Momentum conserving dynamic variational approach for the modeling of fiber-bending stiffness in fiber-reinforced composites

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Motivation
Improving the **numerical modeling** of Fiber-reinforced composites

- **Mesoscopic** *Madeo et al. [2015]*
  - fiber deformations
- **Macroscopic**
  - bending stiffness
- **Constitutive equation**
  - to capture fiber curvature
- **Goals**
  - Stability and accuracy
  - Fiber curvature effect
  - Locking free FE
- **Mixed variational approach**
- **Principle of virtual power**
- **Energy-Momentum scheme** *Gross et al. [2018]*
- **Energy-Momentum consistent time integrator**
- **Higher-order gradient**
- **Mixed-Finite Elements**
New extended Cauchy-Boltzmann continuum model

\[ \varphi_t \]

\[ \tilde{F}_t \neq F_t = \nabla[\varphi_t] \]

\[ \tilde{C} \neq C = \tilde{F}_t \cdot \tilde{F} \]

\[ \Lambda \neq \Lambda \]

\[ \bar{a}_0 \]

\[ \partial B_0 \]

\[ \tilde{F} \]

\[ \nabla \tilde{F} \]

\[ G = \nabla_X[a_t] \]

\[ \Lambda = \tilde{F}^t \cdot G \]

\[ ||a_0|| = 1 \]

\[ a_t = \tilde{\lambda}_{F} \bar{a}_t = \tilde{F} \cdot a_0 \]

\[ ||\bar{a}_t|| = 1 \]

| Variable       | Asmanoglo et al. [2017] | This talk         |
|----------------|--------------------------|-------------------|
| System         | Static                   | Dynamic           |
| $\tilde{F}$    | global                   | element-wise      |
| $\nabla \tilde{F}$ | dependent                | element-wise      |
| $G = \nabla_X[a_t]$ | dependent                | dependent         |
| $\Lambda = \tilde{F}^t \cdot G$ | dependent                | element-wise      |
Constitutive Model

- **General Strain energy function**

\[
\Psi_{total}(I_i(\tilde{C}, \tilde{\Lambda})) = \Psi_{iso}(I_1, I_2, I_3) + \Psi_{aniso}(I_4, I_5) + \Psi_{hg}(I_6(\tilde{\Lambda}))
\]

\[
I_1 = \tilde{C} : I \\
I_2 = \text{cof}(\tilde{C}) : I \\
I_3 = \text{det}(\tilde{C}) \\
I_4 = a_0 \cdot \tilde{C} \cdot a_0 \\
I_5 = a_0 \cdot \tilde{C}^2 \cdot a_0 \\
I_6 = (\tilde{\Lambda} \cdot a_0) \cdot (\tilde{\Lambda} \cdot a_0)
\]

with \( \tilde{C} \neq C = \tilde{F}^t \cdot F \)

- **Example: Polyconvex material formulation for the hyperelastic parts**

\[
\Psi_{total}(I_1, I_3, I_6; \lambda, \mu, c) = \lambda \frac{I_3 - 1}{4} - \left[ \frac{\lambda}{2} + \mu \right] \ln \left( \sqrt{I_3} \right) + \frac{\mu}{2} [I_1 - 3] + c I_6
\]

- **Simple Neo-Hookean isotropic part**

- **c** - Fiber stiffness parameter
Hu-Washizu based power functionals

Kinetic power

\[ \dot{\mathcal{T}}_{\text{kin}} := \int_{\mathcal{B}_0} \rho_0 \mathbf{v} \cdot \dot{\mathbf{v}} \, dV - \int_{\mathcal{B}_0} \mathbf{p} \cdot (\dot{\mathbf{v}} - \dot{\mathbf{\phi}}) \, dV - \int_{\mathcal{B}_0} \dot{\mathbf{p}} \cdot (\mathbf{v} - \dot{\mathbf{\phi}}) \, dV \]

