Automation of multiphysics numerical simulations using open-source software

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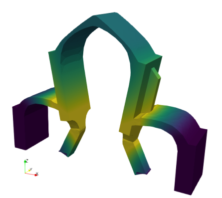
Funded by the European Union

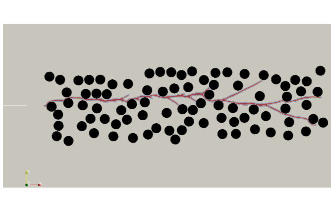
European Research Council
Established by the European Commission

January 22, 2026

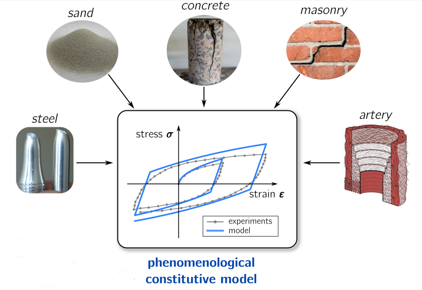
Context

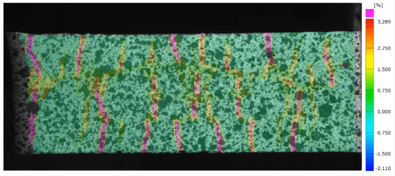
Structural simulations: numerical methods (FE), nonlinearities, complex geometry, time-dependency





Constitutive behavior: elasticity, viscoelasticity, plasticity, damage, temperature effects...





Open-source software for computational mechanics

Advantages/Drawbacks

reproducibility

extensibility

community

user responsibility

learning curve

stability

- code_aster
- deal_ii
- elmer
- Kratos

- Cast3m/Manta
- MOOSE
- MFEM

- OpenFOAM
- Basilisk
- FreeFEM++

- gmsh
- pyvista
- Paraview
- pytorch

Here: FEniCSx – MFront – JAX

FEniCSx

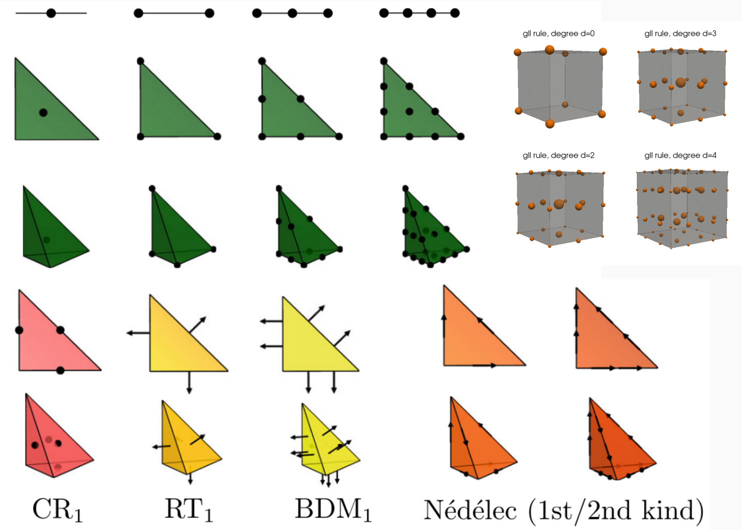
collection of free, open source, software components for **automated solution** of **Partial Differential Equations** (PDEs)

FEniCS PROJECT

Features:

- variational formulation expressed with **math symbolic language**: `ufl.grad`, `ufl.div`, `ufl.derivative`, etc.
- **code-generation** (`C`) and **JIT compilation** of FE kernels
- **extensive library** of finite elements
- designed for **parallel HPC computations**

Element types



A simple elasticity example

Weak form/variational formulation: Find $\boldsymbol{u} \in V$ such that:

$$\int_\Omega \boldsymbol{\sigma}(\boldsymbol{u}) : \nabla^s \boldsymbol{v} \,\mathrm{d}\Omega = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \,\mathrm{d}\Omega \quad \forall \boldsymbol{v} \in V$$

with **isotropic linear elasticity**: $\boldsymbol{\sigma}(\boldsymbol{u}) = \lambda \operatorname{tr}(\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}$ with $\boldsymbol{\varepsilon} = \nabla^s \boldsymbol{u}$.

```
dim, degree = mesh.geometry.dim, 2
V = fem.functionspace(mesh, ("P", degree, dim))

def epsilon(v):
    return ufl.sym(ufl.grad(v))
def sigma(v):
    return lmbda * ufl.tr(epsilon(v)) * ufl.Identity(dim) + 2 * mu * epsilon(v)

u, v = TrialFunction(V), TestFunction(V)

a, L = ufl.inner(sigma(u), epsilon(v)) * dx, ufl.dot(f, v) * dx
```

