A Heterogeneous Model of the Human Knee

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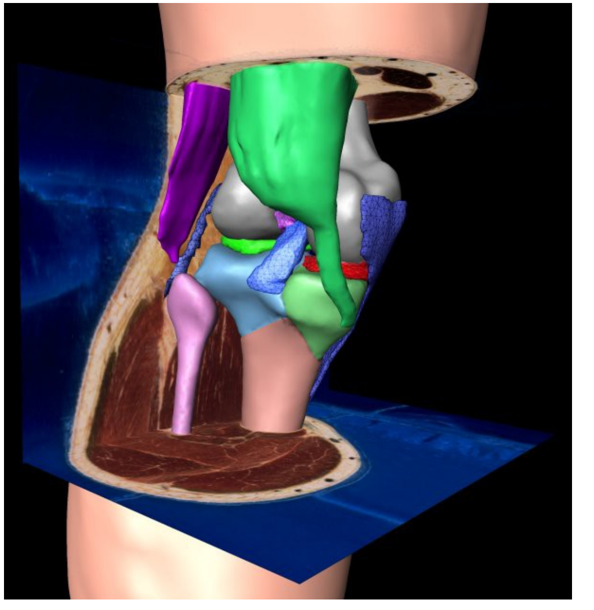
Motivation

Aim: A mechanical model of the human knee



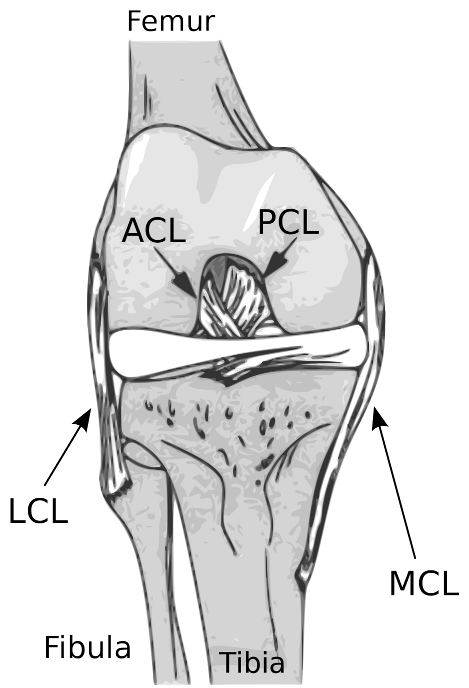
Should:

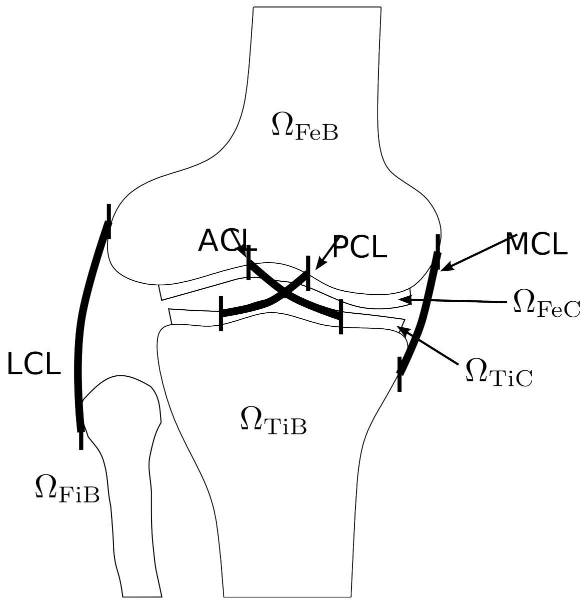
- be fully dynamic
- be patient-specific
- allow high-resolution stress analysis

Overview:

1) Present heterogeneous model
2) Discretize in time and space
3) Solution algorithms
4) Numerical results

Time-dependent heterogeneous model





Components:

- Bones: femur, tibia, fibula
- Articular cartilage on femur and tibia
- Medial and collateral ligaments

Features:

- Fully time-dependent
- Bones and cartilage as 3d continua
- Ligaments as 1d rods with director triads
- Cartilage-cartilage contact

Linear Viscoelasticity and Contact

Bones:

linear elastic material

$$\boldsymbol{\sigma}_{\mathrm{B}}(\mathbf{u}, x) := \mathbf{E}(x) : \boldsymbol{\varepsilon}(\mathbf{u})$$

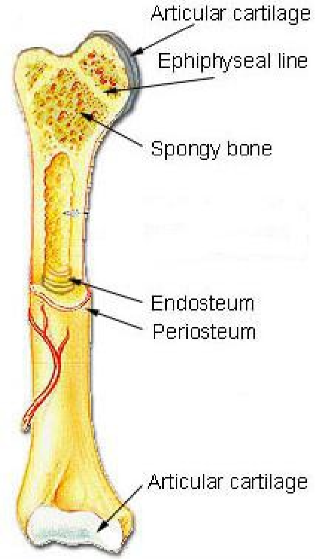


Image: Wikipedia

Cartilage:

linear viscoelastic material

$$\boldsymbol{\sigma}_{\mathrm{V}}(\mathbf{u}, \dot{\mathbf{u}}, x) := \mathbf{E}(x) : \boldsymbol{\varepsilon}(\mathbf{u}) + \mathbf{V}(x) : \boldsymbol{\varepsilon}(\dot{\mathbf{u}})$$

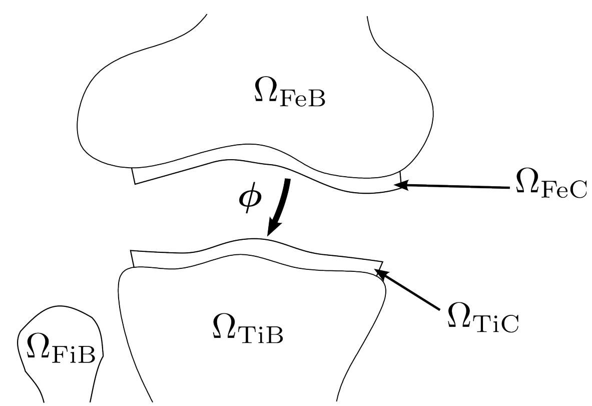
For simplicity: assume materials homogeneous and isotropic

Cartilage-cartilage contact:

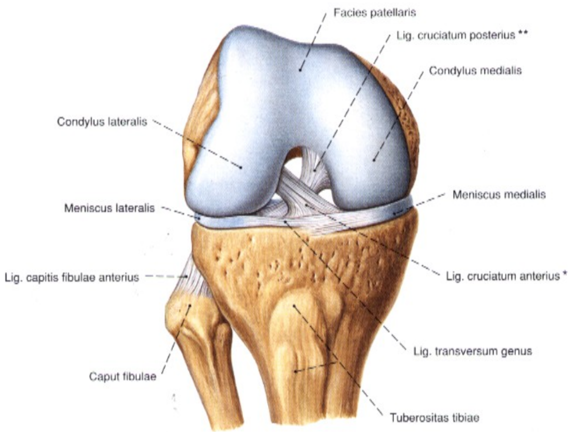
Signorini-type conditions

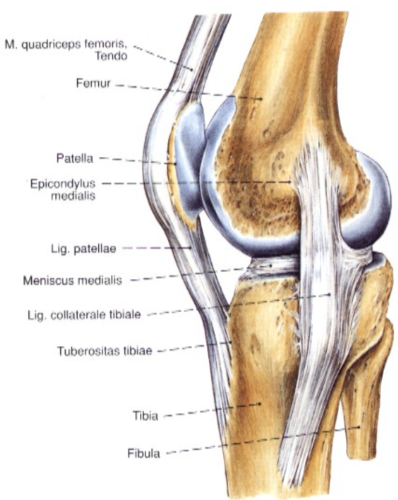
$$\boldsymbol{\phi} : \Gamma_{\mathrm{Fe,C}} \to \Gamma_{\mathrm{Ti,C}}$$

$$[\mathbf{u}(x,t) \cdot \boldsymbol{\nu}]_{\boldsymbol{\phi}} \leq g(x)\,, \quad x \in \Gamma_{\mathrm{Fe,C}}\,,\ t \in [0,T]$$



