University of Stuttgart
Dep. of Mathematics & SC SimTech

DiHu

Towards realistic HPC models of the neuromuscular system

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Our Consortium

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Computational Mathematics for Complex Simulations

Institute of Applied Analysis and Numerical Simulation

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Visualization and Interactive Systems

Visualization Research Center

Thomas Ertl, Michael Krone, Tobias Rau

Continuum Biomechanics and Mechanobiology

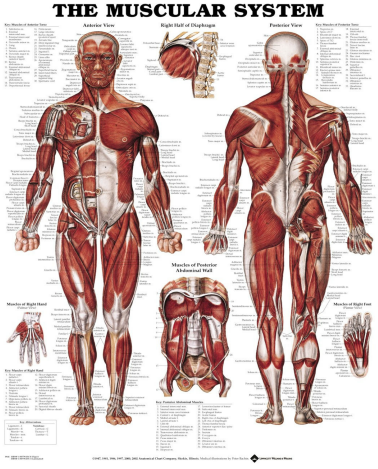
Institute of Applied Mechanics

Oliver Röhrle, Thomas Klotz

The Musculoskeletal System

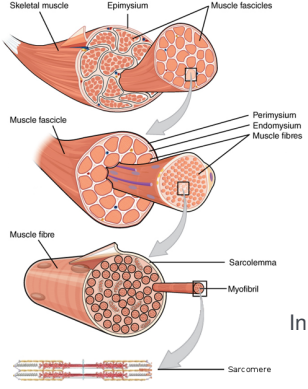
Different Tasks

One System



http://www.physioshop.co.uk/muscular-system-flexible-laminated-chart.html

Anatomy of Skeletal Muscle Tissue



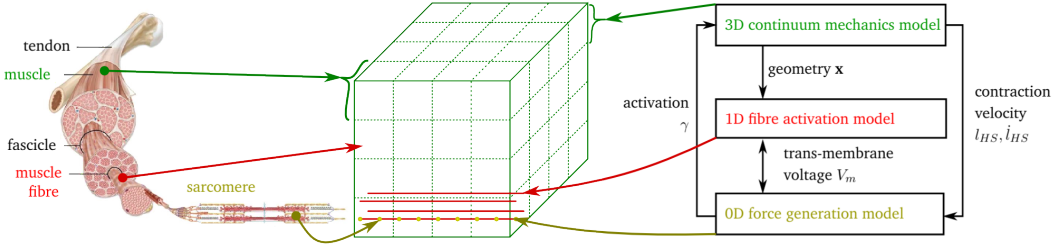
- 639 skeletal muscles (connected via tendons to 206 bones)
- 10–100 fascicles per muscle
- 10–10.000 fibres per fascicle
- Up to 50.000 sarcomeres per fibre

In total: About 10^{12} sarcomeres per body (10^{7}/core on Hazel Hen)

DiHu Project Goals:

- Improve understanding of the neuromuscular system
- Towards patient-specific diagnosis and therapy
- Ultimately, towards neuroprothesis design
- By constructing a multi-X model and simulating it

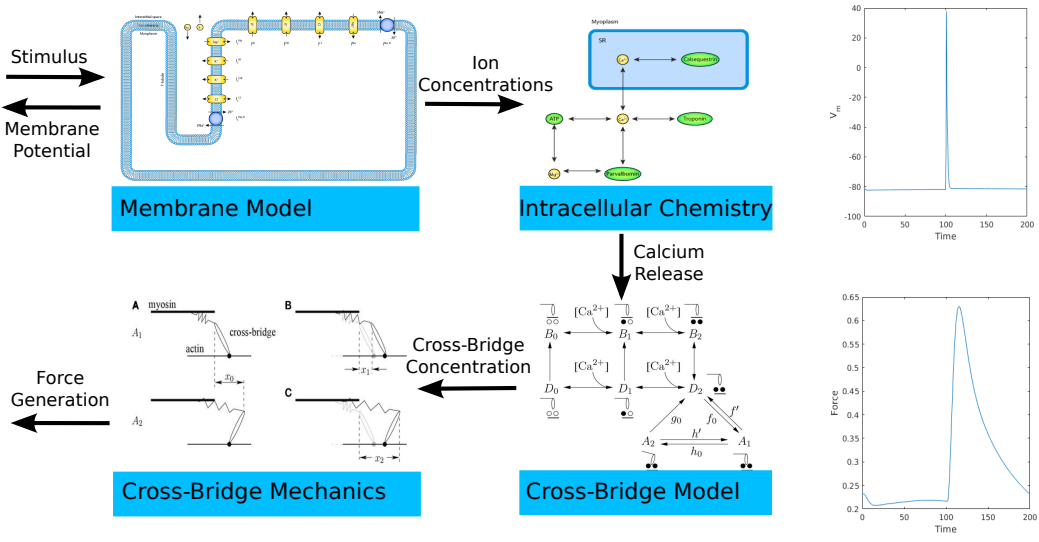
The Multi-scale Multi-physics Model



Sounds doable for a single muscle:

- $O(10^4)$ DOF in 3D mechanics
- $O(10^2)$ DOF in 1D diffusion per fibre, 10^5-10^6 sufficient for physiology
- Problem: sub-cellular dynamics, e.g. exitation-contraction mechanisms

Sub-Cellular Dynamics



Sub-Cellular Dynamics

$$\frac{\partial \phi_S(t)}{\partial t} = -\frac{1}{C_m}\left[I^{Cl}(t) + I^{IR}(t) + I^{DR}(t) + I^{Na}(t) + I^{NaK}(t) - I_{Stim}(t) + \frac{1000}{Ra}\left(\phi_S(t) - \phi_T(t)\right)\right]$$

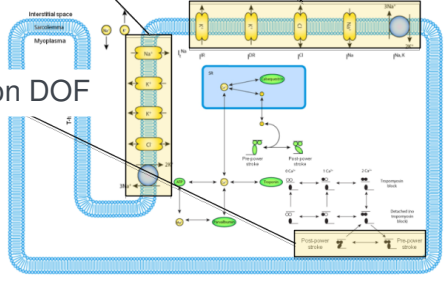
$$\frac{\partial \phi_T(t)}{\partial t} = -\frac{1}{C_m}\left[I_T^{Cl}(t) + I_T^{IR}(t) + I_T^{DR}(t) + I_T^{Na}(t) + I_T^{NaK}(t) + \frac{1000}{Ra \cdot \gamma}\left(\phi_S(t) - \phi_T(t)\right)\right]$$

$$\vdots$$

$$\frac{\partial A_1(t)}{\partial t} = -f_o\, D_2(t) - f_p\, A_1(t) + h_p\, A_2(t) - h_o\, A_1(t)$$

$$\frac{\partial A_2(t)}{\partial t} = -h_p\, A_2(t) + h_o\, A_1(t) - g_o\, A_2(t)$$

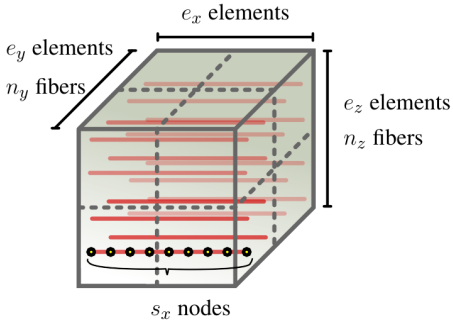
$\sim$56 stiff coupled ODEs per 1D diffusion DOF

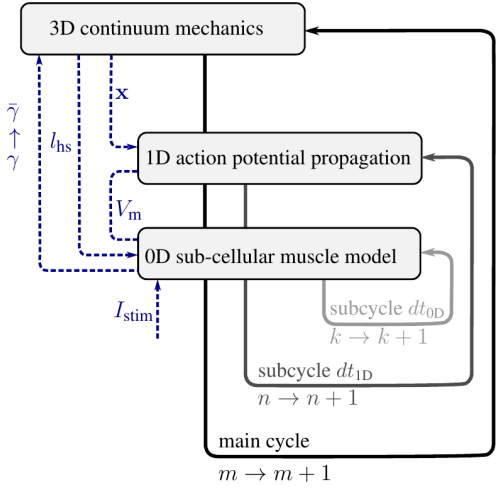


Shorten, P., O'Callaghan P., Davidson J., and Soboleva T., "A mathematical model of fatigue in skeletal muscle force contraction", J. of Muscle Research and Cell Motility, 28(6), 2007, pp. 293-313.

Current state of the project after one year

Domain Decomposition and Multi-Scale Time-Stepping

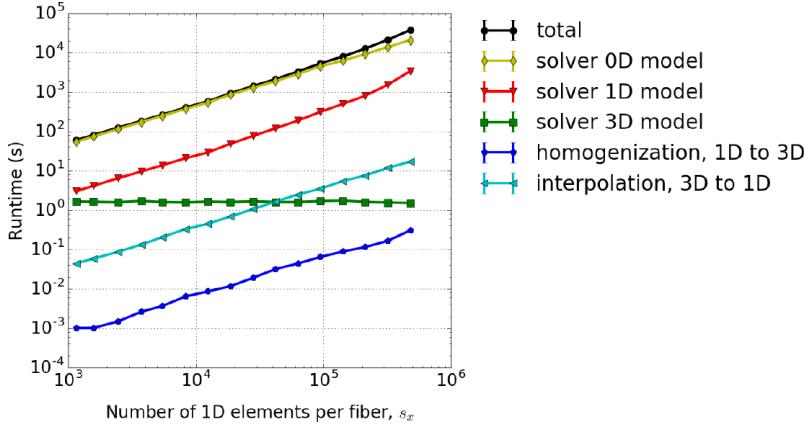




High-Level Bottleneck Analysis

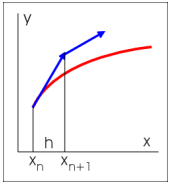
Cellular bio-electro-chemical processes (0D models) dominate runtime