Internal power

\[ \dot{\Pi}_{\text{int}} := \int_{\mathcal{B}_0} \left[ \frac{\partial \Psi_{\text{ela}}}{\partial \tilde{C}} : \dot{\tilde{C}} \right] dV - \int_{\mathcal{B}_0} \frac{1}{2} \left[ \tilde{S} : \left[ \dot{\tilde{C}} - \tilde{F}^t \tilde{F} \right] \right] dV + \int_{\mathcal{B}_0} \left[ \frac{\partial \Psi_{\text{hg}}}{\partial \tilde{\Lambda}} : \dot{\tilde{\Lambda}} \right] dV - \int_{\mathcal{B}_0} \tilde{P} : [\dot{\tilde{F}} - \nabla \dot{\mathbf{\phi}}] \, dV \]

\[ - \int_{\mathcal{B}_0} \tilde{\mathbf{B}} \odot_3 [\dot{\tilde{\Gamma}} - \nabla \dot{\tilde{F}}] \, dV \quad - \int_{\mathcal{B}_0} \tilde{\mathbf{A}} : \left[ \dot{\tilde{\Lambda}} - \frac{\partial \tilde{\Lambda}}{\partial \tilde{F}} : \dot{\tilde{F}} - \frac{\partial \tilde{\Lambda}}{\partial \tilde{\Gamma}} \odot_3 \dot{\tilde{\Gamma}} \right] \, dV \]

External Power

\[ \dot{\Pi}_{\text{ext}} := - \int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \dot{\mathbf{\phi}} \, dV - \int_{\partial T \mathcal{B}_0} \tilde{T} \cdot \dot{\mathbf{\phi}} \, dA - \int_{\partial \mathbf{\phi} \mathcal{B}_0} \mathbf{R} \cdot (\dot{\mathbf{\phi}} - \dot{\hat{\mathbf{\phi}}}) \, dA \]

\[ + \int_{\mathcal{B}_0} \tilde{\mathbf{A}} : \dot{\tilde{\Lambda}} \, dV + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S} : \dot{\tilde{C}} \, dV \]

Principle of Virtual power \((\dot{\mathcal{H}} \equiv \dot{\mathcal{T}}_{\text{kin}} + \dot{\Pi}_{\text{ext}} + \dot{\Pi}_{\text{int}} = 0)\)

\[ \int_{t_n}^{t_{n+1}} \delta \ast \dot{\mathcal{H}} \, dt \equiv \int_{t_n}^{t_{n+1}} \left[ \delta \ast \dot{\mathcal{T}}_{\text{kin}} (\mathbf{\phi}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) + \delta \ast \dot{\Pi}_{\text{ext}} (\mathbf{\phi}, \mathbf{R}) + \delta \ast \dot{\Pi}_{\text{int}} (\mathbf{\phi}, \dot{\tilde{F}}, \tilde{P}, \dot{\tilde{C}}, \tilde{S}, \dot{\tilde{\Gamma}}, \tilde{\mathbf{B}}, \dot{\tilde{\Lambda}}, \tilde{\mathbf{A}}) \right] \, dt \]
Algorithmic stress tensors fulfills the total energy consistence

Gradient theorem with respect to bending curvature deformations

$$G_\bar{\Lambda}(\bar{A}) := \Psi(\bar{\Lambda}_{n+1}) - \Psi(\bar{\Lambda}_n) - \int_{t_n}^{t_{n+1}} \left[ \frac{\partial \Psi(\bar{\Lambda})}{\partial \bar{\Lambda}} + \bar{A} \right] : \dot{\bar{\Lambda}} \, dt = 0$$

Isoperimetric variational problem

$$\mathcal{L} \left( \bar{A}, \lambda_\bar{\Lambda} \right) := \mathcal{F}_\bar{\Lambda} \left( \bar{A} \right) + \lambda_\bar{\Lambda} G_\bar{\Lambda} \left( \bar{A} \right)$$

