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Title: What do we mean by the word “Shock”?

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Intended for: ASC University Liaison activities and technical collaboration in San Antonio, Texas. This presentation will be given at the University of Texas at San Antonio, Trinity University, and Southwest Research Institute, all in San Antonio.

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What do we mean by the word “Shock”?

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Abstract

From one vantage point, a shock is a continuous but drastic change in state variables that occurs over very small time and length scales. These scales and associated changes in state variables can be measured experimentally. From another vantage point, a shock is a mathematical singularity consisting of instantaneous changes in state variables. This more mathematical view gives rise to analytical solutions to idealized problems. And from a third vantage point, a shock is a structure in a hydrocode prediction. Its width depends on the simulation's grid resolution and artificial viscosity. These three vantage points can be in conflict when ideas from the associated fields are combined, and yet combining them is an important goal of an integrated modeling program. This presentation explores an example of how models for real materials in the presence of real shocks react to a hydrocode's numerical shocks of finite width. The presentation will include an introduction to plasticity for the novice, an historical view of plasticity algorithms, a demonstration of how pursuing the meaning of "shock" has resulted in hydrocode improvements, and will conclude by answering some of the questions that arise from that pursuit. After the technical part of the presentation, a few slides advertising LANL's Computational Physics Student Summer Workshop will be shown.

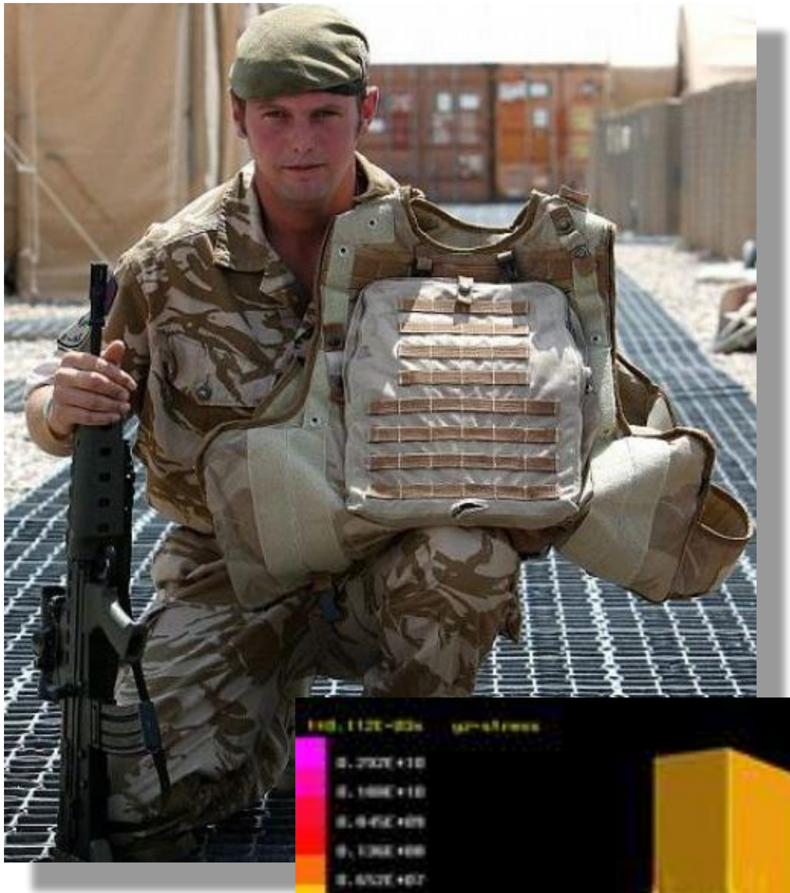
Outline

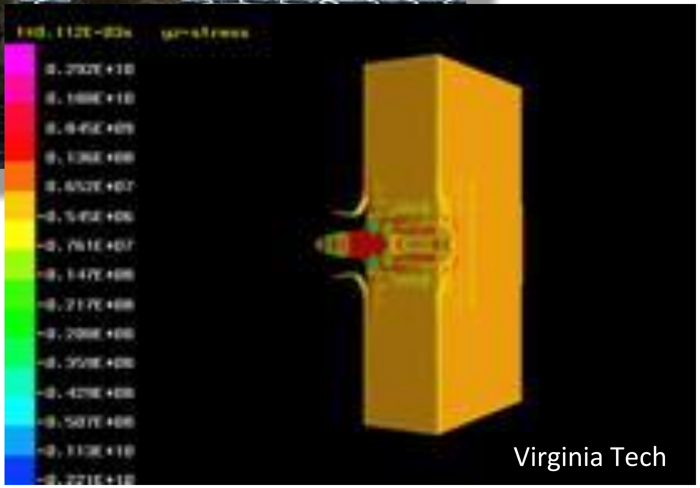
(1)
Motivation: What is strain rate in a shock?

(2)
Introduction to plasticity and historical overview

(3)
Digging into the question: Strain rate, shock, and plasticity

(4)
Benefits to hydrocodes

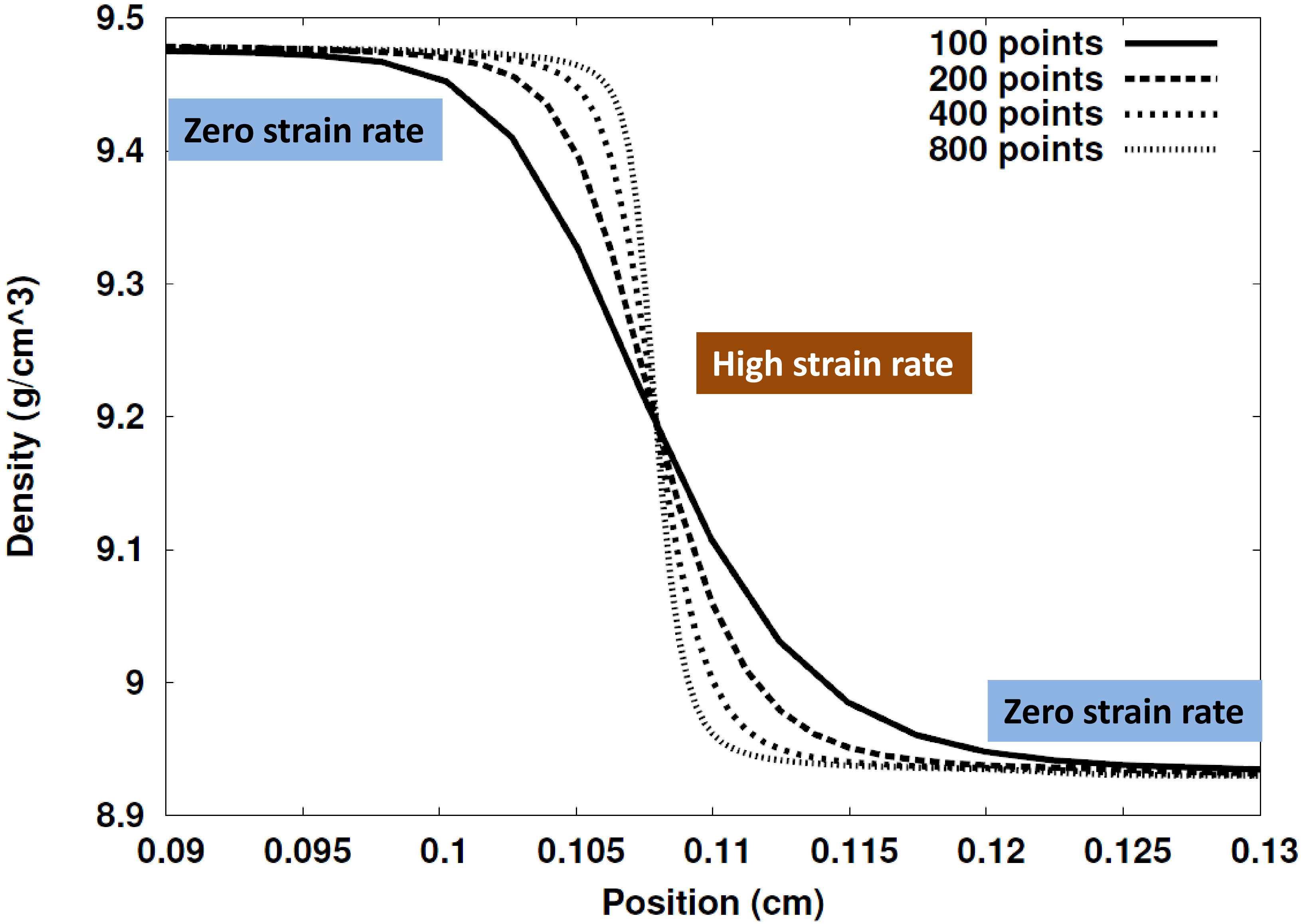




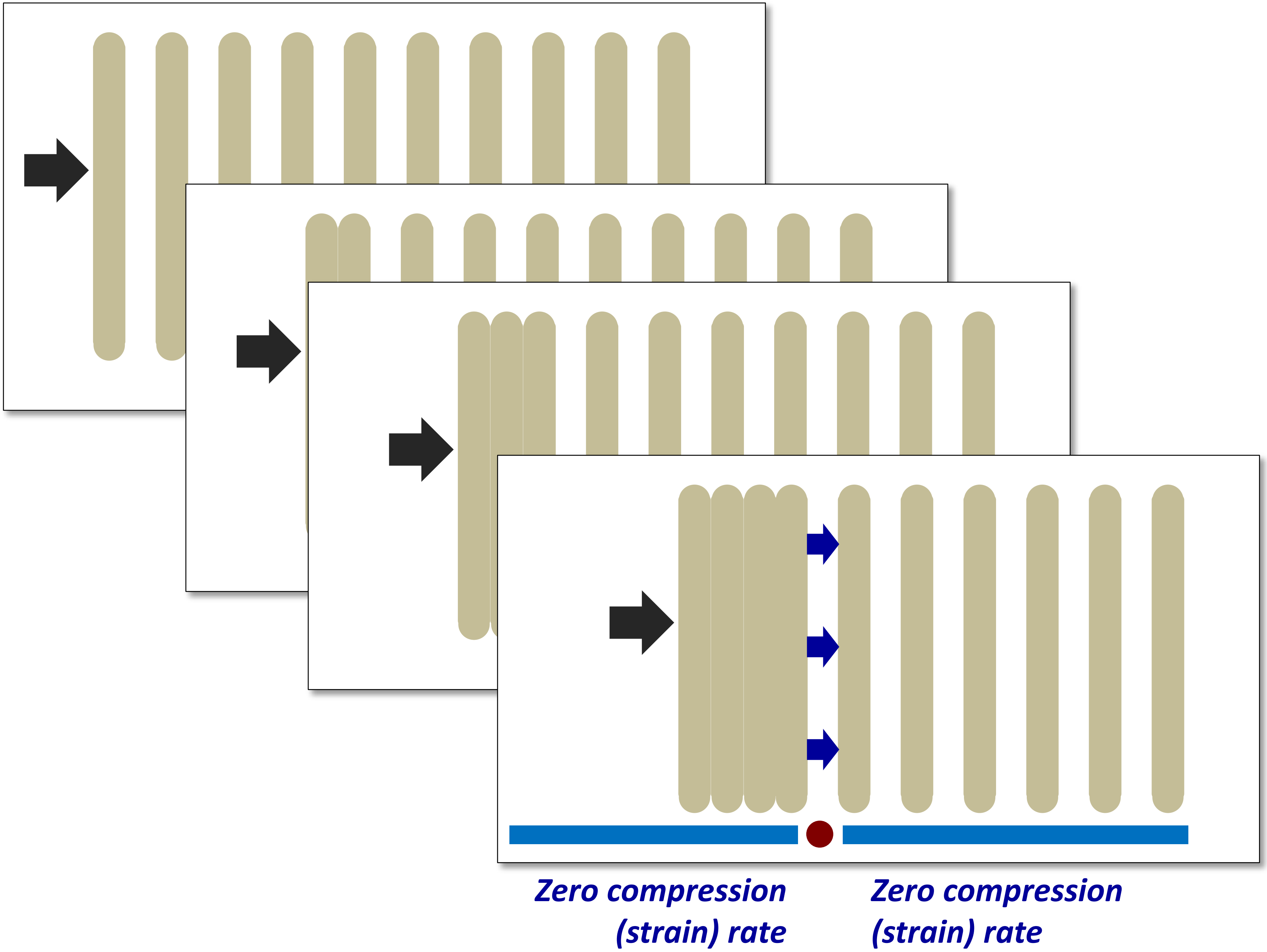
Hydrocodes Converge Toward an Idealized Shock

Underlying plot shown on next slide.

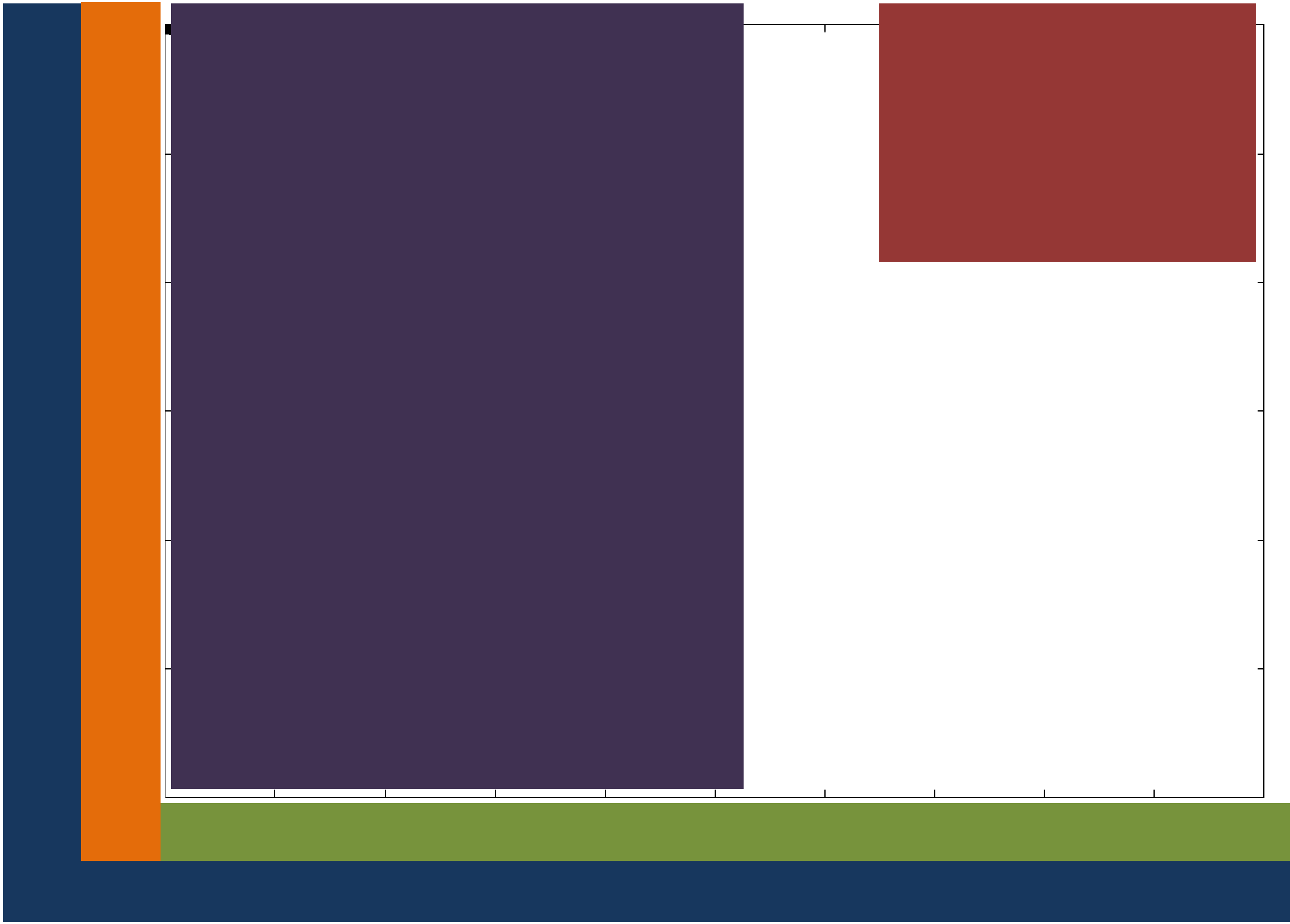
Similar Results when Material is a Solid



Popsicle Analogy of a Shock

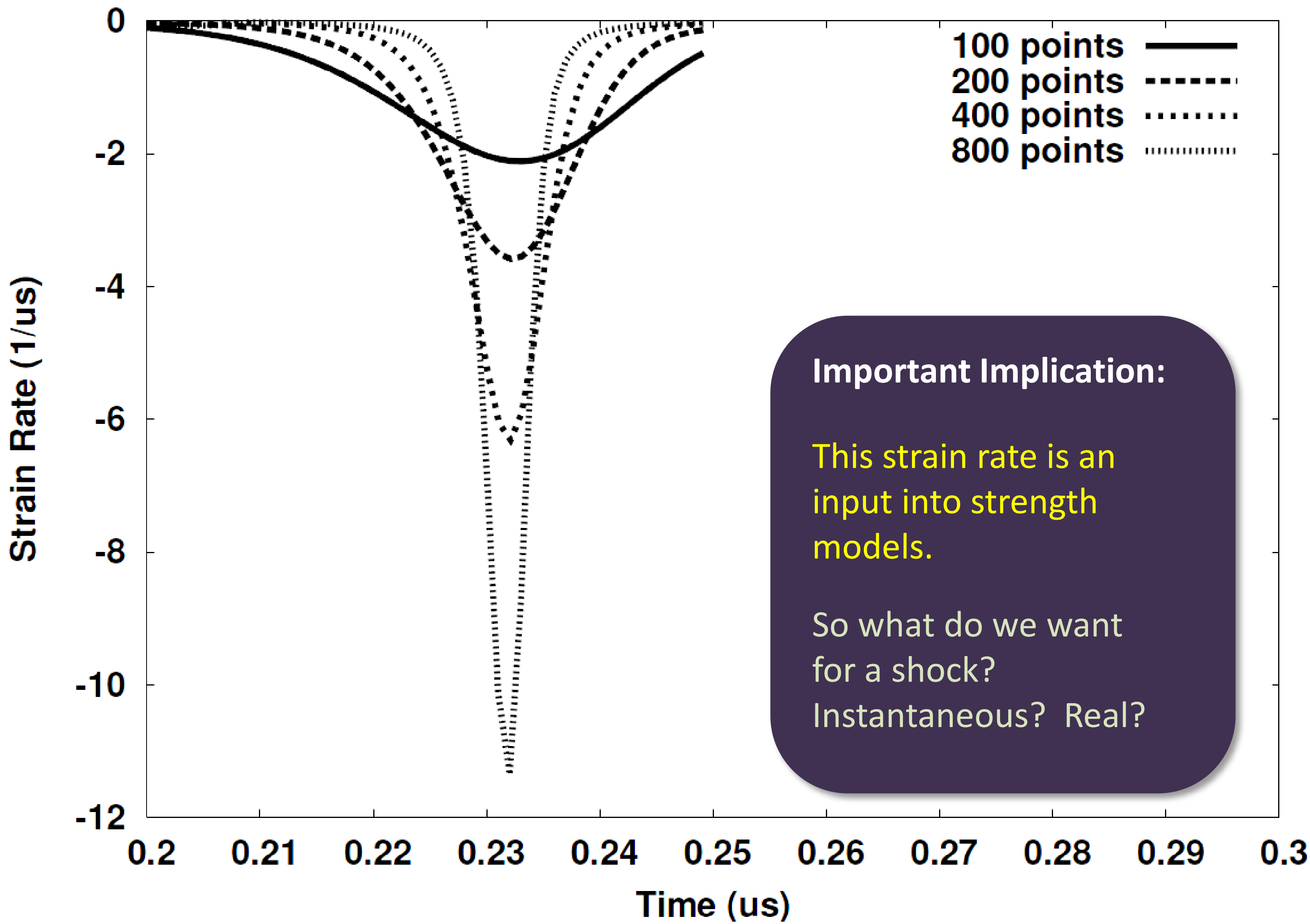


Strain Rate Approaches as Dirac Delta



Underlying plot shown on next slide.

