Addressing Numerical Challenges in Frictional Contact Simulation for Finite-Deformation Solid Mechanics

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Outline

1.1 Quasistatic Compression of Single Crystalline Grains

Experimental Setup

- Apparatus applies uniaxial compression to a single grain
- Platens are made of sapphire to minimize friction
- Invisible to X-rays to allow for in-situ CT imaging

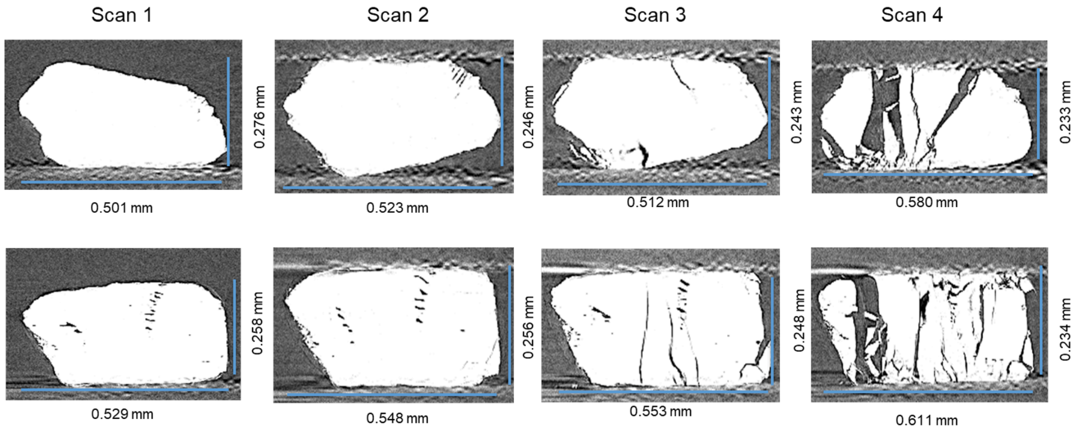
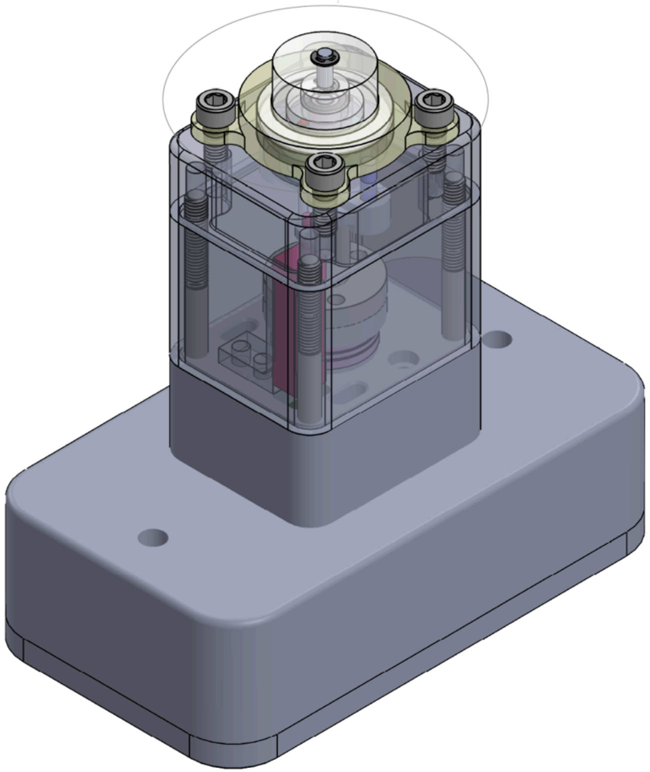


Figure 1: Experiments by Gharaibeh, Alshibli (UTK)



1.2 Material Modeling

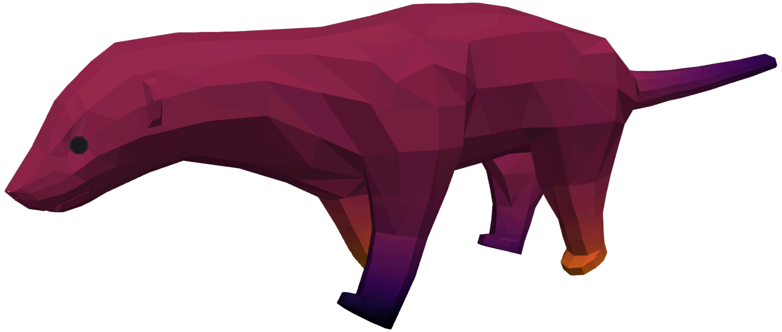
- Grains are brittle and have moderate resistance to compressive load
  - Young's Modulus $E \approx 23.2$ GPa (around high-strength concrete)
  - Critical stress $\sigma_c \approx 1.3$ GPa
- Experiments show vertical cracks in the grain
- Simulations must capture:
  1. Crack initiation and propagation
     - Use phase-field damage model [1]
  2. Large-scale force-displacement behavior
  3. **Contact between platens and grain**

1.3 Modeling Contact

- Experiments use sapphire platens to minimize friction ($\mu_k \approx 0.1$)
- So, why not use frictionless contact (Neumann) or free-slip (Essential) boundary condition?
  - Frictionless contact problems are ill-posed
  - Other methods to prevent rigid-body motion introduce stress singularities
- Modeling frictional contact:
  1. Improves realism of the simulation (some buckling is observed, no contact is truly frictionless)
  2. Stabilizes the numerical solution by constraining motion in the tangent plane

1.4 Software Ecosystem

- Ratel: flexible and fast solid mechanics code [2]
- libCEED: matrix-free high-order finite elements [3]
  - Single kernel for CPU, HIP, CUDA, etc.
- PETSc: scalable and portable solvers and FEM infrastructure [4]



libCEED: Efficient Extensible Discretization

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PETSc TAO

Outline

2.1 General Motions in Finite-Deformation Solid Mechanics

Reference (or initial) configuration Ω_0

- Material points $P \in \Omega_0$ with coordinates $\boldsymbol{X}$

Current (or deformed) configuration Ω_t

- Spatial points $p \in \Omega$ with coordinates $\boldsymbol{x}(\boldsymbol{X})$

Displacement field $\boldsymbol{u} : \Omega_0 \to \Omega_t$

- $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{x} - \boldsymbol{X}(\boldsymbol{x}, t)$

Displacement gradient $\boldsymbol{F} = \nabla_X \boldsymbol{u} + \boldsymbol{I}$, $J = \det(\boldsymbol{F})$

- Length changes: $d\boldsymbol{x} = \boldsymbol{F} d\boldsymbol{X}$
- Areas are related by $da = J\boldsymbol{F}^{-1} dA$
- Volumes are related by $dv = JdV$

