Automatic Differentiation in Solid Mechanics

Interpretation and Composition

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EnzymeCon
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Differentiation in Solid Mechanics

Free energy functional and PDE solvers

$$\psi\left(\boldsymbol{E}\right) = \frac{\lambda}{4}\left(J^2 - 1 - 2\log J\right) - \mu\left(\log J + \operatorname{trace} \boldsymbol{E}\right), \quad J = \sqrt{\left|I_3 + 2\boldsymbol{E}\right|}$$

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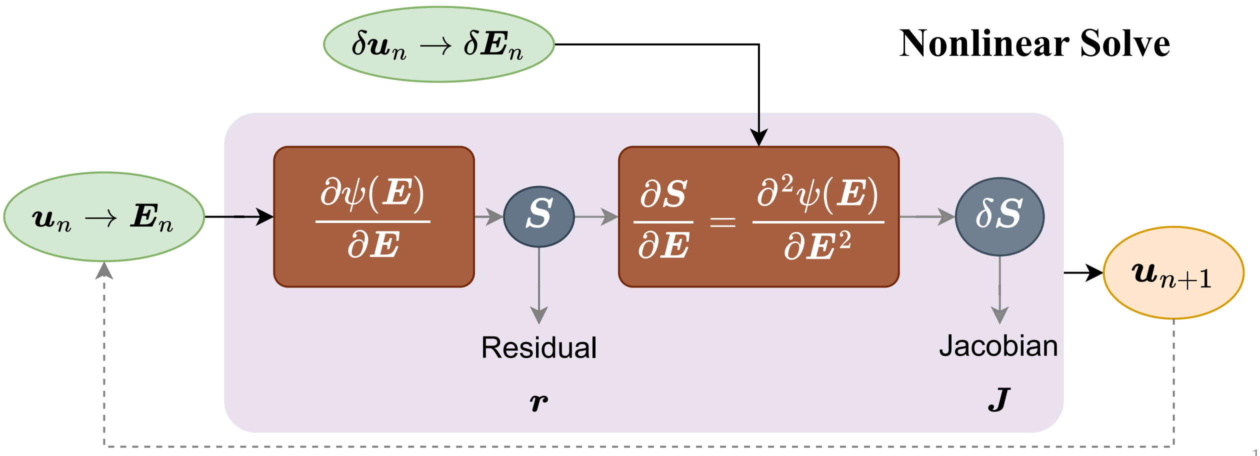

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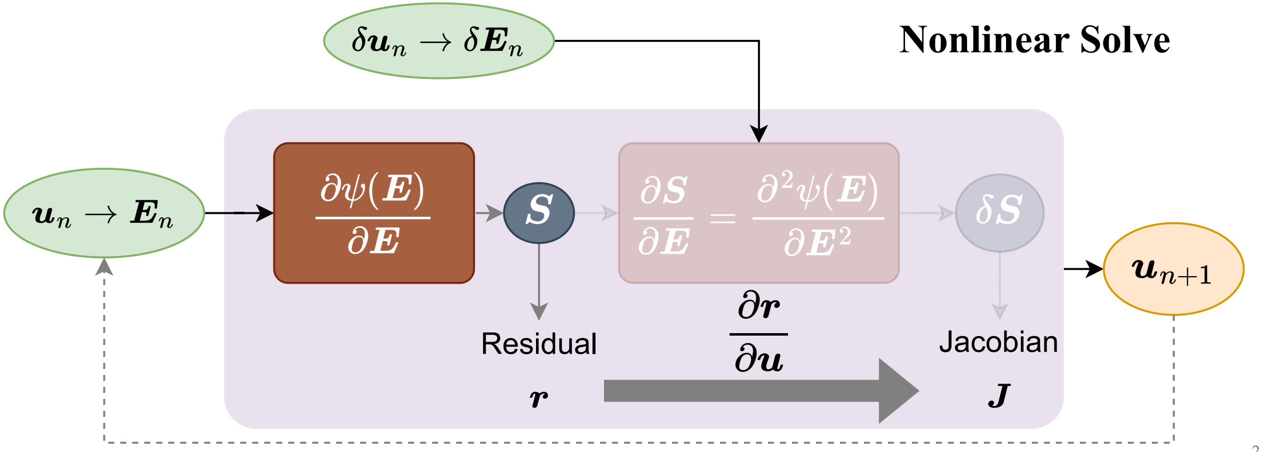

