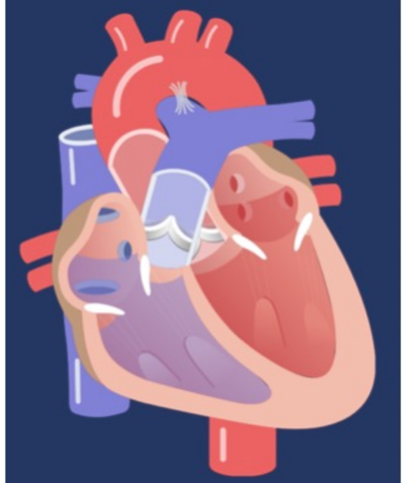
UNIVERSITÀ DI PAVIA
Corso di Dottorato in Computational Mathematics and Decision Sciences

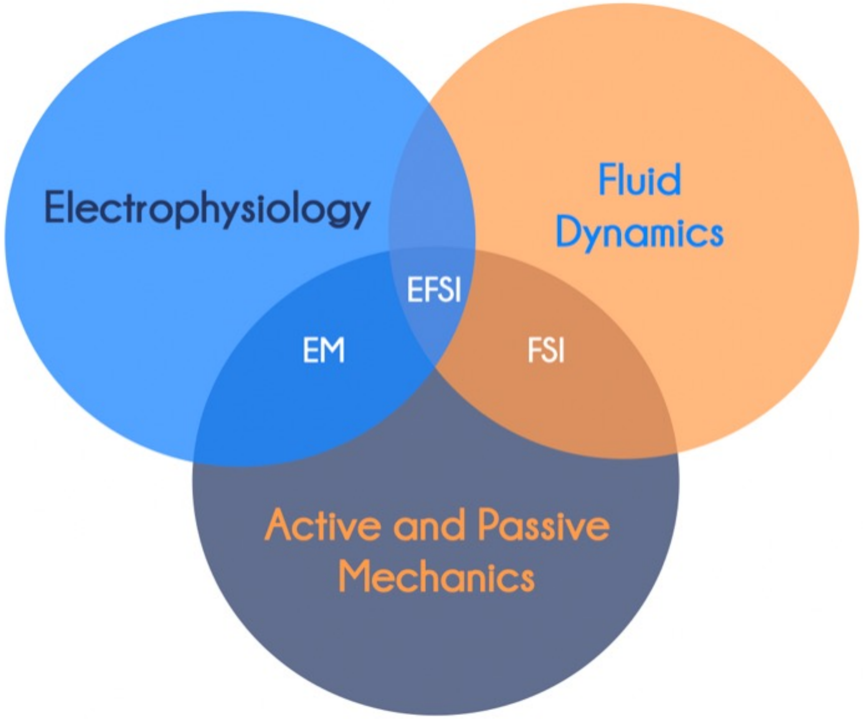
Università della Svizzera italiana

An electro-fluid-structure model based on an embedded strategy with application to cardiac simulations

Silvia Caligari
Supervisor: Prof. Rolf Krause
CoSupervisor: PostDoc Maria Giuseppina Nestola
PostDoc Marco Favino

COMPMAT2022
Spring Workshop 2022
16^{th} – 17^{th} March 2022





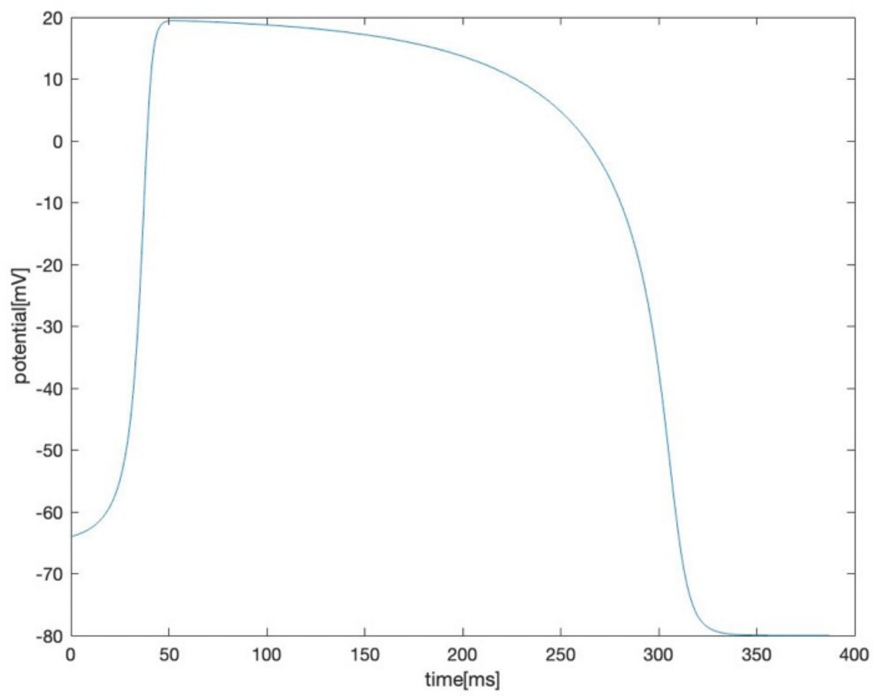
Goal of the Project

Multiphysics Simulation of cardiac tissue

Modeling and computational challenges

- **Multiphysics interactions**: Electrophysiology, Active and Passive Mechanics and Fluid-Dynamics
- **Nonlinear** Coupled Problem
- Numerical systems computationally **expensive** to solve

A fully explicit high order time integrator for the Monodomain system



A simplified complete model of cardiac electrical activity is the anisotropic **Monodomain model**, able to describe the evolution of the transmembrane potential.

$$\chi C_m \frac{\partial v}{\partial t} - \nabla \cdot (D(\mathbf{x}) \nabla v) + F(v,w) = 0 \quad \textbf{on } \Omega \times (0,T)$$

$$\frac{\partial w}{\partial t} = G(v,w) \quad \textbf{on } \Omega \times (0,T)$$

Space Discretization:

Finite Element Method

Examples of Time integrators:

- IMEX
- Splitting Operator

Time integrator proposed:

- Splitting Operator + predictor-corrector

Fractional Step Method:

Consider an initial value problem of the form

$$\frac{\partial u}{\partial t} = \left(L_1 + L_2\right) u \qquad \textbf{for } t \in [0,T]$$
$$u(0) = u_0$$

Godunov (order 1)

1) $\frac{\partial v}{\partial t} = L_1(v)$, $v(0) = u_0$ $\quad [0,\Delta t]$

2) $\frac{\partial \hat{u}}{\partial t} = L_2(\hat{u})$, $\hat{u}(0) = v(\Delta t)$ $\quad [0,\Delta t]$

Strang (order 2)

1) $\frac{\partial v}{\partial t} = L_1(v)$, $v(0) = u_o$ $\quad [0,\Delta t/2]$

2) $\frac{\partial \hat{u}}{\partial t} = L_2(\hat{u})$, $\hat{u}(0) = v(\Delta t/2)$ $\quad [0,\Delta t]$

3) $\frac{\partial v}{\partial t} = L_1(v)$, $v(\Delta t/2) = \hat{u}(\Delta t)$ $\quad [\Delta t/2,\Delta t]$

- Time Discretization L_1 operator (order 2):

1) $\hat{u}(\Delta t) = u_0 + \Delta t F(u_0, w_0)$

$\hat{w}(\Delta t) = w_0 + \Delta t G(u_0, w_0)$

Predictor

2) $u(\Delta t) = u_0 + \Delta t F\left(\frac{u_0 + \hat{u}(\Delta t)}{2}, \frac{w_0 + \hat{w}(\Delta t)}{2}\right)$

