Shear localisation during deformation of reactive thermo-visco-elastic-plastic materials

R. Timms[1], R. Purvis[1], J.P. Curtis[2,3]

[1]School of Mathematics, University of East Anglia, Norwich NR4 7TJ, United Kingdom
[2]AWE, Aldermaston, Berkshire RG7 4PR, United Kingdom
[3]Visiting Professor, Department of Mathematics, University College London, Gower Street, London WC1E 6BT, United Kingdom

Defence and Security Doctoral Symposium

15–16 November 2017

Overview

- Background
- Motivation
- Reactive Shear Band Model
- Conclusion

Background

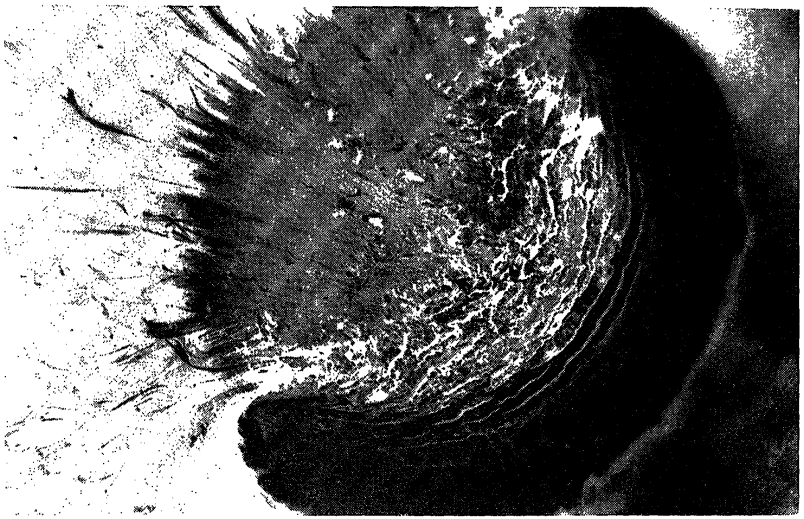


Figure: Heat sensitive film record of impact test with a high explosive. Darker regions correspond to higher temperature.

- Focus on low-speed impacts scenarios - “insults”.
- Accidental ignition is caused by “hot spots”.
- How are these generated?

Image from Hot spot ignition mechanisms for explosives and propellants, Field et al.

Background

- Adiabatic compression of trapped gas spaces.
- Viscous heating of material rapidly extruded between the impacting surfaces.
- Friction between the impacting surfaces, the explosive crystals, and/or grit particles in the explosive layer.
- Localised adiabatic shear of the material during mechanical failure.

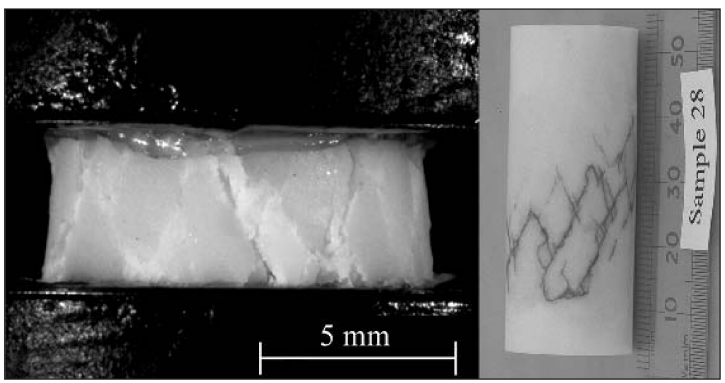


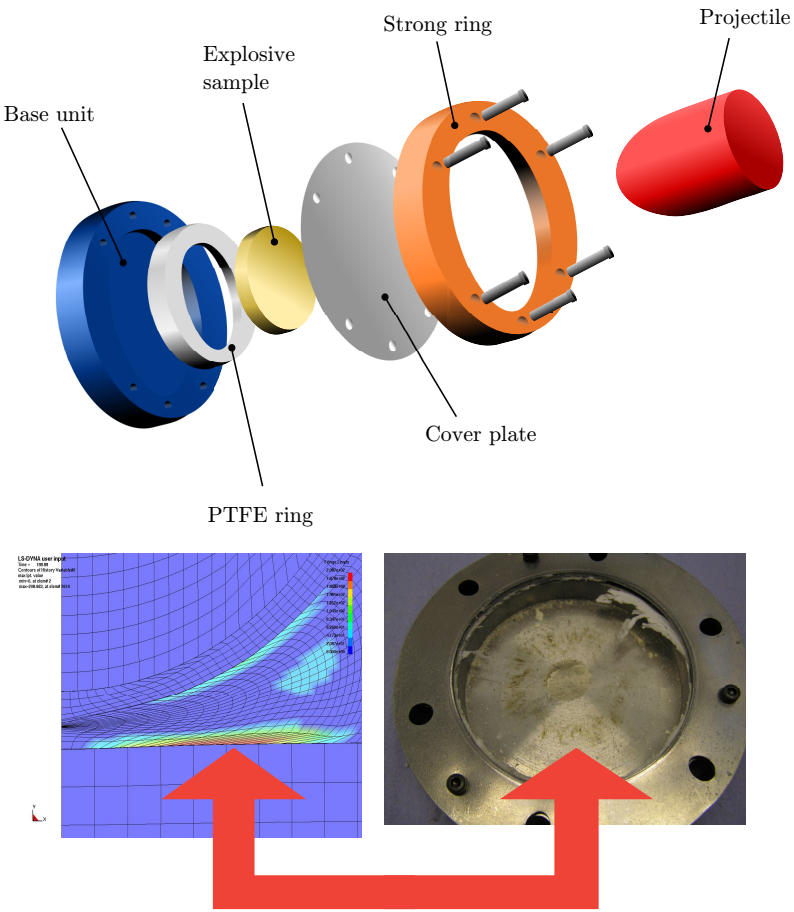
Figure: Photograph of shear bands in a high explosive.

