Modularity and simultaneity in constitutive model applications

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Abstract

Modularity in constitutive model applications.

- Algorithmic and flexible approach for modular assembly of constitutive pieces.
- Reduce number of implemented models and enable automatic combo exploration.

Simultaneity in constitutive model applications.

- Time integration and equation solving are handled simultaneously for all variables.
- Simplify model implementation and enable modular constitutive model generation.
- Increase the efficiency, flexibility, and robustness of mechanics analyses.

Both of these ideas seem possible and could be very useful.

- Constitutive models could be automatically assembled and readily used in analyses.
- There are more details to be worked out for simultaneity across all model types.

Modularity
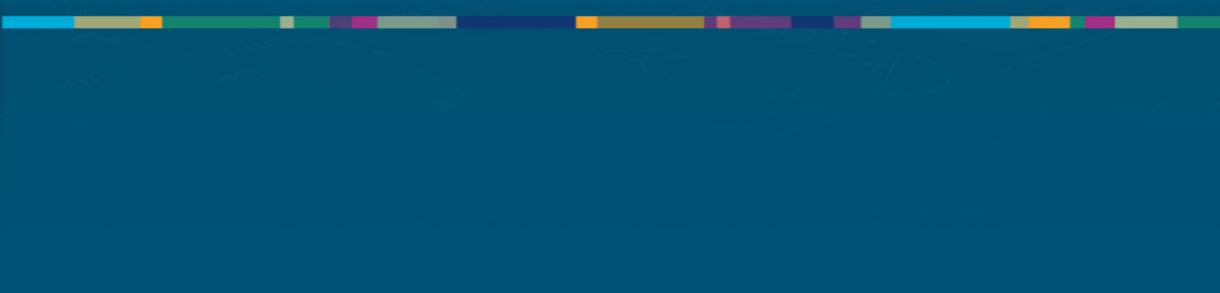
Modularity

Modular assembly of constitutive pieces.

- Algorithmic and flexible approach.
- Readily explore model combinations.
- Reduce number of implemented models.
- May lead to automatic model generation.

Different than current notions of modularity.

- Rules for sequential assembly rather than drop-in replacement.
- Specific combinations of model types create other specific model types.

Some conceptual problems to handle.

- Nested sets of constitutive variables.
- Spooky action (coupling) at a distance.

The constitutive relation for the stress

$$a = a(\mathbf{F}), \quad \boldsymbol{\sigma}(\mathbf{F}) = \frac{1}{J} \frac{\partial a}{\partial \mathbf{F}} \cdot \mathbf{F}^T$$

and that for the viscoplastic flow

$$\dot{\mathbf{F}}_\mathrm{p} = \mathbf{D}_\mathrm{p} \cdot \mathbf{F}_\mathrm{p}, \quad \mathbf{D}_\mathrm{p} = f\left(\frac{|\mathbf{M}'_\mathrm{e}|}{Y(S)}\right) \frac{\mathbf{M}'_\mathrm{e}}{|\mathbf{M}'_\mathrm{e}|}$$

are combined using a kinematic relation

$$\mathbf{F} = \mathbf{F}_\mathrm{e} \cdot \mathbf{F}_\mathrm{p}$$

and other derivable rules for the stresses

$$\mathbf{M}_e = J\mathbf{F}_\mathrm{e}^T \cdot \boldsymbol{\sigma}(F_\mathrm{e}) \cdot \mathbf{F}_\mathrm{e}^{-T}$$

into a hyperelastic-viscoplastic model.

Modularity

Hencky hyperelastic model:

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{2\mu}{J}\,\mathbf{h}' + \frac{\kappa}{J}\,\mathrm{tr}(\mathbf{h})\mathbf{1}, \quad \mathbf{h} = \tfrac{1}{2}\ln(\mathbf{B})$$

Viscoplastic flow [1] models:

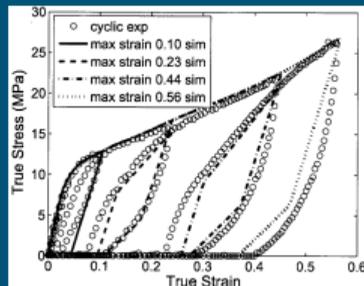$$\mathbf{D}_{\mathrm{p}} = d_0 \exp\left(\frac{-\Delta G}{kT}\right)\sinh\left(\frac{\Delta G}{kT}\frac{|\boldsymbol{\sigma}'|}{Y(S)}\right)\frac{\boldsymbol{\sigma}'}{|\boldsymbol{\sigma}'|}$$

