

## ABSTRACT FACE PAGE

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## MODULAR DESIGN OF MULTISCALE MODELS

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**BACKGROUND:** Reproducibility, usability, and extendibility of multiscale mathematical models are limited by transparency of the model structure, level of documentation, and dependencies across model components. Coding a model from scratch is often more time efficient than re-coding structure from a pre-existing implementation. Further, a high turnover rate of personnel in academic labs exacerbates difficulties of extendibility.

**METHODS:** Separating the dynamic processes into modules that communicate through a standardized interface minimizes interconnections, makes dependencies transparent, and offers an innovative model-building paradigm that addresses the above problems. As a proof-of-concept, we are developing such a design applied to an agent-based model of the innate immune response to fungal pathogens in the lung. In the new structure, a global-state variable that contains data about the simulation space (alveolar duct geometry) and all agents within it (immune cells, fungal spores, hyphae, etc.) is separated from the computations that update it. Each functional module corresponds to an agent type that is responsible only for initializing and modifying the subset of global data related to that agent using a standardized interface. For example, the macrophage module adds and removes macrophages to the simulation space and updates their respective states.

**RESULTS:** Major advantages of the modular implementation are that dependencies between modules are reduced and the tissue geometry contains no functional properties, so adding, deleting, or replacing modules and changing tissue geometry become trivial. Using this structure, simulations can be run for multiple biological variants with any subset of modules or module versions.

**CONCLUSIONS:** The framework allows for crowdsourcing of modeling efforts and its flexibility allows for a wide range of applications in modeling disease.

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