mgis.fenics Part II: Cosserat media in small deformation with mgis.fenics

T. Dancheva[(1)], U. Alonso[(2)], M. Barton[(1)], J. Bleyer[(3)], T. Hefler[(4)], R. Russo[(2)]
(1) BCAM - Basque Center for Applied Mathematics
(2) University of the Basque Country
(3) Laboratoire Navier UMR 8205 (École des Ponts ParisTech-IFSTTAR-CNRS), France
(4) CEA, DES, IRESNE, DEC, SESC, LSC, Cadarache, France

MARIE CURIE ACTIONS
EUROPEAN UNION
This project received funding from the European Union's Marie Skłodowska-Curie Actions (MSCA) Innovative Training Networks (ITN) H2020-MSCA-ITN-2017 under the grant agreement N°764979.

AGENDA

- Introduction
- Cosserat media:
  - Motivation
  - Model
  - Implementation
- Performance
- Conclusion
- Next steps

Introduction

ENABLE H2020 project

This European Training Network actively involves academics and industrial partners in training a new generation of young researchers for the future of **manufacturing**. By developing new solutions for **metallic alloys**, ENABLE proposes a complete rethink of the usual process simulation methods. Innovative **multiscale** (from microscopic to macroscopic scales), and **multi-physics** (strong thermomechanical and microstructural couplings) are addressed.

Cosserat Media - Motivation

- Development of an **Adiabatic Shear Band**
- Localization phenomena & prediction of characteristic length and size effect
- aim to regularize the model and avoid mesh dependency

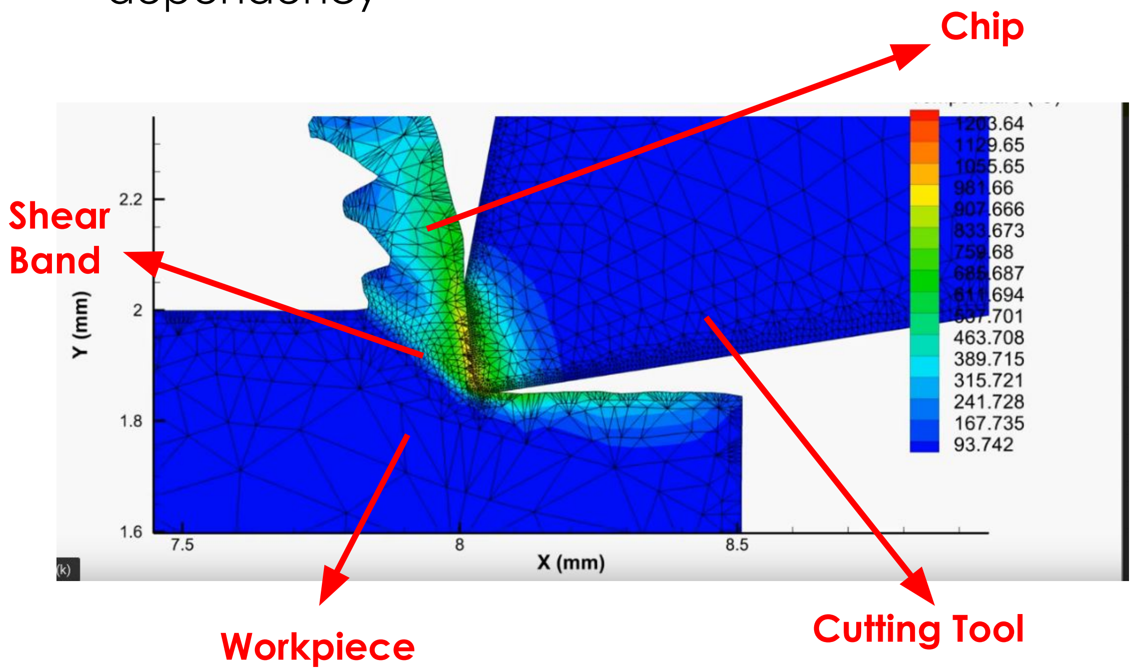


Fig.1 2D machining of Ti-6Al-4V - using Third Wave Systems AdvantEdge - Temperature