Image from Temperature-time response of a polymer bonded explosive in compression (EDC37), Williamson et al.

Low Speed Impact Modelling

Steven Test

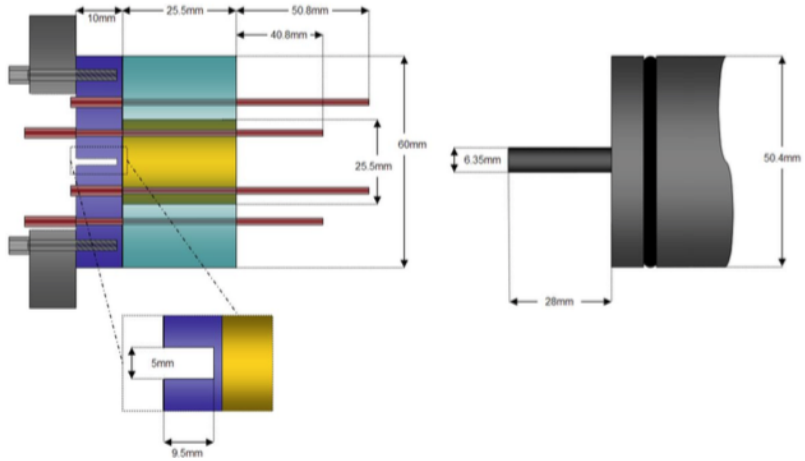
- Experiments conducted at AWE.
- Current LS-Dyna FE model is currently main approach.
- High values of HERMES Ignition parameter seen near confining walls.
- Predicts scorching seen in experiments.



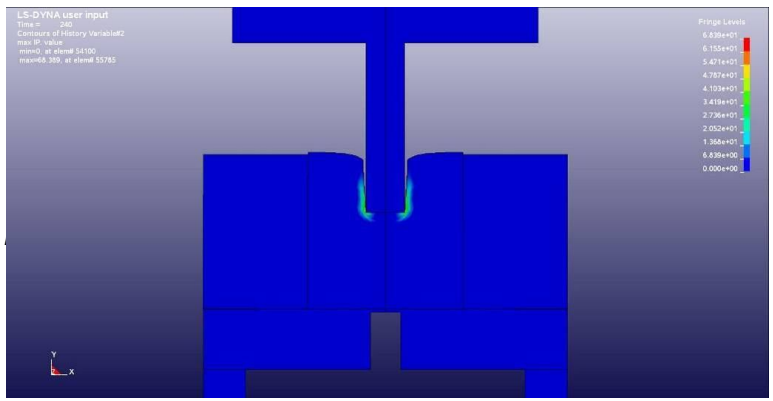
Images courtesy of AWE from CEA Workshop on Explosives, Tours, France

Low Speed Impact Modelling

Spigot Impact



- Localised impact.
- High values of HERMES Ignition parameter at leading edge of spigot.
- Impact velocity ranges from 10 - 40 $\mathrm{m\,s^{-1}}$.



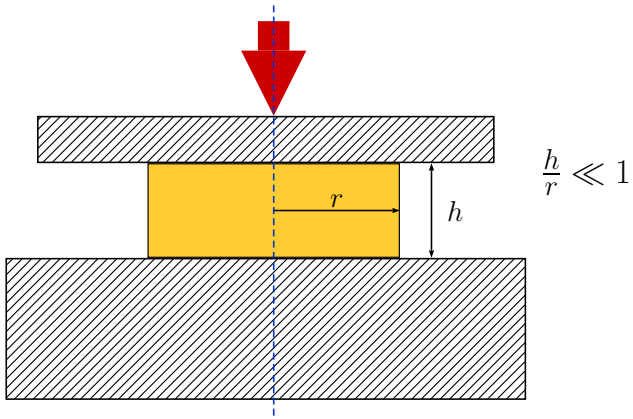
Images courtesy of AWE from CEA Workshop on Explosives, Tours, France

Simplified Low Speed Impact Modelling

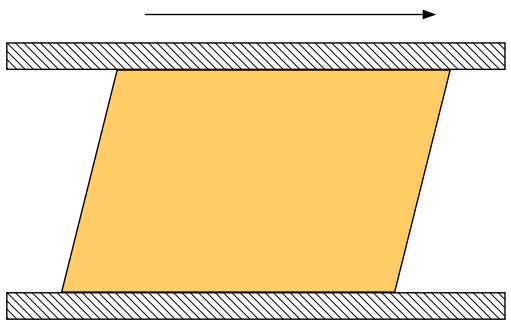
Motivation

- Improve safety during everyday conditions.
- Avoid issues associated with numerical models, e.g.
  - severe mesh deformation,
  - model break down near walls.
- Numerical validation.
- Focus on specific mechanisms/gain physical insight.

Drop test[i.]



Simple shear[ii.]



i. J.P. Curtis, A Model of Explosive Ignition due to Pinch, 38th International Pyrotechnics Seminar, Denver, Colorado, USA.
ii. J.P. Curtis, Explosive Ignition due to Adiabatic Shear, 39th International Pyrotechnics Seminar, Valencia, Spain.