Ligaments





Images: Sobotta

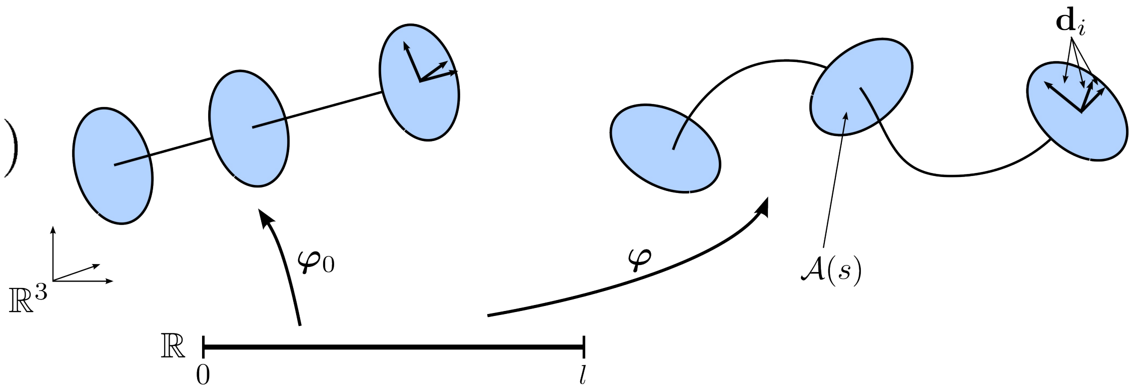
- Ligaments ensure stability of the knee
- Important ligaments:
  - medial and lateral collateral ligament,
  - anterior and posterior cruciate ligaments
- Bundles of collagen fibres
- Can bear very high tensile loads
- For short time scales (few gait cycles): elastic behavior
- Main degrees of freedom:
  - extension, bending, torsion

→ Use a reduced model

Cosserat Rods

A nonlinear Cosserat rod is a map

$$\varphi : [0, l] \to \mathbb{R}^3 \times \mathrm{SO}(3) = \mathrm{SE}(3)$$
$$s \to (r, q)$$



Theorem: [Eliasson '67] The set of configurations

$$\mathcal{C} = \left\{ \varphi : [0, l] \to \mathbb{R}^3 \times \mathrm{SO}(3) \,\middle|\, \varphi \text{ smooth enough} \right\}$$

is a nonlinear manifold.

Strains:

$$(v, u) \in T_{(r,q)}\mathrm{SE}(3)$$
$$T_{(r,q)}\mathrm{SE}(3) \simeq \mathbb{R}^3 \times \mathbb{R}^3$$

Interpretation:

v_1, v_2	: shear	u_1, u_2	: bending
v_3	: extension	u_3	: torsion

Cosserat Rods: Stresses

Stress resultants: on each cross section act

$$\text{a force } \mathbf{n} \in \mathbb{R}^3 \qquad \text{(actually, } (\mathbf{n}, \mathbf{m}) \in T^*\mathrm{SE}(3))$$

$$\text{a moment } \mathbf{m} \in \mathbb{R}^3$$

Assumption: rod is hyperelastic

$$\mathbf{n}_i = \frac{\partial W}{\partial v_i} \qquad \mathbf{m}_i = \frac{\partial W}{\partial u_i}$$

Linear diagonal material:

$$W(\mathsf{u}, \mathsf{v}) = \frac{1}{2} \sum_j K_j (\mathsf{u}_j - \hat{\mathsf{u}}_j)^2 + \frac{1}{2} \sum_j A_j (\mathsf{v}_j - \hat{\mathsf{v}}_j)^2$$

Theorem: Equilibrium states are stationary points of a functional

$$J(\varphi) = \int_{[0,l]} W(\mathsf{u}(s) - \hat{\mathsf{u}}(s), \mathsf{v}(s) - \hat{\mathsf{v}}(s))\, ds$$

Existence of minimizers: [Seidman, Wolfe '88]

Cosserat Rods: Weak Equations of Motion

Functions spaces: Banach manifolds

Configuration space: $Q := H^1([0,l], \mathbb{R}^3 \times \mathrm{SO}(3))$

Lie algebra: $Y := H^1([0,l], \mathbb{R}^3 \times \mathfrak{so}(3))$

Test function space: $T_{\boldsymbol{\varphi}} Q := \{(u, \hat{\theta}\mathbf{q}) : (u,\theta) \in Y\}$

Weak formulation:

Define linear momentum $\mathbf{p}$ and angular momentum $\boldsymbol{\pi}$

$$\int_0^l [\dot{\boldsymbol{\pi}} \cdot \boldsymbol{\mu} + \dot{\mathbf{p}} \cdot \boldsymbol{\eta}]\, ds + \int_0^l [\mathbf{n} \cdot (\boldsymbol{\eta}' - \boldsymbol{\mu} \times \mathbf{r}') + \mathbf{m} \cdot \boldsymbol{\mu}']\, ds = G_{\text{ext}}(\boldsymbol{\eta}, \boldsymbol{\mu})$$

for all $(\boldsymbol{\eta}, \boldsymbol{\mu}) \in Y$

Coupling: Homogeneous Formulation

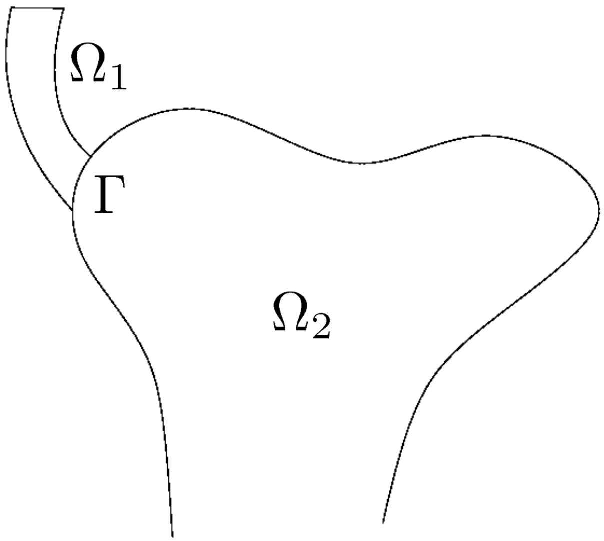
[Quarteroni, Valli '99, S. '08]

