Plasticity and Strain Localisation in the Crust and Lithosphere Models Numerical Aspects

> LAETITIA LE POURHIET ISTEP UPMC PARIS LUCKY 13<sup>TH</sup> CONFERENCE NORWAY

Many thanks to Davidave Mayhem, Joel Frelat, Petsc and my lappy ③

## Typical crust lithosphere problem

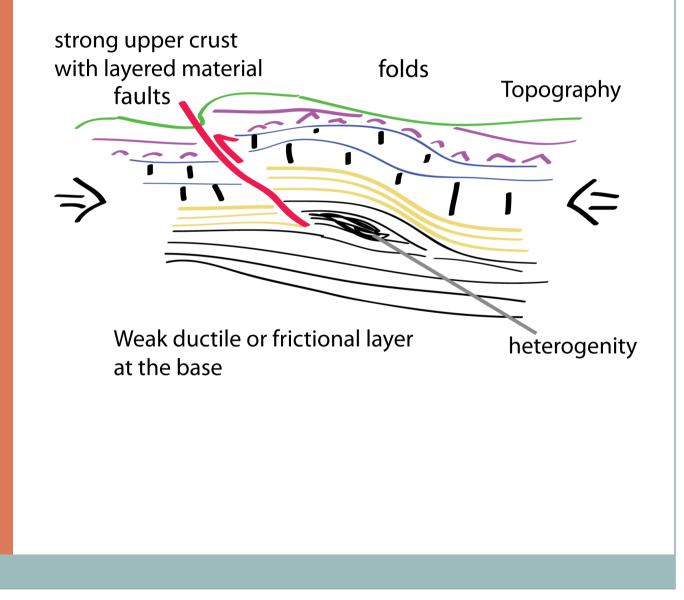
Driven by boundary conditions and mechanical heterogeneities

Weak density contrast

Weak influence of gravity

Large average strength

Length scale of the order of 10's to few 100's km



### Outline ...

What is a long term tectonic fault ?

How we model them in long term tectonics

What are the many and main issues with our model

Clues... new ways ... other approaches... possible solutions.. In one word what's next ? strong upper crust with layered material folds Topography experimentation of the second secon

Today I'll focus on faults....

With faults it is all a matter of scale, long term tectonic faults are faults that are plotted on regional scale maps

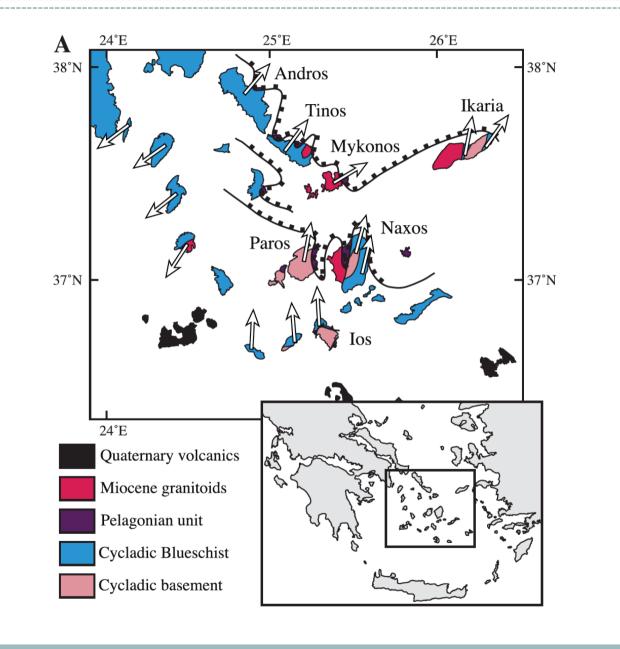
These faults are not straight line infinitely thin...

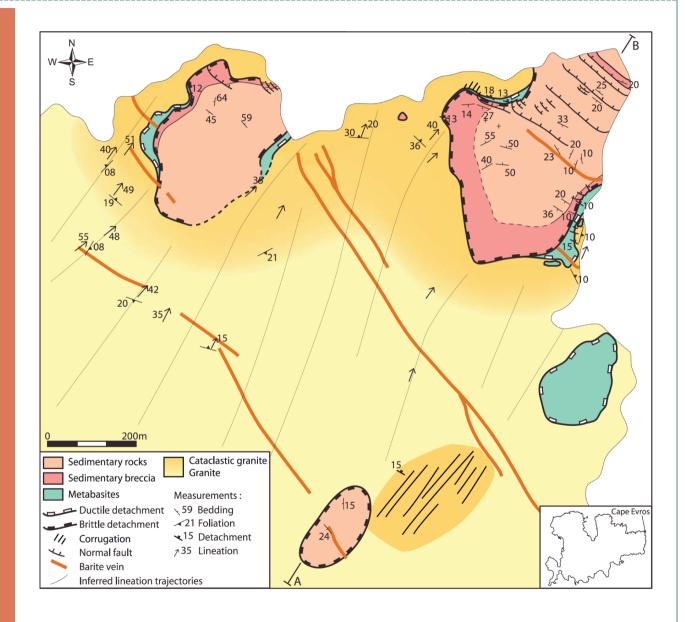
They are networks of 2-3 meter thick cataclasites and most of the time these objects are 100m to 20 km wide.

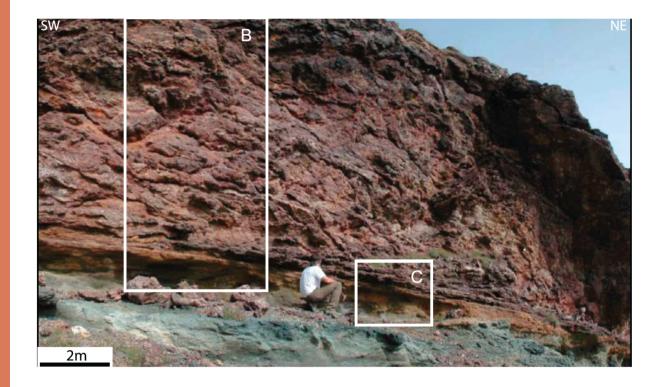
Slip planes are indeed thin but slip planes are not long term faults, they are events... that occur at much smaller time scale than our time steps ! • Some times it is good to put a scale ...

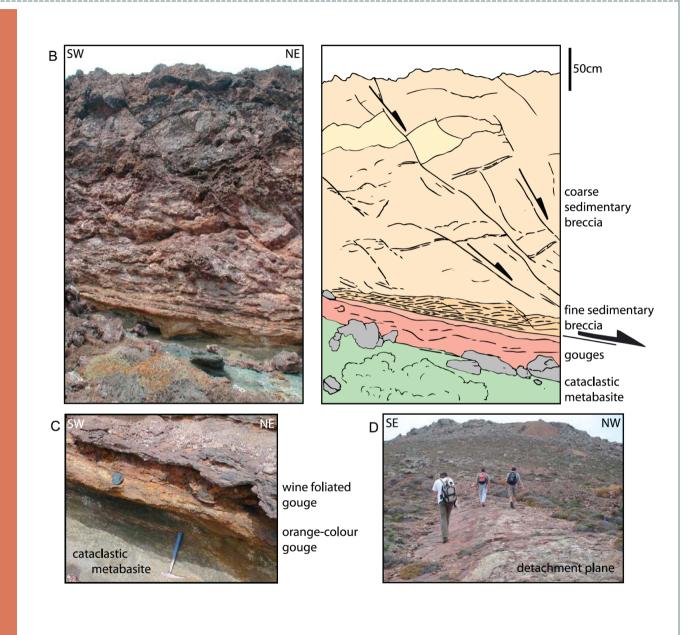
Long term tectonic considers: Time scales that span from couple of Myr to 100's Length scales that span from 10's to 1000 km

So lets go to one of my favourite play ground....

