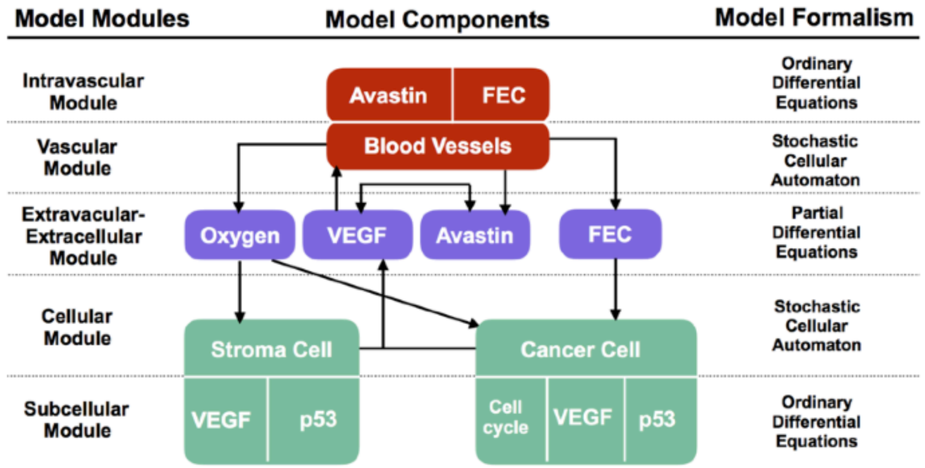
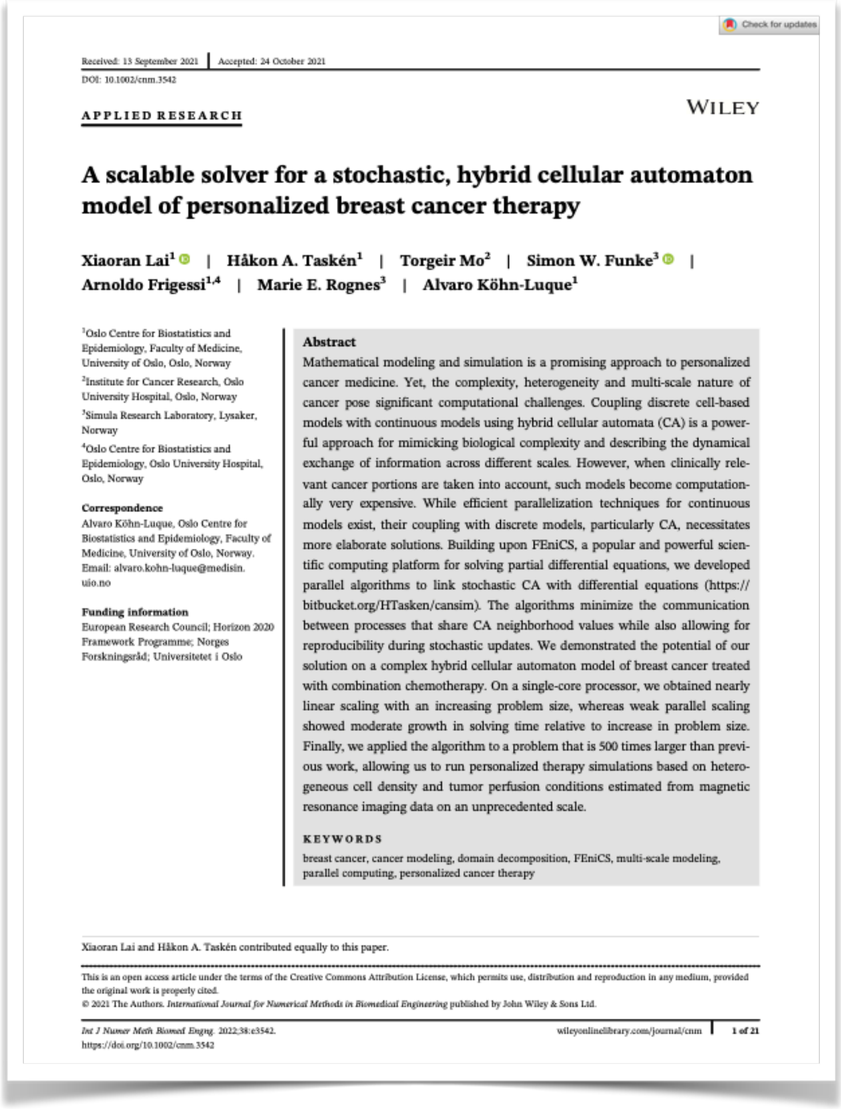
Case study

Cancer simulator

- Model for evolution of breast cancer treated with combination chemotherapy
- Describes the evolution of cancer cells, blood vessels, Oxygen,VEGF and Avastin





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APPLIED RESEARCH

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A scalable solver for a stochastic, hybrid cellular automaton model of personalized breast cancer therapy

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Abstract
Mathematical modeling and simulation is a promising approach to personalized cancer medicine. Yet, the complexity, heterogeneity and multi-scale nature of cancer pose significant computational challenges. Coupling discrete cell-based models with continuous models using hybrid cellular automata (CA) is a powerful approach for mimicking biological complexity and describing the dynamical exchange of information across different scales. However, when clinically relevant cancer portions are taken into account, such models become computationally very expensive. While efficient parallelization techniques for continuous models exist, their coupling with discrete models, particularly CA, necessitates more elaborate solutions. Building upon FEniCS, a popular and powerful scientific computing platform for solving partial differential equations, we developed parallel algorithms to link stochastic CA with differential equations (https://bitbucket.org/HTasken/cansim). The algorithms minimize the communication between processes that share CA neighborhood values while also allowing for reproducibility during stochastic updates. We demonstrated the potential of our solution on a complex hybrid cellular automaton model of breast cancer treated with combination chemotherapy. On a single-core processor, we obtained nearly linear scaling with an increasing problem size, whereas weak parallel scaling showed moderate growth in solving time relative to increase in problem size. Finally, we applied the algorithm to a problem that is 500 times larger than previous work, allowing us to run personalized therapy simulations based on heterogeneous cell density and tumor perfusion conditions estimated from magnetic resonance imaging data on an unprecedented scale.

KEYWORDS
breast cancer, cancer modeling, domain decomposition, FEniCS, multi-scale modeling, parallel computing, personalized cancer therapy

Xiaoran Lai and Håkon A. Taskén contributed equally to this paper.

Case study

Cancer simulator

- Model for the tumour has a large number of parameters
- Many of the parameters can be tuned via directly observing the patient
- In the inference problem we investigate two parameters
  - Sensitivity of cancer cells to the chemotherapy α
  - Minimal cell cycle length of cancer cells T_c