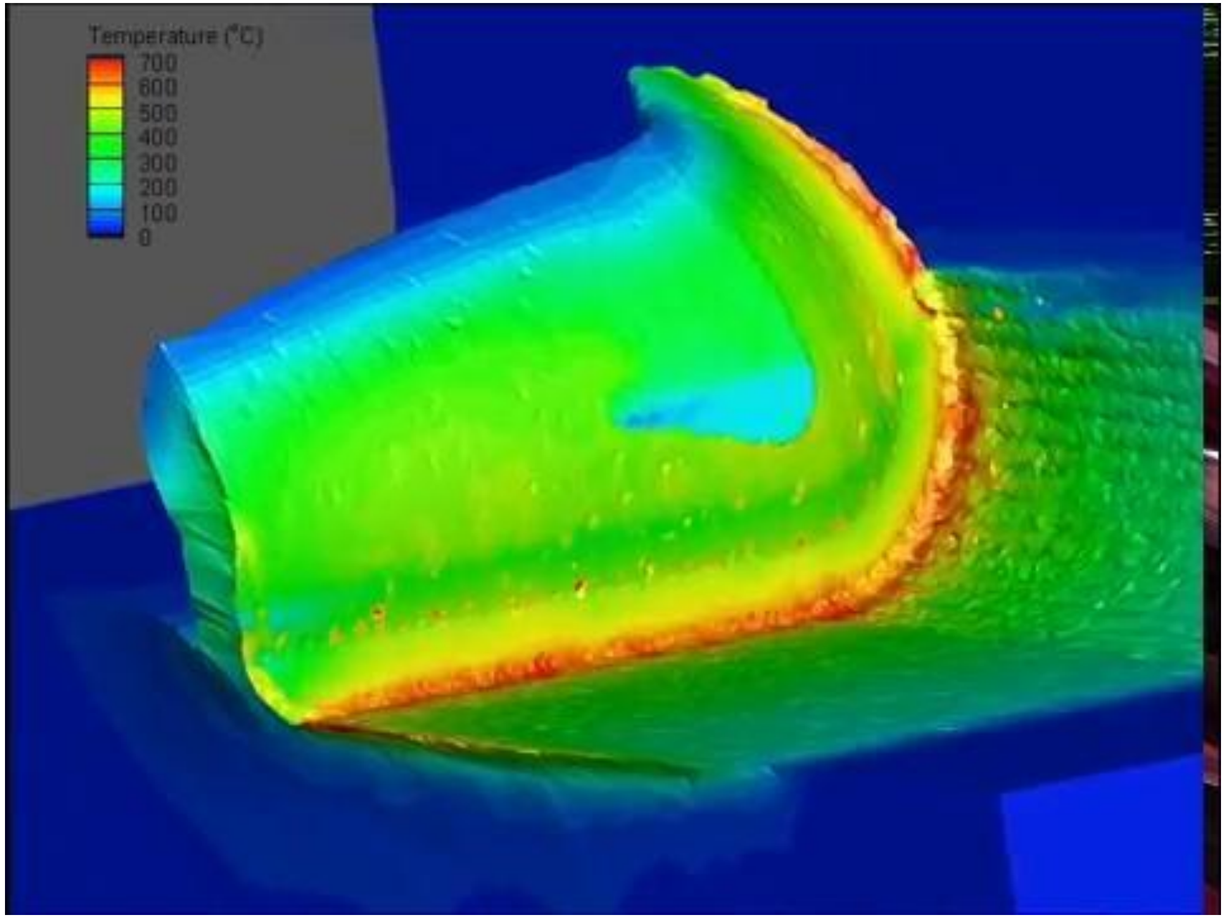


Fig.2 Chip formation during the machining of grade 316L stainless steel - using Third Wave Systems AdvantEdge - Temperature, courtesy of Sandvik Coromant

Cosserat Media in small deformation - model

- the model was initially introduced in 1909 by the Cosserat brothers [Cosserat 1909]
- Raffaele Russo has been working on formulating a thermodynamically consistent model for small deformation and large deformation [Russo et al. 2020]

Displacement — Extra degrees of freedom - the rotation of the microstructure

$$\{u_i,\, \theta_i\}, \quad i = 1,2,3$$

Deformation measures, where $\epsilon_{ijk} = \begin{cases} 1, & \text{if (i,j,k) = (1,2,3),(2,3,1) or (3,1,2);} \\ -1, & \text{if (i,j,k) = (3,2,1),(2,1,3) or (1,3,2);} \\ 0, & \text{otherwise.} \end{cases}$

$\underset{\sim}{\mathbf{e}} = \underline{\mathbf{u}} \otimes \boldsymbol{\nabla} + \underset{\sim}{\epsilon}.\underline{\boldsymbol{\theta}}$ → Cosserat deformation tensor

$\underset{\sim}{\mathbf{k}} = \underline{\boldsymbol{\theta}} \otimes \boldsymbol{\nabla}$ → Cosserat wryness tensor

Balance/equilibrium equation:

$$\int_\Omega \left(\underset{\sim}{\boldsymbol{\sigma}} : \dot{\underset{\sim}{\mathbf{e}}} + \underset{\sim}{\boldsymbol{\mu}} : \dot{\underset{\sim}{\mathbf{k}}}\right) dV = \int_\Omega \left(\underline{\mathbf{f}}.\dot{\underline{\mathbf{u}}} + \underline{\mathbf{c}}.\dot{\underline{\boldsymbol{\theta}}}\right) dV + \int_{\partial\Omega} \left(\underline{\mathbf{t}}.\dot{\underline{\mathbf{u}}} + \underline{\mathbf{m}}.\dot{\underline{\boldsymbol{\theta}}}\right) dS;$$

classical stress — couple stress — body force / couple — external surface / couple traction

Cosserat, Eugene, and François Cosserat. Theorie des corps dédormables. A. Hermann et fils, 1909.
Russo, Raffaele, Samuel Forest, and Franck Andrés Girot Mata. "Thermomechanics of Cosserat medium: modeling adiabatic shear bands in metals." Continuum Mechanics and Thermodynamics (2020): 1-20.