$$\dot{\mathbf{F}}_{\mathrm{p}} = \mathbf{D}_{\mathrm{p}}\cdot\mathbf{F}_{\mathrm{p}}, \quad \dot{\varepsilon}_{\mathrm{p}} = |\mathbf{D}_{\mathrm{p}}|, \quad \dot{Y} = H\left(1 - \frac{Y}{Y_{\infty}}\right)\dot{\varepsilon}_{\mathrm{p}}$$
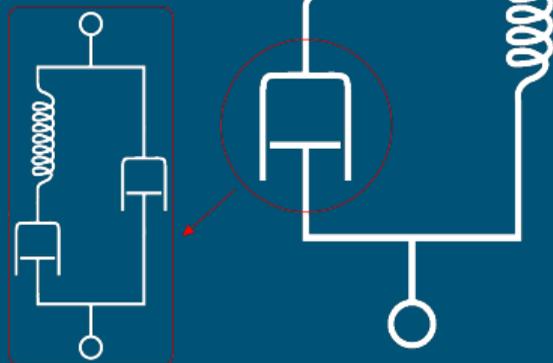
Neo-Hookean [2] hyperelastic model:

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{\mu}{J}\,\mathbf{B}^{*\prime} + \frac{\kappa}{2}\left(J - \frac{1}{J}\right)\mathbf{1}$$

These pieces [3] should be assembled algorithmically.

Silberstein [4] model for Nafion.

Modularity

Additive decomposition:

- Equal deformation gradients.
- Additive Cauchy stresses.

Multiplicative decomposition:

- Multiplicative deformation gradients.
- Also called Kröner-Lee decomposition.
- Certain stress measures are equal, derived
  - variationally for elastic-elastic, and
  - thermodynamically for elastic-plastic.
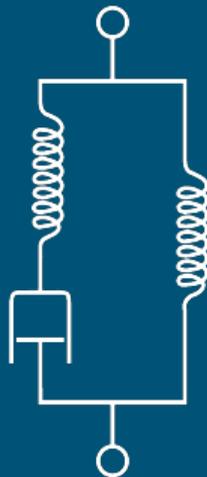
Some apparent challenges:

- Consistent tangents for internal solves.
- Nested sets of internal variables and time-integrated state variables.

Additive

$$\mathbf{F} = \mathbf{F}_1 = \mathbf{F}_2$$
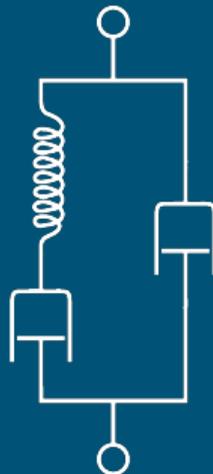$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2$$

Multiplicative

$$\mathbf{F} = \mathbf{F}_1 \cdot \mathbf{F}_2$$
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1$$
$$\boldsymbol{\sigma}_2 = \mathbf{M}_1$$

Simultaneity

Simultaneity

Simultaneous time integration and solving.

- Enables modular constitutive models.
- Model implementation is simpler.
- Extends solver capabilities to models.
- Could be more efficient and robust.

Considerable change to current paradigm.

- Popular iterative approach is a special case sort of like primal-dual solves.
- Existing work assumes time integrator and/or specific constitutive model [5].

Working so far, a few challenges are left.

- Inequality-constraints (plasticity).
- Softening, history, other physics.

Hyperelastic-viscoplastic constitutive model:

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{2\mu}{J}\,\mathbf{h}' + \frac{\kappa}{J}\,\mathrm{tr}(\mathbf{h})\mathbf{1}, \quad \mathbf{h} = \tfrac{1}{2}\ln(\mathbf{B})$$

$$\mathbf{F} = \mathbf{F}_{\mathrm{e}} \cdot \mathbf{F}_{\mathrm{p}}, \quad \dot{\mathbf{F}}_{\mathrm{p}} = \mathbf{D}_{\mathrm{p}} \cdot \mathbf{F}_{\mathrm{p}}, \quad \dot{\varepsilon}_{\mathrm{p}} = |\mathbf{D}_{\mathrm{p}}|$$

$$\Pi(\mathbf{F}, \mathbf{F}_{\mathrm{p}}, \varepsilon_{\mathrm{p}}) = a(\mathbf{F}_{\mathrm{e}}) - \boldsymbol{\lambda} : (\mathbf{F} - \mathbf{F}_0) - \mathbf{P}_0 : \mathbf{F}$$