Set

$$\Omega = \Omega_1 \cup \Omega_2, \qquad \Omega_1 \cap \Omega_2 = \emptyset, \qquad \Gamma = \overline{\Omega}_1 \cap \overline{\Omega}_2, \qquad \operatorname{meas} \Gamma \neq 0$$

Nonlinear elasticity: Find $\mathbf{u} : \Omega \to \mathbb{R}^3$ such that

$$\begin{aligned} -\operatorname{div} \sigma(\mathbf{u}) &= f && \text{in } \Omega_1 \cup \Omega_2 \\ \mathbf{u} &= 0 && \text{on } \Gamma_D \\ \sigma(\mathbf{u})\nu &= p && \text{on } \partial(\Omega_1 \cup \Omega_2) \setminus \Gamma_D \end{aligned}$$



Theorem: This problem is equivalent to

$$\begin{aligned} -\operatorname{div} \sigma(\mathbf{u}_i) &= f_i && \text{in } \Omega_i, \quad i = \{1,2\} \\ \mathbf{u}_1 &= \mathbf{u}_2 && \text{on } \Gamma, \\ \sigma(\mathbf{u}_1)\nu_1 &= -\sigma(\mathbf{u}_2)\nu_2 && \text{on } \Gamma, \end{aligned}$$

plus corresponding BCs on $\partial\Omega_1 \setminus \Gamma$ and $\partial\Omega_2 \setminus \Gamma$.

Abstract Coupling Conditions

Homogeneous coupling conditions:

$$
\begin{aligned}
\mathbf{u}_1 &= \mathbf{u}_2 && \text{on } \Gamma, \\
\sigma(\mathbf{u}_1)\nu_1 &= -\sigma(\mathbf{u}_2)\nu_2 && \text{on } \Gamma,
\end{aligned}
$$

Abstractly: Conditions for primal and dual variables [Quarteroni, Valli '99]

$$
\begin{aligned}
\Phi(\mathbf{u}_1) &= \Phi(\mathbf{u}_2) \\
\Psi(\mathbf{u}_1) &= \Psi(\mathbf{u}_2)
\end{aligned}
$$

3d elasticity:

- Primal variable: $\mathbf{u}$
- Dual variable: σ

Cosserat rods:

- Primal variable: (φ_r, φ_q)
- Dual variable: $(\mathbf{n}, \mathbf{m})$

Multi-Dimensional Coupling

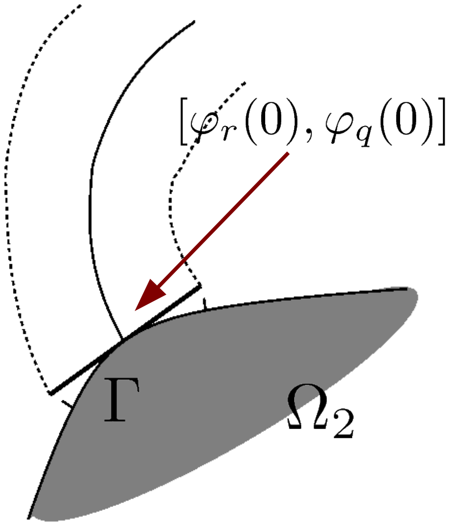
Replace Ω_1 by a Cosserat rod.

Do linear elasticity on Ω_2.

Reduced coupling conditions I: forces and moments

$$\mathbf{n}(0)\nu_0 = -\int_\Gamma \sigma\nu\, ds \qquad \text{Balance of forces}$$

$$\mathbf{m}(0)\nu_0 = -\int_\Gamma (x - \varphi_r(0)) \times \sigma\nu\, ds \qquad \text{Balance of moments}$$



The rod cross section does not match Γ.

Primal Conditions

Average Boundary Orientation:

Average deformation: $\mathcal{F}_\Gamma(\mathbf{u}) = \frac{1}{|\Gamma|}\int_\Gamma \nabla\mathbf{u} + \mathrm{Id}\; ds$

Polar decomposition: $\mathcal{F}_\Gamma(\mathbf{u}) = \mathrm{polar}_\Gamma(\mathbf{u}) R_\Gamma(\mathbf{u})$

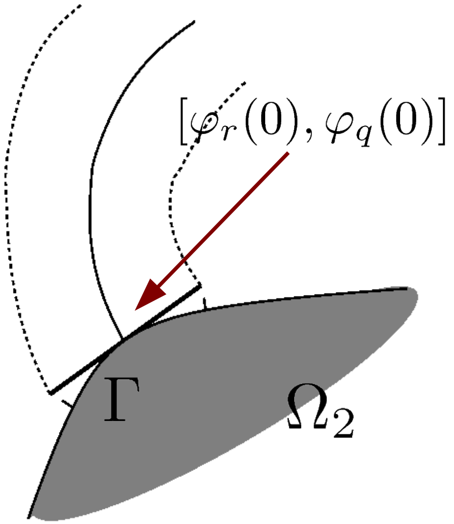
Reference orientation: $\hat{\varphi}_q(0)$ (part of problem definition)

Average orientation: $\mathrm{polar}_\Gamma(\mathbf{u})\hat{\varphi}_q(0)$

Reduced coupling conditions II:

position and orientation

$$r(0) = \frac{1}{|\Gamma|}\int_\Gamma \mathbf{u} + x\, ds \qquad \varphi_q(0) = \mathrm{polar}_\Gamma(\mathbf{u})\hat{\varphi}_q(0)$$



Existence of Solutions

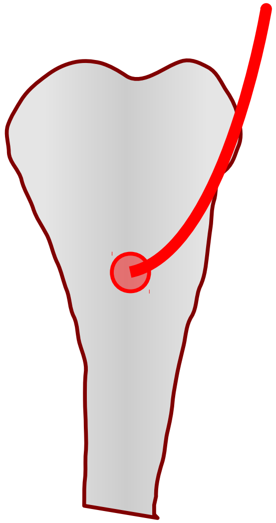
Variety of primal coupling conditions:

Averaged coupling (cond. in $\mathrm{SE}(3)$)

Rigid coupling (cond. in $\mathbf{H}^{1/2}(\Gamma)$)

Theorem: [S, Schiela, 2012] The static coupled system has a solution.

Proof: direct method in the calculus of variations



Kuhn-Tucker conditions yield corresponding dual conditions:

Averaged coupling: dual conditions in $T^*\mathrm{SE}(3)$

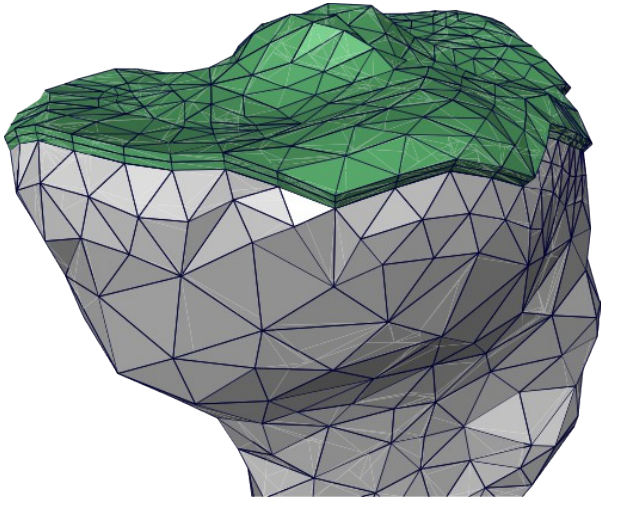
Rigid coupling: dual conditions in $(\mathbf{H}^{1/2}(\Gamma))^*$