Cosserat Media in small deformation - model

❖ <u>Material model for elasto-plasticity</u>

From the Helmholtz free energy and the Clausius-Duhem inequality (2nd thermodynamic law) we can verify the compatibility and derive the following:

- assuming single plastic multiplier we calculate using the consistency condition and the normality rule:

$$\dot{p} = \frac{\underset{\sim}{\mathbf{n}} : \underset{\approx}{\mathbf{\Lambda}} : \underset{\sim}{\dot{\mathbf{e}}} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\dot{\mathbf{k}}}}{\dfrac{\partial A}{\partial p} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\mathbf{\Lambda}} : \underset{\sim}{\mathbf{n}} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\mathbf{n}}};$$

- Normals to the yield surface in the stress and couple stress spaces

$$\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\sigma}}} = \underset{\sim}{\mathbf{n}} = \frac{3}{2}\,\frac{a_1 \underset{\sim}{\boldsymbol{\sigma}}' + a_2 \underset{\sim}{\boldsymbol{\sigma}}'^T}{\sigma_{eq}};$$

$$\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\mu}}} = \underset{\sim}{\mathbf{n}}_c = \frac{3}{2}\,\frac{b_1 \underset{\sim}{\boldsymbol{\mu}} + b_2 \underset{\sim}{\boldsymbol{\mu}}^T}{\sigma_{eq}};$$

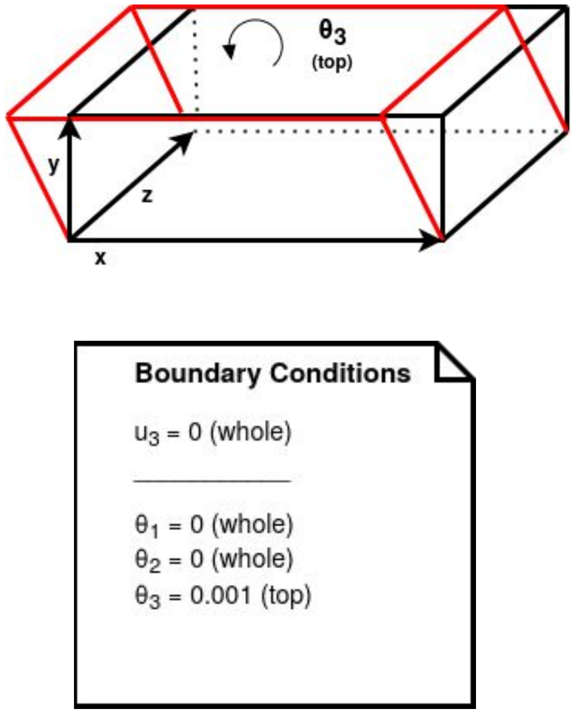
- Equivalent Stress as in [Borst 1991; Lippmann 1969; Mühlhaus and Vardoulakis 1987]