Differential-algebraic equations:

$$x = \mathbf{F}, \quad y = \{\mathbf{F}_{\mathrm{p}}, \ \varepsilon_{\mathrm{p}}\}$$

$$\dot{y} = f(x, y, t), \quad g(t, x, y) = 0$$

Finite elements (and more) are the same:

$$\mathbf{x}^a \text{ for } a \in [1, N], \quad y = \{\mathbf{F}_{\mathrm{p}}^g, \ \varepsilon_{\mathrm{p}}^g\} \text{ for } g \in [1, M]$$

Algebraic equations only:

$$g(t, x, z) = 0$$

$$h(t, x, z) = 0$$

- Elasticity with internal variables.

Standard semi-explicit DAEs:

$$\dot{y} = f(t, x, y, z)$$

$$g(t, x, y, z) = 0$$

$$h(t, x, y, z) = 0$$

- Elasticity with state variables.
- Elasto-plasticity with state variables.

Fully-implicit DAEs:

$$g(t, x, \dot{x}, z) = 0$$

$$h(t, x, \dot{x}, z) = 0$$

- Viscoelasticity with internal variables.

Non-standard semi-explicit DAEs:

$$\dot{y} = f(t, x, \dot{x}, y, z)$$

$$g(t, x, \dot{x}, y, z) = 0$$

$$h(t, x, \dot{x}, y, z) = 0$$

- Viscoelasticity with state variables.

Simultaneity

Time integration (velocities, state variables).

- Explicit methods:
    - Euler, `ode45`, Runge-Kutta, etc.
    - Sometimes called half-explicit.
- Implicit methods:
    - Backward Euler, Runge-Kutta, etc.
    - Coupled with equation solving.

Equation solving (coordinates, internal variables).

- Optimization or root-finding methods:
    - Gradient descent, Newton-Raphson, etc.
    - Many tangents, no consistent tangents.
    - Implicit time integration is root-finding.
- Typically, one solve for each slope evaluation.

Additive
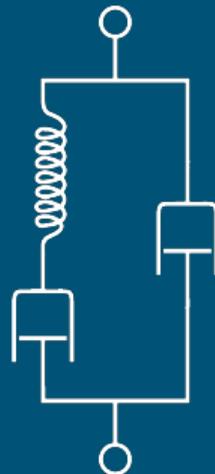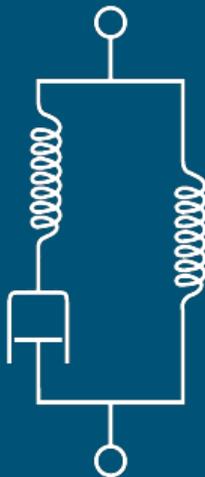$$\mathbf{F} = \mathbf{F}_1 = \mathbf{F}_2$$
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2$$

Multiplicative
$$\mathbf{F} = \mathbf{F}_1 \cdot \mathbf{F}_2$$
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Demonstration

Demonstration

Hencky hyperelastic models:

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{2\mu}{J}\,\mathbf{h}' + \frac{\kappa}{J}\,\mathrm{tr}(\mathbf{h})\mathbf{1}, \quad \mathbf{h} = \tfrac{1}{2}\ln(\mathbf{B})$$
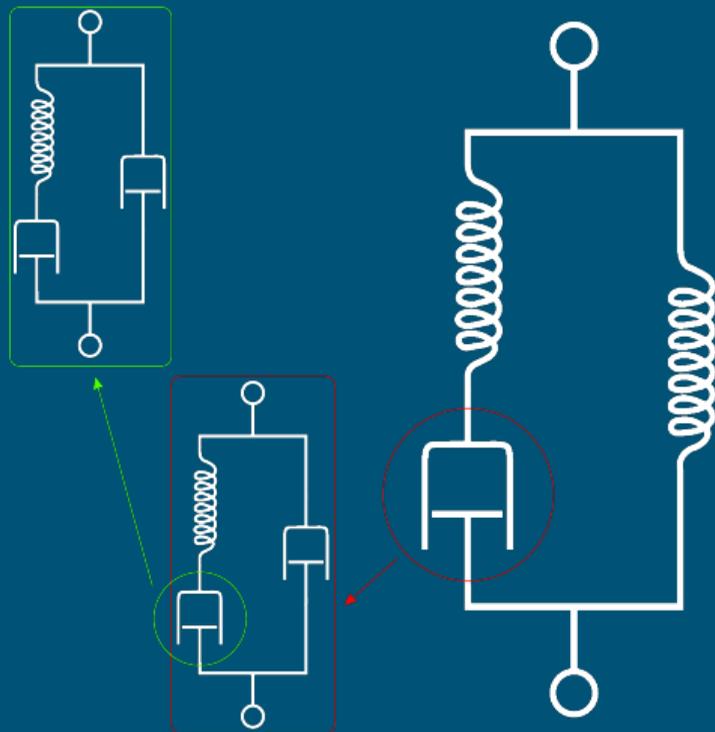
Viscoplastic flow [6] models:

$$\dot{\mathbf{F}}_{\mathrm{p}} = \mathbf{D}_{\mathrm{p}} \cdot \mathbf{F}_{\mathrm{p}}, \quad \mathbf{D}_{\mathrm{p}} = d_0 \left(\frac{|\mathbf{M}'_{\mathrm{e}}|}{Y(S)}\right)^{\frac{1}{m}} \frac{\mathbf{M}'_{\mathrm{e}}}{|\mathbf{M}'_{\mathrm{e}}|}$$

$$\dot{\varepsilon}_{\mathrm{p}} = |\mathbf{D}_{\mathrm{p}}|, \quad Y = Y_0 + H\varepsilon_{\mathrm{p}}, \quad \mathbf{M}_e = J\mathbf{F}_e^T \cdot \boldsymbol{\sigma} \cdot \mathbf{F}_e^{-T}$$

Arruda-Boyce [7] hyperelastic model:

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{\mu\gamma_0\eta}{J\gamma\eta_0}\,\mathbf{B}^{*\prime} + \frac{\kappa}{2}\left(J - \frac{1}{J}\right)\mathbf{1}$$

$$\eta = \mathcal{L}^{-1}(\gamma), \quad \gamma = \sqrt{\mathrm{tr}(\mathbf{B}^*)/3N_b}$$

Demonstration

```rust
let model = ElasticViscoplasticAdditiveElastic::from((
    ElasticMultiplicativeViscoplastic::from((
        Hencky { bulk_modulus: 300.0, shear_modulus: 100.0 },
        ElasticViscoplasticAdditiveViscoplastic::from((
            ElasticMultiplicativeViscoplastic::from((
                Hencky { bulk_modulus: 0.0, shear_modulus: 25.0 },
                ElasticViscoplasticAdditiveViscoplastic::from((
                    ElasticMultiplicativeViscoplastic::from((
                        Hencky { bulk_modulus: 0.0, shear_modulus: 10.0 },
                        ViscoplasticFlow { yield_stress: 3.0, hardening_slope: 0.0, rate_sensitivity: 0.25, reference_flow_rate: 0.04 },
                    )),
                    ViscoplasticFlow { yield_stress: 2.0, hardening_slope: 0.0, rate_sensitivity: 0.25, reference_flow_rate: 0.02 },
                )),
            )),
            ViscoplasticFlow { yield_stress: 1.0, hardening_slope: 1.0, rate_sensitivity: 0.25, reference_flow_rate: 0.01 },
        )),
    )),
    ArrudaBoyce { bulk_modulus: 0.0, shear_modulus: 3.0, number_of_links: 4.0 },
));
let (t, f, s) = model.minimize(
    AppliedLoad::UniaxialStress(|t| 1.0 * t, &[0.0, 1.0]),
    DormandPrince::default(),
    NewtonRaphson::default(),
)?;
```