Strain Rate Approaches as Dirac Delta

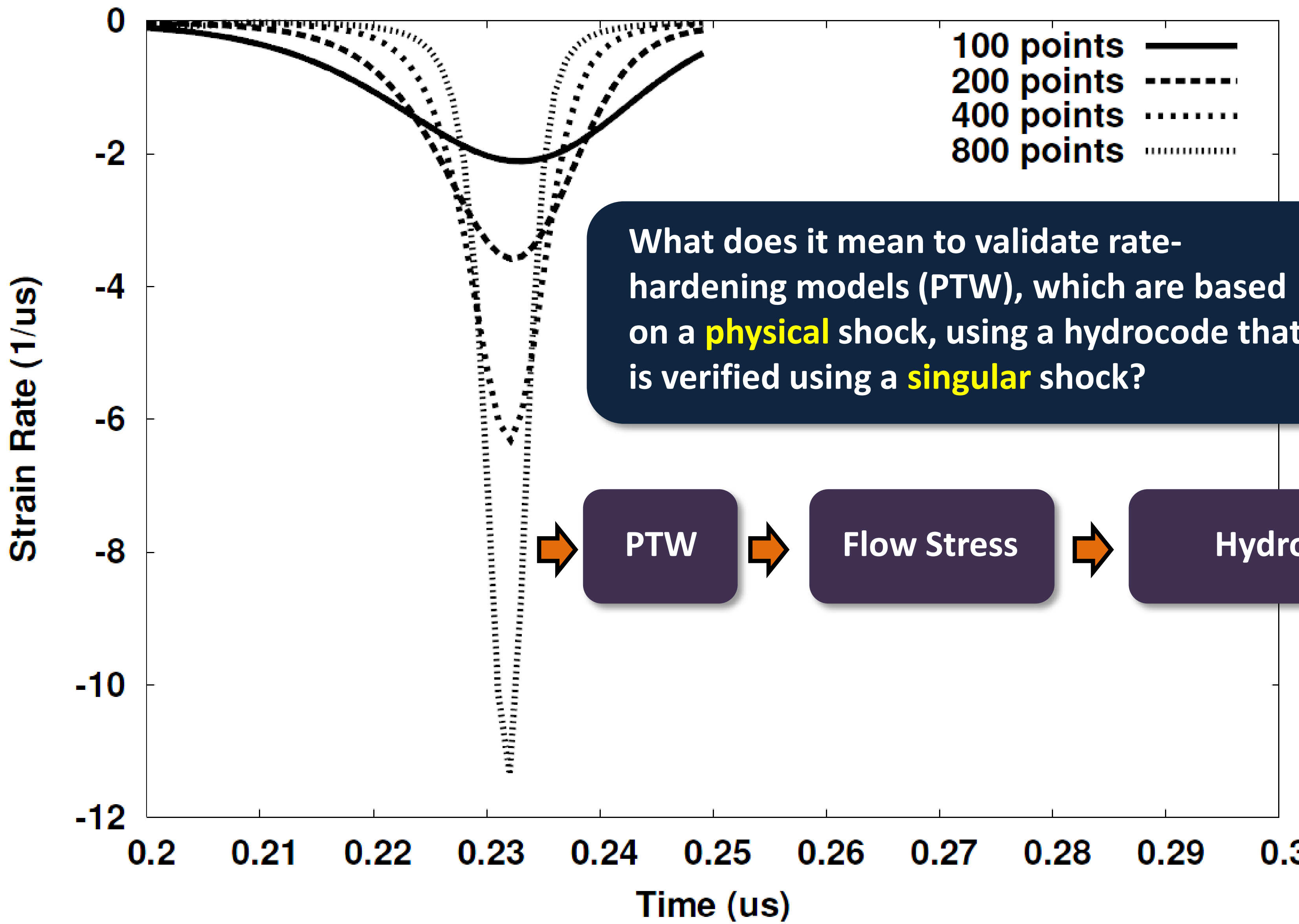


Important Implication:

This strain rate is an input into strength models.

So what do we want for a shock? Instantaneous? Real?

Strain Rate Approaches as Dirac Delta



What does it mean to validate rate-hardening models (PTW), which are based on a **physical** shock, using a hydrocode that is verified using a **singular** shock?

PTW → Flow Stress → Hydro

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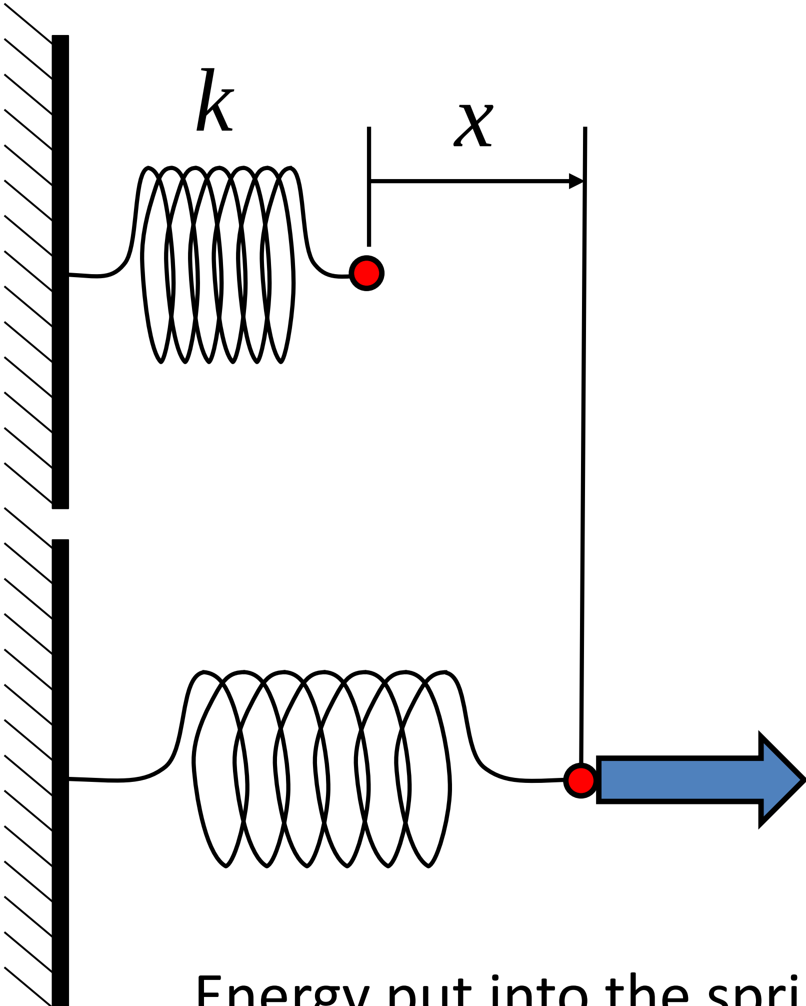
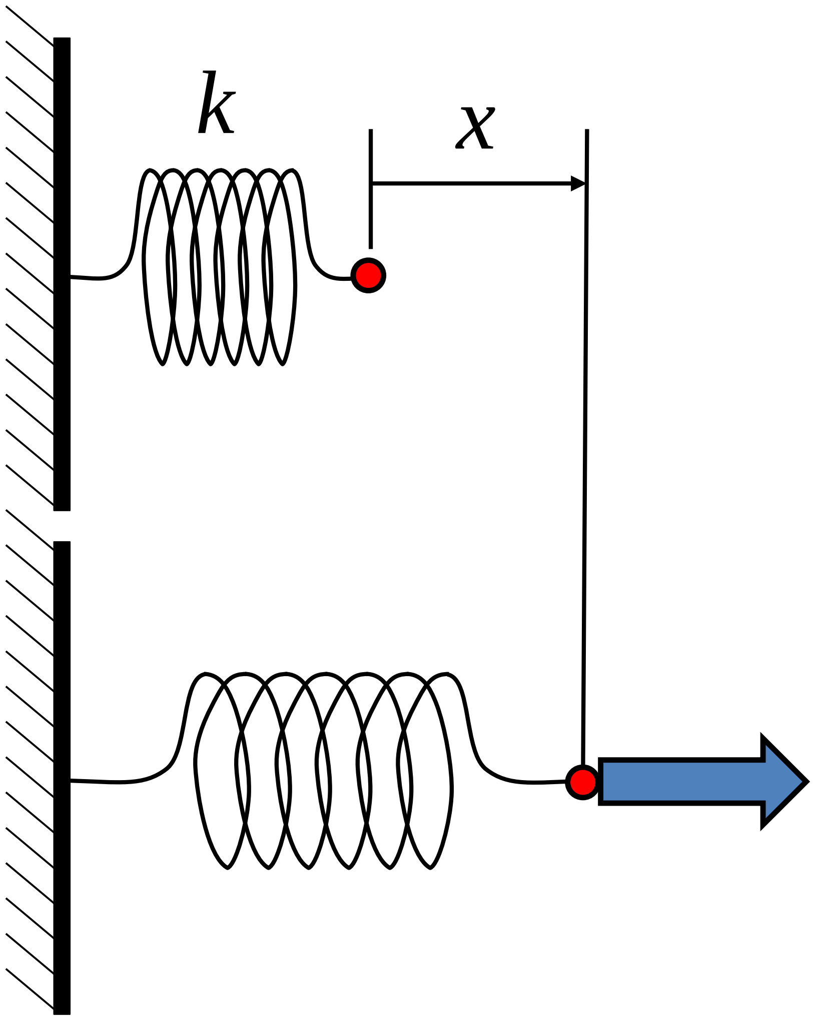


$$F = k \cdot x$$

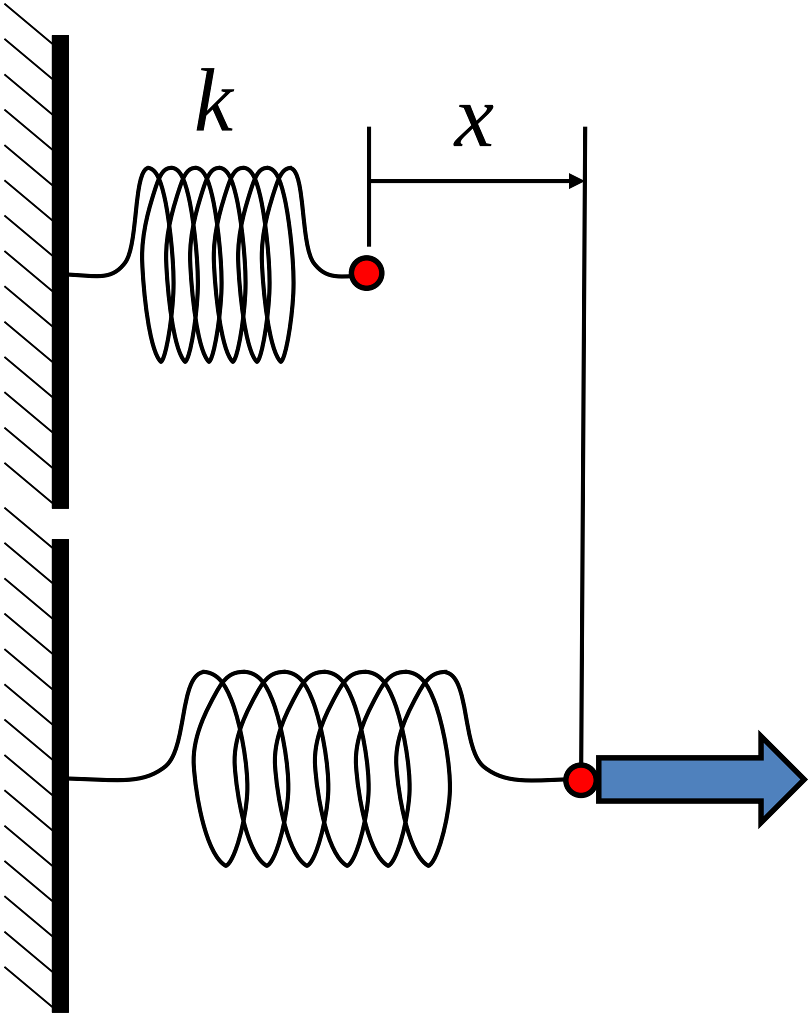
Energy put into the spring = Work = Force x Distance

$$W = \int_0^x F \cdot dx = \frac{1}{2} k x^2$$



$$F = k \cdot x$$

$$W = \frac{1}{2} k x^2$$



The force is the gradient of the energy

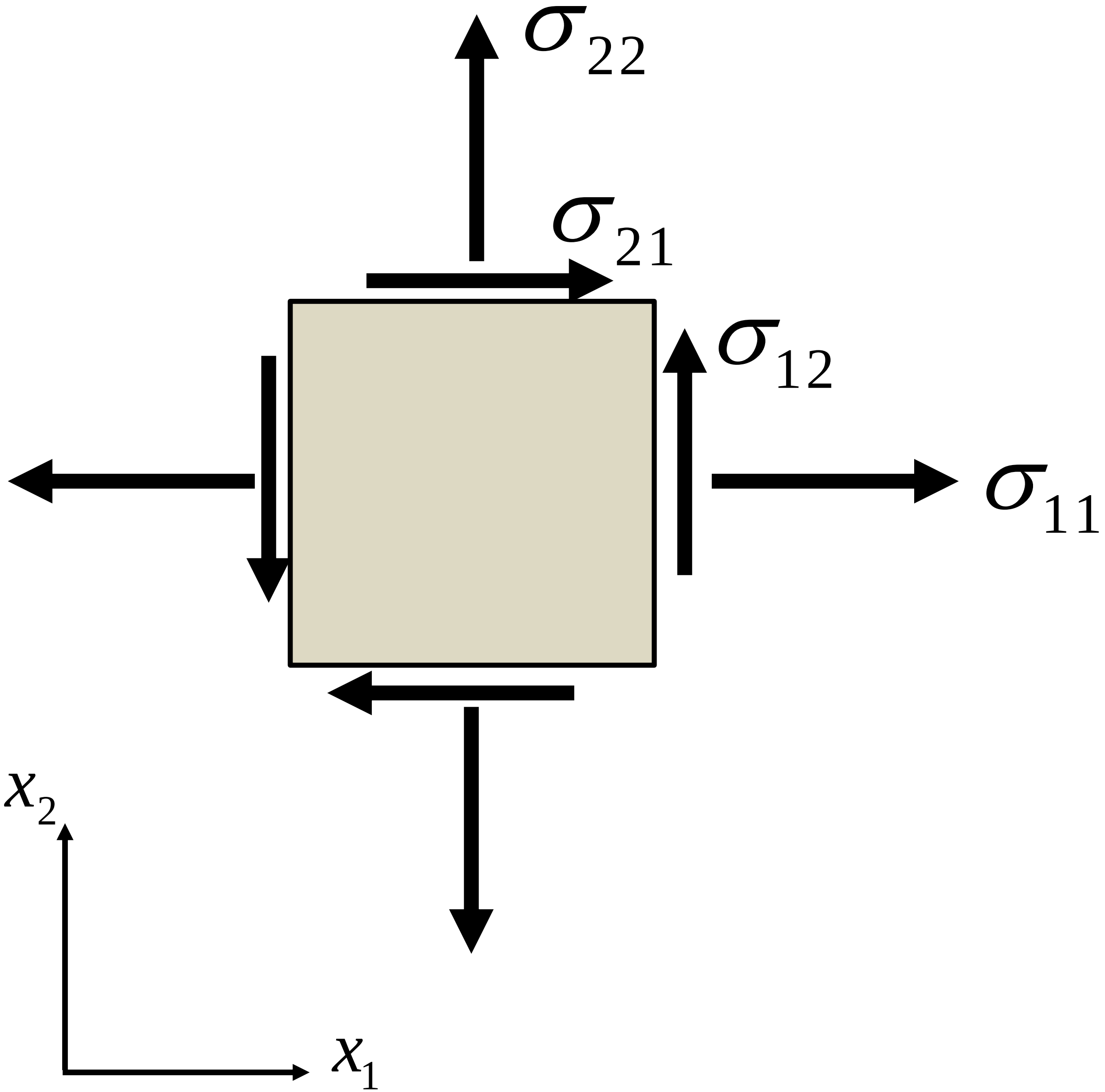
$$F = \frac{d}{dx}W$$

$$F = k \cdot x$$

Relationship

$$W = \frac{1}{2}kx^2$$

In Multi-Dimensional Problems we need a Stress Tensor



Hooke's Law is like a spring but in all directions and including shear. We use a 4th order tensor

$$E_{ijkl}$$

G

Shear Modulus

Indices range from 1-3.

$$F = k \cdot x$$

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl} = \sum_{k=1}^{3}\sum_{l=1}^{3} E_{ijkl}\varepsilon_{kl}$$

Repeated indices imply summation.

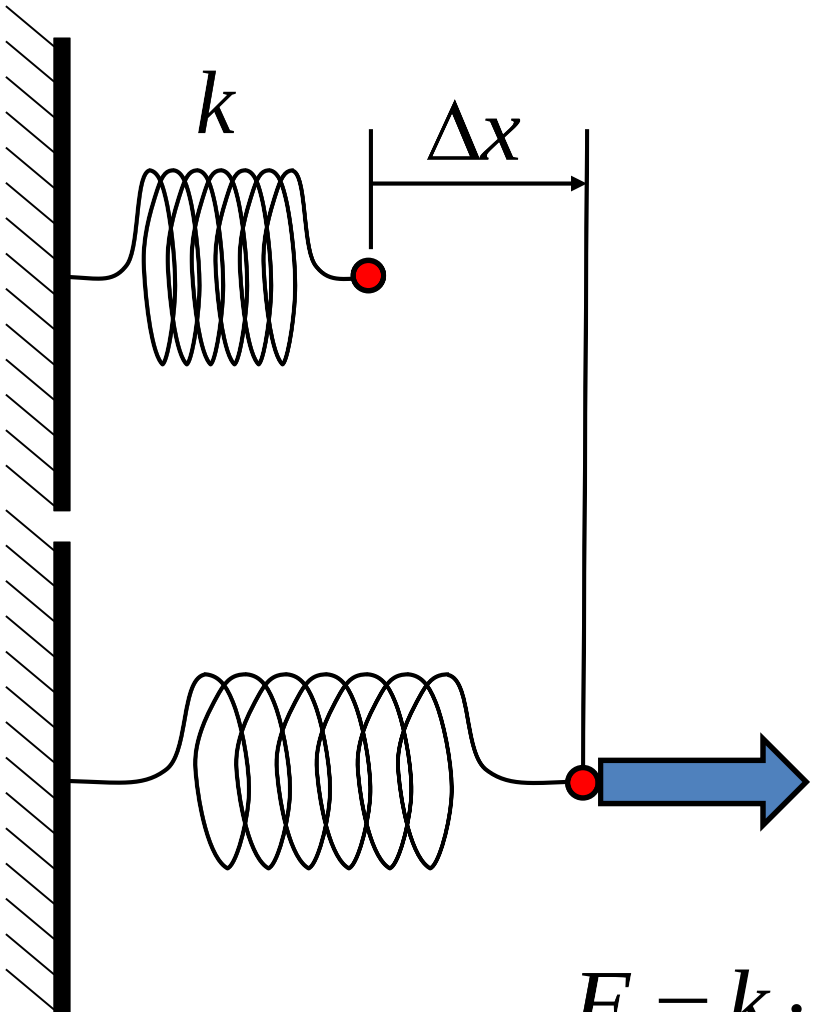
If ε_{kl} is strain

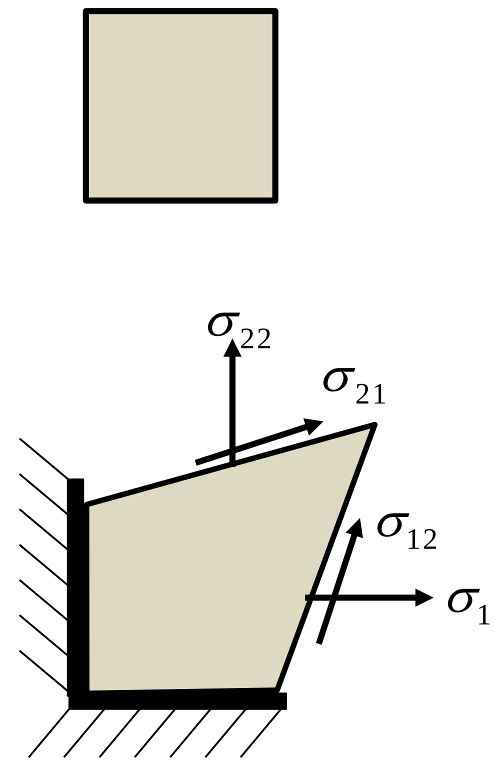
and E_{ijkl} is a constant, then this,

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$$

is the most general form of Hooke's Law for elastic deformation. It can be inverted:

