MULTISIMO LAB

Technical University of Cartagena

Multi-material topology optimization for shape-morphing ultra-soft magneto-active structures

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17th World Congress on Computational Mechanics. Munich,Germany.

Low σ

Stress Field

OUTLINE

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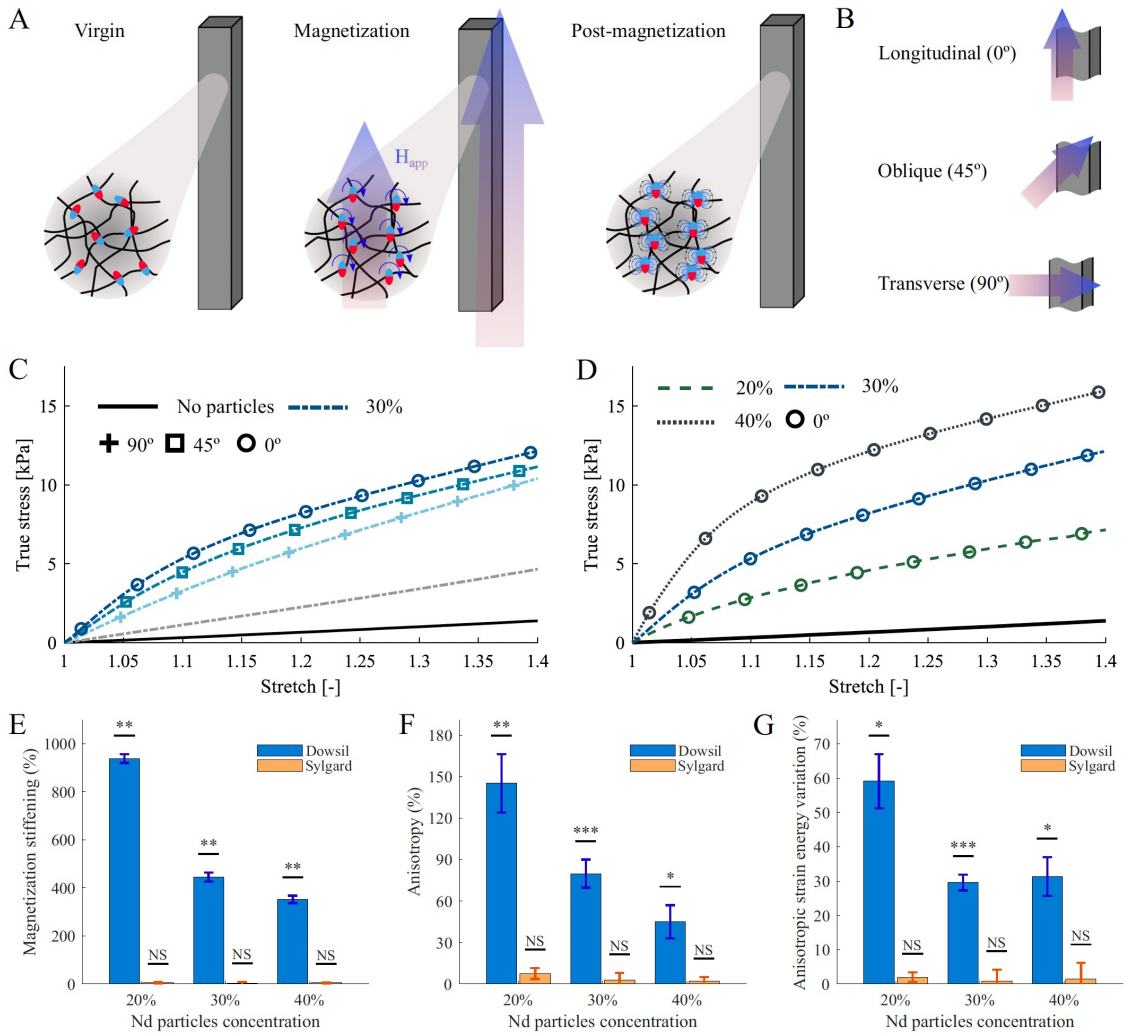
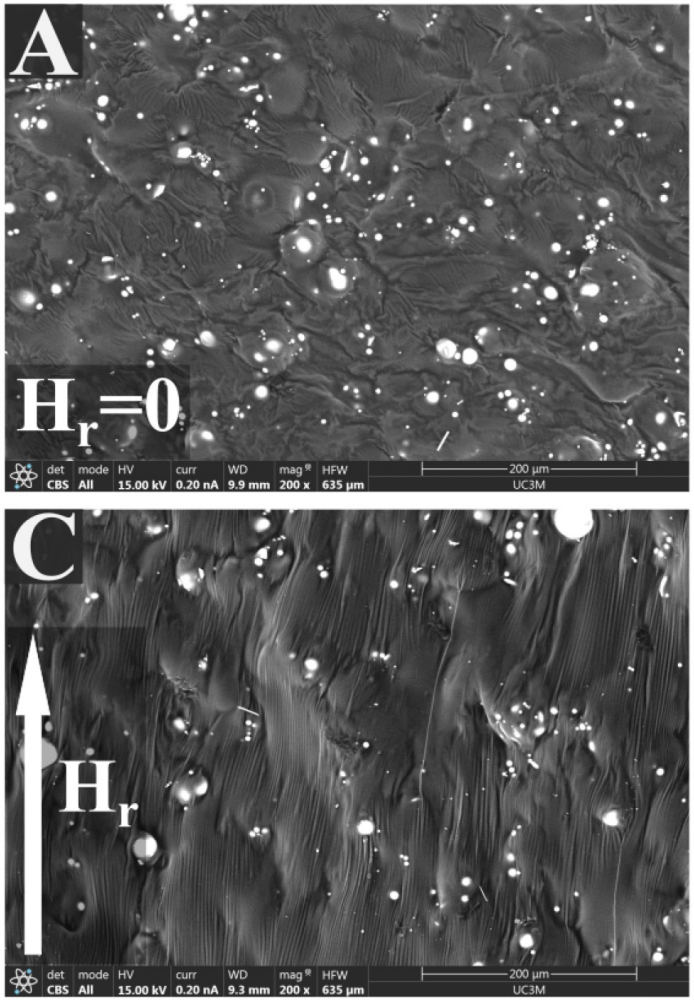
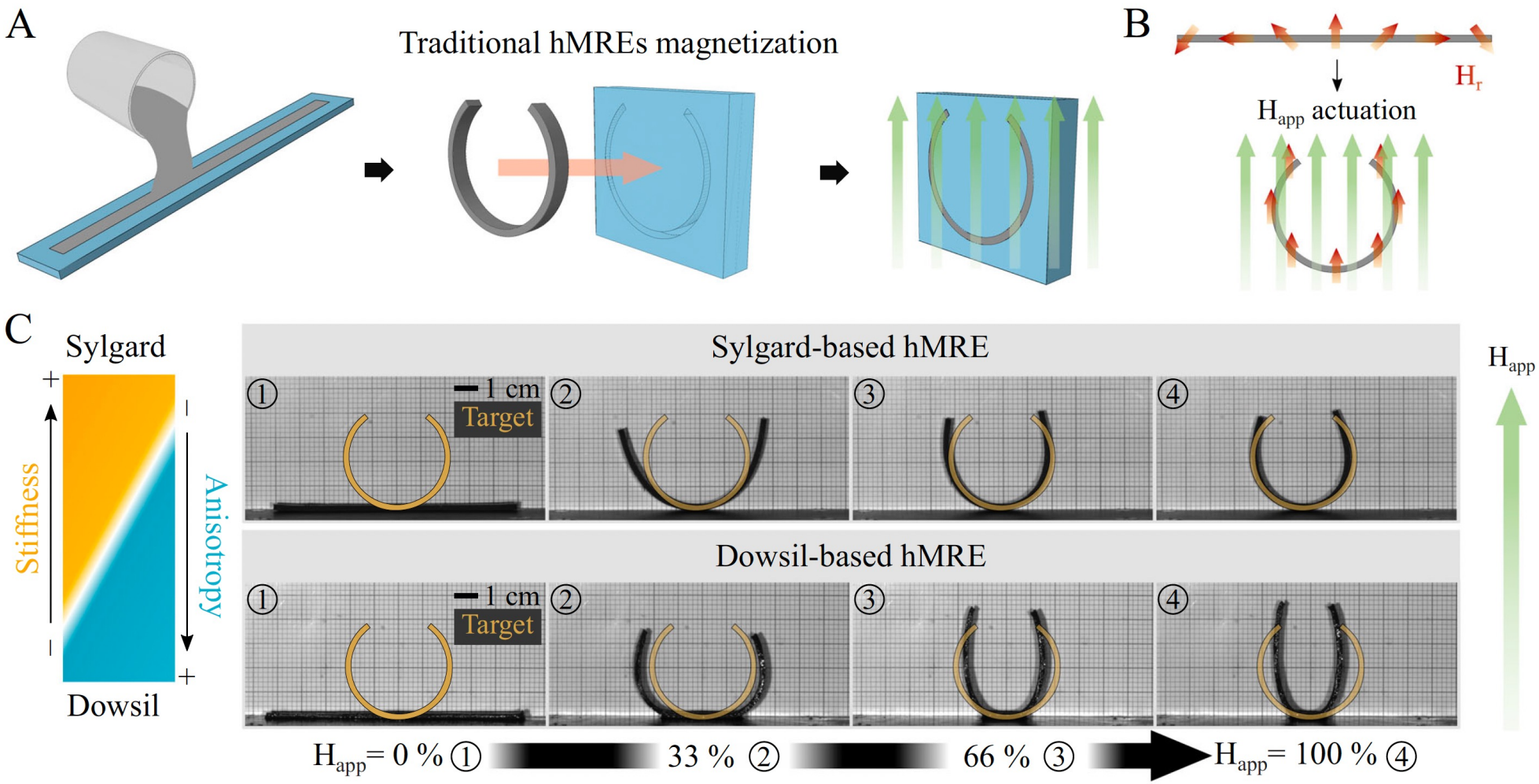
17th World Congress on Computational Mechanics. Munich,Germany.

