White Paper #4: Reporting Finite Element Analysis Studies of Biological Structures

Ahmet Erdemir
Computational Biomodeling Core
Department of Biomedical Engineering
Lerner Research Institute
Cleveland Clinic

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Virtual Discussion
IMAG – MSM 2010

CREDITS

Trent Guess
Jason Halloran
Srinivas Tadepalli
Ganesh Thiagarajan

Working Group 6 members
Working Group 10 members

IMAG members
Biomechanics community

Efficient Methods for Multi-Domain Biomechanical Simulations
R01EB006735

Predicting Cell Deformation from Body Level Mechanical Loads
R01EB009643

Online Access

Online editable version of the white paper

http://www.imagwiki.org/mediawiki/index.php?title=Reporting_in_FEA

Discussion on the white paper

http://www.imagwiki.org/mediawiki/index.php?title=Talk:Reporting_in_FEA

Definitions: Model

The term model in this white paper refers to a **computational model**.

Computational representation of the biological structure for finite element analysis:

- discretized geometric representation
- constitutive relationships of substructures
- interactions between substructures
- loading and boundary conditions

The computational model relies on the

- **mathematical model** – principles of solid mechanics
- **biological model** – deformation of biological structures

For detailed model definitions refer to MSM 2010 – White Paper #1 by Glazier et al.

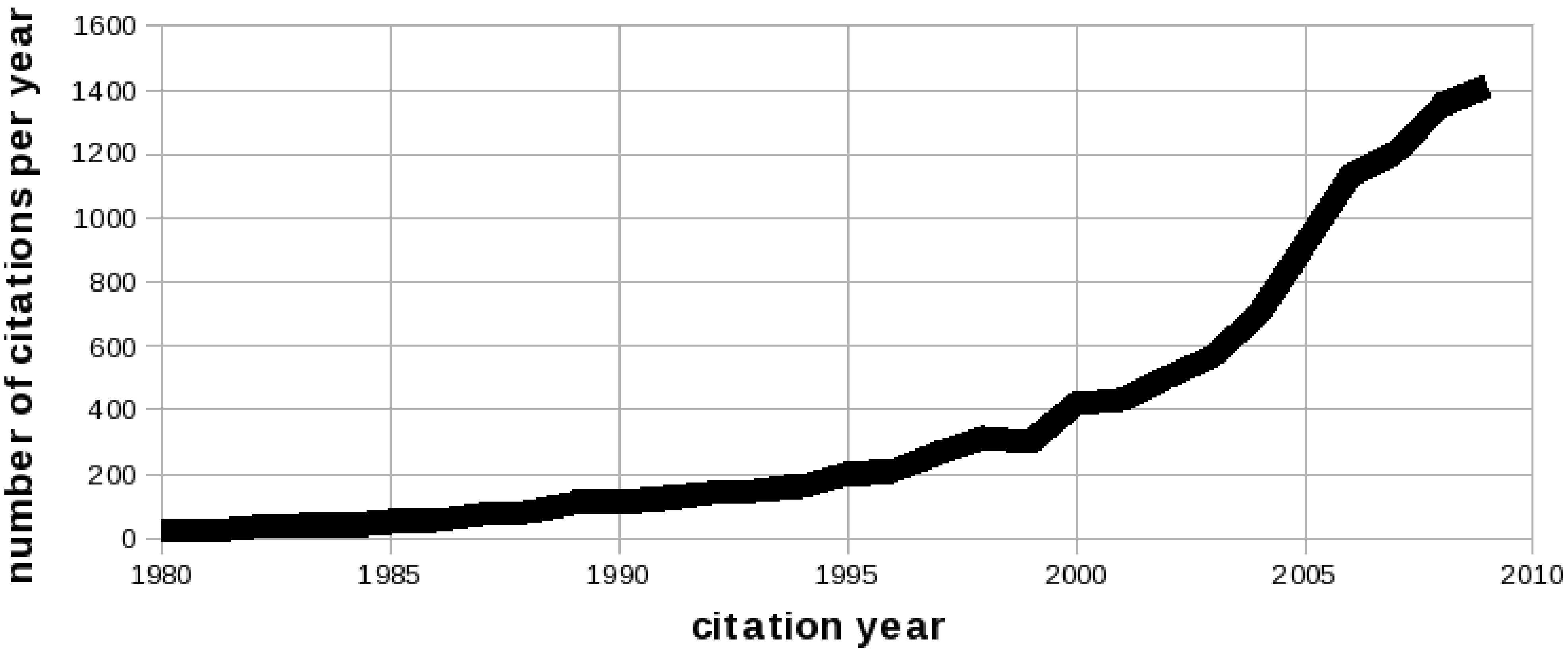
Definitions: Multiscale

The term multiscale in this white paper refers to **interactions between higher spatial scales** of the physiome:

joint/organ biomechanics – tissue mechanics
tissue mechanics – cell biomechanics

For cell scale to macro scale integration refer to MSM 2010 – White Paper #2 by Lin et al.