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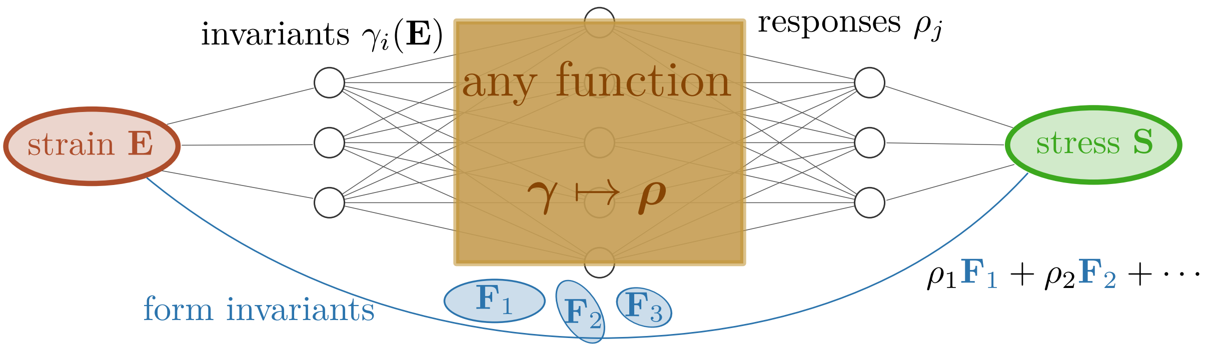
Differentiation in Solid Mechanics

Free energy functional and Inverse problems

$$\psi(\boldsymbol{E}) = \frac{\lambda}{4}\left(J^2 - 1 - 2\log J\right) - \mu\left(\log J + \operatorname{trace}\boldsymbol{E}\right), \quad J = \sqrt{|I_3 + 2\boldsymbol{E}|}$$



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)`

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

`UI1(2)`

$\partial U / \partial \bar{I}_2$.

`UI1(3)`

$\partial U / \partial J$.

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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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∂

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

- Fully automated commercial package (Solid Mechanics, FEM)
- Complex interface ... many inputs)
- ...able for small ...mation due to the ...e of interface design ... $= \boldsymbol{I} + \nabla_X \boldsymbol{u}$
- Not easy to change the interface

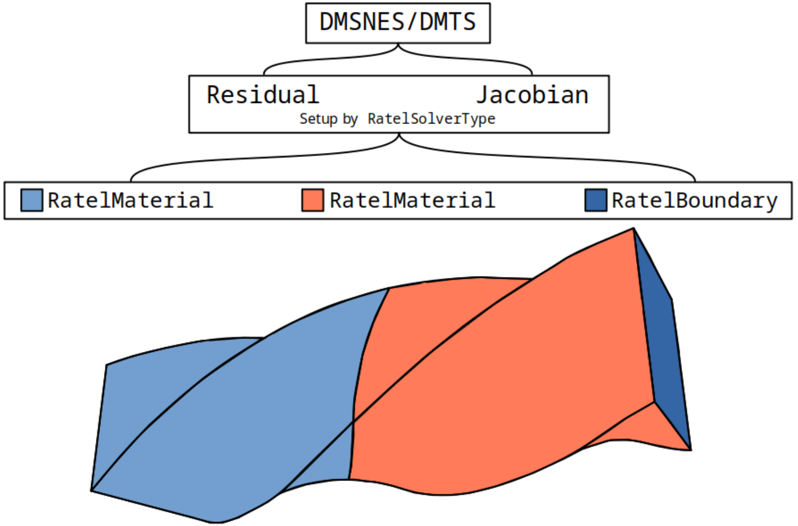
Ratel: Extensible, performance-portable solid mechanics

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



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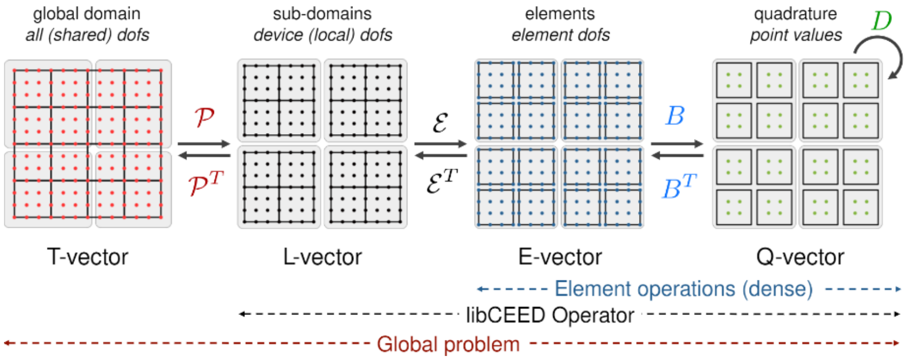
Composition and Abstraction - libCEED: https://libceed.org/en/latest/