Residual Mechanical Anisotropy in ultra-soft hMREs





Shape programming of ultra-soft hMRES



Sylgard 184 (≈2 MPa)

f SéNeCa(+)
Agencia de Ciencia y Tecnología
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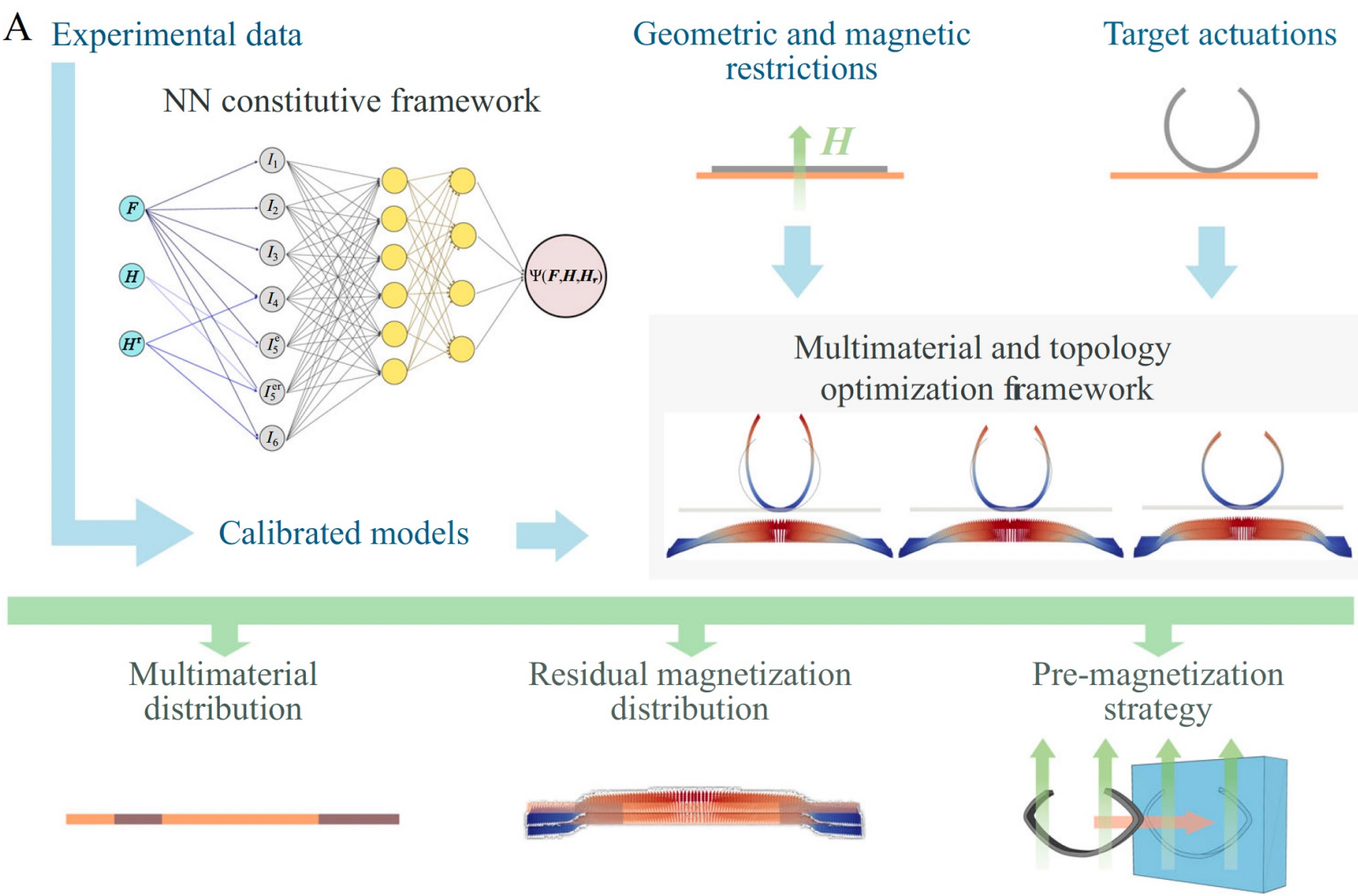
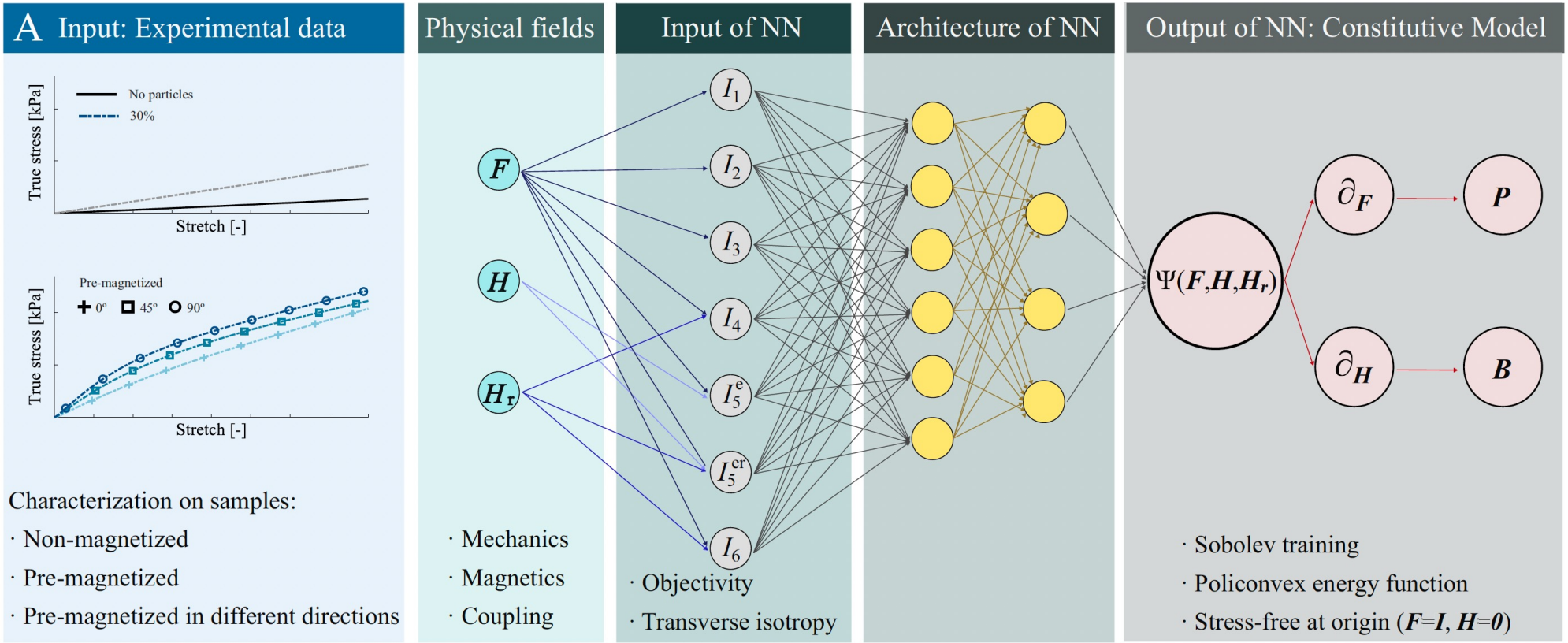
Dowsil CY52-276 (≈3 kPa)

Computational framework



Physics-augmented neural networks constitutive model



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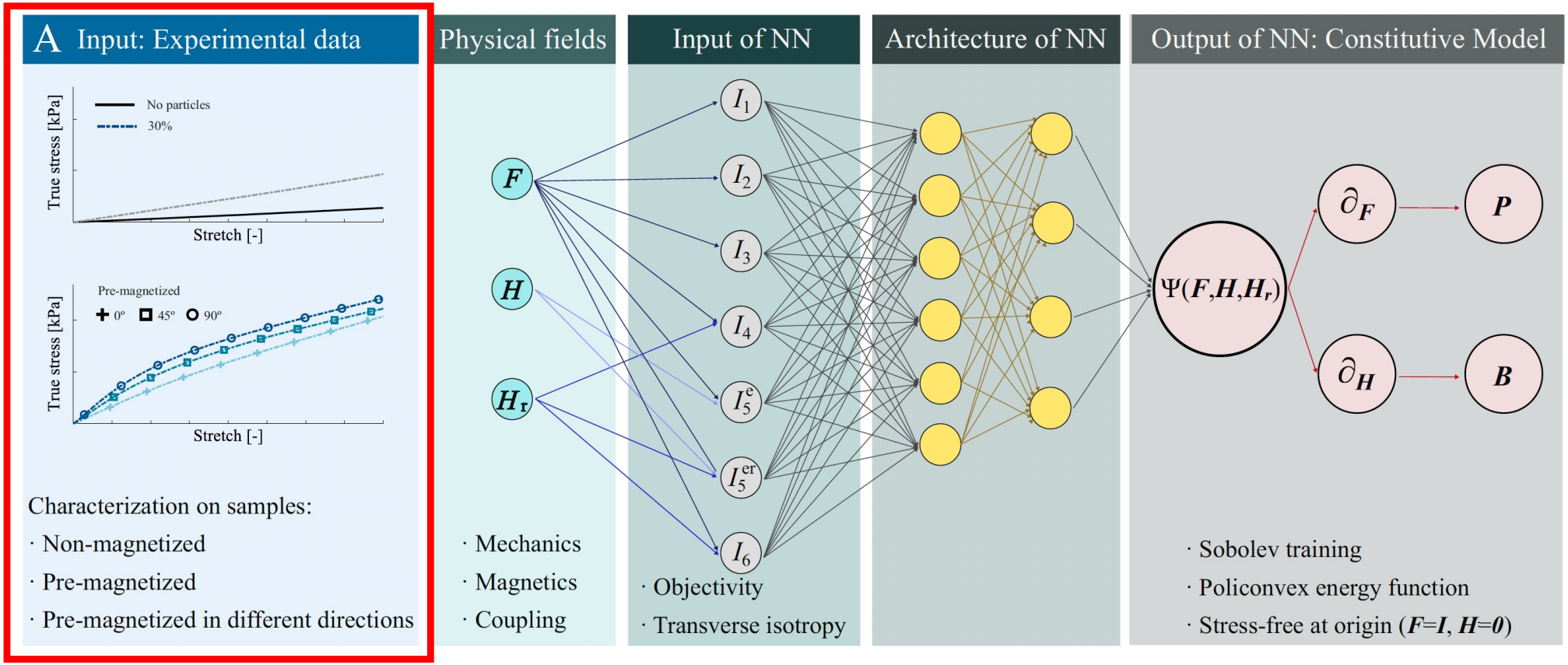
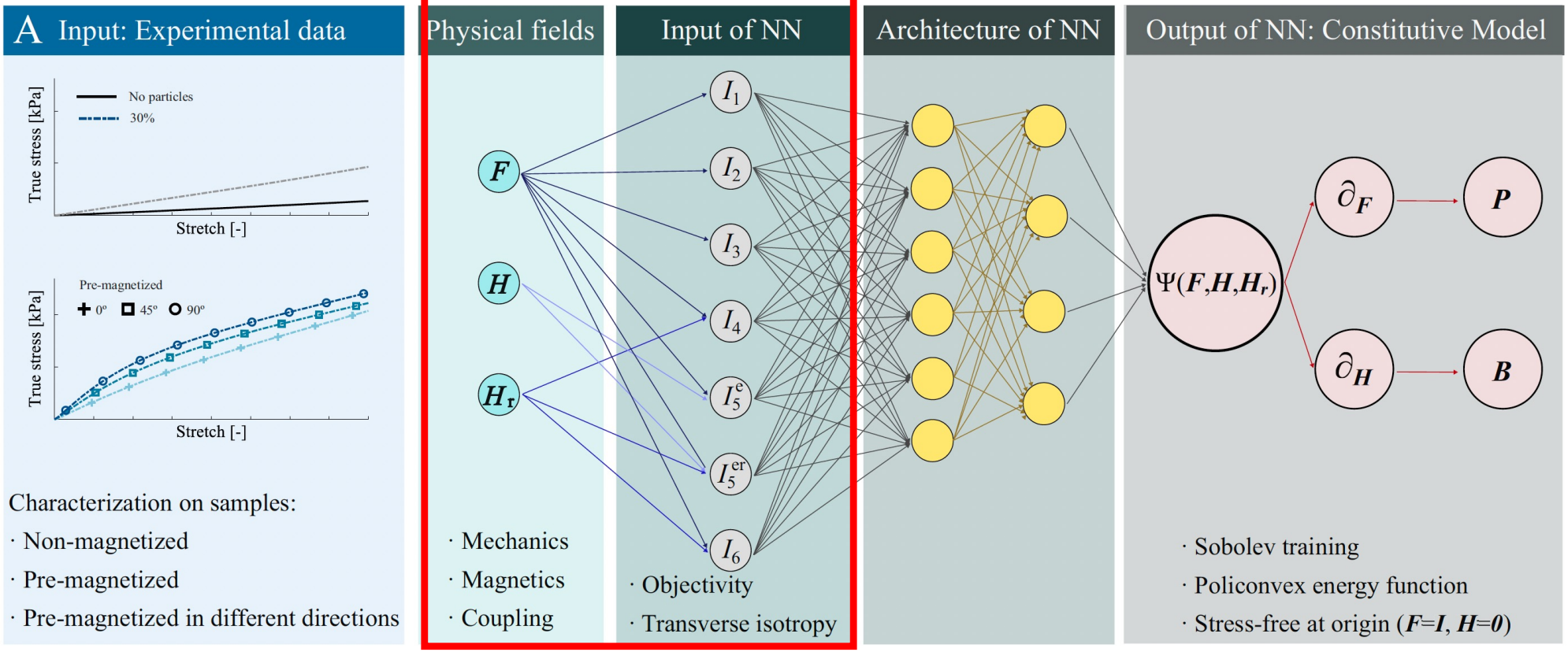