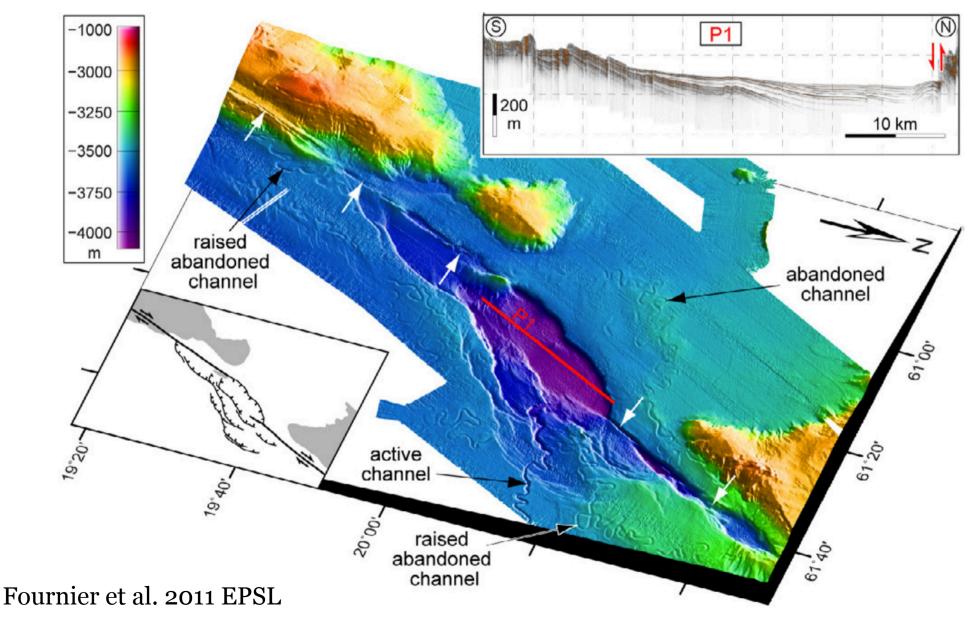








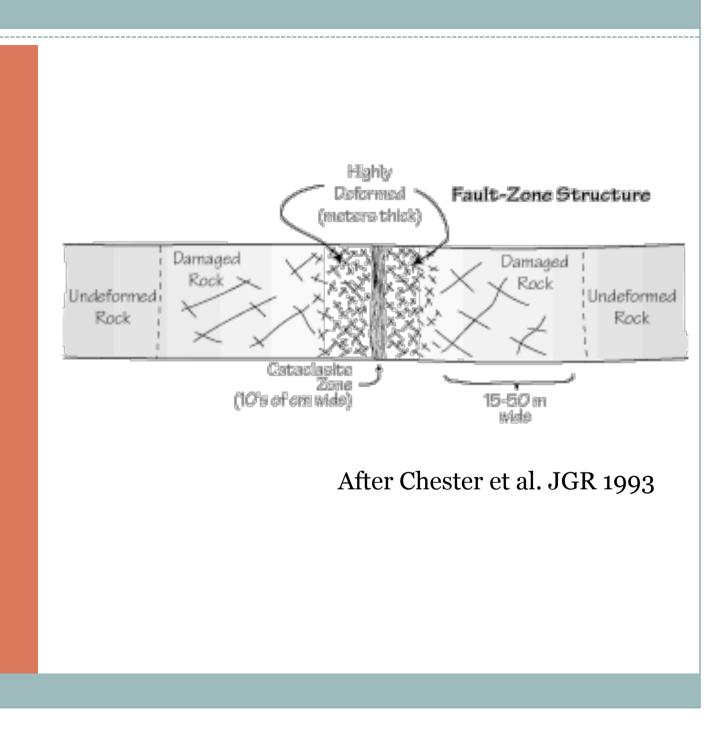
# One can also observe long term structures in the bathymetry ...



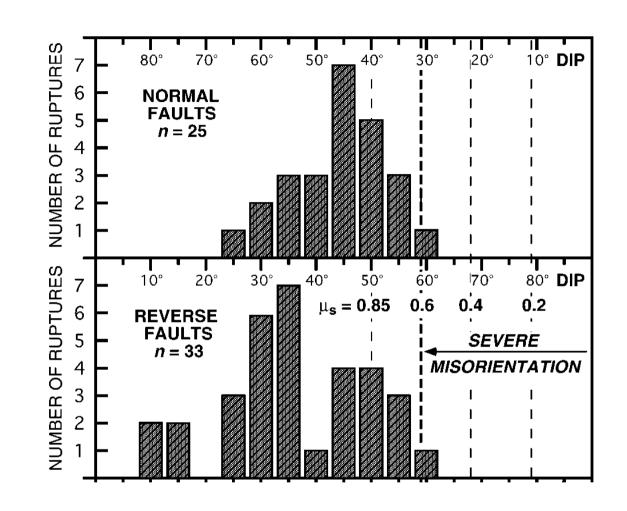
# Or simply in the "real" topography



DEM with J. Saleeby interpreations



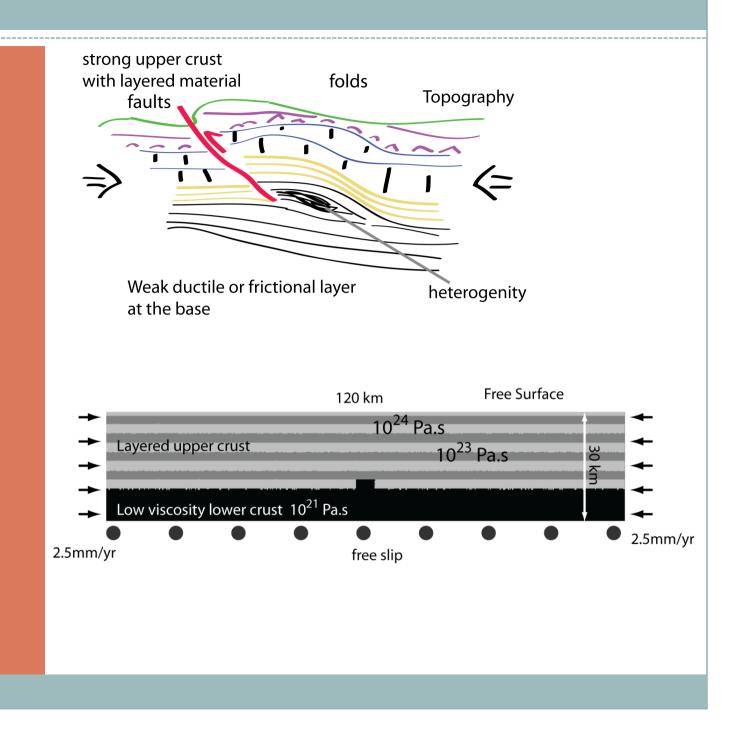
#### What is the orientation of a fault



• What is missing here are the strike slip faults, because they would all probably be severely misoriented.

Colletini 2001 Geology

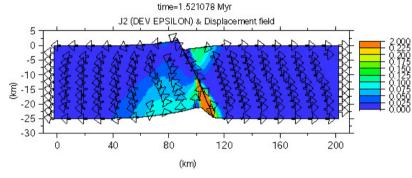
Modeler view of this problem



## Solid Earth: The elastic approach

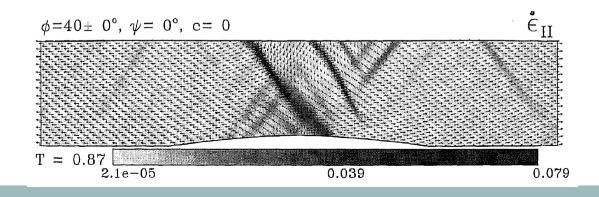
Fractured mechanic approach was find to be very hard to implement for large strain and is now no longer used by the long term tectonic community, however, it is used in code like Pylith (CIG) or Adeli (J. Chéry and R. Hassani) to study earth at the scale of several earth quake cycles.

## The choice Are you o a fractured mechanics person



#### or

#### • a continuum mechanics person Strain rate 2nd Invariant



#### How we model faults in long term tectonics

#### Initiation of salt diapirs with frictional overburdens: numerical experiments

A.N.B. Poliakov <sup>a,b</sup>, Yu. Podladchikov <sup>b</sup> and C. Talbot <sup>b</sup> <sup>a</sup> HLRZ, KFA-Jülich, Postfach 1913, D-5170 Jülich, Germany

<sup>b</sup> Hans Ramberg Tectonic Laboratory, Institute of Earth Sciences, Uppsala University, S-752 36 Uppsala, Sweden (Received July 8, 1993; revised version accepted July 8, 1993) ----- (1

The orientation of shear bands in Coulomb materials with non-associated flow rule is still not well understood. Theories, experiments and numerical simulations give different values for  $\theta$ , the inclination angle subtended by a shear band and the major compressive stress. There are two end-member solutions for shear band inclinations:

$$=\frac{\pi}{4}-\frac{\phi}{2}\tag{1}$$

and:

$$=\frac{\pi}{4} - \frac{\psi}{2} \tag{2}$$

where  $\phi$  and  $\psi$  are the friction and dilation angles, respectively. Eqn. (1) was derived by Coulomb in 1776 and eqn. (2) was obtained by Roscoe (1970).

