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Working towards a modular, fully-coupled phase field fracture model integrating elasticity, plasticity, and damage

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Outline

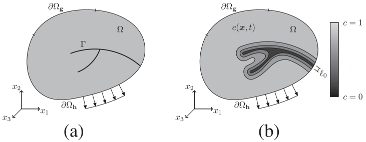
Background

Overview

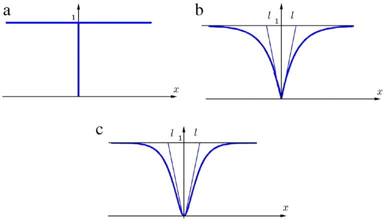
- Phase field methods are a widely used set of techniques used to capture several different types of phenomena
- Initially developed for tracking physical phase changes
- Modified to use a continuous damage variable to track crack propagation in continuum models

Origins of phase field fracture

- Derived from Griffith brittle fracture
- Represent discrete cracks as "smeared" continuum damage models
- Length scale converts infinitesimal crack into finite-width region
- Fracture problem reformulated as coupled PDE system



Borden *et al.* (2014)



Amiri *et al.* (2016)

Phase field fracture models

- Many different phase field fracture models exist
- Different choices for:
  - elastic model
  - inclusion of plasticity (and choice of plastic model)
  - rate-dependence
  - how damage impacts elastic and plastic responses (degradation functions)
  - fracture potential
  - tension-compression split
- Each one has to be derived from scratch based on the assumptions made in that work

Existing formulation within SIERRA

- Existing phase field formulation incorporating plasticity in SIERRA (`PhaseFieldFeFp`) hard-codes many things:
  - elastic, plastic, and fracture models
  - constraints
  - flow rule
  - number of internal variables and phase variables
  - degradation function
  - tension-compression split
- What if we could *generalize* the existing formulation?

Formulation

Guiding Principles

- Potential-based formulation — elastic, plastic, and damage models are all derived from potentials (same for "viscous" parts and kinetic potentials)
- As modular as possible — almost every part has multiple choices (elastic potential, plastic potential, damage potential, degradation function, tension-compression split) and new ones can be implemented as long as they provide the required "bits" (usually: value, jacobian, hessian)
- Generalized — solution method is as general as possible (Sequential Quadratic Programming with Active-Set constraint selection) and almost nothing is assumed about the form of the constraints (can be nonlinear functions of multiple variables)

Derivation

- Start with the usual assumption: $\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p$
- Define potentials $\psi^e\left(\boldsymbol{F}\boldsymbol{F}^{p^{-1}}, \boldsymbol{\phi}\right)$, $\psi^p\left(\boldsymbol{F}^p, \boldsymbol{\phi}, \boldsymbol{Q}\right)$, and $\psi^f\left(\boldsymbol{\phi}, \boldsymbol{\nabla}\boldsymbol{\phi}\right)$
- Further, split the $\boldsymbol{\phi}$ dependence of ψ^e and ψ^p into a multiplicative component:

$$\psi^e\left(\boldsymbol{F}\boldsymbol{F}^{p^{-1}}, \boldsymbol{\phi}\right) = g^e\left(\boldsymbol{\phi}\right)\tilde{\psi}^e\left(\boldsymbol{F}\boldsymbol{F}^{p^{-1}}\right)$$

$$\psi^p\left(\boldsymbol{F}^p, \boldsymbol{\phi}, \boldsymbol{Q}\right) = g^p\left(\boldsymbol{\phi}\right)\tilde{\psi}^p\left(\boldsymbol{F}^p, \boldsymbol{Q}\right)$$

- Define kinetic potentials ψ^*_P, ψ^*_Q, and ψ^*_ϕ that define the viscous response of $\boldsymbol{P}$, $\boldsymbol{Q}$, and $\boldsymbol{\phi}$ respectively
- Split the $\boldsymbol{\phi}$ dependence of ψ^*_P and ψ^*_Q as above

Derivation

- Define generalized flow rule as $\dot{\boldsymbol{F}}^p = \dot{\boldsymbol{Q}}\boldsymbol{M}\left(\boldsymbol{K}\right)\boldsymbol{F}^p$
  - This introduces a *vector* of internal variables $\boldsymbol{Q}$ and a *third-order flow tensor* $\boldsymbol{M}$
    - If $\boldsymbol{Q}$ is size n (n internal variables), then $\boldsymbol{M}$ is $n \times 3 \times 3$
  - Reduces to the standard case when there is only one internal variable (outer dimension of $\boldsymbol{M}$ is 1)
- From now on, we deal only with $\boldsymbol{M}$
  - In the case that $\boldsymbol{M}$ is fully defined (i.e. doesn't need to be solved for), can introduce constraints that fix the components of $\boldsymbol{M}$

Derivation

- At each step, we are given $\{\boldsymbol{F}_n, \phi_n, \boldsymbol{F}^p_n, \boldsymbol{Q}_n\}$ as well as $\boldsymbol{F}_{n+1}$
- We need to find $\left\{\boldsymbol{M}_{n+1}, \boldsymbol{Q}_{n+1}, \boldsymbol{F}^p_{n+1}\right\}$
  - We *also* need to solve for ϕ_{n+1}, but that is done separately due to limitations within SIERRA (alternating minimization approach)
- We have to minimize

$$\Delta A\left(\boldsymbol{F}, \phi, \boldsymbol{\nabla}\phi, \boldsymbol{F}^p, \boldsymbol{Q}\right) + \Delta t g^p\left(\phi_{n+\alpha}\right) \tilde{\psi}^*_Q\left(\frac{\boldsymbol{Q}_{n+1} - \boldsymbol{Q}_n}{\Delta t}; \boldsymbol{Q}_{n+\alpha}\right)$$

with respect to $\boldsymbol{Q}_{n+1}$ and $\boldsymbol{M}_{n+1}$, subject to a system of (possibly non-linear) constraints