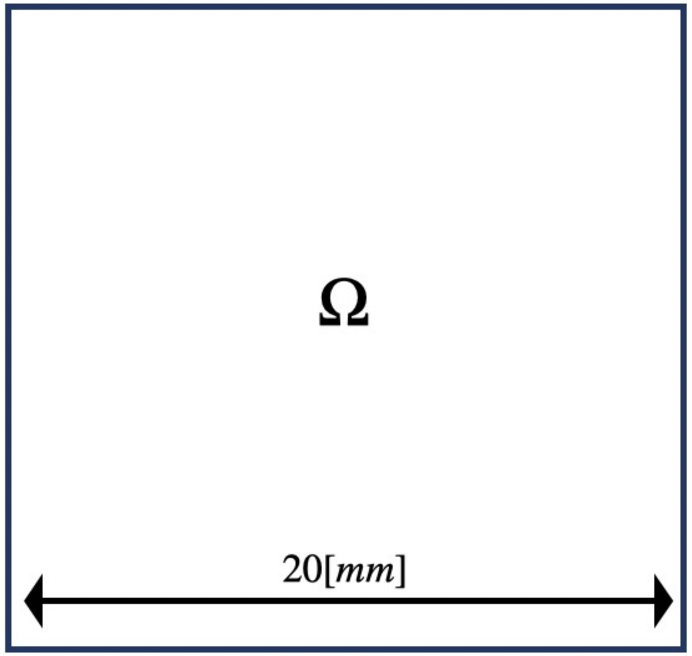
$w(\Delta t) = w_0 + \Delta t G\left(\frac{u_0 + \hat{u}(\Delta t)}{2}, \frac{w_0 + \hat{w}(\Delta t)}{2}\right)$

Corrector

- Time Discretization L_2 operator (Θ-method, order 2):

$$\frac{u^{n+1} - u^n}{\Delta t} = \theta L_i(v^{n+1}) + (1-\theta) L_i(v^n) \quad \text{with} \quad \theta = \frac{1}{2}$$

- Time Discretization L_1 and L_2 order 1: Θ-method



"A Simple Two-variable Model of Cardiac Excitation"

Rubin R. Aliew and Alexander V. Panfilov

$$\frac{\partial u}{\partial t} = d\frac{\partial^2 u}{\partial x^2} - ku(u-a)(u-1) - uw + I_{app}(x,t)$$

$$\frac{\partial w}{\partial t} = (\epsilon_0 + \mu_1 \frac{w}{u+\mu_2})(-w - ku(u-a-1))$$

$k = 8.0$	$d = 0.001$
$a = 0.15$	$\mu_1 = 0.2$
$\epsilon_0 = 0.002$	$\mu_2 = 0.3$

The model involves dimensionless variables ***u***, ***w*** and ***t***. The actual transmembrane potential ***V*** and time ***t*** can be obtained by the formulae:

$$V[mV] = 100.0u - 80.0$$

$$t[ms] = 12.9t[t.u.]$$

Convergence Studies:

- Smooth Initial Condition:

$$V_0 = V(0) = -\frac{1}{\pi}\arctan\left(20 \cdot (x^2 + y^2 - 12.0)\right) + 0.5$$

- Reference configuration: $N_{ref} = 3200 \quad \Delta t = 0.001$

- Convergence results in 1D using Strong splitting:

elements	time step	L_2 error	order_convergence
40	0.25	0.0729	0
80	0.125	0.018	2.0185
160	0.0625	0.0045	2.0011
320	0.03125	0.0011	2.0099

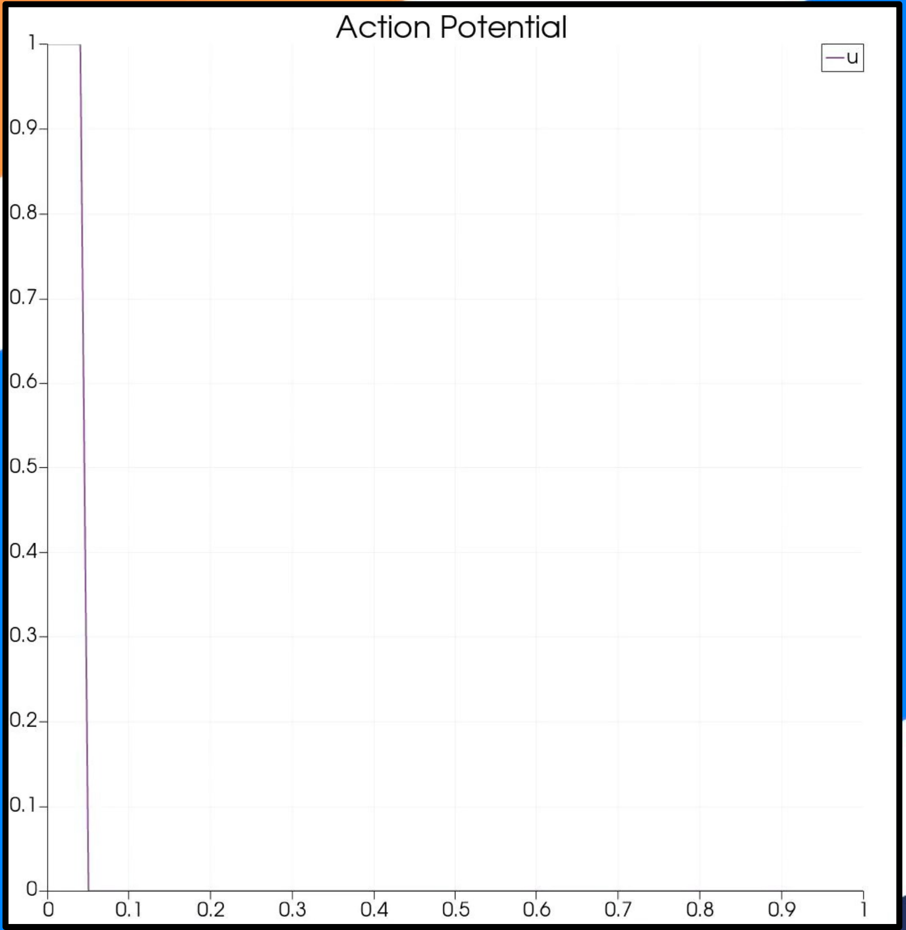
- Convergence results in 2D using Strong splitting:

elements	time step	L_2 error	order_convergence
"40x40"	0.25	0.32768	0
"80x80"	0.125	0.077255	2.0846
"160x160"	0.0625	0.018886	2.0323
"320x320"	0.03125	0.0066277	1.5107
"640x640"	0.015625	0.0011558	2.5196

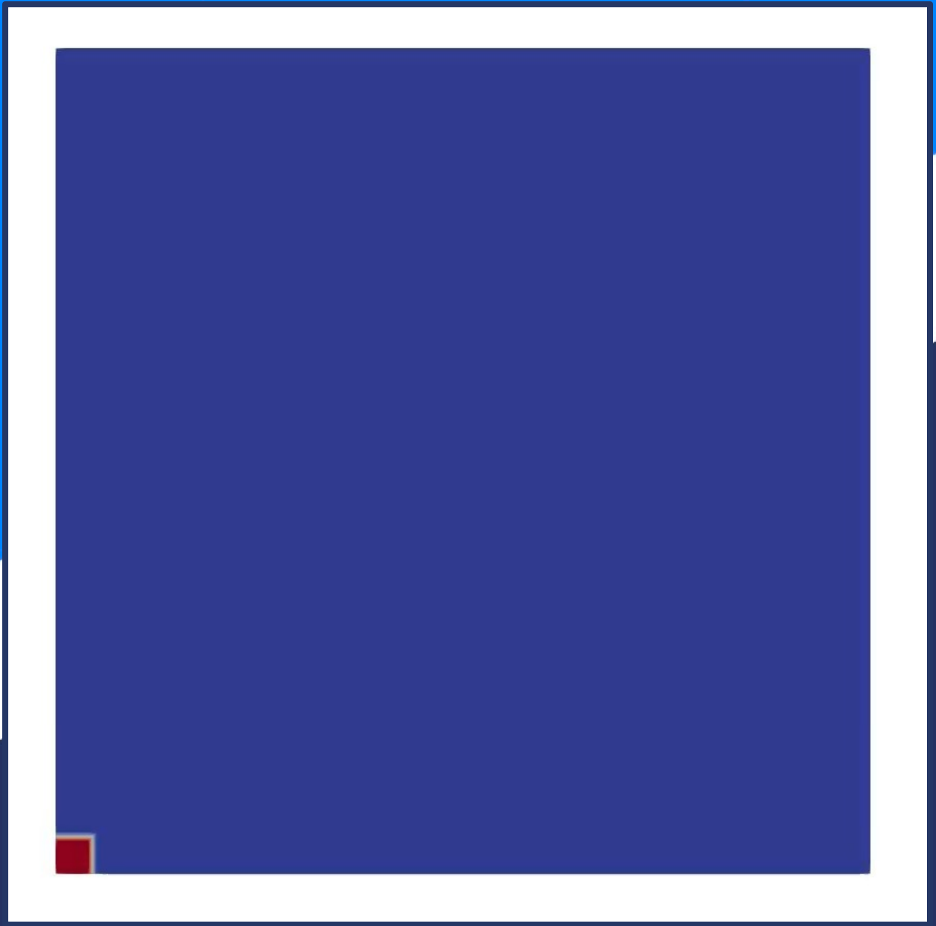
Reference : Computing the Electrical Activity of the Heart
J. Sundnes et al.