(note logscale)

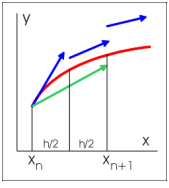


Numerical Improvements

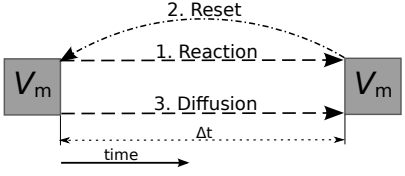
Initial ODE solvers: forward and backward Euler



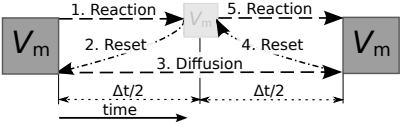
Improved higher order schemes: Heun and Crank-Nicolson



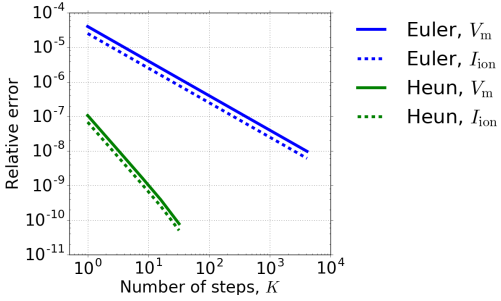
Initial multi-scale time-stepping: 1st order Godunov