Multi-field variational problems

One of the big advantages of **FEniCS**
e.g. **Stokes incompressible fluids**: mixed $u - p$ formulation

Taylor-Hood element (P_2/P_1)

```
# Define function space
P2 =  basix.ufl.element('P', tetrahedron, 2, shape=(dim,))
P1 =  basix.ufl.element('P', tetrahedron, 1)
THe = basix.ufl.mixed_element([P2, P1])
W = fem.functionspace(mesh, THe)
```

```
# Define variational problem
(u, p) = TrialFunctions(W)
(v, q) = TestFunctions(W)
a, L = inner(grad(u), grad(v))*dx - p*div(v)*dx + div(u)*q*dx, dot(f, v)*dx
```

Multi-field variational problems

One of the big advantages of **FEniCS**
e.g. **Stokes incompressible fluids**: mixed $u - p$ formulation

MINI element $(P_1 + \mathcal{B})/P_1$

```
# Define function space
Pv1 = basix.ufl.element('P', tetrahedron, 1)
B = basix.ufl.element('Bubble', tetrahedron, 3)
Mini = basix.ufl.mixed_element([Pv1+B, P1])
W =  fem.functionspace(mesh, Mini)
```

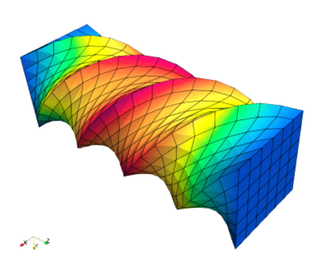
```
# Define variational problem
(u, p) = TrialFunctions(W)
(v, q) = TestFunctions(W)
a, L = inner(grad(u), grad(v))*dx - p*div(v)*dx + div(u)*q*dx, dot(f, v)*dx
```

Finite-strain mechanics

Finite-strain weak equilibrium

$$\int_\Omega \boldsymbol{P}(\boldsymbol{u}) : \nabla \boldsymbol{v}\, \mathrm{d}\Omega = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}\, \mathrm{d}\Omega \quad \forall \boldsymbol{v} \in V$$

$\boldsymbol{P} = \dfrac{\partial \psi}{\partial \boldsymbol{F}}$: first Piola-Kirchhoff stress given by a **hyperelastic potential** $\psi(\boldsymbol{F})$ with $\boldsymbol{F} = \boldsymbol{I} + \nabla \boldsymbol{u}$.



Example: $\psi(\boldsymbol{F}) = \dfrac{\mu}{2}(\bar{I}_1 - 3) + k(J^2 + J^{-2} - 2)$ s.t. $\bar{I}_1 = \mathrm{tr}(\overline{\boldsymbol{C}})$, $\overline{\boldsymbol{C}} = J^{-2/3}\boldsymbol{F}^\mathsf{T}\boldsymbol{F}$, $J = \det \boldsymbol{F}$

Tangent operator

$$a_{\text{tangent}}(\boldsymbol{u}, \boldsymbol{v}) = \int_\Omega \nabla \boldsymbol{u} : \frac{\partial^2 \psi}{\partial \boldsymbol{F} \partial \boldsymbol{F}} : \nabla \boldsymbol{v}\, \mathrm{d}\Omega$$

$\Rightarrow$ **UFL symbolic differentiation**

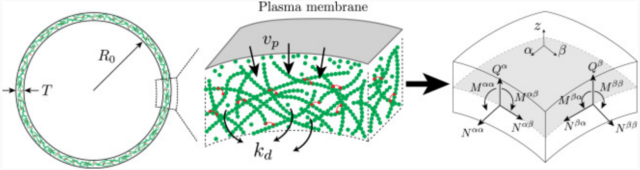
```python
def psi(u):
    ...

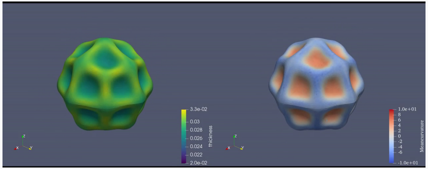
E_pot = psi * dx - ufl.dot(f, u)*dx
Res = ufl.derivative(E_pot, u, v)
Jac = ufl.derivative(Res, u, du)
```