$$\varepsilon_{kl} = D_{ijkl}\sigma_{ij}$$



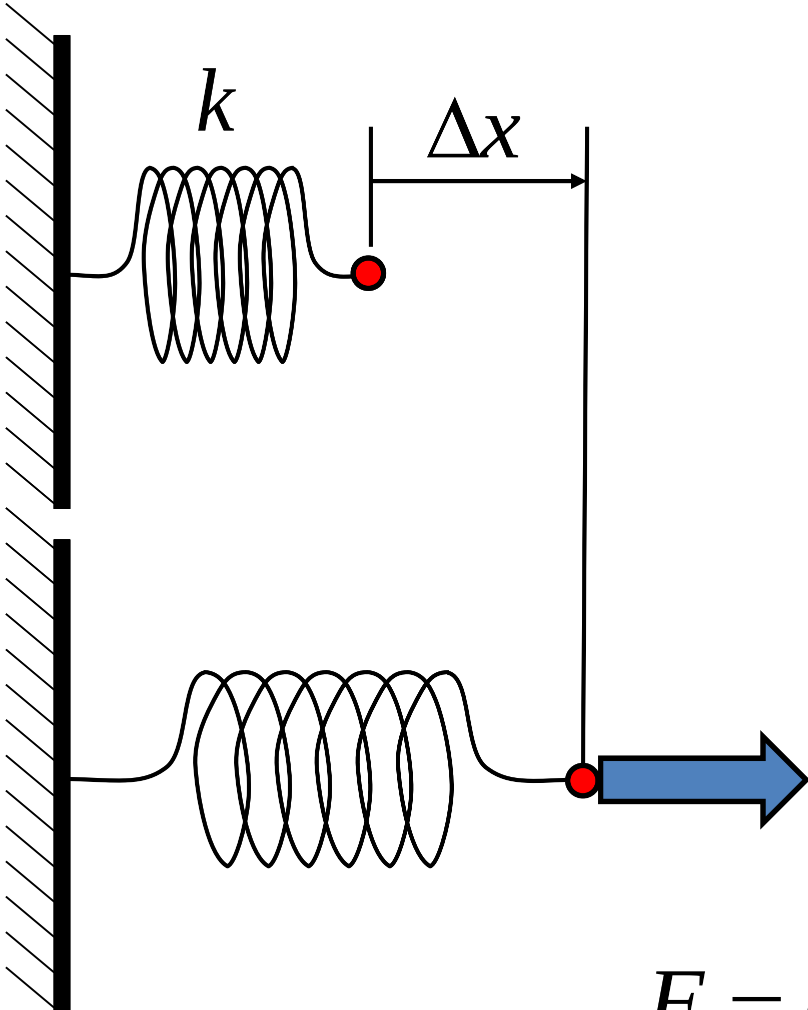


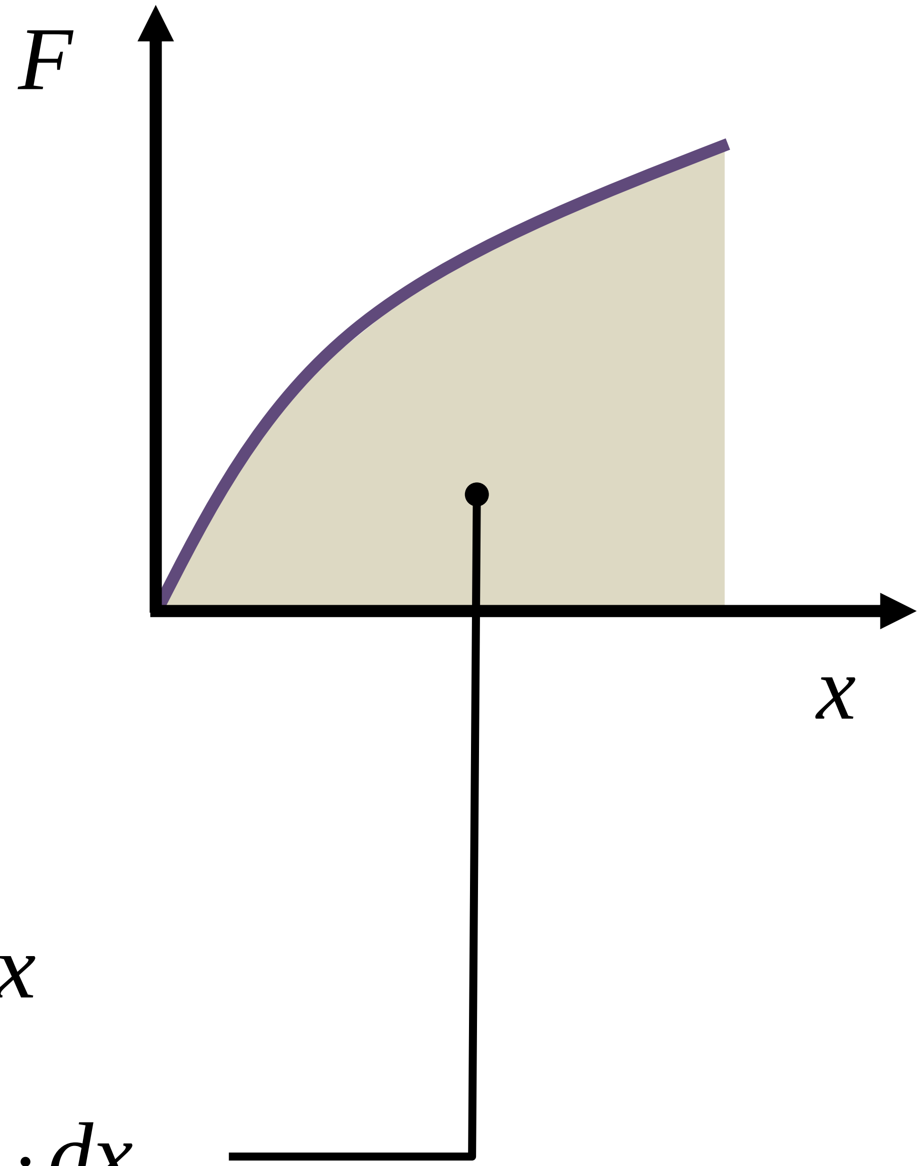
$$F = k \cdot \Delta x$$

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$$

$$F = \frac{dW}{dx}$$

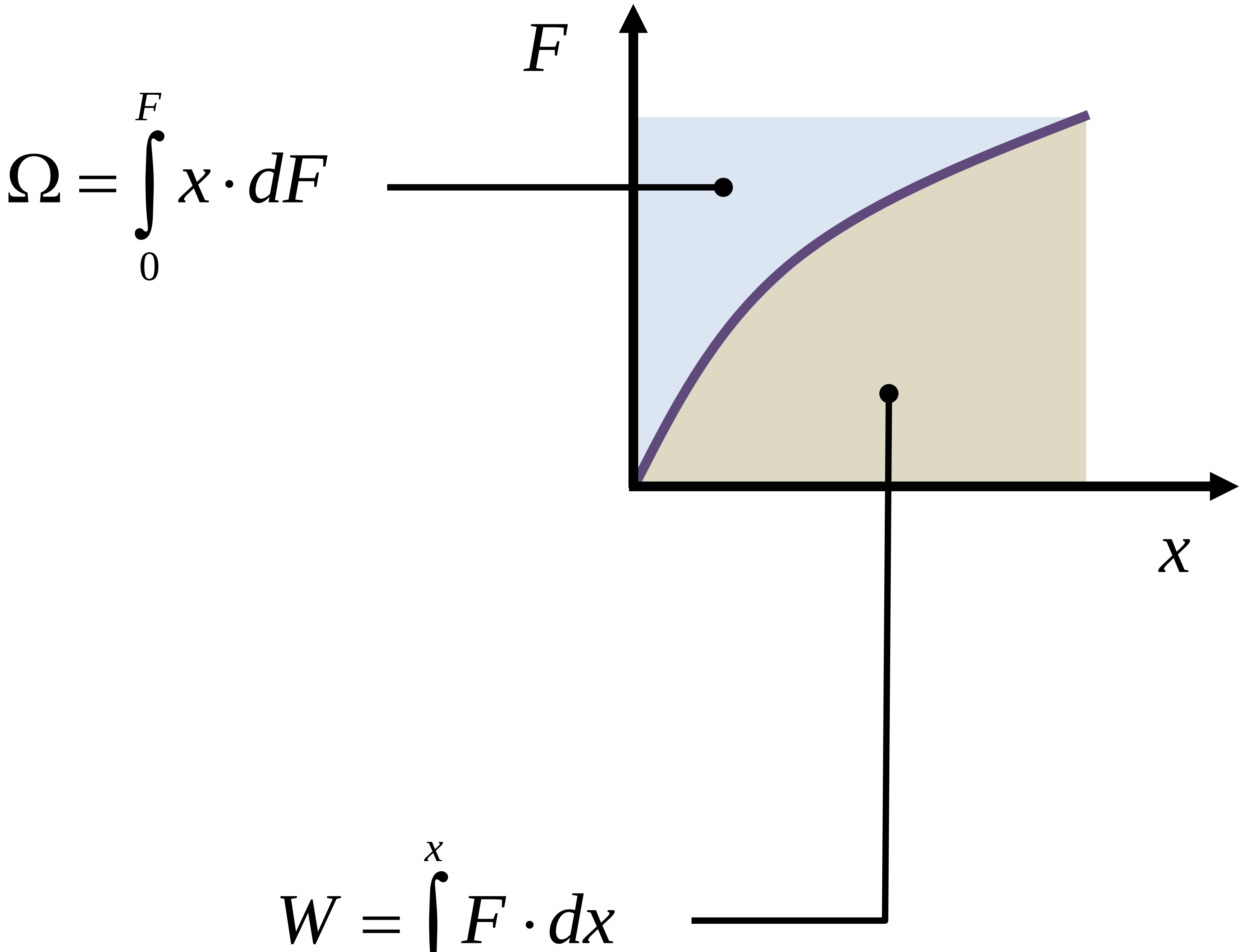
$$\sigma_{ij} = \frac{dW}{d\varepsilon_{ij}}$$



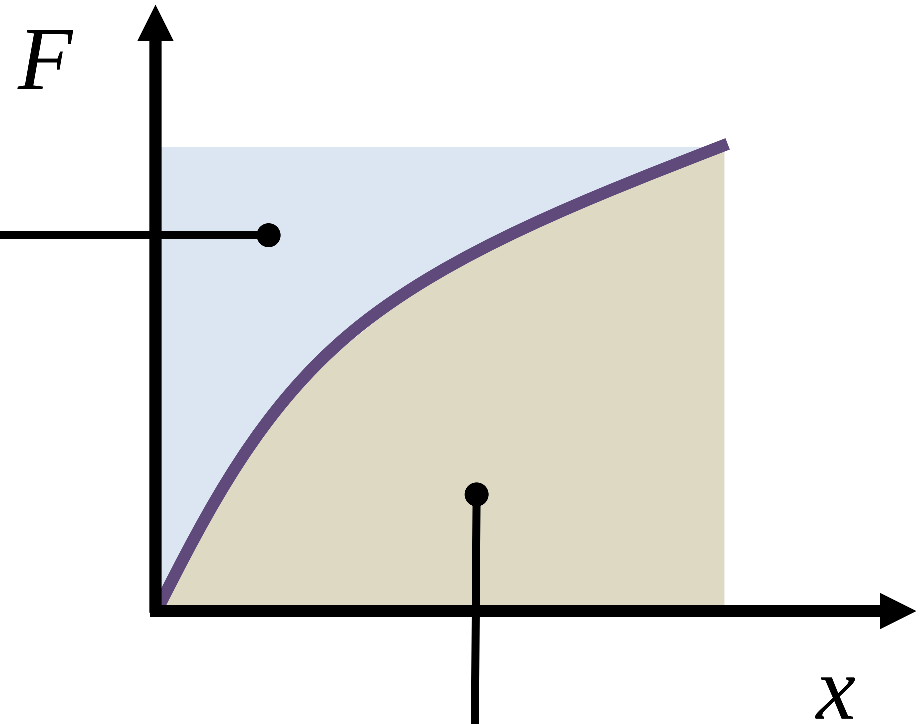


$$F = k \cdot x$$

$$W = \int_0^x F \cdot dx$$

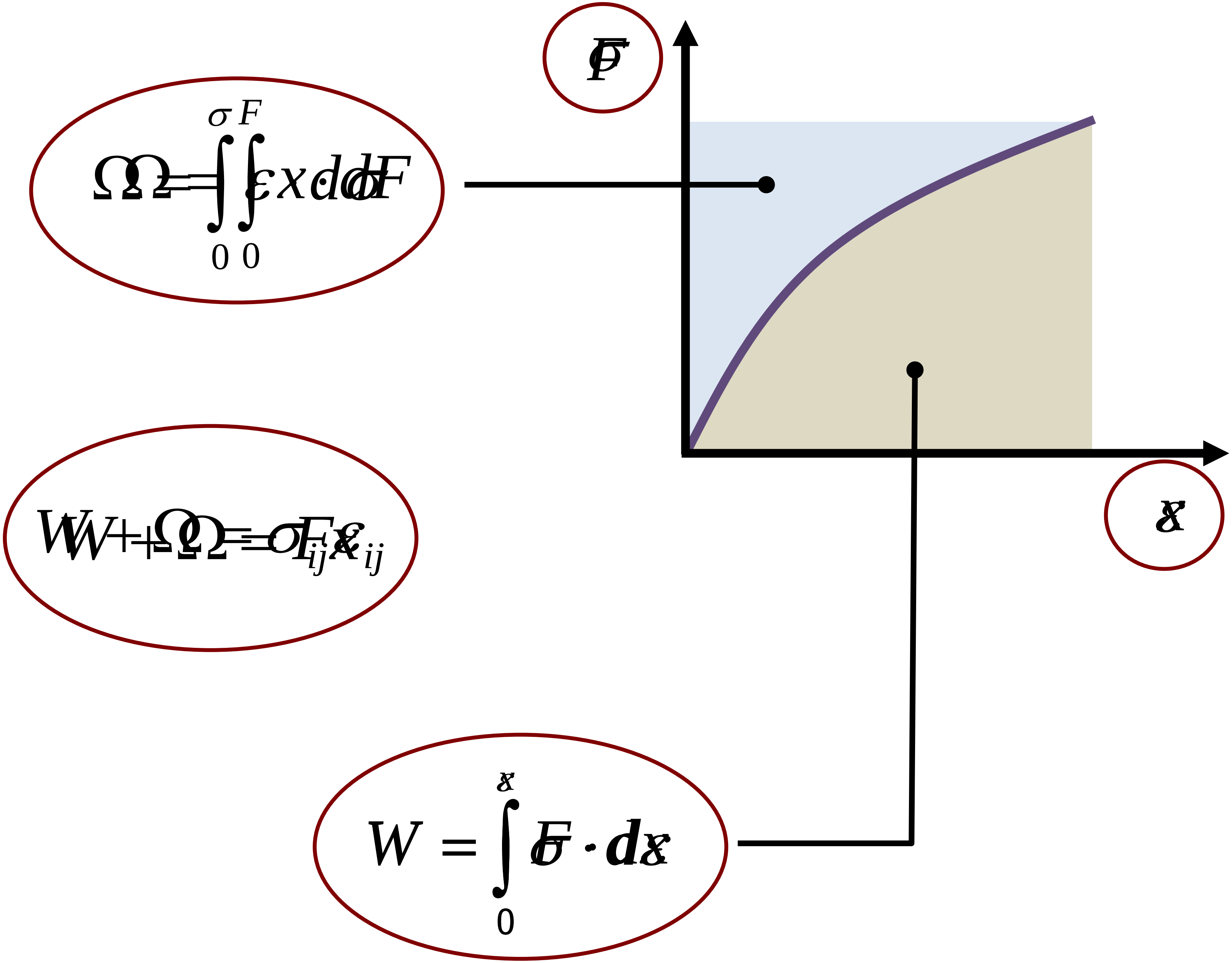

F
x
$\Omega = \int_0^F x \cdot dF$
$W = \int_0^x F \cdot dx$

$$\Omega = \int_0^F x \cdot dF$$



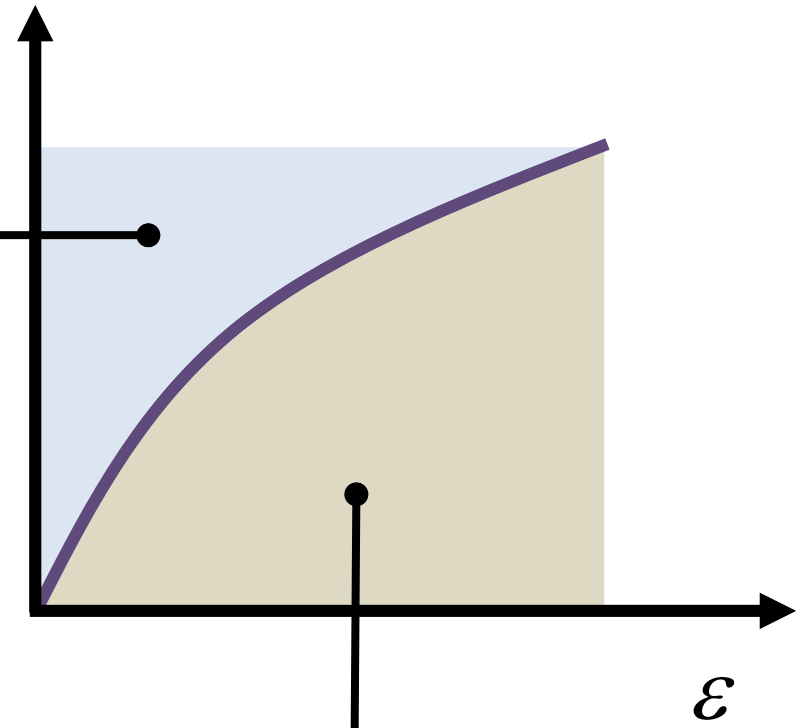
$$W + \Omega = Fx$$

$$W = \int_0^x F \cdot dx$$



$\Omega = \int_0^{\sigma} \varepsilon \, d\sigma$
$\Omega = \int_0^{F} x \, dF$
$W + \Omega = \sigma_{ij} \varepsilon_{ij}$
$W + \Omega = F x$
$W = \int_0^{\varepsilon} \sigma \cdot d\varepsilon$
$W = \int_0^{x} F \cdot dx$
σ / F
ε / x