FEA in Medicine



Search conducted on Pubmed (http://www.pubmed.org) with the search string "finite element".

Why Recommendations for Reporting?

Good reporting practice:

clarifies uncertainty of **reproducibility**
promotes **reusability**
establishes **accountability**

---> CONFIDENCE IN MODELING & SIMULATION

Adequate reporting procedures has the potential to **delineate model and simulation process**.

PATHWAY TO SHARING AND STANDARDS

Why Recommendations for Reporting?

Advances in complex model development and simulation **software** facilitates modeling and simulation but

- Modeler's decision making process is usually **opaque**
- Modeler is sometimes **uninformed**
- Reader/user/reviewer is mostly **uninformed**

Codes & standards for verification & validation are helpful but they

- do not address communication
- are not easy to follow

NEED FOR A CHECKLIST TO BE UTILIZED NOW

Why Recommendations for FEA?

Common tool for simulation of models representative of body/organ/tissue/cell scales

Unfortunately, **models are tightly coupled** to the method of **simulation**

- mathematical models embedded in FEA software
- FEA software specifically designed for biological phenomena
- models sometimes accommodate solver capabilities
- too many simulation software -> too many mark-up languages

Current standards are not readily applicable to complex biomechanical models, need a solution

- to use now
- to inform future

Why Initial Focus on Single Scale?

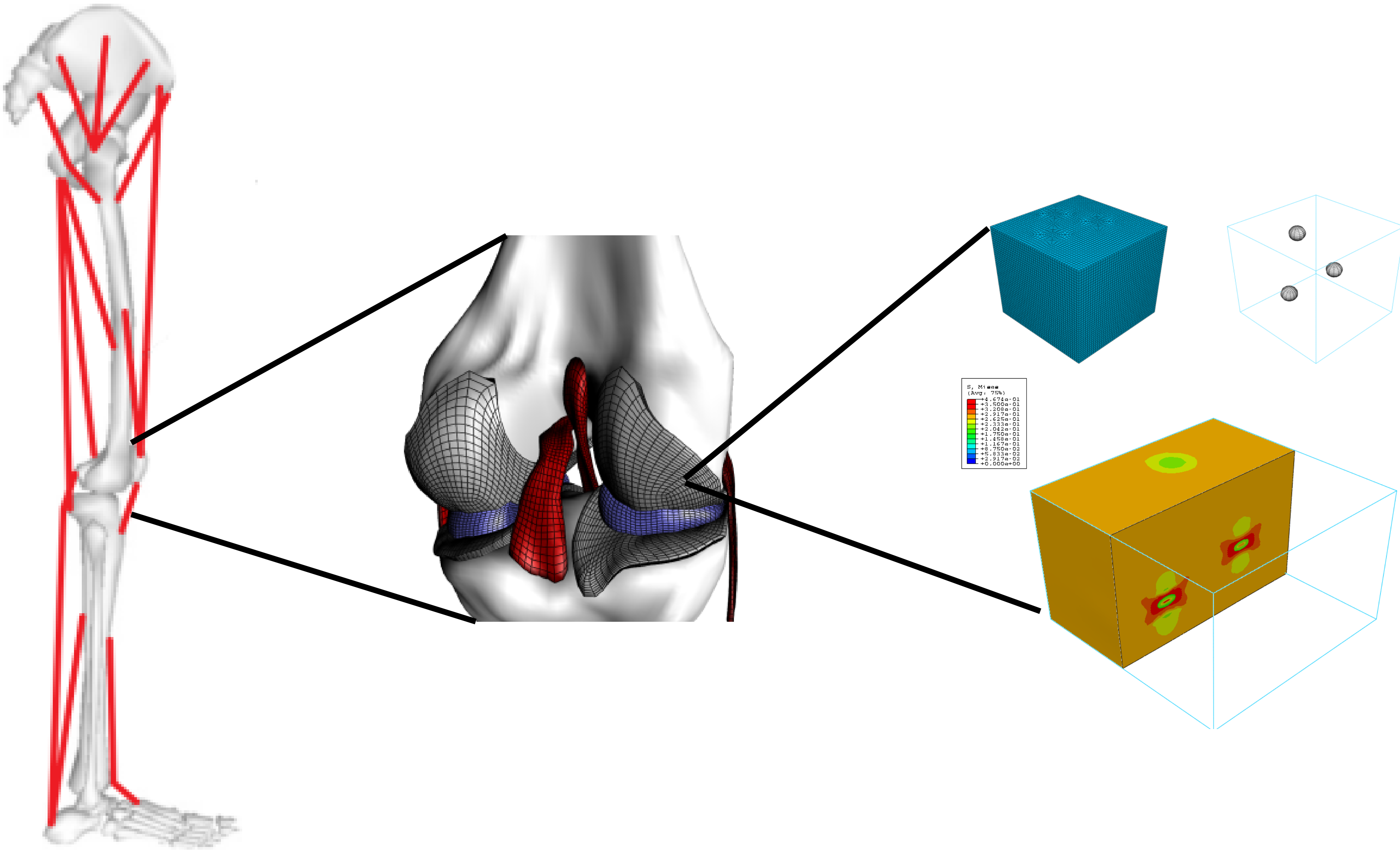
Models of a single spatial scale were and potentially will be used for

