SIMON FRASER UNIVERSITY

Tutorial 1: Introduction to the Flexodeal Framework

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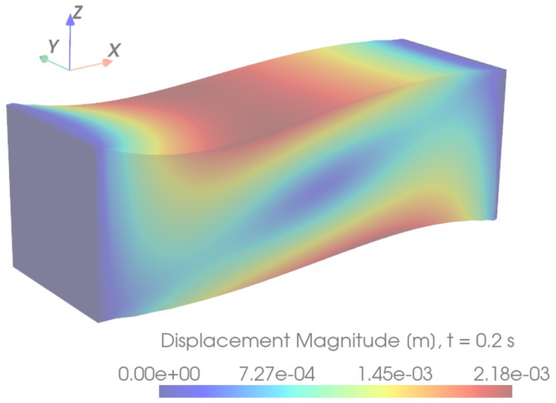
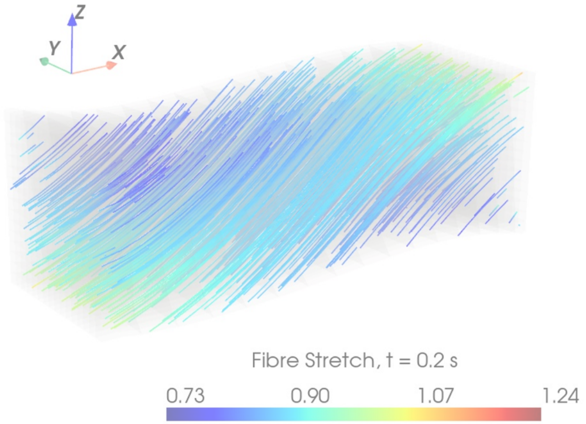
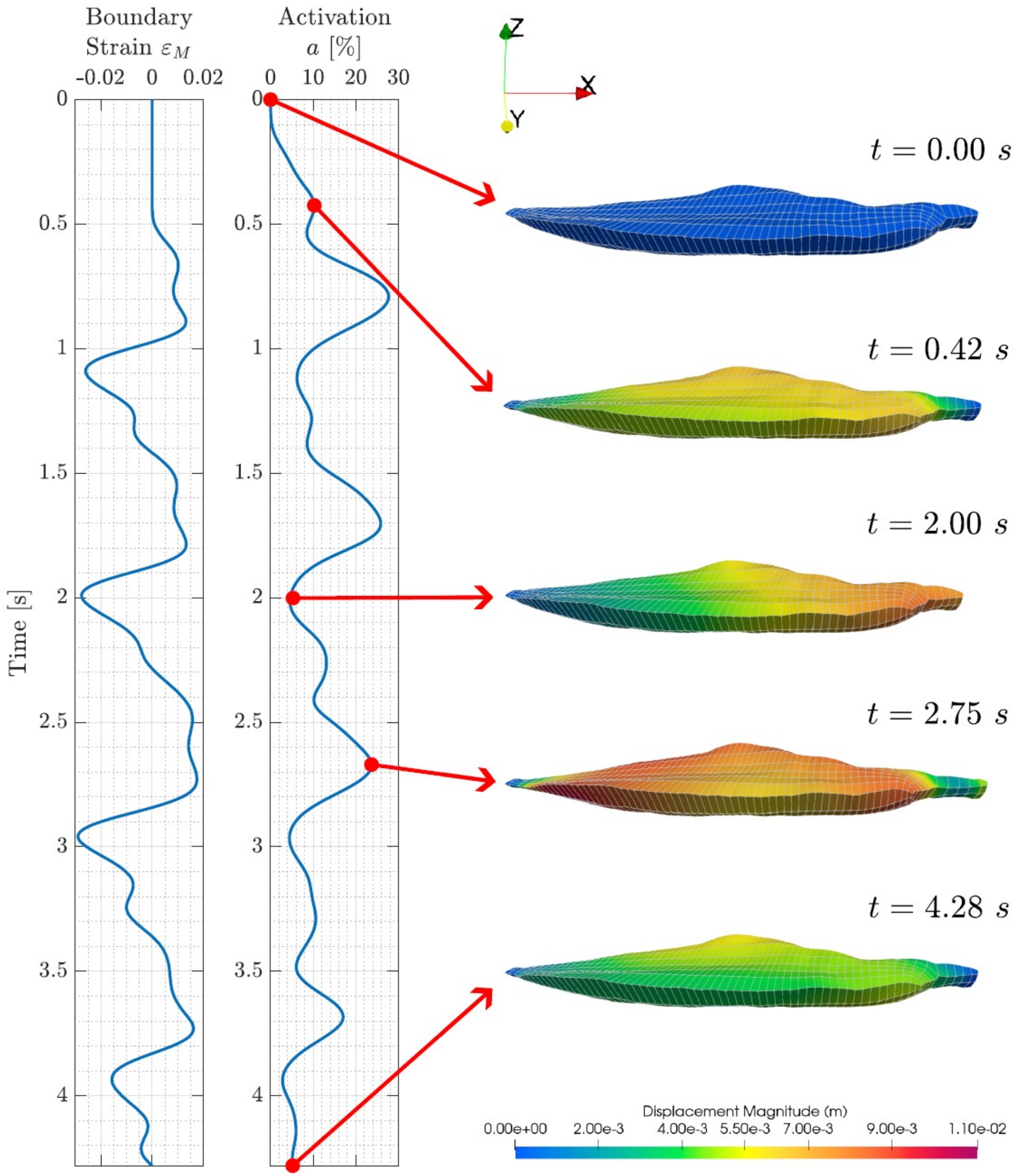