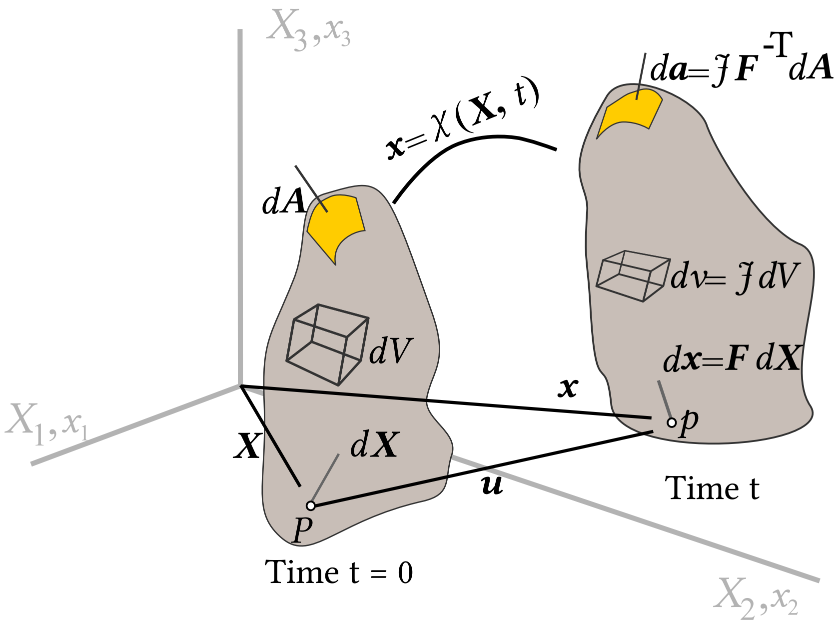


Figure 2: Motion of a material point in a solid body [2]

2.2 Hyperelasticity

Generally, we assume the Cauchy stress $\boldsymbol{\sigma}$ to be a function of the displacement field $\boldsymbol{u}$ and the consitutive model parameters

- In the initial configuration, use the first Piola-Kirchhoff stress $\boldsymbol{P} = J\boldsymbol{\sigma}F^{-T}$

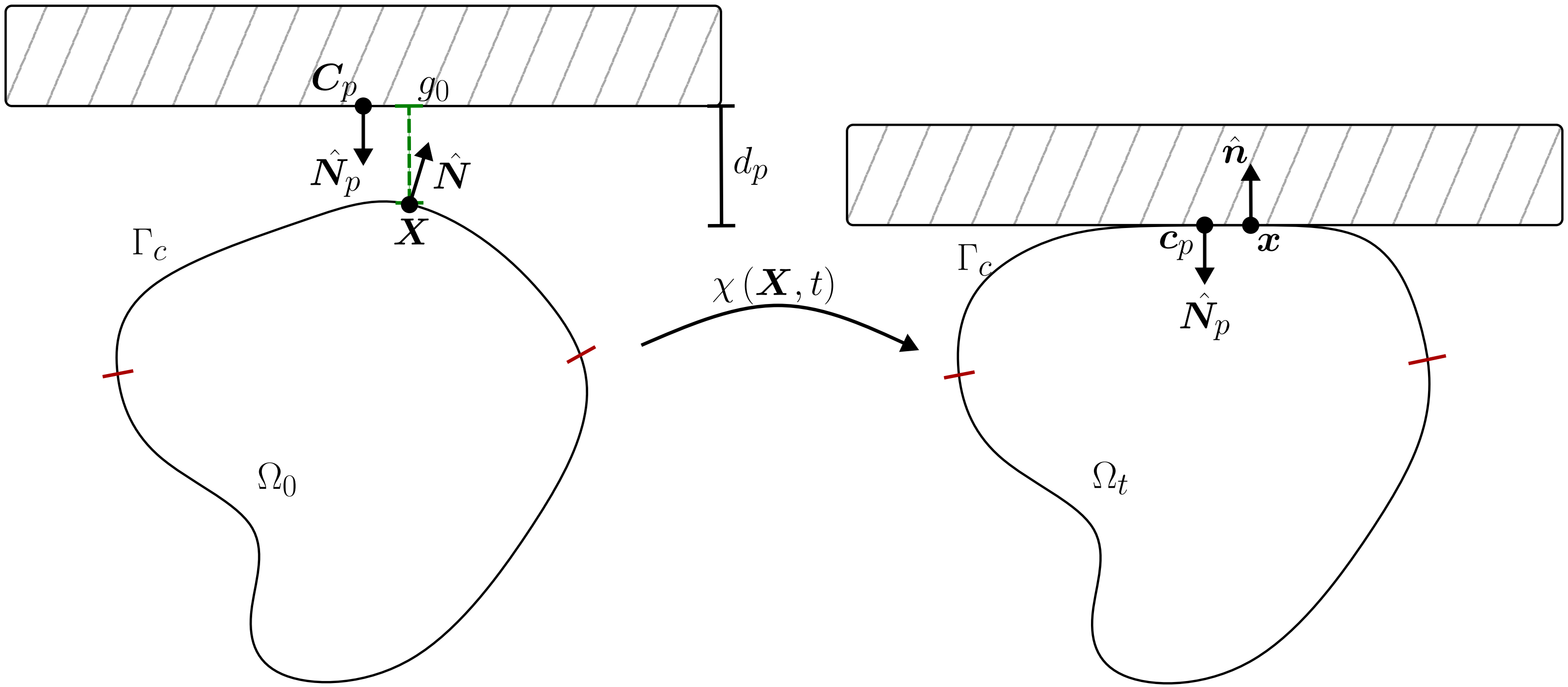
Strong form: Given a body force density $\rho_0\boldsymbol{g}$, Dirichet boundary conditions Γ_D, and applied traction Γ_N, find $\boldsymbol{u} \in \mathcal{V}$, such that

$$\begin{aligned} -\nabla_X \cdot \boldsymbol{P} + \rho_0\boldsymbol{g} &= 0, \quad \text{in } \Omega_0 \\ \boldsymbol{u} &= \overline{\boldsymbol{u}}, \quad \text{on } \Gamma_D \\ \hat{\boldsymbol{\sigma}}(\boldsymbol{u}) := \boldsymbol{P} \cdot \widehat{\boldsymbol{N}} &= \bar{\boldsymbol{t}}, \quad \text{on } \Gamma_N \end{aligned}$$

The term $\hat{\boldsymbol{\sigma}}(\boldsymbol{u})$ is the ***Piola traction vector*** or ***surface forces***.