- decision making
- surgical simulation
- intervention design
- regulatory practice

Models of a single spatial scale will likely be

- reused in multiscale simulations
- dictate response at higher spatial scales

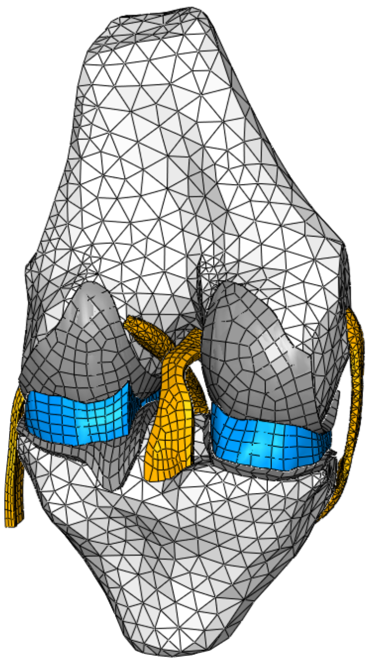
Relevance to Multiscale Analysis



For cell scale to macro scale integration refer to MSM 2010 – White Paper #2 by Lin et al.

Relevance to Modular Modeling

Joint Scale

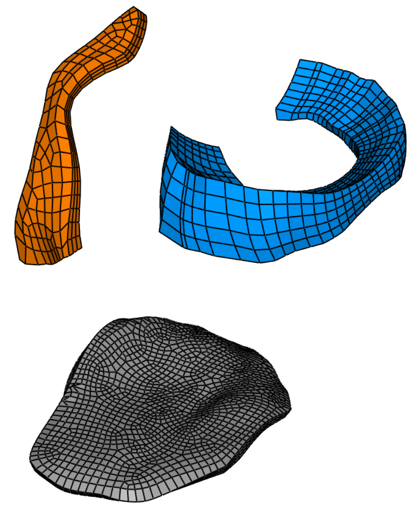


Input/Output:
kinematics/kinetics

Properties:
tissue organization

Module to:
musculoskeletal models