Minimization function

$$\mathcal{F}_\bar{\Lambda} \left( \bar{A} \right) := \frac{1}{2} \int_0^1 \bar{A} : \ddot{\bar{A}} \, d\alpha$$

Algorithmic stress tensors

$$\bar{A} := \frac{\Psi(\bar{\Lambda}_{n+1}) - \Psi(\bar{\Lambda}_n) - \int_0^1 \frac{\partial \Psi(\bar{\Lambda})}{\partial \bar{\Lambda}} : \dot{\bar{\Lambda}} \, d\alpha}{\int_0^1 \dot{\bar{\Lambda}} : \dot{\bar{\Lambda}} \, d\alpha}$$
Variation of power functionals with respect to their dependencies

Virtual internal power

\[
\delta_\ast \Pi_{\text{int}} := \int_{\mathcal{B}_0} \left[ \frac{\partial \Psi^{\text{ela}}(\tilde{C})}{\partial \tilde{C}} - \tilde{S} \right] : \delta_\ast \tilde{C} \, dV - \int_{\mathcal{B}_0} \left[ \tilde{C} - \tilde{F}^t \tilde{F} \right] : \delta_\ast \tilde{S} \, dV - \int_{\mathcal{B}_0} \left[ \tilde{F} - \nabla \dot{\varphi} \right] : \delta_\ast \tilde{P} \, dV
\]

Virtual external power

\[
\delta_\ast \Pi_{\text{ext}} := -\int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \delta_\ast \dot{\varphi} \, dV - \int_{\partial T_{\mathcal{B}_0}} \mathbf{T} \cdot \delta_\ast \dot{\varphi} \, dA - \int_{\partial \varphi_{\mathcal{B}_0}} \mathbf{R} \cdot \delta_\ast \dot{\varphi} \, dA
\]

Virtual kinetic power

\[
\delta_\ast \dot{T} := \int_{\mathcal{B}_0} \left[ \rho_0 \mathbf{v} - \mathbf{p} \right] \cdot \delta_\ast \dot{\mathbf{v}} \, dV - \int_{\mathcal{B}_0} \left[ \mathbf{v} - \dot{\varphi} \right] \cdot \delta_\ast \dot{\mathbf{p}} \, dV + \int_{\mathcal{B}_0} \dot{\mathbf{p}} \cdot \delta_\ast \dot{\varphi} \, dV
\]
Weak momentum balance equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \dot{p} - \rho_0 B \right] \cdot \delta_\dot{\varphi} \, dV \, dt - \int_{t_n}^{t_{n+1}} \int_{\partial B_0} \left[ \tilde{T} + R \right] \cdot \delta_\dot{\varphi} \, dA \, dt + \int_{t_n}^{t_{n+1}} \int_{B_0} \tilde{P} : \nabla [\delta_\dot{\varphi}] \, dV \, dt = 0 \]

Weak first Piola-Kirchoff stress equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \left( \tilde{B} \odot_3 \frac{\partial (\nabla \tilde{F})}{\partial \tilde{F}} \right) + \left( \tilde{A} : \frac{\partial \Lambda}{\partial \tilde{F}} \right) + \left( \tilde{F} \tilde{S} \right) - \tilde{P} \right] : \delta_\dot{\tilde{F}} \, dV \, dt = 0 \]

Weak deformation gradient equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \hat{F} - \nabla \varphi \right] : \delta_\dot{\varphi} \, dV \, dt = 0 \]

Weak curvature equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \hat{\Gamma} - \nabla \hat{\dot{F}} \right] \odot_3 \delta_\dot{\tilde{B}} \, dV \, dt = 0 \]

Weak curvature stress equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \left( \tilde{A} : \frac{\partial \Lambda}{\partial \hat{\Gamma}} \right) - \tilde{B} \right] \odot_3 \delta_\dot{\hat{\Gamma}} \, dV \, dt = 0 \]