$$\Omega = \int_0^{\sigma} \varepsilon \cdot d\sigma$$



$$W + \Omega = \sigma_{ij}\varepsilon_{ij}$$

$$W = \int_0^{\varepsilon} \sigma \cdot d\varepsilon$$

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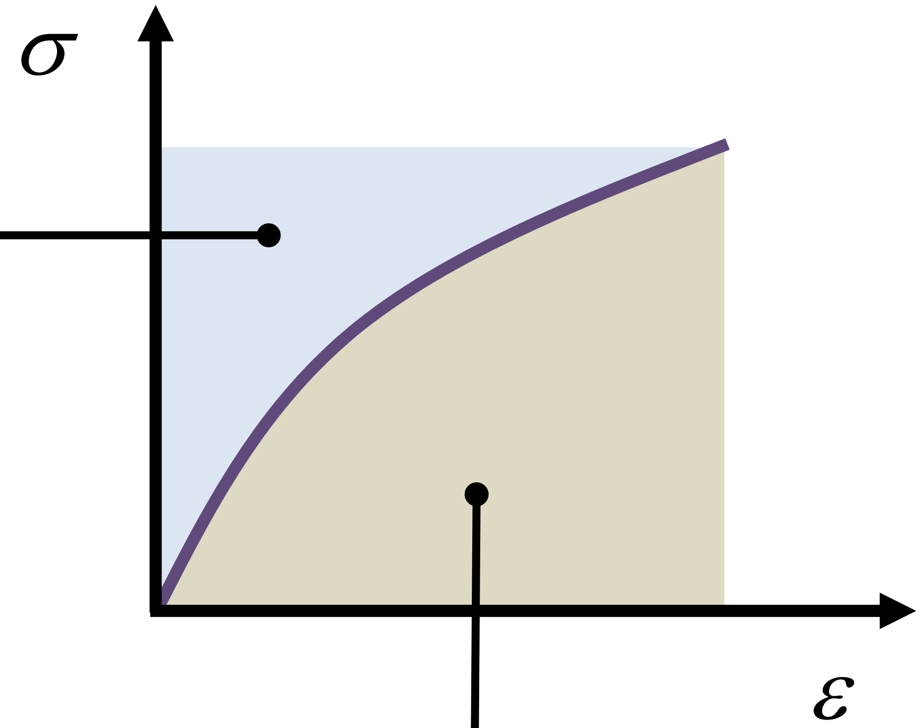


$$W + \Omega = \sigma_{ij}\varepsilon_{ij}$$

$$W = \int_0^{\varepsilon} \sigma \cdot d\varepsilon$$

$$\Omega = \int_0^{\sigma} \varepsilon \cdot d\sigma$$

$$W = \int_0^{\varepsilon} \sigma \cdot d\varepsilon$$

$$W + \Omega = \sigma_{ij}\varepsilon_{ij}$$

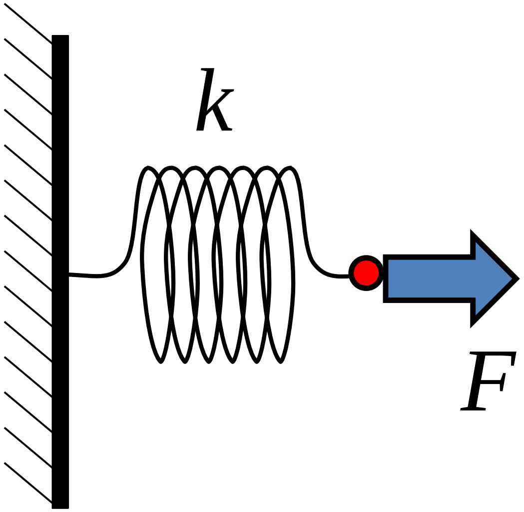
$$\varepsilon_{ij} = \frac{d\Omega}{d\sigma_{ij}}$$

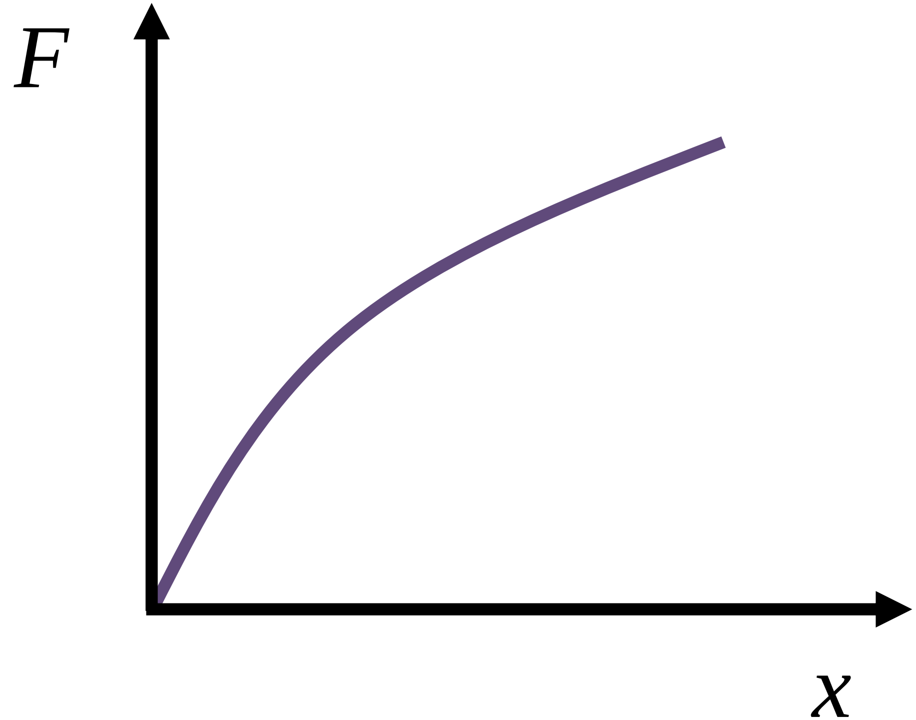
Strain can be expressed as the gradient of its compliment.

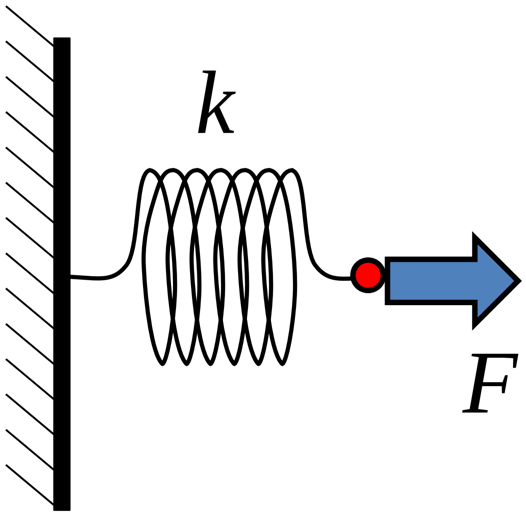
$$\sigma_{ij} = \frac{dW}{d\varepsilon_{ij}}$$

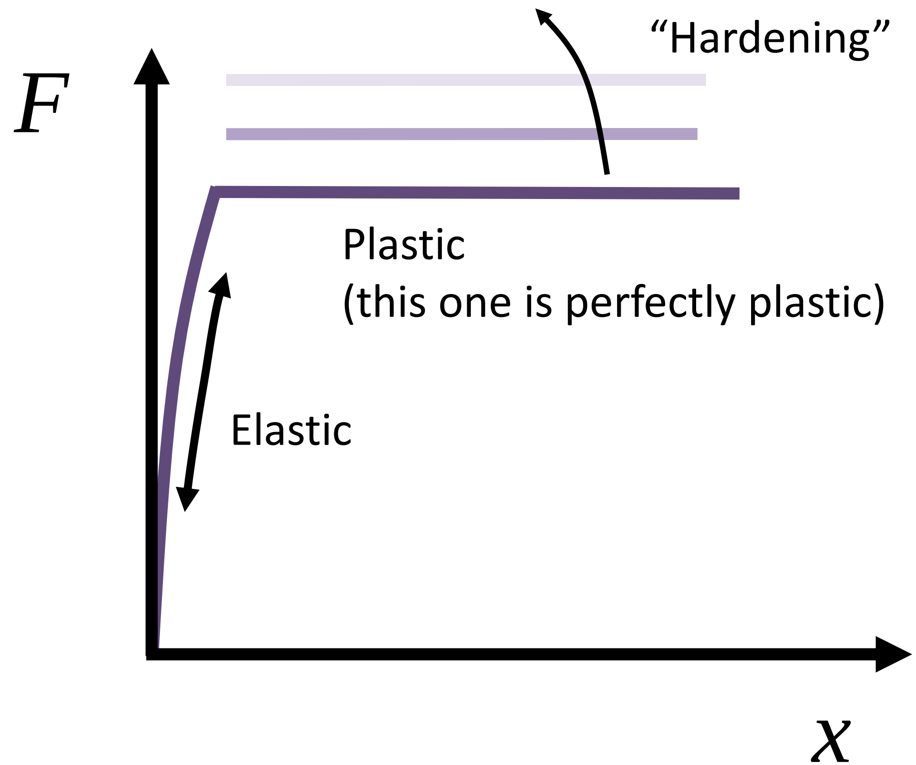
Stress can be expressed as the gradient of the energy density function.

Key point in discussing plasticity…next…


k
F


F
x





<u>In the Plastic Range</u>

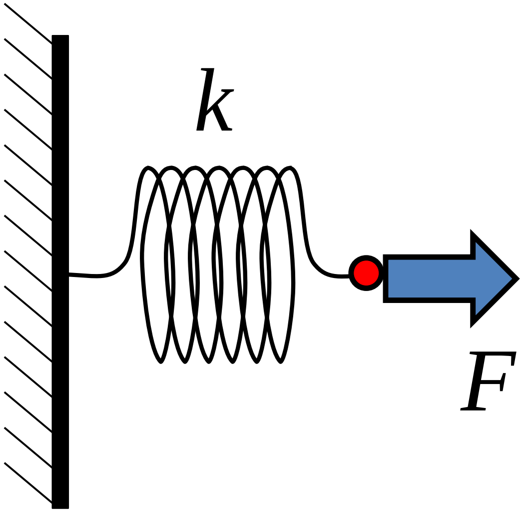
A simple relationship between

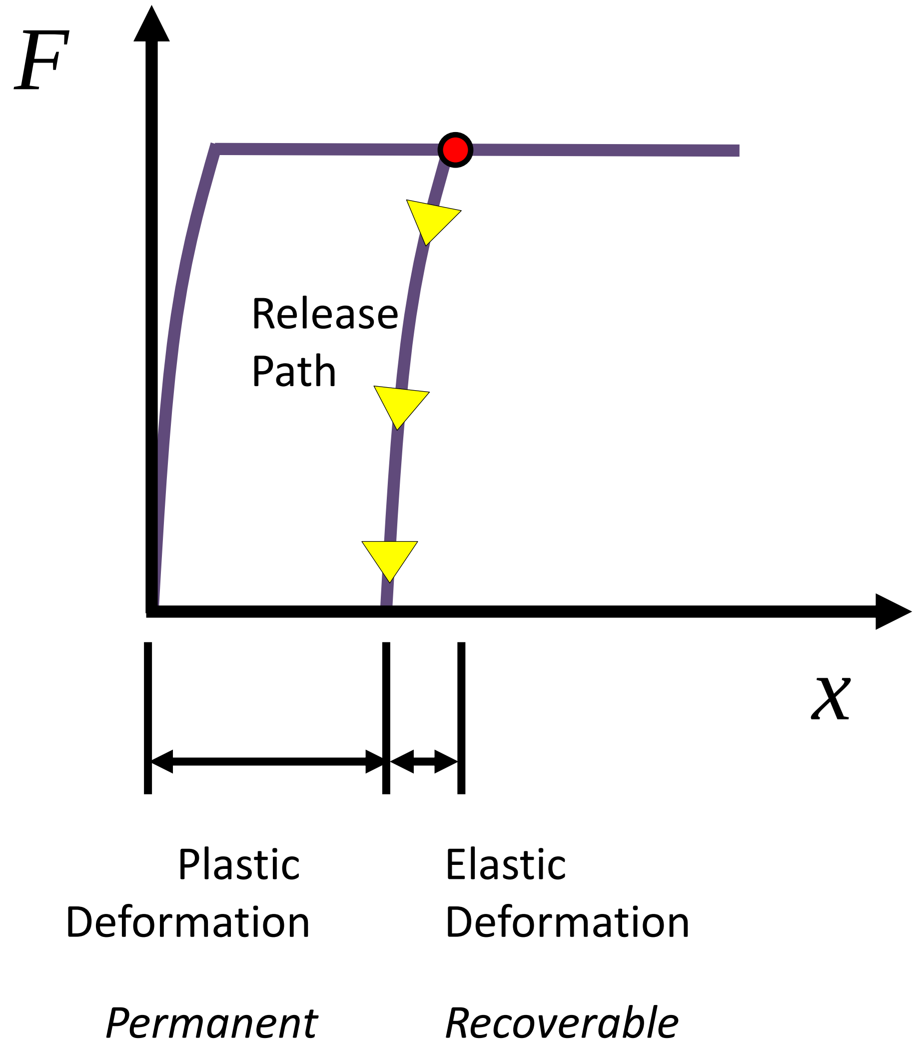
$$F \not\Leftrightarrow x$$

is no longer possible.

<u>Instead we discuss increments</u>

$$dF \Leftrightarrow dx \quad \checkmark$$

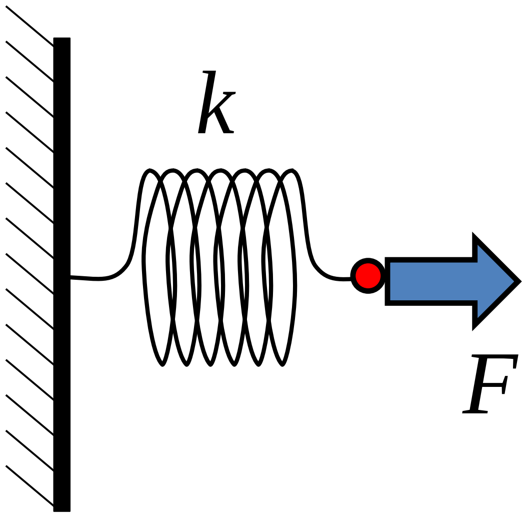


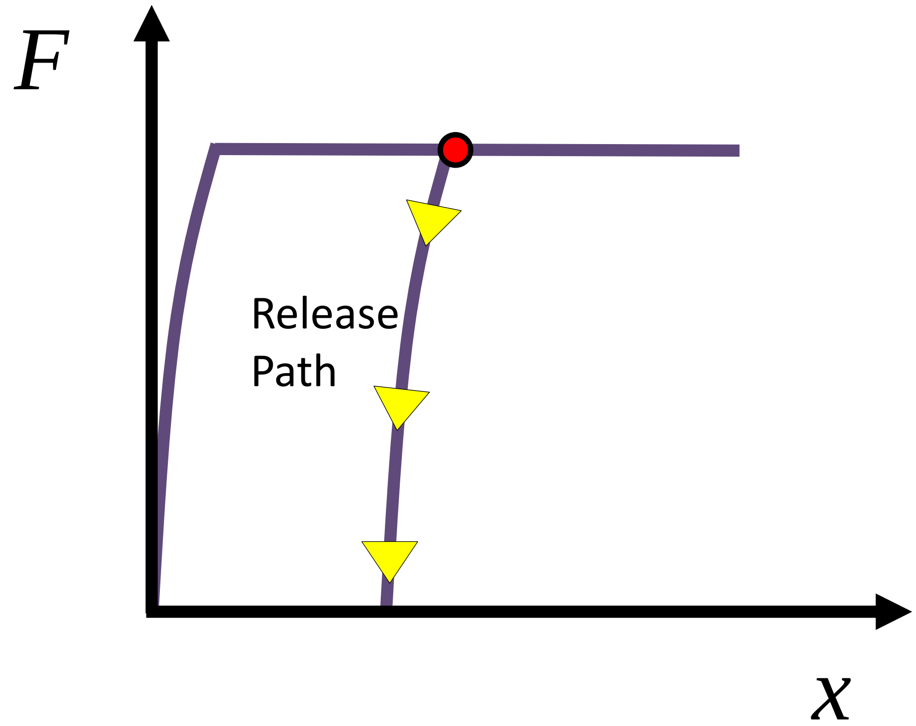


In 3D increments: total = plastic + elastic

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Key point





Handled By

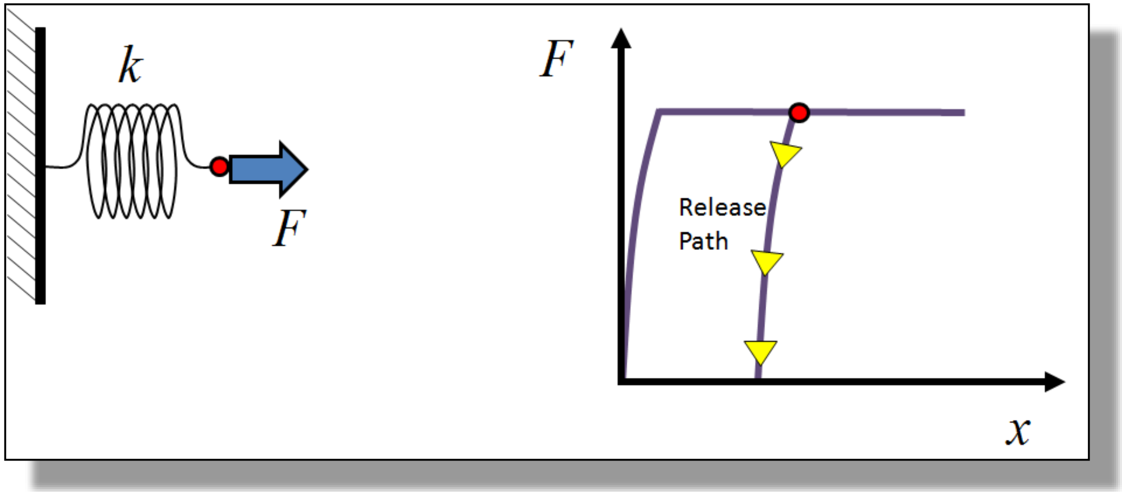
"Flow Rule" Hooke's Law

In 3D increments: total = plastic + elastic

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Key point

First, we need a 3-D solid model for this:



For a tensor with 9 components

$$\sigma_{ij}$$

we need a single value to determine when it yields.

Determining how the plastic strain is related to stress is a central part of plasticity.

"Flow Rule"

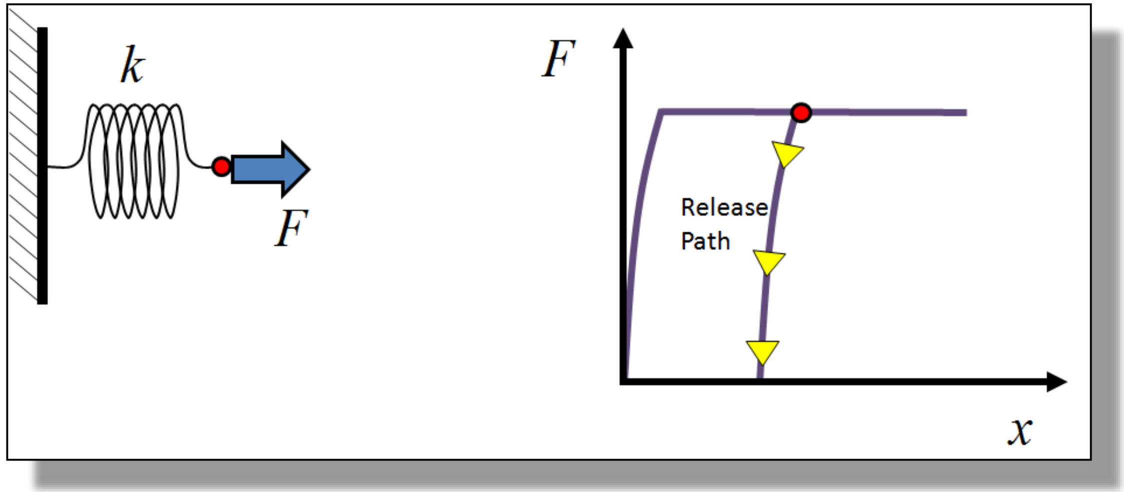
$$d\sigma_{ij} \Leftrightarrow d\varepsilon_{ij}^{p}$$

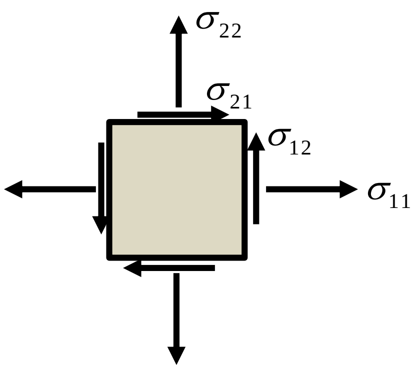
? ? ? ? ? ?