Outline

3. Frictionless Contact Problem



One-sided contact between Ω and a platen

- Platen modeled as a rigid plane with normal $\widehat{\boldsymbol{N}}_p$ and center $\boldsymbol{c}_p(t) = \boldsymbol{C}_p + d_p(t)\widehat{\boldsymbol{N}}_p$

3.1 Key Quantities

The ***normal gap function*** at time t function is defined by

$$g(\boldsymbol{u}) = \widehat{\boldsymbol{N}}_p \cdot \big(\boldsymbol{x} - \boldsymbol{c}_p(t)\big) = \widehat{\boldsymbol{N}}_p \cdot \big(\boldsymbol{u} + \boldsymbol{X} - \boldsymbol{c}_p(t)\big).$$

Decompose $\boldsymbol{u}$ into normal and tangential components:

$$\boldsymbol{u} = u_N \widehat{\boldsymbol{N}}_p + \boldsymbol{u}_{\boldsymbol{t}}, \quad u_N = \widehat{\boldsymbol{N}}_p \cdot \boldsymbol{u}, \quad \boldsymbol{u}_{\boldsymbol{t}} = \boldsymbol{u} - u_N \widehat{\boldsymbol{N}}_p$$

Then, we can rewrite the gap function to emphasize the sole dependence on $\boldsymbol{u}$:

$$g(\boldsymbol{u}) = \underbrace{\widehat{\boldsymbol{N}}_p \cdot \boldsymbol{u}}_{u_N} - d_p(t) + \underbrace{\widehat{\boldsymbol{N}}_p \cdot \big(\boldsymbol{X} - \boldsymbol{C}_p\big)}_{g_0} = u_N + \underbrace{g_0 - d_p(t)}_{\substack{\text{constant for} \\ \text{a given } X, t}}.$$

3.1 Key Quantities

Similarly, the ***surface forces*** $\hat{\boldsymbol{\sigma}}(\boldsymbol{u})$ can be decomposed into normal and tangential components:

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{u}) = \hat{\sigma}_N \widehat{\boldsymbol{N}}_p + \hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}$$

The term $\hat{\sigma}_N$ is the ***normal contact pressure***

Frictionless contact only applies a normal traction $\Rightarrow$ no imposed $\hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}$

Technically, computing $\hat{\boldsymbol{\sigma}}(\boldsymbol{u})$ requires high regularity: $\mathcal{V} \subset H^s$, $s > \frac{3}{2}$

3.2 Karush-Kuhn-Tucker (KKT) Conditions

Then, the frictionless contact conditions for $\boldsymbol{X} \in \Gamma_C$ are

$$
\begin{aligned}
g(\boldsymbol{u}) &\geq 0 && \text{(non-penetration)} \\
\hat{\sigma}_N(\boldsymbol{u}) &\leq 0 && \text{(compressive contact pressure)} \\
g(\boldsymbol{u})\hat{\sigma}_N(\boldsymbol{u}) &= 0 && \text{(complementary condition)}
\end{aligned}
$$

3.2.1 Enforcement

Nitsche's method [5], [6]

Let $\gamma > 0$ be stabilization parameter (or positive integrable function). Prescribe

$$\hat{\sigma}_N(\boldsymbol{u}) = \underbrace{[\hat{\sigma}_N(\boldsymbol{u}) + \gamma g(\boldsymbol{u})]_{\mathbb{R}^-}}_{\text{computed}}, \quad [v]_{\mathbb{R}^-} = \min(v, 0)$$

- Stabilization parameter γ is material dependent
  - γ is typically around $100 \times$ Young's modulus
- ***Variationally consistent***: KKT-conditions are weakly satisfied
- **But**, introduces asymmetry in the tangent system
  - $\Rightarrow$ requires GMRES instead of CG
- Requires computing surface forces – can be expensive

Outline

4.1 Tangent (Slip) Velocity

The frame-indifferent slip velocity $\boldsymbol{v}$ is defined as

$$\boldsymbol{v} = \dot{\boldsymbol{u}} - g(\boldsymbol{u})\underbrace{\dot{\widehat{\boldsymbol{N}}}_p}_{=0}$$

Of interest for friction is the tangential component:

$$\boldsymbol{v}_t = \boldsymbol{v} - \left(\widehat{\boldsymbol{N}}_p \cdot \boldsymbol{v}\right)\widehat{\boldsymbol{N}}_p$$

Note, $\dot{\boldsymbol{u}}$ is determined by the time discretization scheme chosen

- In our case, backward Euler: At t_{n+1}, $\dot{\boldsymbol{u}} = \frac{1}{\Delta t_{n+1}}\left(\boldsymbol{u}_{n+1}^{(k)} - \boldsymbol{u}_n\right)$

4.2 Coulomb Friction Model

The Coulomb friction force is defined by [7] as

$$\boldsymbol{F} = \begin{cases} F_C \operatorname{sgn}(\boldsymbol{v}_t), & \|\boldsymbol{v}_t\| > 0 \\ \min(F_C, \|\hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}\|) \operatorname{sgn}(\hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}), & \|\boldsymbol{v}_t\| = 0 \end{cases}$$

where $F_C = -\mu_k \hat{\sigma}_N$ and

$$\operatorname{sgn}(\boldsymbol{v}) = \begin{cases} \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|}, & \text{if } \|\boldsymbol{v}\| \neq 0 \\ \boldsymbol{0}, & \text{otherwise} \end{cases}$$

$\Rightarrow$ discontinuous and non-differentiable at $\|\boldsymbol{v}\|_t = 0$

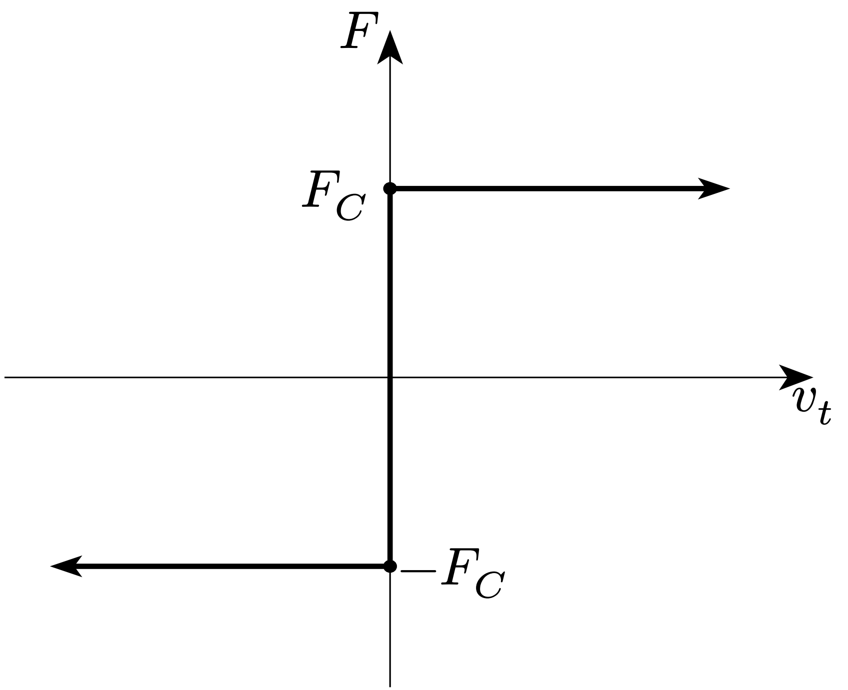


Figure 3: Coulomb friction model, 1D

4.2.1 Numerical Challenges

Newton Convergence

- Newton's method fails to converge for frictional contact problems
- **Why?**
  - Step discontinuity in Coulomb friction model
  - Oscillating force direction near $\|\boldsymbol{v}\|_t = 0$
- **How to address?**
  - Regularized friction model
  - Viscous damping
  - Line-search methods:
    - Critical-point line-search: pseudo-energy minimizer (doesn't work for Coulomb)
    - Backtracking line-search: works for all models, but fails to capture snap-through
  - Semi-smooth Newton methods (not currently used)

