Forward-Mode Enzyme in Developing Constitutive Models with Ratel

Leila Ghaffari, William Moses, Jeremy L Thompson, Karen Stengel, Rezgar Shakeri, and Jed Brown

Department of Computer Science
University of Colorado Boulder

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Differentiation in Solid Mechanics

Free energy functional and PDE solvers

$$\psi\left(\boldsymbol{E}\right) = \frac{\lambda}{4}\left(J^2 - 1 - 2\log J\right) - \mu\left(\log J + \operatorname{trace}\boldsymbol{E}\right), \quad J = \sqrt{\left|\boldsymbol{I} + 2\boldsymbol{E}\right|}$$

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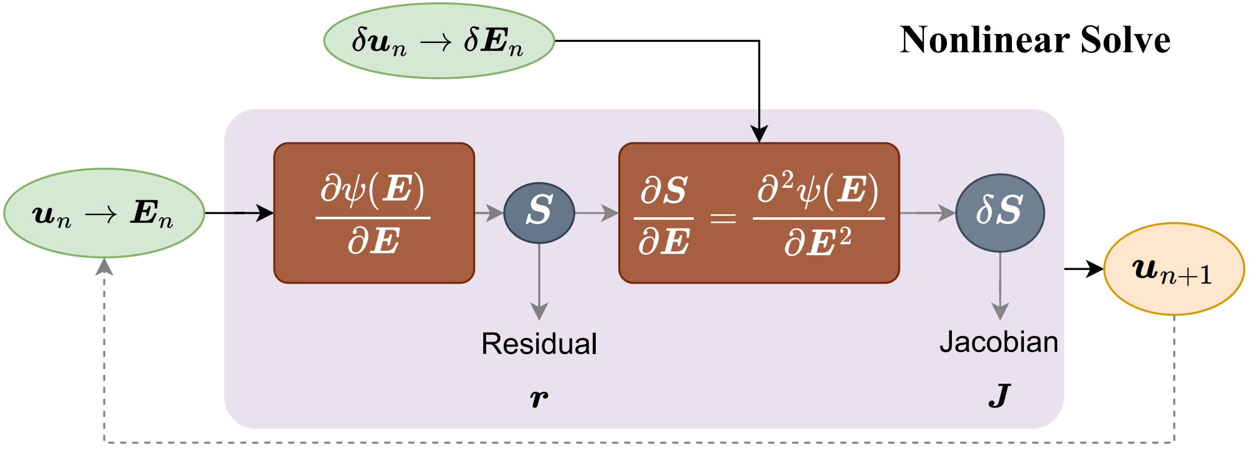

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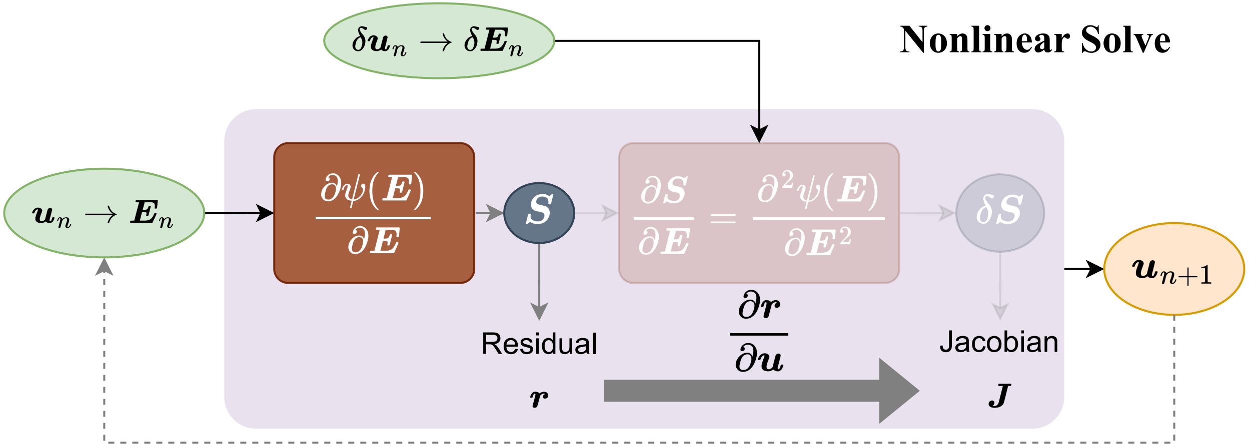

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Differentiation in Solid Mechanics

Free energy functional and Inverse problems

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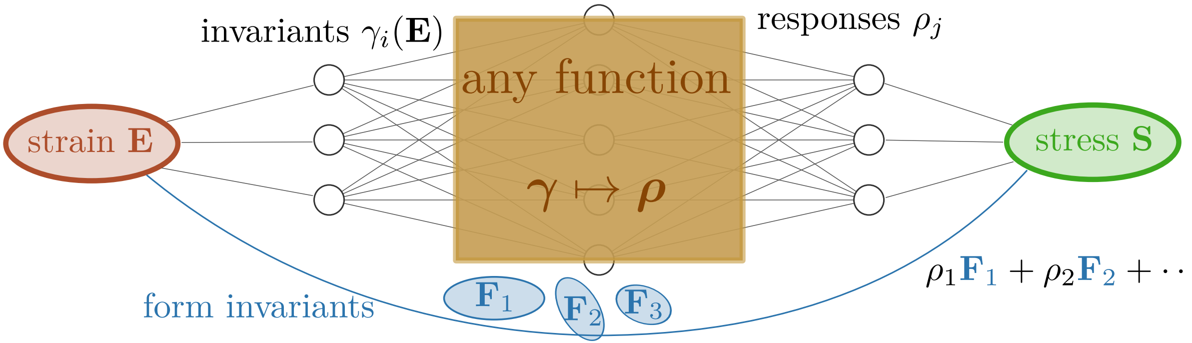

ABAQUS

UHYPER: USER SUBROUTINE

Variables to be defined

`U(1)`

U, strain energy density function. For a compressible material, at least one derivative involving J should be nonzero. For an incompressible material, all derivatives involving J will be ignored. The strain invariants—$\bar{I}_1$, $\bar{I}_2$, and J—are defined in Hyperelastic behavior of rubberlike materials.