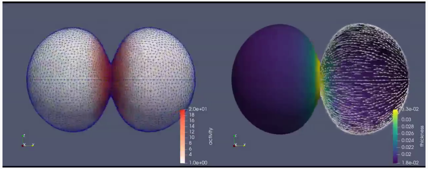
A biomechanics application [with Hudson Borja da Rocha and Hervé Turlier (Collège de France)]

Mechanics of biological cells

- The **cell cortex** is a very thin layer under the membrane that controls cell shape.
- It **actively generates forces and flows** (e.g. during cell division or deformation).
- We model its mechanics using an **active viscous shell model** [JMPS, 2022]







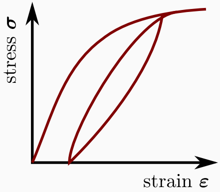
MFront

Material constitutive modeling

Constitutive model = a **stress-strain** relation

$$\boldsymbol{\varepsilon} \longrightarrow \boxed{\text{CONSTITUTIVE RELATION}} \longrightarrow \boldsymbol{\sigma}$$

generally with **custom implementation** in a FE solver



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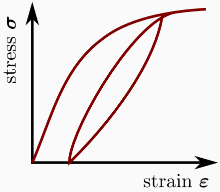
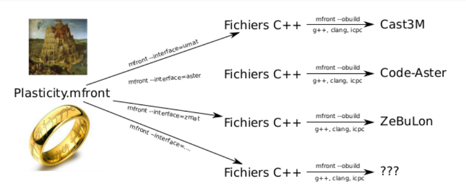


- **decouple** material library from structural solvers
- **inter-operability**: **material knowledge** can be **shared** across various solvers (industrial and academic)
- improve quality assurance, long-term sustainability, collaboration

MFront

`MFront` = a **code generation tool** dedicated to **material knowledge**
Main developer: Thomas Helfer (CEA Cadarache) + many other contributors

- Numerical **efficiency**
- **Inter-operability**: specific (`Cast3M`, `code_aster`, `Europlexus`, `Abaqus`, `Zebulon`, `Ansys`, etc.) and *generic* interfaces (`python`, `fortran`, `c`, `julia`, etc.)
- Ease of use (**Domain-Specific Languages**)



Features

- C++ code, text file input to be compiled for a given interface
- **Typical mechanical behaviors**: elasticity, viscoelasticity, plasticity, damage, temperature dependence, finite strains, cohesive zone models, *homogenized behaviors*
- **solvers**: implicit/explicit time integrators, (quasi)-Newton
- `mtest`: testing tool

Examples

Pre-defined modular bricks

```
@DSL Implicit;
@Behaviour PerfectPlasticity;
@Epsilon 1.e-14;
@Theta 1;
@Brick StandardElastoViscoPlasticity{
  stress_potential : "Hooke" {young_modulus : 200e9,
      poisson_ratio : 0.3},
  inelastic_flow : "Plastic" {
    criterion : "Mises",
    isotropic_hardening : "Linear" {R0 : 150e6},
}
};
```

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    criterion : "Mises",
    isotropic_hardening : "Linear" {R0 : 150e6},
}
};
```

```
@DSL Implicit;
@Behaviour Norton;
@Brick StandardElasticity;

@MaterialProperty stress E;
E.setGlossaryName("YoungModulus");
@MaterialProperty real ν, A, nn;
ν.setGlossaryName("PoissonRatio");
A.setEntryName("NortonCoefficient");
nn.setEntryName("NortonExponent");

@StateVariable real    p;
p.setGlossaryName("EquivalentViscoplasticStrain");