Reactive Shear Bands

Shear band schematic

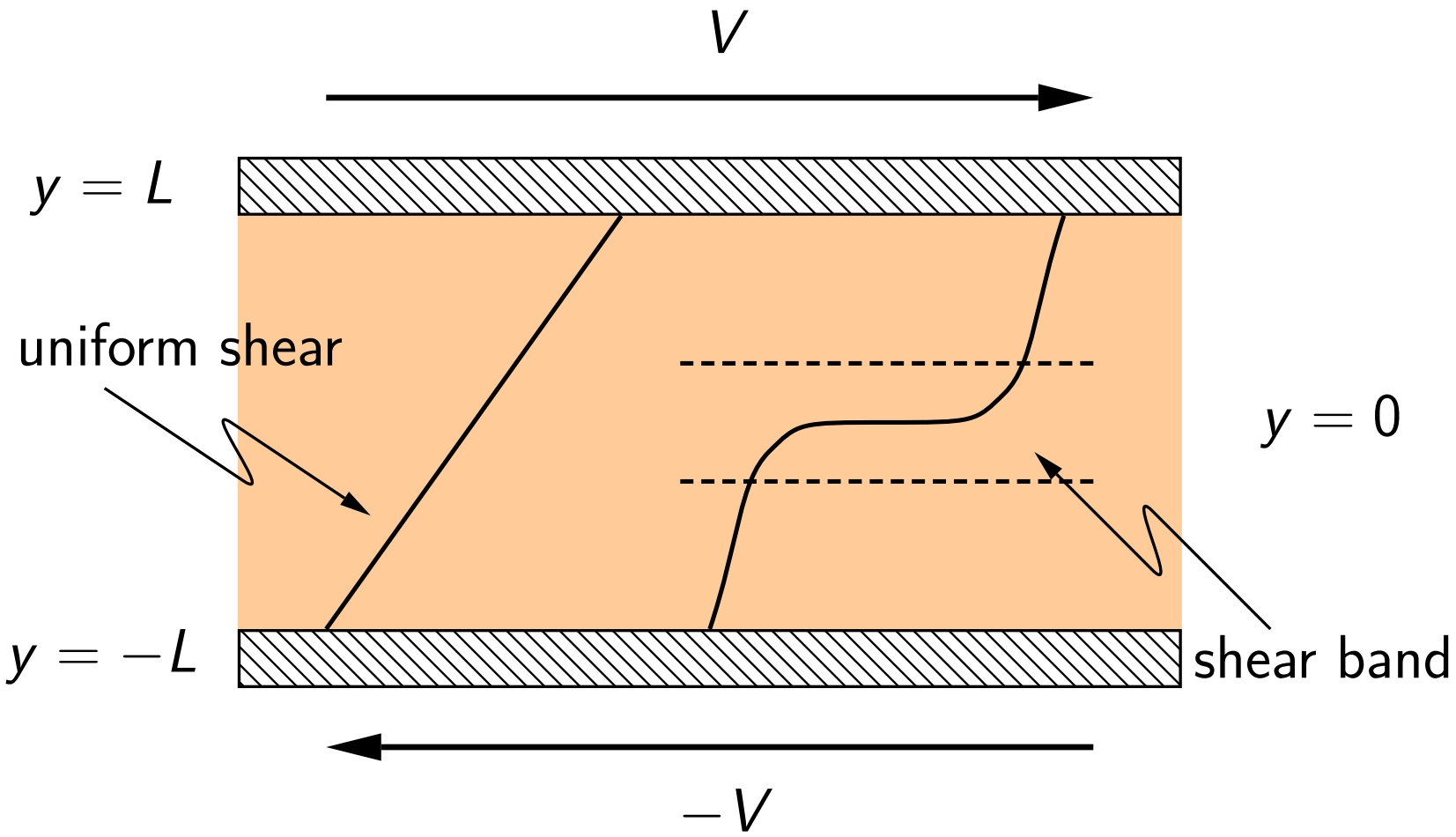


Figure: uniform shearing vs. shear banding

Reactive Shear Bands

Governing equations

One-dimensional model of shear band:

$$
\begin{aligned}
\rho v_t &= s_y, && \text{momentum balance;}\\
\rho c T_t &= \kappa T_{yy} + \beta s \dot{\gamma} + \rho \Omega A \mathrm{e}^{-\frac{E}{RT}}, && \text{energy balance;}\\
s_t &= G(v_y - \dot{\gamma}), && \text{elastic relationship;}\\
\dot{\gamma} &= \dot{\gamma}(s, T, \gamma), && \text{plastic flow law;}\\
\gamma &= \int_0^t \dot{\gamma}(t')\,\mathrm{d}t', && \text{plastic strain.}
\end{aligned}
$$

Here the dependent variables are velocity v, stress s, temperature T, and plastic strain rate $\dot{\gamma}$. The plastic strain γ is determined by integration of strain rate. The material constants ρ, G, c, κ, β, Ω, A, E and R, are the density, elastic shear modulus, specific heat, thermal conductivity, Taylor-Quinney coefficient, heat of reaction, rate constant, activation energy and molar gas constant, respectively.

Reactive Shear Bands

Constitutive law

Exponential strain-rate law

$$\dot{\gamma}(s, T) = \dot{\Gamma}^* \exp\{-[B_1^{-1}(T_p - T) + B_2^{-1}(s_p - s)]\},$$

where $\dot{\Gamma}^*$, T_p and s_p are the reference strain-rate, temperature and stress, respectively. The parameters B_1, B_2 are related to strain-rate sensitivity M and thermal sensitivity P via the definitions

$$M \equiv \frac{1}{s_\mathrm{p}} \frac{\partial s}{\partial \log \dot{\Gamma}} = \frac{B_2}{s_\mathrm{p}}, \quad P \equiv -\frac{T_\mathrm{p}}{s_\mathrm{p}} \frac{\partial s}{\partial T} = \left(\frac{B_2}{s_\mathrm{p}}\right) \Big/ \left(\frac{B_1}{T_\mathrm{p}}\right).$$

Shear band formation due to a thermal flux inhomogeneity, DiLellio, J.A. and Olmstead, W.E.