Discretization: Bones and Cartilage

Time discretization: Contact-Stabilized Newmark Method

[Deuflhard, Klapproth, Krause, Schiela]

- Energy-dissipative
- No numerical oscillations
- Each spatial problem is a minimization problem



Space discretization:

- First-order Lagrangian finite elements
- Bones: tetrahedra, Cartilage: prisms

Mortar coupling:

- Contact and bone-cartilage coupling
- Dual basis mortar elements [Wohlmuth, Krause '03]
- Exact evaluation of contact integrals [Krause, S. '05, S. '08]

Rods: Time discretization

Energy-Momentum Method: [Simo, Tarnow '92, Simo, Tarnow, Doblaré '95]

At each time step *n* solve for the increment

$$(\mathbf{u}, \boldsymbol{\theta}) \in Y := H^1([0,l], \mathbb{R}^3 \times \mathfrak{so}(3))$$

$$\frac{1}{\tau}\,\mathrm{dyn}_{(\mathbf{r}^n,\mathbf{q}^n)}[(\mathbf{u},\boldsymbol{\theta});(\boldsymbol{\eta},\boldsymbol{\mu})] + \mathrm{pot}_{(\mathbf{r}^n,\mathbf{q}^n)}[(\mathbf{u},\boldsymbol{\theta});(\boldsymbol{\eta},\boldsymbol{\mu})] = G(\boldsymbol{\eta},\boldsymbol{\mu}) \qquad \forall(\boldsymbol{\eta},\hat{\boldsymbol{\mu}}) \in Y$$

Update configuration

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{u} \qquad \text{and} \qquad \mathbf{q}^{n+1} = \mathrm{cay}[\boldsymbol{\theta}]\mathbf{q}^n,$$

Conservation properties:

- Linear and angular momentum
- Total energy

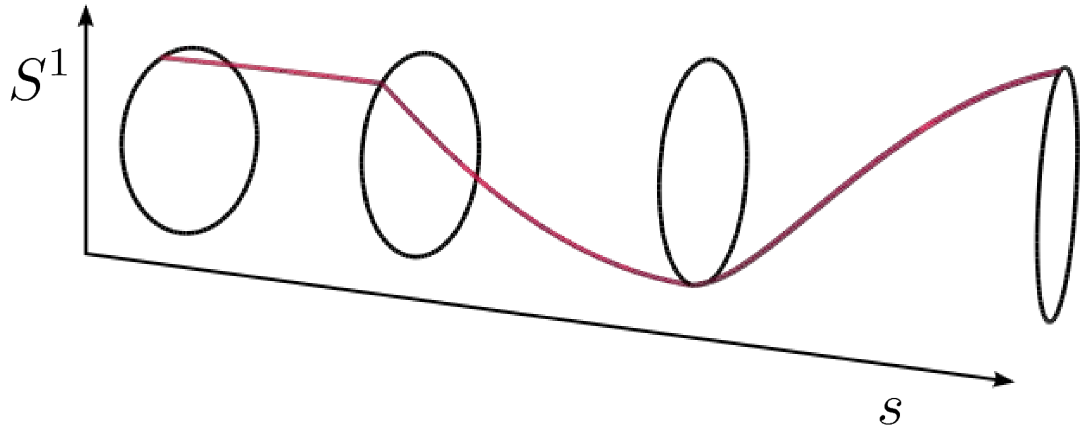
Discretization: Geodesic Finite Elements

How do you discretize 1d functions with values on a Riemannian manifold?

→ piecewise interpolation along geodesics

Definition: Geodesic finite elements [S '10]

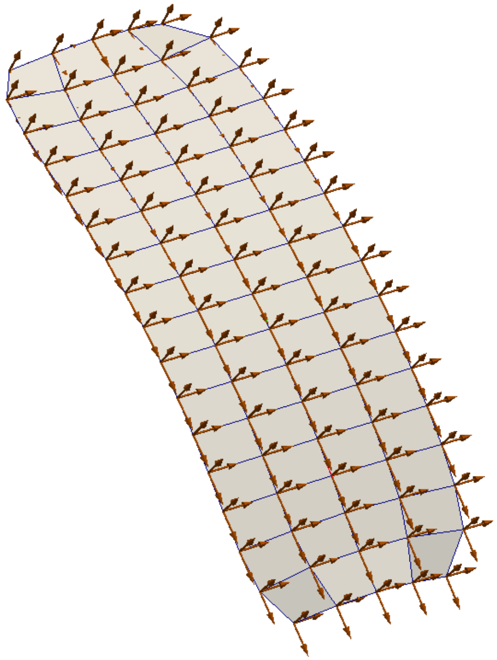
Let M be a Riemannian manifold and G be a one-dimensional grid.
A geodesic finite element function is a continuous function $\phi : [0, l] \to M$ such that for each element $[l_i, l_{i+1}]$, $\phi(t)$ is a minimizing geodesic.



Properties of Geodesic Finite Elements

- Works for general Riemannian manifolds M
- Conforming: $V_h^M \subset H^1([0,l], M)$
- Nodal evaluation $\mathcal{E} : V_h^M \to M^n$ is well defined.
- For each $\varphi : [0,l] \to M$ Lipschitz, the nodal prolongation $\mathcal{E}^{-1} : M^n \to V_h^M$ is well-defined in a neighborhood of φ if the grid is fine enough.
- Invariant under isometries Q of M (frame invariance)

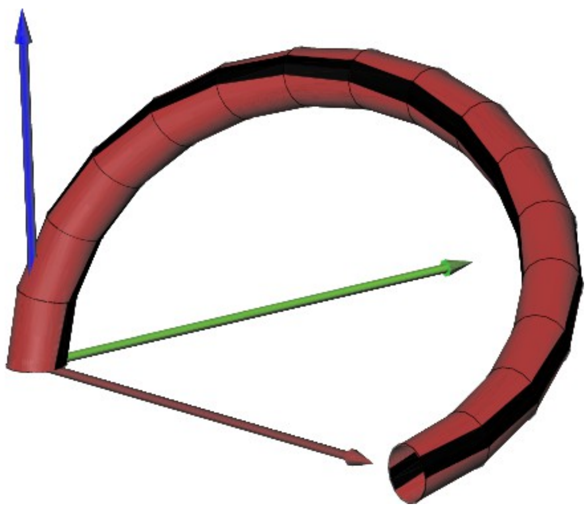
$$Q\mathcal{E}^{-1}v = \mathcal{E}^{-1}Qv, \quad v \in M^n$$

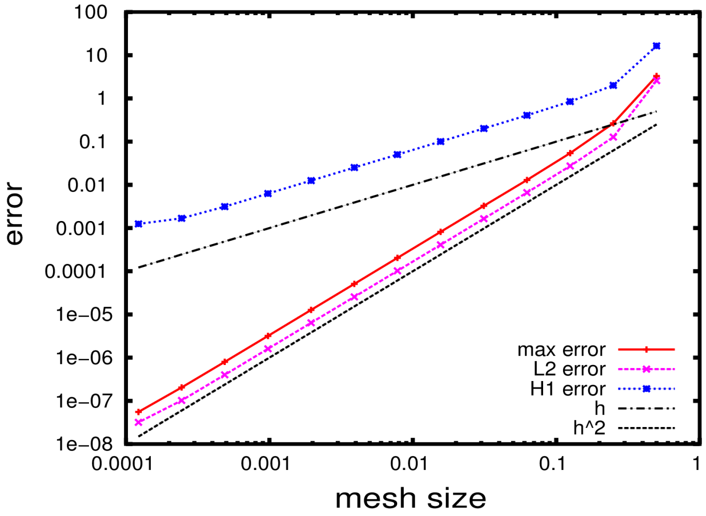


Generalization to higher dimensions

- Riemannian center of mass
- 2d Cosserat shells [with P. Neff] as models for ligaments
- Higher-order interpolation

Optimal Discretization Errors





“Theorem” [Grohs, Hardering, S]: Geodesic finite elements for the harmonic map problem from R^d into a Riemannian manifold M fulfill the same Sobolev-type error bounds as regular finite elements for linear elliptic problems.