`U(2)`

$\tilde{U}_{dev}$, the deviatoric part of the strain energy density of the primary material response. This quantity is needed only if the current material definition also includes Mullins effect (see Mullins effect).

`UI1(1)`

$\partial U / \partial \bar{I}_1$.

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- Complex interface (too many inputs)
- Unstable for small deformation due to the choice of interface design

$$\boldsymbol{F} = \boldsymbol{I} + \nabla_X \boldsymbol{u}$$

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$$\boldsymbol{F} = \boldsymbol{I} + \nabla_X \boldsymbol{u}$$

- Not easy to change the interface

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AD helps us to create a more generic interface (one input function, $\psi(\mathbf{E})$).

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  e of interface design
  $= \boldsymbol{I} + \nabla_X \boldsymbol{u}$
- Not easy to change the interface

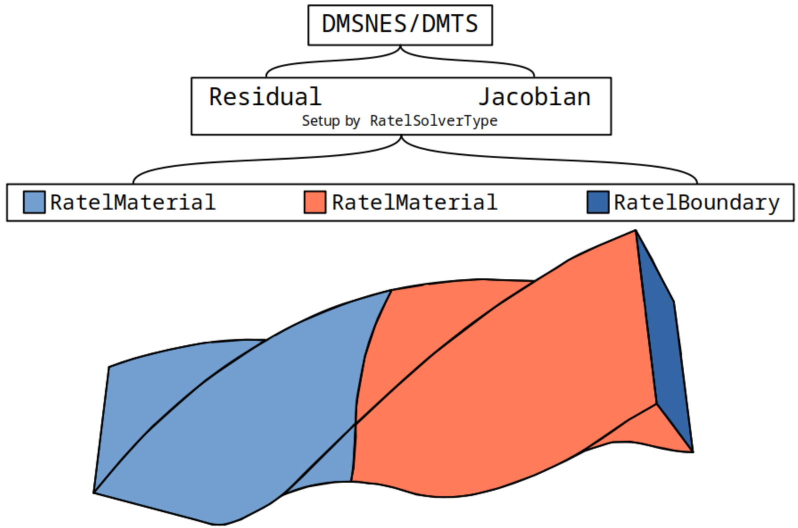
RATEL: EXTENSIBLE, PERFORMANCE-PORTABLE SOLID MECHANICS

HTTPS://GITLAB.COM/MICROMORPH/RATEL

GitLab-CI passed | License BSD 2-Clause | Documentation latest | coverage 96.05%

Features:

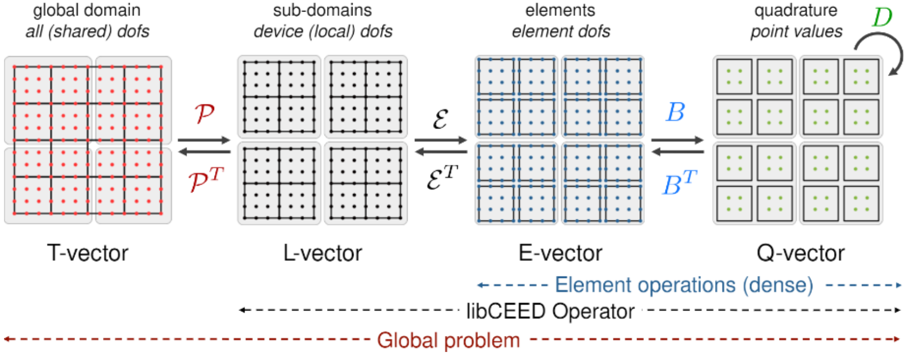
- Linear elasticity
- Neo-Hookean and Mooney-Rivlin Hyperelasticity
- Multi-material
- Static, Quasistatic, Dynamic
- Initial and Current configurations



Ratel: Extensible, performance-portable solid mechanics

Composition and Abstraction - libCEED: https://libceed.org/en/latest/

$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$



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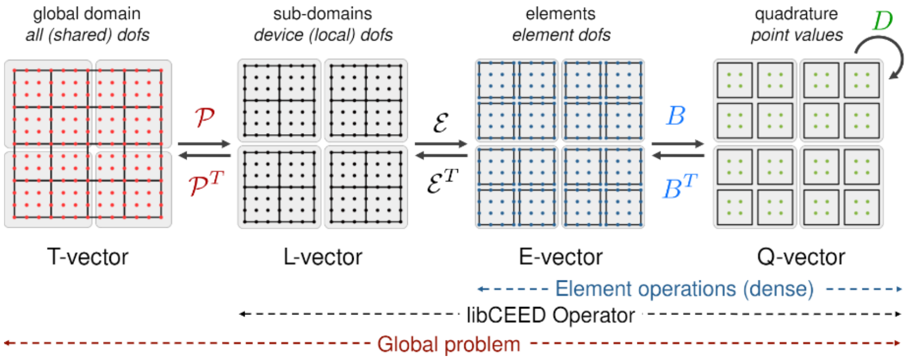

- Purely algebraic high-order FEM

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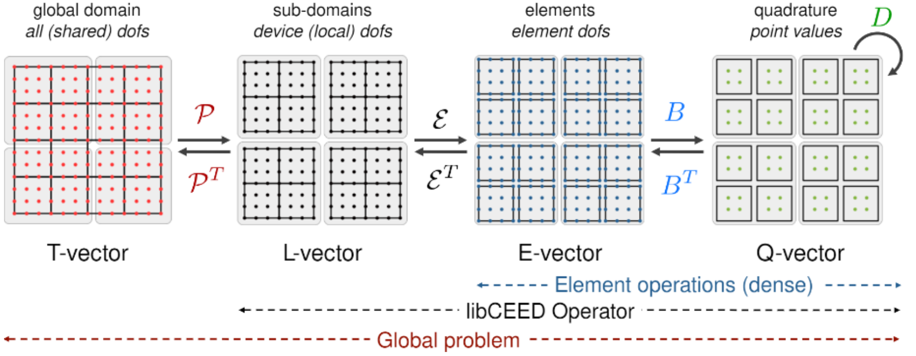