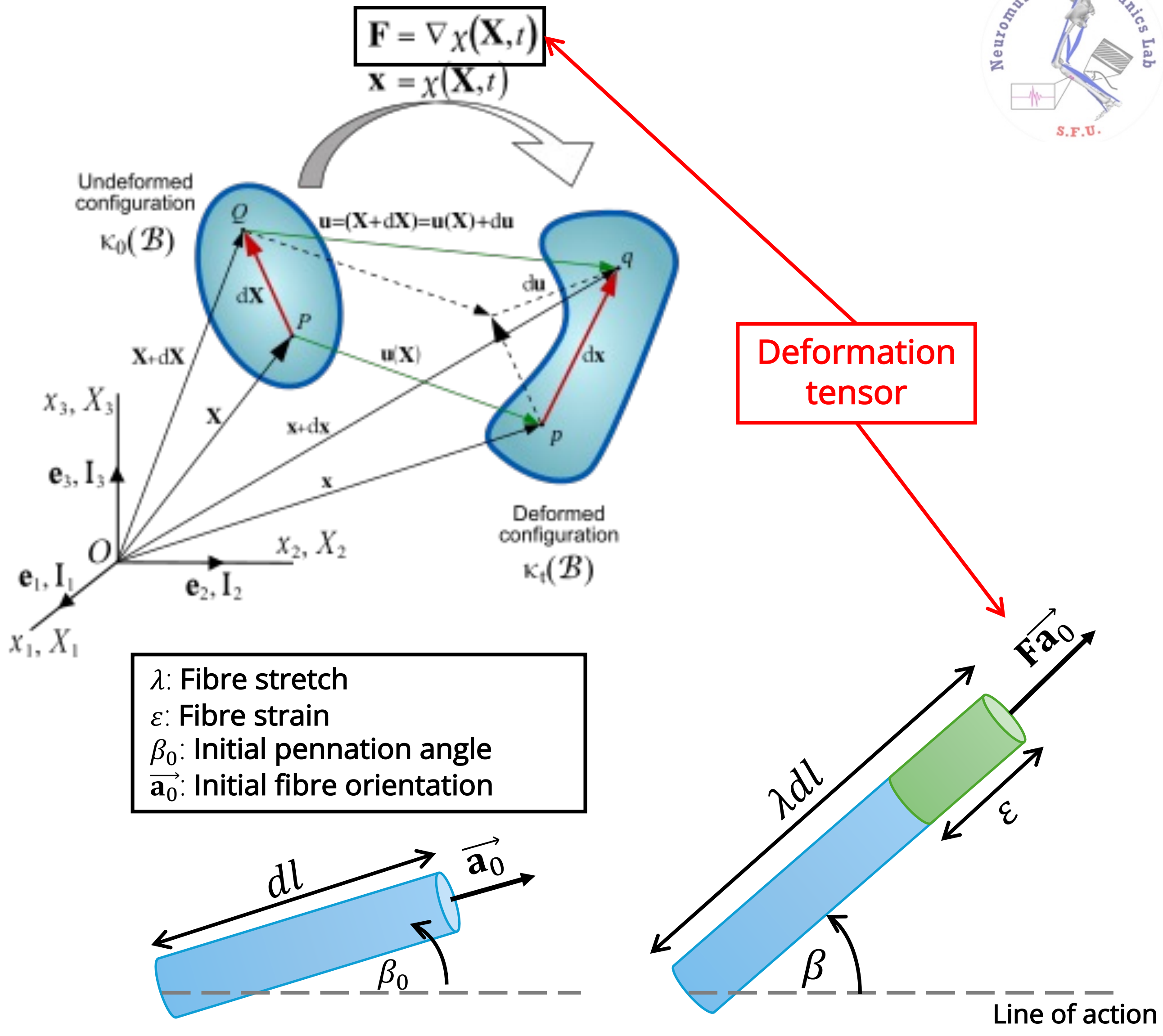
What is Flexodeal?