4.3.1 Threlfall Friction Model

Goal: Remove force discontinuity from the Coulomb model

Let v_0 be a threshold velocity, then the Threlfall friction model is

$$\boldsymbol{F} = \begin{cases} F_C \frac{1-\exp\left(-\frac{3\|\boldsymbol{v}_t\|}{v_0}\right)}{1-\exp(-3)} \operatorname{sgn}(\boldsymbol{v}_t), & \|\boldsymbol{v}_t\| \leq v_0 \\ F_C \operatorname{sgn}(\boldsymbol{v}_t), & \|\boldsymbol{v}_t\| > v_0 \end{cases}$$

- Continuous and differentiable at low $\|\boldsymbol{v}\|$
- Reduces to Coulomb model at high $\|\boldsymbol{v}\|$

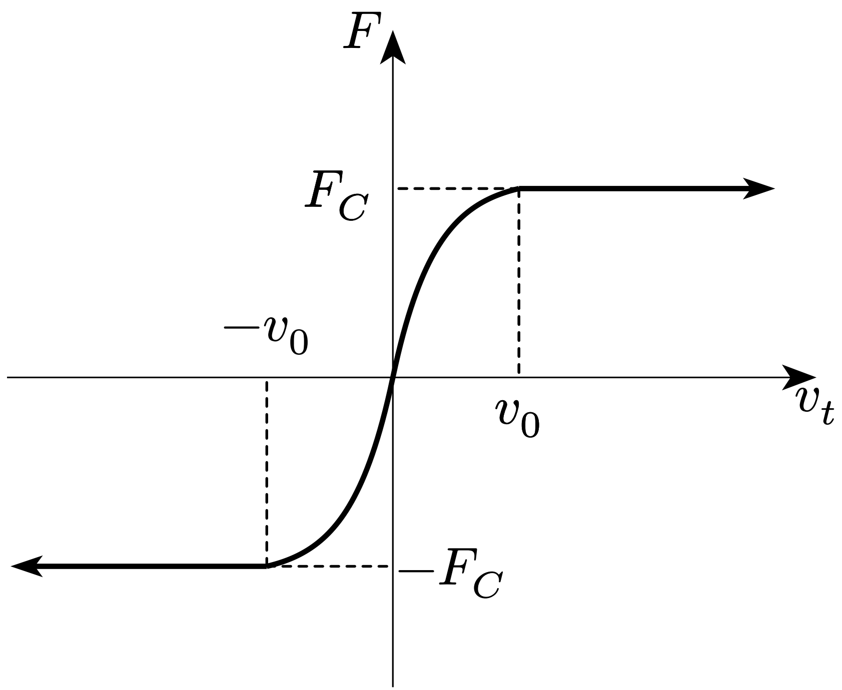


Figure 4: Threlfall friction model, 1D

4.3.1 Threlfall Friction Model

Much better than Coulomb model in some cases:

- Low velocities
- Low friction coefficients

Better emulates the behavior of lubricated contact

- Allows slip at low velocities
- Better matches experimental results

Better numerical stability

- Can use critical-point line-search
- Requires far fewer Newton iterations
- Better behavior for small time steps

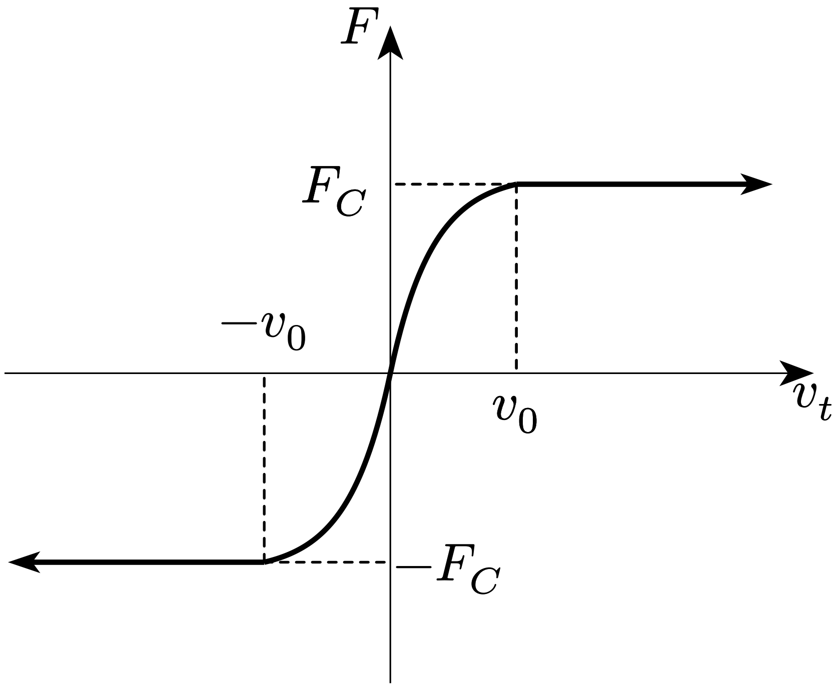


Figure 5: Threlfall friction model, 1D

4.3.2 Viscous Friction Model

Goal: Simulate lubricated contact

Let F_v be the viscous damping coefficient, then the Coulomb model with viscous damping is

$$\boldsymbol{F} = \begin{cases} F_C \operatorname{sgn}(\boldsymbol{v}_t) + F_v \boldsymbol{v}_t, & \|\boldsymbol{v}_t\| > 0 \\ \min(F_C, \|\hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}\|) \operatorname{sgn}(\hat{\boldsymbol{\sigma}}_{\boldsymbol{t}}), & \|\boldsymbol{v}_t\| = 0 \end{cases}$$