- Purely algebraic high-order FEM
- Single source Vanilla C for physics

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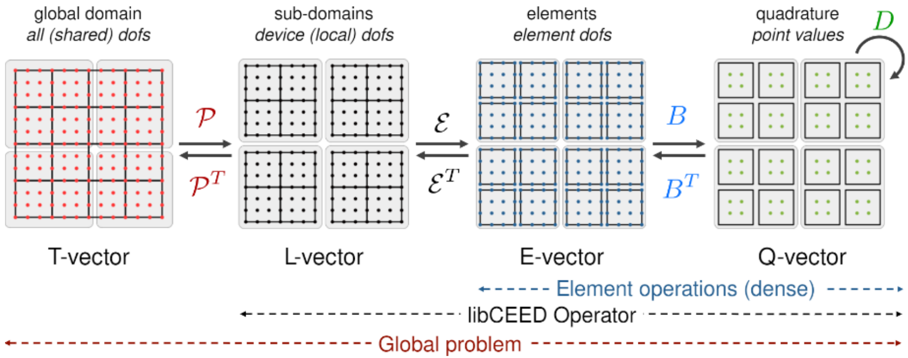

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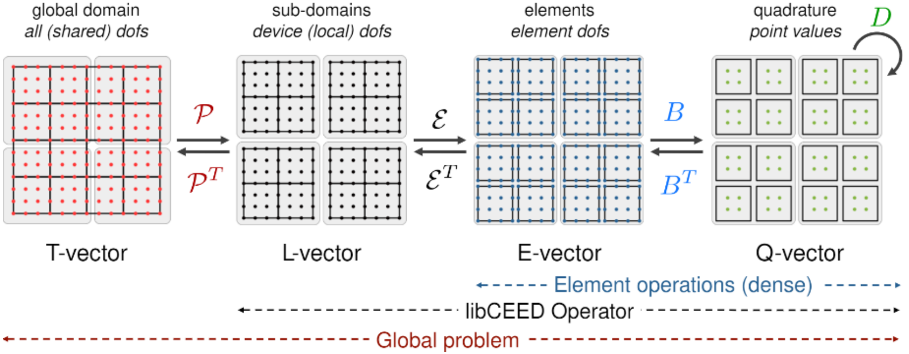

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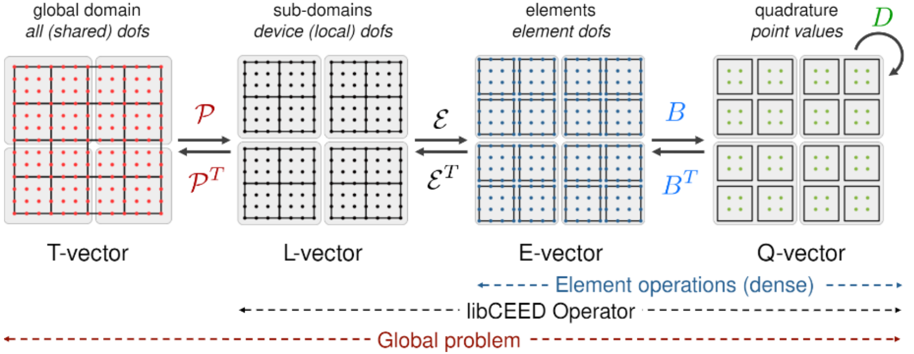

- Purely algebraic high-order FEM
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- Backend plugins with run-time selection `./bps -ceed /gpu/cuda`
- Support for Matrix-assembly and Matrix-free

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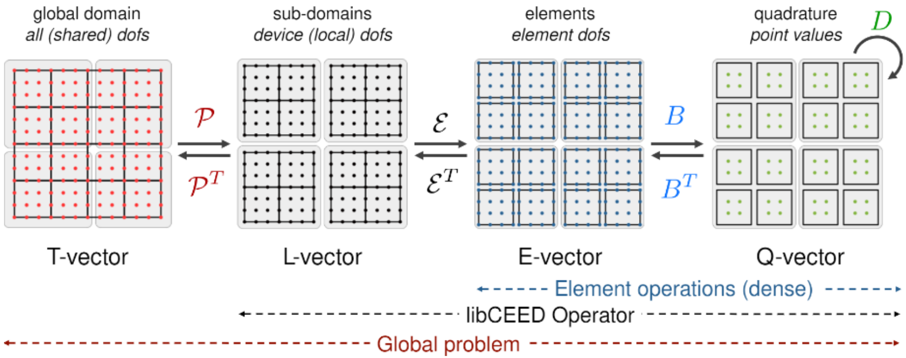

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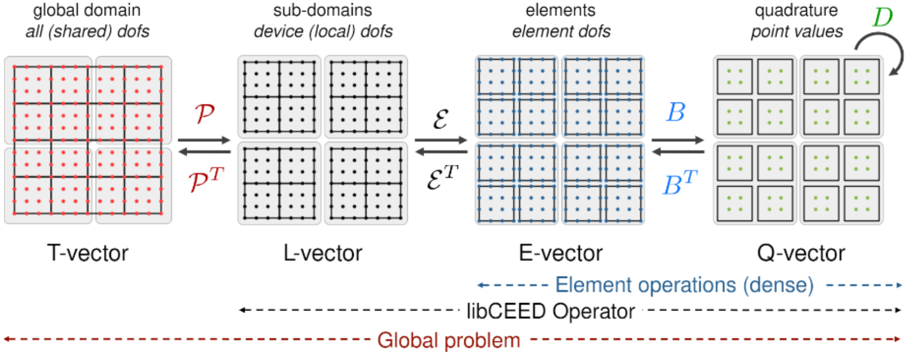