Physics-augmented neural networks constitutive model

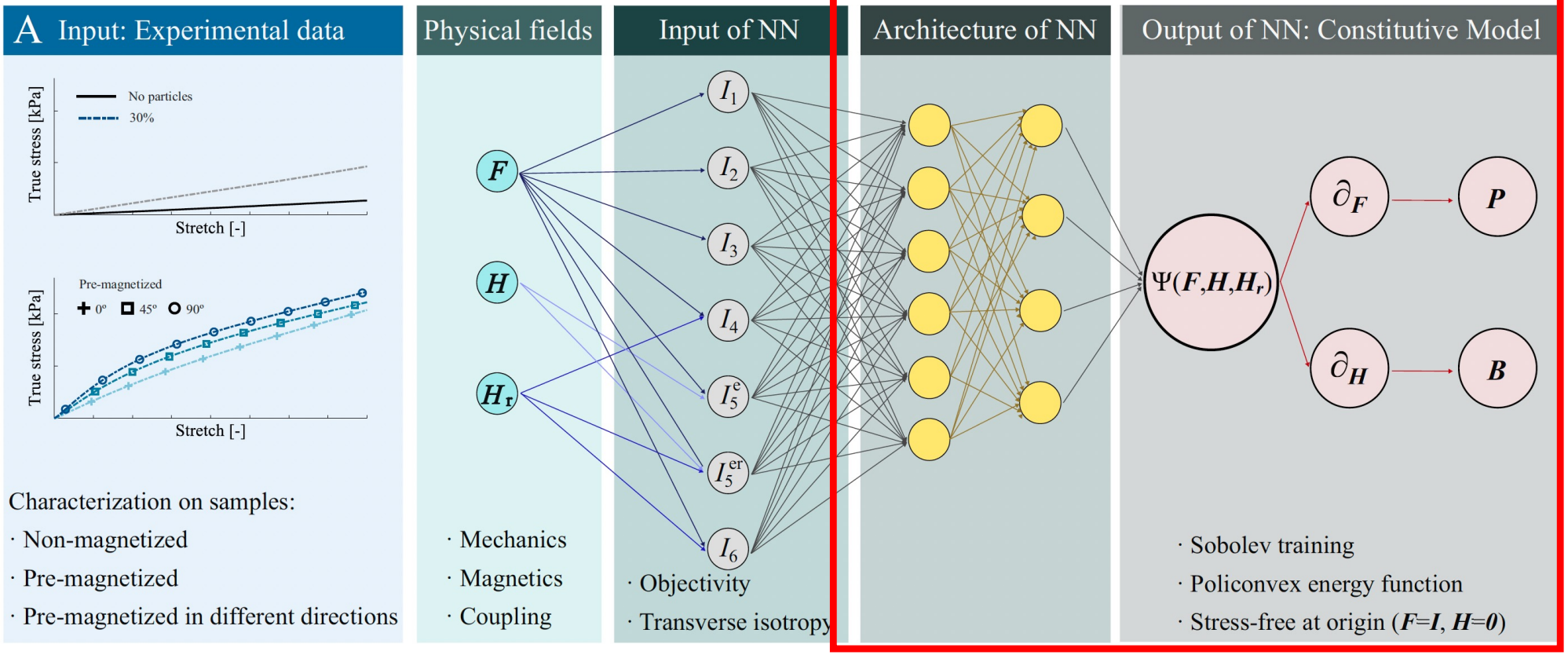


$$I_1 = \boldsymbol{F} : \boldsymbol{F}; \qquad I_2 = \mathrm{Cof}\boldsymbol{F} : \mathrm{Cof}\boldsymbol{F}; \qquad I_3 = \det \boldsymbol{F};$$

$$I_4 = \boldsymbol{F}\boldsymbol{H}_r \cdot \boldsymbol{F}\boldsymbol{H}_r; \qquad I_6 = \mathrm{Cof}\boldsymbol{F}\boldsymbol{H}_r \cdot \mathrm{Cof}\boldsymbol{F}\boldsymbol{H}_r;$$

$$I_5^e = \boldsymbol{H} \cdot \boldsymbol{C}^{-1} \cdot \boldsymbol{H} \qquad I_5^{er} = \boldsymbol{H} \cdot \boldsymbol{C}^{1/2} \cdot \boldsymbol{H}_r$$

Physics-augmented neural networks constitutive model

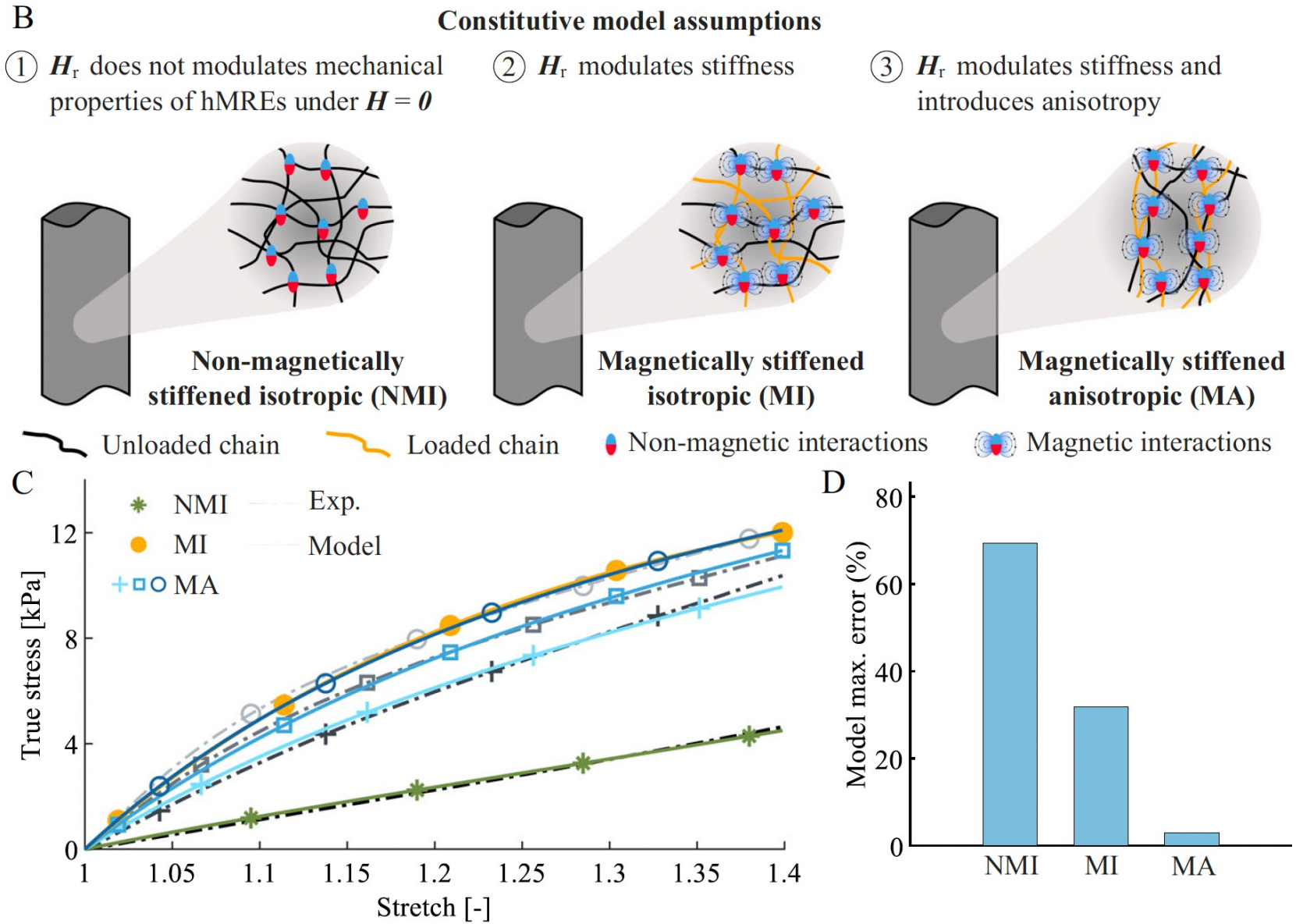


$$\Psi(\mathbf{F}, \mathbf{H}, \mathcal{W}) = \mathbb{U}(I_1, I_2, I_3, I_4, I_5, I_5^{er}, I_6; \mathcal{W})$$

$$\mathcal{W} = \{\mathbf{W}_1, \ldots, \mathbf{W}_{L+1}, \mathbf{b}_1, \ldots, \mathbf{b}_{L+1}\}$$

$$\mathcal{L}(\mathcal{W}) = \frac{\sum_{i=1}^{n_d} \left\| \mathbf{P}^i - \partial_{\mathbf{F}} \Psi(\mathbf{F}^i, \mathbf{0}, \mathcal{W}) \right\|^2}{\sum_{i=1}^{n_d} \left\| \mathbf{P}^i \right\|^2} + \frac{\kappa_r}{2} \sum_i \left(\min((\mathcal{W}_\nu)_i, 0)\right)^2$$