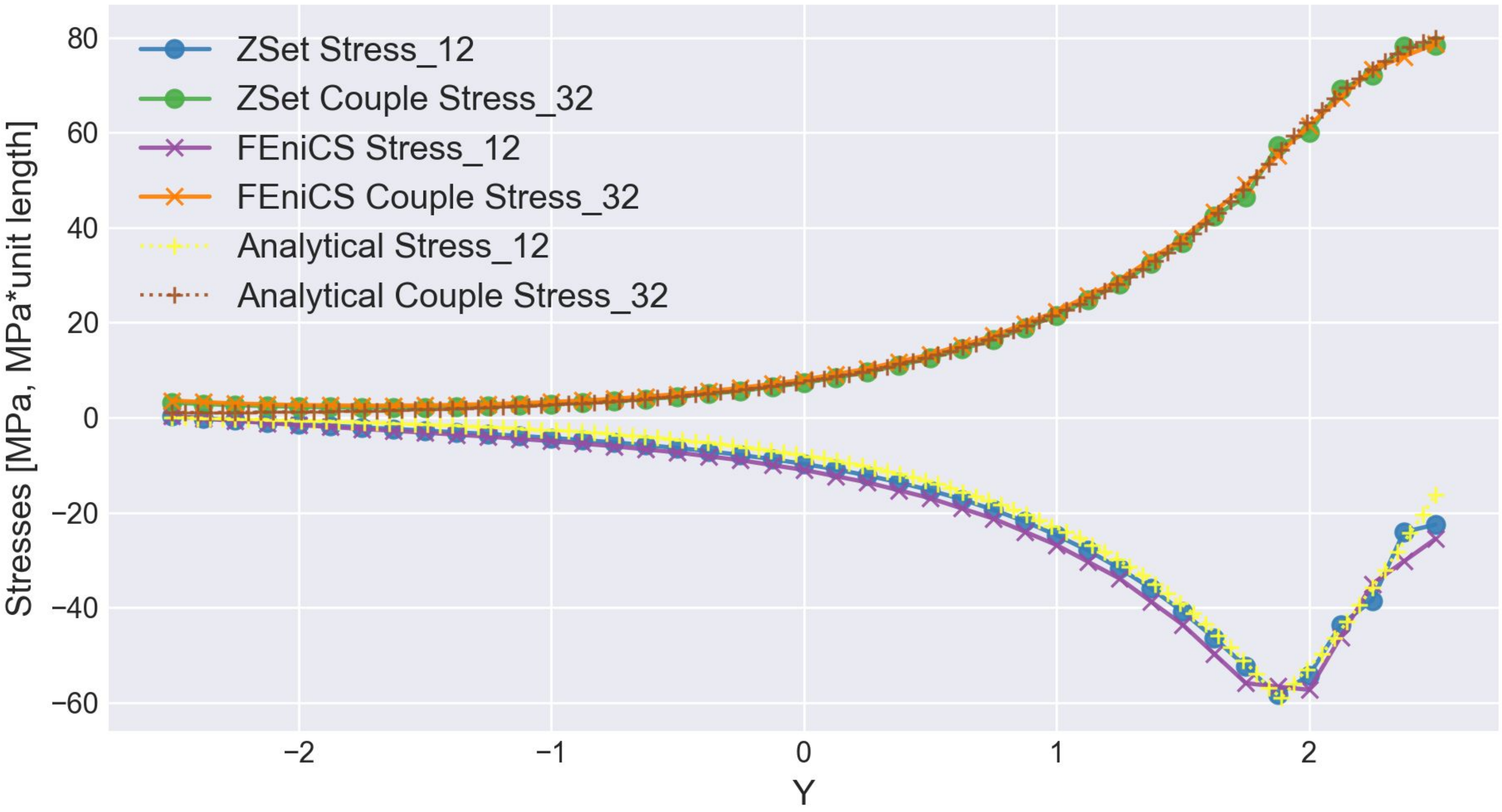
$$\sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2}\left(\mathrm{a}_1\, \underset{\sim}{\boldsymbol{\sigma}}' : \underset{\sim}{\boldsymbol{\sigma}}' + \mathrm{a}_2\, \underset{\sim}{\boldsymbol{\sigma}}' : \underset{\sim}{\boldsymbol{\sigma}}'^{\mathrm{T}} + \mathrm{b}_1\, \underset{\sim}{\boldsymbol{\mu}} : \underset{\sim}{\boldsymbol{\mu}} + \mathrm{b}_2\, \underset{\sim}{\boldsymbol{\mu}} : \underset{\sim}{\boldsymbol{\mu}}^{\mathrm{T}}\right)};$$

Characteristic length: $l_p = \sqrt{\dfrac{\mathrm{a}}{\mathrm{b}}};$

De Borst, R. E. N. É. "Simulation of strain localization: a reappraisal of the Cosserat continuum." Engineering computations (1991).
Lippmann, H. "Eine Cosserat-Theorie des plastischen Fliessens." Acta Mechanica 8.3 (1969): 255-284.
Mühlhaus, Hans-Bernd and I. Vardoulakis (1987). "The thickness of shear bands in granular". In: Géotechnique

Cosserat Media Implementation - Glide test





Iterations to converge - equilibrium:

- FEniCS: [1,1,1,1,1,1,3,7,8,8,9,10,10,11,12,13,15,16,18]
- Zset:[1,1,1,1,1,1,4,5,6,6,6,7,7,8,9,10,10,9]

Fig.3 Comparison MFront+FEniCS with ZSet and the analytical solution [S.Forest et al.]

Forest, S. and R. Sievert (Jan. 2003). "Elastoviscoplastic constitutive frameworks for generalized continua". In: Acta Mechanica 160.1-2, pp. 71–111.

Cosserat Media Implementation

Fig. 4 Explicit Implementation MFront

```
// Note @InitLocalVariables is called before @PredictionOperator and
// @TangentOperator and @Derivative, so we can define the elastic operator here
// to factorize the code a little bit
@InitLocalVariables {
  ∂σ/∂Δeto = lambda * t2tot2<N, real>::IxI() +
             (mu + mu_c) * t2tot2<N, real>::Id() +
             (mu - mu_c) * t2tot2<N, real>::transpose_derivative();
  ∂μₖ/∂Δκ = alpha * t2tot2<N, real>::IxI() +
            (beta + gamma) * t2tot2<N, real>::Id() +
            (beta - gamma) * t2tot2<N, real>::transpose_derivative();
}

@ComputeThermodynamicForces {
  σ = lambda * trace(εᵉˡ) * Tensor::Id() + 2 * mu * syme(εᵉˡ) +
      mu_c * (εᵉˡ - transpose(εᵉˡ));
  μₖ = alpha * trace(κᵉˡ) * Tensor::Id() + 2 * beta * syme(κᵉˡ) +
      gamma * (κᵉˡ - transpose(κᵉˡ));
}
```