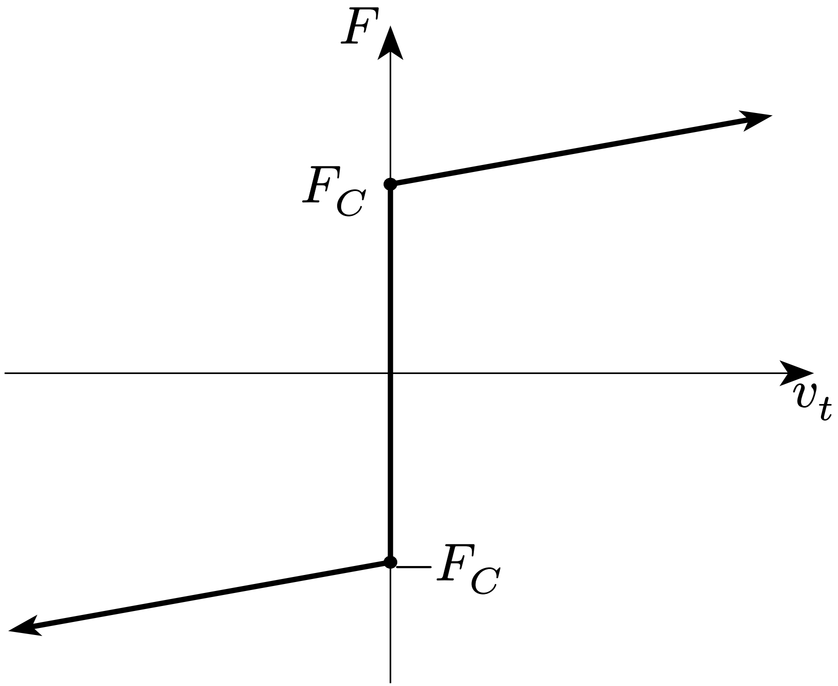


Figure 6: Coulomb with viscous friction, 1D

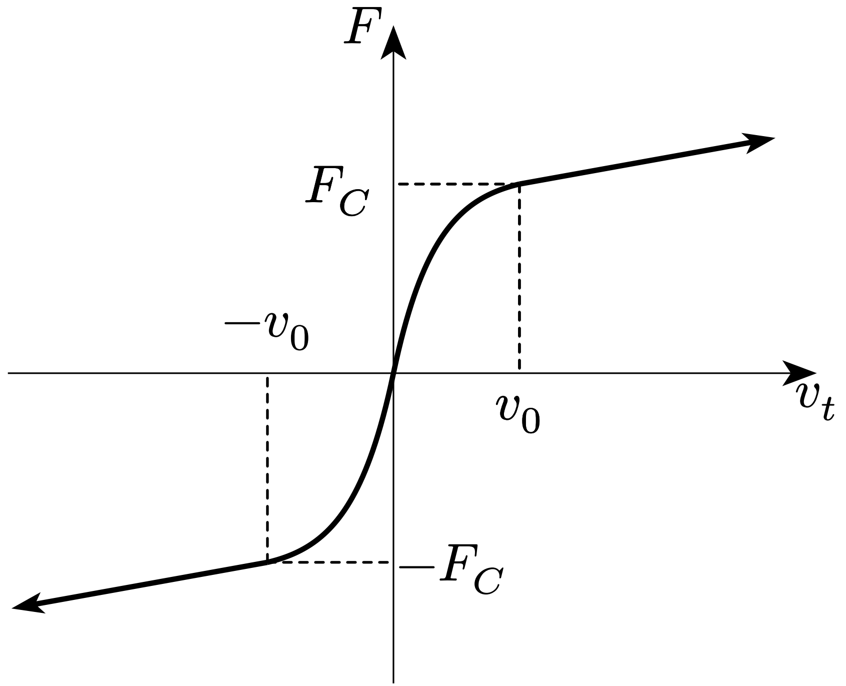


Figure 7: Threlfall with viscous friction, 1D

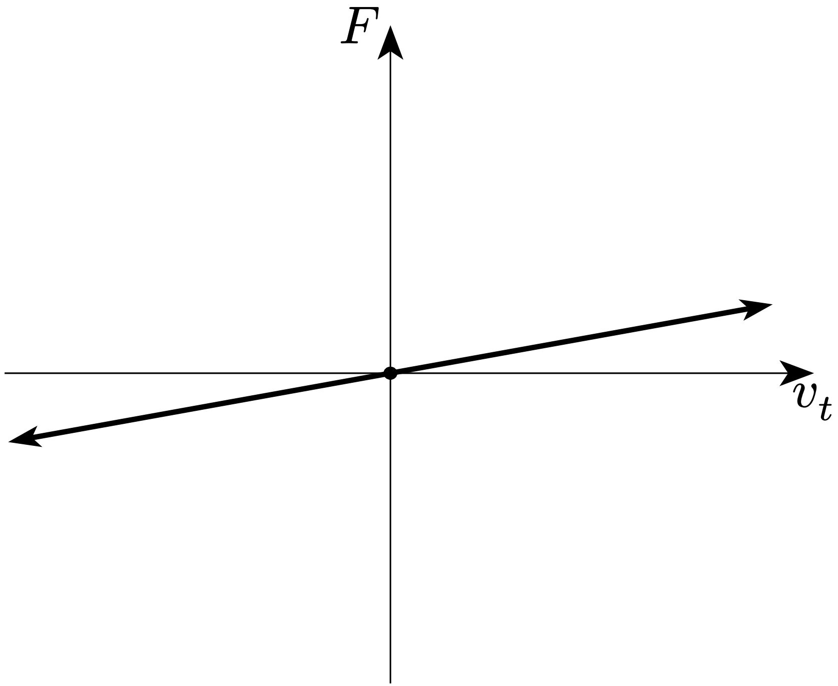


Figure 8: Pure viscous friction, 1D

4.3.2 Viscous Friction Model

Pure viscous friction works shockingly well

- Particularly for conformal contact
- Can use critical-point line-search
- Less physically accurate, but sufficient to stabilize the numerics
- Better convergence for conformal contact