Attempts to prove either of the results have not been successful because there is experimental evidence for both the Coulomb and the Roscoe orientations. Vermeer (1990) showed that orientation of shear bands may depend on the grain size of granular material and that Coulomb-type shear bands occur in fine sands, whereas Roscoe-type shear bands are observed in coarse materials. Arthur et al. (1977) and Vardoulakis (1980) each reported experimental evidence for an intermediate orientation of shear bands:

$$=\frac{\pi}{4} - \frac{\phi + \psi}{4} \tag{3}$$

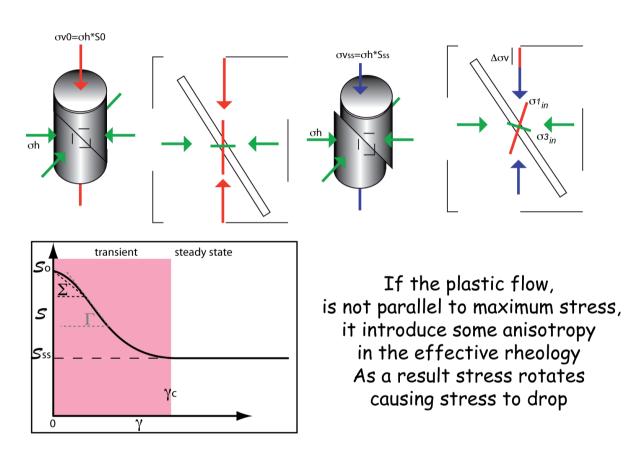
A theoretical explanation of this observation was given by Vermeer (1982). Later, Vermeer (1990) analysed the post-bifuricational behaviour of frictional material, allowing it to unload elastically outside of the shear band. He found that that there is a wide range of admissible orientations of shear bands in between the two limits (1) and (2).

Systematical numerical experiments on shear band inclinations in a compressional uniaxial test were carried out by Hobbs and Ord (1989) using a FLAC program. They obtained a broad range of shear band inclinations, not predicted by eqns. (1), (2), or (3). However, they demonstrated that the angle  $\theta$  decreases, as both  $\phi$  and  $\psi$  increase.

The scattering of inclination angles in experiments may be due to friction at the end platens, which can delay the inception of a shear band (Vermeer and De Borst, 1984) or produce kinking (Dawson, 1993). In numerical experiments, a similar effect can occur due to the finite size of a model (i.e. influence of boundaries) which affects the inclination angles.

For these reasons, we do not expect to find unique shear band orientation. It is more instructive to study relative changes in shear orientation, rather than absolute values.

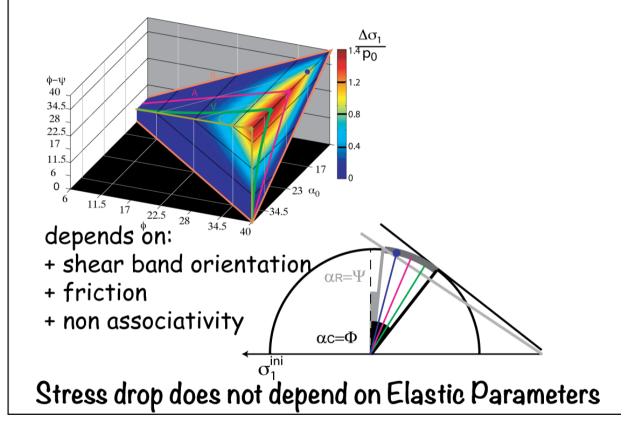
Non associated flow rule and so called structural softening as used in long term tectonics community follows more or less Vermeer 1990 paper (14 pages)



Vermeer 1990 géotechnique, Le Pourhiet 2013 BSGF

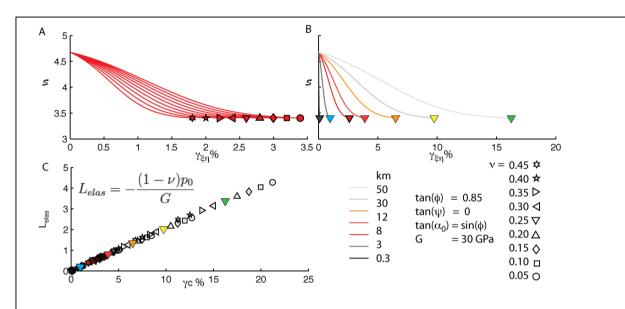
Non associated flow rule and so called structural softening predicts that a wide range of orientation are acceptable...

#### Stress drop is obtained analytically



Vermeer 1990 géotechnique, Le Pourhiet 2013 BSGF

Characteristic elastic strain during the transient is very small



Critical strain depends almost linearly on elastic Parameters Considering a fault at 12 km depth full softening is obtained for: - 25 cm of slip for a 10 m thick gouge - 2.5mm of dlip for a 10cm thick gouge

#### Le Pourhiet 2013 BSGF

## How we model faults in long term tectonics

Much Later when I was a phd student...

People started to compare numerical code for plasticity problem... Geological Society, London, Special Publications

# The numerical sandbox: comparison of model results for a shortening and an extension experiment

Susanne J. H. Buiter, Andrey Yu. Babeyko, Susan Ellis, Taras V. Gerya, Boris J. P. Kaus, Antje Kellner, Guido Schreurs and Yasuhiro Yamada

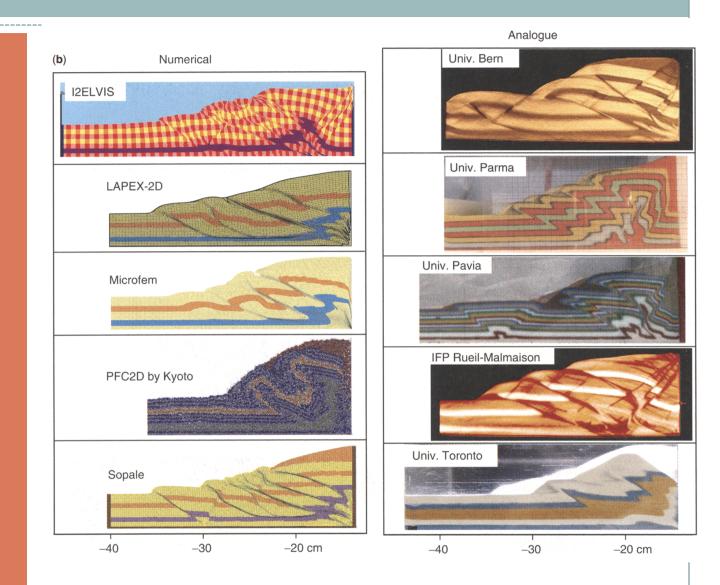
*Geological Society, London, Special Publications* 2006, v.253; p29-64. doi: 10.1144/GSL.SP.2006.253.01.02

## How we model faults in long term tectonics

Much Later when I was a phd student...

People started to compare numerical code for plasticity problem...

AND GOT REALLY SCARED



And the forbidden question re-emerged ... What is the correct orientation for shear band ...

## Visco – Plastic approach

Since the residual stress does only depends on shear band orientation

And

The elastic strain is small

It is possible to find an effective viscosity that reach a similar orientation instantaneously.

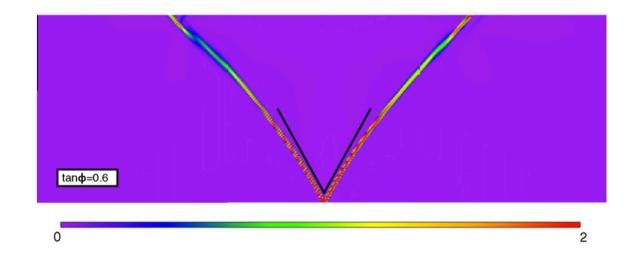
# Physics of the Earth and Planetary Interiors 171 (2008) 177–186 Contents lists available at ScienceDirect Physics of the Earth and Planetary Interiors journal homepage: www.elsevier.com/locate/pepi

Shear banding analysis of plastic models formulated for incompressible viscous flows

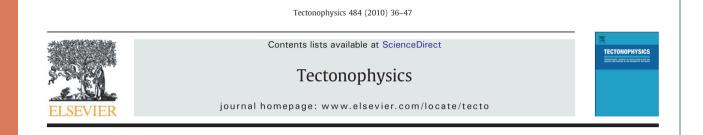
V. Lemiale<sup>a,\*</sup>, H.-B. Mühlhaus<sup>b</sup>, L. Moresi<sup>a</sup>, J. Stafford<sup>a</sup>

<sup>a</sup> School of Mathematical Sciences, Monash University, Melbourne, Victoria, 3800, Australia
<sup>b</sup> Earth Systems Science Computational Centre (ESSCC) The University of Queensland, St. Lucia, QLD 4072, Australia

$$\eta_{\rm eff}^{I} = \eta \frac{3\alpha p^{I} + k}{\bar{\tau}^{\upsilon, I}} \tag{34}$$