@Integrator{
  constexpr const auto Mᵉ = Stensor4::M();
  const auto μ = computeMu(E, ν);
  const auto σᵉ = sigmaeq(σ);
  const auto iσᵉ = 1 / (max(σᵉ, real(1.e-12) ⋅ E));
  const auto vᵖ = A ⋅ pow(σᵉ, nn);
  const auto ∂vᵖ/∂σᵉ = nn ⋅ vᵖ ⋅ iσᵉ;
  const auto n = 3 ⋅ deviator(σ) ⋅ (iσᵉ / 2);
  // Implicit system
  fεᵉˡ += Δp ⋅ n;
  fp -= vᵖ ⋅ Δt;
  // jacobian
  ∂fεᵉˡ/∂Δεᵉˡ += 2 ⋅ μ ⋅ θ ⋅ dp ⋅ iσᵉ ⋅ (Mᵉ - (n ⊗ n));
  ∂fεᵉˡ/∂Δp = n;
  ∂fp/∂Δεᵉˡ = -2 ⋅ μ ⋅ θ ⋅ ∂vᵖ/∂σᵉ ⋅ Δt ⋅ n;
} // end of @Integrator
```

Advanced aspects

- **Finite strain**: solvers require different "forms" of the tangent operator e.g. $\frac{d\boldsymbol{\sigma}}{d\boldsymbol{d}}$, $\frac{d\boldsymbol{P}}{d\boldsymbol{F}}$, $\frac{d\boldsymbol{S}}{d\boldsymbol{E}}$ and many others... $\Rightarrow$ `MFront` provides conversion methods
- support for different modeling hypotheses: `PlaneStrain`, `Tridimensional`, `Axisymmetric`, etc. (optimized code/hypothesis)
- **numerical jacobian** (finite-differences) for implicit systems
- compile-time dimensional analysis
- recently, support for generalized behaviors (**multi-physics**)

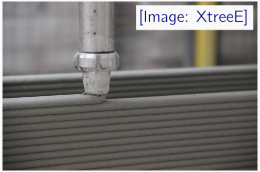
Mechanics

$$\Delta\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\sigma}_n, \boldsymbol{\alpha}_n \to \boxed{\texttt{MFront}} \to \boldsymbol{\sigma}_{n+1}, \boldsymbol{\alpha}_{n+1}, \frac{d\boldsymbol{\sigma}_{n+1}}{d\boldsymbol{\varepsilon}_{n+1}}$$

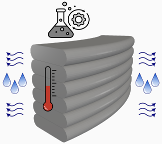
Multiphysics

$$(\Delta\boldsymbol{g}^1, \ldots, \Delta\boldsymbol{g}^p)_{n+1}, (\boldsymbol{\sigma}^1, \ldots, \boldsymbol{\sigma}^p)_n, \boldsymbol{\alpha}_n \to \boxed{\texttt{MFront}} \to (\boldsymbol{\sigma}^1, \ldots, \boldsymbol{\sigma}^p)_{n+1}, \boldsymbol{\alpha}_{n+1}, \frac{\partial \boldsymbol{\sigma}^i_{n+1}}{\partial \boldsymbol{g}^j_{n+1}}$$

Early age concrete = a **thermo-poro-chemo-mechanical** model [M. Pierre et al.]



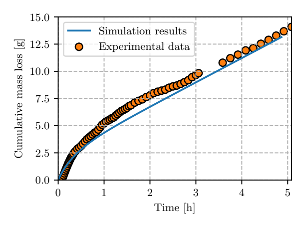
$$
\begin{cases}
\mathrm{d}\boldsymbol{\sigma} = \mathbb{C}(\xi) : \mathrm{d}\boldsymbol{\varepsilon} - b(\xi) S_\ell \mathrm{d}p \mathbf{1} - 3\alpha K(\xi) \mathrm{d}T \mathbf{1} \\
\mathrm{d}\phi = b(\xi) \mathrm{tr}(\mathrm{d}\boldsymbol{\varepsilon}) + \frac{b(\xi) - \phi_0(\xi)}{K_s} S_\ell \mathrm{d}p - 3\alpha \left(b(\xi) - \phi_0(\xi)\right) \mathrm{d}T - \Delta \overline{V}_s \mathrm{d}\xi \\
\mathrm{d}S_s = 3\alpha K(\xi) \mathrm{tr}(\mathrm{d}\boldsymbol{\varepsilon}) - 3\alpha \left(b(\xi) - \phi_0(\xi)\right) S_\ell \mathrm{d}p + \frac{C(1-\phi_0(\xi))}{T_0} \mathrm{d}T - \frac{\mathcal{L}}{T_0} \mathrm{d}\xi
\end{cases}
$$

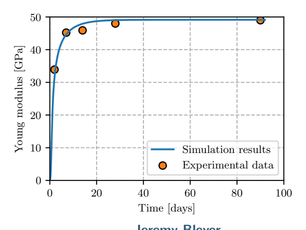