- Purely algebraic high-order FEM
- Single source Vanilla C for physics
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- Support for Matrix-assembly and Matrix-free
- Operator abstraction
- User choice of data storage at quadrature point

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https://petsc.org/release/

- Parallel solution of PDEs

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- Optimization (PETSc/Tao)

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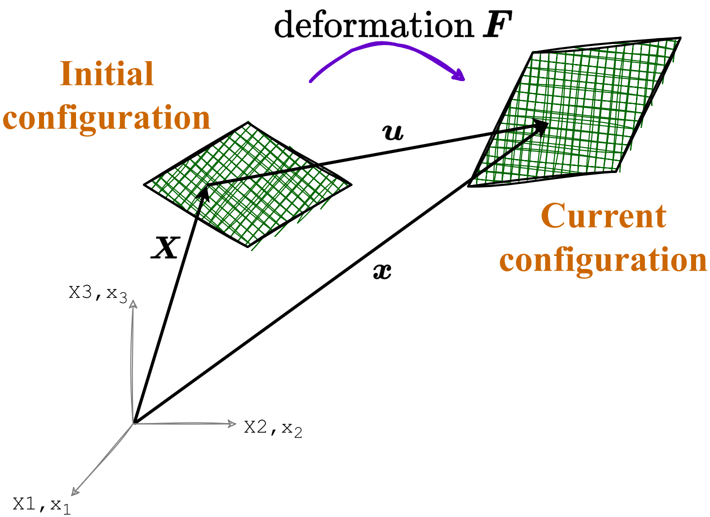
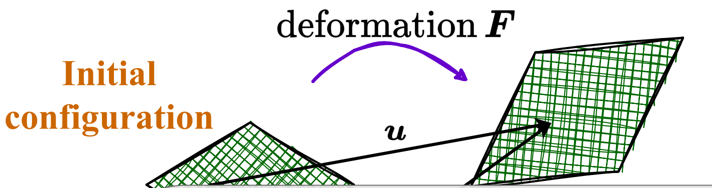
- *reverse* and *forward* mode AD

Initial vs Current configuration





$$\overbrace{\nabla_X \boldsymbol{v} : \boldsymbol{F}\boldsymbol{S}}^{\text{Initial Residual}} \xrightarrow{\text{push forward}} \overbrace{\nabla_x \boldsymbol{v} : \boldsymbol{\tau}}^{\text{Current Residual}}$$

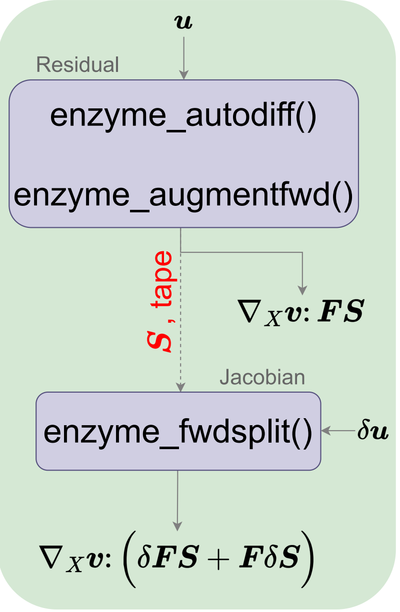
$$\Big\downarrow \text{linearize} \qquad\qquad\qquad\qquad \Big\downarrow \text{linearize}$$

$$\underbrace{\nabla_X \boldsymbol{v} : \left(\delta \boldsymbol{F}\boldsymbol{S} + \boldsymbol{F}\delta\boldsymbol{S}\right)}_{\text{Initial Jacobian}} \xrightarrow{\text{push forward}} \underbrace{\nabla_x \boldsymbol{v} : \left(\delta\boldsymbol{\tau} - \boldsymbol{\tau}(\nabla_x \delta\boldsymbol{u})^T\right)}_{\text{Current Jacobian}}$$

Ratel - Enzyme AD

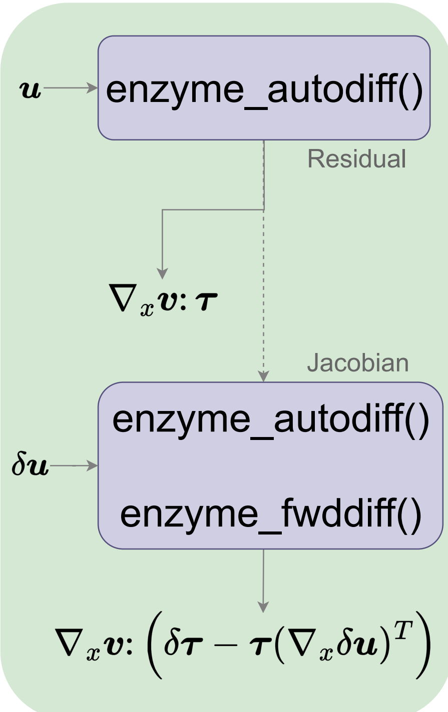
Initial configuration - Reverse and Forward Split

```
// S = d(\psi) / d(E) [Reverse mode]
void SecondPiolaKirchhoffStress_NeoHookean_AD(...) {
  __enzyme_autodiff((void *)StrainEnergy, ...);
}

// Call forward S and return tape
__enzyme_augmentfwd(
(void *)SecondPiolaKirchhoffStress_NeoHookean_AD,
enzyme_allocated, tape_bytes, enzyme_tape, tape,
enzyme_nofree, ...);

// Compute dS using the stored tape [Forward-split]
__enzyme_fwdsplit(
(void *)SecondPiolaKirchhoffStress_NeoHookean_AD,
enzyme_allocated, tape_bytes, enzyme_tape, tape, ...);
```