Simple to implement

- No dependence on tangent surface forces

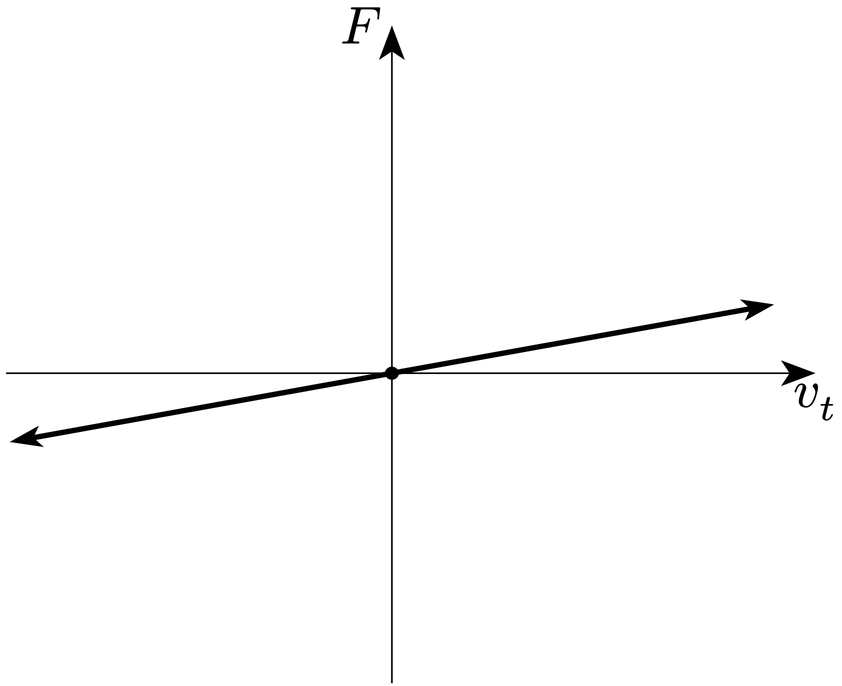
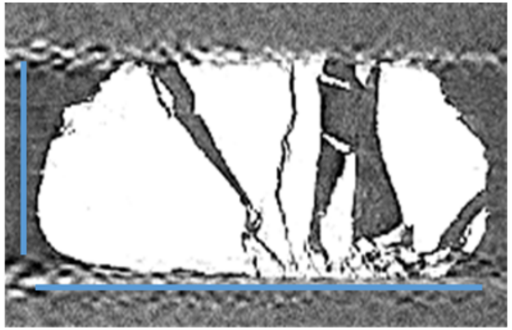