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



- Purely algebraic high-order FEM
- Single source Vanilla C for physics
- Various CPU and GPU backends
- Backend plugins with run-time selection `./bps -ceed /gpu/cuda`
- Support for Matrix-assembly and Matrix-free
- Operator abstraction
- User choice of data storage at quadrature point

PETSc:

https://petsc.org/release/

- Parallel solution of PDEs
- CPUs (MPI)
- GPUs
  - CUDA
  - HIP
  - OpenCL
- Hybrid MPI-GPU
- Optimization (PETSc/Tao)

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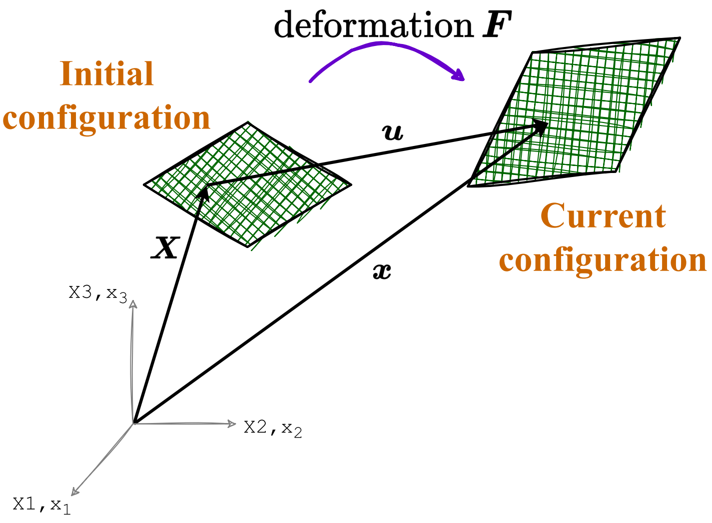
Enzyme AD:

https://enzyme.mit.edu/

- High-Performance Automatic Differentiation
- Work at the LLVM level
- Support for variety of languages (C/C++, Julia, Rust, Fortran, etc)
- *reverse* and *forward* mode AD

Initial vs Current configuration



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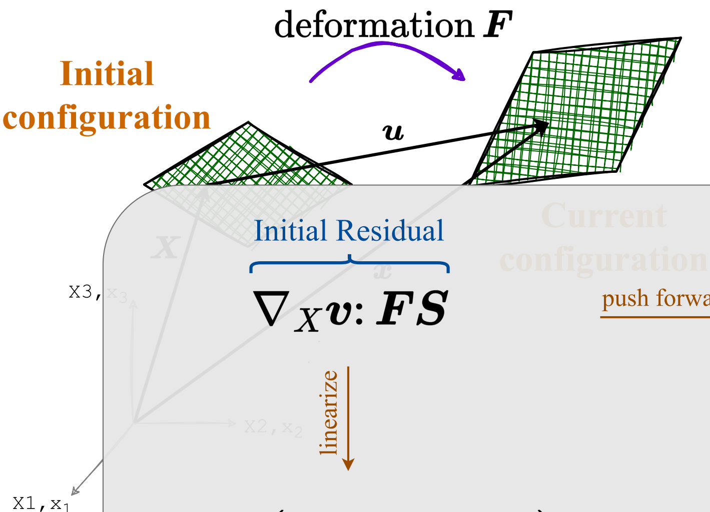
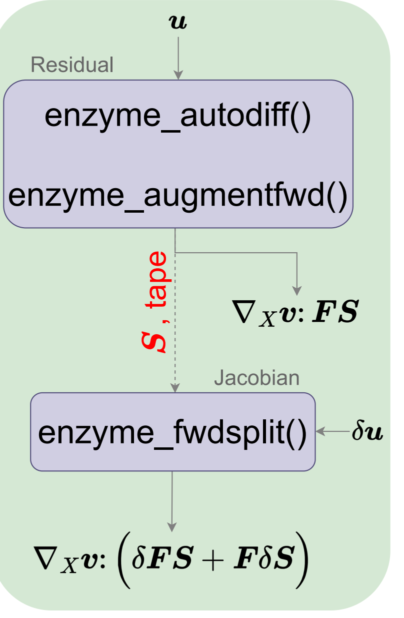