- It is a computational framework developed by the NML to simulate the dynamic deformation of active muscle tissue in 3D based on commonly-accepted physiological principles.
- Written in C++, powered by deal.II.
- Discretization based on finite elements.
- Geometries are meshed using hexahedral elements (voxels).



Main Features

- Local minimization of the total energy leads to a system of nonlinear PDEs in a **three-field formulation** (Simo et al. 1985).
- Stress modelled as the additive response of:
  - An **along-fibre** component (Hill's model),
  - Base material,
  - Intramuscular fat,
  - Tendon,
  - Aponeurosis.

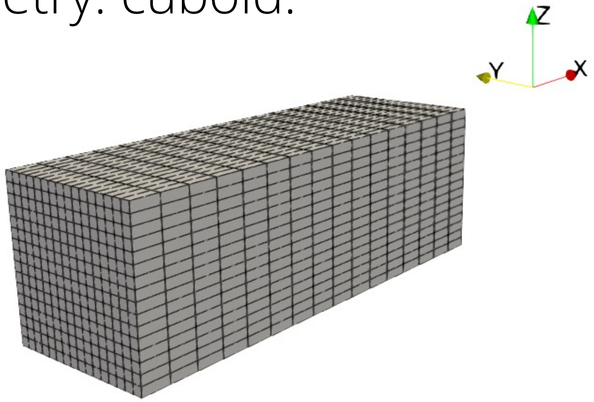


Undeformed configuration $\longrightarrow$ $\mathbf{x} = \chi(\mathbf{X}, t)$ $\longrightarrow$ Deformed configuration

Available in two versions

Flexodeal Lite (Tutorial 1)
github.com/sfu-nml/flexodeal-lite

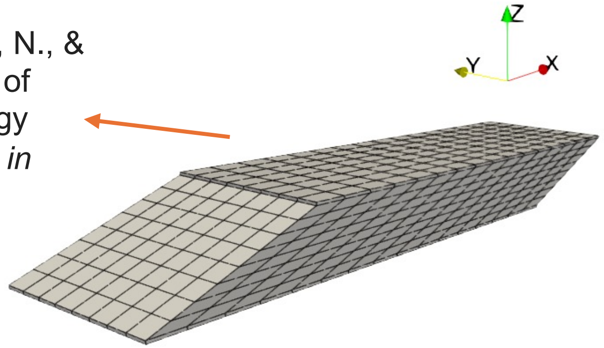
- A simpler code suitable for numerical developments or simple experiments.
- Supports muscle tissue only (no tendon or aponeurosis).
- Fat-free muscle (by default).
- Default geometry: cuboid.