Physics-augmented neural networks constitutive model

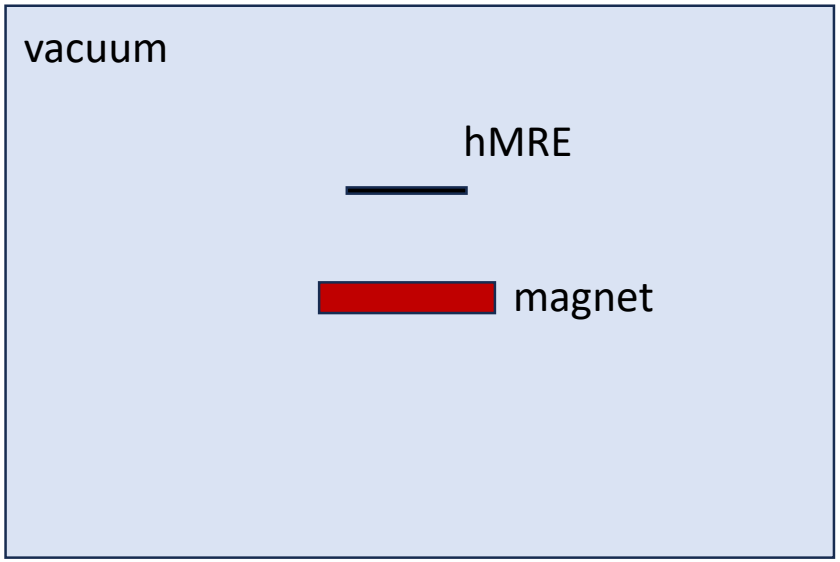


Staggered solver for magneto-mechanics in vacuum

The numerical resolution of the coupled magneto-mechanical problem was performed via a custom finite element implementation using a **staggered scheme.**

Step 1: Magnetostatic problem (scalar potential)
Solve for $\varphi \in \mathbb{V}^{\varphi}$ in $\Omega_0 \cup \Omega_{v0}$:

$$
\begin{aligned}
\mathrm{DIV}\,\mathbf{B}(\boldsymbol{X},\mathbf{F},\mathbf{H}) &= 0, \\
\mathbf{H} &= -\nabla_0 \varphi, \\
\mathbf{B} &= -\frac{\partial \Psi}{\partial \mathbf{H}} \quad \text{in } \Omega_0, \\
\mathbf{B} &= -\frac{\partial \Psi_{Maxw}}{\partial \mathbf{H}} \quad \text{in } \Omega_{v0}, \\
\varphi &= \varphi^{\star} \quad \text{on } \partial\Omega_{v0\varphi}.
\end{aligned}
$$



The scalar magnetic potential φ was computed in the entire domain (hMRE and vacuum). Continuity and boundary conditions were imposed across interfaces and on the boundary.

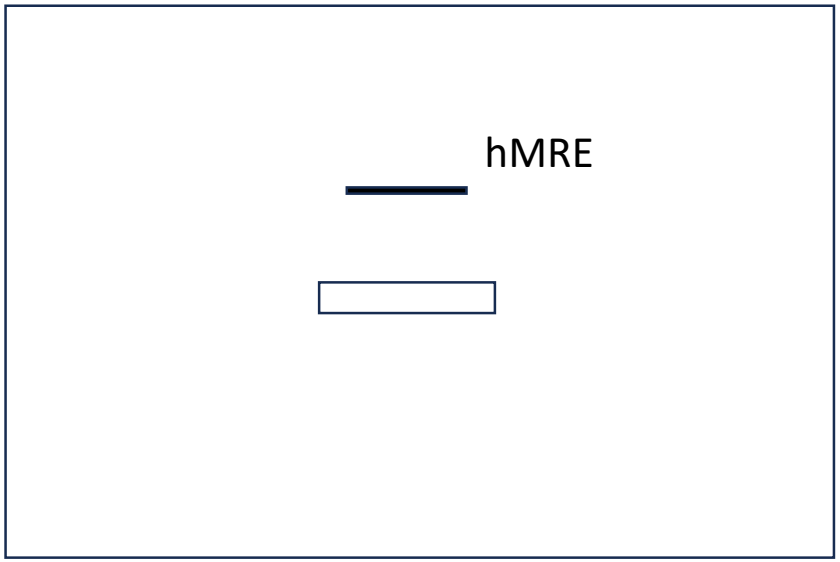
Staggered solver for magneto-mechanics in vacuum

The numerical resolution of the coupled magneto-mechanical problem was performed via a custom finite element implementation using a **staggered scheme.**

Step 2: Mechanical problem in the solid

Using $\mathbf{H}$ from Step 1, solve for $\boldsymbol{\phi} \in \mathbb{V}_s^{\boldsymbol{\phi}}$ in Ω_0:

$$
\begin{aligned}
\mathrm{DIV}\,\mathbf{P}(\boldsymbol{X}, \mathbf{F}, \mathbf{H}) &= \mathbf{F}_0, \\
\mathbf{F} &= \nabla_0 \boldsymbol{\phi}, \\
\boldsymbol{\phi} &= \boldsymbol{\phi}^\star \quad \text{on } \partial\Omega_{0\boldsymbol{\phi}}, \\
[\![\mathbf{P}]\!]\mathbf{N} &= \mathbf{0} \quad \text{on } \partial\Omega_0 \cap \partial\Omega_{v0}, \\
\mathbf{P} &= \frac{\partial \Psi}{\partial \mathbf{F}} \quad \text{in } \Omega_0.
\end{aligned}
$$



The deformation mapping $\boldsymbol{\phi}$ *was computed in the solid domain by solving the equilibrium equation. Dirichlet and Neumann boundary conditions were applied as appropriate, and* ***H is taken from Step 1.***

Staggered solver for magneto-mechanics in vacuum

The numerical resolution of the coupled magneto-mechanical problem was performed via a custom finite element implementation using a **staggered scheme.**

Step 3: Mechanical problem in the vacuum

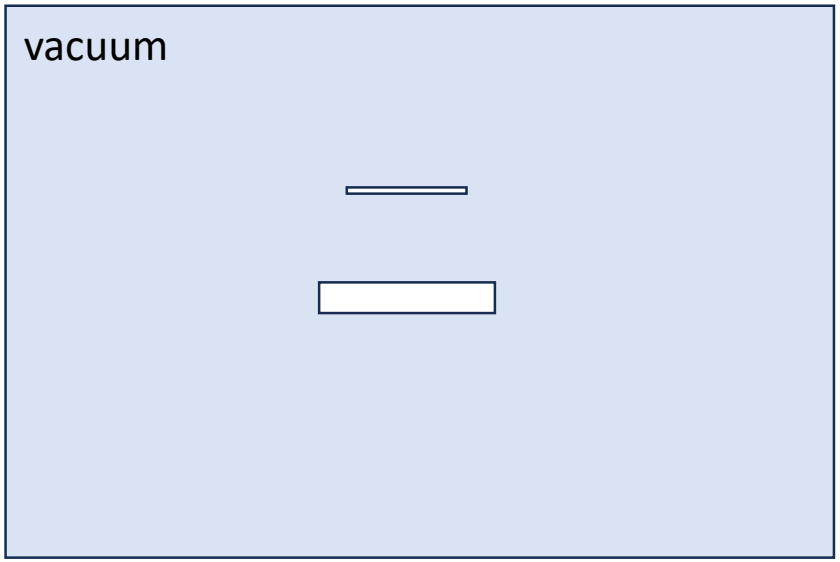
Enforce continuity with $\boldsymbol{\phi}$ and solve for $\boldsymbol{\phi}_v \in \mathbb{V}_v^{\boldsymbol{\phi}}$ in Ω_{v0}:

$$\mathrm{DIV}\left(\frac{\partial \Psi_{vm}}{\partial \mathbf{F}}(\mathbf{F})\right) = \mathbf{0},$$

$$\mathbf{F} = \nabla_0 \boldsymbol{\phi}_v,$$

$$\boldsymbol{\phi}_v = \mathbf{0} \quad \text{on } \partial\Omega_{v0\boldsymbol{\phi}},$$

$$\boldsymbol{\phi}_v = \boldsymbol{\phi} \quad \text{on } \partial\Omega_0 \cap \partial\Omega_{v0}.$$



A nonlinear elastic problem was solved in the vacuum region using a potential $\boldsymbol{\phi}$v, enforcing continuity with the solid deformation and applying clamped boundary conditions on its boundary.

Mesh movement stabilization

1) Fictitious energy model

$$\Psi_{vm}(\mathbf{F}) = \frac{\mu_1}{2p_1 3^{p_1-1}}\left(\hat{I}_1\right)^{p_1} + \frac{\mu_2}{2p_2 3^{p_2-1}}\left(\hat{I}_2\right)^{p_2} + \frac{\kappa}{2}\left(J^{p_3} + J^{-p_3}\right)$$

$\{\mu_1, \mu_2, \kappa\}$ represent fictitious elastic properties of Ω_{v0}

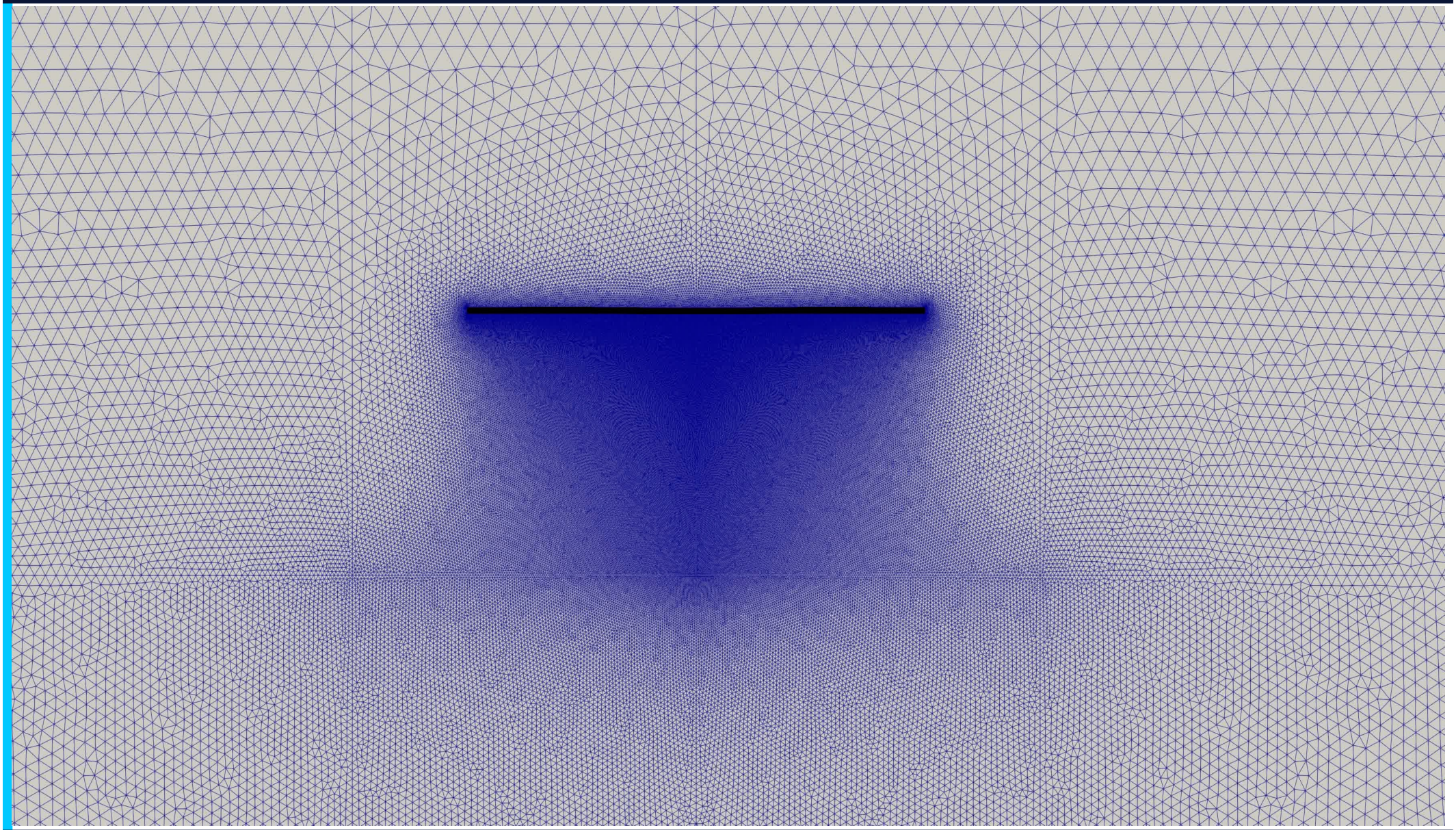
$\{p_1, p_2, p_3\}$ penalise in a nonlinear fashion the isochoric invariants and the volumetric invariant J