Numerical Results

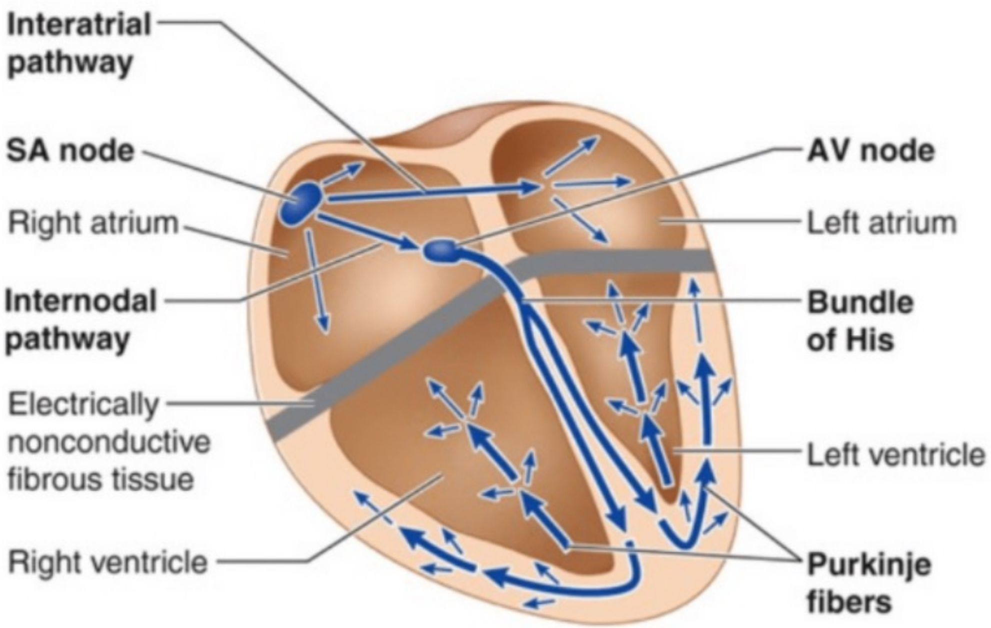
Panfilov Model in 1D



Panfilov Model in 2D



Pony: a software library for Electrophysiology



- FHN model
- Monodomain Model with LuoRudy ionic Model (including Calcium dynamics)
- FHN model with operator splitting (predictor-corrector)
- Panfilov model (FHN modified) with operator splitting (predictor corrector)
- Diffusion model with operator splitting (Halley and Newton methods)

Luo-Rudy Model

We coupled the **Monodomain** equation with **Luo-Rudy Ionic Model** , where ionic current I_{ion} is the sum of six ionic currents.

$$\chi C_m \frac{\partial v}{\partial t} - \nabla \cdot (D(\mathbf{x}) \nabla v) + \chi I_{ion}(v, w) = I_{app} \quad \textbf{on } \Omega \times (0,T)$$

$$\frac{\partial w}{\partial t} = R(v, w) \quad \textbf{on } \Omega \times (0,T)$$

with $\quad I_{ion} = I_{Na} + I_{si} + I_K + I_{K1} + I_{KP} + I_b$

- **Space Discretization:**

  Finite Element Method

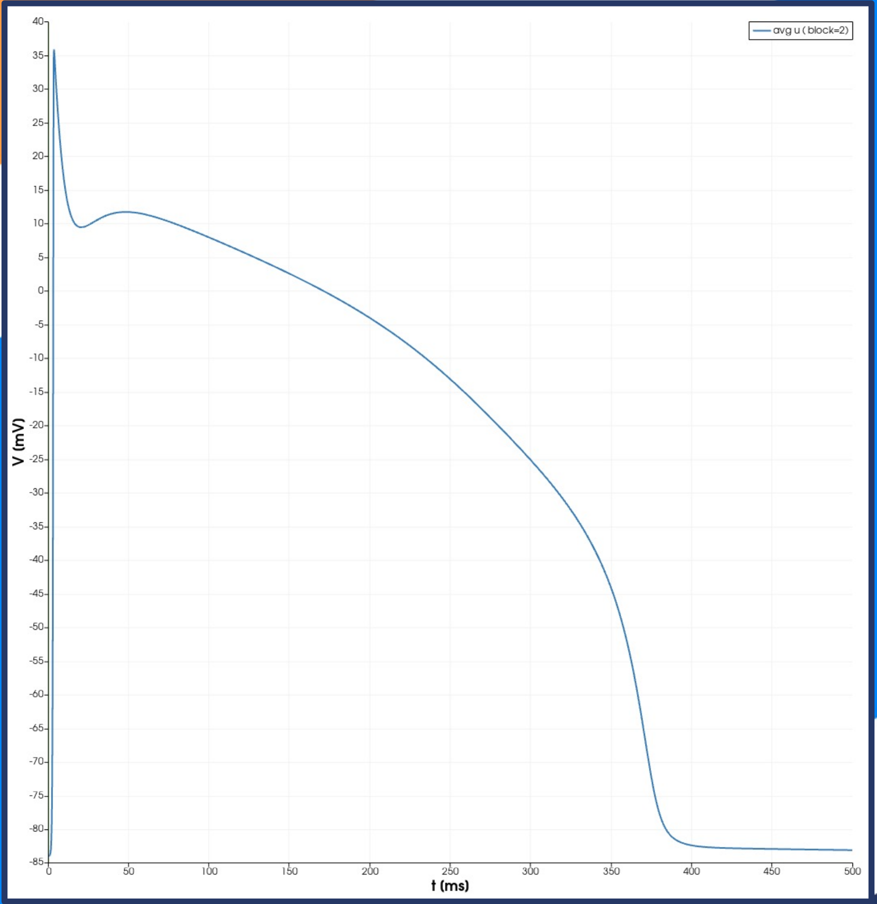
- **Time Discretization:**

  Gating equations, associated with ionic currents, are implemented with **Rush-Larsen Method**, using the potential at the previous time step v^{n-1}.
  Then we can use w^n for obtaining the solution of the Monodomain equation v^n:

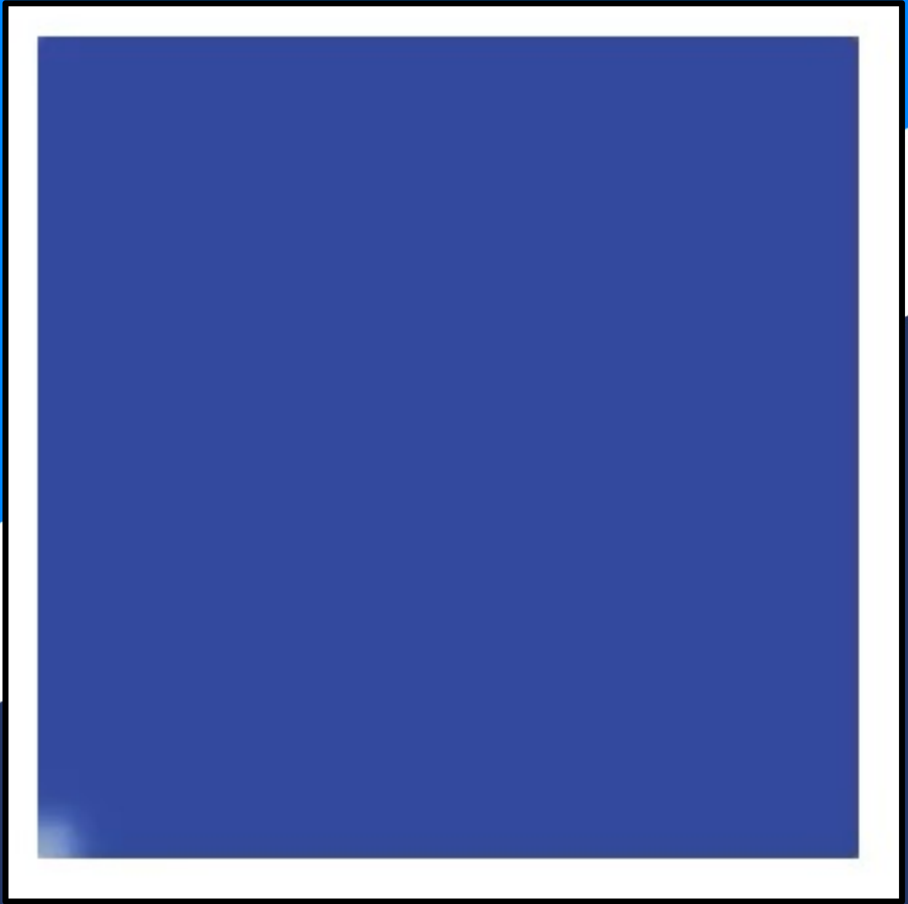
$$\chi C_m \frac{v^n - v^{n-1}}{dt} - Dv^n + \chi I_{ion}(v^{n-1}, w^n) = I_{app}(t_n)$$

Numerical Results

LuoRudy Action Potential



LuoRudy Model in 2D



Fluid Structure Interaction Problem

Main **difficulties** related to numerical simulation FSI problems:

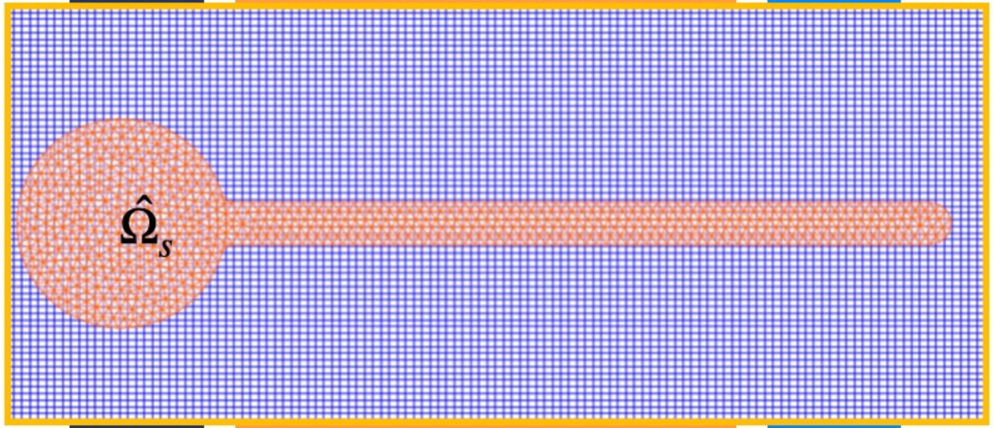
- **Two-field problem** where the two phases are separated by a common boundary whose position is an unknown of the problem
- Thin and/or bulky solid structures which may exhibit **large deformations**
- Simulations involving **transition** from **laminar** to **turbulent** flow
- The treatment of the **interface conditions** ensuring the **continuity** of the **velocity** and the **stress**

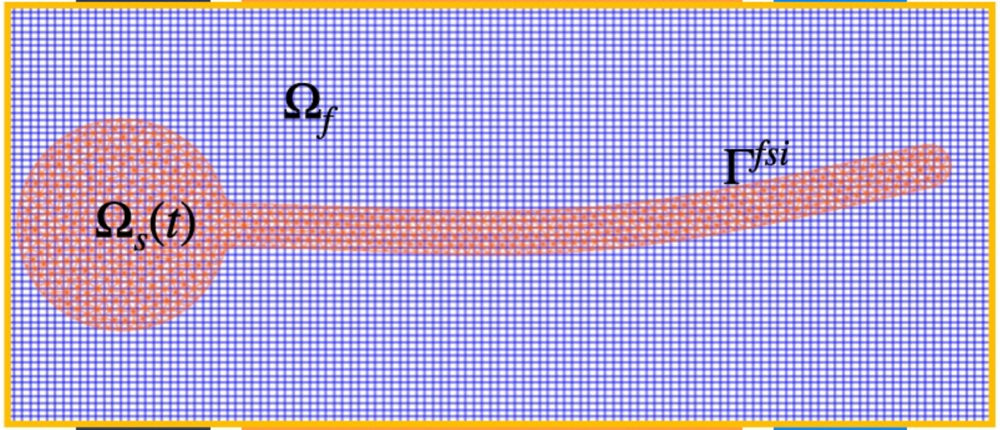
The **main feature** of the proposed methodology is the combination of:

☑ A high-order Navier-Stokes solver

☑ An L^2-projection approach for coupling the Eulerian and the Lagrangian variables

☑ The solution of the elastodynamics equation





FSI: Mathematical Model

The **strong formulation** of FSI problem reads as follow:

Solid subproblem:

$$\hat{\rho}_s \frac{\partial^2 \hat{\mathbf{u}}_\mathbf{s}}{\partial t^2} - \hat{\nabla} \cdot \hat{\mathbf{P}} = \mathbf{0} \qquad \text{in } \hat{\Omega}_s \times (0,T)$$

$$\hat{\mathbf{u}}_\mathbf{s} = \hat{\mathbf{u}}_\mathbf{b} \qquad \text{on } \hat{\Gamma}_s^d$$

Fluid subproblem:

$$\rho_f \frac{\partial \mathbf{v}_\mathbf{f}}{\partial t} + \rho_f(\mathbf{v}_\mathbf{f} \cdot \nabla)\mathbf{v}_\mathbf{f} + \nabla p_f - \mu_f \Delta \mathbf{v}_\mathbf{f} = \mathbf{0} \qquad \text{in } \Omega_f \times (0,T)$$

$$\nabla \cdot \mathbf{v}_\mathbf{f} = \mathbf{0} \qquad \text{in } \Omega_f \times (0,T)$$

$$\mathbf{v}_\mathbf{f} = \mathbf{v}_\mathbf{b} \qquad \text{on } \Gamma_f^d$$

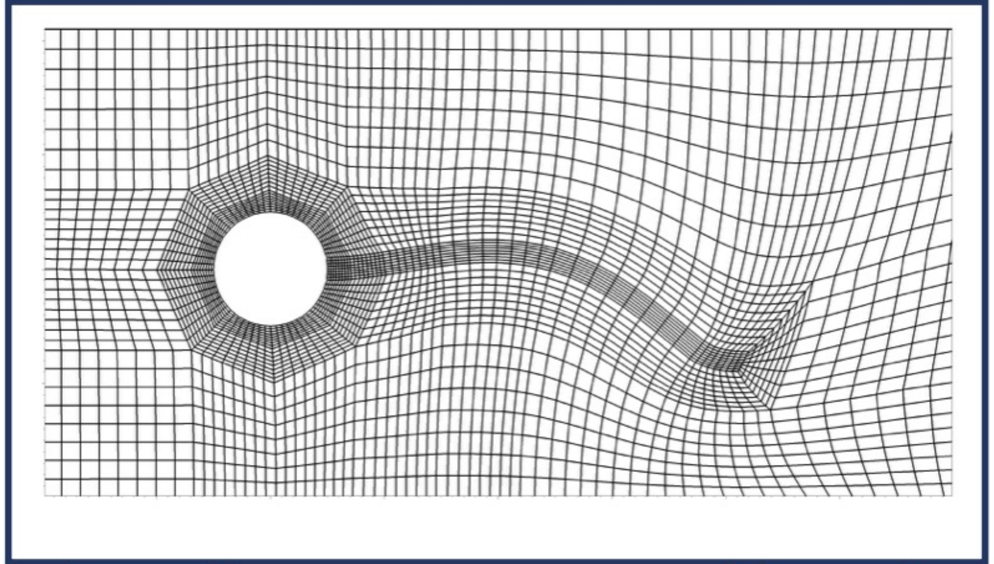
Fsi coupling:

$$\mathbf{v}_\mathbf{f} = \frac{\partial \mathbf{u}_\mathbf{s}}{\partial t} \qquad \text{on } \Gamma^{fsi}$$

$$\hat{J}^{-1}\hat{\mathbf{P}}\hat{\mathbf{F}}^\mathbf{T}\mathbf{n} = \sigma_\mathbf{f}\mathbf{n} \qquad \text{on } \Gamma^{fsi}$$