$$\begin{array}{ccc}
\overbrace{\nabla_X \boldsymbol{v} : \boldsymbol{F}\boldsymbol{S}}^{\text{Initial Residual}} & \xrightarrow{\text{push forward}} & \overbrace{\nabla_x \boldsymbol{v} : \boldsymbol{\tau}}^{\text{Current Residual}} \\
\Big\downarrow \text{linearize} & & \Big\downarrow \text{linearize} \\
\underbrace{\nabla_X \boldsymbol{v} : \left(\delta\boldsymbol{F}\boldsymbol{S} + \boldsymbol{F}\delta\boldsymbol{S}\right)}_{\text{Initial Jacobian}} & \xrightarrow{\text{push forward}} & \underbrace{\nabla_x \boldsymbol{v} : \left(\delta\boldsymbol{\tau} - \boldsymbol{\tau}(\nabla_x \delta\boldsymbol{u})^T\right)}_{\text{Current Jacobian}}
\end{array}$$

Ratel - Enzyme AD

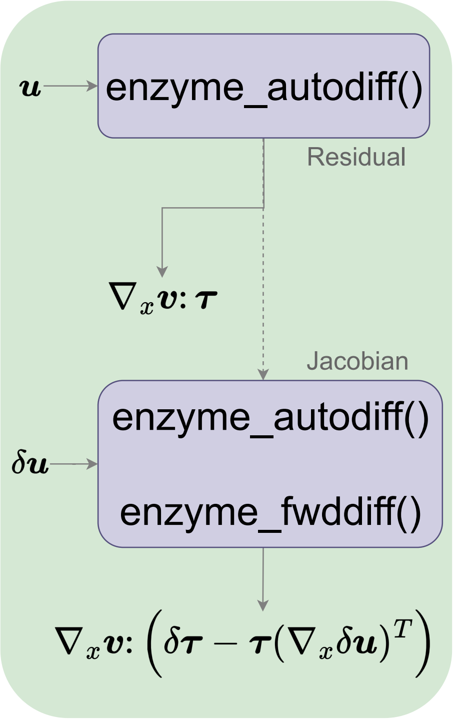
Initial configuration - Forward Split

```
// 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



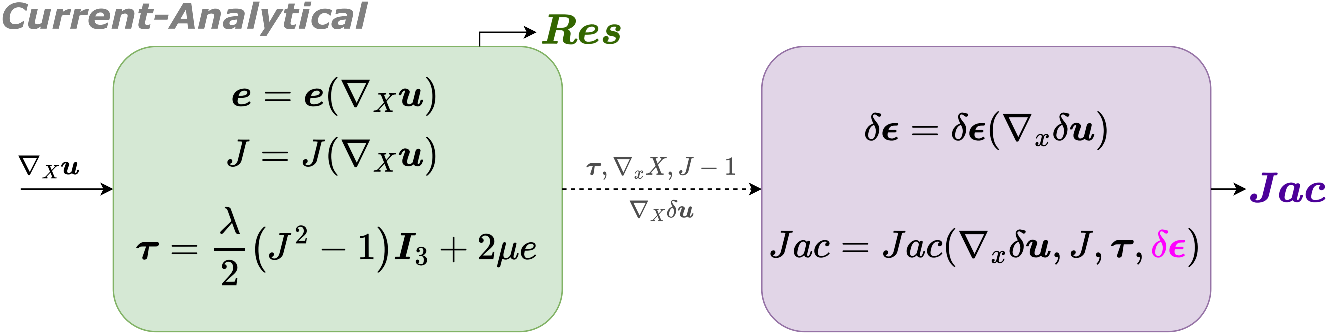

```
// Compute tau = (dPsi / de) * (2 e + I) [Reverse]
void Kirchhofftau_Voigt_NeoHookean_AD(...) {
  __enzyme_autodiff((void *)StrainEnergy, ...);
  ...
  for (int j = 0; j < 6; j++)
    b_Voigt[j] = 2 * e_Voigt[j] + (j < 3);
  ...
  RatelMatMatMult(1., dPsi, b, tau);
}