## **Comparison...** and parametric approach

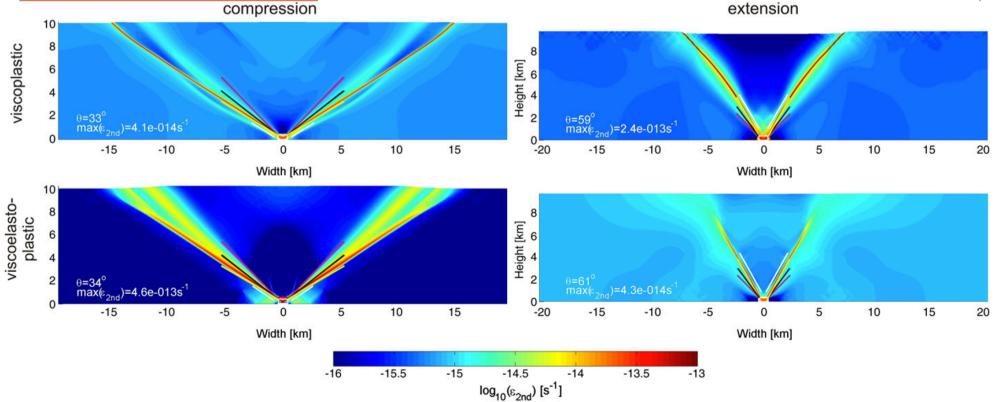


Factors that control the angle of shear bands in geodynamic numerical models of brittle deformation

Boris J.P. Kaus \*

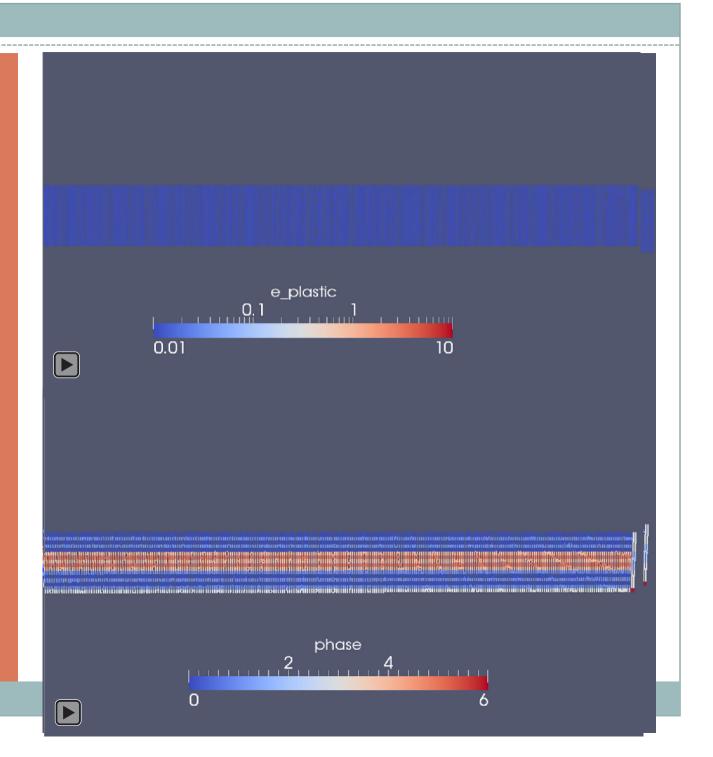
Geophysical Fluid Dynamics, Department of Earth Sciences, ETH Zurich, Switzerland University of Southern California, Los Angeles, USA





And last year I started to play the game of comparisons using our (Dave and I) new code pTatin

And got really unhappy with the results what was so different about pTatin that brought this effectively weaker rheology ?



# pTatin

- Fully parallel 2D/3D marker + FE methodology.
- Library code providing support for FE meshes and marker treatment.
- Extremely flexible solver configuration AMG, GMG with configurable assembled / unassembled operators on each level.
- Extensible + multi-physics support provided.
- Model definition is decoupled from solver (isolating users from unnecessary code).
- Solver support provided by PETSc (<u>www.mcs.anl.gov/petsc</u>)

#### Library provides

FE Meshes Q2,P1,Q1

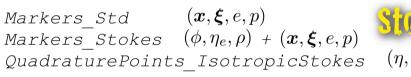
#### **Quadrature utilities**

- line, surface, volume rules
- extensible data types

#### Marker utilities

- extensible data types
- advection
- re-population
- projection operators

#### Example: Stokes support



 $(\eta, Fu_x, Fu_y, Fu_z, Fp)$ 

FormFunction\_IsotropicStokes()
FormJacobian\_IsotropicStokes()
MatMultMF\_A\_IsotropicStokes()

Apply\_MeshGeometry\_IC()
Apply\_MaterialGeometry\_IC()
Apply\_X\_BC()
Apply\_X\_IC()
Output()



Mixed Finite Element Method (FEM)

$$\begin{bmatrix} A & G \\ D & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} \hat{f} \\ \hat{h} \end{bmatrix} \longrightarrow \mathcal{A}x = b$$

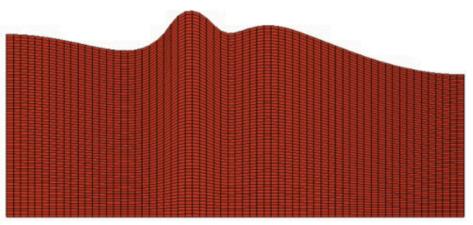
# Discretisation (u,p)

A: discrete stress gradient operatorG: discrete gradient operatorD: discrete divergence operator

Quadrilateral (hexahedral) elements

Simple  $M_x x M_y x M_z$  structured mesh

 $Q_2P_1$  basis functions for velocity and pressure



- + Inf-sup stable.
- + Total (not differential) density can be used.
- + Efficient solvers can be developed which exploit the structured mesh.
- + Free surface boundary condition (or coupled SPM's) is easy to include.

# pTatin

#### PDE

$$\left[\eta(\boldsymbol{u}, p) D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i(\boldsymbol{u}, p)$$
$$u_{k,k} = 0$$

**STOKES NON-LINEAR RESIDUALS**  $F_{u_i} := \left[ \eta(\boldsymbol{u}, p) D_{ij}(\boldsymbol{u}) \right]_i - p_{,i} - f_i(\boldsymbol{u}, p)$ 

NON-LINEAR UPDATE

$$\begin{bmatrix} A + \delta A & B + \delta B \\ B^T + \delta B^T & 0 \end{bmatrix} \begin{bmatrix} \delta u \\ \delta p \end{bmatrix} = - \begin{bmatrix} F_u \\ F_c \end{bmatrix}$$

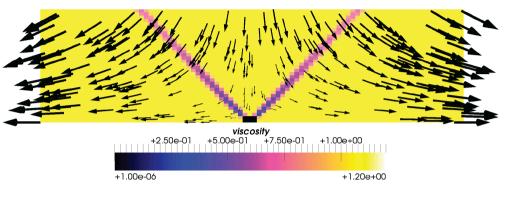
JACUE

 $F_{k,k} = u_{k,k}$ 

$$\mathcal{J}_s = \begin{bmatrix} A + \delta A & B + \delta B \\ B^T + \delta B^T & 0 \end{bmatrix}$$

#### **ELMAN-STYLE PRECONDITIONER**

$$\mathcal{P}_s = \begin{bmatrix} A' & B\\ 0 & -S \end{bmatrix}$$



#### void FormFunction(Vec X,void \*ctx) {

- Extract u,p from X
- Update nonlinearities on markers  $f:=\tau_{II}-\tau_y\leq 0$

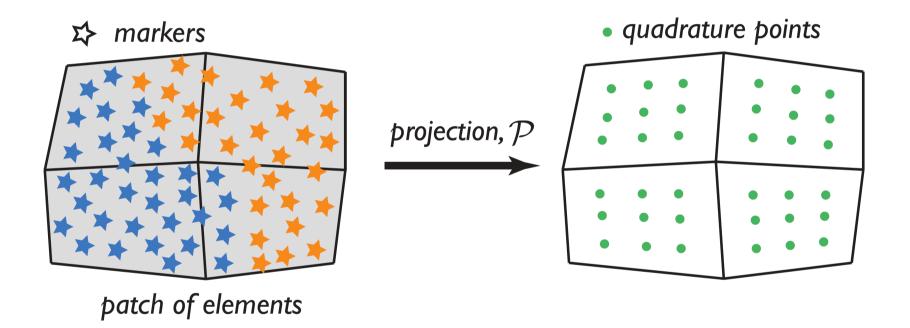
$$\tau_{II} := \sqrt{\frac{1}{2}\tau_{ij}\tau_{ij}}$$
$$\eta_{vp} = \begin{cases} \frac{\tau_y}{\sqrt{2\epsilon_{ij}\epsilon_{ij}}} & \text{if } \tau_{II} > \tau_y \\ \eta & \text{otherwise} \end{cases}$$