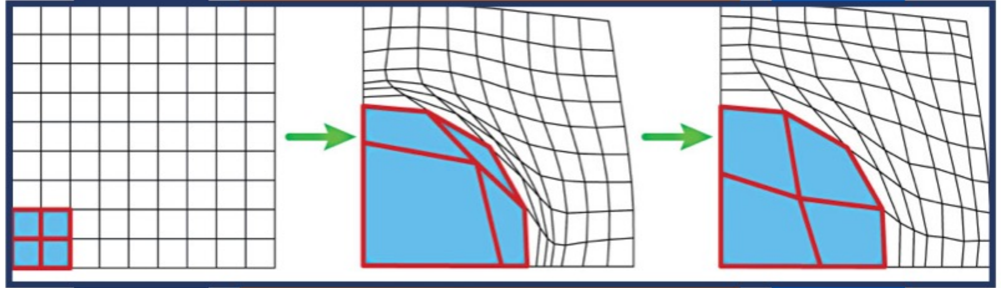
+ Initial Conditions

Boundary-Fitted Methods

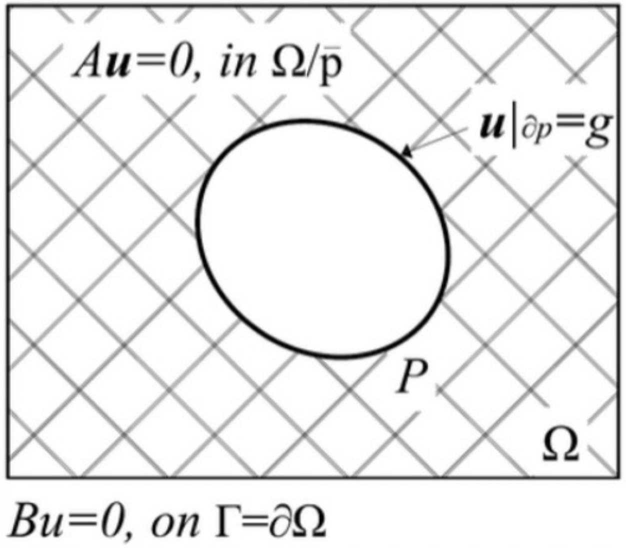


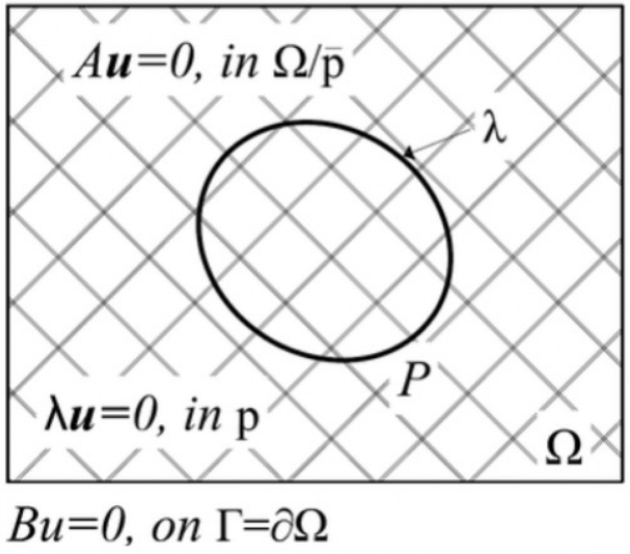
- Fluid subproblem is solved in a **moving spatial domain**
- Navier-Stokes equations are formulated in an **Arbitrary Lagrangian Eulerian** framework
- Solid structure is usually analysed in a Lagrangian fashion

☑ **Accurate results at the interface**



- **Large displacements** and/or rotations may involve distortions of the fluid grid.
- The generation of a body-fitted grid is **time consuming** and **computationally expensive**





Immersed Boundary Methods

- The presence of the immersed solid is accounted by a force term in the Navier-Stokes equations
- Combination with Mortar Method
- L^2-projection approach for handling the interface conditions: the velocity continuity and force exchange.

Solid subproblem:

$$\hat{\rho}_s \frac{\partial^2 \hat{\mathbf{u}}_\mathbf{s}}{\partial t^2} - \hat{\nabla} \cdot \hat{\mathbf{P}} = \mathbf{0} \qquad \text{in } \hat{\Omega}_s$$

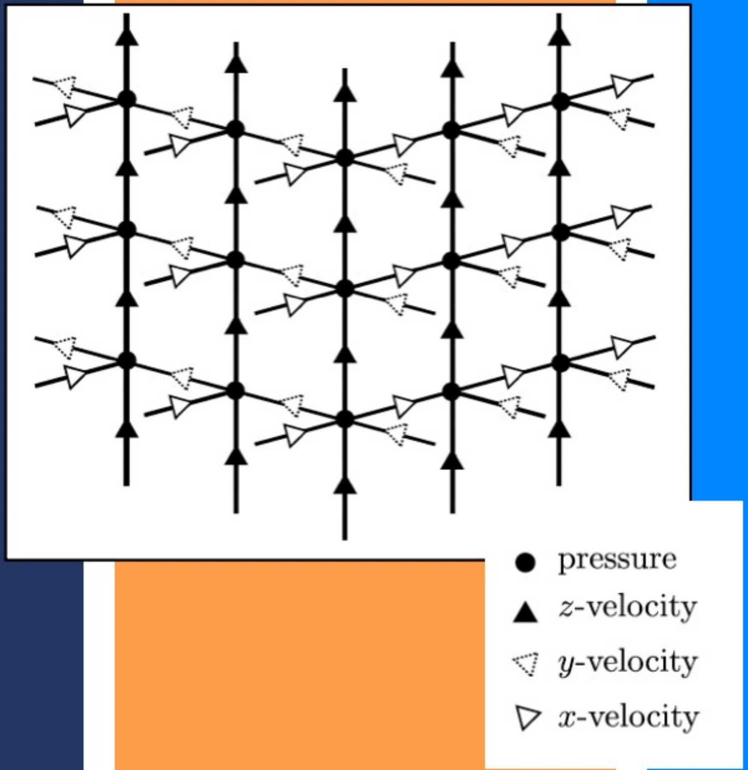
$$\hat{\mathbf{u}}_\mathbf{s} = \hat{\mathbf{u}}_\mathbf{b} \qquad \text{on } \hat{\Gamma}_s^d$$

Fluid subproblem:

$$\rho_f \frac{\partial \mathbf{v_f}}{\partial t} + \rho_f(\mathbf{v_f} \cdot \nabla)\mathbf{v_f} + \nabla p_f - \mu_f \Delta \mathbf{v_f} = \mathbf{f}_{fsi} \qquad \text{in } \Omega_f$$

$$\nabla \cdot \mathbf{v_f} = \mathbf{0} \qquad \text{in } \Omega_f$$

$$\mathbf{v_f} = \mathbf{v_b} \qquad \text{on } \Gamma_f^d$$



An Immersed Boundary method for Fluid-Structure interaction based on variational transfer,
Maria Giuseppina Chiara Nestola et al., Journal of Computational Physics , 2019

- **Spatial Discretization of the Solid Subproblem**

Adopted Method: **Finite Element.**

Let $\{\hat{\varphi}^h_{s,i}\}_{i\in J_s}$ the Lagrange basis of the function space $\hat{V}^h_s := \{H^1_{\hat{\Gamma}^d_2}(\hat{\Omega}^h_s) \cap \hat{X}^h_s\}$.