Flexodeal (Tutorial 2)
github.com/sfu-nml/flexodeal

- A more complex code suitable for realistic experiments of the muscle-tendon unit.
- Support muscle tissue, tendon, and aponeurosis.
- Spatially-variable intramuscular fat.
- Spatially-variable initial fibre orientations.
- Default geometry: idealized MG.

Ross, S. A., Domínguez, S., Nigam, N., & Wakeling, J. M. (2021). The energy of muscle contraction. III. Kinetic energy during cyclic contractions. *Frontiers in physiology*, *12*, 628819



Downloading and compiling Flexodeal Lite

Description	UNIX Command
Download the latest release of Flexodeal Lite from: https://github.com/sfu-nml/flexodeal-lite/releases	wget https://github.com/sfu-nml/flexodeal-lite/archive/refs/tags/v1.6.1.zip
Unzip the downloaded file	unzip v1.6.1.zip
Navigate to the flexodeal-lite-1.6.1 folder	cd flexodeal-lite-1.6.1
Compile the software	cmake . -DCMAKE_BUILD_TYPE=Release -DDEAL_II_DIR=<path/to/deal.II>
Call "make"	make
If "make" was successful, you should now have an executable called "flexodeal-lite".	./flexodeal-lite

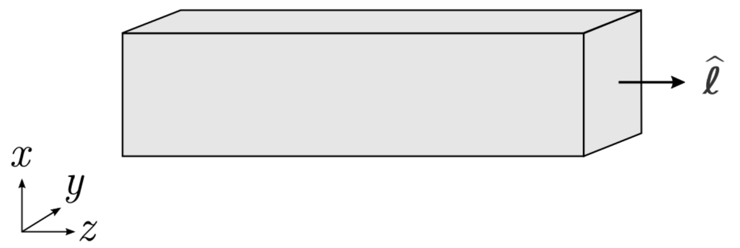
The default experiment

How to set up a computational experiment?

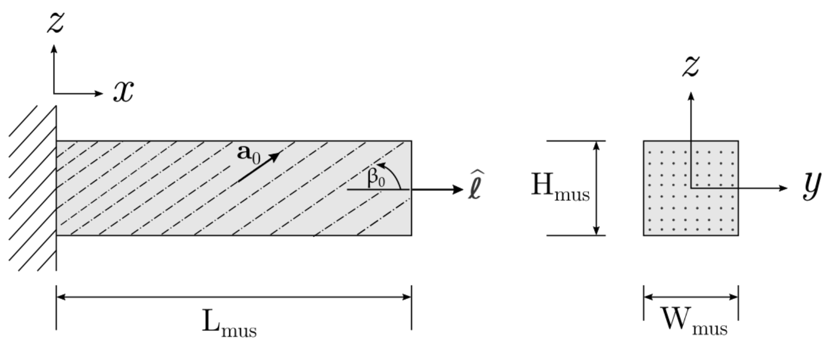
- In the Flexodeal framework, we follow the principles of computational mechanics.
- To set an experiment, you will need:
  1. A mesh of your geometry (computational domain).
  2. Model and simulation (numerical) parameters.
  3. A time-dependent boundary strain -> this controls the length of the muscle.
  4. A time-dependent activation profile.
- We will go over the details of the default experiment in Flexodeal Lite, i.e. the one you obtain when simply running in your terminal:

`./flexodeal-lite`.

Geometry (computational domain)

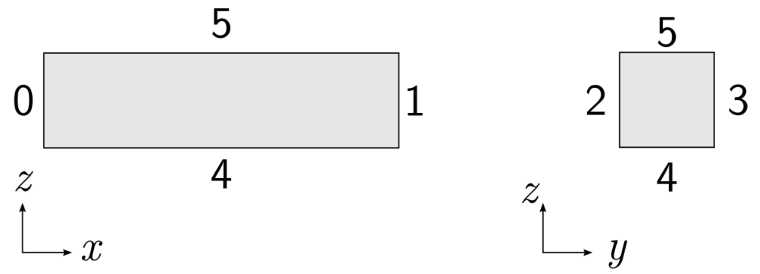


3D view. Geometry contains **muscle tissue only** (no aponeurosis or tendon).