2) Stabilization of the elasticity tensor

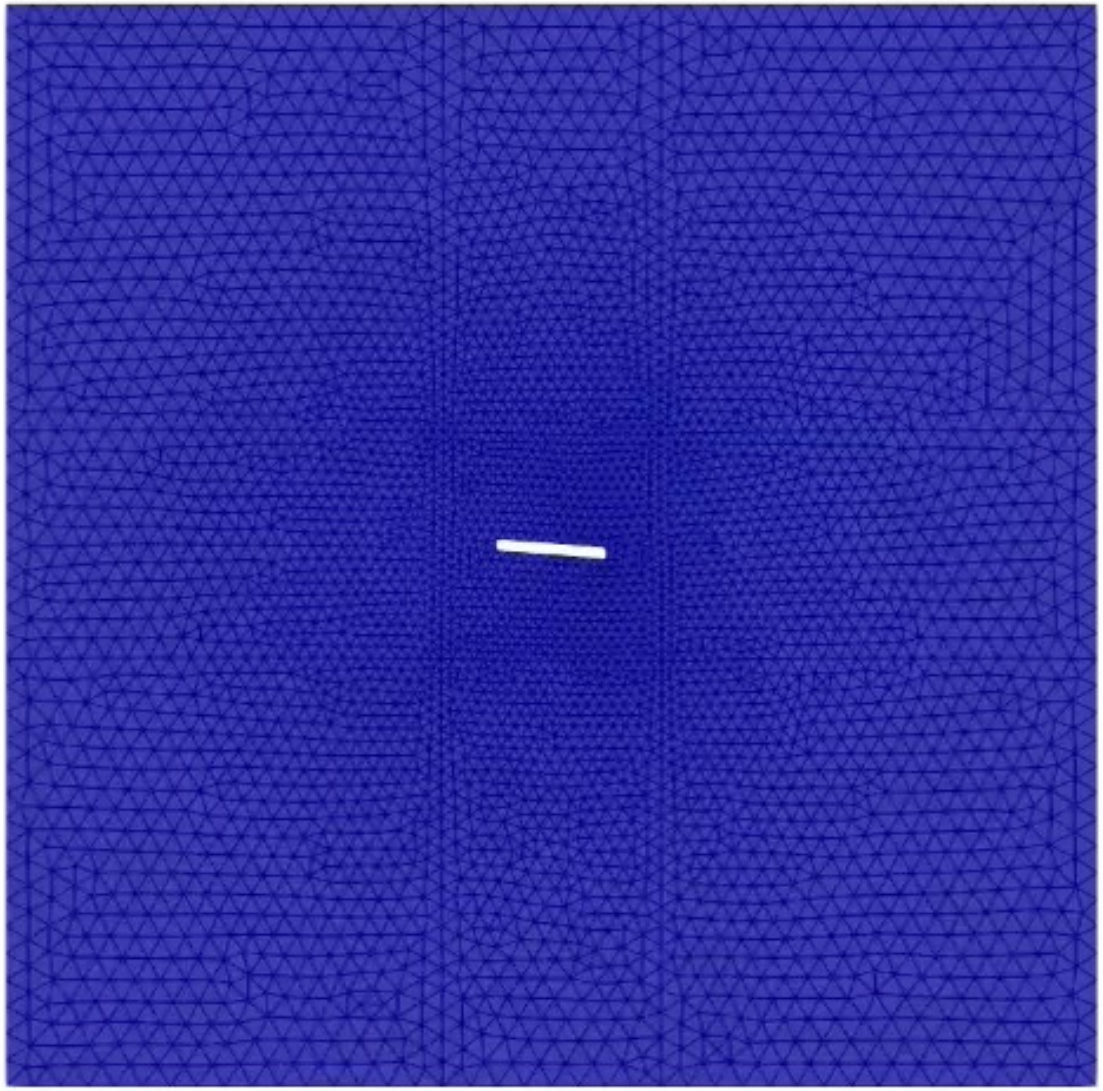
$$D\mathcal{W}_{\phi_v}(\boldsymbol{\phi}_v|_k)[\Delta\boldsymbol{\phi}_v] = \int_{\Omega_0} \boldsymbol{\nabla}_0\boldsymbol{v} : \boldsymbol{\mathcal{C}}_{\text{reg}}(\mathbf{F}) : \boldsymbol{\nabla}_0\Delta\boldsymbol{\phi}_v \, dV$$

$$\boldsymbol{\mathcal{C}}_{\text{reg}} = \sum_{i=1}^{9} \max\left(\lambda_i, 0\right) \boldsymbol{V}_i \otimes \boldsymbol{V}_i,$$

