### Scalable solver for a multi-scale model of personalised breast cancer therapy

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# State of personalised medicine

- Data-driven approach Find the 'right' biomarkers, validate and apply
- Knowledge-driven approach
  - phenotypic
  - mechanistic







Multiple active regimens

# Clinical problem

Variation in response to therapy

Unpredictable toxicity



Mechanistic Mathematical Models of Treatment Response



## Multi-scale hybrid CA model







2000

2500

Time

3000

3500

4000

1500

100-

0.

τ

500

1000

FEC100 + Avastin

4500

# Testing optimal anti-angiogenetic drug dose



Lai et. al (2019), Cancer Research

# Simulating whole section of biopsy



2.4 million points numerical grid

12 weeks of treatment

Approx. 50 days in a single core

## Scalable solver for hybrid CA model

#### • Design goal:

- Simulating biologically relevant size in cluster environment
- Module-wise easy to implement and can be solved efficiently
- Balance between arithmetic and communication
- Reproducible
- Features
  - Modular design
  - FEniCS: efficient PDE solver framework with PETSc and ParMETIS backend
  - High-throughput-ready (sim\_db Simulation database)
  - Open MPI parallelisation
  - Minimal communication during discrete CA update
  - RNG for each cell ensuring reproducibility across different machine





### Heterogenous perfusion profile





## **Challenges and Outlook**

- Incorporate more (or fewer) tumour mechanisms
- Describe the multiscale dynamics better at a molecular model
- Systematically evaluate models against observational data Uncertainty quantification (Approx. Bayesian Computation)
- Improve PDE solver performance
- Generalisation of the hybrid model framework
- Better clinical trial Standardization of longitudinal data collection to fulfill the need of modelling
- Preprint soon!





#### simula



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#### Funding

BigInsight, Center for Research-Based Innovation (SFI) funded by Norwegian Research Council

PerCaThe, convergent environment funded by UiO:Life Sciences