Solving Subdomain Problems

Spatial bone-cartilage problem:

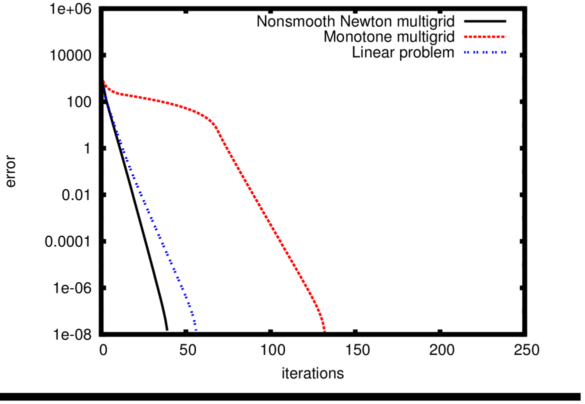
Basically one constrained minimization problem

$$\mathbf{u}_h^{n+1} = \operatorname*{arg\,min}_{\mathbf{v}_h \in \mathcal{K}_h} \left[\frac{1}{2} g(\mathbf{v}_h, \mathbf{v}_h) - \tau^2 f_{\text{ext}}(\mathbf{u}_h^n + \mathbf{v}_h) \right]$$

$$g(\mathbf{v}_h, \mathbf{v}_h) = \left\| \mathbf{v}_h - \mathbf{u}_{h,\text{pred}}^{n+1} \right\|_{\mathbf{L}_2}^2 + \tau^2 a\left(\frac{\mathbf{u}_h^n + \mathbf{v}_h}{2}, \frac{\mathbf{u}_h^n + \mathbf{v}_h}{2} \right) + \frac{\tau}{2} b\left(\frac{\mathbf{v}_h - \mathbf{u}_h^n}{\tau}, \frac{\mathbf{v}_h - \mathbf{u}_h^n}{\tau} \right)$$

Truncated Nonsmooth Newton MG [Gräser, Kornhuber '08, Gräser, S., Sack '08]

- Global convergence
- No regularization
- Asymptotic multigrid rates
- Very short preasymptotic phase (beats monotone multigrid)



Solving Subdomain Problems

Spatial ligament problems:

Given $\boldsymbol{\varphi}_h^n$, find $(\mathbf{u}_h^n, \boldsymbol{\theta}_h^n)$ such that

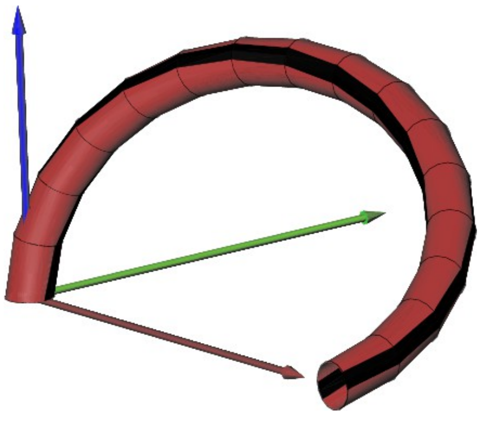
$$\frac{1}{\tau}\,\mathrm{dyn}_{\boldsymbol{\varphi}_h^n}[(\mathbf{u}_h^n, \boldsymbol{\theta}_h^n); (\boldsymbol{\eta}_h, \boldsymbol{\mu}_h)] + \mathrm{pot}_{\boldsymbol{\varphi}_h^n}[(\mathbf{u}_h^n, \boldsymbol{\theta}_h^n); (\boldsymbol{\eta}_h, \boldsymbol{\mu}_h)] = G(\boldsymbol{\eta}_h, \boldsymbol{\mu}_h)$$

for all test functions

$$(\boldsymbol{\eta}_h, \boldsymbol{\mu}_h) \in Y_{h,0} := \{y_h \in Y_h \mid y_h(0) = y_h(l) = 0\}$$

Effectively, $(\mathbf{u}_h^n, \boldsymbol{\theta}_h^n)$ and $(\boldsymbol{\eta}_h, \boldsymbol{\mu}_h)$ from 6-valued first-order FE space

- Nonlinear equation in a linear space
- No minimization formulation



Damped Newton Solver:

- Hesse matrices are block-tridiagonal

Dirichlet-Neumann Algorithm

Choose $\lambda_r^0 \in \mathbb{R}^3$, $\lambda_q^0 \in SO(3)$.

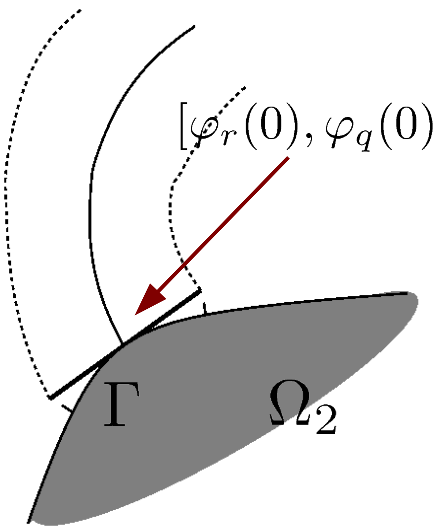
Dirichlet step:

For each rod φ and all $k \geq 0$ solve

$$\varphi^{k+1} = \text{solution of E–M increment problem}$$

$$\varphi_r^{k+1}(l) = r_D \qquad \varphi_q^{k+1}(l) = q_D$$

$$\varphi_r^{k+1}(0) = \lambda_r^k \qquad \varphi_q^{k+1}(0) = \lambda_q^k$$



This yields:

- Stress resultant: $\mathbf{n}^k(0) \in \mathbb{R}^3$
- Moment resultant: $\mathbf{m}^k(0) \in \mathbb{R}^3$

Dirichlet-Neumann Algorithm

Neumann step:

Define a traction field $\tau^k : \Gamma \to \mathbb{R}^3$ such that

$$\int_\Gamma \tau^k \, ds = \mathbf{n}^k(0)\nu_0 \qquad \int_\Gamma (x - \varphi_q(0)) \times \tau^k \, ds = \mathbf{m}^k(0)\nu_0$$

Solve

$$\begin{aligned} -\operatorname{div}\sigma(\mathbf{u}^{k+1}) &= \mathbf{f} && \text{in } \Omega_2 \\ \sigma\nu &= -\tau^k && \text{on } \Gamma \end{aligned}$$

plus further boundary conditions.

