Perspectives on Sharing Models and Related Resources in Computational Biomechanics Research

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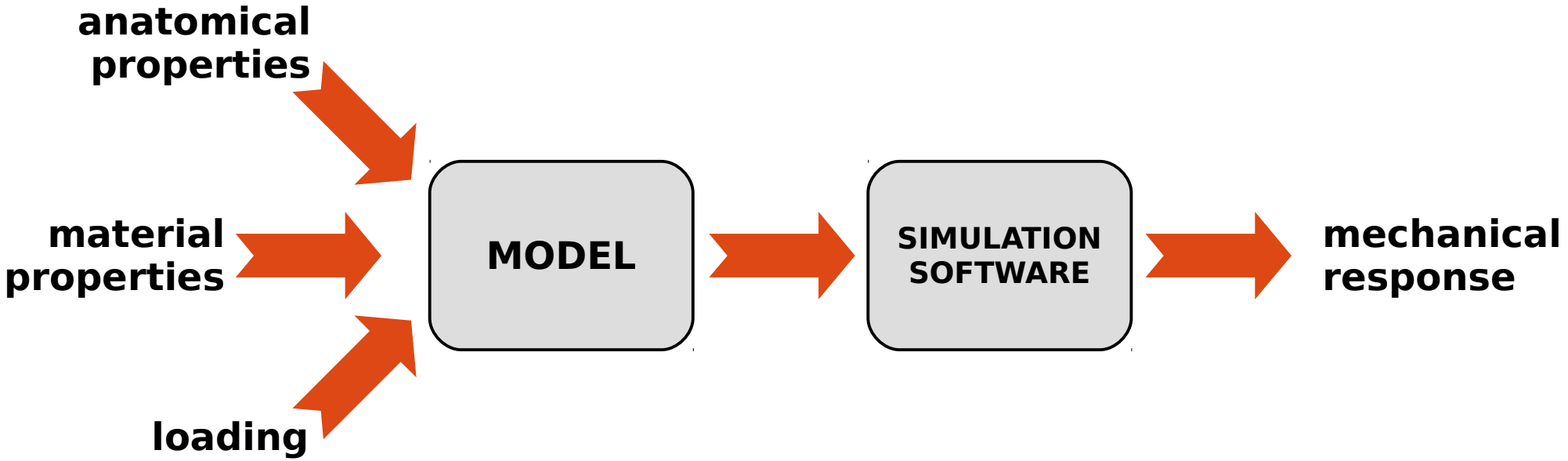
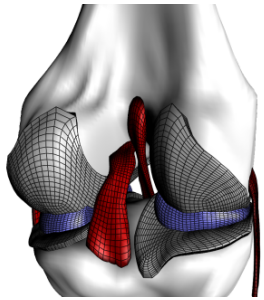
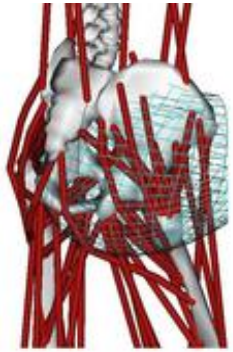
M&S WORKFLOW IN BIOMECHANICS



CHALLENGES OF SHARING





What, where, when, how?
Multi-level information

- Raw data
  medical imaging
  physiology
- Derivative data
  segmentation / geometry
  constitutive relations
- Model components
  mesh
  constitutive models
- Working model
- Simulation software
  binary or source code
- Simulation results

Issues

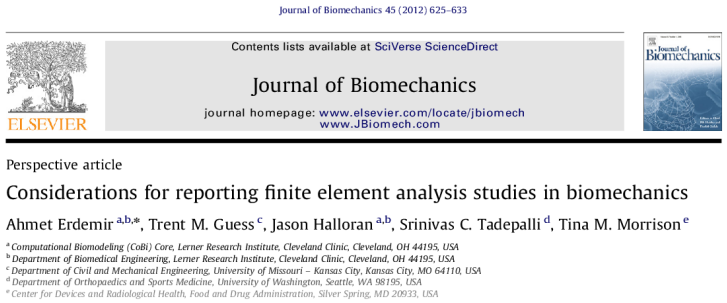
- Heterogeneous data
- Fragmented formats
- Detached model description and phenomena formulation
- Large variety of simulation software
- Mark-ups specific to software
- Coupled models - multiscale, multiphysics
- Nested models - constitutive

OpenSim FEBio python ABAQUS SimVascular MATLAB

SHARE TO REPRODUCE & REUSE

Publish
~80 reporting parameters

- Model identification
- Model structure
- Simulation structure
- Verification
- Validation
- Availability