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

Ratel - Enzyme AD

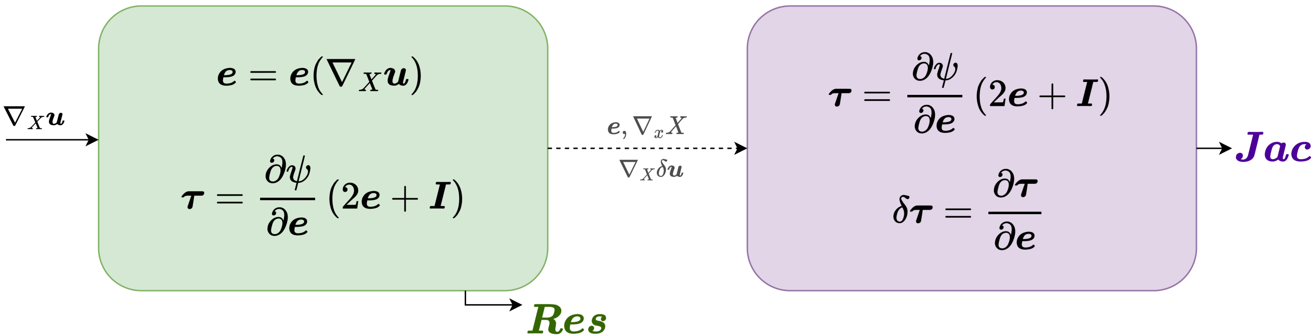
Performance for different Jacobian representations

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



Current-AD



Current-Analytical

$\nabla_X \boldsymbol{u} \rightarrow$

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

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

$$\boldsymbol{\tau} = \frac{\lambda}{2}\left(J^2 - 1\right)\boldsymbol{I}_3 + 2\mu e$$

$\rightarrow$ ***Res***

$\boldsymbol{\tau}, \nabla_x X, J-1$ / $\nabla_X \delta\boldsymbol{u}$ $\dashrightarrow$

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

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

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

$\rightarrow$ ***Jac***

Current-AD

$\nabla_X \boldsymbol{u} \rightarrow$

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

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

$\rightarrow$ ***Res***

$\boldsymbol{e}, \nabla_x X$ / $\nabla_X \delta\boldsymbol{u}$ $\dashrightarrow$

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$\boldsymbol{e}, \nabla_x X$

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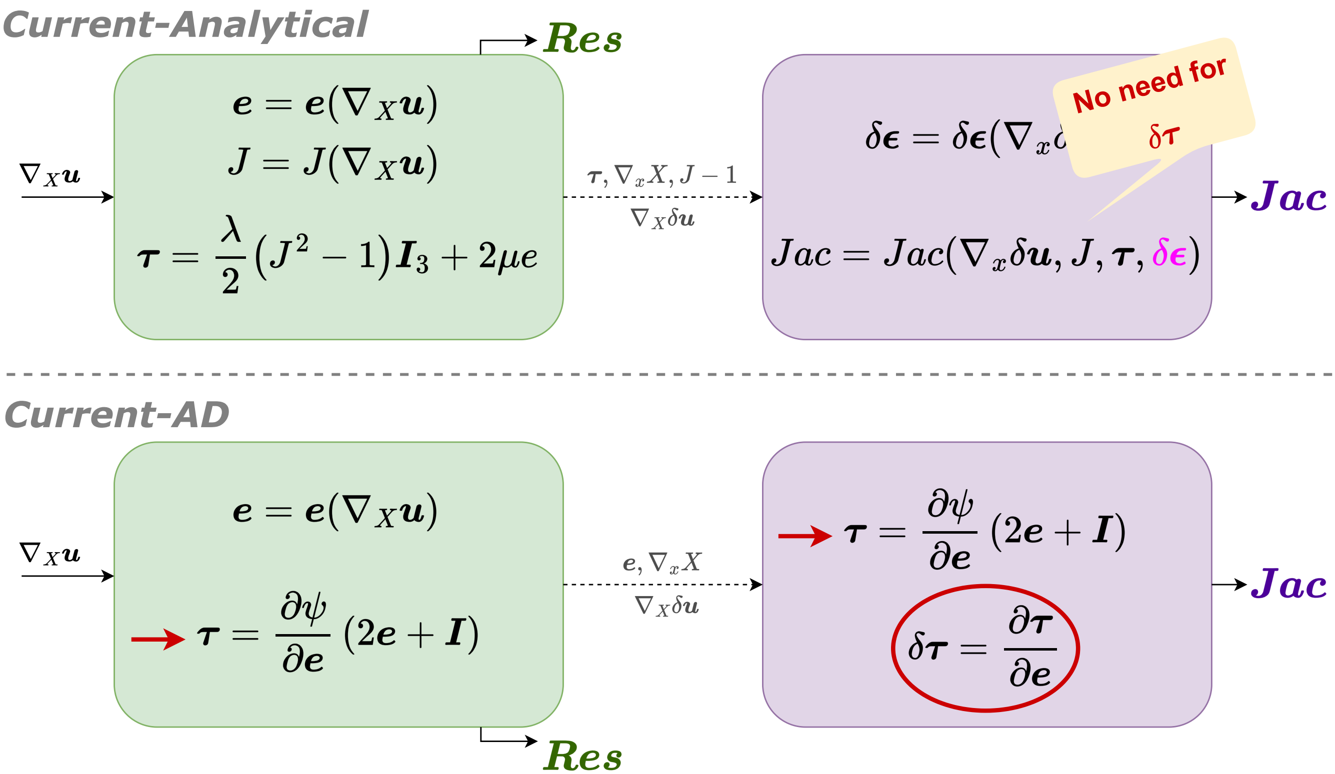