Dirichlet-Neumann Algorithm

Geodesic damped update on SE(3)

$\theta \in (0, \infty)$ damping parameter.

Position update:

$$\lambda_r^{k+1} = \theta|\Gamma|^{-1} \int_\Gamma (\mathbf{u}^{k+1} + x)\, dx + (1-\theta)\lambda_r^k$$

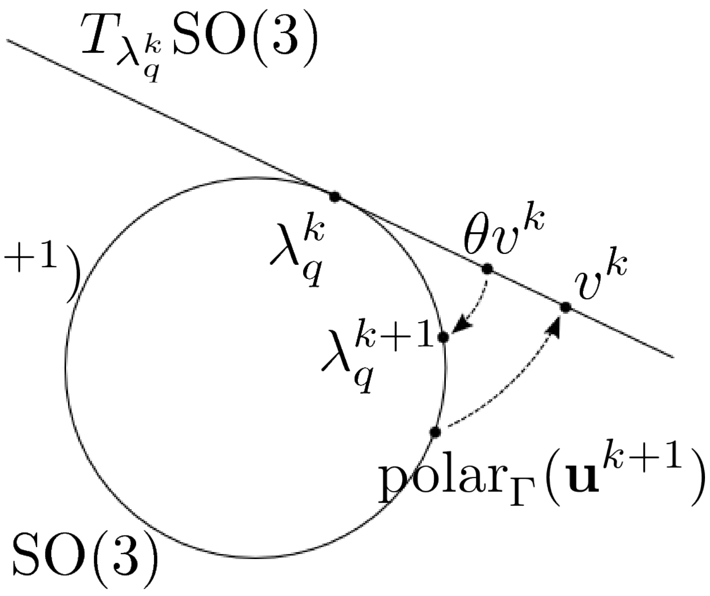
Orientation update:

New average orientation: $\mathrm{polar}_\Gamma(\mathbf{u}^{k+1})$

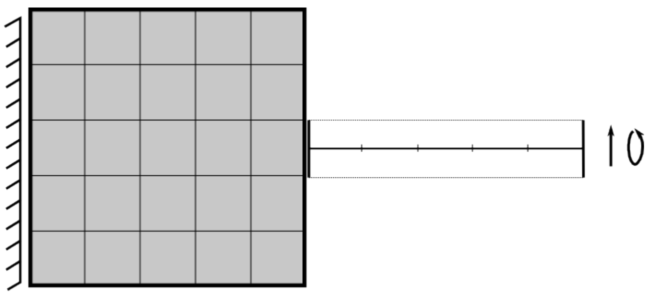
Interpolate on the geodesic from λ_q^k to $\mathrm{polar}_\Gamma(\mathbf{u}^{k+1})$

$$v^k = \exp^{-1}_{\lambda_q^k} \mathrm{polar}_\Gamma(\mathbf{u}^{k+1})$$

$$\lambda_q^{k+1} = \exp_{\lambda_q^k} \theta v^k$$



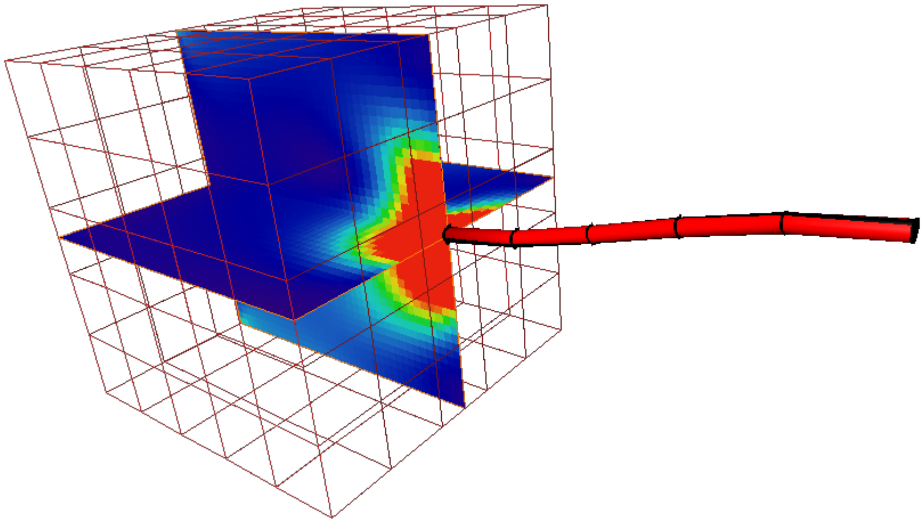
D.-N.: Numerical Results

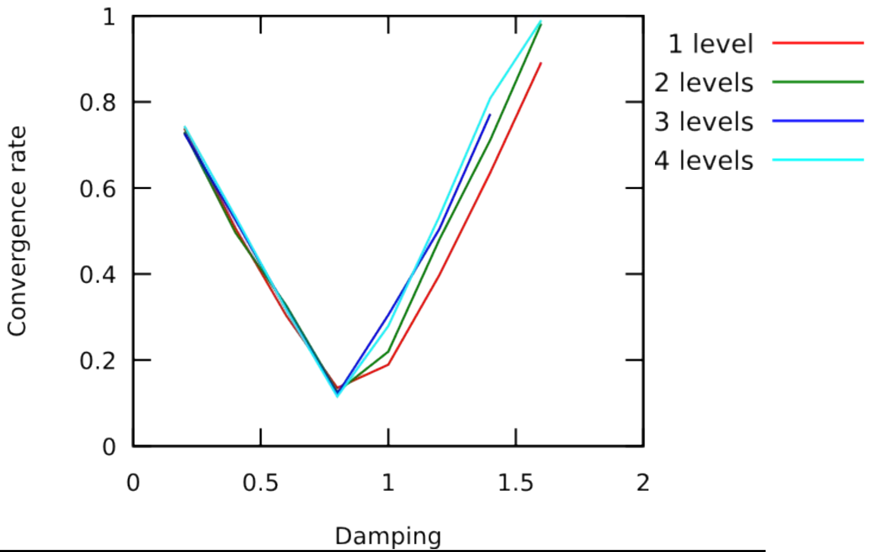


- Dirichlet boundary conditions:
  upward displacement and 90° torsion
- Cross-section area: 1 units
- Material parameters: $E = 2.5 \cdot 10^5, \nu = 0.3$

Level-independent convergence rates!

Level-independent optimal damping parameter!