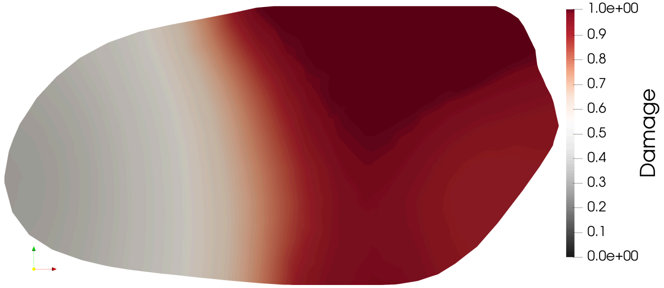
Figure 9: Pure viscous friction, 1D

Outline

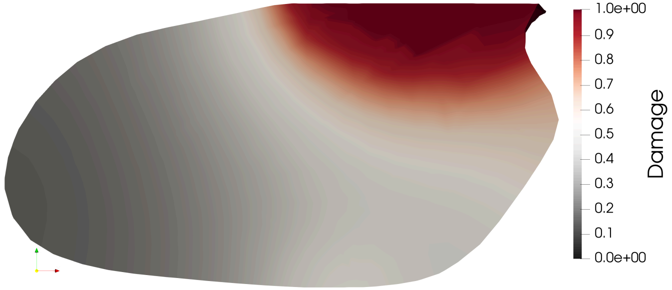
5.1 Qualitative Comparison



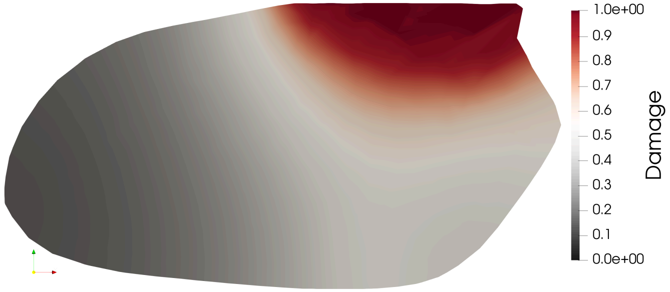
Experiment



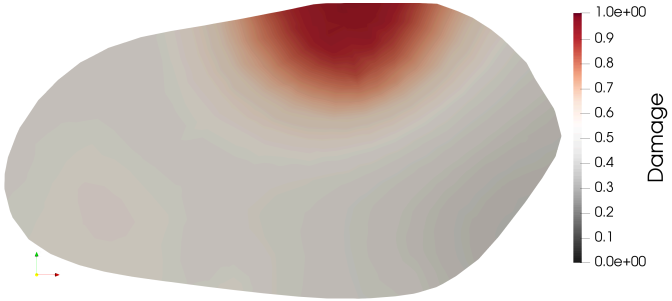
Viscous Threlfall



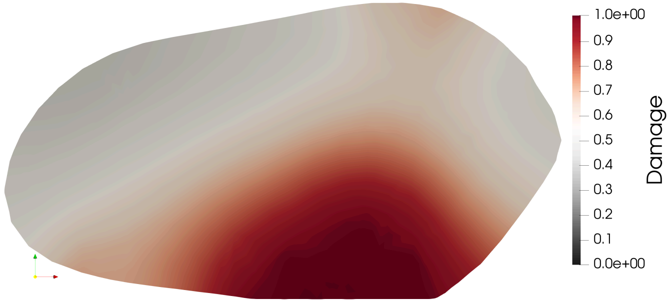
Threlfall



Viscous

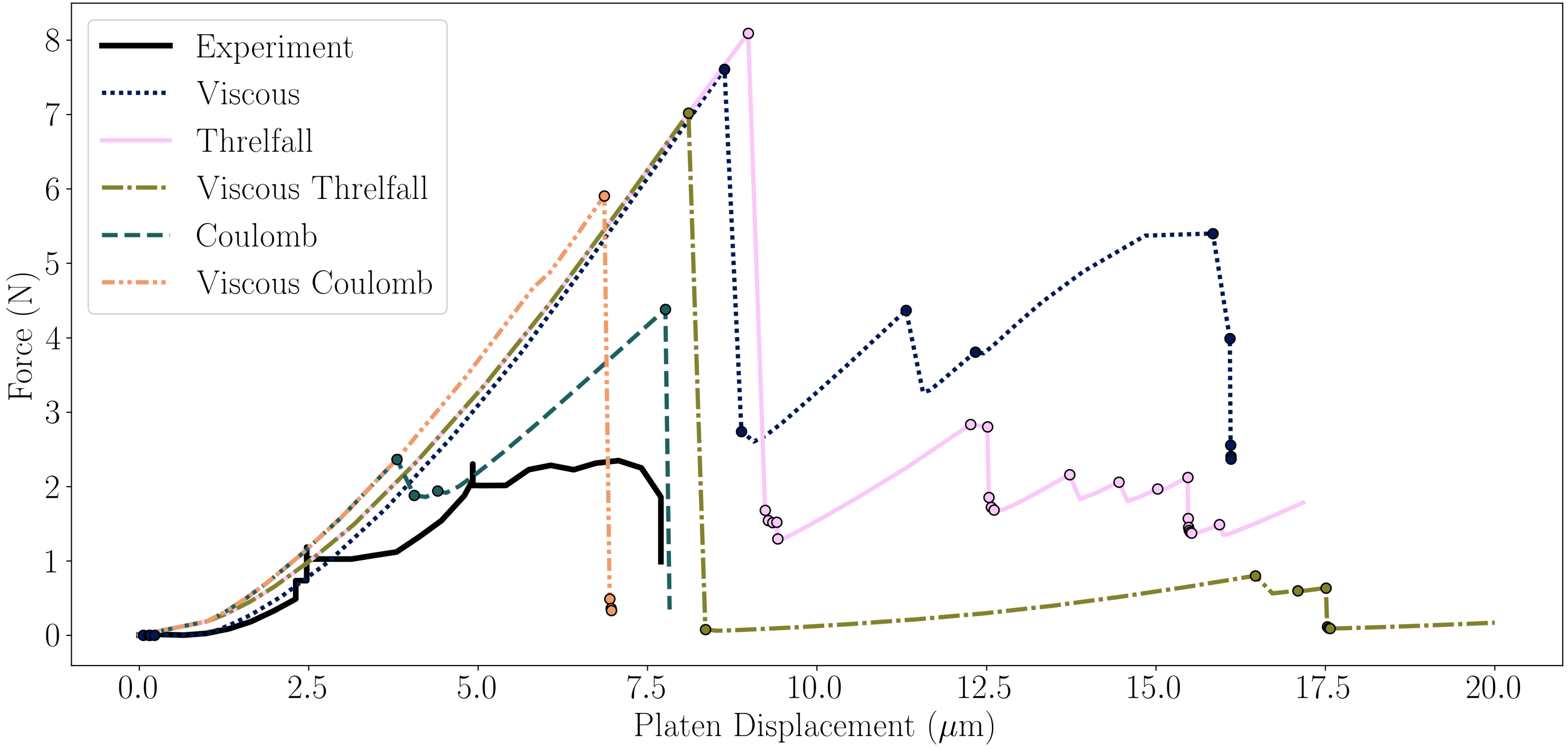