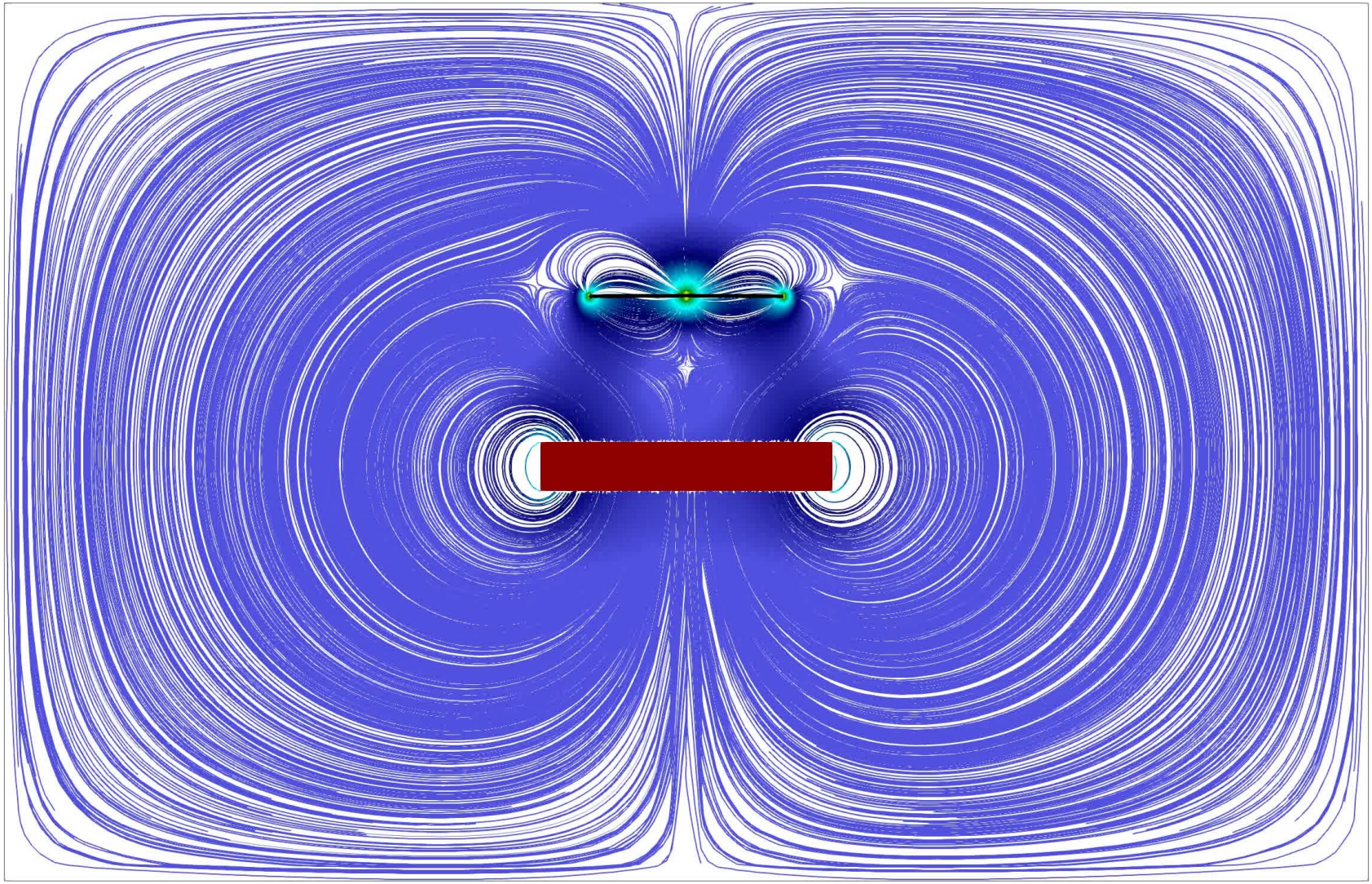
Mesh movement stabilization



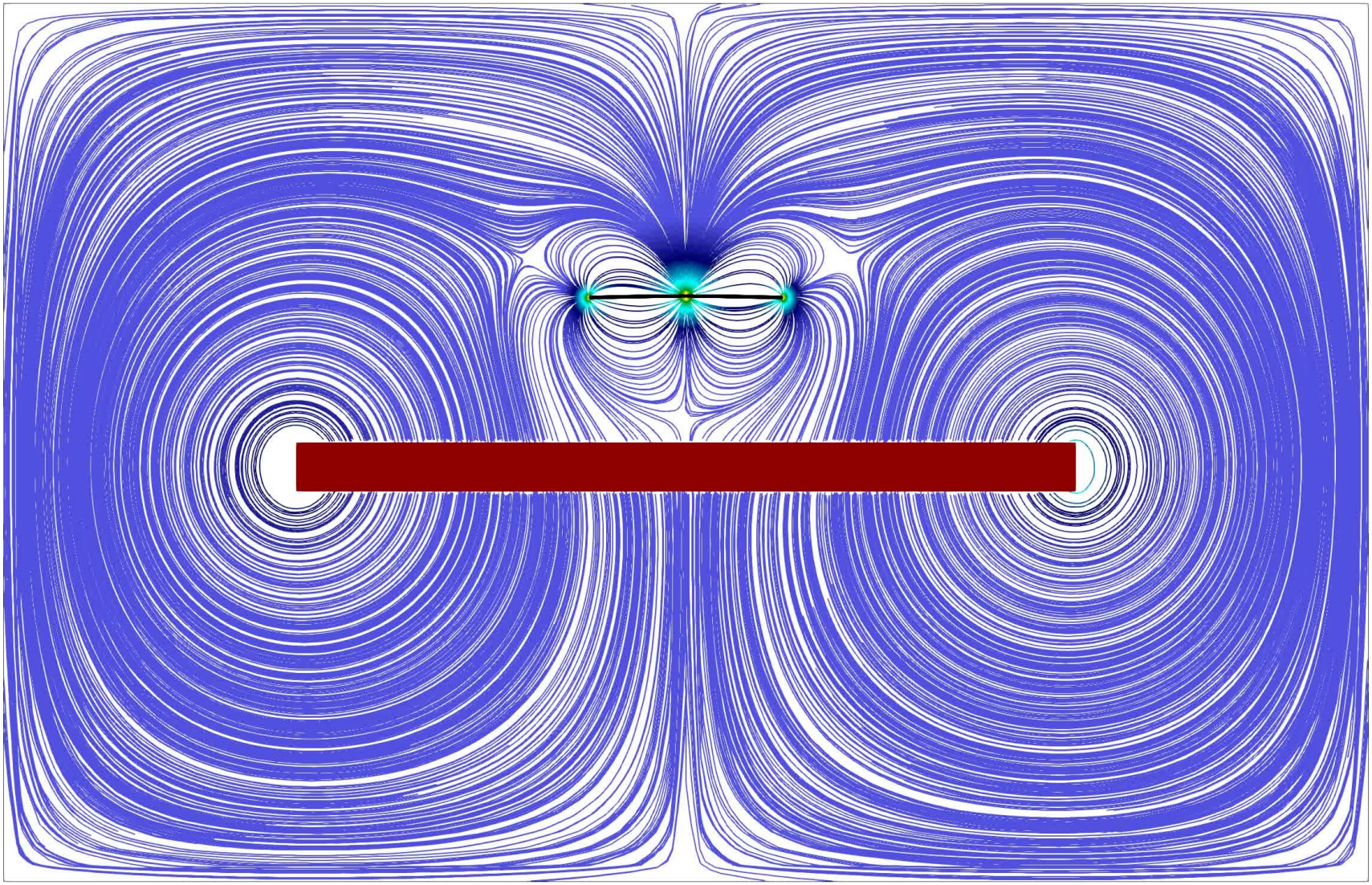
Mesh movement stabilization



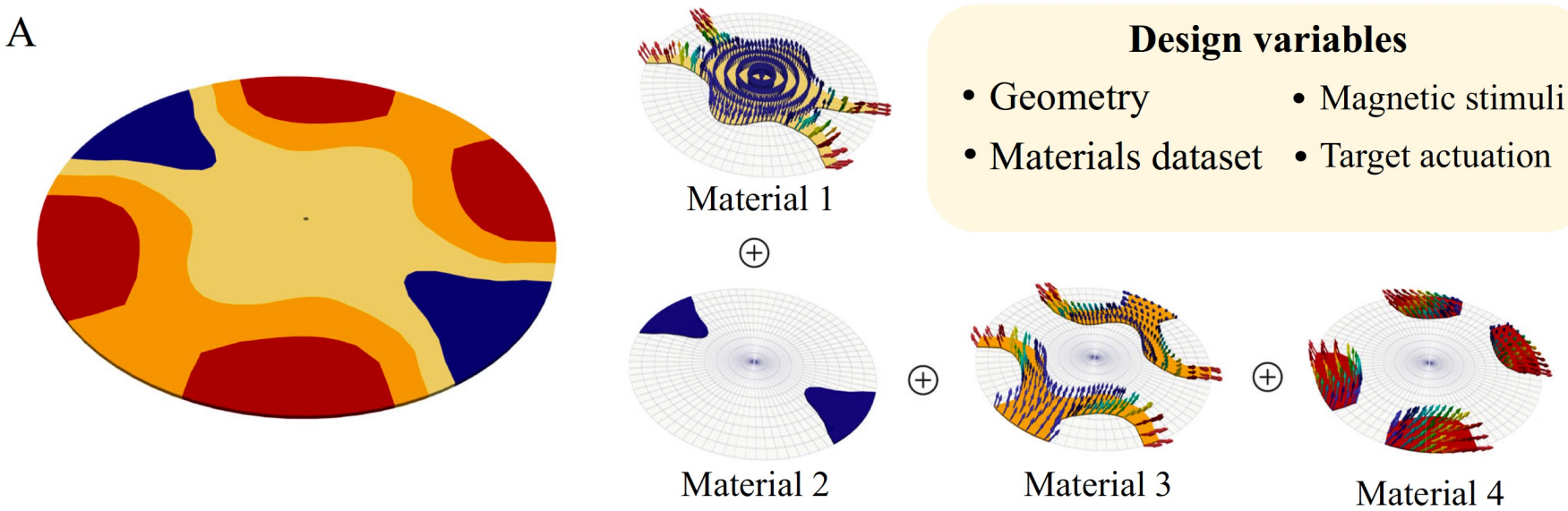
Staggered solver for magneto-mechanics in vacuum



Examples



Optimization framework



Design variables

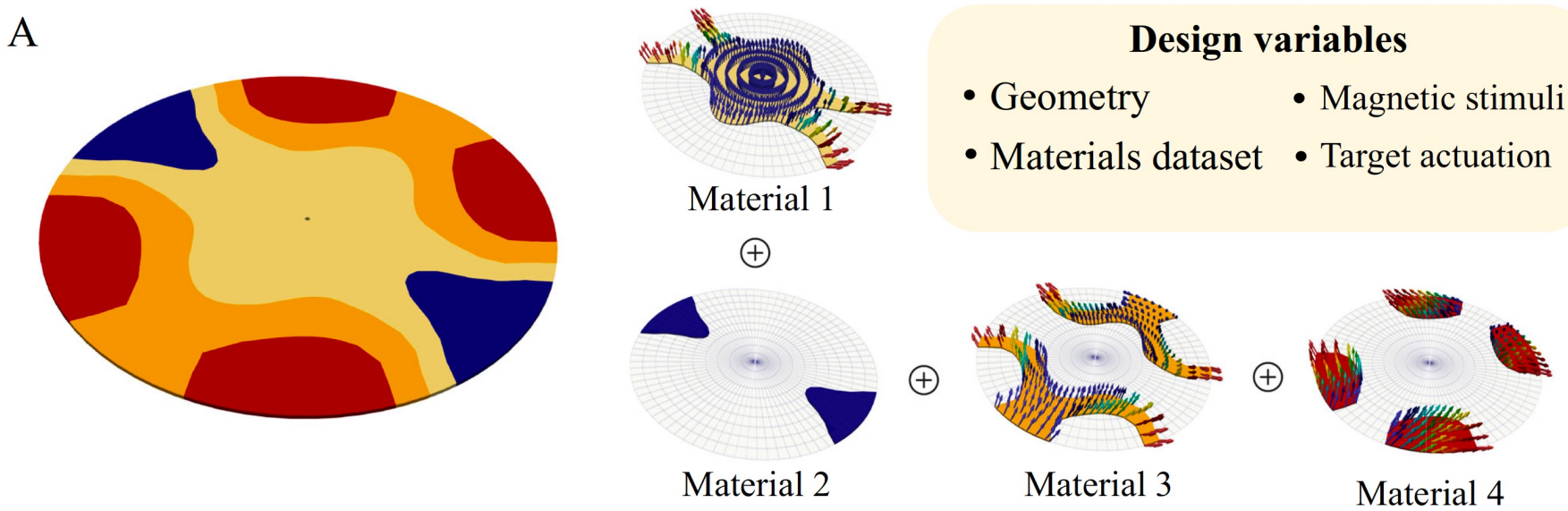
- Geometry
- Materials dataset
- Magnetic stimuli
- Target actuation

$$\mathbf{H}_r = H_r \mathbf{N}(\theta, \varphi), \qquad \mathbf{N}(\theta, \varphi) = \begin{bmatrix} \cos(\theta)\sin(\varphi) & \sin(\theta)\sin(\varphi) & \cos(\varphi) \end{bmatrix}$$

$$\Psi(\xi, c, \theta, \varphi, H_{app}, \mathbf{F}) = (1 - \xi^{p_\xi})\, \Psi_p(\mathbf{F}) + \xi^{p_\xi}\, \Psi_a(c, \theta, \varphi, H_{app}, \mathbf{F})$$

$$\Psi_a(c, \theta, \varphi, H_{app}, \mathbf{F}) = (1 - c^{p_c})\ \Psi|_{c=0.2}\,(\mathbf{F}, \mathbf{H}_r(\theta, \varphi), H_{app}) + c^{p_c}\ \Psi|_{c=0.3}\,(\mathbf{F}, \mathbf{H}_r(\theta, \varphi), H_{app})$$

Optimization framework



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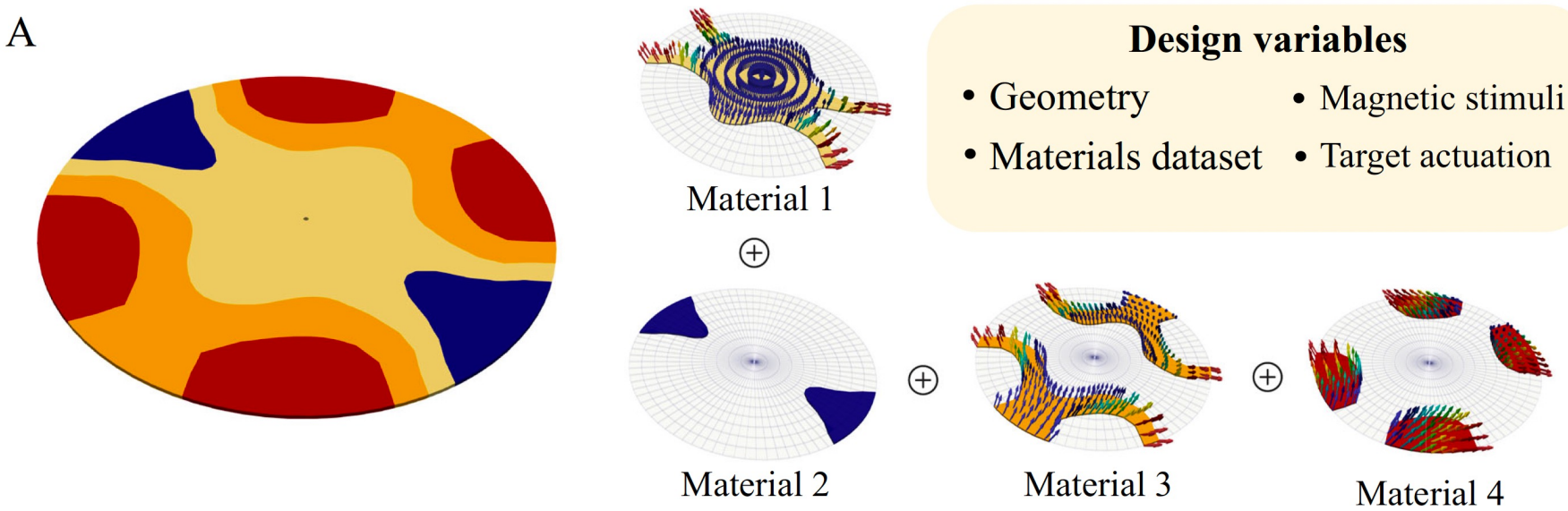
Optimization framework