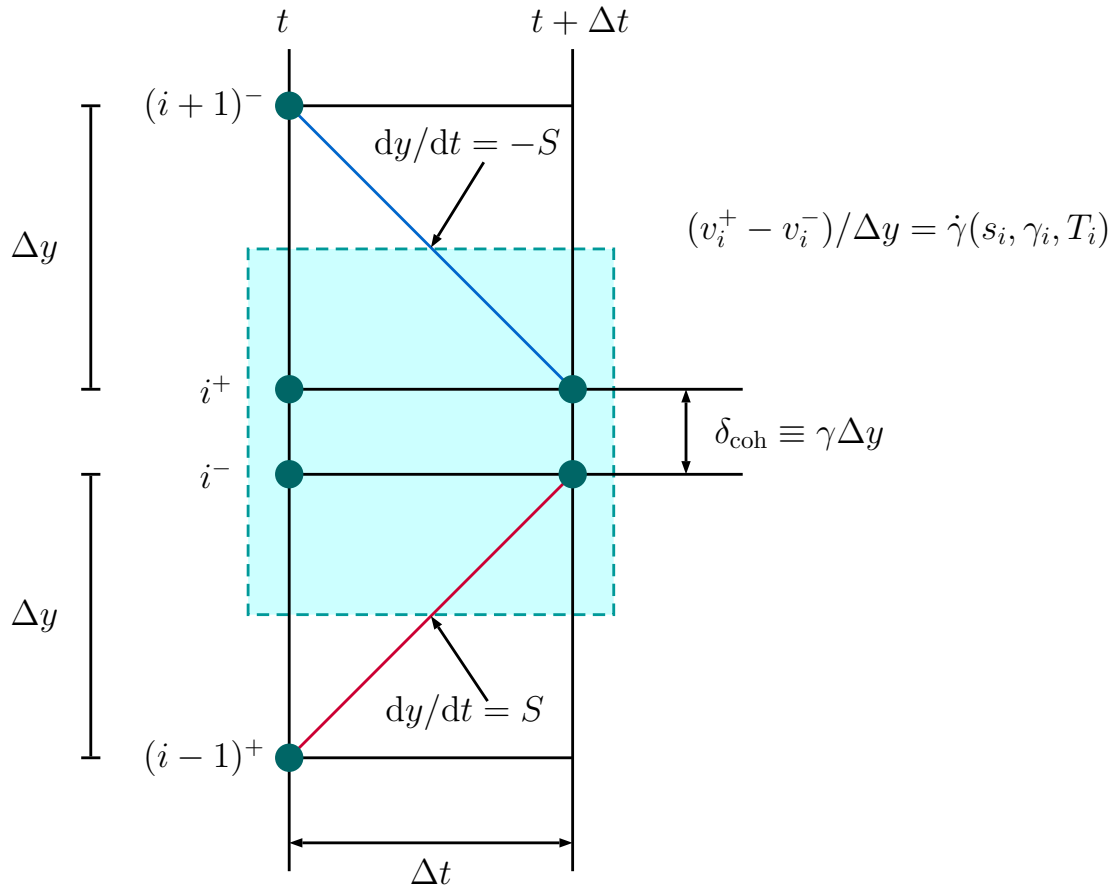
Reactive Shear Bands

Numerical solution – “cohesive scheme”

Elastic wave speed:

$$S = \sqrt{G/\rho}.$$

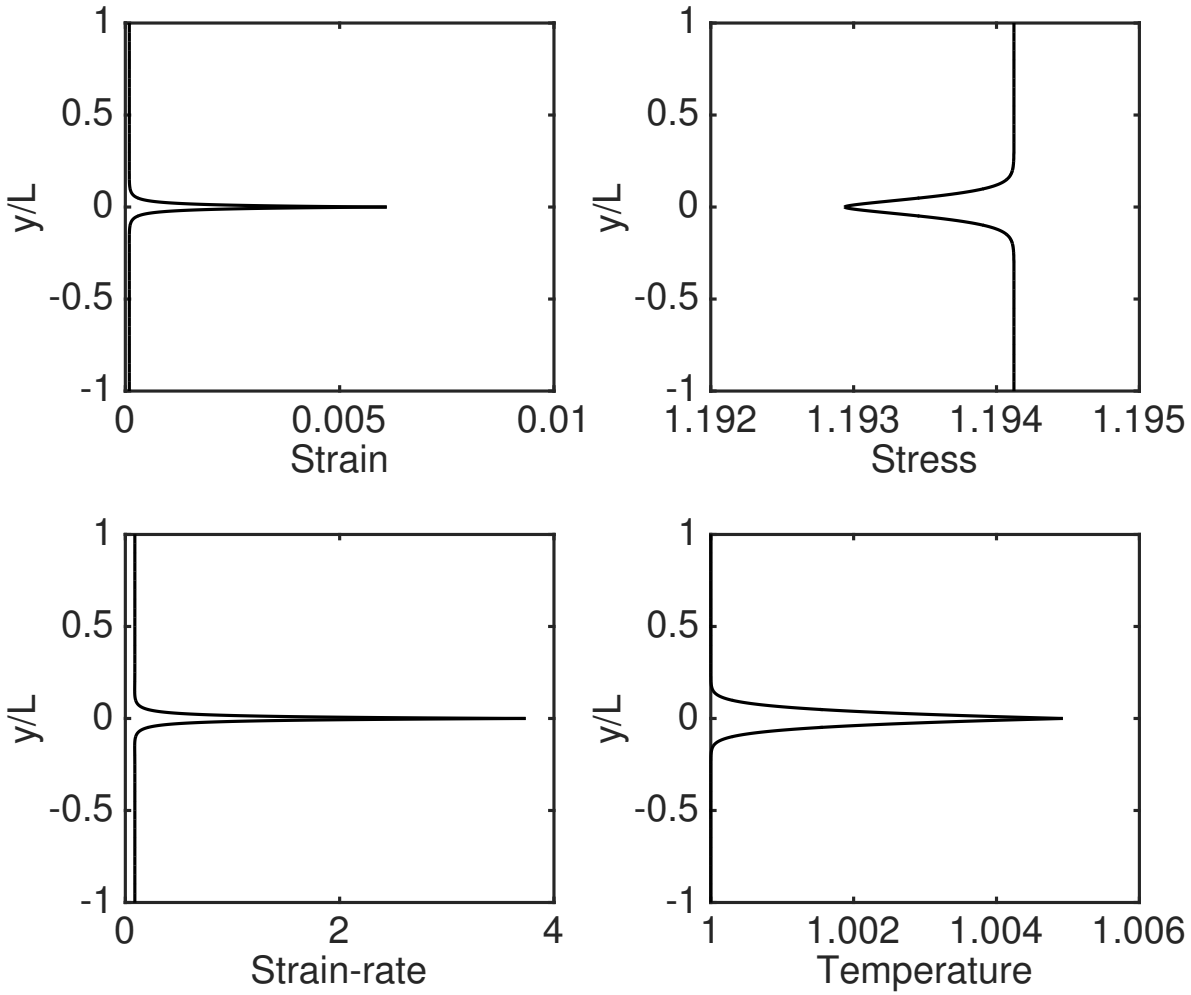
Grid size: Δy.
Time step: $\Delta t = \Delta y / S$.