Weak curvature stress equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ 2 \frac{\partial \Psi_{ela} (\tilde{C})}{\partial \tilde{C}} + \tilde{S} - \tilde{S} \right] : \delta_\dot{\tilde{C}} \, dV \, dt = 0 \]

Weak fiber curvature stress equation
\[ \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \frac{\partial \Psi_{hg}(\Lambda)}{\partial \Lambda} + \tilde{A} - \tilde{A} \right] : \delta_\dot{\Lambda} \, dV \, dt = 0 = \int_{t_n}^{t_{n+1}} \int_{B_0} \left[ \hat{\Lambda} - \frac{\partial \Lambda}{\partial \hat{F}} : \hat{F} - \frac{\partial \Lambda}{\partial \hat{\Gamma}} \odot_3 \hat{\Gamma} \right] : \delta_\dot{\hat{A}} \, dV \, dt \]
Theory

Conserving total angular momentum with an additive term of higher order gradient

Angular momentum balance law

\[ \mathcal{J} := \int_{\mathcal{B}_0} \varphi \times p \, dV \]

\[
\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \mathcal{J} \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \varphi \times \dot{p} \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \mathcal{J} \, dV \, dt = 0
\]

Employing the test function \( \delta_\ast \dot{\varphi} = c \times \varphi \) in weak momentum balance equation

Axial vector \( c = \text{const.} \)

\[
\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} c \cdot [\varphi \times \dot{p}] \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} c \cdot [\varphi \times \rho_0 B] \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} c \cdot [\mathcal{P} \times \mathcal{F}] \, dV \, dt
\]

\[+ \int_{t_n}^{t_{n+1}} \int_{\partial \mathcal{B}_0} c \cdot [\varphi \times (\mathcal{T} + \mathcal{R})] \, dA \, dt \]

\[
\mathcal{J}_{n+1} - \mathcal{J}_n = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} [\varphi \times \rho_0 B] \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\partial \mathcal{B}_0} [\varphi \times (\mathcal{T} + \mathcal{R})] \, dA \, dt
\]

\[+ \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \epsilon \cdot \left[ \left( \nabla \mathcal{B} \otimes_3 \frac{\partial(\mathcal{F} \mathcal{F}^t)}{\partial \mathcal{F}} \right) + \left( \mathcal{A} : \frac{\partial \mathcal{A}}{\partial \mathcal{F}} \right) + \left( \mathcal{F} \mathcal{S} \right) \right] \mathcal{F}^t \, dV \, dt \]
Conserving total energy with an additive term of higher order gradient

**Kinetic energy balance**

\[ \mathcal{K} := \frac{1}{2} \rho_0 \mathbf{v} \cdot \mathbf{v} \]

\[
\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \mathcal{K} \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \mathbf{v} \cdot \rho_0 \dot{\mathbf{v}} \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \dot{\mathbf{\varphi}} \cdot \dot{\mathbf{p}} \, dV \, dt
\]

**Employing the test function** \( \delta_\ast \dot{\varphi} = \dot{\varphi} \) **in weak momentum balance equation**

\[
\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \dot{\varphi} \cdot \dot{\mathbf{p}} \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \dot{\varphi} \cdot \rho_0 \mathbf{B} \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\partial \mathcal{B}_0} \varphi \cdot (\overline{\mathbf{T}} + \mathbf{R}) \, dA \, dt
\]

\[ - \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \overline{\mathbf{P}} : \nabla \varphi \, dV \, dt \]

\[
\mathcal{K}_{n+1} - \mathcal{K}_n = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \dot{\varphi} \cdot \rho_0 \mathbf{B} \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\partial \mathcal{B}_0} \varphi \cdot (\overline{\mathbf{T}} + \mathbf{R}) \, dA \, dt
\]

\[ - \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \left[ \left( \mathcal{B}_3 \cdot \frac{\partial (\nabla \mathbf{F})}{\partial \mathbf{F}} \right) + (\mathbf{A} : \frac{\partial \mathbf{\Lambda}}{\partial \mathbf{F}}) + (\mathbf{F} \mathbf{S}) \right] : \dot{\mathbf{F}} \, dV \, dt \]
Lagrangian ansatz functions in space ($N$) and time ($M, M', \tilde{M}$)  
Gross et al. [2018]