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$\nabla_X u$
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Current-AD
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$\tau = \frac{\partial\psi}{\partial e}(2e + I)$
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$\boldsymbol{\tau}, \nabla_x X, J-1$

$\nabla_X \delta \boldsymbol{u}$

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

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

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

$\boldsymbol{Jac}$

AD is great but not as smart as human beings!!!

Current-AD

$\nabla_X \boldsymbol{u}$

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

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

$\boldsymbol{e}, \nabla_x X$

$\nabla_X \delta \boldsymbol{u}$

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

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

$\boldsymbol{Jac}$

$\boldsymbol{Res}$

Enzyme Wishlist

- Enzyme-aware clangd

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research under Award Number DE-SC0016140.

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$\boldsymbol{A}\boldsymbol{A}^{-1}$

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- Compile code with `-O0`
- Calling Enzyme in a debugger
- Internal cancellation of tensor operations

$$d(\cancel{\boldsymbol{A}\boldsymbol{A}^{-1}}) = d(\boldsymbol{I}) = \boldsymbol{0}$$

$$d(\boldsymbol{A}\boldsymbol{A}^{-1}) = d(\boldsymbol{A})\boldsymbol{A}^{-1} + \boldsymbol{A}d(\boldsymbol{A}^{-1})$$

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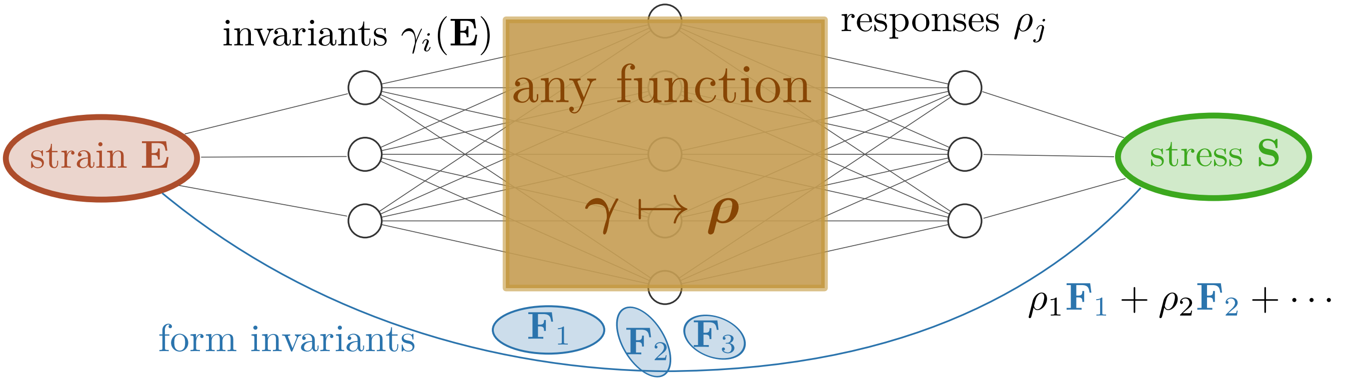
Outlook

Towards Plasticity



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