Ratel - Enzyme AD

Current configuration - Reverse and Forward




```
// Compute tau = (dPsi / de) * (2 e + I) [Reverse]
void Kirchhofftau_Voigt_NeoHookean_AD(...) {
  __enzyme_autodiff((void *)StrainEnergy, ...);
  ...
  for (int j = 0; j < 6; j++)
    b_Voigt[j] = 2 * e_Voigt[j] + (j < 3);
  ...
  RatelMatMatMult(1., dPsi, b, tau);
}

// Compute dtau [Forward]
CEED_QFUNCTION_HELPER void dtau_fwd(...) {
  __enzyme_fwddiff(
  (void *)Kirchhofftau_Voigt_NeoHookean_AD, ...);
}
```

Ratel - Enzyme AD

Performance for different Jacobian representations

Problem	Storage	Scalars	Time (s)
`current`	$W; \nabla_x \boldsymbol{\xi}, \boldsymbol{\tau}, J-1$	17	36.2
`initial`	$W, \nabla_X \boldsymbol{\xi}; \nabla_X \boldsymbol{u}$	19	48.4
`initial-AD`	$W, \nabla_X \boldsymbol{\xi}; \nabla_X \boldsymbol{u}, S,$ `tape`	31	53.9
`current-AD`	$W; \nabla_x \boldsymbol{\xi}, \boldsymbol{e}$	16	55.8

Current-Analytical

$\nabla_X \boldsymbol{u}$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$J = J(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I} + 2\mu e$$

Res

$\boldsymbol{\tau}, \nabla_x X, J - 1$

$\nabla_X \delta \boldsymbol{u}$

$$\delta \boldsymbol{\epsilon} = \delta \boldsymbol{\epsilon}(\nabla_x \delta \boldsymbol{u})$$

$$Jac = Jac(\nabla_x \delta \boldsymbol{u}, J, \boldsymbol{\tau}, \delta \boldsymbol{\epsilon})$$

Jac

Current-AD

$\nabla_X \boldsymbol{u}$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}\,(2\boldsymbol{e} + \boldsymbol{I})$$

Res

$\boldsymbol{e}, \nabla_x X$

$\nabla_X \delta \boldsymbol{u}$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}\,(2\boldsymbol{e} + \boldsymbol{I})$$

$$\delta \boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{e}}$$

Jac

Current-Analytical

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$$J = J(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I} + 2\mu e$$

Res

$\boldsymbol{\tau}, \nabla_x X, J - 1$

$\nabla_X \delta\boldsymbol{u}$

$$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta\boldsymbol{u},$$

No need for $\delta\boldsymbol{\tau}$

$$Jac = Jac(\nabla_x \delta\boldsymbol{u}, J, \boldsymbol{\tau}, \delta\boldsymbol{\epsilon})$$

Jac

Current-AD

$\nabla_X \boldsymbol{u}$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}\left(2\boldsymbol{e} + \boldsymbol{I}\right)$$

Res

$\boldsymbol{e}, \nabla_x X$

$\nabla_X \delta\boldsymbol{u}$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}\left(2\boldsymbol{e} + \boldsymbol{I}\right)$$

$$\delta\boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{e}}$$

Jac

Current-Analytical

$\nabla_X \boldsymbol{u}$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$J = J(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I} + 2\mu e$$

Res

$\boldsymbol{\tau}, \nabla_x X, J-1$

$\nabla_X \delta \boldsymbol{u}$

$$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta \boldsymbol{u},$$

No need for

$\delta\boldsymbol{\tau}$

$$Jac = Jac(\nabla_x \delta \boldsymbol{u}, J, \boldsymbol{\tau}, \delta\boldsymbol{\epsilon})$$

Jac

Current-AD

$\nabla_X \boldsymbol{u}$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}(2\boldsymbol{e} + \boldsymbol{I})$$