Main parameters (can be modified in parameters file):

- L_{mus}: muscle length
- H_{mus}: muscle height
- W_{mus}: muscle width
- $\boldsymbol{a_0} = \langle cos(\beta_0), 0, sin(\beta_0) \rangle$: fibre orientation
- $\hat{\ell}$: line of action



Boundary IDs:

- 0: Fixed (no displacement)
- 1: Moving boundary (prescribed strain)
- 2-5: Traction free.

Parameters file

- A file with extension `.prm` containing several model and simulation parameters.
- Some important parameters in this file are:
  - Type of simulation (dynamic or quasi-static),
  - Simulation time and time step size,
  - Muscle block dimensions,
  - Fibre orientations,
  - Markers (to track selected point displacements),
  - Solver type (“Direct” for coarse meshes, “CG” for finer meshes),
  - Error tolerances.
- Open the **`parameters.prm`** file to see the complete list of parameters.

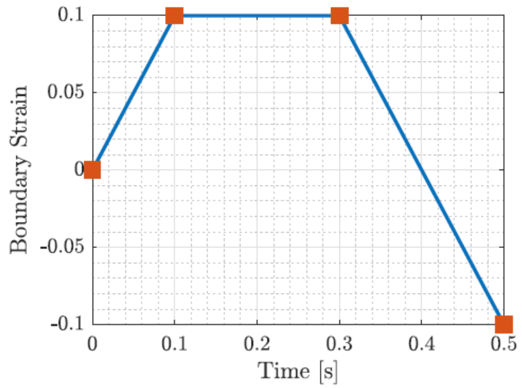
Boundary strain and activation files

- They provide the time-dependent prescribed boundary strain (on boundary ID 1 for the default experiment) and the time-dependent activation profile to the simulation.
- Each file is a table of coordinate pairs.
- Flexodeal uses linear interpolation to evaluate these functions between control points.

Strain
(e.g., 0.1 = 10% strain = lengthen muscle to 1.1L_{mus}

control_points_strain.dat	
0.0	0.0
0.1	0.1
0.3	0.1
0.5	−0.1

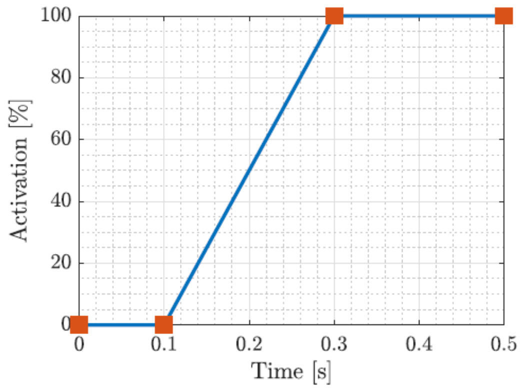
⇒



Time
(in seconds)