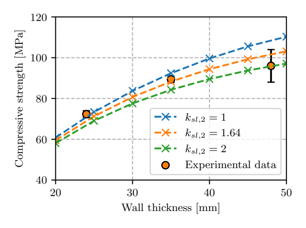
3D-printed concrete

Evolution of material properties with hydration, **change of solid volume** + **heat** due to **chemical reaction(s)**

[A. Gribonval et al.]: influence of **environmental conditions** on **compressive strength**

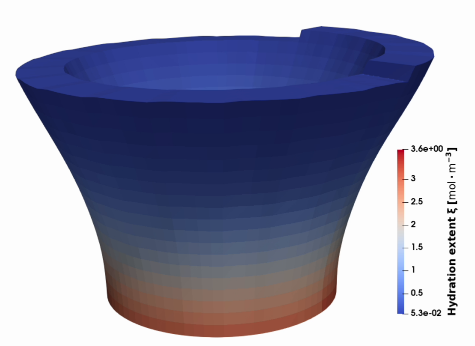






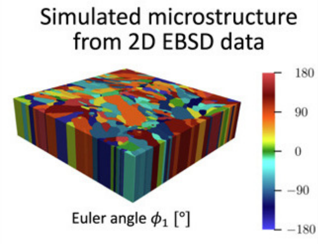
3D-printing concrete modeling

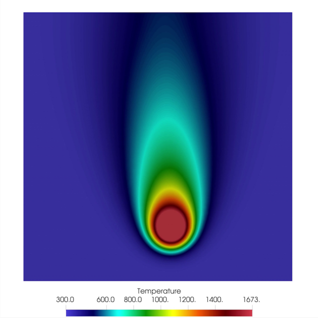
[M. Pierre]: `gmsh` - `FEniCSx` - `MFront` pipeline with mesh activation
THCM model with elastoplastic Cam-Clay behavior

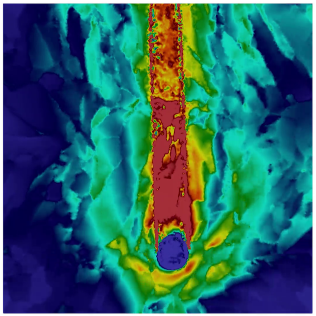


Residual stresses after laser scanning of additively manufactured stainless steel

coll. Nikhil Mohanan, Manas Upadhyay (LMS, Ecole Polytechnique)







MFront: thermo elastoviscoplastic polycrystal model
FEniCSx: weakly coupled thermomechanics on polycrystal mesh

JAX

Constitutive models as ML models

Constitutive models can be formalized as **parametrized functions** (stress update):

$$\boxed{\boldsymbol{\sigma}_{n+1}, \boldsymbol{\alpha}_{n+1} = \mathcal{M}_{\boldsymbol{\theta}}(\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\alpha}_n)}$$

where $\boldsymbol{\theta}$ are the model **material parameters** and $\mathcal{M}_\theta = \mathcal{O}_1 \circ \mathcal{O}_2 \circ \cdot \circ \mathcal{O}_n$

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Formally equivalent with ML, main **differences** are:

- **internal state** not **observable** from data
- **sequential evaluation of the model** in time:

$$\boldsymbol{\sigma}_1, \boldsymbol{\alpha}_1 = \mathcal{M}_{\boldsymbol{\theta}}(\boldsymbol{\varepsilon}_1, \boldsymbol{\alpha}_0) \to \boldsymbol{\sigma}_2, \boldsymbol{\alpha}_2 = \mathcal{M}_{\boldsymbol{\theta}}(\boldsymbol{\varepsilon}_2, \boldsymbol{\alpha}_1) \to \cdots \to \boldsymbol{\sigma}_{n+1}, \boldsymbol{\alpha}_{n+1} = \mathcal{M}_{\boldsymbol{\theta}}(\boldsymbol{\varepsilon}_n, \boldsymbol{\alpha}_n)$$

- some **elementary operations** $\mathcal{O}_i$ may not have **closed-form** expressions

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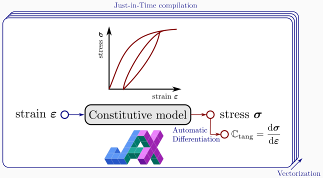
Opportunities

- **phenomenological** or **NN-based** models can be treated in a **unifying framework**
- they can be **seamlessly hybridized**!
- material parameter **identification** can benefit from **ML gradient-based algorithms**
- **practical implementation** can benefit from **modern ML frameworks**

JAX for constitutive modeling



JAX = accelerated (GPU) array computation and program transformation designed for **HPC** and large-scale **machine learning**