Tissue Scale

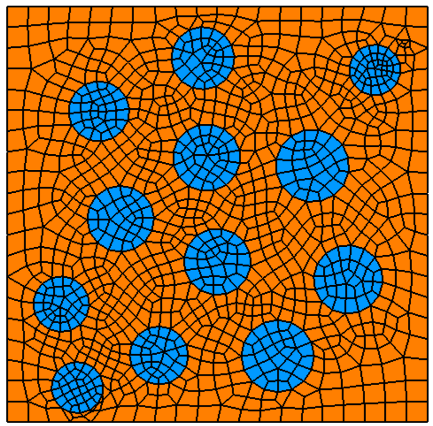


Input/Output:
loading & BCs (attachment)
tissue deformation

Properties:
constitutive relation

Module to:
joint models

Cell Scale



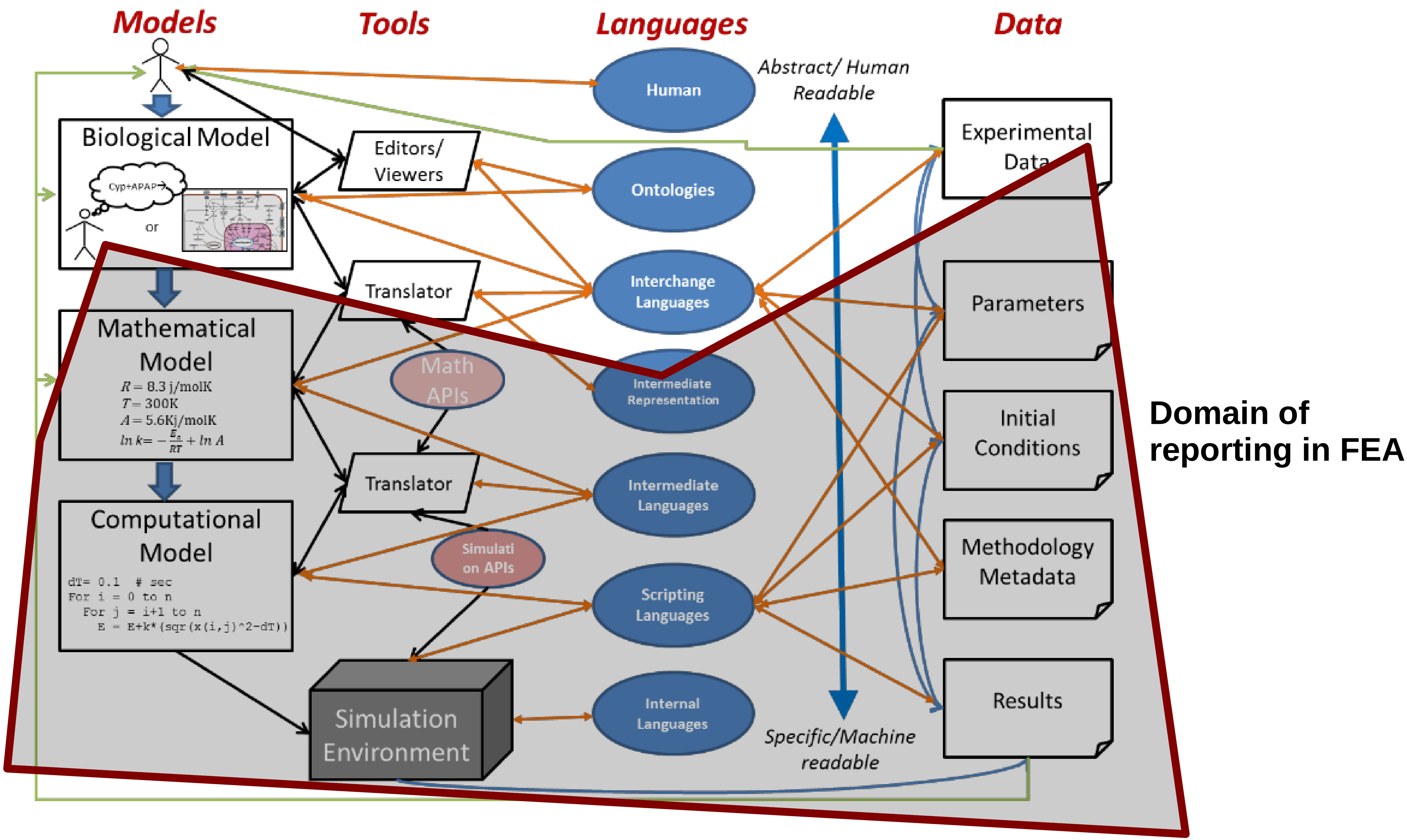
Input/Output:
constitutive relation
microstructural deformation

Properties:
microstructural organization

Module to:
tissue models

For modular modeling refer to MSM 2010 – White Paper #3 by Bassingthwaighte et al.

Relevance to Model Abstraction



For levels of model abstraction refer to MSM 2010 – White Paper #1 by Glazier et al.