control_points_activation.dat	
0.0	0.0
0.1	0.0
0.3	1.0
0.5	1.0

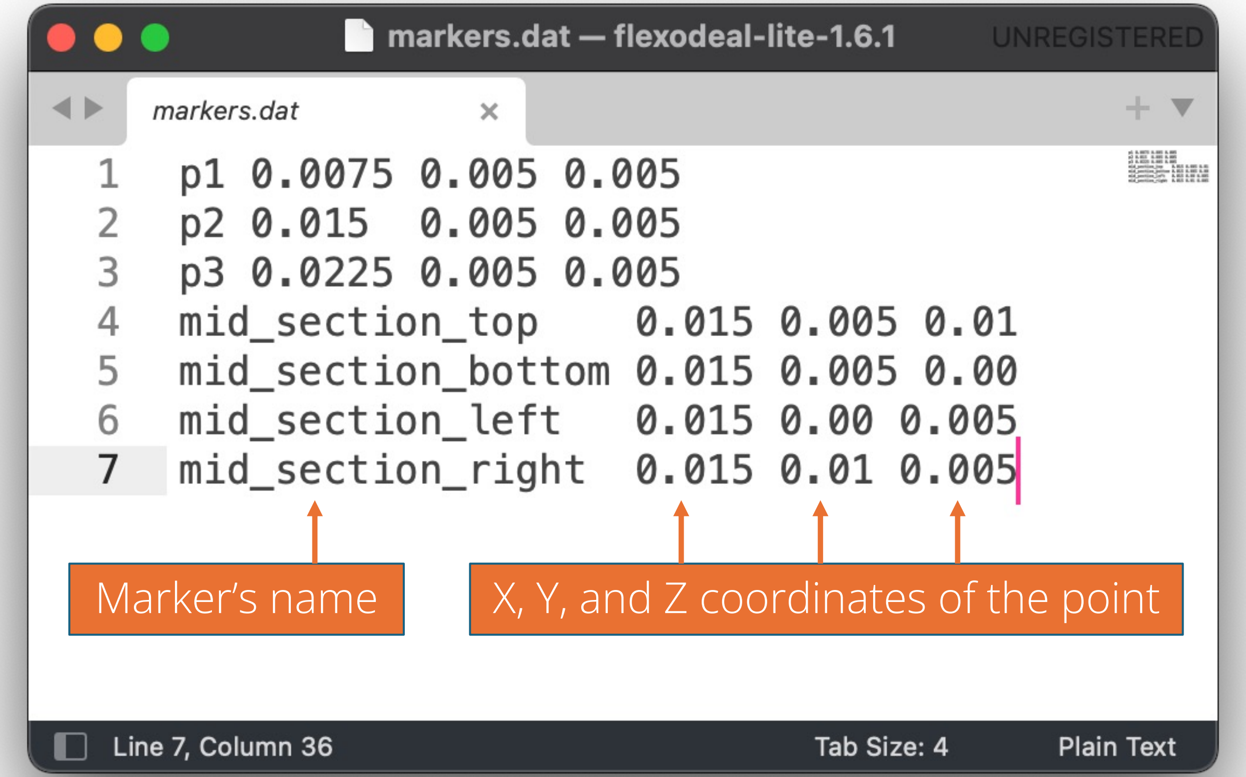
⇒



Activation
(e.g., 0.5 = 50%, 1.0 = 100%)

Markers (displacement trackers, optional)

- Although the entire 3D displacement field is available as a VTU file, we can also track this variable at point locations in the mesh.
- Markers **must correspond to** mesh vertices.
- If you do not require this feature, this file can be left empty.



Some notes

- CMake compiles a machine-dependent version of Flexodeal.
- Unless you modified the `flexodeal-lite.cc` file directly, you do not need to call `make` (or `cmake`) every time you run `./flexodeal-lite`
- The call to `./flexodeal-lite` accepts the following command-line arguments:

Argument	Default value	Description
`-PARAMETERS`	`parameters.prm`	Parameter file
`-BDY_STRAIN`	`control_points_strain.dat`	Boundary strain profile
`-ACTIVATION`	`control_points_activation.dat`	Activation profile
`-OUTPUT_DIR`	Directory name based on current time and date	Folder where the simulation results will be stored

Output files & visualization

CSV files

Description	File
Time series of activation and muscle length.	`activation_muscle_length-3d.csv`
Time series of selected point displacements (markers).	`displacements-3d.csv`
Time series of energies (kinetic, internal, volumetric, isochoric, ...).	`energy_data-3d.csv`
Time series of force at the moving end of muscle in the direction of the line of action	`force_data-3d.csv`

Vectorial force at each boundary ID at each time step	`force_data-3d-000.csv`
	`force_data-3d-001.csv`
	…

Time series of velocity averages	`gearing_info-3d.csv`
Time series of mean stretch and mean pennation angle	`mean_stretch_pennation_data-3d.csv`

ParaView files (3D fields)

Description	File

Main model unknowns: muscle displacement, pressure, dilatation.	`solution-3d-000.vtu`
	`solution-3d-001.vtu`
	…

Muscle velocity	`velocity-3d-000.vtu`
	`velocity-3d-001.vtu`
	…

Fibre stretch and fibre orientations	`stretch-3d-000.csv`
	`stretch-3d-001.csv`
	…

Fibre strain rate	`strain-rate-3d-000.csv`
	`strain-rate-3d-001.csv`
	…

Kirchhoff stress tensor	`stress-3d-000.vtu`
	`stress-3d-001.vtu`
	…

Visualization in ParaView

- Task: Open and explore any of the VTU files.
- Suggested: Rescale data range over all timesteps.
- Discussion of visualization techniques and presentation.