Polynomial degree in time($k$)

- Time rate variables and mixed fields ($\varphi, v, p, \tilde{F}, \tilde{\Gamma}$)

\[
\begin{align*}
\dot{(\bullet)}^{e,h} &= \sum_{I=1}^{k+1} \sum_{A=1}^{n_{n.o}} M_I(\alpha) N^A(\xi)(\bullet)_I^{eA} \\
\dot{(\bullet)}^{e,h} &= \frac{1}{h_n} \sum_{I=1}^{k+1} \sum_{A=1}^{n_{n.o}} M'_I(\alpha) N^A(\xi)(\bullet)_I^{eA}
\end{align*}
\]

- Lagrange multiplier and variation fields ($\tilde{P}, \tilde{B}, \delta_* \bullet$)

\[
\begin{align*}
\dot{(\bullet)}^{e,h} &= \sum_{I=1}^{k} \sum_{A=1}^{n_{n.o}} \tilde{M}_I(\alpha) N^A(\xi)(\bullet)_I^{eA} \\
\tilde{M}_i(\alpha) &= \prod_{j=1 \atop j \neq i}^{k} \frac{\alpha - \alpha_j}{\alpha_i - \alpha_j}, \quad 1 \leq i \leq k
\end{align*}
\]

- Lagrange multipliers are approximated with the same shape functions as their corresponding mixed fields e.g. ($\tilde{F} & \tilde{P}$), ($\tilde{\Gamma} & \tilde{B}$)
Numerical studies
Model setup - Simple beam

Initial conditions

\[ \rho_0 = 1000 \]
\[ \varphi_0 = X \]
\[ \mathbf{v}_0 = \mathbf{0} \]
\[ \mathbf{a}_0^T = [1 \; 0 \; 0]^T \]
\[ \hat{p} = 200 \hat{f} \]

Material parameters

\[ \mu = 0.1 \cdot 10^6 \]
\[ K = 100 \cdot 10^6 \]
\[ c = [0, 12 \cdot 10^6] \]

Temporal parameters

\[ h_n = 0.002 \]
\[ T = 1 \]
\[ \text{Tol} = 1e^{-4} \]

Dirichlet: Fixed support  Neumann: In-plane load

Fiber orientation along X-axis
Numerical studies
Maximum deflection vs. $c$ and $\alpha$

Varying fiber stiffness $c$, with $\alpha_0 = e_1$

Varying fiber orientation $\alpha$, with $c = 1 \cdot 10^6$

Displacement of a point $P$ at the free end of the beam
Numerical studies
Total momenta and energy consistence

Angular momentum error plot

Energy error plot

For $c = 1 \cdot 10^6$, $a_0 = e_1$ and a Newton-Raphson tolerance TOL
1. Motivation
   ▶ Capture fiber bending stiffness in fiber-reinforced composites
   ▶ Stable and accurate dynamical FE simulations

2. Approach
   ▶ Higher-order gradient based independent field for the fiber curvature
   ▶ Variational-based mixed finite element formulation
   ▶ Energy-Momentum scheme (enhanced Galerkin method - eG)

3. Important results
   ▶ Fiber curvature effect captured by the element-wise fields $\tilde{F}$, $\tilde{\Gamma}$, $\tilde{\Lambda}$
   ▶ Time integrator conserves total momenta and energy consistently
   ▶ Gradient shape functions can be approximated with different polynomials

4. Further steps
   ▶ Use different polynomials for mixed fields to study the locking behaviour
   ▶ Extend the continuum to thermo-mechanical setting