```
def constitutive_update(eps, state, dt):
    [...]
    return stress, new_state
```

- **JIT** and **automatic vectorization**

```
batch_constitutive_update = jax.jit(jax.vmap(constitutive_update, in_axes=(0, 0, None))
```

- **Automatic Differentiation**

```
constitutive_update_tangent = jax.jacfwd(constitutive_update, argnums=0, has_aux=True)
```

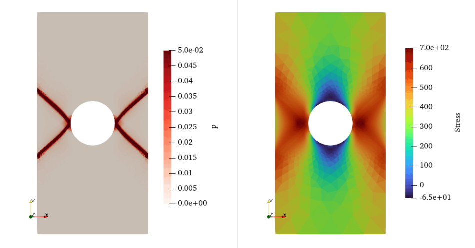
`jaxmat` – an open-source material modeling library

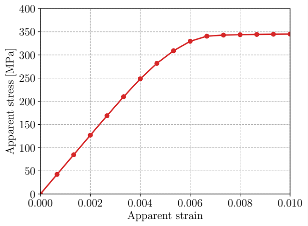
First release end of 2025: `https://github.com/bleyerj/jaxmat`

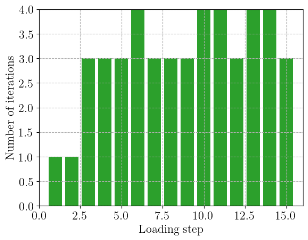
Features

- based on `JAX` and `equinox` (NN models), `optimistix` (optimization solvers), `diffrax` (ODE solvers)
- models as **PyTrees** $\Rightarrow$ allows **modularity** and **hierarchical composition**:
  $\boldsymbol{\theta} = \{\boldsymbol{\theta}_{\text{elastic}}, \{\boldsymbol{\theta}_{\text{plastic}}, \boldsymbol{\theta}_{\text{hardening}}\}\}$
- prototype **material models**: elastoplasticity, viscoplasticity, hyperelasticity, finite strain plasticity, viscoelasticity, Generalized Standard Materials, damage, etc.
- **hybrid NN-phenomenological** models
- **differentiable solvers** using **implicit differentiation**
- **gradient-based** identification
- **CPU** or **GPU** acceleration
- **compatibility** with FEniCSx (`v.0.10`)

Small-strain elastoplasticity








```
E, nu = 70e3, 0.3
elastic_model = LinearElasticIsotropic(E, nu)

class VoceHardening(equinox.Module):
    sig0 = 350.0
    sigu = 500.0
    b = 1e3
    def __call__(self, p):
        return self.sig0 + (self.sigu - self.sig0) * (1 - jnp.exp(-self.b *
      p))

