

Draft Computational M&S Workflow

1. Domain and Context
 - 1.1. Specify the biomedical R&D context - e.g. [fracture union/nonunion in adults](#)
 - 1.2. Describe broad biomedical issues/questions/needs
 - 1.3. Identify referent experimental systems
 - 1.4. From a very broadly computational M&S perspective: how is it envisioned that M&S approaches may contribute to 1.2?
2. Objectives
 - 2.1. Spanning wet-lab and computational M&S perspective: state scientific objectives (immediate, near-term, longer-term)
 - 2.2. From a broad M&S perspective: what model usage type might be needed to approach 1.4? E.g.: predictive, analysis, heuristic, reproduce another lab's computational M&S work, challenge a hypothesis, etc.
 - 2.3. What criteria will be used to recognize outcomes (that progress is being made in achieving 2.1? E.g.: visualizations, validations, falsified hypotheses, iteration logging, etc.
3. Usage patterns (a pattern = similar use cases)
 - 3.1. Identify wet-lab experimental system usage patterns from 1.3
 - 3.2. Detail planned & envisioned (immediate, near-term, longer-term) model usage patterns
 - 3.3. Identify targeted attributes (TAs)
 - 3.4. How will 3.2 synergize with 3.1?
 - 3.5. Metrics: for a given usage pattern, how will model outputs and TAs be mapped to outcome criteria?
 - 3.6. Design concrete verification cases for each usage pattern.
4. Survey
 - 4.1. What prior modeling approaches have been used for one or more usage pattern from (3)?
 - 4.2. Can an available (external or internal) model be repurposed?
 - 4.3. Given (2) & (3), are there standard formats and model structures? Should they be adopted?
5. Requirements
 - 5.1. Given 2–4, list immediate, near-term, and longer-term requirements
6. Implementation
 - 6.1. Decide on M&S approaches and structures needed to actualize (3) & (5).
temporary end