Relevance to Mark-Up Languages

Identify information to incorporate as metadata for storage of models and simulation results

Generate specifics for mark-up languages to extract key model information (automated-reporting)

Clarify model exchange parameters to translate between open mark-up languages and commercial ones used by proprietary simulation software

Implementation

For a model to be useful

the model itself does not need to be complete

the **reporting** of the model should be

complete
explicit

Adaptations of **standards for model sharing and unified simulations** should be a **long term goal** but it may not be practical

Adaptation of **reporting standards** can be implemented **at this moment** and facilitate transition to higher level modeling standards

A Spin-Off from Standards Proposal

Checklist of model standards

CHECKLIST FOR MODEL AGAINST DESIRED STANDARDS: CHECK X FOR THOSE MET			
Check YES (either manual or auto if standard met)	YES		
model author = checked by author; checked within model code by math?	model author	checked in code?	Problem? Limit? Other?.
Group 1: Identification and Description			
1. Model Name, Key words (generic and specific)			
2, Brief one or two line description			
3. Detailed description, diagrams, equations			
4. Reference to Publication describing the model			
5. Pointer to the publication or pdf			
6. Related Models, antecedents, comparables, and successors			
Group 2. Model Structure and Content			
1. Domain definition (cells, mito, tissues, organ system, organism)			
2. Main variables (chemicals, pressures, etc.), with units			
3. Parameters, with units, and with source references			
4. Descriptions and references for subsidiary models			
5. Source Code: Clear, deeply commented, explained, referenced.			
6. Inputs and outputs defined. All nodes and edges defined.			
7. Define linkage type (Chemical, electrical, mechanical,etc.)			
8. Ontology base for notation			
9. Numerical solvers used, and conditions set			
Group 3. Verification: math of model and solution methods are sound			
1. Unitary Balance: (units on all variables and parameters)			
2. Mass balance: (list constituents whose conservation is checked)			
3. Charge balance: (ion currents, membrane potential)			
4. Osmotic balance: (volume, total activities, fluxes)			
5. Thermodynamic Balance (Haldane constraints on reactions)			
6. All equations correct, units balance, with all terms defined			
7. Numerical solutions checked against analytical solutions			
8. Running code supplied in a common format			
9. Solutions show little dependence on time or space step size			
10. Methods for verification defined. Reference model solution?			
Group 4. Validation: model is physiologically realistic			
1. Initial and boundary conditions in accord with physiology			
2. Data provided, and fitted by model			
3. Model is predictive, shown to fit other data not used as basis			
4. Parameters justified (sources provided) and evaluated			
Group 5: Availability of Source Code and Forum for critiques			
1. Website source from which to download model code and data			
2. Website or email or address to accept queries			
3. Website for public commentary and responses			
4. References to subsequent publications or alternative models			
Revised 12sep09 by JBBassingthwaighte			

Working Group 10

Standards for Modeling

Targeted at biophysical/biochemical models

Customized for complex biomechanical models simulated using finite element analysis

Customized for model reporting rather than model development

For the WG10 Standards Proposal, refer to http://www.imagwiki.org/mediawiki/index.php?title=Working_Group_10#Standards_Proposal.

Single Scale

Identification & Description

- Model name, keywords (generic and specific)
- Version
- Simulation software
- Brief description
- Summary of utility
- Summary of highlights
- Summary of limitations
- Reference to publication
- Pointer to publication
- Related models

Single Scale

Model Structure & Content

- Physics and domains
- Assumptions
- Loading and boundary conditions
- Primary output variables
- Secondary output variables
- Reference configuration
- Components (subsidiary models)
  - Geometry
  - Mesh
  - Constitutive relationships
- Interactions
  - Interacting components
  - Interaction properties
- Solution strategy
- Simulation settings

Single Scale

Verification

Methods of verification

Correctness of formulation

Comparisons with analytical solutions

Sensitivity to simulation settings

Mesh convergence

Assessment of repeatability

Single Scale

Validation

Physiological relevance of loading and BCs

Justification of parameters

Data used for model development

Data used for model comparison

Validation procedures (direct, indirect)

Sensitivity analysis

Predictive capacity

Single Scale

Availability

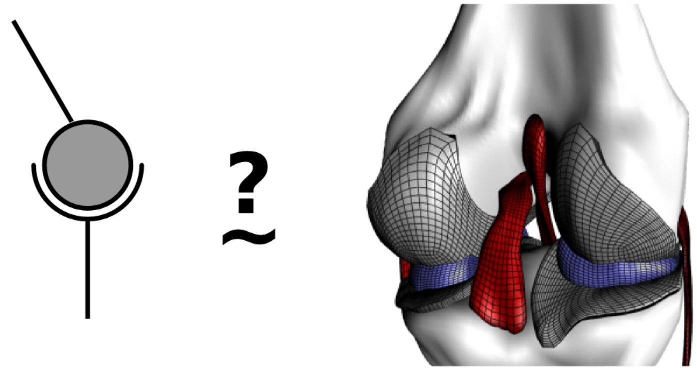
- Website for downloads
- Website (or contact) for queries
- Website for public commentary, responses, and rating
- Licensing
- Follow-up