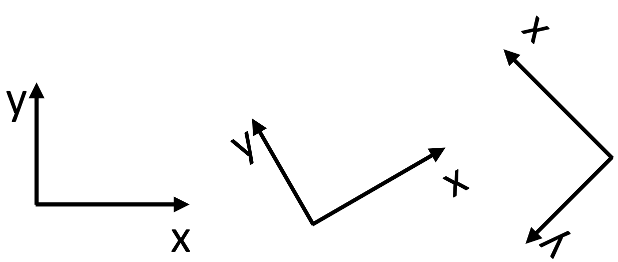
For a tensor with 9 components

$$\sigma_{ij}$$

we need a single value to determine when it yields.







It must be invariant with respect to the choice of coordinate system.

Here is one that works:

$$J_2 = (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6\left(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{32}^2\right)$$

von Mises Yield Criteria

$$J_2(\sigma) = Y^2$$

Yield Stress

…give or take some multipliers (i.e., how we define Y – some divide by 3).

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$$J_2 = (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6\left(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{32}^2\right)$$

von Mises Yield Criteria

$$J_2(\sigma) = Y^2$$

Yield Stress

…give or take some multipliers (i.e., how we define Y – some divide by 3).

It is helpful to separate pressure.

Average, bulk pressure + Deviations from the average

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix} + \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}$$

Here is one that works:

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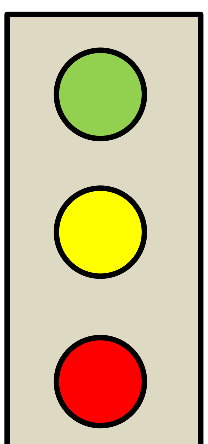
von Mises Yield Criteria

$$J_2(\sigma) = Y^2$$

Yield Stress

So we have a "Yield Function":

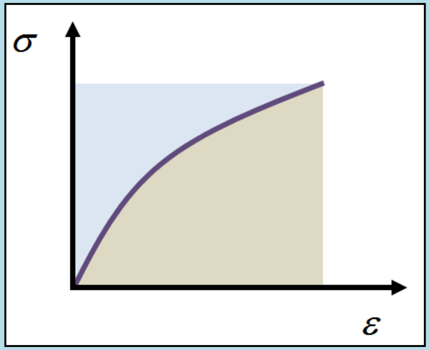
$$f(\sigma) = J_2(\sigma) - Y^2$$



< 0	Elastic	*Hooke's Law Only*
$= 0$	Plastic	*Flow Rule*
> 0	Impossible	*We make sure of this*

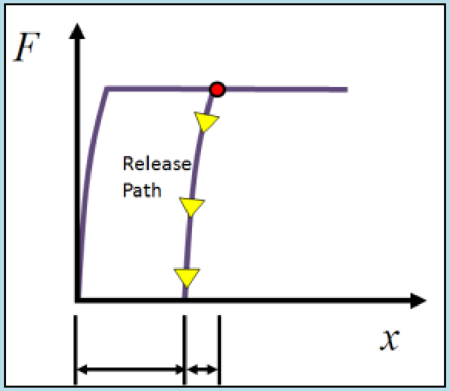
Review

$$\varepsilon_{ij} = \frac{d\Omega}{d\sigma_{ij}}$$



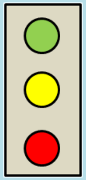
Elastic Strain: Gradient of a complimentary energy density function.

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$



Total strain: Sum of **elastic strain** and **plastic strain**.

$$f(\sigma) = J_2(\sigma) - Y^2$$



We have **a yield function** that describes when yielding occurs.

Next Step

$$\varepsilon_{ij} = \frac{d\Omega}{d\sigma_{ij}} \qquad d\varepsilon_{ij} = D_{ijkl} d\sigma_{kl}$$

Hooke's Law

√ √

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Assert: Plastic strain must be the gradient of *something*. But what?

$$f(\sigma) = J_2(\sigma) - Y^2$$

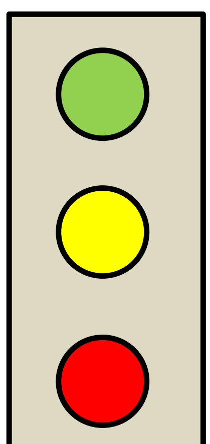
$$d\varepsilon_{ij}^{p} \propto \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

Choosing the yield function for the gradient makes what's called the **Associated Flow Rule**.

$$d\varepsilon_{ij}^{p} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$d\varepsilon_{ij}^{p} \propto \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

Finding that multiplicative constant requires another equation.



< 0

$= 0$

It's this one → > 0 Impossible

Next Step

$$\varepsilon_{ij}^{e} = \frac{d\Omega}{d\sigma_{ij}} \qquad d\varepsilon_{ij}^{e} = D_{ijkl}\, d\sigma_{kl}$$

Hooke's Law

$$d\varepsilon_{ij}^{p} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Associated Flow Rule

$$d\varepsilon_{ij}^{p} \propto \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$f(\sigma) = J_2(\sigma) - Y^2$$

Next Step

$$\varepsilon_{ij}^{e} = \frac{d\Omega}{d\sigma_{ij}} \qquad d\varepsilon_{ij}^{e} = D_{ijkl}\, d\sigma_{kl}$$

Hooke’s Law

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Associated Flow Rule

$$d\varepsilon_{ij}^{p} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$d\varepsilon_{ij}^{p} \propto \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$f(\sigma) = J_2(\sigma) - Y^2$$

$$d\varepsilon_{ij}^{e} = D_{ijkl} d\sigma_{ij}$$

$$d\varepsilon_{ij}^{p} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}}$$

$$d\varepsilon_{ij} = d\varepsilon_{ij}^{p} + d\varepsilon_{ij}^{e}$$

Two Equations/Two Unknowns

$$d\varepsilon_{ij} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}} + D_{ijkl} d\sigma_{ij}$$

Strain = Plastic + Elastic

Plastic strain is the gradient of the yield surface

$$df = \frac{\partial f(\sigma)}{\partial \sigma_{ij}} d\sigma_{ij} = 0$$

We must not go off (beyond) the yield surface.

Solving, and…

(1) Assuming isotropic material (shear and bulk modulus)
(2) Using deviatoric strain e and stress s

Produces the Prandlt-Reuss Material Model

$$d\sigma_{ij} = 2G de_{ij} + K de_{ij}\delta_{ij} - \frac{G s_{mn} de_{mn}}{Y^2} s_{ij}$$

<u>Two Equations/Two Unknowns</u>

$$d\varepsilon_{ij} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}} + D_{ijkl} d\sigma_{ij}$$

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<u>Two Equations/Two Unknowns</u>

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Solving, and…

(1) Assuming isotropic material (shear and bulk modulus)
(2) Using deviatoric strain e and stress s

Produces the Prandlt-Reuss Material Model

$$\dot{s}_{ij} = 2G\dot{e}_{ij} - \frac{G s_{mn}\dot{e}_{mn}}{Y^2} s_{ij}$$

<u>Two Equations/Two Unknowns</u>

$$d\varepsilon_{ij} = d\lambda \frac{\partial f(\sigma)}{\partial \sigma_{ij}} + D_{ijkl}\, d\sigma_{ij}$$

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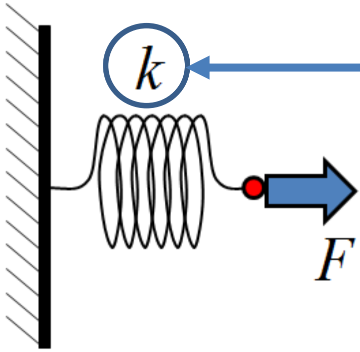
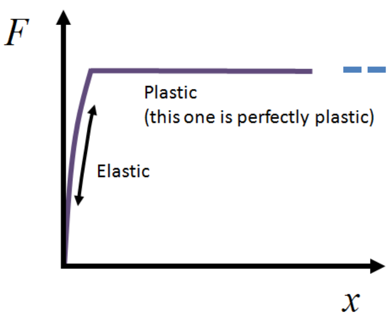
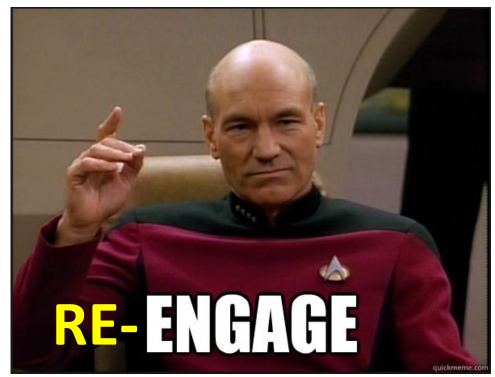


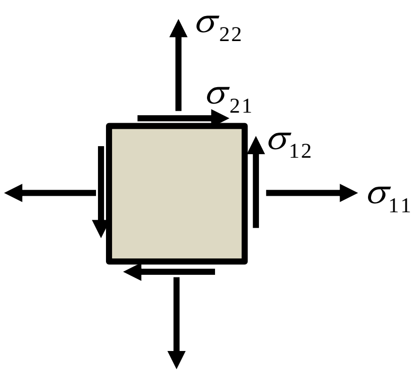
$$s_{ij} = Ge_{ij}$$

You can reengage by choosing to believe the following…that we have this ODE…

$$\dot{s}_{ij} = 2G\dot{e}_{ij} - \frac{Gs_{mn}\dot{e}_{mn}}{Y^2} s_{ij}$$







Stress tensor = Average, bulk pressure + Deviations from the average

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix} + \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}$$

$$\dot{s}_{ij} = 2G\dot{e}_{ij} - \frac{G s_{mn} \dot{e}_{mn}}{Y^2} s_{ij}$$

Prandlt-Reuss ("P-R") Material Model

$$\dot{s}_{ij} = 2G\dot{e}_{ij} - \frac{G s_{mn}\dot{e}_{mn}}{Y^2} s_{ij}$$

Ortiz & Popov: Generalized framework for numerical methods, including radial return

Kreig & Kreig: Analytical solution and comparison to numerical methods

Saint-Venant
von Mises
Prandtl
Levy

Emphasis on numerical accuracy

1930 | 1940s/WW2 | 1977 | 1985

Focus largely on low speed deformation

High-speed deformation begins

Other analytical solutions and numerical methods follow. Time Step a Factor.

In a code the strain rate is constant during a time step.

This enables integration of the P-R ODE either analytically or numerically.

Prandlt-Reuss ("P-R") Material Model

$$\dot{s}_{ij} = 2G\dot{e}_{ij} - \frac{G s_{mn}\dot{e}_{mn}}{Y^2} s_{ij}$$

1964: Wilkins' Radial Return Algorithm

Solves the above ODE at each time step in a hydrocode.

Given strain rate (circled), produce new estimates of stress at each time step.

Does not look like an ODE solver, though.

Radial Return Algorithm

Three Pieces

(1) Split the stress tensor

Average, bulk pressure + Deviations from the average

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix} + \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}$$

(2) Use a scalar metric of σ

$$J_2 \equiv \frac{1}{6}\left[(\sigma_{11}-\sigma_{22})^2+(\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2\right]+\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2$$

Notice that p does ***not*** play a role. Only s_{ij} plays a role.

(3) Ensure J_2 respects Y

$$J_2 \le \frac{Y^2}{3}$$

This is the job of the radial return algorithm.

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix} + \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}$$

$$J_2 \equiv \frac{1}{6}\left[(\sigma_{11}-\sigma_{22})^2 + (\sigma_{22}-\sigma_{33})^2 + (\sigma_{33}-\sigma_{11})^2\right] + \sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2$$

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(1) Split the stress tensor

Average, bulk pressure + **Deviations from the average**

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix} + \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}$$

$$J_2\left(s_{ij}\right) \leq \frac{Y^2}{3}$$

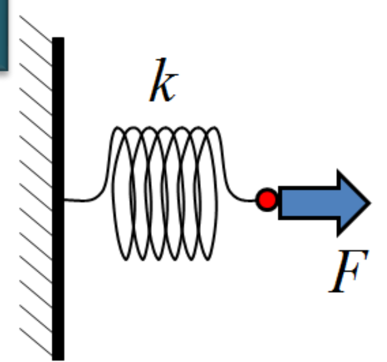
Must Obey

$$J_2 \equiv \frac{1}{6}\left[\left(s_{11}-s_{22}\right)^2+\left(s_{22}-s_{33}\right)^2+\left(s_{33}-s_{11}\right)^2\right]+s_{12}^2+s_{23}^2+s_{31}^2$$

Hooke's Law using "deviatoric" stress and strain.

Shear modulus **Deviatoric strain**

$$s_{ij} = 2Ge_{ij}$$



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Must Obey

Shear modulus

Deviatoric strain

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Shear modulus

Deviatoric strain

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$$s_{ij} = 2Ge_{ij}$$

Transient version

$$\dot{s}_{ij} = 2G\dot{e}_{ij}$$

$$J_2(s_{ij}) \le \frac{Y^2}{3}$$

Must Obey

$$s_{ij}^{\mathrm{new}} = s_{ij}^{\mathrm{old}} + \Delta t \, 2G\dot{e}_{ij}$$

Transient version

$$\dot{s}_{ij} = 2G\dot{e}_{ij}$$

$$J_2(s_{ij}) \le \frac{Y^2}{3}$$

Must Obey

$$s_{ij}^{\text{trial}} = s_{ij}^{\text{old}} + \Delta t 2G\dot{e}_{ij}$$

$$s_{ij}^{\text{new}} = \alpha\, s_{ij}^{\text{trial}}$$

Radial Return Algorithm

1. Compute trial deviatoric stress

$$s_{ij}^{\text{trial}} = s_{ij}^{\text{old}} + \Delta t 2G\dot{e}_{ij}$$

$$J_2\left(s_{ij}\right) \leq \frac{Y^2}{3}$$

Must Obey

2. Compute its J_2

3. Scale it back so that it obeys the yield criteria

$$s_{ij}^{\text{new}} = \alpha\ s_{ij}^{\text{trial}}$$

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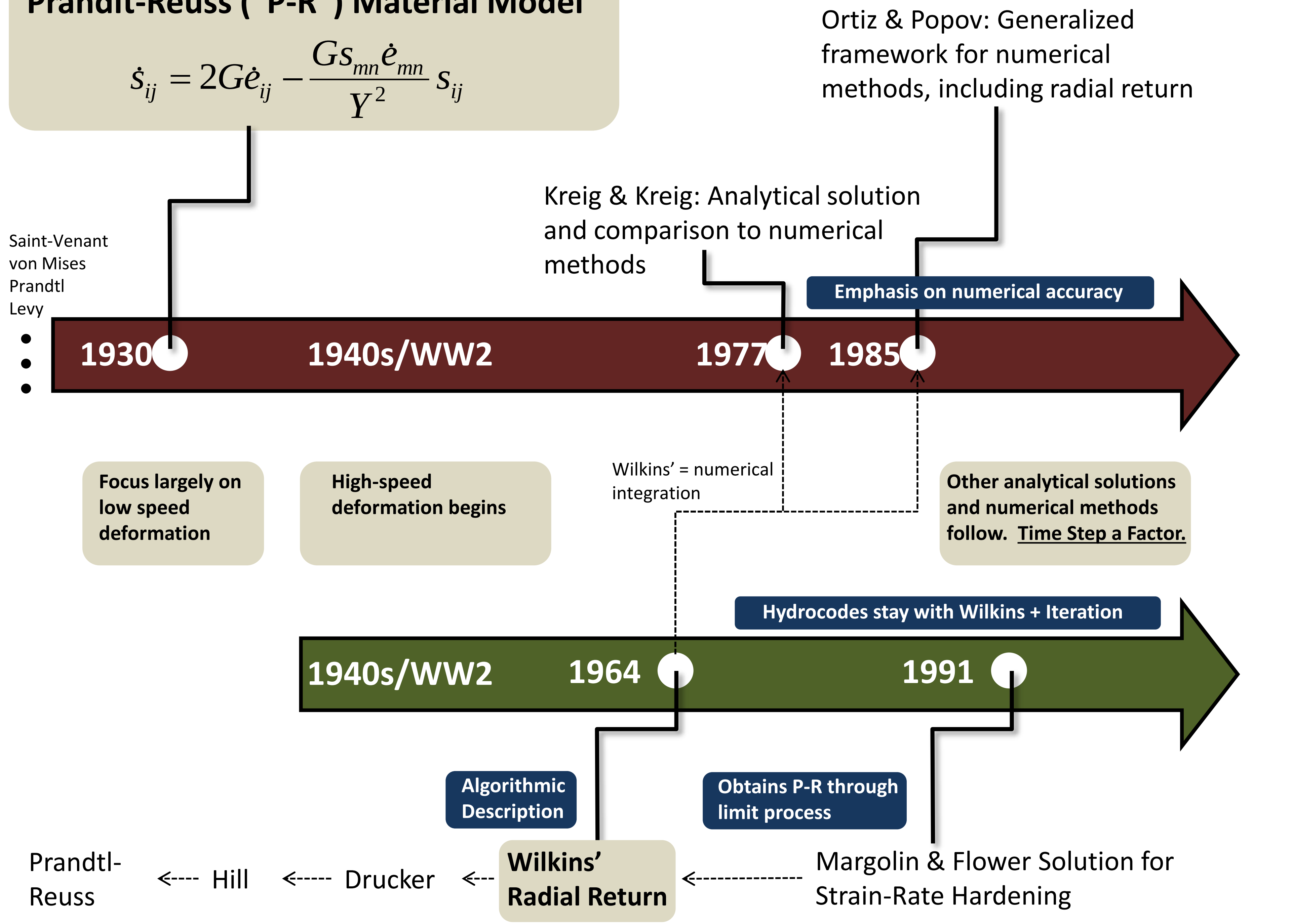


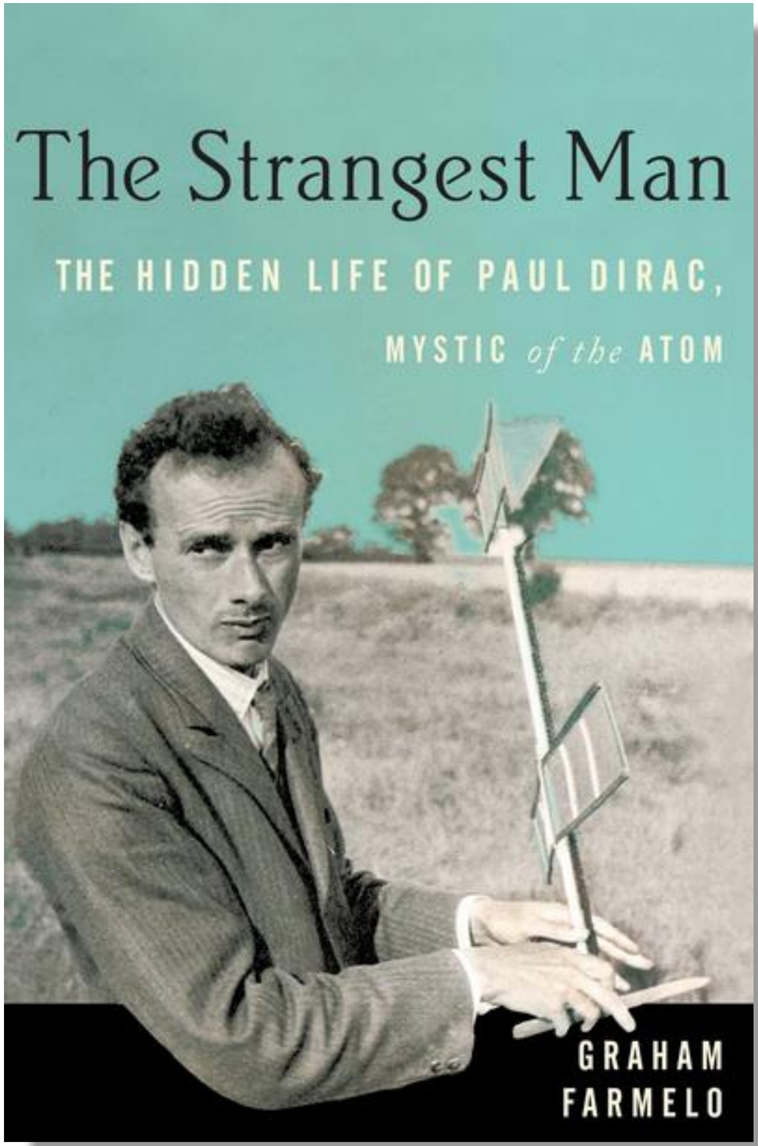
Outline

(1)
Motivation: What is strain rate in a shock?