Res

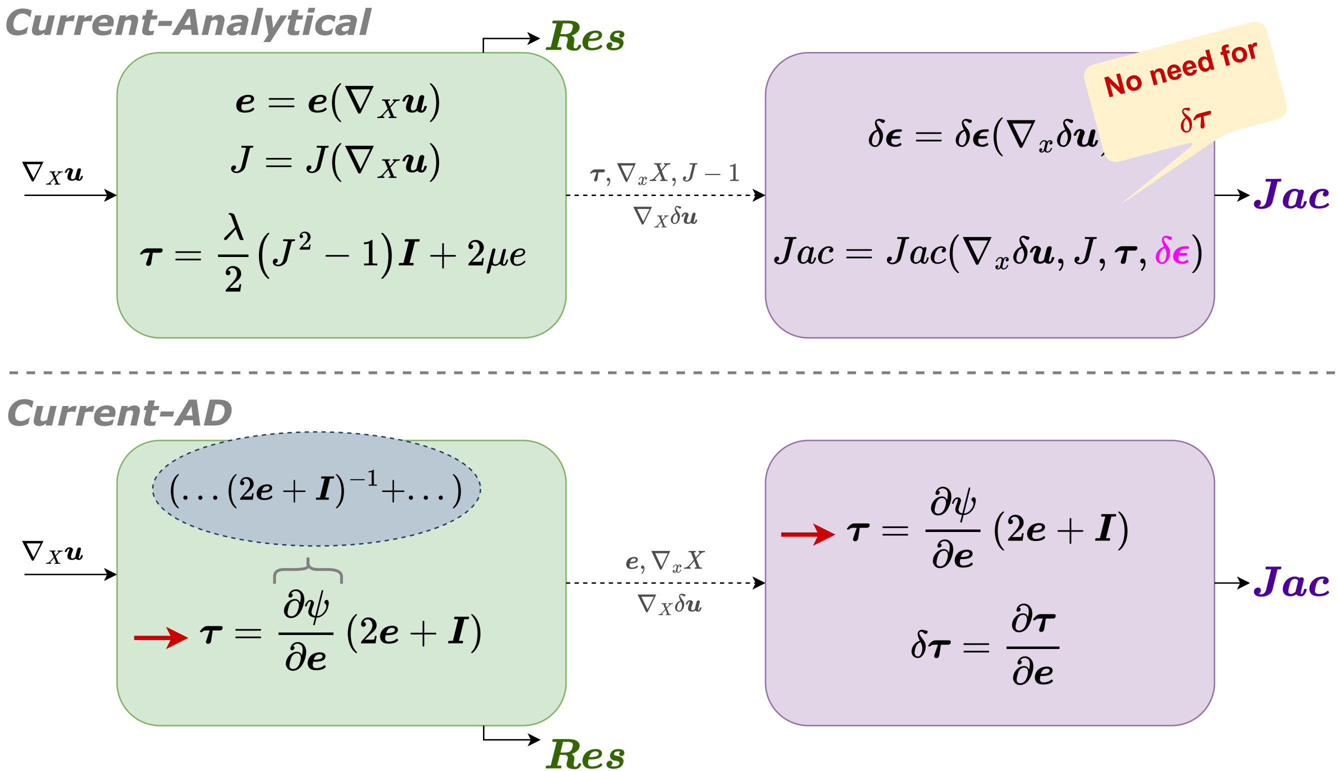
$\boldsymbol{e}, \nabla_x X$

$\nabla_X \delta \boldsymbol{u}$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}(2\boldsymbol{e} + \boldsymbol{I})$$

$$\delta\boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{e}}$$

Jac


Current-Analytical
$\nabla_X \boldsymbol{u}$
$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$
$J = J(\nabla_X \boldsymbol{u})$
$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I} + 2\mu e$
Res
$\boldsymbol{\tau}, \nabla_x X, J-1$
$\nabla_X \delta\boldsymbol{u}$
$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta\boldsymbol{u})$
No need for
$\delta\boldsymbol{\tau}$
$Jac = Jac(\nabla_x \delta\boldsymbol{u}, J, \boldsymbol{\tau}, \delta\boldsymbol{\epsilon})$
Jac
Current-AD
$\nabla_X \boldsymbol{u}$
$(\ldots(2\boldsymbol{e}+\boldsymbol{I})^{-1}+\ldots)$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial\boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
Res
$\boldsymbol{e}, \nabla_x X$
$\nabla_X \delta\boldsymbol{u}$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial\boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
$\delta\boldsymbol{\tau} = \frac{\partial\boldsymbol{\tau}}{\partial\boldsymbol{e}}$
Jac

Current-Analytical

$\nabla_X \boldsymbol{u} \rightarrow$

$$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$$

$$J = J(\nabla_X \boldsymbol{u})$$

$$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I} + 2\mu e$$

$\rightarrow$ ***Res***

$\xrightarrow[\nabla_X \delta\boldsymbol{u}]{\boldsymbol{\tau},\, \nabla_x X,\, J-1}$

$$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta\boldsymbol{u},$$

No need for $\delta\boldsymbol{\tau}$

$$Jac = Jac(\nabla_x \delta\boldsymbol{u}, J, \boldsymbol{\tau}, \delta\boldsymbol{\epsilon})$$

$\rightarrow$ ***Jac***

Current-AD

$\nabla_X \boldsymbol{u} \rightarrow$

$$\boldsymbol{\tau} = \overbrace{\frac{\partial \psi}{\partial \boldsymbol{e}}}^{(\dots(2\boldsymbol{e}+\boldsymbol{I})^{-1}+\dots)}(2\boldsymbol{e}+\boldsymbol{I})$$