Multiscale Issues

Mechanical Consistency

Post-processing problem

Equivalence between higher and lower scale representations

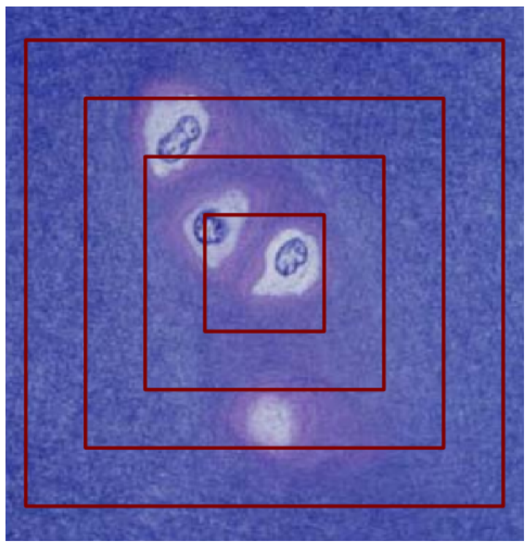


Representative Volume Element Convergence

Underlying geometry

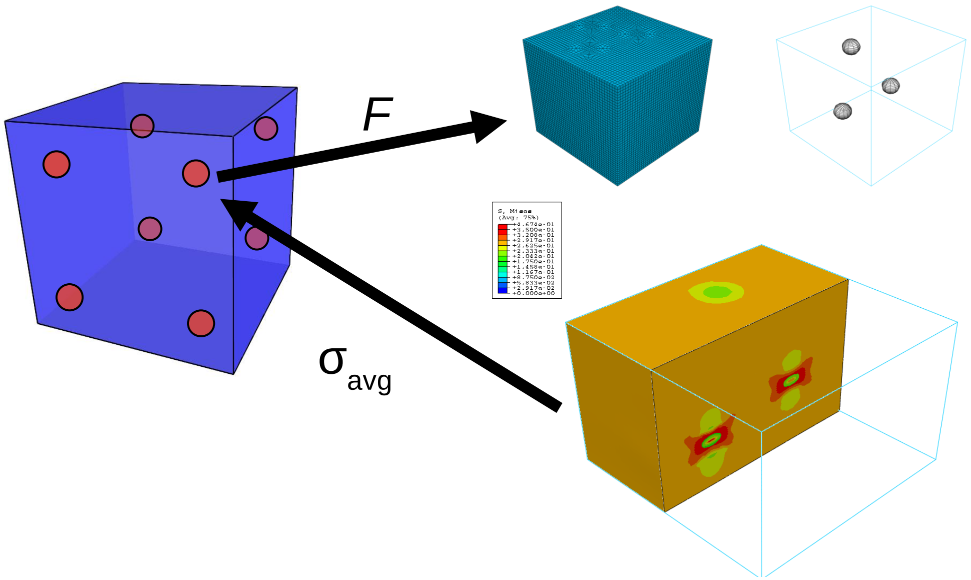
Constitutive response

Variable of interest



Multiscale Issues

Scale Separation



Assumptions of computational homogenization

Assumptions of post-processing

Modularity

Assumptions for hierarchical coupling

Case Study

Fill-in form to illustrate and understand boundaries of a given model

Yao J, Snibbe J, Maloney M, Lerner AL. Stresses and strains in the medial meniscus of an ACL deficient knee under anterior loading: a finite element analysis with image-based experimental validation. J Biomech Eng. 2006 Feb;128(1):135-41.

Short-Term Directions

Collaborative evolution and adoption by

- investigators
- journals
- funding agencies
- societies

to

- document
- review

with the ultimate goal of establishing

- confidence
- reproducibility
- reusability

Long-Term Directions

Customization to other discipline specific modeling modalities, for example

- movement analysis
- multiphysics investigations

Collaborative evolution to move from reporting standards to

- model exchange & sharing standards
- implementation in mark-up languages
- incorporation in multiscale modeling frameworks
- storage with models as metadata

Contact

Ahmet Erdemir
erdemira@ccf.org
+1 (216) 445 9523

http://www.lerner.ccf.org/bme/cobi
http://www.lerner.ccf.org/bme/erdemir