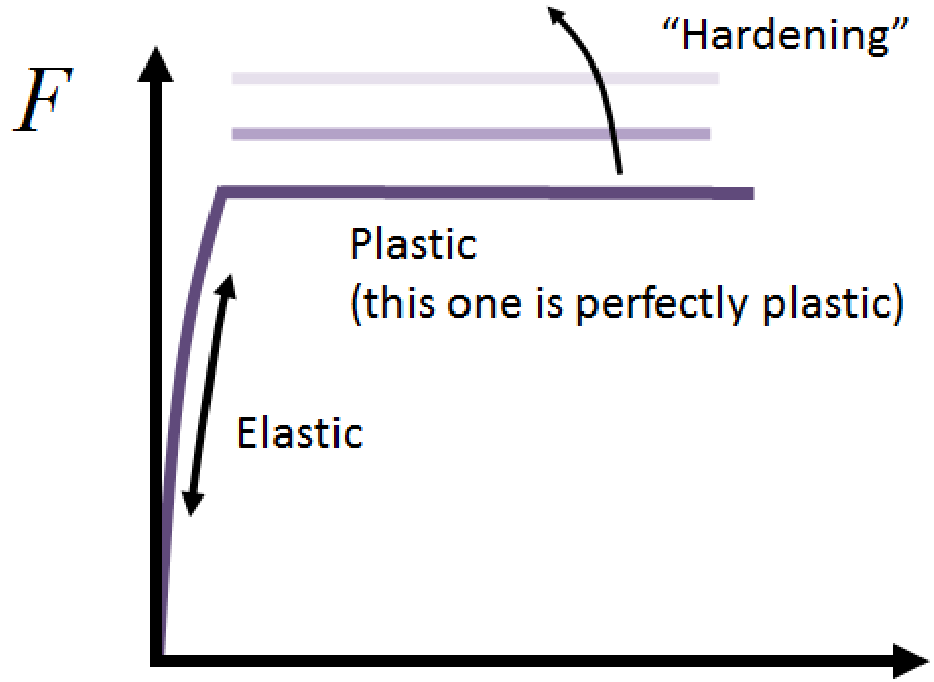
(2)
Introduction to plasticity and historical overview

(3)
Digging into the question: Strain rate, shock, and plasticity

(4)
Benefits to hydrocodes



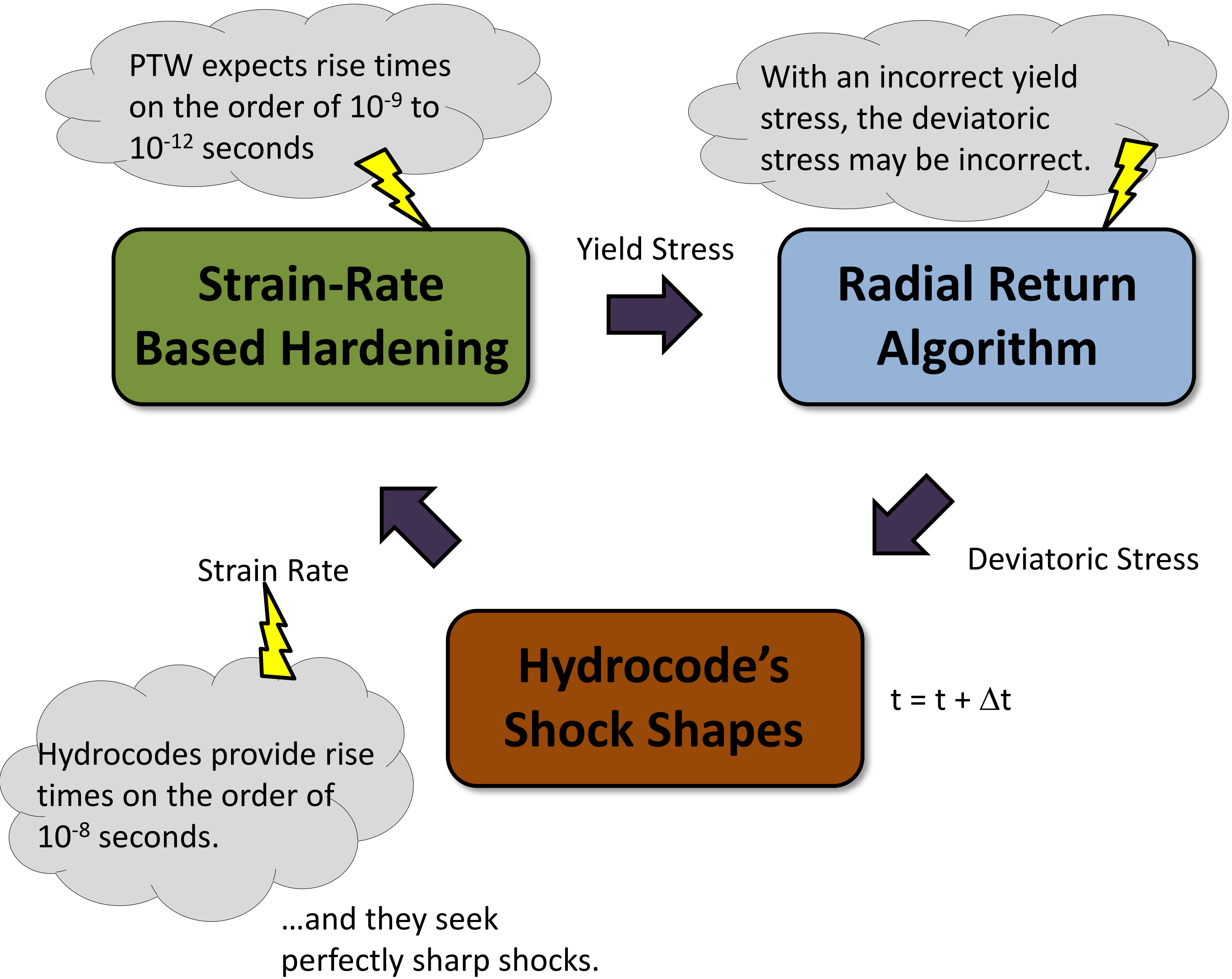
Strain-Rate Based Hardening

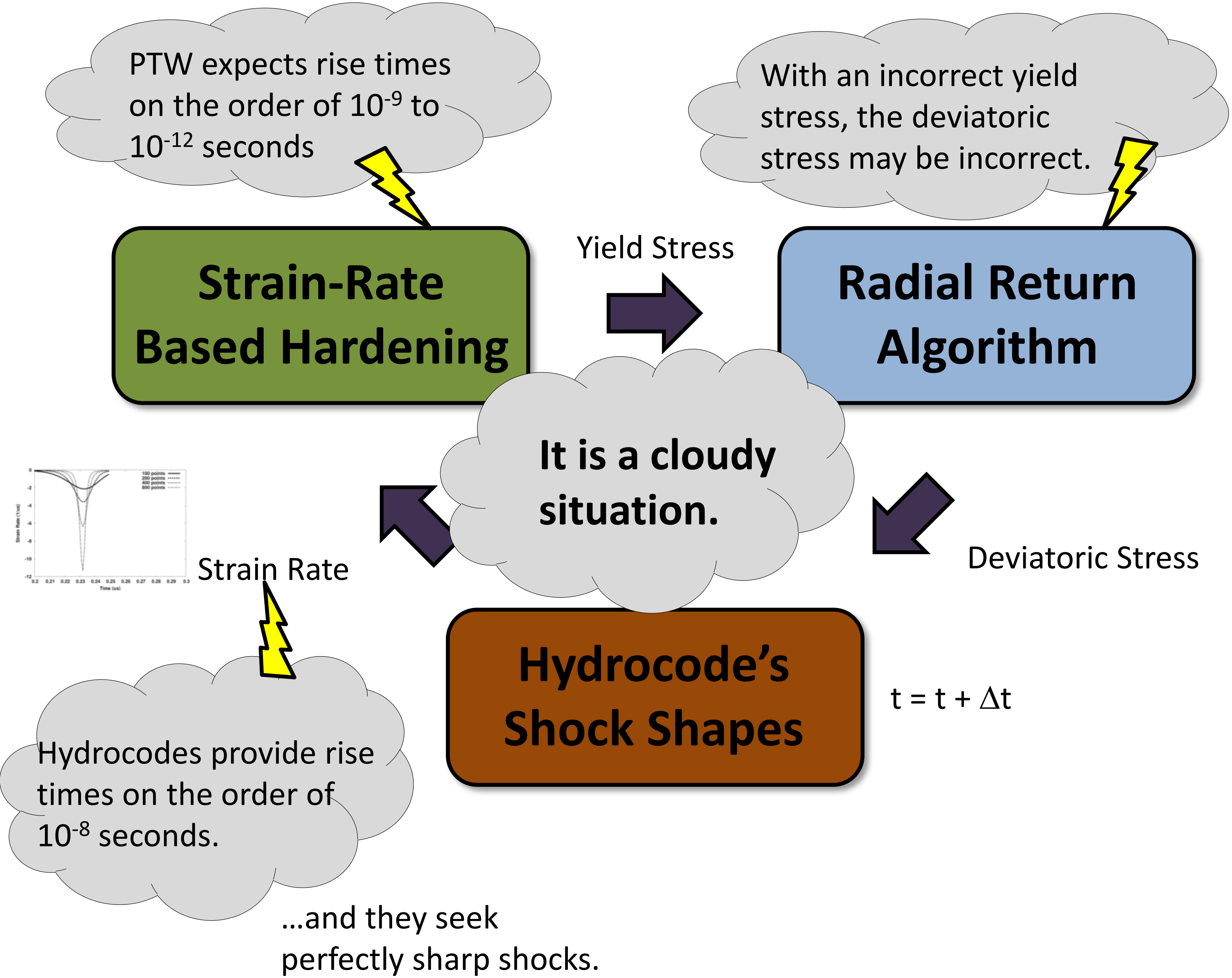


Strain Rate

Hydrocode's Shock Shapes

$t = t + \Delta t$


PTW expects rise times on the order of 10^{-9} to 10^{-12} seconds
With an incorrect yield stress, the deviatoric stress may be incorrect.
Strain-Rate Based Hardening
Yield Stress
Radial Return Algorithm
Deviatoric Stress
Strain Rate
Hydrocode's Shock Shapes
$t = t + \Delta t$
Hydrocodes provide rise times on the order of 10^{-8} seconds.
...and they seek perfectly sharp shocks.


PTW expects rise times on the order of 10^{-9} to 10^{-12} seconds
With an incorrect yield stress, the deviatoric stress may be incorrect.
Strain-Rate Based Hardening
Yield Stress
Radial Return Algorithm
It is a cloudy situation.
Strain Rate (1/us)
Time (us)
100 points
200 points
400 points
800 points
0
-2
-4
-6
-8
-10
-12
0.2
0.21
0.22
0.23
0.24
0.25
0.26
0.27
0.28
0.29
0.3
Strain Rate
Deviatoric Stress
Hydrocode's Shock Shapes
$t = t + \Delta t$
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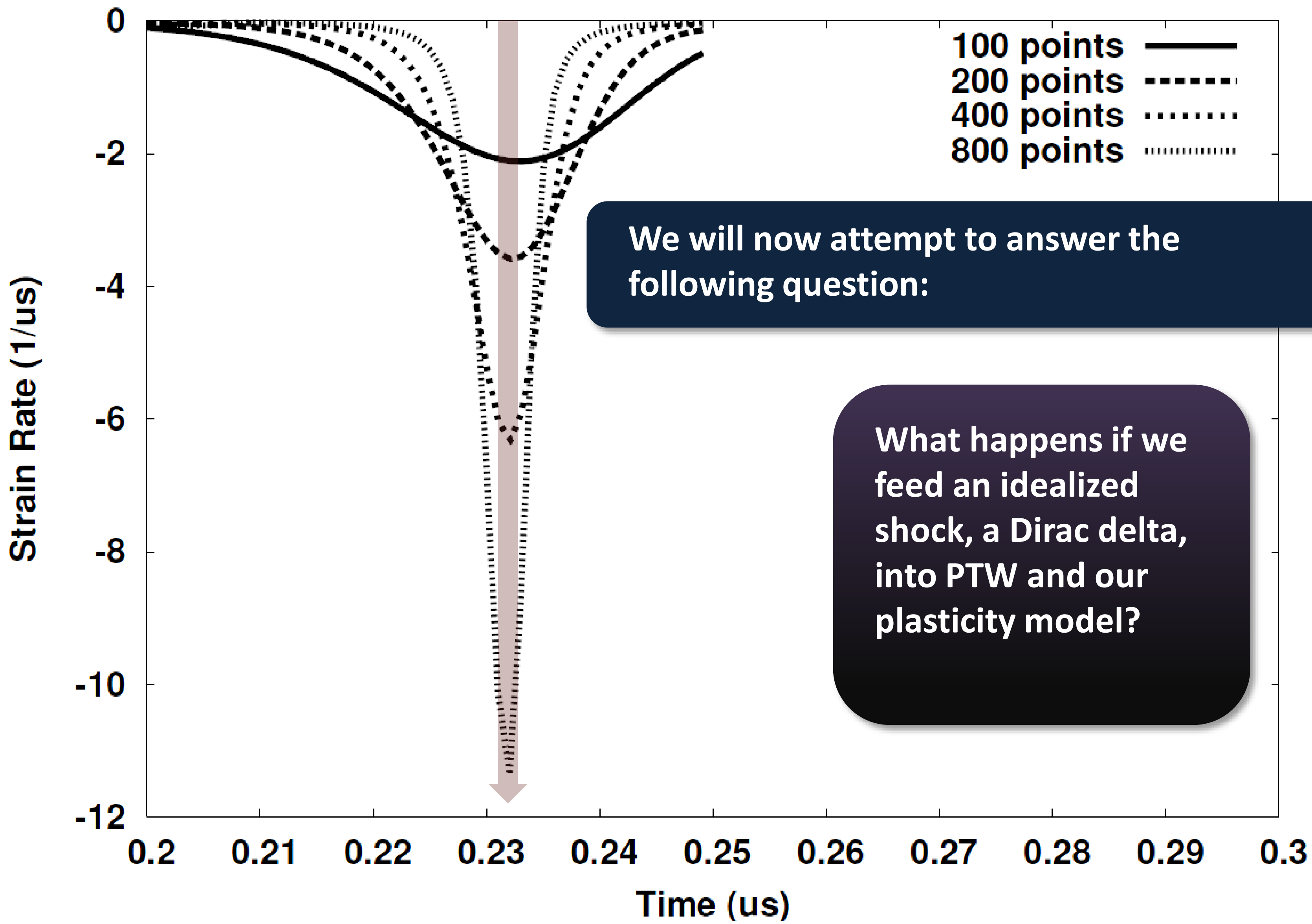
…and they seek perfectly sharp shocks.

Strain Rate Approaches as Dirac Delta



We will now attempt to answer the following question:

What happens if we feed an idealized shock, a Dirac delta, into PTW and our plasticity model?

Radial Return Algorithm

In 1991 Margolin and Flower let $\Delta t \rightarrow 0$ in the algorithm.

The result was a Prandtl-Reuss like equation.

1. Compute trial deviatoric stress

$$S_{ij}^{\text{trial}} = S_{ij}^{\text{old}} + \Delta t 2G\dot{e}_{ij}$$

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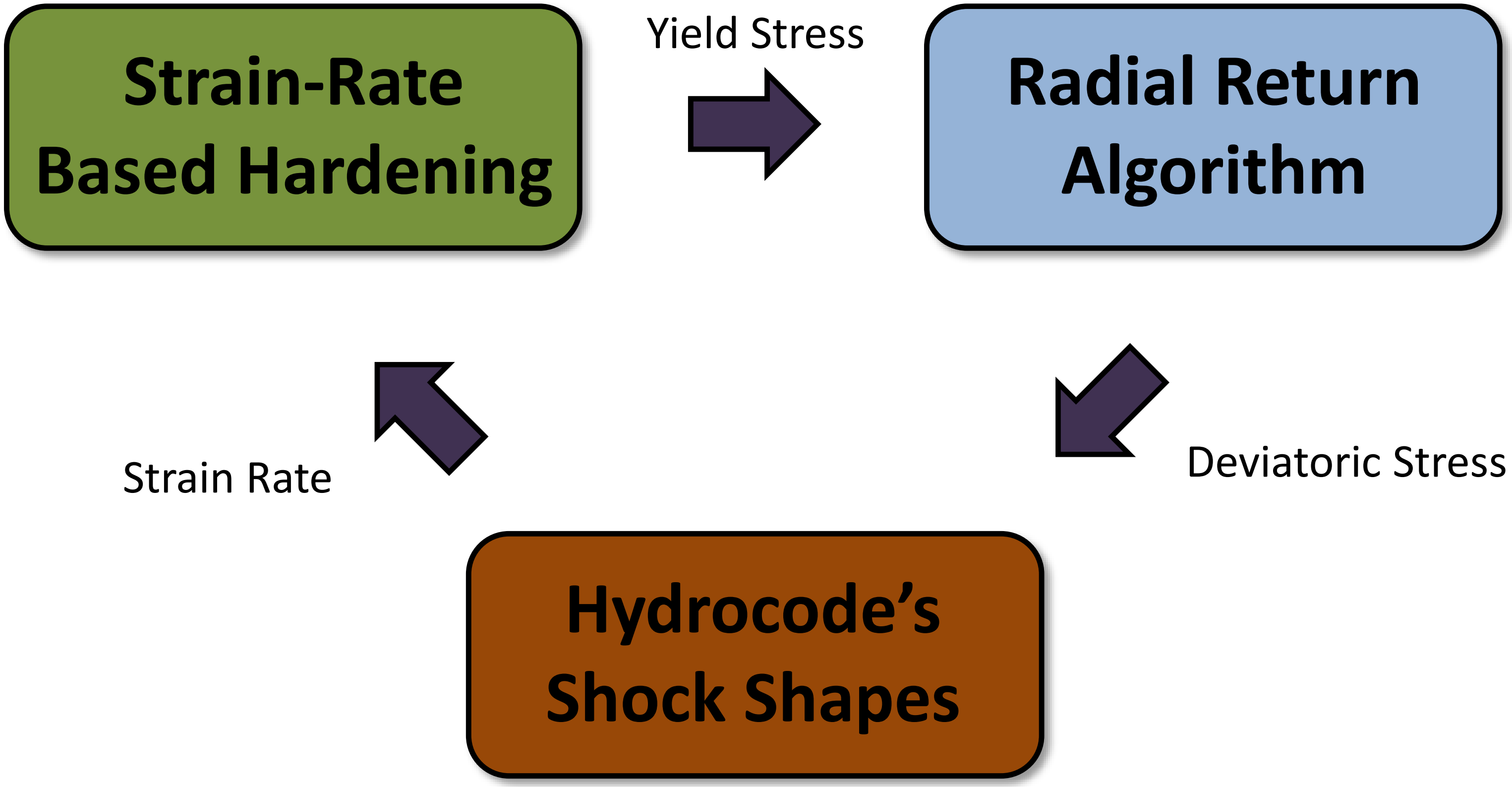
The result was a Prandtl-Reuss like equation.