Coulomb

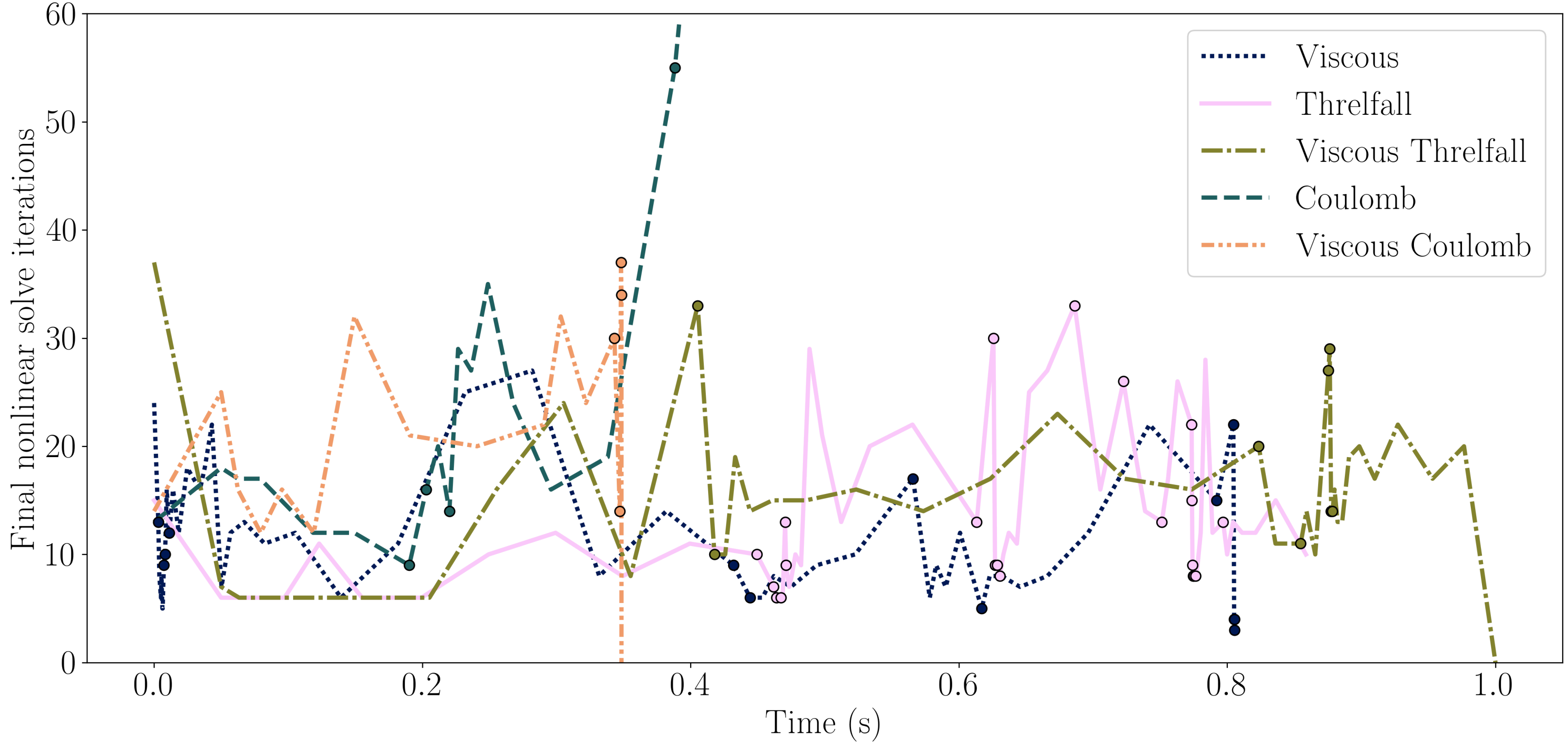


Viscous Coulomb

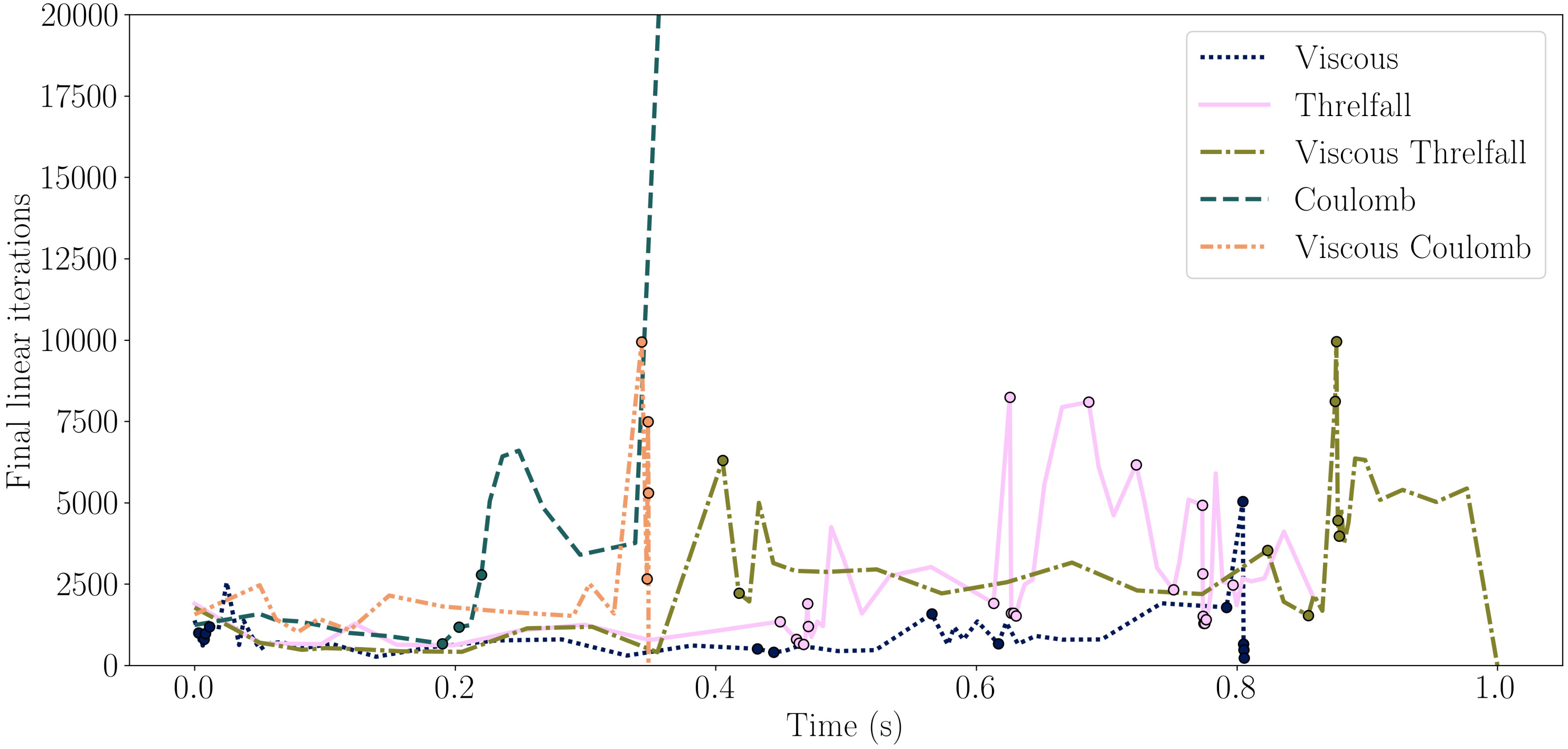
5.2 Force-Displacement Comparison



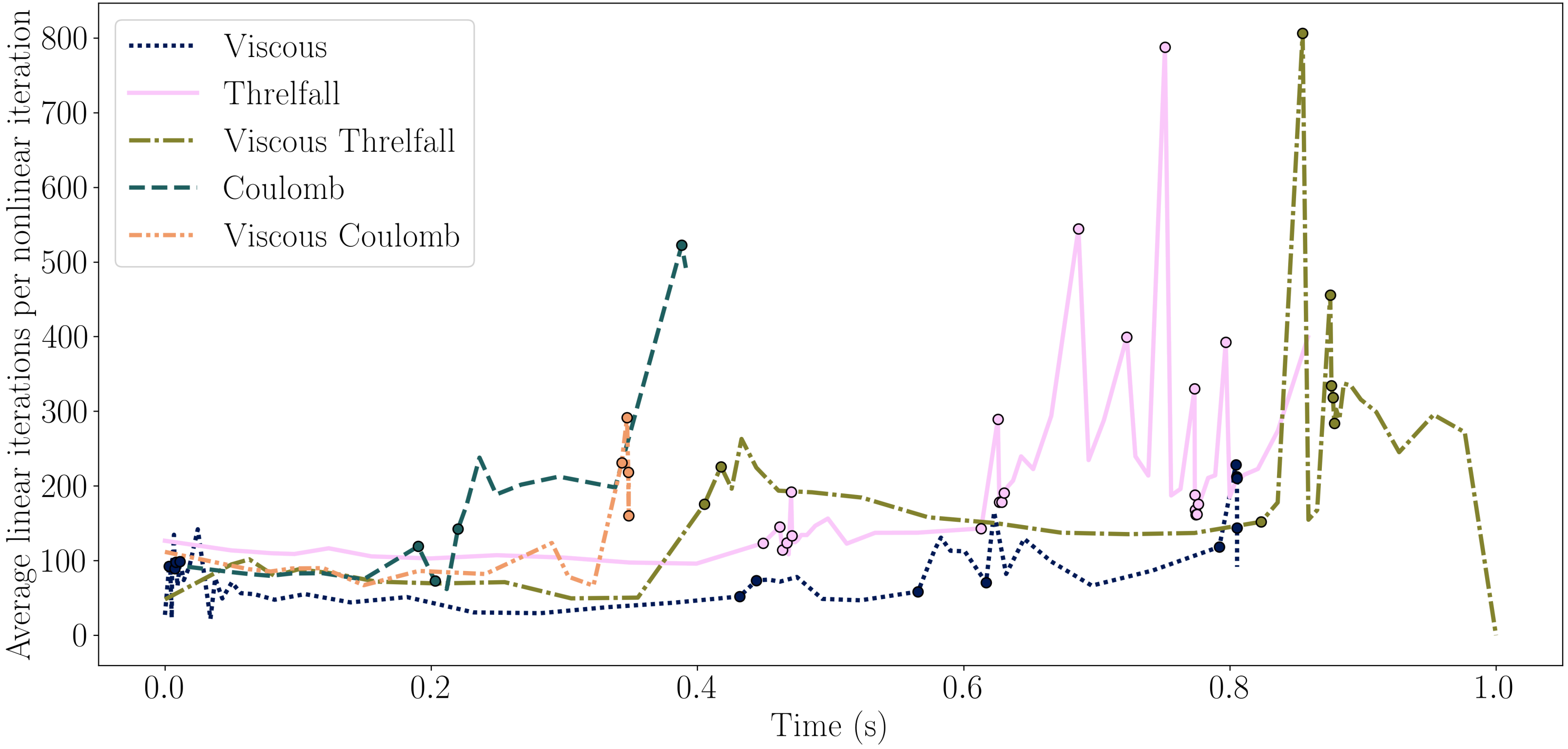
5.3.1 Nonlinear Solver Iterations



5.3.2 Linear Solver Iterations



5.3.3 Linear Solver Iterations Per Nonlinear Iteration



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