- Project marker properties to QP
- Evaluate FE Stokes residuals

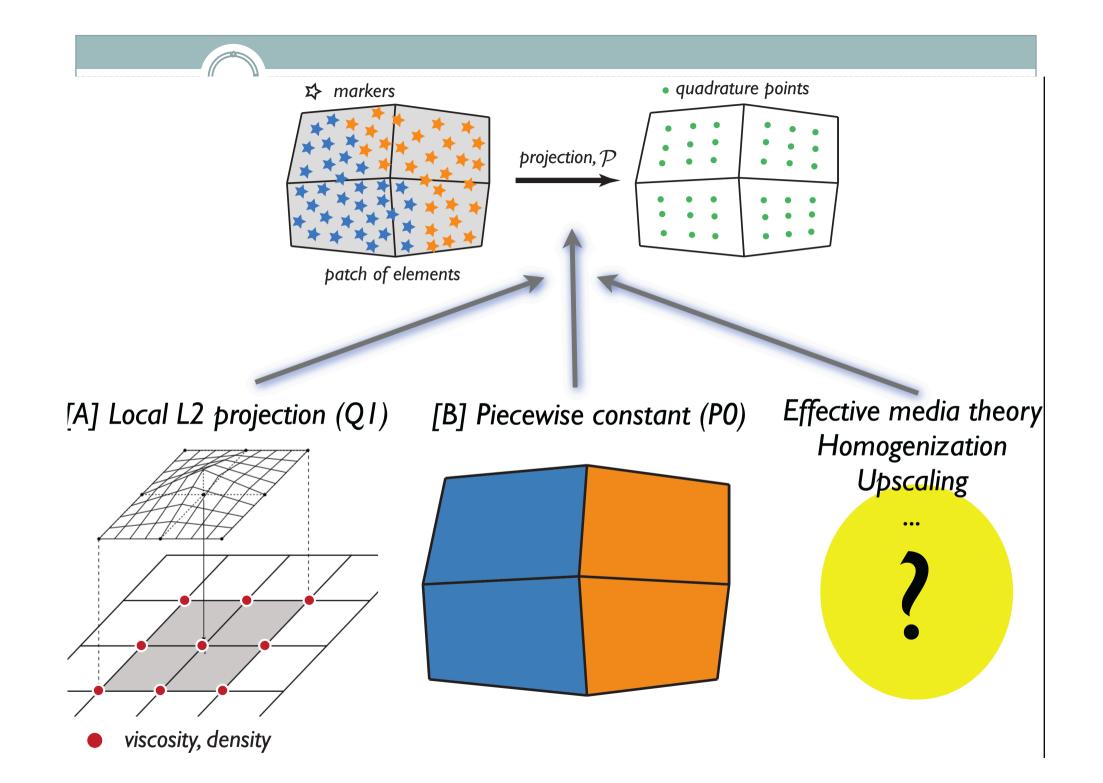
$$F_u = A^e u^e - G^e p^e - \hat{f}^e$$
$$F_c^e = D^e u^e - \hat{h}^e$$



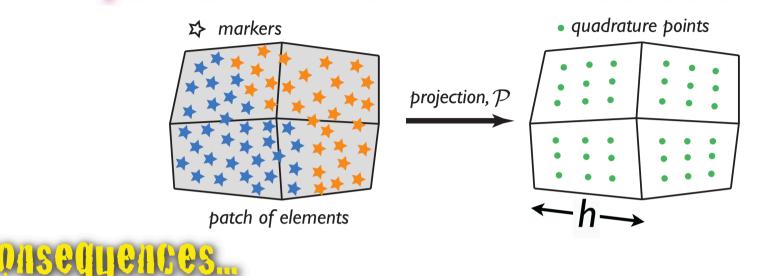
- Basis functions for flow problem: velocity u, pressure p
- Basis functions for coefficients: effective viscosity; density



Projection P maps marker properties onto the quadrature points used to evaluate the integrals within the FE weak form



# **Hybrid Marker-FEM Discretisation**

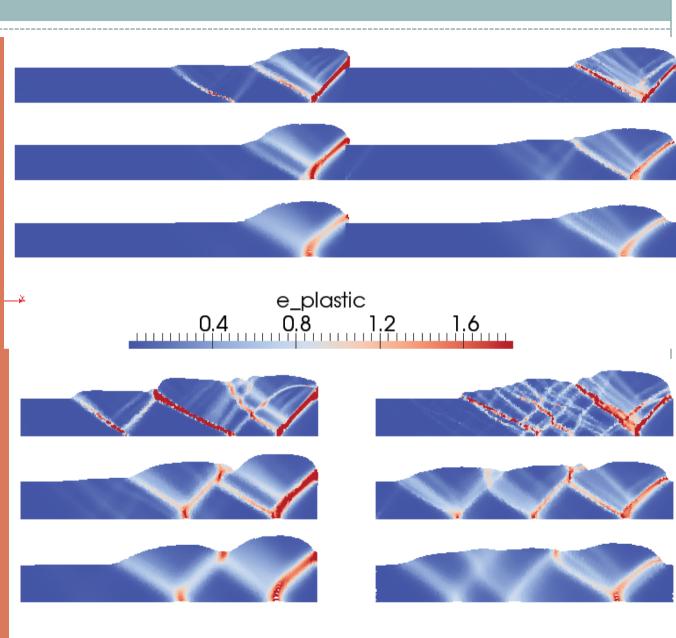


- With smooth coefficients, projection [A] preserves optimal of accuracy for u, p (via Strangs second lemma).
- Discontinuous coefficients reduces u, p order of accuracy to O(h) for both u, p in L2 using either projection [A] or [B].
- No integration error.
- Completely decoupled FE discretisation from marker discretisation.
   There is NO sub-grid resolution achieved using markers w.r.t errors in u, p