[i] F. Zhou et. al. A numerical methodology for investigating the formation of adiabatic shear bands. Journal of the Mechanics and Physics of Solids, 2006.

Reactive Shear Bands

Numerical solution – onset of shear band



Reactive Shear Bands

Boundary Layer Analysis

- Heat flux inhomogeneity $q(t)$ at $y = 0$ initiates a zone of localised shearing.
- Plastic localisation zone is identified as a *boundary layer*.
- The typical length scale is taken to be the *thermal length scale*

$$l = \left(\frac{\kappa s_0}{\rho c G \dot{\Gamma}_0} \right)^{1/2},$$

effectively placing the boundary at an infinite distance from the shear band.

Reactive Shear Bands

Boundary Layer Analysis

The non-dimensional governing equations are recast in the form

$$s_t = \hat{\rho}^{-1} \int_0^t s_{yy}(y, t')\, \mathrm{d}t' + \omega - \dot{\gamma},$$

$$T_t = T_{yy} + \lambda s \dot{\gamma} + \hat{\Omega} \hat{A} \exp\left(-\frac{\hat{E}}{T}\right),$$

where

$$t^* = \frac{s_0}{G\dot{\Gamma}_0}, \quad l = \left(\frac{\kappa s_0}{\rho c G \dot{\Gamma}_0}\right)^{1/2}, \quad \dot{\Gamma}_0 = \frac{v_0}{l}, \quad \omega = \frac{w}{\dot{\Gamma}_0},$$

$$\hat{\rho} = \frac{\kappa \dot{\Gamma}_0}{c s_0}, \quad \lambda = \frac{\beta s_0^2}{\rho c G T_0}, \quad \hat{E} = \frac{E}{R T_0}, \quad \hat{\Omega} = \frac{\Omega}{c T_0}, \quad \hat{A} = A t^*.$$

Reactive Shear Bands

Boundary Layer Analysis

For early times the inert elastic solution given by

$$T_e(y,t) = 1 + \delta \int_0^t \frac{e^{-\frac{y^2}{4(t-t')}}}{[\pi(t-t')]^{1/2}} h(t')\,\mathrm{d}t',$$
$$s_e(y,t) = 1 + \omega t,$$

is appropriate. Here the heat flux inhomogeneity used to initiate a shear band is represented as

$$q(t) = \delta h(t), \quad 0 \leq h(t) \leq 1.$$

Reactive Shear Bands

Boundary Layer Analysis

- Identify small parameter ε:

$$\frac{B_1}{T_0} = \beta_1^{-1}\varepsilon, \quad \frac{B_2}{s_0} = \beta_2^{-1}\varepsilon, \quad 0 < \varepsilon \ll 1,$$

  where β_1 and β_2 are $O(1)$ constants.

- Exploit the largeness of the (non-dimensional) pre-exponential factor $\hat{A}$:

$$\hat{A} = \hat{A}_0 \frac{\hat{E}^{1/2}}{T_R} \exp\left(\frac{\hat{E}}{T_R}\right), \quad \frac{T_R}{\hat{E}^{1/2}} \sim \varepsilon^{1/2},$$

  where T_R is the critical reaction temperature, $\hat{E}$ is the non-dimensional activation energy, and $\hat{A}_0$ is $O(1)$.

Reactive Shear Bands

Boundary Layer Analysis

Boundary layer variables:

$$y = \varepsilon\xi, \quad t = t_p + \varepsilon\tau, \quad \xi > 0, \quad \tau > -\frac{t_p}{\varepsilon} \to -\infty,$$

with t_p the critical plastic time.
Look for solution as a perturbation to the elastic solution:

$$T = T_e(\varepsilon\xi, t_p + \varepsilon\tau) + \varepsilon T_1(\xi, \tau) + \varepsilon^{3/2} T_2(\xi, \tau) + \cdots,$$
$$s = s_e(\varepsilon\xi, t_p + \varepsilon\tau) + \varepsilon s_1(\xi, \tau) + \varepsilon^{3/2} s_2(\xi, \tau) + \cdots.$$

Define critical reaction time τ_R as the solution of

$$T_R = T_e(0, t_p + \varepsilon\tau_R) + \varepsilon T_1(0, \tau_R) + o(\varepsilon),$$

where the function T_1 is to be determined as part of the solution.

