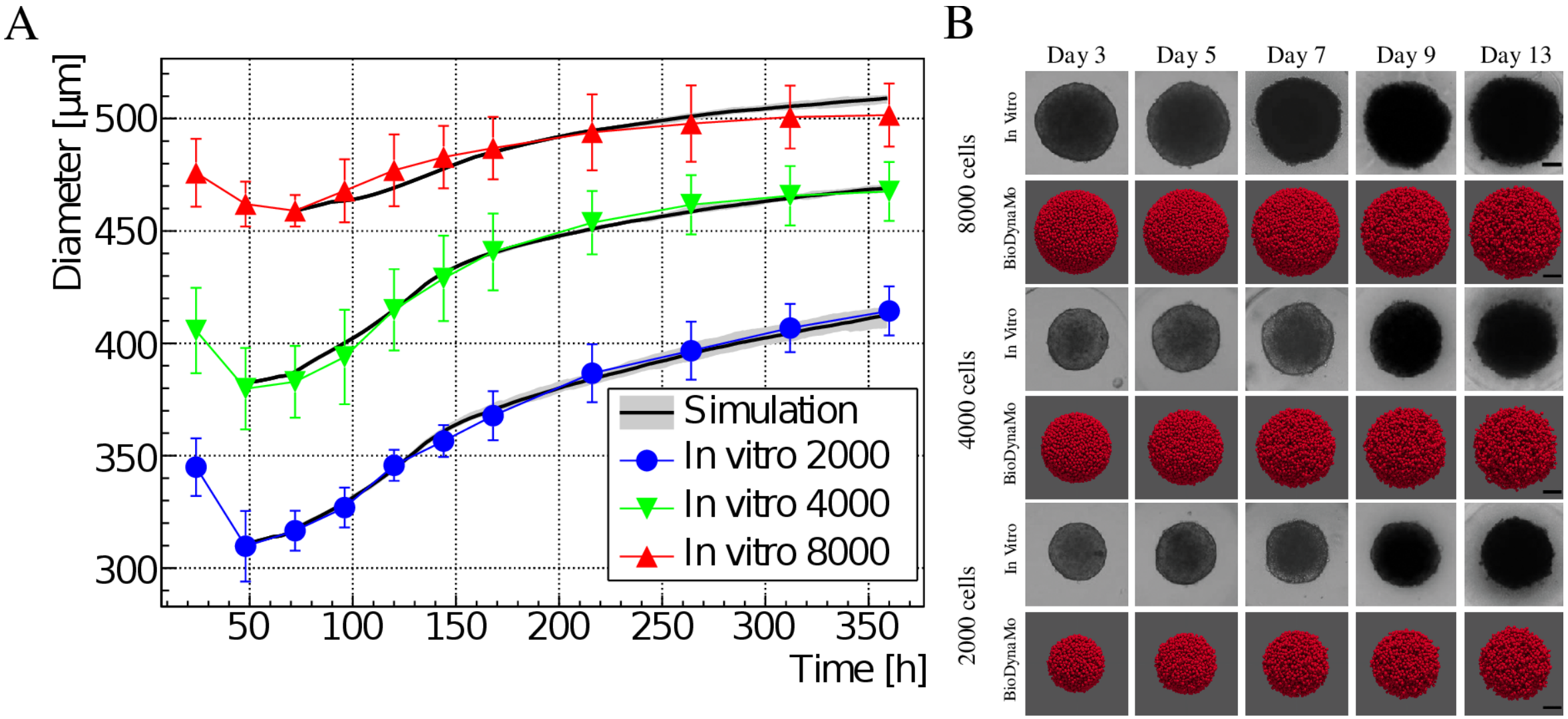
References

- Lukas Breitwieser, Ahmad Hesam, Jean de Montigny, Vasileios Vavourakis, Alexandros Iosif, Jack Jennings, Marcus Kaiser, Marco Manca, Alberto Di Meglio, Zaid Al-Ars, Fons Rademakers, Onur Mutlu, Roman Bauer
  BioDynaMo: A General Platform for Scalable Agent-based Simulation
  https://arxiv.org/abs/2006.06775, 5 February 2021.
- Project Website
  https://biodynamo.org/
- Source Code
  https://github.com/BioDynaMo/biodynamo
- Single-pyramidal cell simulation:
  https://www.youtube.com/watch?v=taWMFs5D5Pg
- Large-scale pyramidal cell simulation :
  https://www.youtube.com/watch?v=MA74wZbhO7w
- Tumor spheroid simulation :
  https://www.youtube.com/watch?v=Q9UkpLuLnkU

Appendix

Oncology Use Case



Further Information : Breitwieser et al. 2021