Other consequences

... We do not get the same results as the others ©

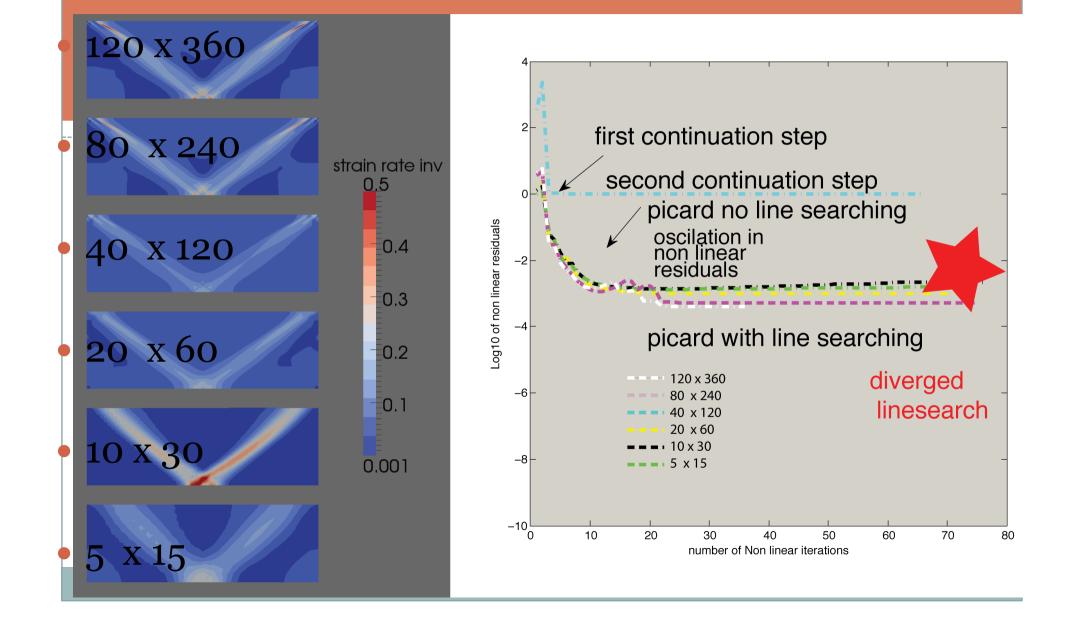
or even with our selves

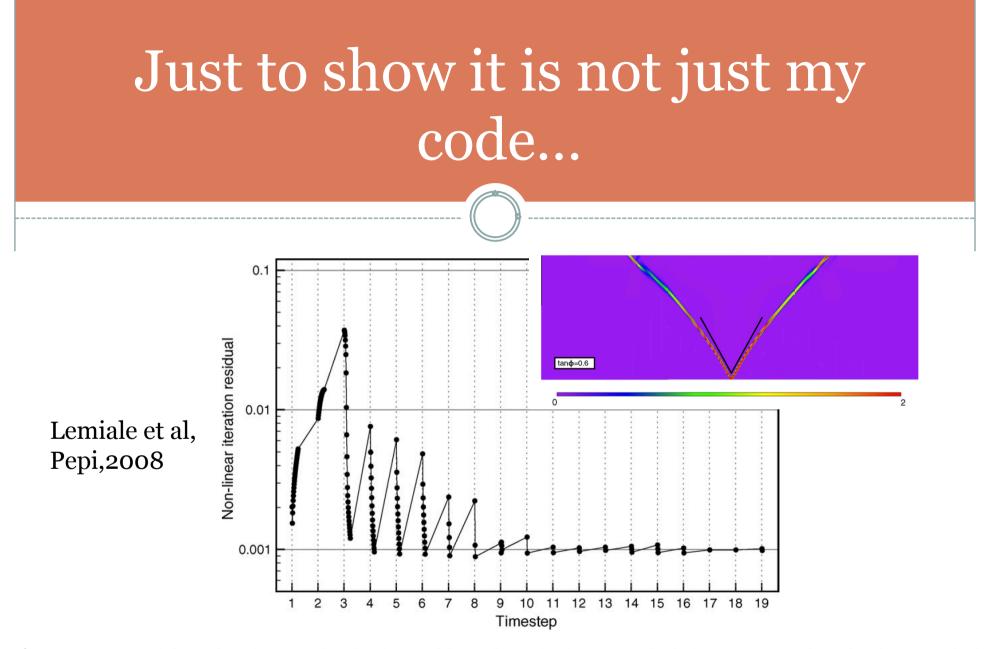


e\_plastic 0.4 0.8 1.2 1.6



# What's the issue with our model?



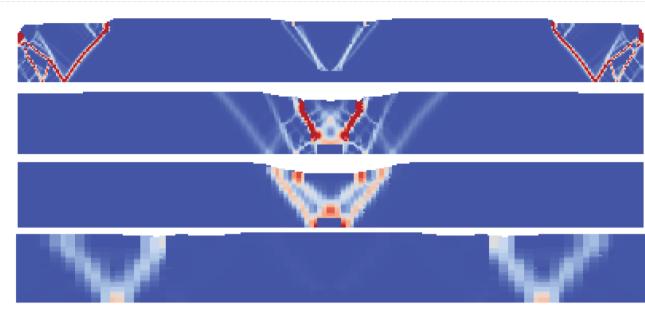


**Fig. 9.** Convergence graph for tan  $\phi$  = 0.6 in compression. The tolerance of the non linear solver is set to 0.001 but is also set to truncate after 25 iterations. Truncation is observed in the first two timesteps but stops once the shear bands are locked in place by strain softening.

## What's the issue with our model ?

Lack of convergence of the non linear solve

Lack of convergence of the solution with resolution



## plas\_sr 10 2.5 5 7.5 10 בר

Particulary sick case to illustrate the problem, i.e. Instead of using benchmarks parameters, I now use typical production tolerances and run 50 time step... Gauss point projection,

Dirty non linear solve (maximum number of non linear iterations limited to 7)

Time stepping continues if non linear solves fails.

#### What's the issue with our model ?

Problem 1 : The non linear solver either: 1) Oscilates with picard and no line searching 2) Diverges with Picard and line searching 3) Causes the number of linear iterations to explode with Newton (>10000, Diverge due to max it) As a result even on the first time step we don't know what is the solution.

## Solution to the non linear equation

Non linear solver strategy :

Change from exact to inexact newton

And make use of ew algorithm to compute ksp

Was that hard to implement?

Nope, we are using petsc snes ©

SIAM J. SCI. COMPUT. Vol. 17, No. 1, pp. 16-32, January 1996 © 1996 Society for Industrial and Applied Mathematics 002

#### CHOOSING THE FORCING TERMS IN AN INEXACT NEWTON METHOD\*

#### STANLEY C. EISENSTAT<sup>†</sup> AND HOMER F. WALKER<sup>‡</sup>

Abstract. An inexact Newton method is a generalization of Newton's method for solving F(x) = 0,  $F : \mathbb{R}^n \to \mathbb{R}^n$ , in which, at the *k*th iteration, the step  $s_k$  from the current approximate solution  $x_k$  is required to satisfy a condition  $||F(x_k) + F'(x_k) s_k|| \le \eta_k ||F(x_k)||$  for a "forcing term"  $\eta_k \in [0, 1)$ . In typical applications, the choice of the forcing terms is critical to the efficiency of the method and can affect robustness as well. Promising choices of the forcing terms are given, their local convergence properties are analyzed, and their practical performance is shown on a representative set of test problems.

While the Newton systems must be solved well enough to retain fast local convergence of the Newton's iterates, use of excessive inner iterations, particularly when  $||x_k - x_*||$  is large, is neither necessary nor economical. Thus, the number of required inner iterations typically increases as the Newton process progresses, so that the truncated iterates approach the true Newton iterates.

A sequence of nonnegative numbers  $\{\eta_k\}$  can be used to indicate the variable convergence criterion. In this case, when solving a system of nonlinear equations, the update step of the Newton process remains unchanged, and direct solution of the linear system is replaced by iteration on the system until the residuals

$$oldsymbol{r}_k^{(i)} = oldsymbol{F}'(oldsymbol{x}_k) \Delta oldsymbol{x}_k + oldsymbol{F}(oldsymbol{x}_k)$$

PETSC MANUAL

satisfy

$$\frac{\|\boldsymbol{r}_k^{(i)}\|}{|\boldsymbol{F}(\boldsymbol{x}_k)\|} \le \eta_k \le \eta < 1.$$

Here  $x_0$  is an initial approximation of the solution, and  $\|\cdot\|$  denotes an arbitrary norm in  $\Re^n$ .

# Solution to the non linear equation

Projection of viscosity on gausspoint

Makes a smoother solution...

Picard now works with linesearching and oscilation disapear

Yet for large viscosity contrast exact newton fails because the pb is too hard While the Newton systems must be solved well enough to retain fast local convergence of the Newton's iterates, use of excessive inner iterations, particularly when  $||x_k - x_*||$  is large, is neither necessary nor economical. Thus, the number of required inner iterations typically increases as the Newton process progresses, so that the truncated iterates approach the true Newton iterates.

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$$oldsymbol{r}_k^{(i)} = oldsymbol{F}'(oldsymbol{x}_k) \Delta oldsymbol{x}_k + oldsymbol{F}(oldsymbol{x}_k)$$

PETSC MANUAL

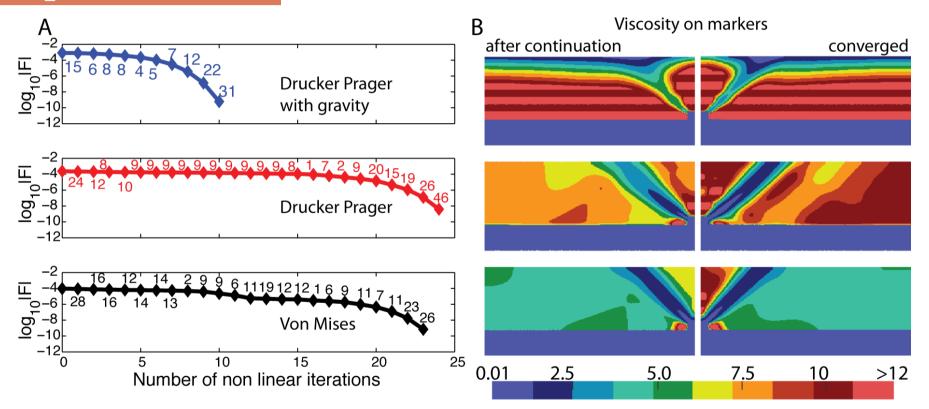
satisfy

 $\frac{\|\boldsymbol{r}_{k}^{(i)}\|}{\|\boldsymbol{F}(\boldsymbol{x}_{k})\|} \leq \eta_{k} \leq \eta < 1.$ 

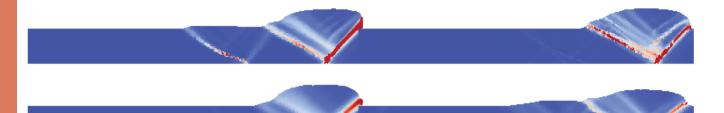
Here  $x_0$  is an initial approximation of the solution, and  $\|\cdot\|$  denotes an arbitrary norm in  $\Re^n$ .

# Solution to the non linear equation

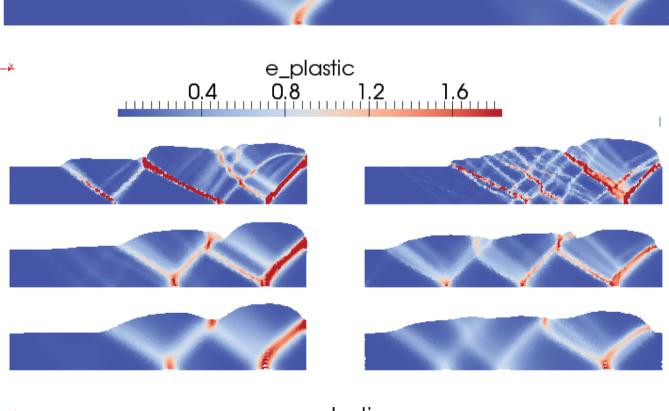
#### May & Le Pourhiet, in prep, JCP



Unfortunately, this only works with markers, not with gauss points, So we loose the pseudo sub element accuracy, shear bands are thicker And we need more grid resolution... ..... ((

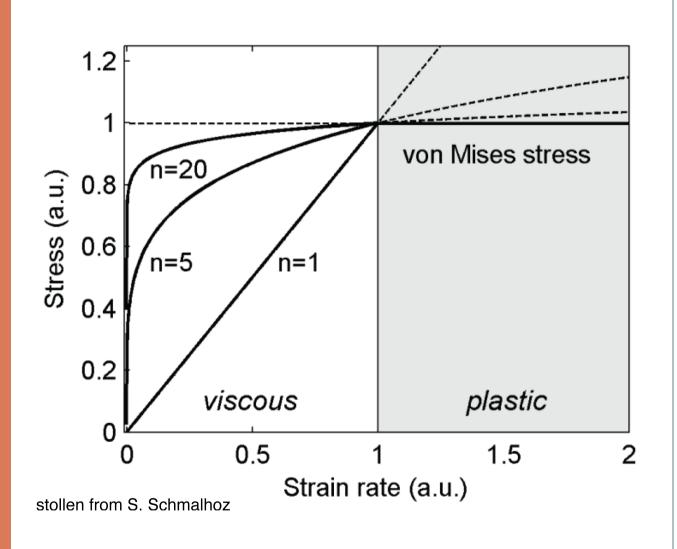


And just as a reminder... it does not solve the issue with convergence with grid resolution...



e\_plastic 0.4 0.8 1.2 1.6

**One might now** ask, why the other rheologies we use in earth science to localize strain do not have this issue? **Even when** they are very non linear?