$$\underset{\sim}{\Lambda} = \begin{bmatrix} (\lambda+2\mu) & \lambda & \lambda & & & & & & \\ \lambda & (\lambda+2\mu) & \lambda & & & & & & \\ \lambda & \lambda & (\lambda+2\mu) & & & & & & \\ & & & (\mu+\mu_c) & (\mu-\mu_c) & & & & \\ & & & (\mu+\mu_c) & (\mu-\mu_c) & & & & \\ & & & & & (\mu+\mu_c) & (\mu-\mu_c) & & \\ & & & & & (\mu+\mu_c) & (\mu-\mu_c) & & \\ & & & & & & & (\mu+\mu_c) & (\mu-\mu_c) \\ & & & & & & & (\mu+\mu_c) & (\mu-\mu_c) \end{bmatrix}$$

$$\underset{\sim}{C} = \begin{bmatrix} (\alpha+2\beta) & \alpha & \alpha & & & & & & \\ \alpha & (\alpha+2\beta) & \alpha & & & & & & \\ \alpha & \alpha & (\alpha+2\beta) & & & & & & \\ & & & (\beta+\gamma) & (\beta-\gamma) & & & & \\ & & & (\beta+\gamma) & (\beta-\gamma) & & & & \\ & & & & & (\beta+\gamma) & (\beta-\gamma) & & \\ & & & & & (\beta+\gamma) & (\beta-\gamma) & & \\ & & & & & & & (\beta+\gamma) & (\beta-\gamma) \\ & & & & & & & (\beta+\gamma) & (\beta-\gamma) \end{bmatrix}$$

$$\underset{\sim}{\sigma} = \lambda \,\mathrm{trace}\left(\underset{\sim}{e}^{e}\right) \underset{\sim}{I} + 2\mu \left(\underset{\sim}{e}^{e}\right)^{sym} + 2\mu_c \left(\underset{\sim}{e}^{e}\right)^{skew}$$

$$\underset{\sim}{\mu} = \alpha \,\mathrm{trace}\left(\underset{\sim}{k}\right) \underset{\sim}{I} + 2\beta \left(\underset{\sim}{k}^{e}\right)^{sym} + 2\gamma \left(\underset{\sim}{k}^{e}\right)^{skew}$$

Fig.4 .mfront file for the Cosserat glide test

Cosserat Media Implementation

Fig. 5 Explicit Implementation MFront

```
@Derivative {
  const auto se = 2 * mu * deviator(syme(εᵉˡ)) + mu_c * (εᵉˡ - transpose(εᵉˡ));
  const auto seq = sqrt(3 * (a_1 * (se | se) + a_2 * (se | transpose(se)) +
                             b_1 * (μₖ | μₖ) + b_2 * (μₖ | transpose(μₖ))) /
                        2);
  dₜεᵉˡ = dₜeto;
  dₜκᵉˡ = dₜκ;
  if (seq - R0 - H * p > 0) {
    const auto n = eval(3 * (a_1 * se + a_2 * transpose(se)) / (2 * seq));
    const auto n_c = eval(3 * (b_1 * μₖ + b_2 * transpose(μₖ)) / (2 * seq));
    const auto cste = 1 / (H + (n |∂σ/∂Δeto | n) + (n_c |∂μₖ/∂Δκ | n_c));
    dₜp = ((n |∂σ/∂Δeto | dₜeto) + (n_c |∂μₖ/∂Δκ | dₜκ)) * cste;
    dₜεᵉˡ -= dₜp * n;
    dₜκᵉˡ -= dₜp * n_c;
  }
}
```

$$\sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2}\left(\mathrm{a}_1\, \underset{\sim}{\boldsymbol{\sigma}}' : \underset{\sim}{\boldsymbol{\sigma}}' + \mathrm{a}_2\, \underset{\sim}{\boldsymbol{\sigma}}' : \underset{\sim}{\boldsymbol{\sigma}}'^{\mathrm{T}} + \mathrm{b}_1\, \underset{\sim}{\boldsymbol{\mu}} : \underset{\sim}{\boldsymbol{\mu}} + \mathrm{b}_2\, \underset{\sim}{\boldsymbol{\mu}} : \underset{\sim}{\boldsymbol{\mu}}^{\mathrm{T}}\right)};$$

$$\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\sigma}}} = \underset{\sim}{\mathbf{n}} = \frac{3}{2}\, \frac{a_1 \underset{\sim}{\boldsymbol{\sigma}}' + a_2 \underset{\sim}{\boldsymbol{\sigma}}'^{T}}{\sigma_{eq}};$$

$$\frac{\partial f}{\partial \underset{\sim}{\boldsymbol{\mu}}} = \underset{\sim}{\mathbf{n}}_c = \frac{3}{2}\, \frac{b_1 \underset{\sim}{\boldsymbol{\mu}} + b_2 \underset{\sim}{\boldsymbol{\mu}}^{T}}{\sigma_{eq}};$$

$$\dot{p} = \frac{\underset{\sim}{\mathbf{n}} : \underset{\approx}{\boldsymbol{\Lambda}} : \dot{\underset{\sim}{\mathbf{e}}} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\mathbf{C}} : \dot{\underset{\sim}{\mathbf{k}}}}{\dfrac{\partial A}{\partial p} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\boldsymbol{\Lambda}} : \underset{\sim}{\mathbf{n}} + \underset{\sim}{\mathbf{n}}_c : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\mathbf{n}}};$$