Design variables

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$$\Psi(\xi, c, \theta, \varphi, H_{app}, \mathbf{F}) = (1 - \boxed{\xi^{p_\xi}})\, \Psi_p(\mathbf{F}) + \xi^{p_\xi}\, \Psi_a(c, \theta, \varphi, H_{app}, \mathbf{F})$$

$$\Psi_a(c, \theta, \varphi, H_{app}, \mathbf{F}) = (1 - \boxed{c^{p_c}})\, \Psi|_{0.2} \quad (\mathbf{F}, \mathbf{H}_r(\theta, \varphi), H_{app}) + c^{p_c}\, \Psi|_{0.3} \quad (\mathbf{F}, \mathbf{H}_r(\theta, \varphi), H_{app})$$

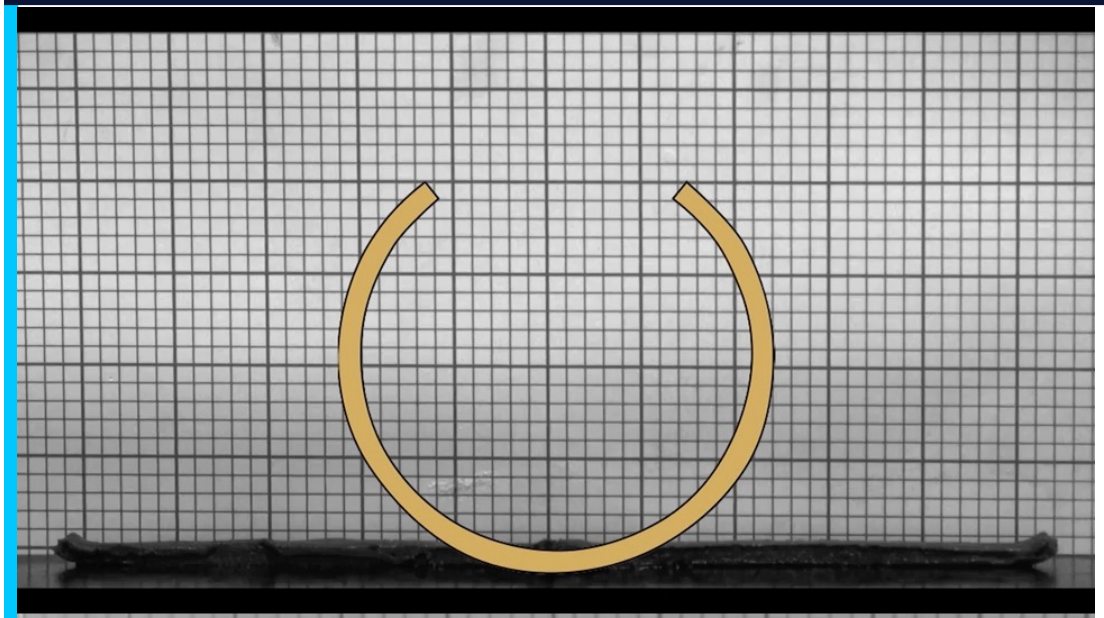
Optimization formulation

$$\text{Minimize in } (\xi, c, \theta, \varphi, H_r): \ \mathcal{J}(\xi, c, \theta, \varphi, H_{app}) := \int_{\Omega_0} \|\boldsymbol{\phi}(\xi, c, \theta, \varphi, H_{app}) - \boldsymbol{\phi}_d\|^2 \, dV$$

$$\text{subject to} \begin{cases} \begin{cases} \mathrm{DIV}\mathbf{P}(\xi, c, \theta, \psi, H_{app}, \mathbf{F}) = \mathbf{F}_0; & \text{in } \Omega_0; \\ \mathbf{F} = \boldsymbol{\nabla}_0 \boldsymbol{\phi} \Rightarrow \mathrm{CURL}\mathbf{F} = \mathbf{0}; & \text{in } \Omega_0 \\ \boldsymbol{\phi} = \boldsymbol{\phi}^\star; & \text{on } \partial\Omega_{0\boldsymbol{\phi}} \end{cases} \\ \begin{cases} \Psi(\xi, c, \theta, \psi, H_{app}, \mathbf{F}) = (1 - \xi^{p_\xi})\Psi_p(\mathbf{F}) + \xi^{p_\xi}\Psi_a(c, \theta, \psi, H_{app}, \mathbf{F}) \\ \Psi_a(c, \theta, \psi, H_{app}, \mathbf{F}) = \begin{cases} (1 - c^{p_c}) \ \Psi|_{c=0.2} (\mathbf{F}, \mathbf{H}_r(\theta, \psi), H_{app}) \\ + c^{p_c} \ \Psi|_{c=0.3} (\mathbf{F}, \mathbf{H}_r(\theta, \psi), H_{app}) \end{cases} \\ \mathbf{P}(\xi, c, \theta, \psi, H_{app}, \mathbf{F}) = \dfrac{\partial \Psi(\xi, c, \theta, \psi, \mathbf{F}, H_{app})}{\partial \mathbf{F}} \end{cases} \\ \xi \in [0, 1] \\ c \in [0, 1] \\ \theta \in [-2\pi, 2\pi] \\ \psi \in [-2\pi, 2\pi] \\ H_{app} \in [0, H_{app,max}] \end{cases}$$

Optimized Dowsil C-shape

Optimized Dowsil C-shape



Topology and material optimization

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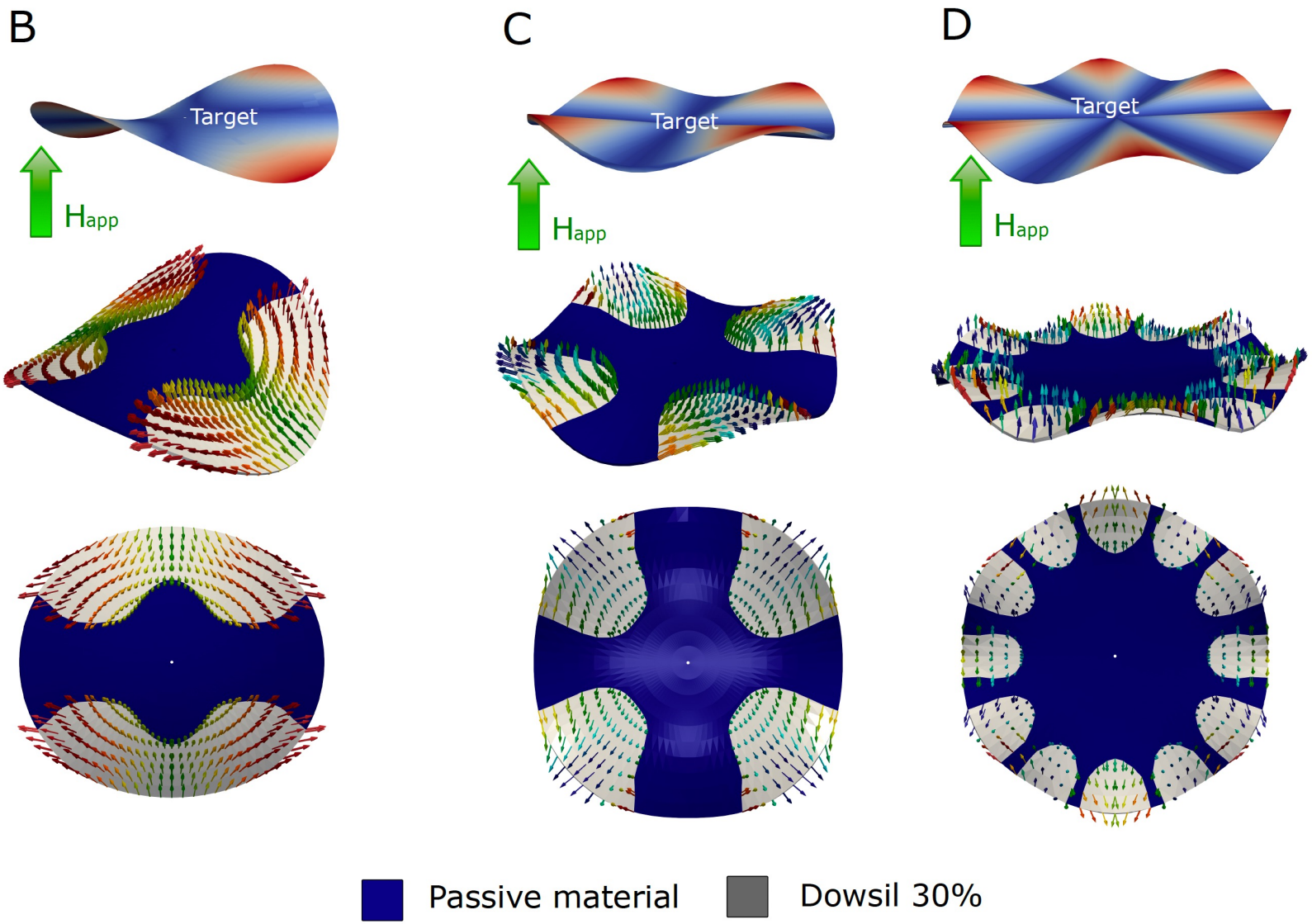
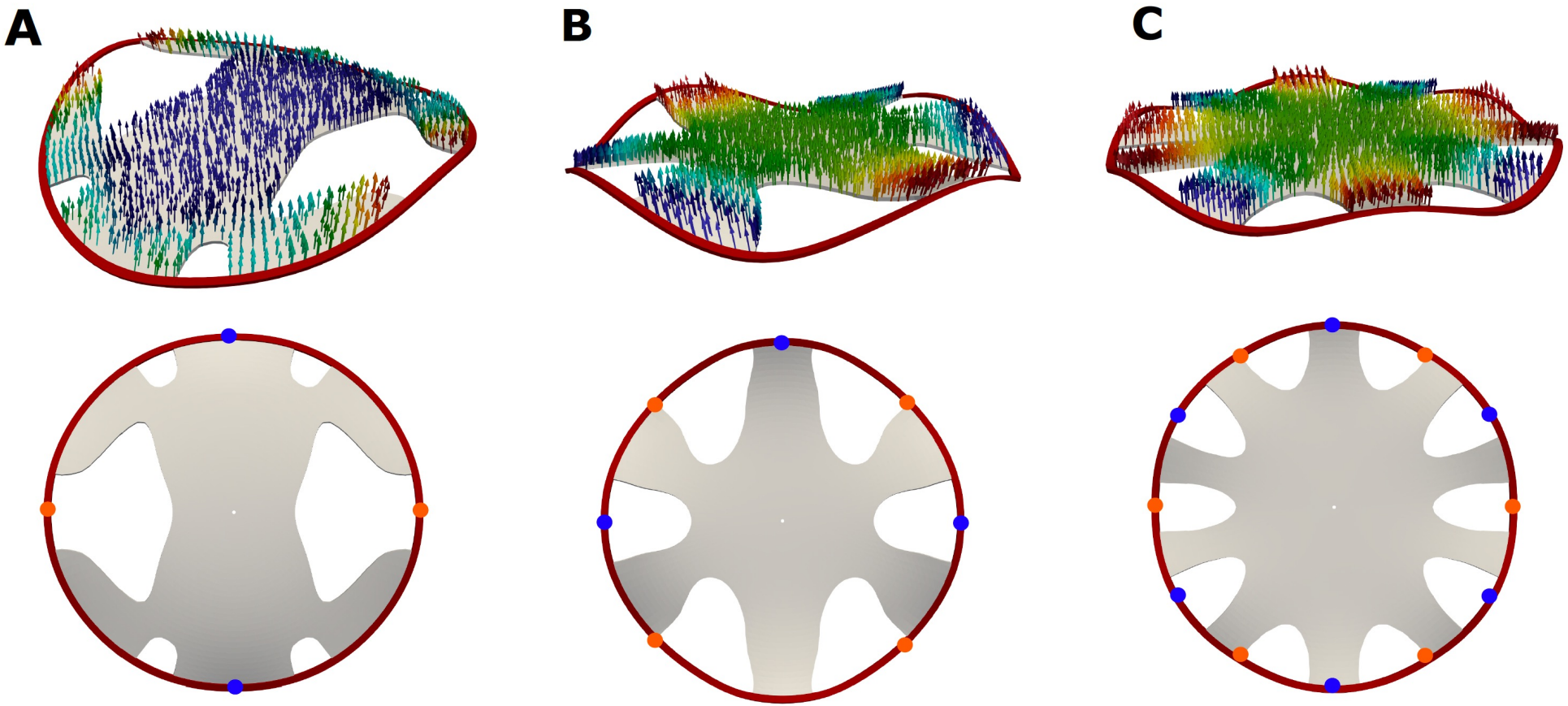
Staggered Approach