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journal homepage: www.elsevier.com/locate/jbiomech
www.JBiomech.com

Perspective article

Considerations for reporting finite element analysis studies in biomechanics

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adapted from Erdemir et al. (2012)

VS

Share model

- To examine formal description
- To repeat simulations
- To customize
- Exact, complete, usable

Share software

- To examine formulation
- To repeat simulations
- Describes phenomena

Share data

- To reproduce modeling
- Grounding

HISTORICAL BACKGROUND

2006

Tissue Mechanics Working Group

Discussions in working groups
e.g., Journal for Dissemination

Model Sharing Working Group

Biomechanics Working Group

2010

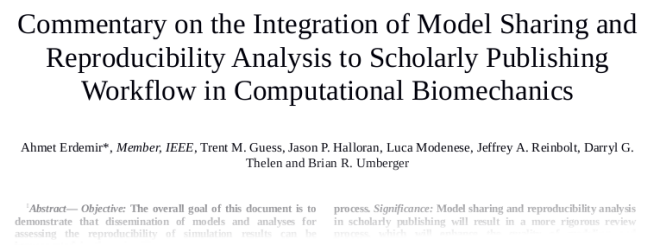
Committee on Credible Practice of Modeling & Simulation in Healthcare

2014

IEEE EMBS Computational Biology and the Physiome Technical Committee

WCB 2014 Journal Editors Meeting

IEEE Special Section on Model Reproducibility & Sharing


Commentary on the Integration of Model Sharing and Reproducibility Analysis to Scholarly Publishing Workflow in Computational Biomechanics

Ahmet Erdemir*, *Member, IEEE*, Trent M. Guess, Jason P. Halloran, Luca Modenese, Jeffrey A. Reinbolt, Darryl G. Thelen and Brian R. Umberger

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ARTICLE

Journal of Biomechanical Engineering

Expert View

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Perspectives on Sharing Models and Related Resources in Computational Biomechanics Research

The role of computational modeling for biomechanics research and related clinical care will be increasingly prominent. The biomechanics community has been developing computational models routinely for exploration of the mechanics and mechanobiology of diverse biological structures. As a result, a large array of models, data, and discipline-specific simulation software has emerged to support endeavors in computational biomechanics. Sharing computational models and related data and simulation software has first

Erdemir A, Hunter PJ, Holzapfel GA, Loew LM, Middleton J, Jacobs CR, Nithiarasu P, Löhner R, Wei G, Winkelstein BA, Barocas VH, Guilak F, Ku JP, Hicks JL, Delp SL, Sacks M, Weiss JA, Ateshian GA, Maas SA, McCulloch AD, Peng GCY. *Perspectives on Sharing Models and Related Resources in Computational Biomechanics Research*. J Biomech Eng. 2018; 140(2), 024701. **http://dx.doi.org/10.1115/1.4038768**.

GOALS

- To document current **perspectives** in **biomechanics community** for **sharing** of computational models and related resources

  Journal editors
  Key stakeholders, e.g., resource providers

- To identify **commonalities** and **differences** of **opinions** in regard to model sharing in biomechanics

- To understand potential impact of model sharing on **reproducibility** and **reuse**

SOLICITATION OF PERSPECTIVES

Invitation to

- 8 groups of journal editors
  primarily biomechanics
- 6 stakeholders from community
  resource providers in biomechanics

Invitation for

- 300-500 words opinion piece
  plus references
- To be published verbatim

Opinion pieces to consider

- opportunities, challenges, success stories
- incorporating model sharing into scientific workflow
- impact on of research, translation, training
- envision a sustainable ecosystem

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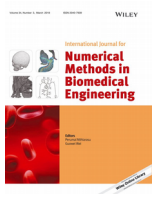

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THEMES FROM CONTRIBUTORS

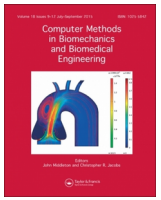
Clarity on terminology
Role of standards
Need for databases

Need for increased ability
Journal tools for rich content
Evolve standards of reporting
Associating data to manuscripts

Journal guidance
Use of repositories or supporting materials
Avoiding rigid requirements

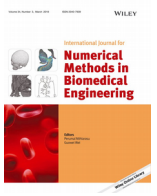
Examples of impact of sharing
Available infrastructure
Cultural and behavioral issues
Academia's award structure
Need for leaders

Challenges of reproducing FEA
Concerns about source code



Initiative for a library
Potential workflow for sharing

Benchmarking before sharing
Sharing with all inputs
Special issue on benchmarking
Need for standard for sharing