Demonstration

Conclusion
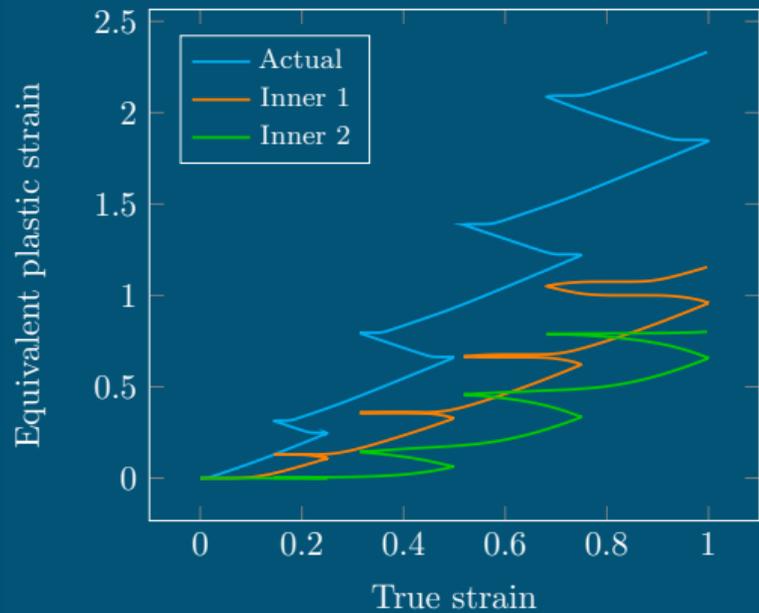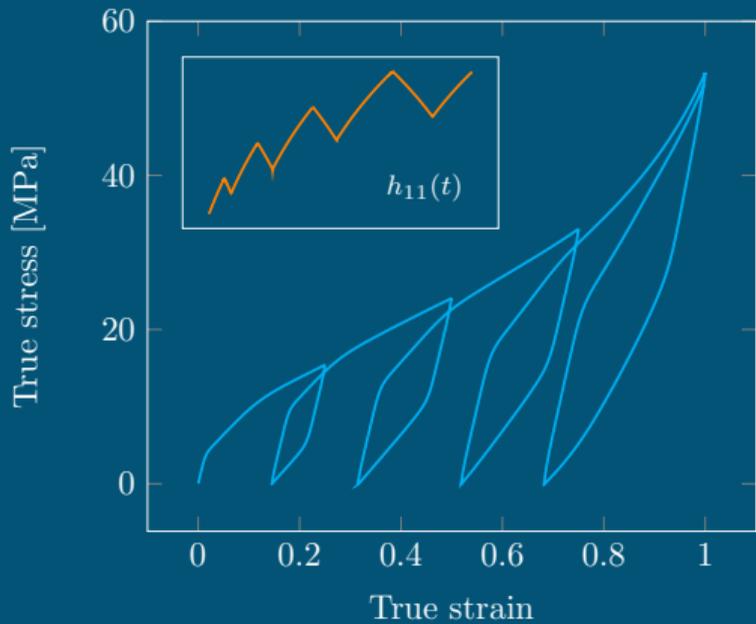
Modularity

- Flexible and practical implementations.
- Support more models but develop less.
- Genetic algorithms or AI/ML assistance.

Simultaneity

- Enables modularity in constitutive models.
- More efficient and robust implementation.
- Same theme as constraints, multi-physics.
- Could this increase parallel performance?

Considerations

- Constitutive models integral type [8–10].
- Cohesive zone, damage, other models.
- Complexity for modern [11] or older tools.

$$\mathbf{F} = \mathbf{F}_1 \cdot \mathbf{F}_2$$
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1$$
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References
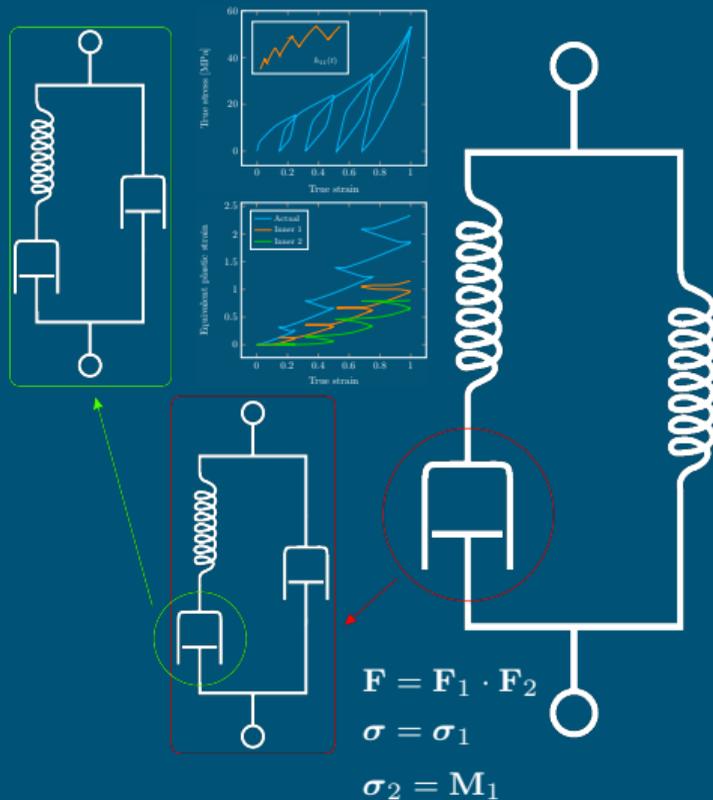
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