Reactive Shear Bands

Boundary Layer Analysis

Coupled equations for magnitudes of temperature and stress perturbations at the centre of the shear band:

$$f(\eta) = \int_{-\infty}^{\eta} [\pi(\eta - \eta')]^{-1/2} \Big\{ \exp\left[\eta' + f(\eta') - g(\eta')\right] + \Lambda_R \exp\left[\Lambda_\tau(\eta' - \eta'_R) + f(\eta') - f(\eta'_R)\right] \Big\} \mathrm{d}\eta',$$

$$g(\eta) = \Lambda_p \exp\left[\eta + f(\eta) - g(\eta)\right],$$

where $\eta = \beta_3 \tau + \log\left[\frac{\lambda\dot{\gamma}_0(1+\omega t_p)}{b\beta_3^{1/2}}\right]$, and

$$\Lambda_p = \frac{\beta_2(\hat{\rho}_0\beta_3)^{1/2}}{\beta_1\lambda(1+\omega t_p)}, \quad \Lambda_R = \frac{\hat{\Omega}\hat{A}_0}{b\beta_3^{1/2}}, \quad \Lambda_t = \frac{a}{\beta_3}.$$

Here $\beta_3 = \beta_1 a + \beta_2\omega$ and $a = T_{e_t}(0, t_p)$.

Reactive Shear Bands

Boundary Layer Analysis

In terms of dimensional quantities the parameters are approximately given by:

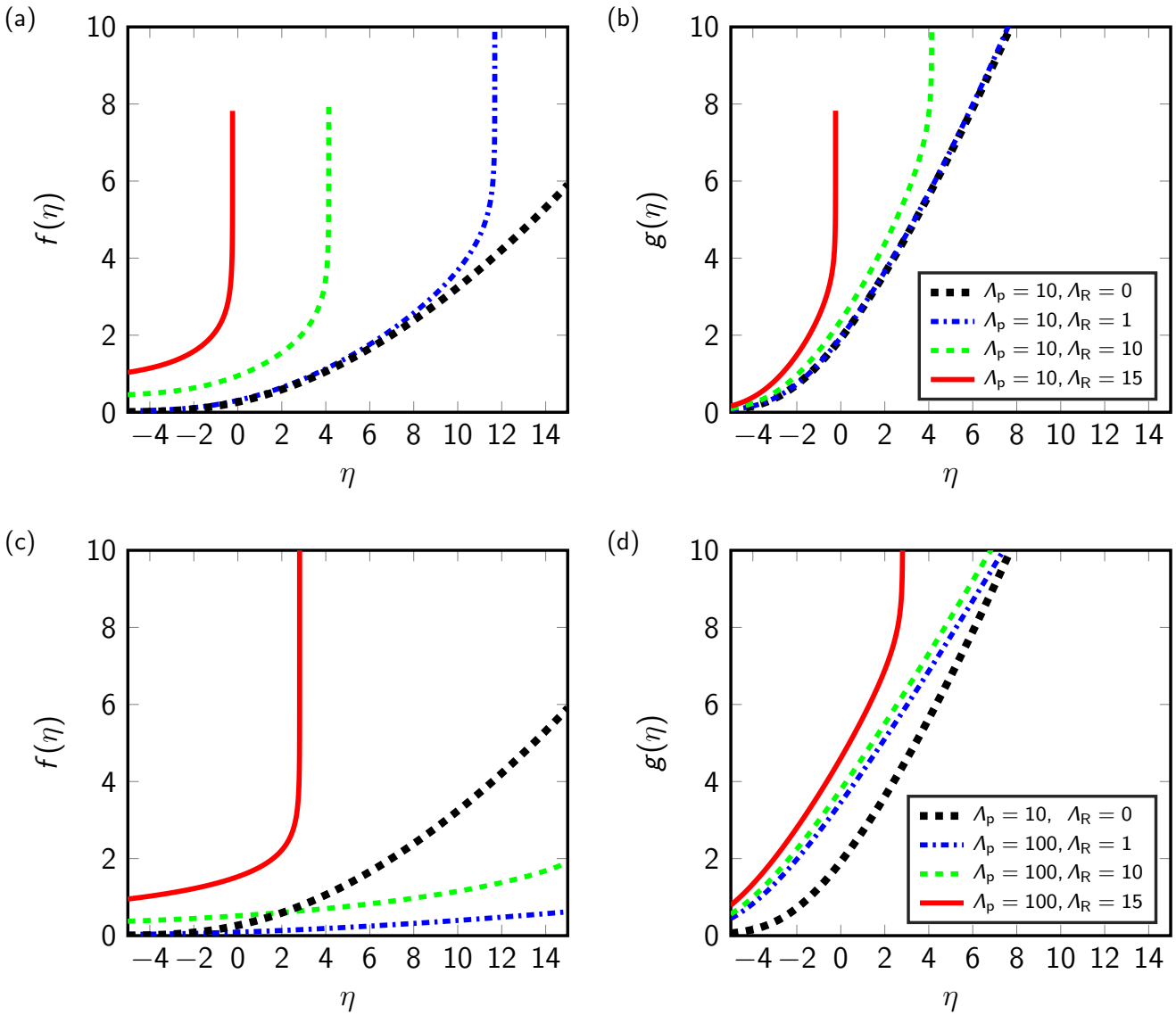
$$\Lambda_p \approx \frac{\rho G T_p (\kappa c w)^{1/2}}{P M^{1/2} s_P^{5/2}} \approx 1\text{–}100,$$