Running simple examples

Example 1: Isometric contraction

- Run the experiment (write everything in one line):

```
./flexodeal-lite -PARAMETERS=examples/IC_parameters.prm
-BDY_STRAIN=examples/IC_strain.dat -ACTIVATION=examples/IC_activation.dat
-OUTPUT_DIR=results_ic
```

- We consider a 3 x 1 x 1 cm block of parallel-fibred muscle tissue (no pennation).
- Fully activate the block over a span of 1 s.
- This is a quasi-static experiment. No velocity or fibre strain rate data is exported.
- This is also a benchmark experiment. At any of the fixed ends, when the activation reaches 100%:

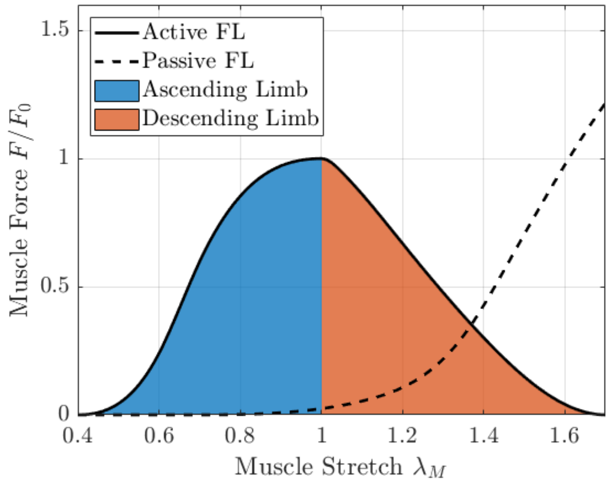
$$\text{Force} = \text{F}_0 = \sigma_0 \times \text{CSA} = 200{,}000 \text{ Pa} \times 0.01^2 \text{ m}^2 = 20 \text{ N}$$

- Hence, we expect a force of ~20 N at any of the fixed ends.

