

Model Credibility - A modular approach to multiscale modeling of the innate immune response to invasive aspergillosis



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Summary

Core Principles

Accessibility

- Software that is hard to use is hard to test
- Model must be easy to use by a non-computer scientist
- Carefully identify system specifications, and guarantee functionality on systems meeting specs
- "Wet lab" team will be first testers/validators, community-based approach to post-release validation
- Strong visualization component and high performance essential in to facilitate engagement

Transparency

- All source published in whole as early as possible to allow anyone to inspect/ challenge model
- Strict usage of version control to allow free inspection of past iterations and permit easy branching & modification

Standardization

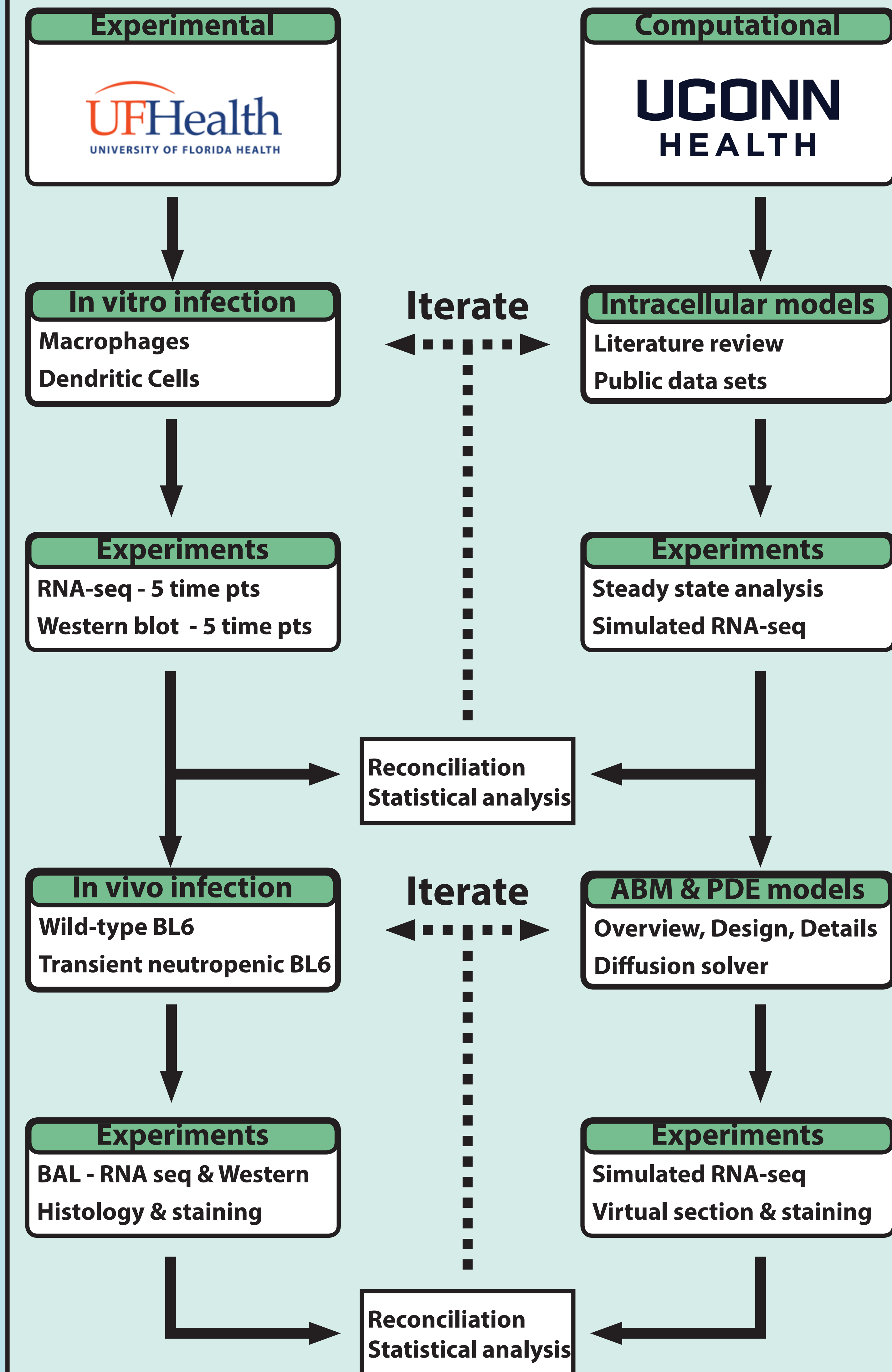
- Agent-based model (tissue-level) specified by Overview, Design Concepts, Details (ODD) protocol
- Boolean network-based model and finite state machine (FSM) specified for intracellular level
- Source code strictly adherent to ISO standards - e.g. C99, Fortran 90, VHDL-93