$$\int_{\hat{\Omega}_s} \hat{\rho}_s \frac{\partial^2 \hat{\mathbf{u}}^h_s}{\partial t^2} \cdot \hat{\varphi}^h_{s,i} d\hat{V} + \int_{\hat{\Omega}^h_s} \hat{\mathbf{P}}(\hat{\mathbf{u}}^h_s) : \hat{\nabla} \hat{\varphi}^h_{s,i} d\hat{V} = \int_{\hat{\Gamma}^{fsi}} \hat{\mathbf{P}}(\hat{\mathbf{u}}^h_s)\hat{\mathbf{n}} \cdot \hat{\varphi}^h_{s,i} d\hat{S} \quad \forall \hat{\varphi}^h_{s,i}$$

Let us define the force exerted from the solid structure to the fluid

$$(\mathbf{F}^h_{fsi}, \cdot)_{L^2(\hat{\Omega}_s)} = (\hat{\mathbf{P}}(\hat{\mathbf{u}}^h_s)\hat{\mathbf{n}}, \cdot)_{L^2(\hat{\Gamma}^{fsi})}$$

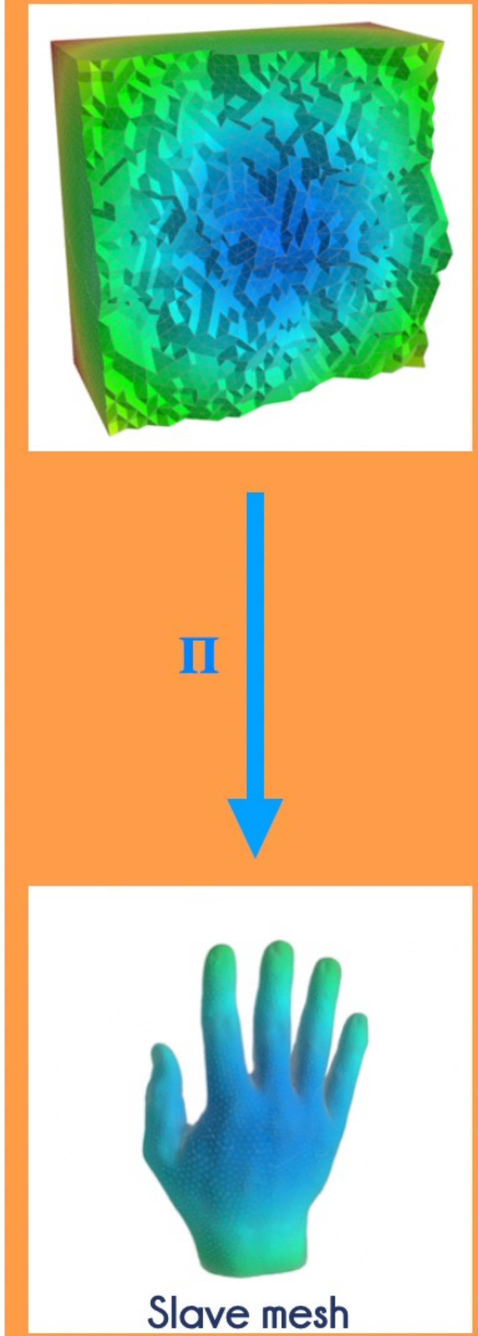
- **Spatial Discretization of the Fluid Subproblem**

Adopted Method: **Finite Difference**

Navier-Stokes equations for incompressible flow can be written in the following matrix form:

$$\rho_f \frac{\partial}{\partial t} \begin{bmatrix} \mathbf{v}^h_f \\ 0 \end{bmatrix} + \begin{bmatrix} -L & G \\ D & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^h_f \\ p_f \end{bmatrix} = \begin{bmatrix} N(\mathbf{v}^h_f) + \mathbf{f}^h_{fsi} \\ 0 \end{bmatrix}, \qquad f_{fsi}(\boldsymbol{x}, t) = \int_{\Omega_s} F_{fsi}(\boldsymbol{X}, t)\delta(\boldsymbol{X} - \chi(\boldsymbol{X}, t))\, d\Omega$$

The discretisation in space is done by using finite-difference on a staggered grid setup with individual grids for the pressure and each velocity component.



- **Spatial Discretization of the Fluid-Structure coupling:**

The Navier-Stokes equations and the solid dynamics are coupled by means of L^2**-projections** over the whole overlapping domain I_h.

Let introduce a discrete space of Lagrange Multipliers M^h_{fsi} ,based on the current configuration of the **slave mesh** $T^h_s(t)$, and the FSI **projection operator**

$$\Pi : V^h_f(T^h_f) \rightarrow V^h_s(T^h_s(t))$$
$$v^h_f \rightarrow w^h_s$$

Let $\{\varphi^h_{s,i}\}_{i\in J_s}$, $\{\varphi^h_{f,j}\}_{j\in J_f}$ and $\{\varphi^h_{fsi,k}\}_{k\in J_{si}}$ the Lagrange basis function of the spaces V^h_s, V^h_s and M^h_{fsi} . The projected velocity field $\mathbf{w}^h_s$ can be found as:

$$\int_{I_h} (v^h_f - \Pi(v^h_f))\lambda^h_{fsi} dV = \int_{I_h} (v^h_f - w^h_s)\lambda^h_{fsi} dV = 0 \quad \forall \lambda^h_{fsi} \in M^h_{fsi}$$

In matrix form:

$$\mathbf{R}\mathbf{w}_s = \mathbf{B}\mathbf{v}_f$$

where $R_{k,i} = \int_{I_h} \varphi^h_{s,i}\varphi^h_{sfi,k} dV \quad B_{k,j} = \int_{I_h} \varphi^h_{j,f}\varphi_{fsi,k} dV$

- A **fully implicit** treatment of the coupling is used for the **time** discretization .

  For the time discretisation of the **elastodynamics equation** the following scheme is adopted (**Newmark scheme**)

$$\hat{\rho}_s \mathbf{m} \frac{\hat{\mathbf{u}}_\mathbf{s}^{\mathbf{n+1}}}{\Delta t^2} + \mathbf{k}(\hat{\mathbf{u}}_\mathbf{s}^{\mathbf{n+1}}) = \mathbf{m}\mathbf{F}_\mathbf{fsi}^{\mathbf{n+1}} + \hat{\rho}_s \mathbf{m} \left(\frac{2\hat{\mathbf{u}}_\mathbf{s}^{\mathbf{n}}}{\Delta t^2} - \frac{\hat{\mathbf{u}}_\mathbf{s}^{\mathbf{n-1}}}{\Delta t^2} \right)$$

  For the discretization of the **Navier-Stokes equations** we use a **third order Runge-Kutta** scheme:

$$\begin{bmatrix} \mathbf{J} & \mathbf{G}^m \\ \mathbf{0} & \mathbf{D}\mathbf{J}^{-1}\mathbf{G}^m \end{bmatrix} \begin{bmatrix} \mathbf{v}_f^m \\ p_f^m \end{bmatrix} = \begin{bmatrix} \mathbf{q}(\mathbf{v}_f^{m-1}, \mathbf{v}_f^{m-2}, \mathbf{f}_{fsi}^{n+1}) \\ \mathbf{D}\mathbf{J}^{-1}\mathbf{q}(\mathbf{v}_f^{m-1}, \mathbf{v}_f^{m-2}, \mathbf{f}_{fsi}^{n+1}) \end{bmatrix}$$

  where $\mathbf{v}_f^{m=0} = \mathbf{v}_f^n$ and $\mathbf{v}_f^{m=3} = \mathbf{v}_f^{n+1}$.