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

This has enabled an analytical study of shocks with plastic deformation.

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$



Strain-Rate Based Hardening

For overdriven (strong) shocks…

PTW

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

- Yield stress (Y)
- Shear modulus (G)
- Plastic strain rate ($\dot{e}$)
- Based on material constants and density ($\dot{\xi}$)
- Adjustable parameter (β)

Strain-Rate Based Hardening

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^{2}}$$

Strain-Rate Based Hardening

Yield Stress

Radial Return Algorithm

Deviatoric Stress

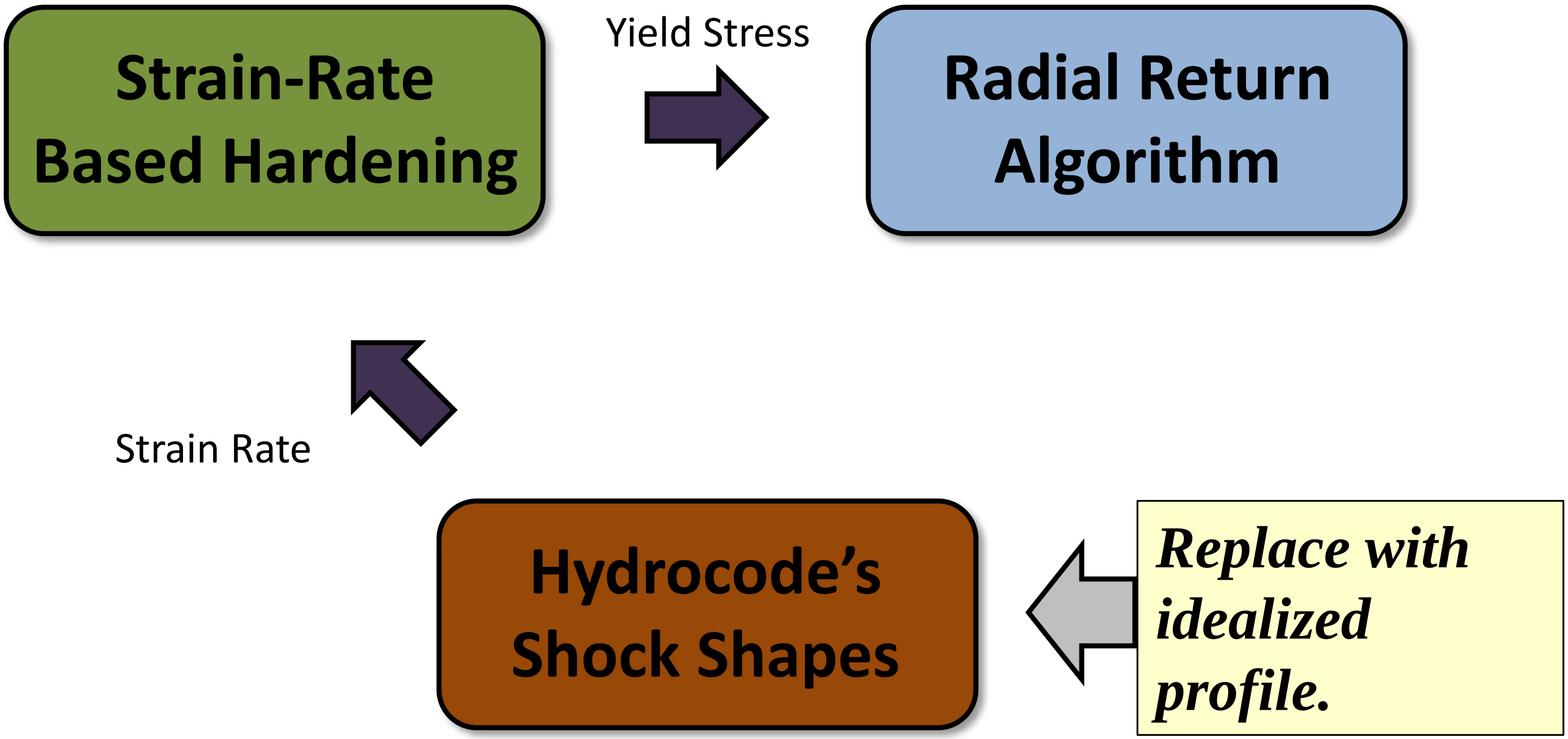
Strain Rate

Hydrocode's Shock Shapes

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = -\underbrace{\begin{bmatrix} p & & \\ & p & \\ & & p \end{bmatrix}}_{\text{EOS}} + \underbrace{\begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix}}_{\text{Radial Return}}$$

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$



$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

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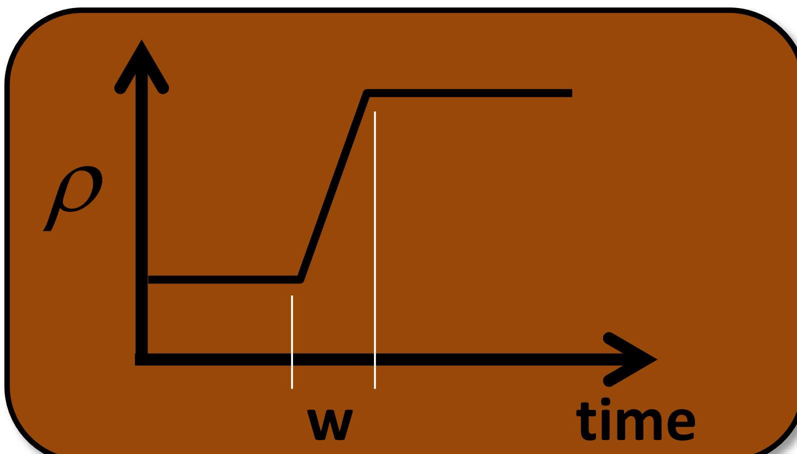
Strain-Rate Based Hardening

Yield Stress →

Radial Return Algorithm

Strain Rate ↖



Linear density rise

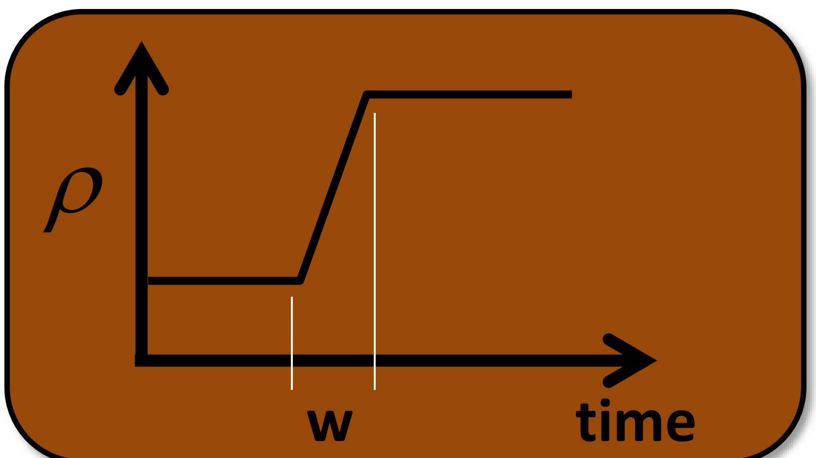
$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

Analytical expressions for $Y, \dot{Y}$

ODE can be solved analytically with special choice for β.

Analytical expressions for $\dot{e}, \dot{\xi}$



PTW Strength Model

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

Radial Return as an ODE

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

This is: Deviatoric stress during the linear density rise.

Result:

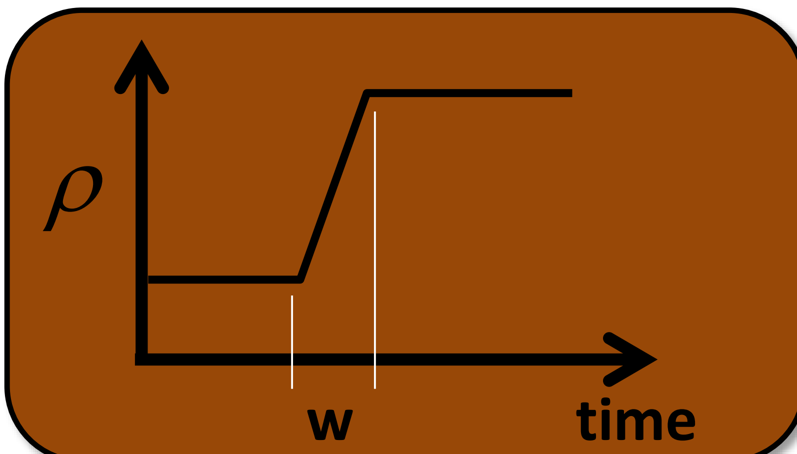
$$s_{ij} = -\frac{1}{C}(k\dot{\rho})\frac{\rho(t)^{k-1} - \rho_o^{2k}\rho(t)^{-k-1}}{\rho(t)^{k} + \rho_o^{2k}\rho(t)^{-k}}$$

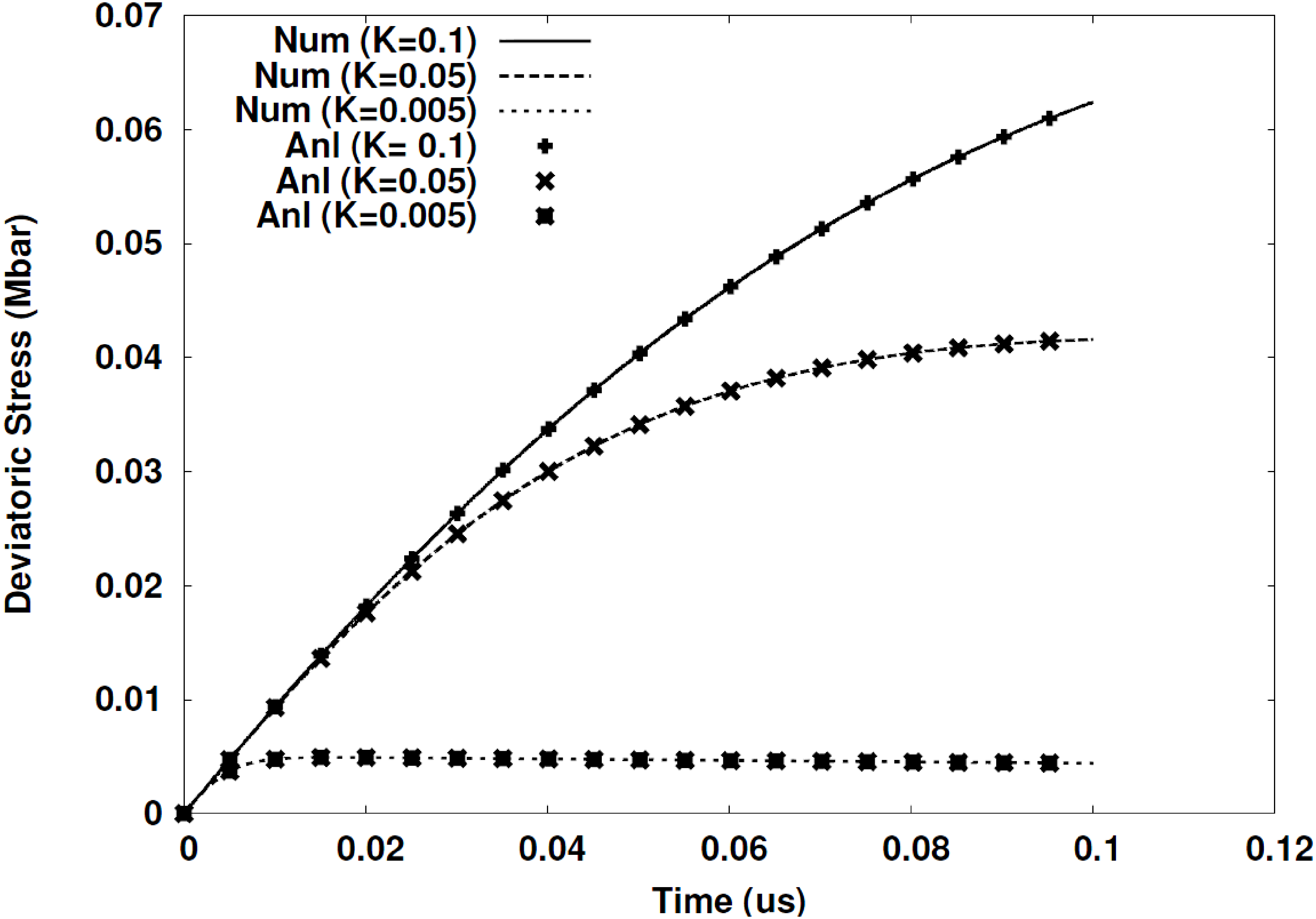
“Analytical”

versus

“Numerical”

Hydrocode shock shape




Num (K=0.1)
Num (K=0.05)
Num (K=0.005)
Anl (K= 0.1)
Anl (K=0.05)
Anl (K=0.005)
Deviatoric Stress (Mbar)
Time (us)
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0
0.02
0.04
0.06
0.08
0.1
0.12

PTW Strength Model

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

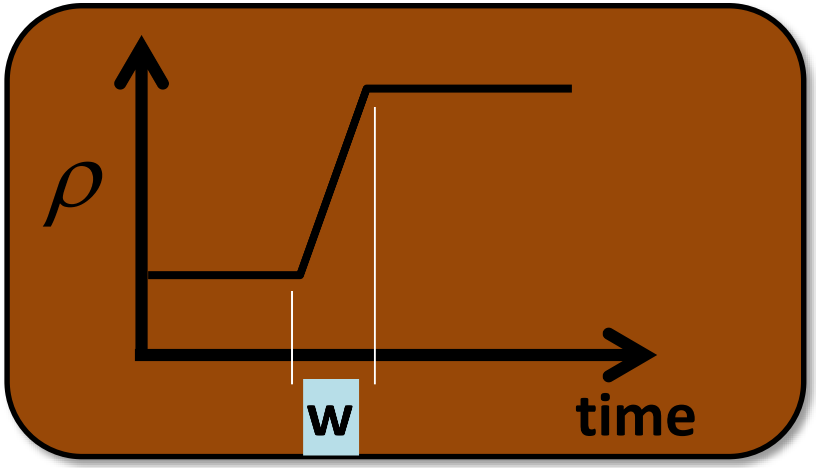
Radial Return

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - G\dot{s}_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

$$s_{ij} = -\frac{1}{C}(k\dot{\rho})\frac{\rho(t)^{k-1} - \rho_o^{2k}\rho(t)^{-k-1}}{\rho(t)^{k} + \rho_o^{2k}\rho(t)^{-k}}$$

k is a function of shock width, w.

Hydrocode shock shape



We can take $\lim_{w \to 0}$ of s_{ij}.

$$s_{ij} = -\frac{1}{C}(k\dot{\rho})\frac{\rho(t)^{k-1} - \rho_o^{2k}\rho(t)^{-k-1}}{\rho(t)^{k} + \rho_o^{2k}\rho(t)^{-k}}$$

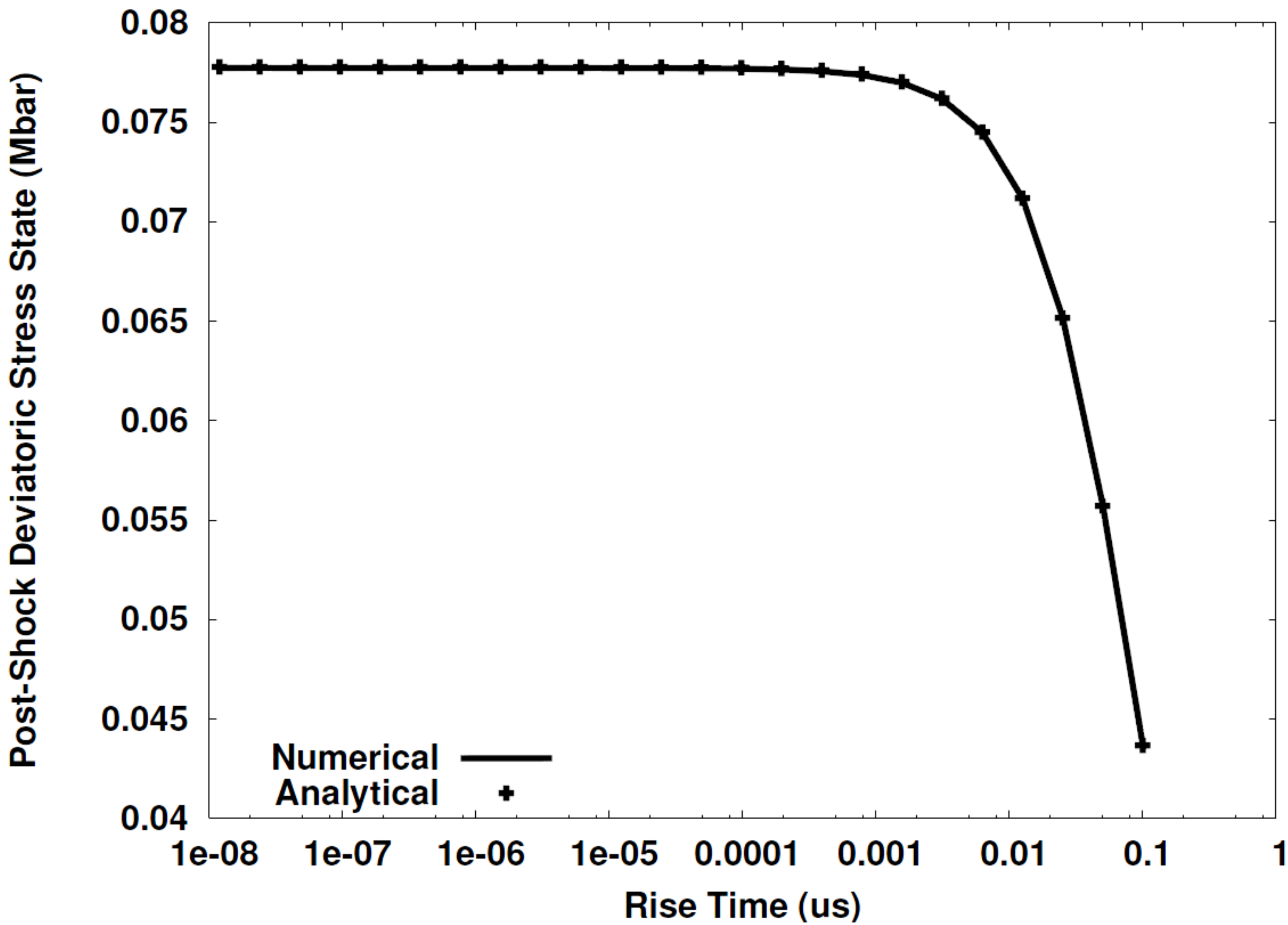
The Result:

$$\lim_{\mathrm{w}\to 0} s_{ij} \propto \frac{1}{\rho_{\text{final}}}\ln\left(\rho_{\text{final}} / \rho_{\text{initial}}\right)$$

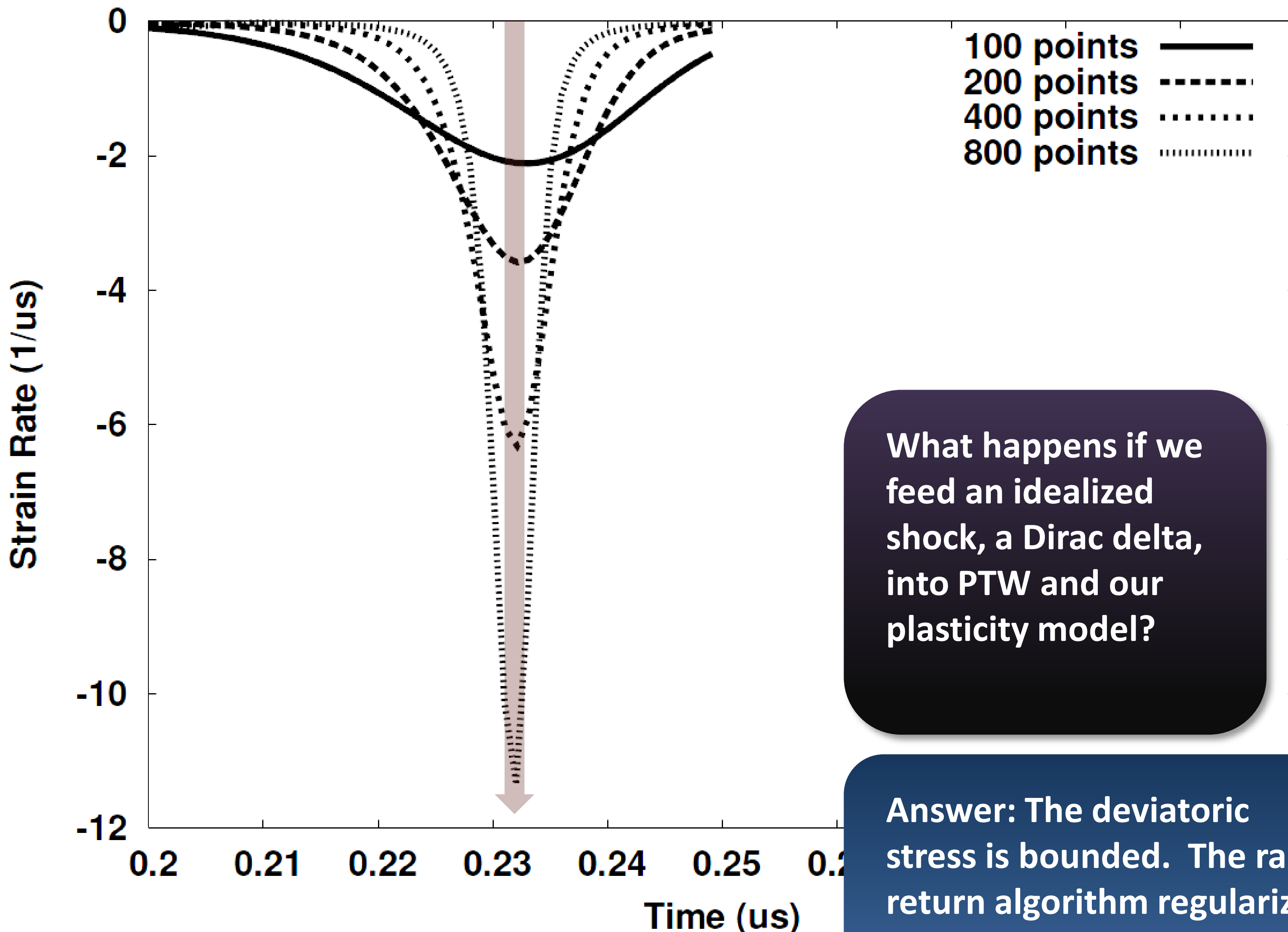
It is finite.