Fig.5 .mfront file for the Cosserat glide test - continuation

Optimization: converting to an implicit implementation

Cosserat Media Implementation

FEniCS + MFront

Zset

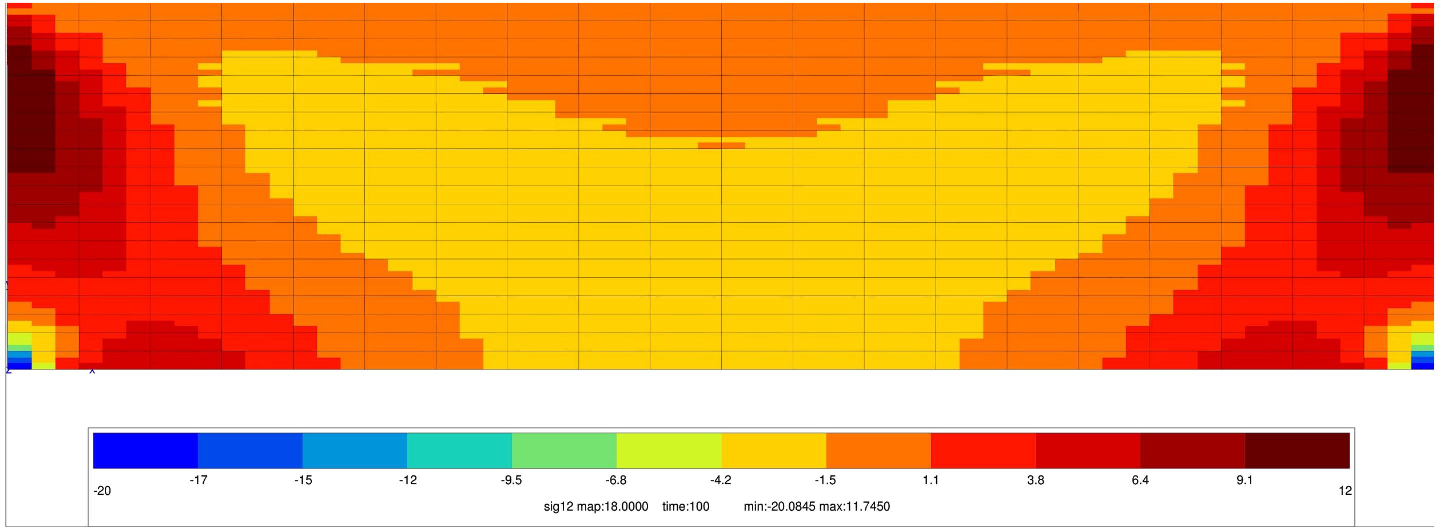


Fig.6
Glide test - Result for the stress, σ_{12}

Cosserat Media Implementation

FEniCS + MFront

Zset

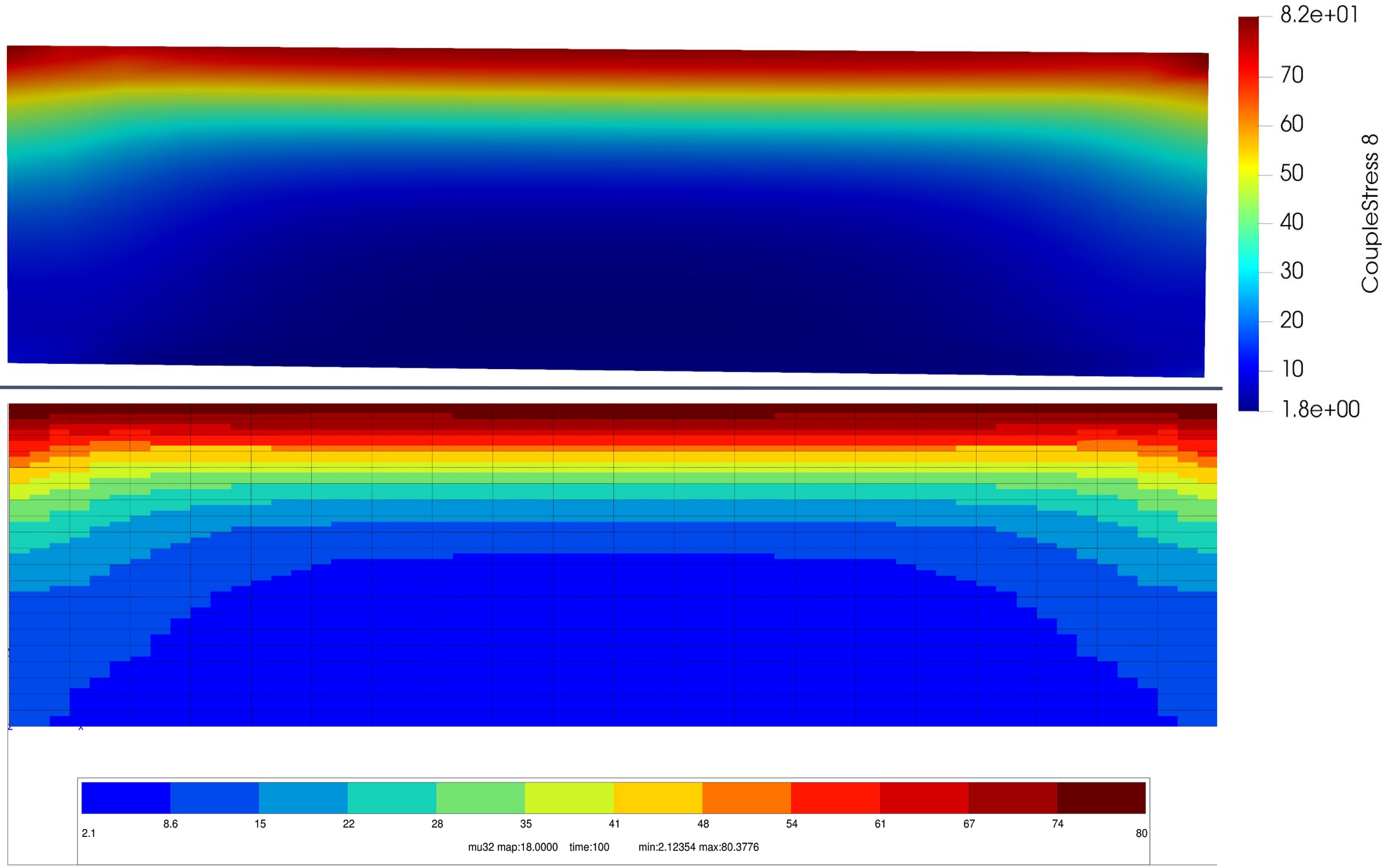


Fig.7
Glide test - Result for the couple stress, μ_{32}

Performance

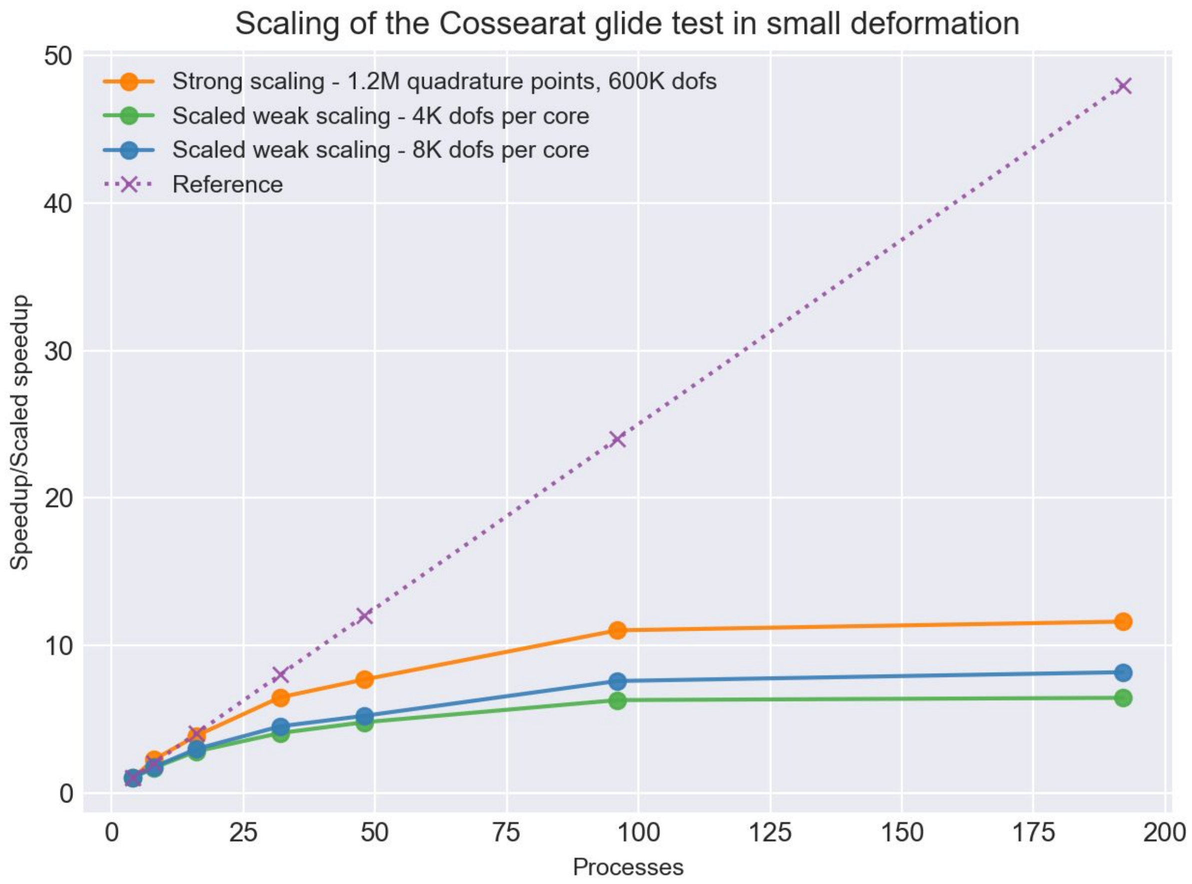


Fig.8 Strong and weak scaling plot for the glide test

ATLAS EDR @ Donostia International Physics Center