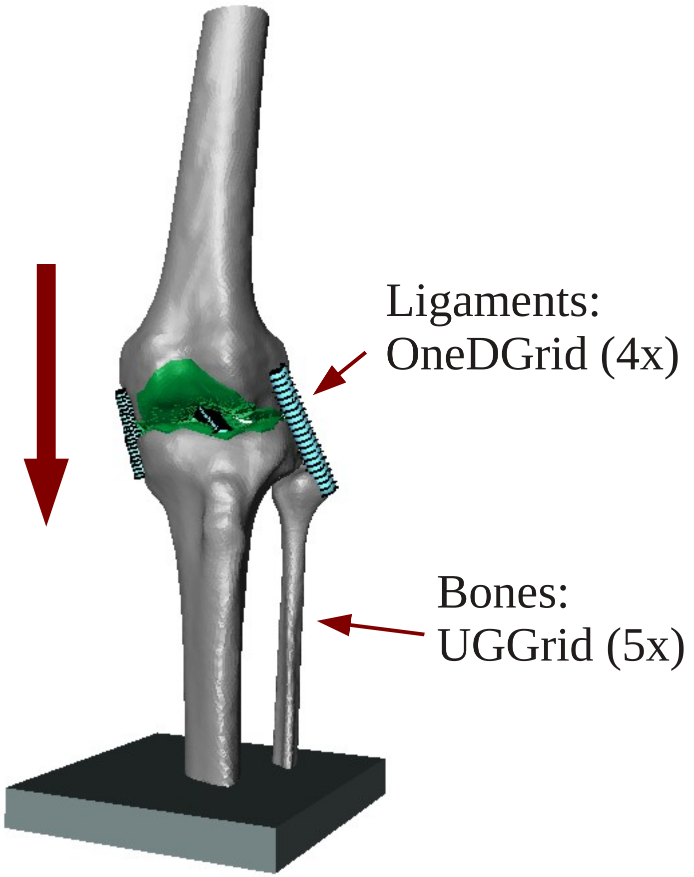
Putting it all together

Full modell:

- Bones: distal femur, proximal tibia and fibula
- Bone data from Visible Human data set
- Articular cartilage from anatomy atlas
- Ligaments: cruciate and collateral ligaments
- Insertion sites from anatomy atlas

Fully dynamic simulation:

- initially: uniform downward movement
- lower obstacle
- Grids twice uniformly refined
- Automatically constructed boundary parametrizations [Krause, S. '06]



Implementation: Dune

Putting it all together

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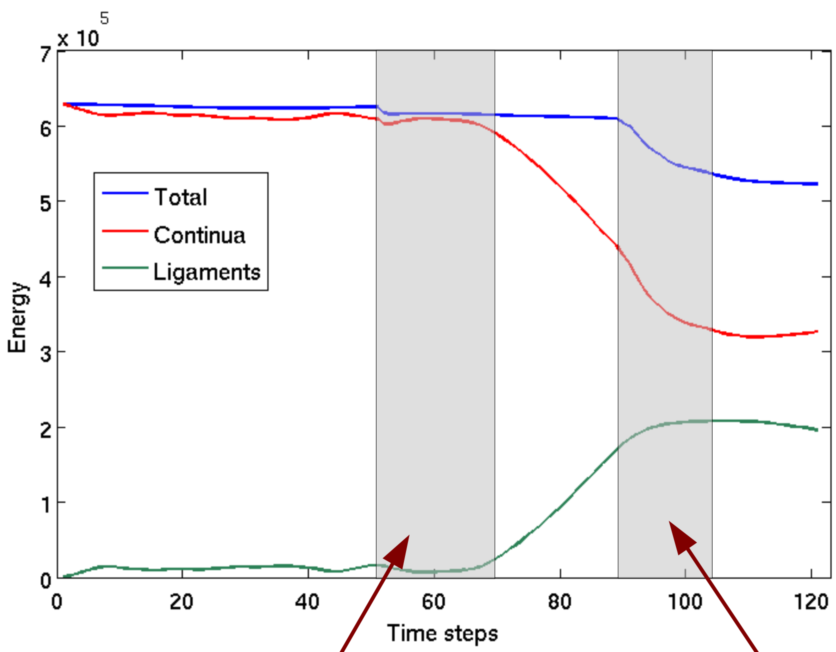
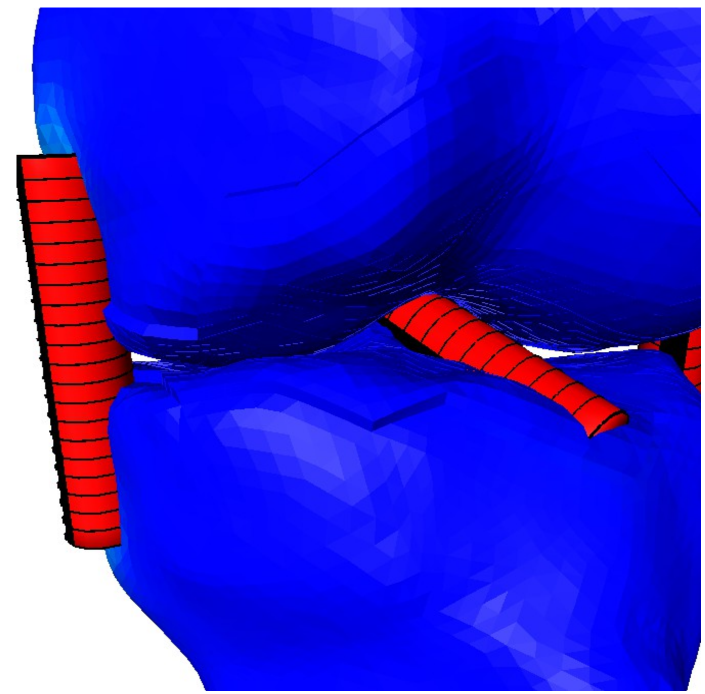
Energy behavior

Dune
http://dune-project.org/

Energy dissipative:





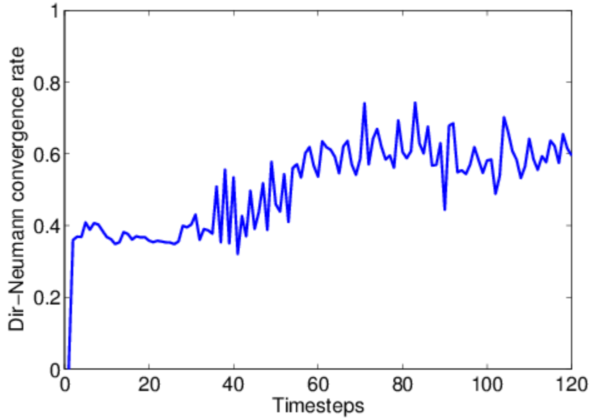
tibia-obstacle contact

femur-tibia contact

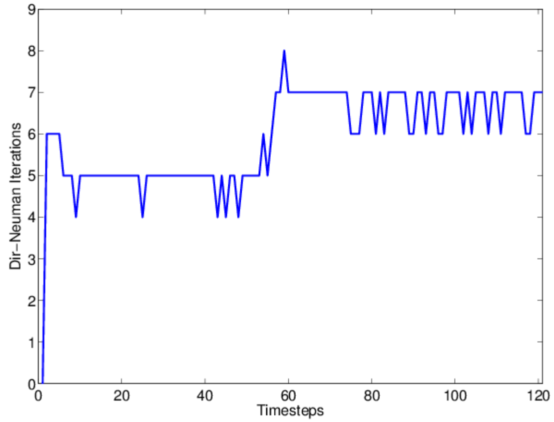
Solver Performance

Dirichlet-Neumann:

converge rate

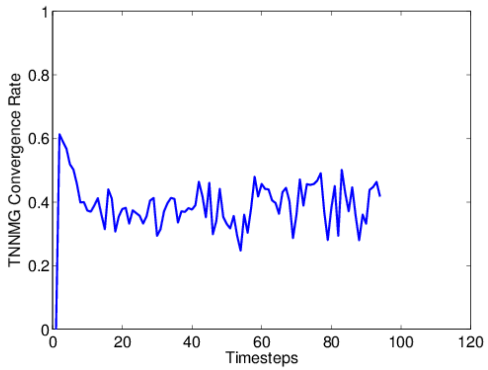


iteration numbers

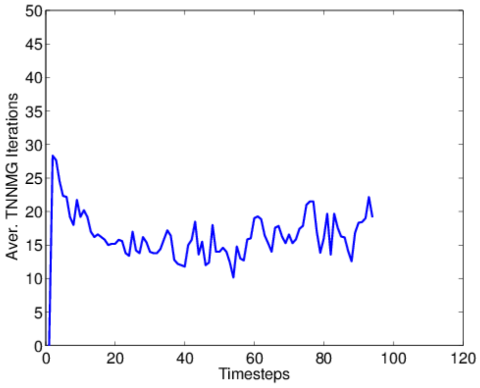


Truncated Nonsmooth Newton Multigrid:

converge rate



iteration numbers



Outlook: Towards complete gait cycles

Geometric nonlinearity:

$$\varepsilon(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T + \nabla\mathbf{u}^T\nabla\mathbf{u})$$

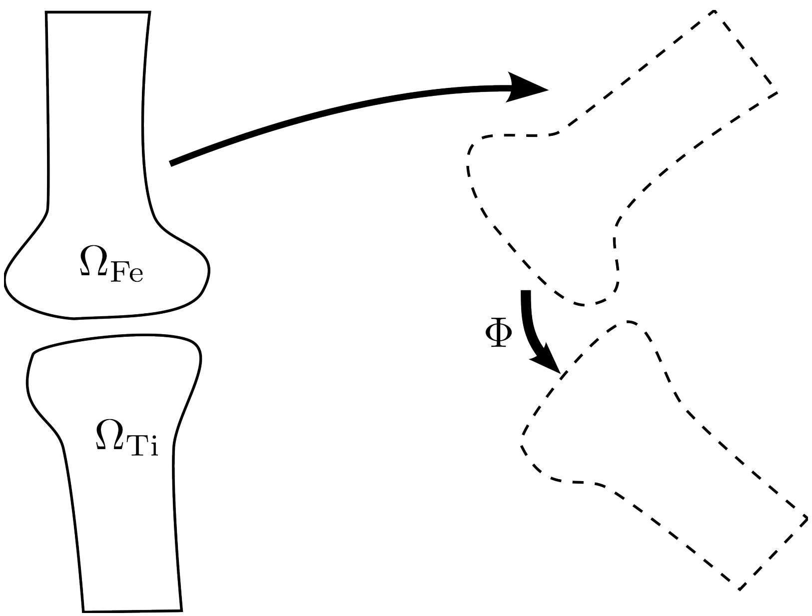
material remains linear

Time discretization: enhance contact-stabilized Newmark framework

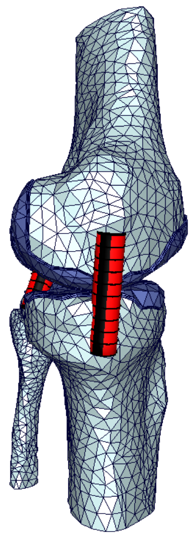
- Keep energy dissipativity
- Minimization problems as spatial problems

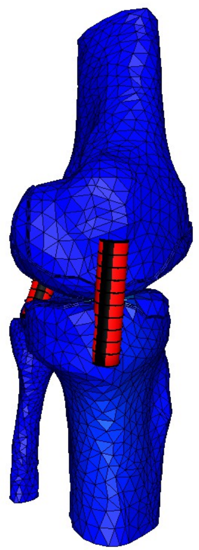
Assemble linearized contact conditions:

- Contact conditions for a deformed configuration



Outlook: Towards complete gait cycles





Problem setting:

- Bones: femur, tibia, fibula
- Cartilage on femur, tibia
- Ligaments: two cruciate, two collateral ligaments

Boundary/initial conditions:

- Tibia and fibula are clamped
- Femur falls subject to gravity

Outlook: Towards complete gait cycles

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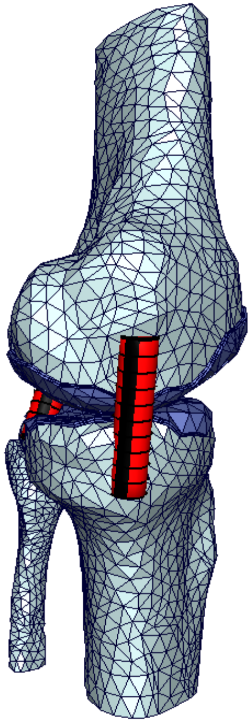
Limits of the model? ⟶ try longer simulations:

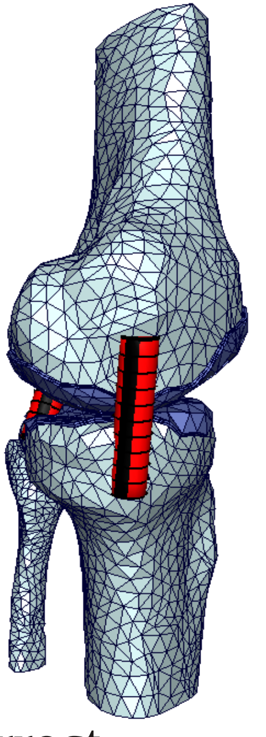


Outlook: Towards complete gait cycles

Limits of the model? ⟶ try longer simulations:

Outlook: Towards complete gait cycles

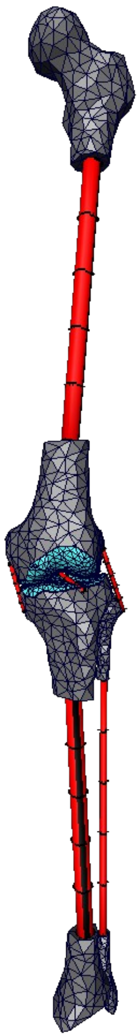
Limits of the model? → try longer simulations:



Conclusions:

- Implementation (presumably) correct
- Limits of the model exceeded
- Next goal: patella and patella tendon

Current Work / Open Problems

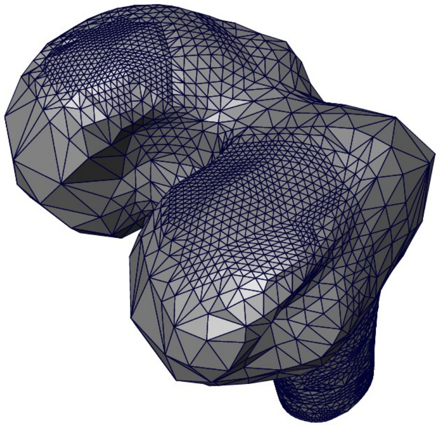


Analysis/Algorithms

- Space-adaptivity
- Geometrically exact bone/cartilage models
- Heterogeneous bone models
- Convergence of the Dirichlet-Neumann algorithm
- Alternative Steklov-Poincaré type solvers
- Two-dimensional ligament models
- Bone-ligament contact

Application:

- Patella, menisci
- Validation with real-world data
- Implant wear testing



Thank you for your attention!