Requirements from simulation software end
Interacting with infrastructure
Commitment to facilitate model sharing

Fragmentation of journal requirements
Varying format requirements
Definition of a sharable model
Sustainable archiving

Available infrastructure
Available simulation software
Multiple domain/physics/scale integration

CONSOLIDATION & CONSIDERATIONS

Benefits of sharing

- assessment of reproducibility
- innovation by reuse
- repurpose for new publications
- training
  new method
  modeling technique
- outreach
  downloads and visibility

Extent of sharing

- complete model markup
- foundational data
- simulation software
  if model is not standalone
- submodels
- simulation results
- simpler models with similar abstraction

Platforms for sharing

- federally funded & publicly available repositories
- journal sites
  supplementary material
- general purpose data repositories
- institutional sites
- laboratory sites
- dedicated sites

CONSOLIDATION & CONSIDERATIONS

Support from Journals

- supplementary material
- recommendation to use existing repositories
- online journal tools for rich content
- encouragement to use and evolve existing standards
- digital object identifiers
- clarify terminology

Burden of sharing - infrastructure

- development, maintenance, expansion
- repositories that co-exist and cross-reference
- centralized curation
- access to simulation software
- components for coupled simulations

Burden of sharing – developers, users, reviewers

- prepare & disseminate
- maintain packages
- document model
- review markup
- repeat simulations

CONSOLIDATION & CONSIDERATIONS

Risk of sharing

- low quality of models
- controlled release
  benchmark & disseminate
  time delays
- early release
  disseminate & certify
  balance quality vs early adoption

Management of intellectual property

- incompatible licensing
  when blending models
  model vs simulation software
- unintentional limitations on broad dissemination
- pay wall problem

Promotion of sharing

- incentives and recognition
  self-motivated
  visibility and increased citations
- mandates
  journals & funding agencies
- need for official recognition
  academic promotion
  awards

IN SUMMARY

Where are we now?

- **Value** of model sharing for reproducibility and reuse
- **Examples** of model, data, and software sharing
- Availability of **infrastructure**
- Support from **journals** - editorial and infrastructure

Yet

- Difficulties to recognize model sharing as a common component of scholarly workflow remain

What can we do

- Promote and demonstrate model sharing and its utility
- Try new strategies
- Communicate in an organized fashion

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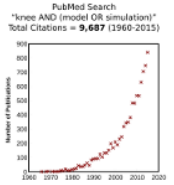
A collaborative pathway to establish credible practice of modeling and simulation in knee biomechanics in conformance with community recommendations

by Erdemir, Besier, Imhauser, Laz, Morrison, Shelburne, Halloran

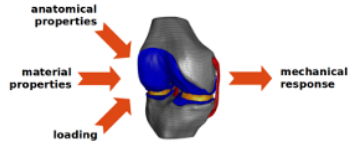
BACKGROUND

Computational modeling and simulation (M&S) has become a routine strategy in knee biomechanics for

- scientific knowledge
  joint and tissue function
  impact of pathology
  injury mechanisms
  surgical interventions
- clinical guidance
  osteoarthritis
  meniscal tears
  ligament injuries
  joint pain
  rehabilitation



Abstraction and fundamental components of knee M&S to explore biomechanical function are unified.



Implementation of knee M&S, however, is highly fragmented due to modelers' decisions, specifically their art.

*Do the **predictions** of natural knee biomechanics **depend** on **modeling decisions** of separate development teams **when** the target simulation scenarios and the **source data** to build models remain the **same**?*

Our multi-team collaboration aims to understand the **"art"** of M&S in knee biomechanics:

- To quantify the influence of variations in M&S workflows on the reproducibility of joint level predictions
- To quantify the influence of variations in M&S workflows on the reproducibility of tissue level predictions

This document establishes the correspondence between the design of our **reproducibility study on knee M&S** and the broad **guidance** from biomedical community **on credible practice of M&S**.

- To summarize our study design to understand, document, and review multiple M&S workflows in knee biomechanics.
- To establish mapping of the components of our knee M&S project to Ten "Not" So Simple Rules of Credible Practice of M&S in healthcare.