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Maybe, we might have read more carefully the original review (68 pages)

#### HERÓN VOI. 29 1984 no. 3

Contents

#### NON-ASSOCIATED PLASTICITY FOR SOILS, CONCRETE AND ROCK

P. A. Vermeer Department of Civil Engineering, Geotechnical Laboratory Delft University of Technology

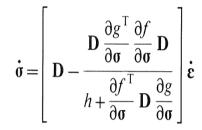
R. de Borst

Software Engineering Department/Section DIANA Institute TNO for Building Materials and Building Structures

# **Original formulation**

#### Note :

- There is a hardening modulus h
- This localisation with this rheology is triggered by unstability, unless h is adjusted to compensate for stress drop...
- 3) Remember FLAC is an inertial method.



The most striking numerical result is

the occurrence of post-peak softening as a consequence entirely of the non-associated flow rule. This can be explained from the violation of Drucker's stability postulate.

# **Solutions ?**

Is it possible to actually find a method for which we might obtain the solution of the non linear problem ?

What can we do to make sure the solution does not change when we increase the resolution ? Problem :

Non associated flow rule does not yield a unique possible shear band orientation...

The stress drop depends sollaly on orientation of the band... which in turns depend on resolution and numerics we never describe in papers...

For visco-plastic case it does not even depends on strain....

It is mechanically unstable (rupture Drucker Postulates) The derivative of work with displacement is negative and our formulation does not have a term too store the energy released by strain localisation.... (no elasticity / no inertia )

The problem is just badly paused...

We can benchmark codes as much as we want they will never reach the same results

# Looking closer at the Original formulation

The hardening modulus h, permits to select a initial orientation...

This parameter depends on mobilised friction and dilation and therefore might be used as a state variable to introduce softening/ damage. For large values of the hardening modulus h, that is in the beginning of loading, shear bands cannot develop, as this can take place only if equation (8.6b) has a real solution. The critical value of the hardening modulus  $h_c$  for which shear-band formation is first possible is derived from the condition that the expression under the square root has a non-negative sign, yielding:

$$h_{\rm c} = \frac{E(\sin \phi^* - \sin \psi^*)^2}{16(1 - \nu^2)}$$
(8.7)

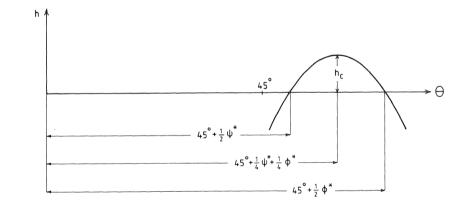


Fig. 8.7 Relation between hardening modulus and inclination angle of the shear band.

"The" orientation should be Arthur if we would used this hardening formulation.

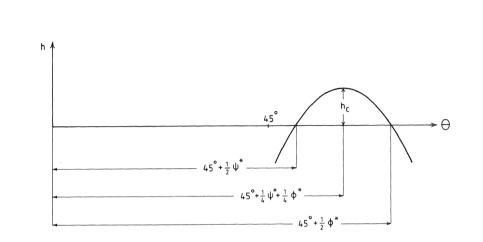


Fig. 8.7 Relation between hardening modulus and inclination angle of the shear band.

Then, that is for  $h = h_c$ , equation (8.6b) gives one unique solution for the inclination angle  $\theta$  of the shear band

$$\cos 2\theta = -\frac{1}{2}(\sin \phi^* + \sin \psi^*) = -\sin \left(\frac{1}{2}\phi^* + \frac{1}{2}\psi^*\right) \cos \left(\frac{1}{2}\phi^* - \frac{1}{2}\psi^*\right)$$

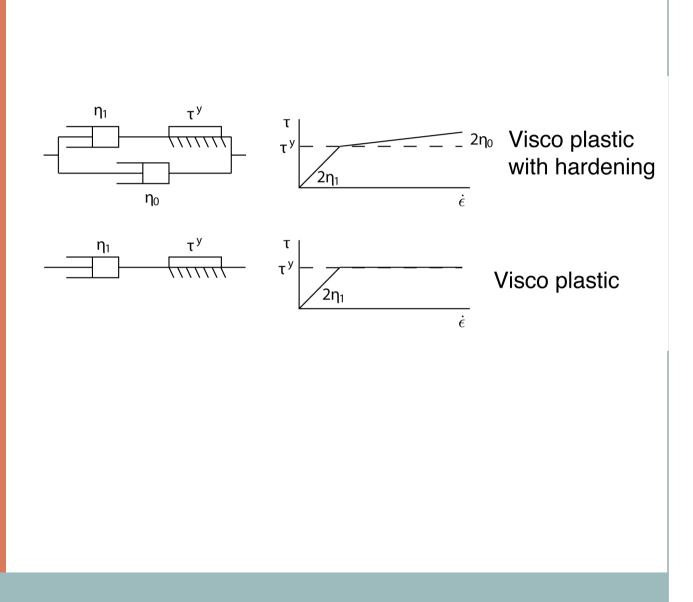
or

$$\sin (90^{\circ} - 2\theta) = -\sin \left( \frac{1}{2} \phi^* + \frac{1}{2} \psi^* \right) \cos \left( \frac{1}{2} \phi^* - \frac{1}{2} \psi^* \right)$$

This equation can further be simplified by noting that the difference between the mobilised friction angle and the mobilised dilatancy angle seldom exceeds 30°. Hence,  $\cos(\frac{1}{2}\phi^* - \frac{1}{2}\psi^*)$  is in the range between 0.96 and 1.0. We can thus omit the cosine term in the above equation, so that we obtain for the inclination angle  $\theta$ :

$$\theta \approx 45^{\circ} + \frac{1}{4}(\phi^* + \psi^*) \text{ for } h = h_c$$
(8.8)

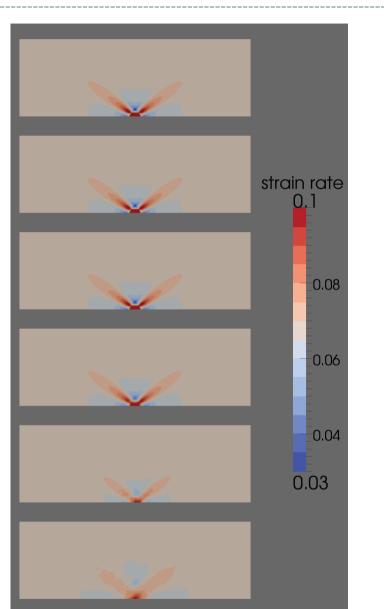
What if the secret would be to find a rheology that localises strain with the "right" angle without rupturing Drucker postulate?



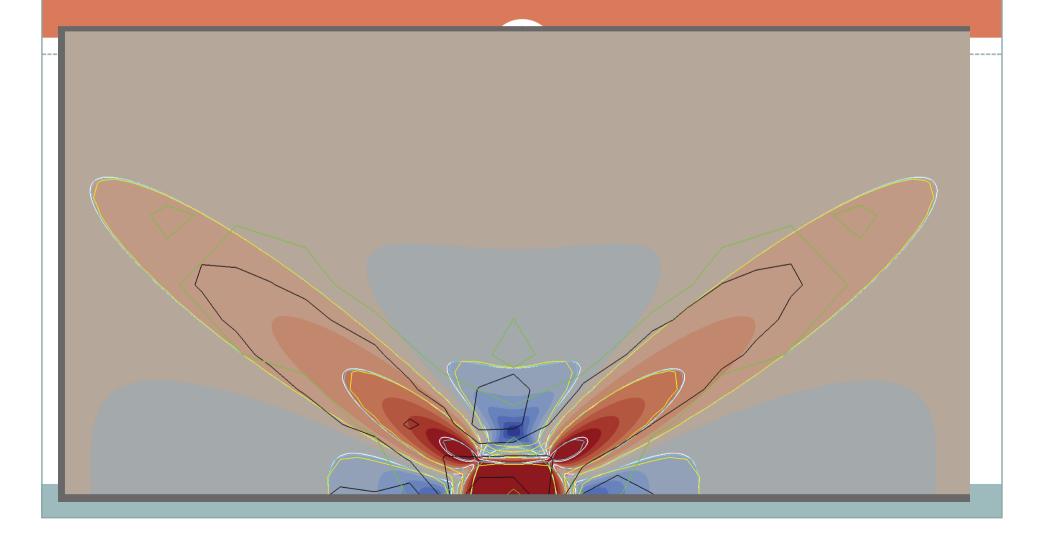
## Convergence with the grid resolution

What Do I mean by convergence....