Staggered Approach



Optimizable region

Non optimizable region

Maximize out of plane displacement

Minimize out of plane displacement

HyperFEM (julia)

github.com

README MIT license

HyperFEM

docs stable | docs dev | Tests passing | codecov unknown

Multiphysics Simulation of Multifunctional Soft Materials

HyperFEM is a library within the Gridap ecosystem designed for the simulation of multiphysics problems involving multifunctional hyperelastic materials. The ultimate goal of HyperFEM is to provide a **high-level, expressive, and rapid prototyping tool** that accelerates the modeling stages of **Thermo–Electro–Magneto–Mechanical** multiphysics problems. To this end, it includes a comprehensive library of **analytically derived constitutive models** formulated through tensor algebra. In addition, HyperFEM provides abstractions for **monolithic and staggered solution schemes**, extending Gridap's capabilities in the context of **nonlinear solid mechanics**.

Installation

Open the Julia REPL, type `]` to enter package mode, and install as follows

```
pkg> add HyperFEM
```

Usage

First, include the main HyperFEM module:

```
using HyperFEM
```

Example of a Monolithic implementation for the simulation of Nonlinear ElectroMechanical deformation of dielectric elastomers

https://github.com/MultiSimOLab/Adv_Mater_Ultra_Soft_Magnet

HyperFEM (julia)

- **High-level multiphysics framework** within the Gridap ecosystem for nonlinear hyperelastic materials

- Designed to **bridge the gap between continuum-level modeling and algorithms based on PDEs** (optimization, control, ML, UQ...).

- Rapid prototyping of **thermo-electro-magneto-mechanical-acoustic-fluid** problems using analytically derived constitutive models

- Dedicated abstractions for **monolithic and staggered solution** schemes in nonlinear solid mechanics

HyperFEM (julia)

TensorAlgebra: high-level tensor operations generated through multiple dispatch and metaprogramming

```
"""
    ⊗₁₃²⁴(A::TensorValue{D}, B::TensorValue{D})::TensorValue{D*D}

Outer product of two second-order tensors (matrices), returning a fourth-order tensor
represented in a `D² x D²` flattened matrix using combined indices.
"""
@generated function (⊗₁₂³⁴)(A::TensorValue{D,D,Float64}, B::TensorValue{D,D,Float64}) where {D}
  str = ""
  for iB in 1:D*D
    for iA in 1:D*D
      str *= "A.data[$iA] * B.data[$iB], "
    end
  end
  Meta.parse("TensorValue{D*D,D*D, Float64}($str)")
end


"""
```

$$(I3 \otimes_{13}^{24} (N \otimes N))$$

HyperFEM (julia)

PhysicalModels: a high-level abstraction for constitutive models, providing analytically defined continuum energy functions and consistent derivatives

```julia
struct NeoHookean3D <: IsoElastic
  λ::Float64
  μ::Float64
  ρ::Float64

  function NeoHookean3D(; λ::Float64, μ::Float64, ρ::Float64=0.0)
    new(λ, μ, ρ)
  end

  function (obj::NeoHookean3D)(Threshold=0.01)
    λ, μ = obj.λ, obj.μ
    J(F) = det(F)
    H(F) = det(F) * inv(F)'
    Ψ(F) = μ / 2 * tr((F)' * F) - μ * logreg(J(F)) + (λ / 2) * (J(F) - 1)^2 - 3.0 * (μ / 2.0)

    ∂log∂J(J) = J >= Threshold ? 1 / J : (2 / Threshold - J / (Threshold^2))
    ∂log2∂J2(J) = J >= Threshold ? -1 / (J^2) : (-1 / (Threshold^2))

    ∂Ψ_∂J(F) = -μ * ∂log∂J(J(F)) + λ * (J(F) - 1)
    ∂Ψu(F) = μ * F + ∂Ψ_∂J(F) * H(F)
    ∂Ψ2_∂J2(F) = -μ * ∂log2∂J2(J(F)) + λ
    ∂Ψuu(F) = μ * I9 + ∂Ψ2_∂J2(F) * (H(F) ⊗ H(F)) + ∂Ψ_∂J(F) * ×ᵢ⁴(F)
    return (Ψ, ∂Ψu, ∂Ψuu)
  end
end
```

HyperFEM (julia)

PhysicalModels: a high-level abstraction for constitutive models, providing analytically defined continuum energy functions and consistent derivatives

```
modeliso = MooneyRivlin3D(λ=(1e5, μ1=1e3, μ2=1e3)
fibra1 = HGO_1Fiber(c1=c1[1], c2=c2[1])
fibra2 = HGO_1Fiber(c1=c1[2], c2=c2[2])
fibra3 = HGO_1Fiber(c1=c1[3], c2=c2[3])
fibra4 = HGO_1Fiber(c1=c1[4], c2=c2[4])
modelelec = IdealDielectric(ε=4.0)

constitutive_model= modeliso +[fibra1 fibra2 fibra3 fibra4]+ modelelec
```

C. Perez-Garcia, R. Ortigosa, J. Martínez-Frutos, and D. Garcia-Gonzalez, ***Topology and material optimization in ultra-soft magnetoactive structures: making advantage of residual anisotropies.*** *Adv. Mater. (2025)*

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GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

UNIÓN EUROPEA
FONDO EUROPEO DE DESARROLLO REGIONAL
"Una manera de hacer Europa"

AGENCIA ESTATAL DE INVESTIGACIÓN

Low σ

Stress Field

HyperFEM (julia)

ComputationalModels: an abstraction of numerical problem classes (e.g., static linear, static nonlinear, dynamic nonlinear, staggered schemes) designed to encapsulate PDE solvers and enable their integration within outer-loop workflows such as control, optimization, and machine learning

```
# Problem 1: residual and jacobian
res_mag(Λ) = (φ, vφ) -> -1.0 * ∫((∇(vφ) ⋅ (∂Ψs∂H0 ∘ (F ∘ (∇(uhsolid(Λ))'), ℋ₀ ∘ (∇(φ)), Nh))))dΩsolid -
                                ∫((∇(vφ) ⋅ (∂Ψv∂H0 ∘ (F ∘ (∇(uhvacuum(Λ))'), ℋ₀ ∘ (∇(φ))))))dΩvacuum_mag

jac_mag(Λ) = (φ, dφ, vφ) -> ∫(∇(vφ)' ⋅ ((∂Ψs∂H0H0 ∘ (F ∘ (∇(uhsolid(Λ))'), ℋ₀ ∘ (∇(φ)), Nh)) ⋅ ∇(dφ)))dΩsolid +
                                ∫(∇(vφ)' ⋅ ((∂Ψv∂H0H0 ∘ (F ∘ (∇(uhvacuum(Λ))'), ℋ₀ ∘ (∇(φ)))) ⋅ ∇(dφ)))dΩvacuum_mag

# Problem 2: residual and jacobian
res_mech(Λ) = (u, v) -> ∫((∇(v)' ⊙ (∂Ψs∂F ∘ (F ∘ (∇(u)'), ℋ₀ ∘ (∇(φh(Λ))), Nh))))dΩsolid -
                                ∫((v.⁺ ⋅ ((∂Ψv∂F ∘ (F ∘ (∇(uhvacuum(Λ))'), ℋ₀ ∘ (∇(φh(Λ))))).⁻ ⋅ nΓsf.⁺)))dΓsf

jac_mech(Λ) = (u, du, v) -> ∫(∇(v)' ⊙ ((∂Ψs∂FF ∘ (F ∘ (∇(u)'), ℋ₀ ∘ (∇(φh(Λ))), Nh)) ⊙ (∇(du)')))dΩsolid

# Problem 3: residual and jacobian
res_vacmech(Λ) = (u, v) -> ∫((∇(v)' ⊙ (∂Ψvm∂F ∘ (F ∘ (∇(u)')))))dΩvacuum_mec
jac_vacmech(Λ) = (u, du, v) -> ∫(∇(v)' ⊙ ((∂Ψvm∂FF ∘ (F ∘ (∇(u)'))) ⊙ (∇(du)')))dΩvacuum_mec
```

HyperFEM (julia)

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```
# ******************************************************
#             Computational problems
#******************************************************

# Problem 1
nls_mag = NewtonSolver(LUSolver(); maxiter=20, atol=1.e-9, rtol=1.e-8, verbose=true)
comp_model_mag = StaticNonlinearModel(res_mag, jac_mag, Uφ⁺, Vφ, Dφ; nls=nls_mag, xh=φh⁺)

# Problem 2
nls_mech = NewtonSolver(LUSolver(); maxiter=20, atol=1.e-6, rtol=1.e-2, verbose=true)
comp_model_mech = StaticNonlinearModel(res_mech, jac_mech, Uu_solid⁺, Vu_solid, Du_solid; nls=nls_mech, xh=uh_solid⁺)

# Problem 3
nls_vacmech = NewtonSolver(LUSolver(); maxiter=10,  rtol=2, verbose=true)
comp_model_vacmech = StaticNonlinearModel(res_vacmech, jac_vacmech, Uu_vacuum⁺, Vu_vacuum, Du_vacuum; nls=nls_vacmech, xh=uh_vacuum⁺)

# Staggered resolution:  Problem1-> Problem2-> Problem3
comp_model = StaggeredModel((comp_model_mag, comp_model_mech, comp_model_vacmech), (φh⁺, uh_solid⁺, uh_vacuum⁺), (φh⁻, uh_solid⁻, uh_vacuum⁻))
```