Delegation

- Three main teams with domain experts:
 - **Computation** (UConn Health)
 - **Experimentation/testing** (UFHealth)
 - **Visualization/UI** (Kitware, Inc.)
- Each team performs detailed uncertainty & validation - e.g. precision estimates for computation, biological/technical replicates for wet lab, I/O functionality for visualization
- Teams work in parallel on design, test, iterate cycles with weekly discussions and shared digital lab notebook

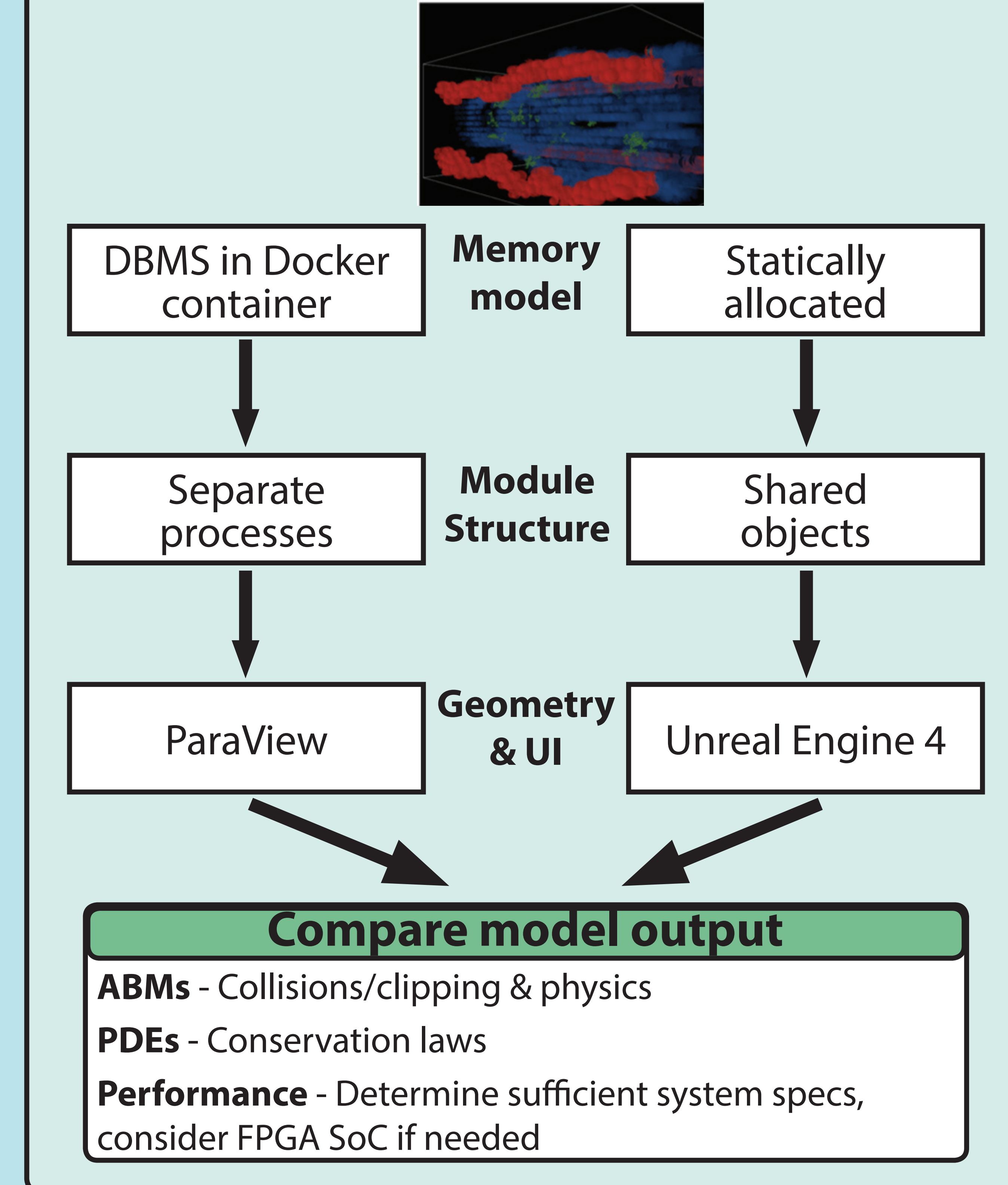
Parallel Design Approach

Two sites: Experimental/Clinical & Mathematical/Computational



Competing Implementations

Two paths: High-level & Mid-level
Initial evaluations using previously published model



Crossover validation