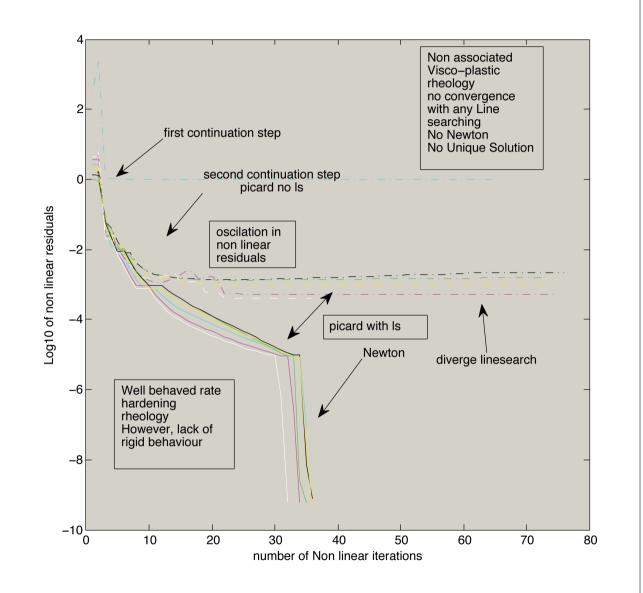
Simply that results do not change when I increase the resolution ! • 120 x 360 • 80 x 240 • 40 x 120 • 20 x 60 • 10 x 30 • 5 X 15

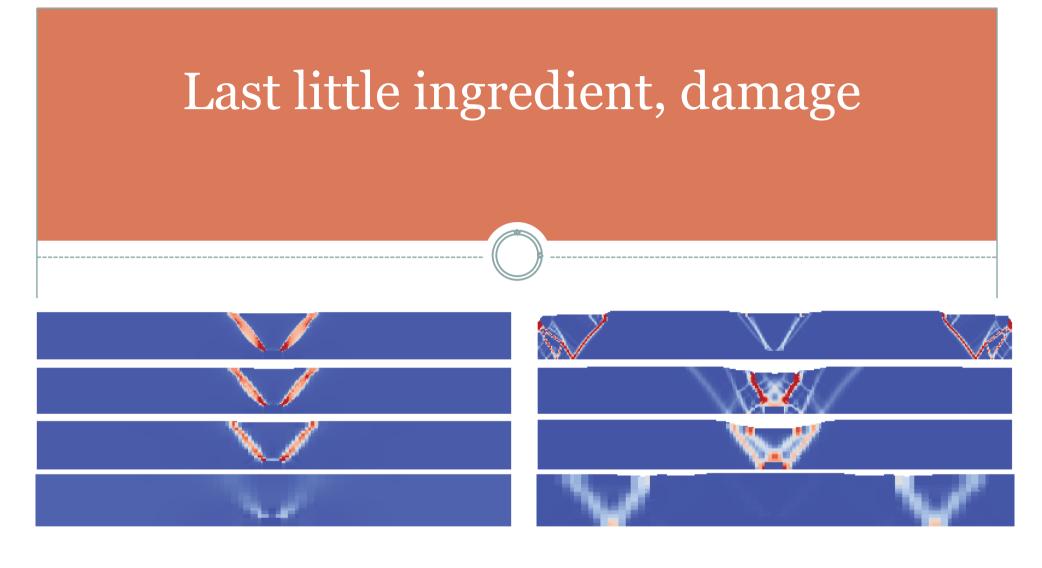


With increasing grid resolution, the solution changes, only in the places of the model with high strain rate, but not in the far field.With this type of rheology, it becomes possible to use AMR to workout the details within high strain rate zone, being sure it will not affect the solution in the low strain rate zone



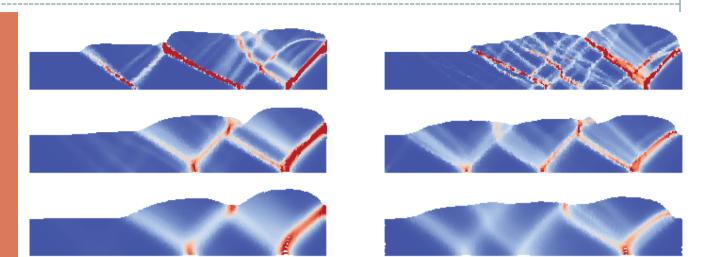
Now, even with gauss point projection, the line searching works, picard converges and Newton too.







## Take away messages



#### e\_plastic 0.4 0.8 1.2 1.6

We need to better describe projections, boundary conditions, error evaluation, non linear algorithm in our publications...

These details are always missing when trying to compare results between code and largely influence the results.

#### Non linear problems:

# Exact jacobian are extremely difficult to write for plasticity or multiphysics problems.

Picard linearisation is very slow to converge Approximate Jacobian are very efficient when over solving is avoid Eisentat-walker works very well for regularised/smoothed visco-plasticity

3 Physics $x = [x_a, x_b, x_c]$ 

**Non-linear residual**  $F_i(x) = 0$ 

"Jacobian" (physics coupling)

$$J^* = \begin{bmatrix} J_{aa} & J_{ab} & J_{ac} \\ J_{ba} & J_{bb} & J_{bc} \\ J_{ca} & J_{cb} & J_{cc} \end{bmatrix}$$

#### Non-linear solver

Given initial guess ,  $x^0$ while not converged Solve  $J^*(x^k)\delta x = -F(x^k)$ Step  $x^{k+1} = x^k + \delta x$ 

#### Types of Jacobian

$$J^* = \frac{\partial F}{\partial x}$$

[2] Approximate Jacobian (JFNK)  
$$J^*y \approx \frac{F(x + \epsilon y) - F(x)}{\epsilon}$$

#### [3] Picard linerisation

- Lag the non-linearity within the operator.

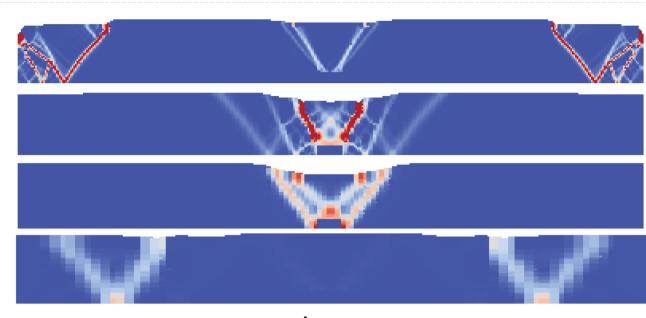
$$oldsymbol{A}(oldsymbol{x}^k)oldsymbol{\delta} x = -oldsymbol{F}(oldsymbol{x}^k)$$

## Take away messages

All of this was done in 2D, where we can always afford higher resolution and a lot of non linear iterations...

But we all wanna have fast 3D codes that scale on massively parallel machine.

If we do not have fast converging algorithm for faulting, we will end up with the bottom picture !





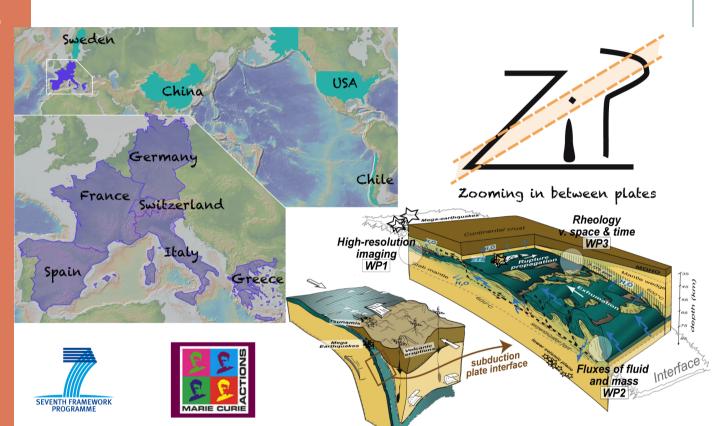
Not converged non linear solve + time stepping = PIXAR\*

\* Fast obtained solution that look realistic enough for people to like the movie. Special effects indeed!

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