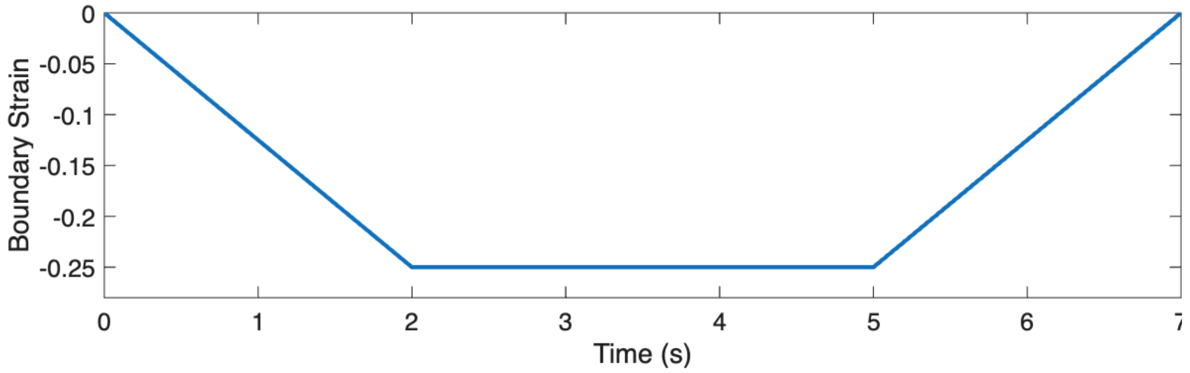
Example 2: Ascending limb contraction

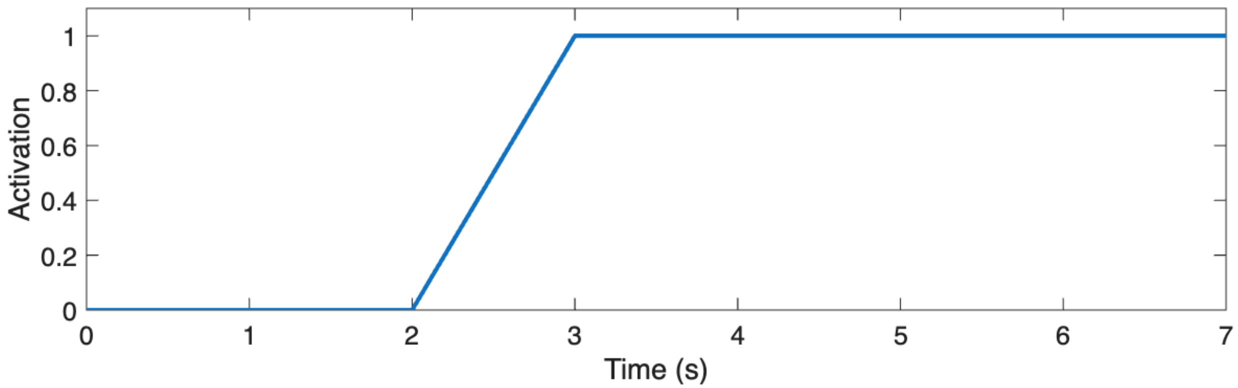
- Run the experiment (write everything in one line):

```
./flexodeal-lite -PARAMETERS=examples/AL_parameters.prm
-BDY_STRAIN=examples/AL_strain.dat
-ACTIVATION=examples/AL_activation.dat
-OUTPUT_DIR=results_al
```



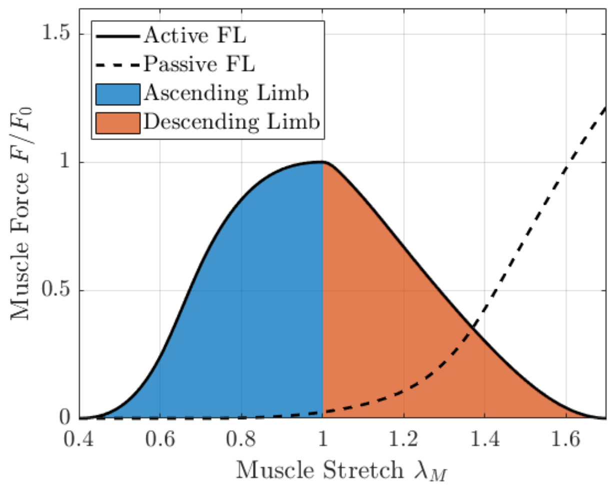
- We consider a 3 x 1 x 1 cm block of muscle-tissue, 30 deg. pennation. This is a dynamic experiment.
- Strain and activation profiles:





Try it yourself!

- Set up a contraction on the descending limb of the force-length curve as follows:
  1. Lengthen the muscle block to 1.1 times its initial length (or +10% strain) over 2 seconds.
  2. Then, perform an isometric contraction over 1 second, activating the muscle to 50%.
  3. Shorten the muscle back to its initial length over 2 seconds.
- You can assume the same geometry and muscle architecture as for the ascending limb contraction.



More Resources

- Finite element simulation using deal.II: https://www.dealii.org/current/doxygen/deal.II/Tutorial.html
- Mathematical details of Flexodeal:
  - Almonacid, J. A., Domínguez-Rivera, S. A., Konno, R. N., Nigam, N., Ross, S. A., Tam, C., & Wakeling, J. M. (2024). A three-dimensional model of skeletal muscle tissues. *SIAM journal on applied mathematics*, *84*(3), S538-S566.
  - Almonacid Paredes, J. A. (2025). On the nonlinear elastodynamics of skeletal muscle (Chapters 5 and 6). PhD Thesis, Simon Fraser University (available at www.sfu.ca/~javiera).
- ParaView documentation: https://docs.paraview.org/en/v5.13.1/UsersGuide/introduction.html

www.github.com/sfu-nml

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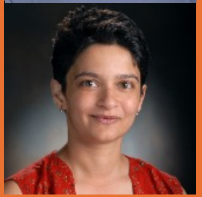
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