Derivation

$$\mathcal{L} = g^e\left(\boldsymbol{\phi}_{n+1}\right)\tilde{\psi}^e\left(\boldsymbol{F}^e_{n+1}\right) + g^p\left(\boldsymbol{\phi}_{n+1}\right)\tilde{\psi}^p\left(\boldsymbol{F}^p_{n+1}, \boldsymbol{Q}_{n+1}\right)$$
$$+ \Delta t g^p\left(\boldsymbol{\phi}_{n+\alpha}\right)\tilde{\psi}^*_p\left(\frac{\boldsymbol{Q}_{n+1} - \boldsymbol{Q}_n}{\Delta t}; \boldsymbol{Q}_{n+\alpha}\right) - \lambda_i c_i$$

- Minimize to solve for updated $\boldsymbol{Q}_{n+1}$ and $\boldsymbol{M}_{n+1}$
- Easy to solve if all constraints are equalities (Newton-Raphson or such would work nicely)
- Active-Set methods can be utilized for constraint selection

Derivation

$$\begin{pmatrix} \mathcal{L}_{,\boldsymbol{xx}} & -\boldsymbol{c}_{,\boldsymbol{x}} \\ \boldsymbol{c}_{,\boldsymbol{x}} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{p}_k \\ \boldsymbol{\lambda}_{n+1} \end{pmatrix} = \begin{pmatrix} -F_{,\boldsymbol{x}} \\ -\boldsymbol{c} \end{pmatrix}$$

- We convert it to a quadratic problem and utilize SQP with Active-Set constraint selection
- Derivation is involved but fairly straight-forward
- To use this method, we need the Hessian of the Lagrangian as well as derivatives of the constraint equations

Examples

- Pure elasticity
  - Elastic potential turned on, all other potentials and kinetic potentials disabled, degradation functions turned off
  - $\mathcal{L} = \tilde{\psi}^e \left(\boldsymbol{F}_{n+1} \right)$
- Elasto-plasticity, isotropic plasticity
  - Elastic and plastic potentials turned on, all other potentials and kinetic potentials disabled, degradation functions turned off
  - $\mathcal{L} = \tilde{\psi}^e \left(\boldsymbol{F}_{n+1} \boldsymbol{F}^{p^{-1}}_{n+1} \right) + \tilde{\psi}^p \left(\boldsymbol{F}^p_{n+1}, Q_{n+1} \right) - \lambda_i c_i$, with $M_{ii} = 0$, $M_{ij} M_{ij} = \frac{3}{2}$, $M_{ij} = M_{ji}$, and $Q_{n+1} - Q_n \geq 0$
- Elasto-plasticity, isotropic + kinematic + rate-dependent plasticity with damage
  - All potentials enabled, plastic kinetic potential enabled, all other kinetic potentials disabled, degradation functions turned on
  - $\mathcal{L} = g^e \left(\boldsymbol{\phi}_{n+1} \right) \tilde{\psi}^e \left(\boldsymbol{F}^e_{n+1} \right) + g^p \left(\boldsymbol{\phi}_{n+1} \right) \tilde{\psi}^p \left(\boldsymbol{F}^p_{n+1}, Q_{n+1} \right) + \Delta t g^p \left(\boldsymbol{\phi}_{n+\alpha} \right) \tilde{\psi}^*_p \left(\frac{\Delta Q}{\Delta t}; Q_{n+\alpha} \right) - \lambda_i c_i$ with the same constraints as before

Challenges

- No generalized n-dimensional tensor library available in SIERRA...so created one!
- Finding relevant derivatives of the log strain tensor was highly non-trivial
- Implementing the tension-compression split in a generic way, especially the spectral tension-compression split, was non-trivial
- Numerical sensitivities
- Efficiency concerns

Dealing with the TCS

$$\frac{\mathrm{d}\tilde{\psi}^{e\pm}}{\mathrm{d}F^e_{kl}} = \frac{\partial\tilde{\psi}^{e\pm}}{\partial E^{e\pm}_{uv}} \frac{\partial E^{e\pm}_{uv}}{\partial E^e_{mn}} \frac{\partial E^e_{mn}}{\partial C^e_{pq}} \frac{\partial C^e_{pq}}{\partial F^e_{kl}}$$

- $\frac{\partial E^{e\pm}_{uv}}{\partial E^e_{mn}}$ will be different for each tension-compression split
- Fairly straightforward for the deviatoric-volumetric tension-compression split
- A bit more involved for the spectral tension-compression split

Example problem

- Uses the developed *framework* (`Potential` classes, TCS handling, etc) within the earlier (specialized) formulation
- Does *not* use generalized solver (yet)

Costs and Benefits

Costs

- SQP can be slower than more specialized methods (e.g. return-mapping)
- May need stronger guarantees on potentials or other components than with more specialized solvers (most components need at least C^2)
- Derivations can be tricky

Benefits

- Can implement material models whose constraints are not independent
- Can investigate alternative flow rules
- Converts the existing formulation into a *framework* rather than one specific model
    - As long as requirements for material models are met, can be used within this framework

Conclusions

Current State

- Preliminary implementation of `GeneralizedPhaseFieldFeFp`
- Phase field solver has also been mostly modularized
- Designing correctness and regression tests
- Further optimization of n-dimensional tensor library may be needed
- Comparison of old and new formulations to verify correctness of behavior

Next Steps

- New elastic, plastic, and damage models can be developed, explored, and compared against experimental data to better model materials of interest
- Inclusion of void mechanics and void nucleation, potentially through development of a surrogate model
- Exploration of ways to model crack initiation while being consistent with our variational formulation

Questions?