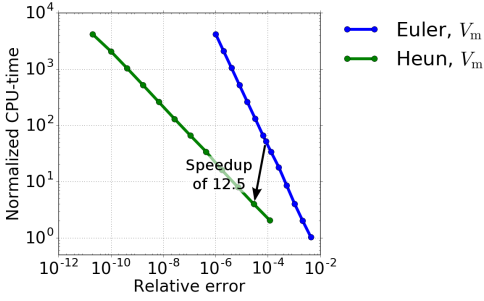


Improved higher order scheme 2nd order Strang splitting



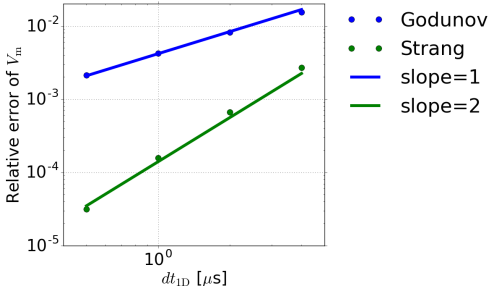
Numerical Improvements

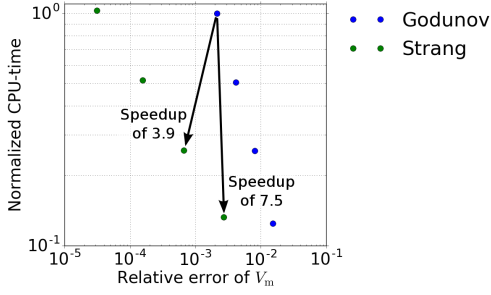




Improvements as expected, translates to runtime

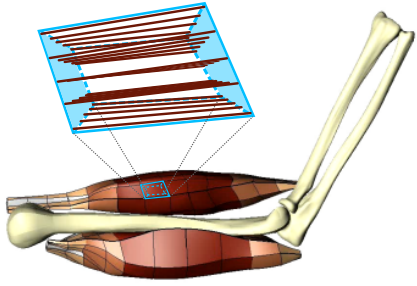
Numerical Improvements



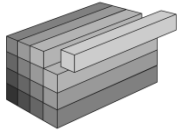


Improvements as expected, translates to runtime

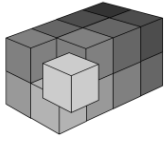
Domain Decomposition Improvements



Pillar-shaped DD

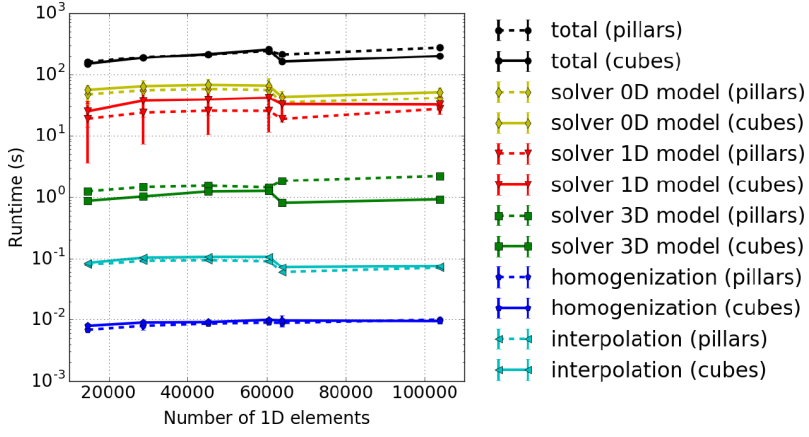


Cube-shaped DD

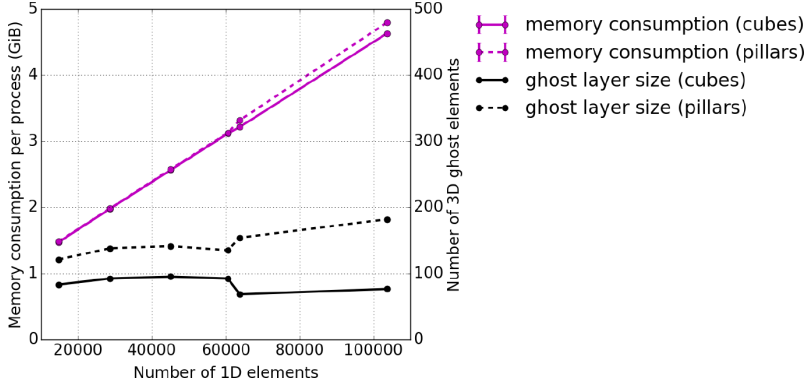


- Goal: minimize communication
- Pillar-shaped DD more suitable for 1D (local per fibre)
- Cube-shaped DD more suitable for 3D (local for mechanics)
- Unclear which is better (cut fibres or not)

Domain Decomposition Improvements

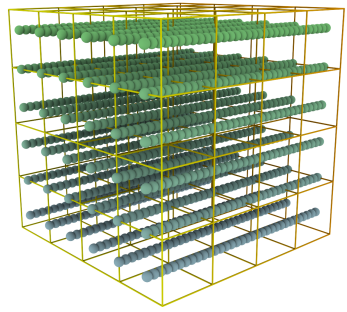


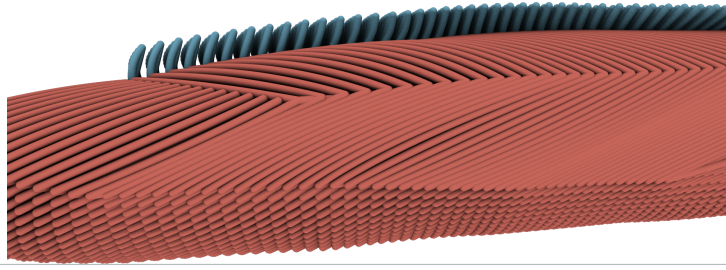
Current Limiting Factor



Visualisation

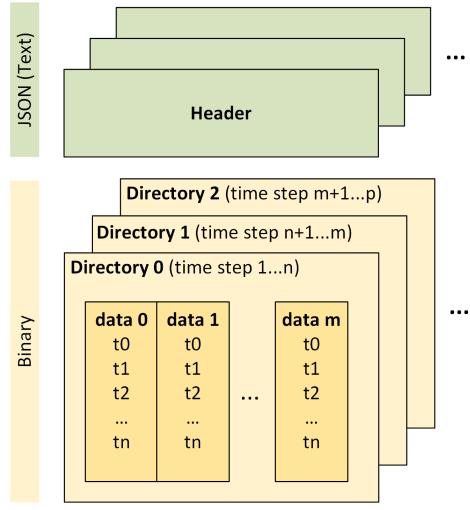
- MegaMol framework as basis for new visualization methods
- CPU-based rendering with OSPRay for HPC: interactive RT and preparation for in-situ vis.
- First muscle fibre renderers integrated into MegaMol





IO Bottlenecks

- Efficient file format based on data separation
- Human-readable JSON headers
- Compressed binary-encoded raw data blocks
- Abstraction layer for parallel file IO



Summary and Outlook

Progress after one year:

- From 1 to 768 cores
- From 5000 to 180000 muscle fibres
- Additional 0D models
- From zero code knowledge to substantial speedups

Outlook:

- Per-node performance close to peak
- 1M muscle fibres
- Feedback loop in the model
- True in-situ visualization, streaming from HLRS to VISUS

Acknowledgements