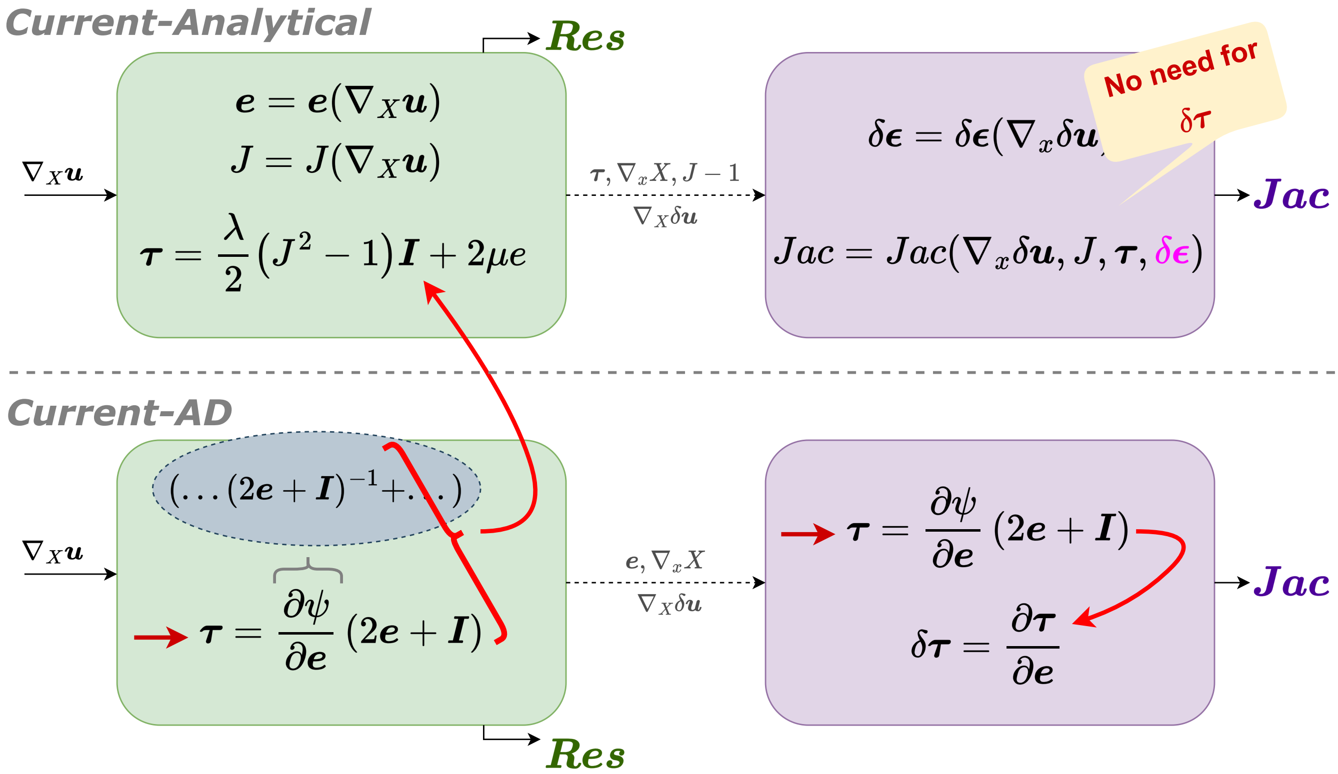
$\rightarrow$ ***Res***

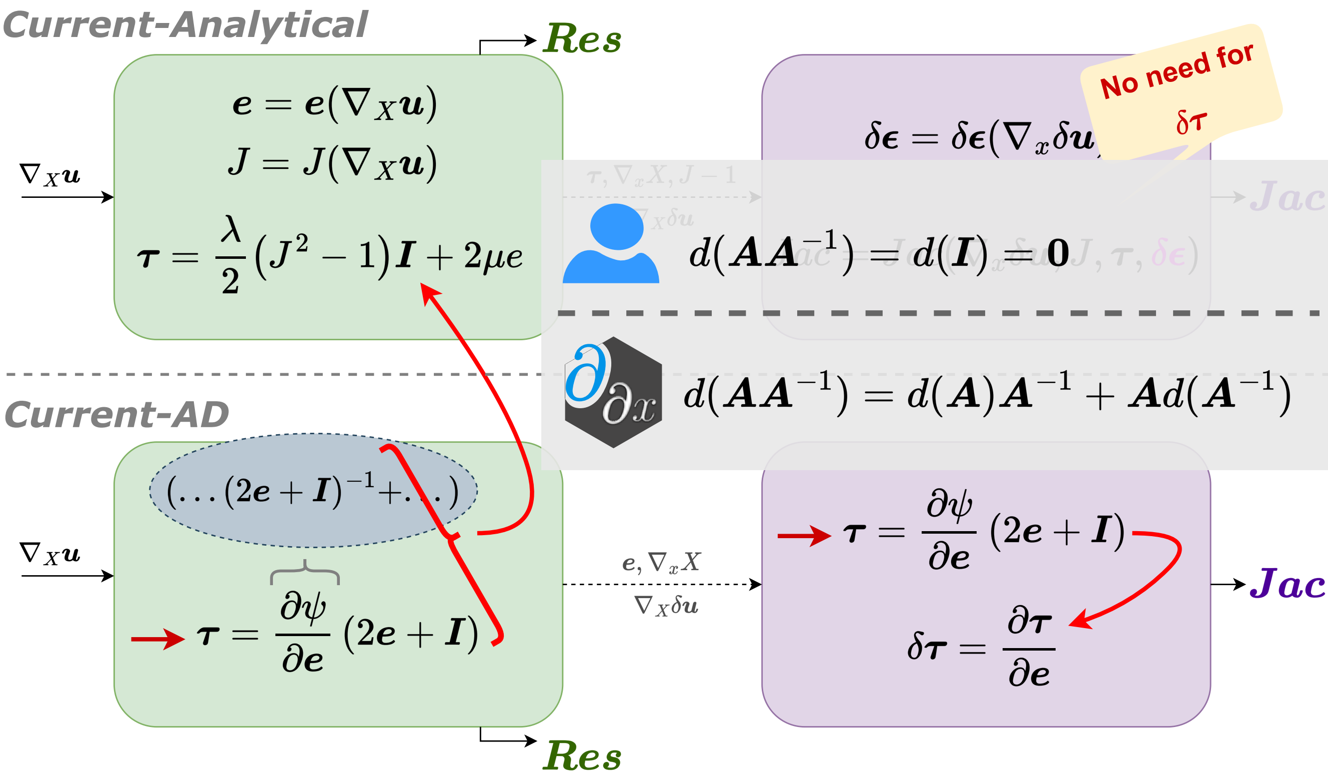
$\xrightarrow[\nabla_X \delta\boldsymbol{u}]{\boldsymbol{e},\, \nabla_x X}$