$$\Lambda_R \approx \frac{\Omega M^{1/2}}{c T_p} \approx 0\text{–}20,$$

$$\Lambda_t \approx \frac{a}{\beta_3} \sim \delta \ll 1.$$

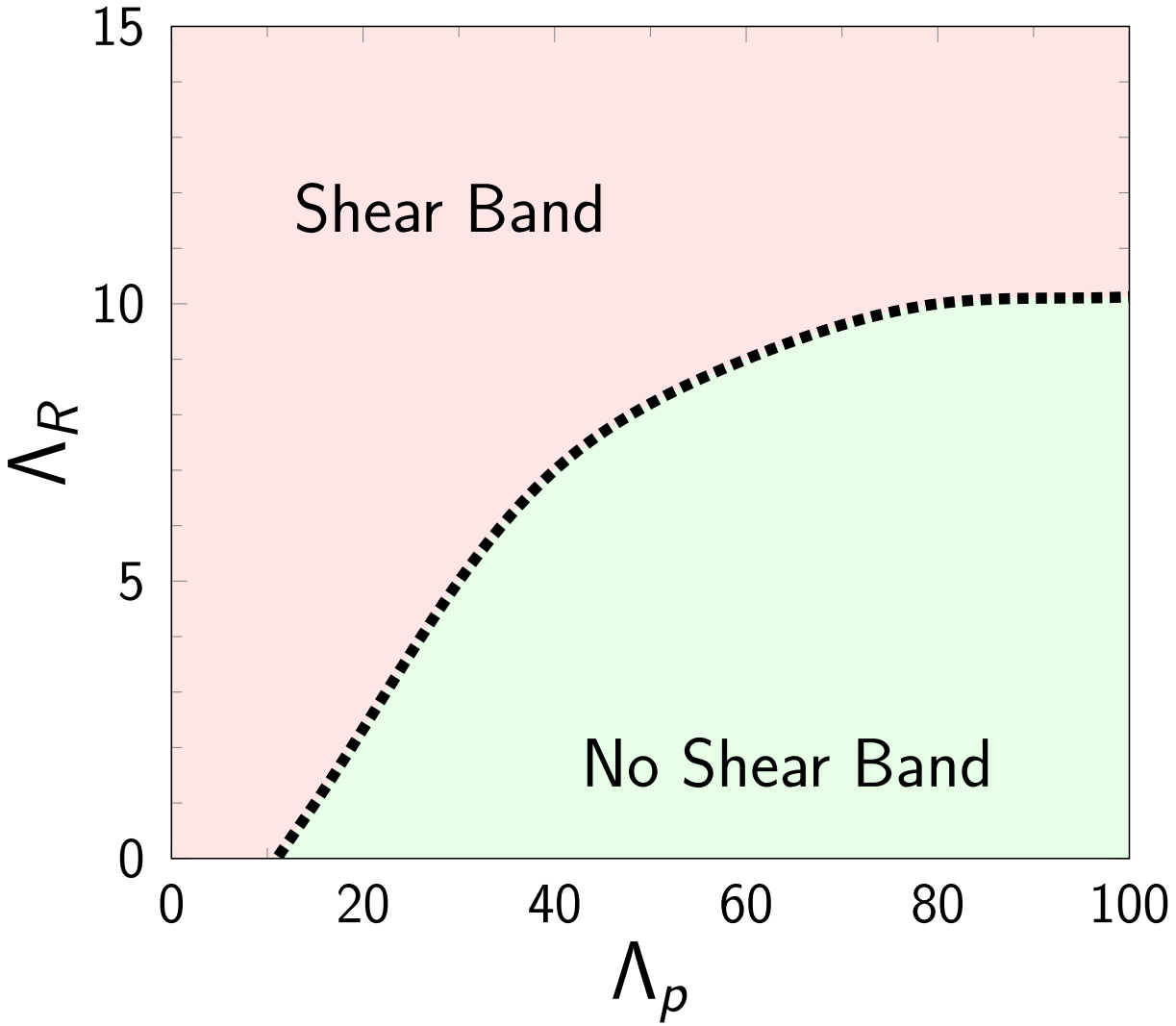
Reactive Shear Bands

Boundary Layer Analysis



Reactive Shear Bands

Boundary Layer Analysis



Elastic-plastic Model

Boundary Layer Analysis

The reactive solution may be matched onto the earlier plastic solution:

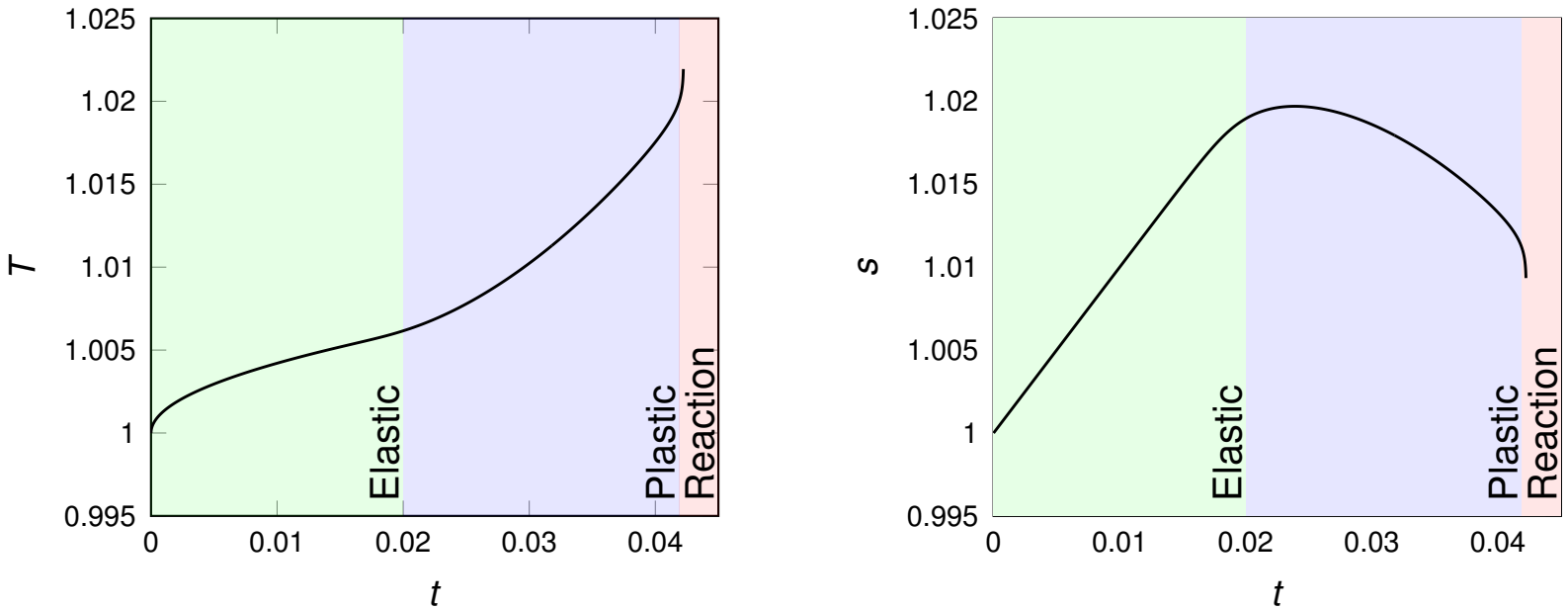


Figure: The centreline temperature $T = T_e + \varepsilon T_1$ and stress $s = s_e + \varepsilon s_1$ for $t = t_p + \varepsilon\tau$. Here the critical plastic and reaction temperatures are $T_p = 1.01$ and $T_R = 1.02$, giving critical times $t_p = 0.02$ and $t_R = 0.0419$, respectively. The value of the small parameter was $\varepsilon = 10^{-2}$.

Reactive Shear Bands

Boundary layer analysis – numerical comparison

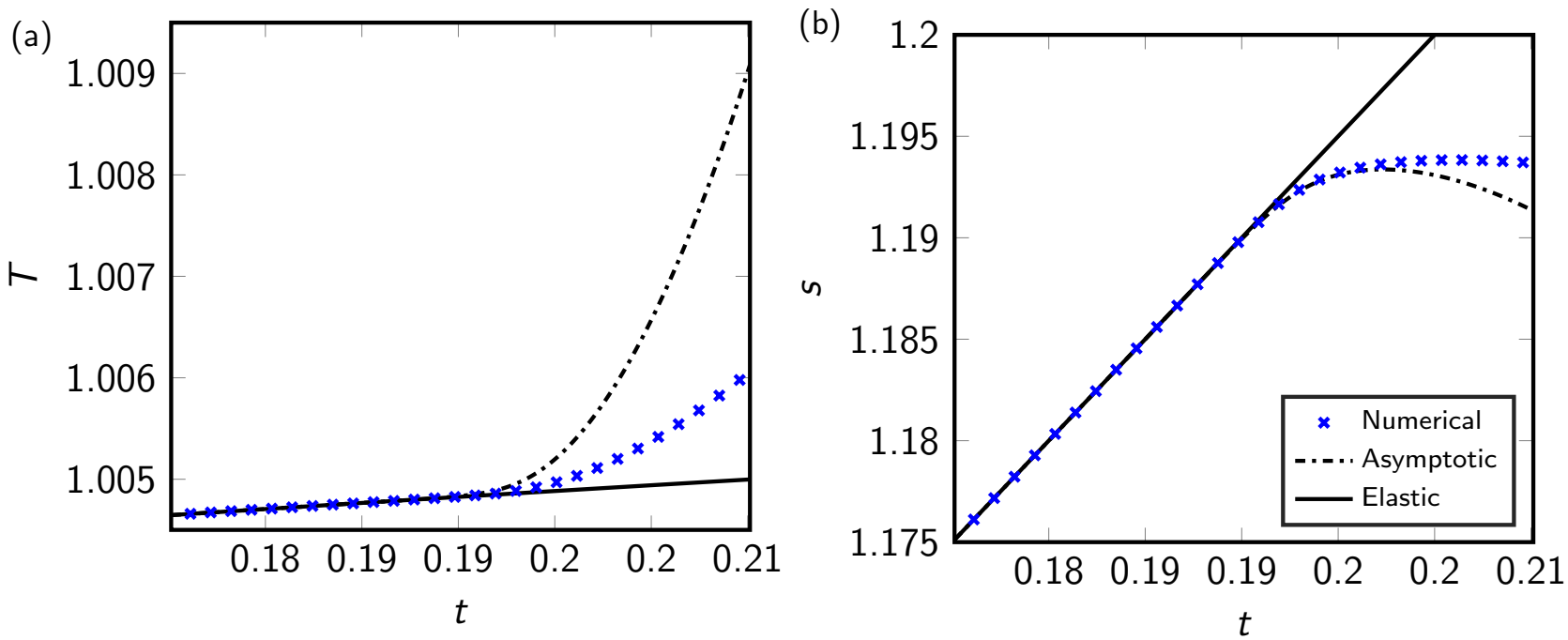


Figure: Comparison of the numerical and asymptotic solutions for the centreline temperature and stress near to the critical plastic time scale $t_p = 0.195$. Note that $\varepsilon = 10^{-3}$.

Reactive Shear Bands

Conclusions

- Numerical solution of Thermo-Viscoplastic model suggest boundary layer.
- Elastic-plastic model more amenable to boundary layer methods.
- Plastic and reaction timescales allow for asymptotic solution near to critical plastic and reaction times t_p and t_R.
- Key features of asymptotic solution compare well with numerical solution using so-called "cohesive" scheme[i].
- Can a similar approach model the onset of reaction in a fully-formed shear band?

[i] F. Zhou et. al. A numerical methodology for investigating the formation of adiabatic shear bands. Journal of the Mechanics and Physics of Solids, 2006.

Acknowledgements

This work was supported by an Engineering and Physical Sciences Research Council industrial CASE partnership with AWE [grant number EP/L505729/1]. Thanks to colleagues at AWE and UEA for useful scientific discussion.