A strategy for solving the FSI system is the **Block-Gauss-Seidel method** iterating between the fluid and solid subproblems.
The iterative procedure terminates at $l = L$ when one of the following two convergence criteria is satisfied:

Absolute convergence criterion

$$\| \mathbf{f}_{s\to f}^{l+1} - \mathbf{f}_{s\to f}^{l} \|_\infty < \epsilon_A$$

Relative convergence criterion

$$\frac{\| \mathbf{f}_{s\to f}^{l+1} - \mathbf{f}_{s\to f}^{l} \|_\infty}{\| \mathbf{f}_{s\to f}^{0} \|} < \epsilon_R$$

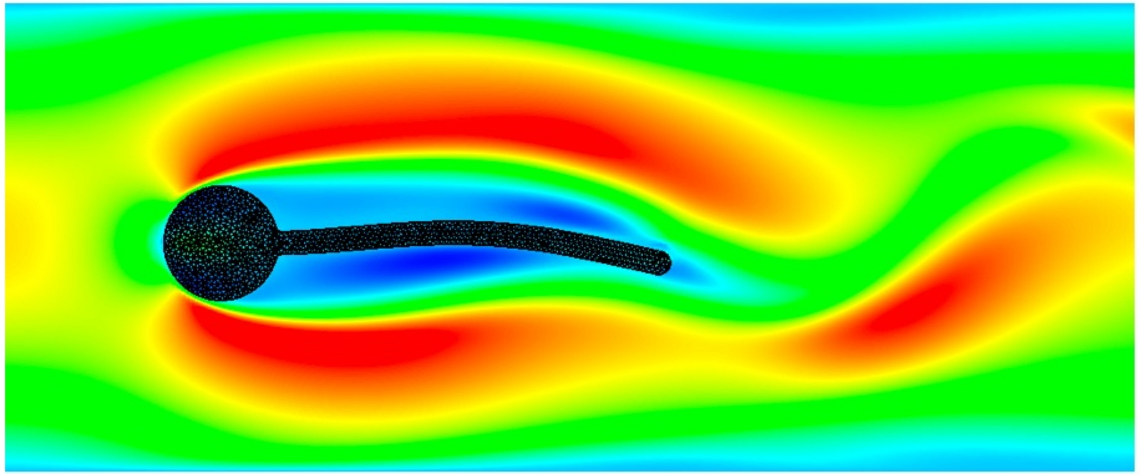
Algorithm Scheme

STEP 7:

if one of the two convergence criteria is satisfied

$$\hat{\mathbf{u}}_s^{n+1} = \hat{\mathbf{u}}_s^{l+1}, \quad \mathbf{v}_f^{n+1} = \mathbf{v}_f^{l+1}, \quad p_f^{n+1} = p_f^{l+1}$$

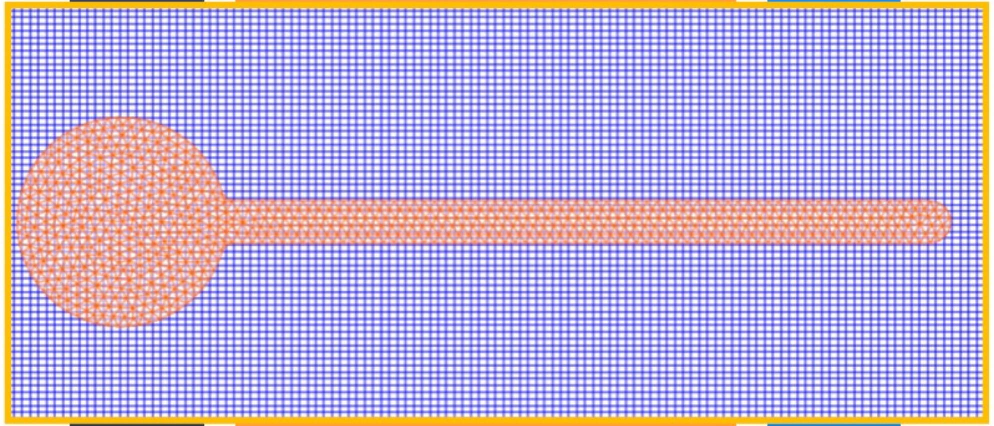
FSI Framework + Active Stress



- Updating Pony's Moose Version
- Storing Fluid Mass Matrix
- Fixed bug for restarting option
- Adding Active Stress term

FSI + Active Term: Mathematical Model

We would like to add an **active stress** to the solid structure behaviour in order to simulate muscle contraction.



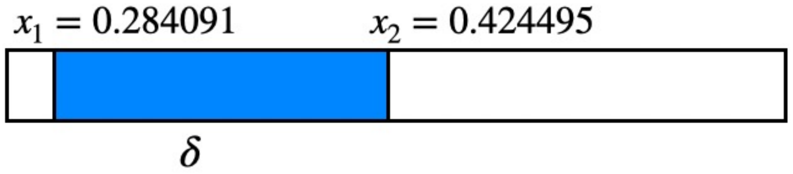
Solid subproblem:

$$\hat{\rho}_s \frac{\partial^2 \hat{\mathbf{u}}_\mathbf{s}}{\partial t^2} - \hat{\nabla} \cdot (\mathbf{P_m} + \mathbf{P_a}) = \mathbf{0} \qquad \text{in } \hat{\Omega}_s \qquad \text{where} \quad P_a = \alpha \mathbf{F} \mathbf{g} \otimes \mathbf{g}$$

$$\hat{\mathbf{u}}_\mathbf{s} = \hat{\mathbf{u}}_\mathbf{b} \qquad \text{on } \hat{\Gamma}_s^d$$

- **Active Stress Function applied along the fibres :**

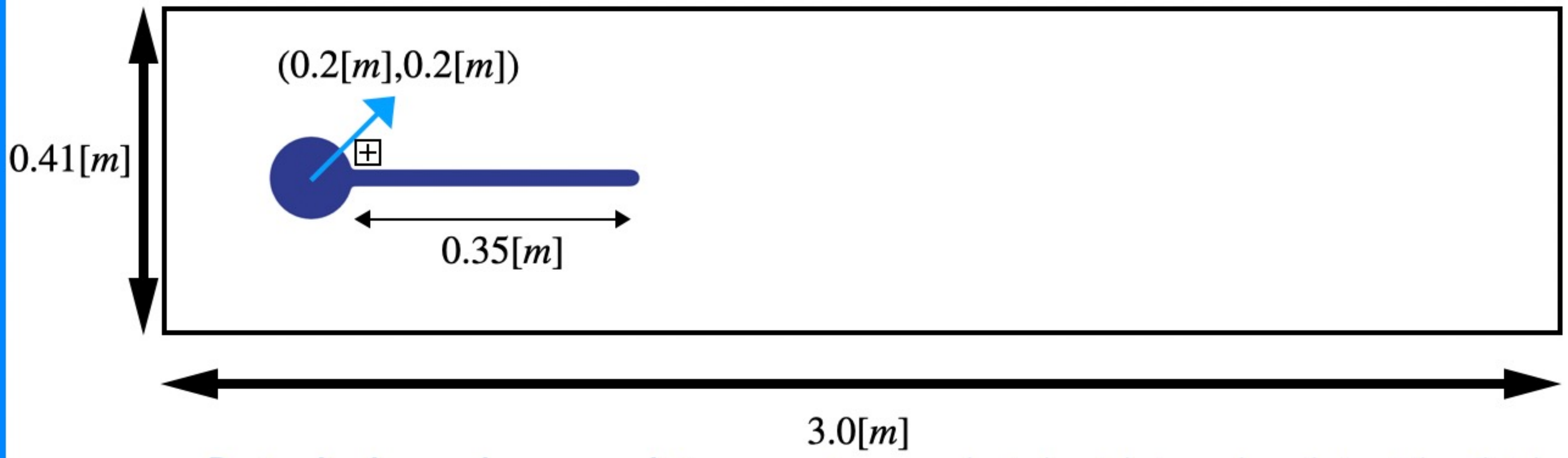
$$\alpha = \begin{cases} 5 \cdot 10^5 \cdot \sin\left(\frac{2\pi t}{T}\right) \cdot \exp\left(-\frac{0.21 - y}{0.006667}\right) & 0 \leq t \leq T/2 \\ 5 \cdot 10^5 \cdot \sin\left(\frac{2\pi t}{T}\right) \cdot \exp\left(-\frac{y - 0.19}{0.006667}\right) & T/2 < t \leq T \end{cases}$$



Reference : *A fluid-structure interaction study of soft robotic swimmer using a fictitious domain/active strain method*
Z. Lin et al.

Numerical Results

We present an FSI example by using the **Truck-Horn FSI Benchmark** of an incompressible flow past an elastic solid structure.



- **Periodic boundary conditions** are imposed at the inlet and outlet of the fluid channel together with no-slip boundary conditions on the top and the bottom wall.