material = vonMisesIsotropicHardening(elastic_model,
    yield_stress)
```

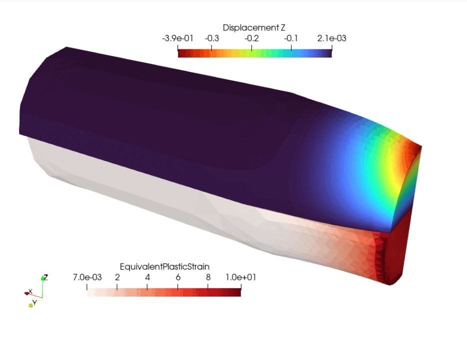
$\boldsymbol{F}^{\text{e}}\boldsymbol{F}^{\text{p}}$ finite-strain plasticity

$$\boldsymbol{F} = \boldsymbol{F}^{\text{e}}\boldsymbol{F}^{\text{p}}\,; \quad \bar{\boldsymbol{b}}^{\text{e}} = J^{-2/3}\boldsymbol{F}^{\text{e}}(\boldsymbol{F}^{\text{e}})^{\text{T}}$$

$$\boldsymbol{\tau} = \mu\,\text{dev}(\bar{\boldsymbol{b}}^{\text{e}}) + \frac{\kappa}{2}(J^2 - 1)\boldsymbol{I}$$

$$f(\bar{\boldsymbol{b}}^{\text{e}}) = \mu\|\boldsymbol{s}\| - \sqrt{\frac{2}{3}}R(p_n + \Delta p) \leq 0$$

$$0 = \text{dev}(\bar{\boldsymbol{b}}^{\text{e}} - \bar{\boldsymbol{b}}^{\text{e}}_{\text{trial}}) + \sqrt{\frac{2}{3}}\Delta p\,\text{tr}(\bar{\boldsymbol{b}}^{\text{e}})\frac{\boldsymbol{s}}{\|\boldsymbol{s}\|}$$

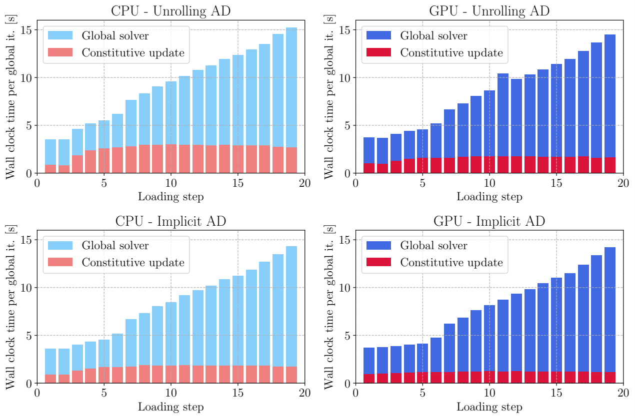


Resolution involves local solving of a Newton system of size 7
Tangent operator in $PK1/F$ using **implicit AD**:

$$\boldsymbol{P} = \boldsymbol{\tau}\boldsymbol{F}^{-1} \qquad \mathbb{C}_{\text{tang}} = \frac{\partial \boldsymbol{P}}{\partial \boldsymbol{F}}$$

$F^e F^p$ finite-strain plasticity

Constitutive equation: `jax[cpu]` or `jax[gpu]` on `NVIDIA RTX A1000`
Linear solver: PETSc `gmres` + `gamg`



Global linear solves – Constitutive behavior integration

Material model identification

Identification

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \frac{1}{M}\sum_{k=1}^{M} \|\boldsymbol{\sigma}^{(k)} - \boldsymbol{\sigma}_{\text{data}}^{(k)}\|^2$$

gradient-based optimisation, needs **material parameters sensitivities**

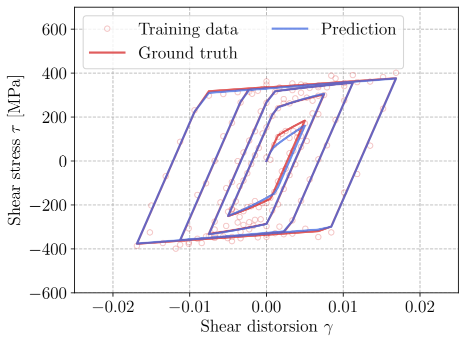
$$\frac{\partial \boldsymbol{\sigma}^{(k)}}{\partial \boldsymbol{\theta}} \to \frac{\partial \mathsf{F}}{\partial \boldsymbol{\theta}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}; \boldsymbol{\theta})$$

easy to obtain with **JAX**

```
@jax.jit
def loss(material, sig_data, loading):
    sig_hat = compute_evolution(material, loading)
    loss = optax.l2_loss(sig_hat, sig_data)
    return loss.mean()
```

differentiable time loop with `jax.lax.scan`

Armstrong-Frederick type hardening plasticity with **noisy data**



Open source and industry

Undabit: an Italian vibro-acoustic company

Simvia: subsidiary of **EDF**

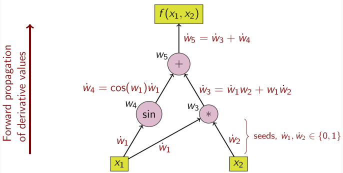
- training, technical support
- software projects, cloud & HPC

At Simvia, we believe that open-source [...] give industrial companies control over their simulation solutions, by offering them reactivity, performance, and scalability.

Thank you for your attention!

What is Automatic Differentiation ?

- **Numerical Differentiation**: $f'(x) = \dfrac{f(x+h) - f(x)}{h}$ with e.g. $h = 10^{-6}$
  truncation/rounding errors, $O(dim)$ evaluations
- **Symbolic differentiation**: f represented as an **expression graph**, generates **another expression graph** of the derivative
  expression swell, duplicate operations, no-closed form expression
- **Automatic differentiation**: operates directly on the **computer program**, no symbolic representation (numerical evaluation only), **exact**
  forward and **reverse** mode (**back-propagation** in ML)



[Wikipedia]