$$\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$$

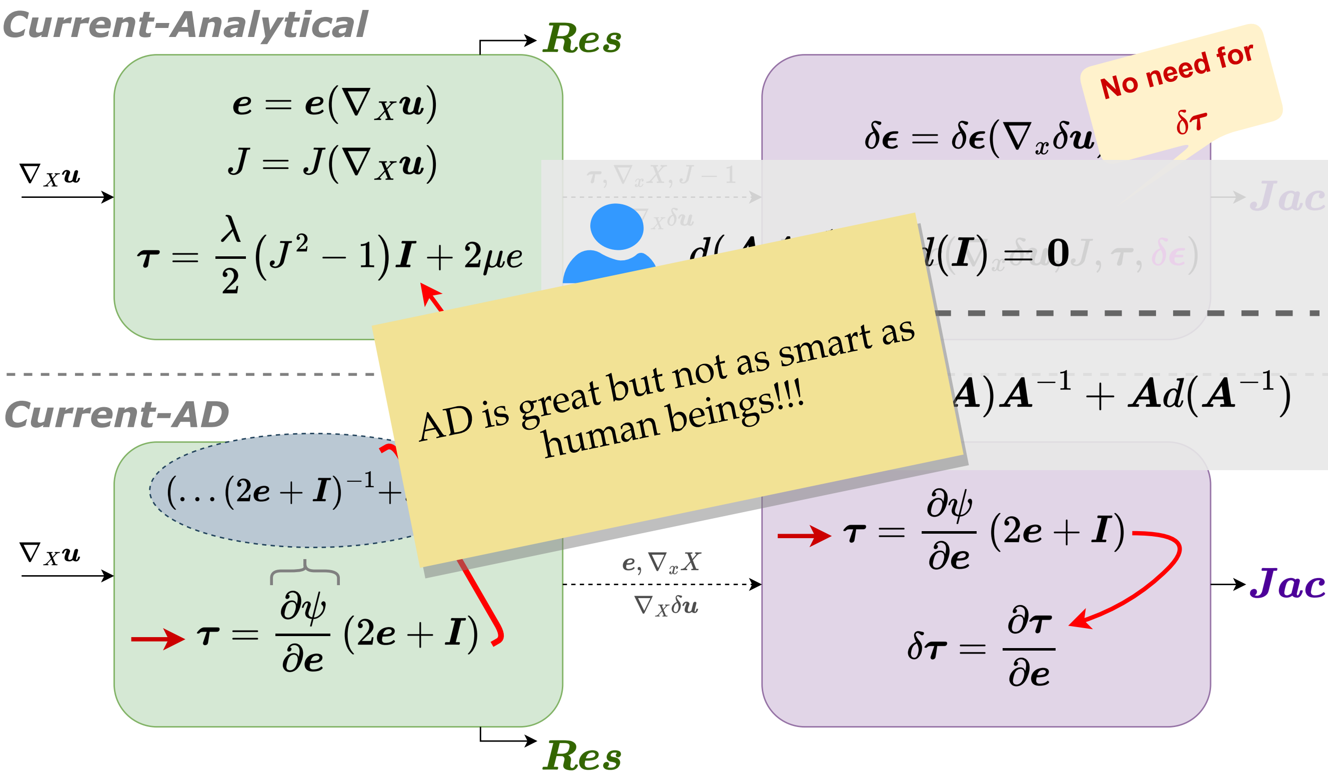
$$\delta\boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{e}}$$

$\rightarrow$ ***Jac***


Current-Analytical
Res
$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$
$J = J(\nabla_X \boldsymbol{u})$
$\boldsymbol{\tau} = \frac{\lambda}{2}\big(J^2 - 1\big)\boldsymbol{I} + 2\mu e$
$\nabla_X \boldsymbol{u}$
$\boldsymbol{\tau}, \nabla_x X, J-1$
$\nabla_X \delta \boldsymbol{u}$
$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta \boldsymbol{u})$
No need for $\delta\boldsymbol{\tau}$
$Jac = Jac(\nabla_x \delta \boldsymbol{u}, J, \boldsymbol{\tau}, \delta\boldsymbol{\epsilon})$
Jac
Current-AD
$(\ldots(2\boldsymbol{e}+\boldsymbol{I})^{-1}+\ldots)$
$\nabla_X \boldsymbol{u}$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial \boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
$\boldsymbol{e}, \nabla_x X$
$\nabla_X \delta \boldsymbol{u}$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial \boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
$\delta\boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{e}}$
Jac
Res



Current-Analytical
Res
$e = e(\nabla_X u)$
$J = J(\nabla_X u)$
$\tau = \frac{\lambda}{2}(J^2-1)I + 2\mu e$
$\nabla_X u$
No need for $\delta\tau$
$\delta\epsilon = \delta\epsilon(\nabla_x \delta u)$
Jac
$d(AA^{-1}) = d(I) = 0$
$d(AA^{-1}) = d(A)A^{-1} + Ad(A^{-1})$
Current-AD
$(\dots(2e+I)^{-1}+\dots)$
$\tau = \frac{\partial\psi}{\partial e}(2e+I)$
$e, \nabla_x X$
$\nabla_X \delta u$
$\tau = \frac{\partial\psi}{\partial e}(2e+I)$
$\delta\tau = \frac{\partial\tau}{\partial e}$
Jac
Res



Current-Analytical
Res
$\boldsymbol{e} = \boldsymbol{e}(\nabla_X \boldsymbol{u})$
$J = J(\nabla_X \boldsymbol{u})$
$\boldsymbol{\tau} = \frac{\lambda}{2}(J^2 - 1)\boldsymbol{I} + 2\mu e$
$\nabla_X \boldsymbol{u}$
$\delta\boldsymbol{\epsilon} = \delta\boldsymbol{\epsilon}(\nabla_x \delta\boldsymbol{u}$
No need for $\delta\boldsymbol{\tau}$
$\boldsymbol{\tau}, \nabla_x X, J-1$
$\nabla_X \delta u$
Jac
$d(\boldsymbol{I}) = \boldsymbol{0}$
$\boldsymbol{A})\boldsymbol{A}^{-1} + \boldsymbol{A}d(\boldsymbol{A}^{-1})$
AD is great but not as smart as human beings!!!
Current-AD
$(\ldots(2\boldsymbol{e}+\boldsymbol{I})^{-1}+$
$\nabla_X \boldsymbol{u}$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial\boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
$\boldsymbol{e}, \nabla_x X$
$\nabla_X \delta\boldsymbol{u}$
$\boldsymbol{\tau} = \frac{\partial\psi}{\partial\boldsymbol{e}}(2\boldsymbol{e}+\boldsymbol{I})$
$\delta\boldsymbol{\tau} = \frac{\partial\boldsymbol{\tau}}{\partial\boldsymbol{e}}$
Jac
Res

OUTLOOK

TOWARDS PLASTICITY

$$\text{Input Scalar Functions} = \begin{cases} \psi(\boldsymbol{E}; \mathbb{I}) & \leftarrow \text{ free energy} \\ \phi(\boldsymbol{S}; \mathbb{I}) & \leftarrow \text{ dissipation potential} \\ f(\boldsymbol{S}; \mathbb{I}) & \leftarrow \text{ yield surface} \end{cases}$$

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