TEN "NOT SO" SIMPLE RULES

By Committee on Credible Practice of Modeling & Simulation in Healthcare.
To learn more about the Committee, refer to https://simtk.org/plugins/moinmoin/cpms/

1. *Define context clearly* — Plan and develop the M&S activity with clear definition of the intended purpose or context accommodating end-users needs.
2. *Use appropriate data* — Use data relevant to the M&S activity, which can ideally be traced back to the source.
3. *Evaluate within context* — Evaluate the M&S activity through verification & validation, uncertainty quantification, and sensitivity analysis faithful to the context/purpose/scope of the M&S efforts, with clear and a-priori definition of evaluation metrics and including test cases.
4. *List limitations explicitly* — Provide an explicit disclaimer on the limitations of the M&S to indicate under what conditions or applications the M&S may or may not be relied on.
5. *Use version control* — Implement a version control system to trace the time history of the M&S activities, including delineation of contributors' efforts.
6. *Document adequately* — Document all M&S activities, including simulation code, model markup, scope and intended use of M&S activities, users' and developers' guides.
7. *Disseminate broadly* — Disseminate appropriate components of M&S activities, including simulation software, models, simulation scenarios and results.
8. *Get independent reviews* — Have the M&S activity reviewed by independent third-party users and developers, essentially by any interested member of the community.
9. *Test competing implementations* — Use competition of multiple implementations to check the conclusions of different implementations of the M&S processes against each other.
10. *Conform to standards* — Adopt and promote generally applicable and discipline specific operating procedures, guidelines, and standards accepted as best practices.

For additional details, refer to Erdemir, A., Mulugeta, L. and Lytton, W. W. Ten "not so" simple rules for credible practice of modeling and simulation in healthcare: a multidisciplinary committee perspective. 2015 Biomedical Engineering Society / Food and Drug Administration Frontiers in Medical Devices Conference: Innovations in Modeling and Simulation, May 18-20, 2015, Washington, DC.

DATA

Reuse of existing data on knee anatomy and mechanics

1 knee from Open Knee(s)
- 8 cadaver knees from 8 donors
- Medical imaging (MRI)
- Joint kinematics-kinetics
- Tissue testing

1 knee from Natural Knee Data
- 7 cadaver knees from 5 donors
- Medical imaging (CT, MRI)
- Joint kinematics-kinetics

Open Knee(s)

Natural Knee Data

M&S PHASE: CALIBRATION

Start with

Initial specimen-specific knee model
Specimen-specific joint kinematics-kinetics
- laxity datasets
Literature

Deliver

Calibrated specimen-specific knee model
Calibration fit error (before & after)
Loading and boundary conditions
Changes in anatomical representation
Changes in tissue representation

M&S PHASE: REUSE

Start with

Benchmarked specimen-specific knee model
Simulation cases
- Passive flexion
- Pivot shift
- Weight-bearing standing (x-ray)
- Sit-to-stand motion

Deliver

Loading and boundary conditions
Joint mechanics predictions
Tissue mechanics predictions

OPERATING PROCEDURES
(for each M&S phase)

Group consensus on
- Deliverables
- Earmarked specimen-specific data

Activities of individual teams to
- Prepare specifications
- Submit/disseminate specifications
- Execute specifications
- Document protocol deviations
- Submit/disseminate protocol deviations
- Submit/disseminate deliverables
- Submit cost estimate

Group review (completeness) of
- Specifications
- Protocol deviations
- Deliverables
- Costs

M&S PHASE: DEVELOPMENT

Start with

Specimen-specific medial imaging datasets
Literature

Deliver

Initial specimen-specific knee model

Representation of anatomy
- Segmentation
- Geometry
- Mesh

Representation of tissue behavior
- Constitutive models
- Tissue stress-strain response
- Tissue bulk response

5 M&S teams

M&S PHASE: BENCHMARKING

Start with

Calibrated specimen-specific knee model
Specimen-specific joint kinematics-kinetics
- combined loading datasets
- datasets from resected joint

Deliver

Benchmarked specimen-specific knee model
Benchmark error
Loading and boundary conditions

THIRD-PARTY REVIEW & COMPARISON

Deliverables
- Models
- Model components
- Simulation results

Modeling & simulation workflows
- Specifications
- Protocol deviations
- Reporting

Predictive capacity
- Calibration results
- Benchmarking results

Model reuse credibility and criticality assessment

collaboration with US FDA for independent review

POSTER GOALS

STUDY DESIGN ON "ART" OF MODELING

From project Reproducibility in Simulation-Based Prediction of Natural Knee Mechanics.
For a copy of the grant proposal, refer to https://simtk.org/svn/kneehub/doc/grant_resubmission.pdf.

Project Title: Reproducibility in simulation-based prediction of natural knee mechanics
Project Funding: NIBIB, NIH (R01EB024573; PI: Erdemir)
Project Website: https://simtk.org/projects/kneehub
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