- A **parabolic velocity profile** is enforced upstream of the structure. This fringe forcing term acts in the region $x_{start} = 2.5[m] < x < x_{end} = 3.0[m]$

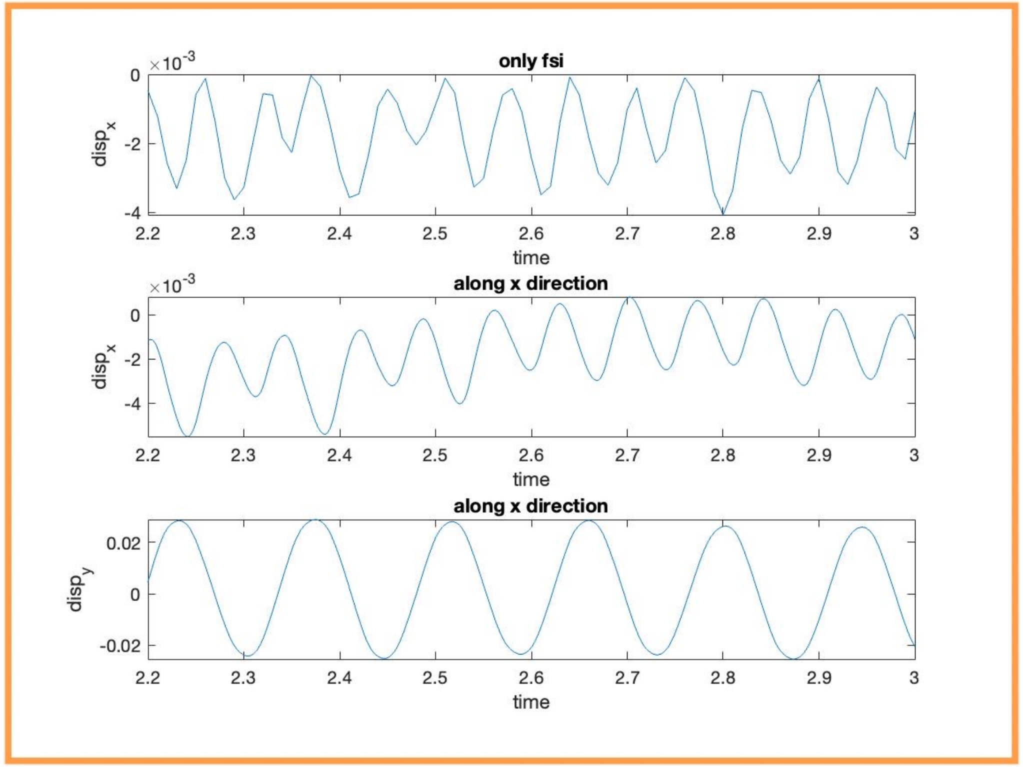
- **Material Model for Structure : Saint-Venant**

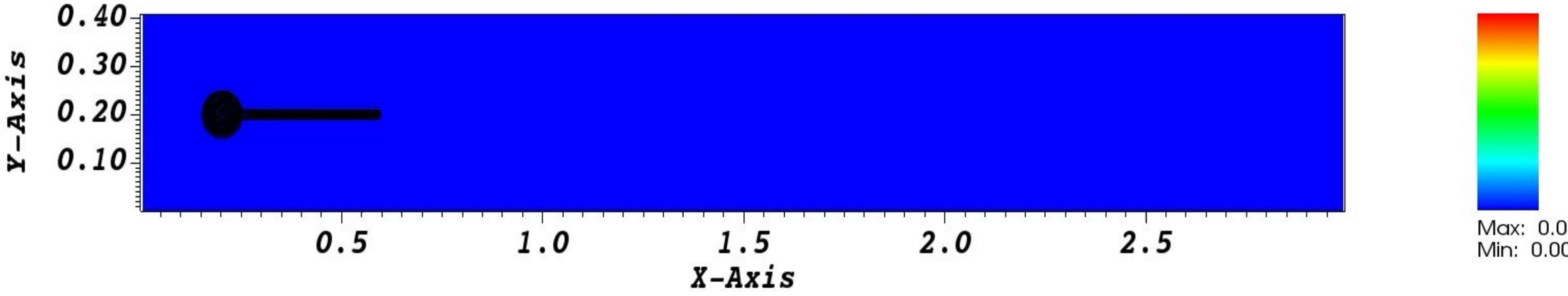
  Second Piola-Kirchiff Stress $\mathbf{S}_m = \lambda_s Tr(\mathbf{E}) + 2\mu_s \mathbf{E}$

  $\mu_s = 2000000 \quad \lambda_s = k_s - 2\frac{\mu_s}{d} \quad k_s = 4666667$

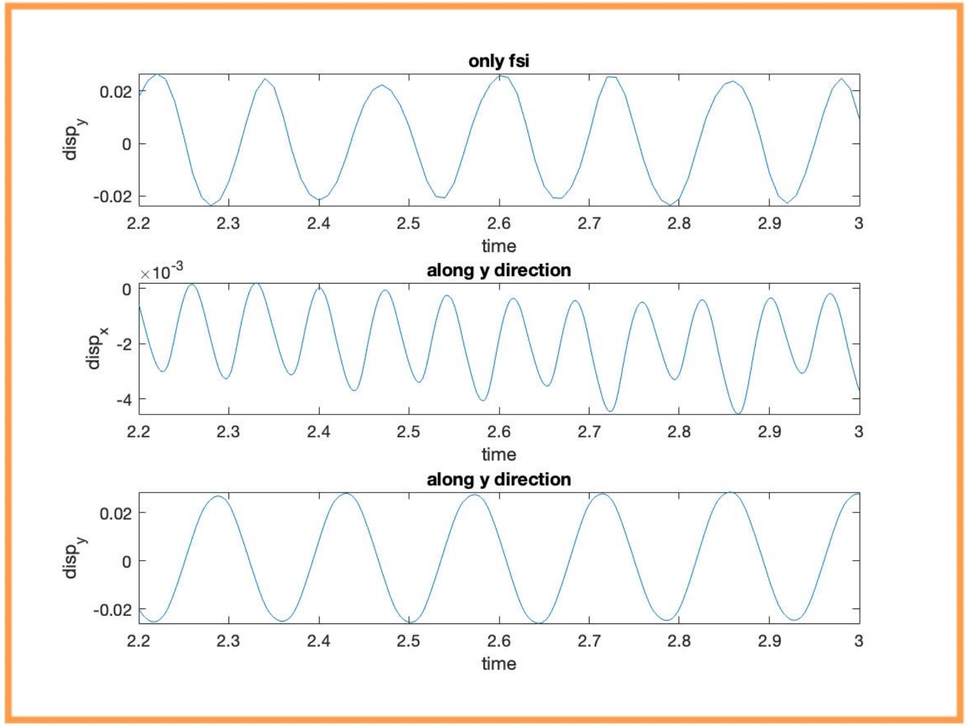
  d mesh dimension

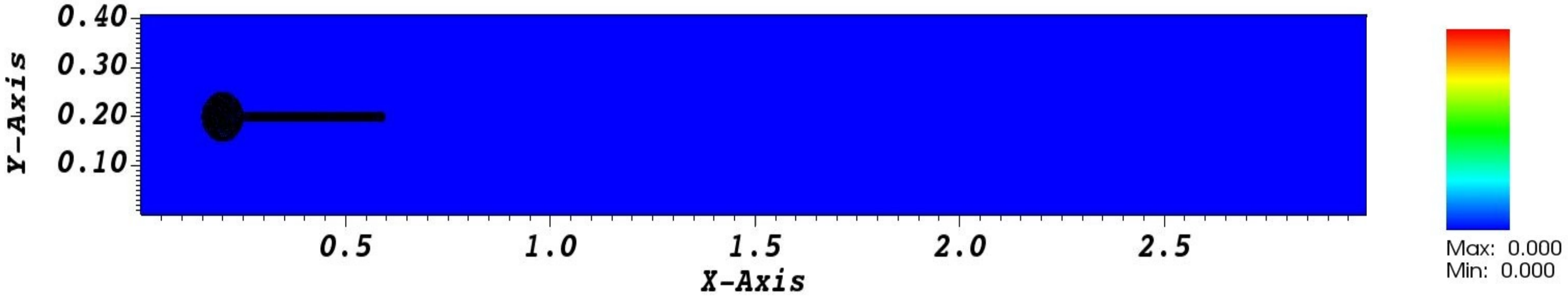
FSI active term along x direction





FSI active term along y direction





Current work

Convergence Studies in 2D

Future work

Application to a Ventricular Geometry