```
def f(x):
    [...]
    for i in range(n):
        [...]
```

```
def f(x):
    if cond:
        [...]
    else:
        [...]
```

```
def f(x):
    [...]
    while cond:
        [...]
```

Differentiating through elastoplasticity

Return mapping algorithm

Elastic predictor $\boldsymbol{\sigma}_{\text{elas}} = \boldsymbol{\sigma}_n + \mathbb{C} : \Delta\boldsymbol{\varepsilon}$

$f_{\text{elast}} = \sigma_{\text{eq}} - R(p_n)$

- if $f_{\text{elas}} < 0$: $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{\text{elas}}$ and $\Delta p = 0$
- else: $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{\text{elas}} - 2\mu\Delta\boldsymbol{\varepsilon}^{\text{p}}$ with $\Delta\boldsymbol{\varepsilon}^{\text{p}} = \Delta p \dfrac{3}{2\sigma_{\text{eq}}^{\text{elas}}}\boldsymbol{s}_{\text{elas}}$

$$\textbf{Solve } r(\Delta p) = \sigma_{\text{eq}}^{\text{elas}} - 3\mu\Delta p - R(p_n + \Delta p) = 0 \tag{1}$$

implement **Solve** using fixed-point algorithm, Newton method, bisection, etc.

Every step is differentiable with AD *a priori*, **except** (1).

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Algorithm unrolling

Any algorithm used to solve (1) can be written in JAX using loops, conditionals, etc. We can **differentiate through the algorithm** (*unrolling the algorithm iterations*).

Implicit automatic differentiation [Blondel et al., 2022]

We can leverage instead the **implicit function theorem**

e.g. root finding: Find x_θ s.t. $F(x_\theta;\theta) = 0$

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To find $\partial_\theta x_\theta$, we differentiate the equation so that:

$$
\begin{aligned}
&[\partial_x F]\partial_\theta x_\theta + \partial_\theta F = 0 \\
\Rightarrow \quad &\partial_\theta x_\theta = -[\partial_x F]^{-1}\partial_\theta F
\end{aligned}
$$

need only to solve a **linear system** for the **jacobian matrix** $[\partial_x F]$

the derivative computation becomes **independent from the algorithm** used to solve the nonlinear system, can use AD to form the jacobian $[\partial_x F]$

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Can be implemented for any function using `jax.lax.custom_root`
Available in `optimistix`:

```
solver = optimistix.Newton(rtol=1e-8, atol=1e-8)
solution = optimistix.root_find(fun, solver, y0, adjoint=optimistix.ImplicitAdjoint())
```

PANN models for data-driven hyperelasticity

Isotropic hyperelastic potential

$$\psi(\boldsymbol{F}) = \Psi(I_1, I_2, I_3)$$

polyconvexity guaranteed if Ψ is **convex**

Physics-Augmented Neural Networks [Linden et al., 2023] approximate

$$\psi_{\boldsymbol{\theta}}(\boldsymbol{F}) = \Psi_{\boldsymbol{\theta}}(I_1, I_2, I_3, -2J)$$

where $\Psi_{\boldsymbol{\theta}}(\mathcal{I})$ is an **Input Convex Neural Network** (ICNN) [Amos et al., 2017] (positive weights, `softplus` activation)

Important: enforce stress-free initial configuration

$$\Psi_{\boldsymbol{\theta}}^{\text{PANN}}(\boldsymbol{C}) = \Psi_{\boldsymbol{\theta}}(\mathcal{I}) - \left.\frac{\partial \Psi_{\boldsymbol{\theta}}}{\partial \mathcal{I}}\right|_{\boldsymbol{C}=\boldsymbol{I}} 2(J-1)$$

```
class PANN(ICNN):
    def nn_energy(self, lambC):
        I3 = jnp.prod(lambC)
        I1 = jnp.sum(lambC)
        I2 = jnp.sum(I3 / lambC)
        return super().__call__(jnp.asarray([I1, I2,
  I3, -2*jnp.sqrt(I3)]))
```

```
    def pann_energy(self, lambC):
        J = jnp.sqrt(jnp.prod(lambC))
        dpsi_dC =
  jax.jacfwd(self.nn_energy)(jnp.ones((3,)))[0]
        return self.nn_energy(lambC) - 2 * dpsi_dC *
  (J - 1)
```

PANN model on rubber elasticity data [Treloar, 1944]

PANN with 4 inputs, 10 neurons in 1 hidden layer