- Infiniband EDR network
- 37 nodes with Intel Xeon Platinum 8168 (24 cores per node x 2 threads)
- 8 nodes with Intel Xeon Platinum 8280 (28 cores per node x 2 threads)
- 2x NVIDIA Tesla P40, 1x NVIDIA Tesla P40

Current setup:

- using Singularity container
- using MPICH using the UCX network framework

Conclusions

- From the profiling and scaling results we can conclude that the major bottleneck is the resolution of the system of nonlinear equations (quasi Newton line search) using MUMPS as a linear solver

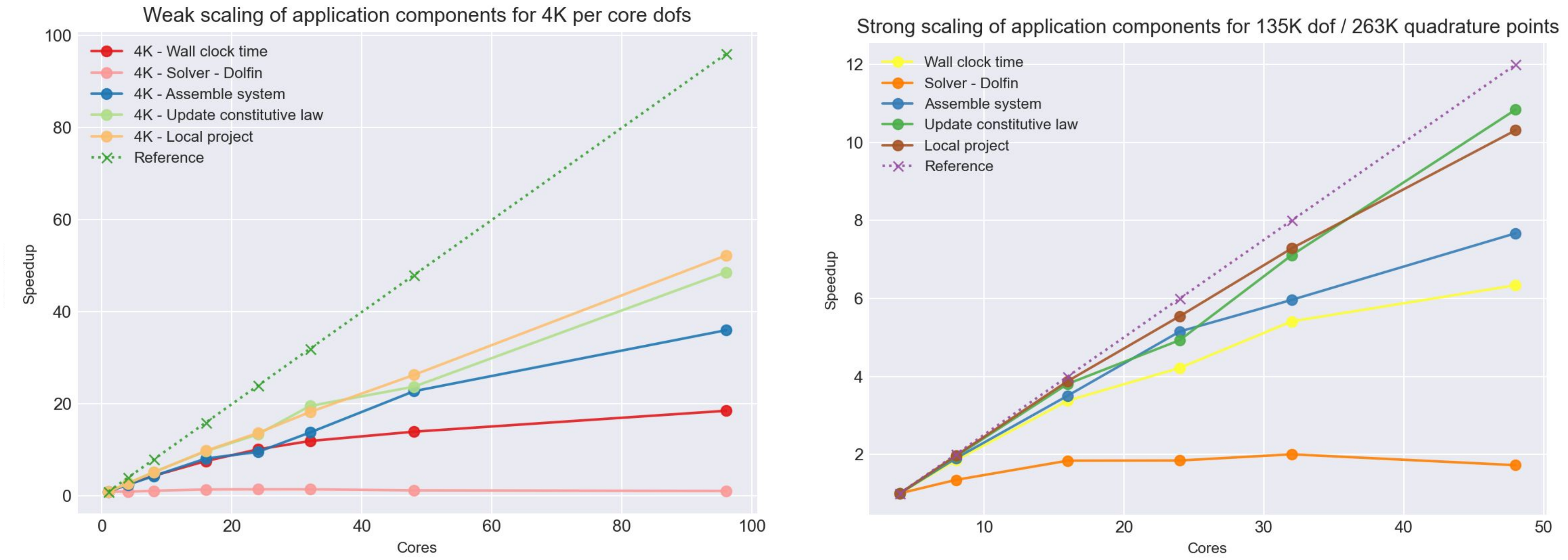


Fig.9 Strong and weak scaling plot for various routines part of the simulation

Next steps

- Increase problem size
- Native installation of the software stack on ATLAS-EDR
- Profiling with EXTRAE for MPI statistics, DCRAB for node statistics
- Exploring other linear solvers (and nonlinear)
- Implicit scheme implementation
- Porting to dolfin-x
- Further HPC analysis and code optimizations
- Implementation of the full thermodynamically consistent Cosserat model in Large deformation - elasto viscoplasticity

Questions

Thank you for your attention!