The radial return algorithm regularizes the singularity.

Computations confirm it.



Strain Rate Approaches as Dirac Delta



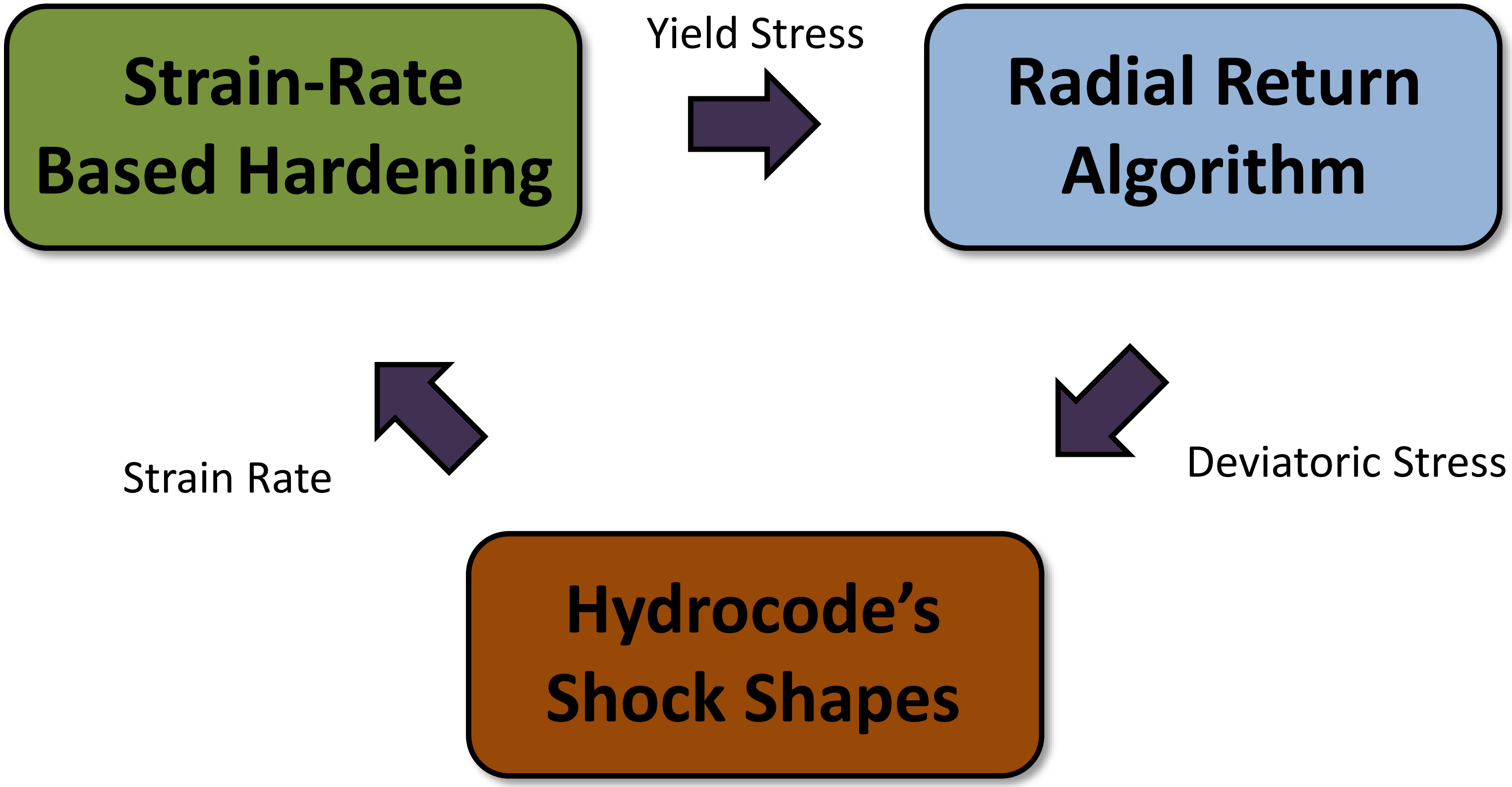
What happens if we feed an idealized shock, a Dirac delta, into PTW and our plasticity model?

Answer: The deviatoric stress is bounded. The radial return algorithm regularizes the singularity.

Like integrating a Dirac-delta

$$\int f(x)\delta(x-c)dx = f(c)$$

Answer: Radial return regularizes the singularity

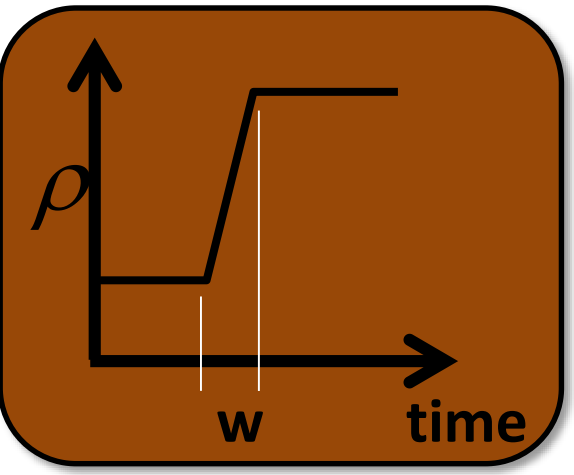


Question: What if the idealized shock were produced (infinite strain rate)?

Like integrating a Dirac-delta

$$\int f(x)\delta(x-c)dx = f(c)$$

Answer: Radial return regularizes the singularity



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Analytical shock shape

PTW

ODE Form of Radial Return

Solved that ODE and took

limit w→0

Question: What if the idealized shock were produced (infinite strain rate)?

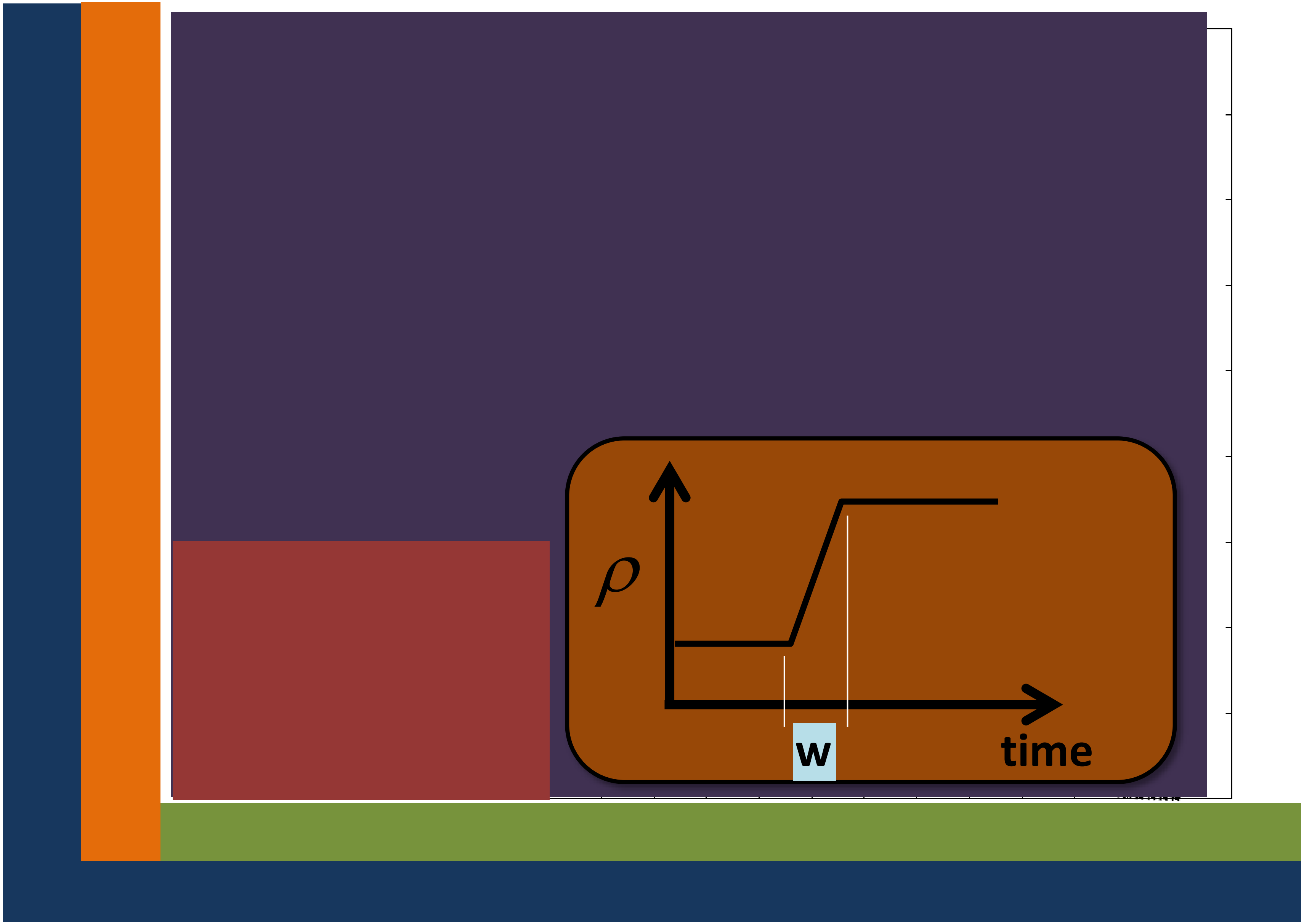
Strain-Rate Based Hardening

Radial Return Algorithm

Next Question: How do the hydrocode shock and the idealized shock relate in the context of plasticity?

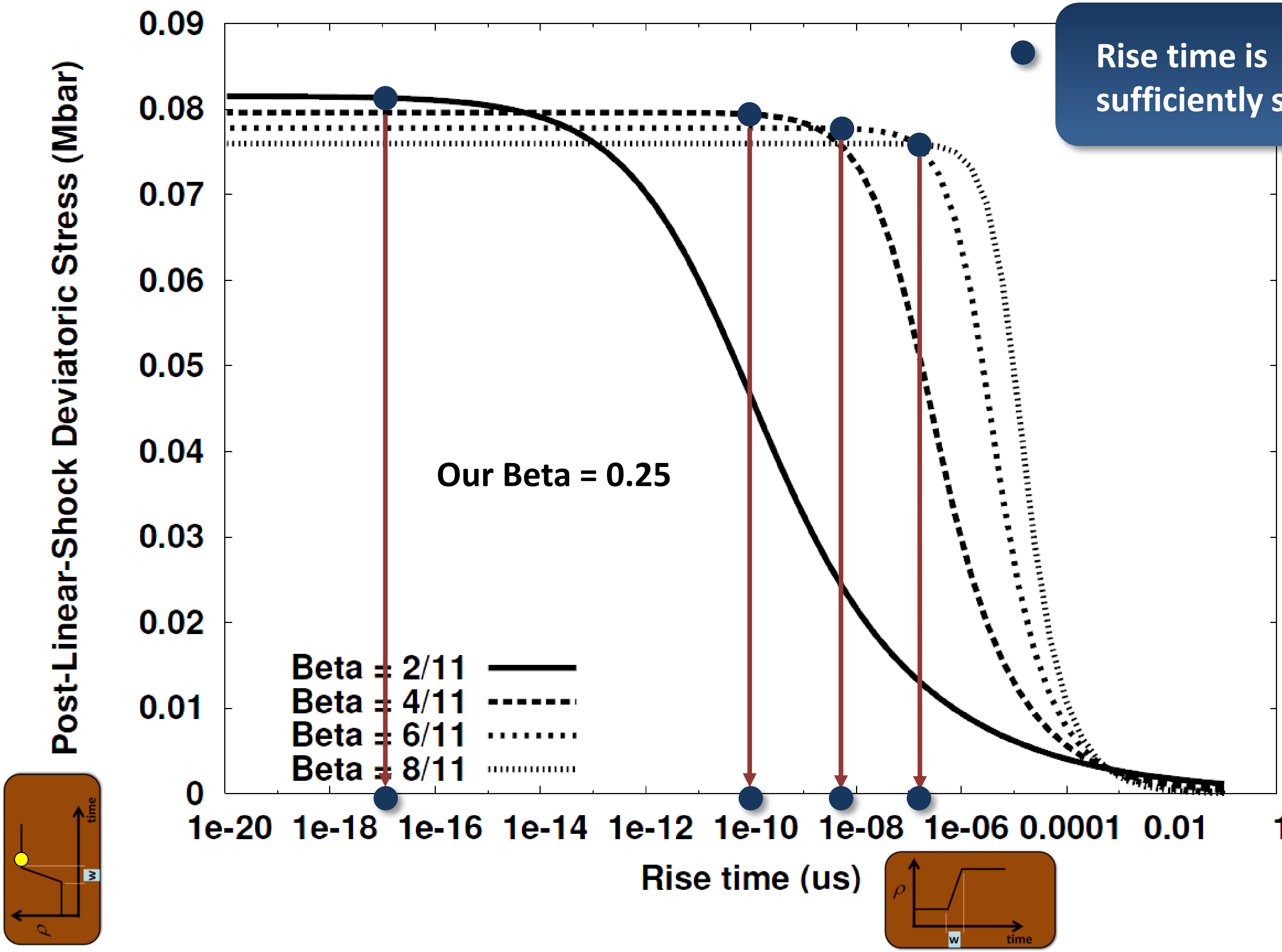
Hydrocode's Shock Shapes

Shock Rise Time Required for Convergence can be Very Small



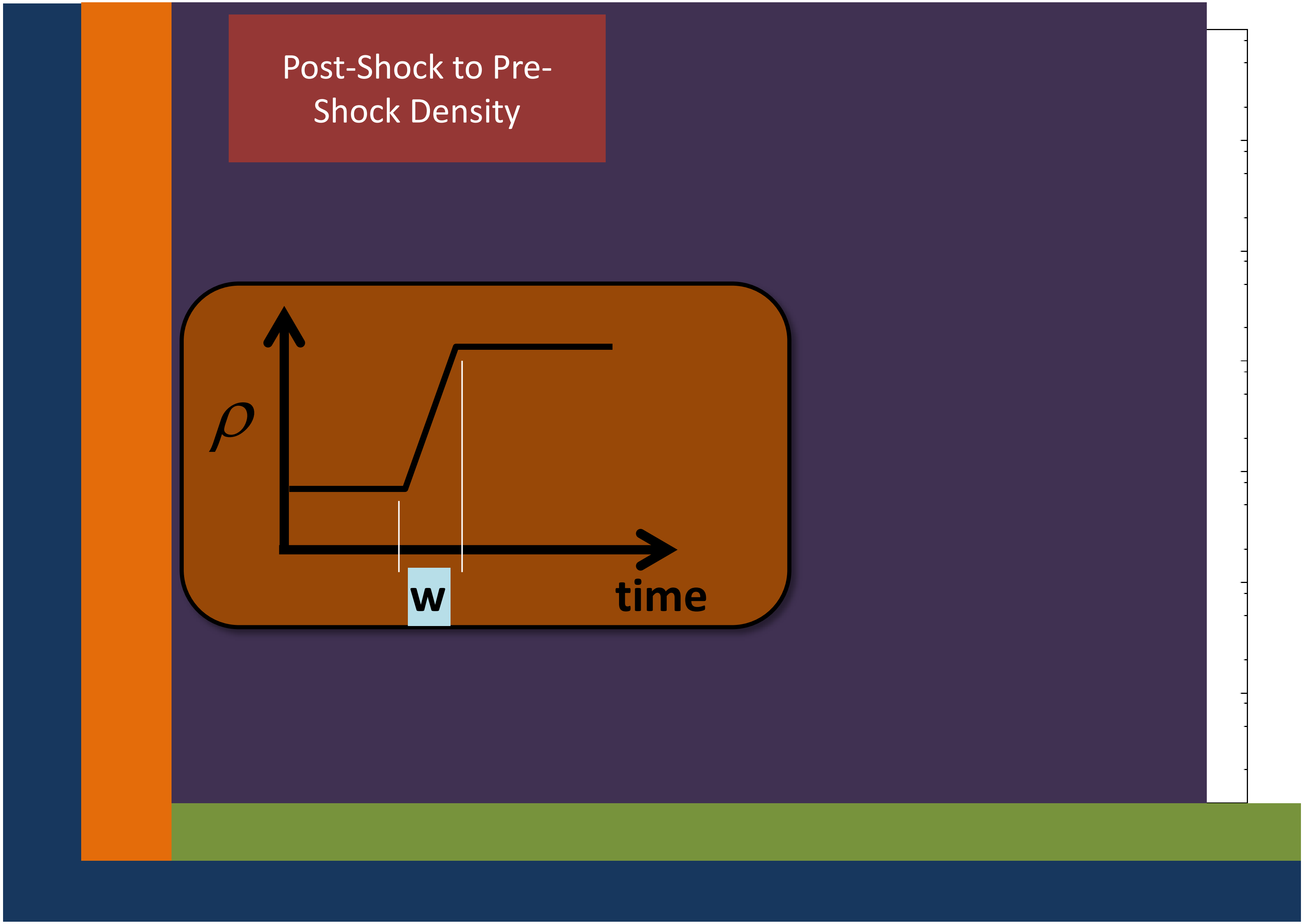
Underlying plot shown on next slide.

Shock Rise Time Required for Convergence can be Very Small



Rise time is sufficiently small

Shock Rise Time Required for Convergence can be Very Small



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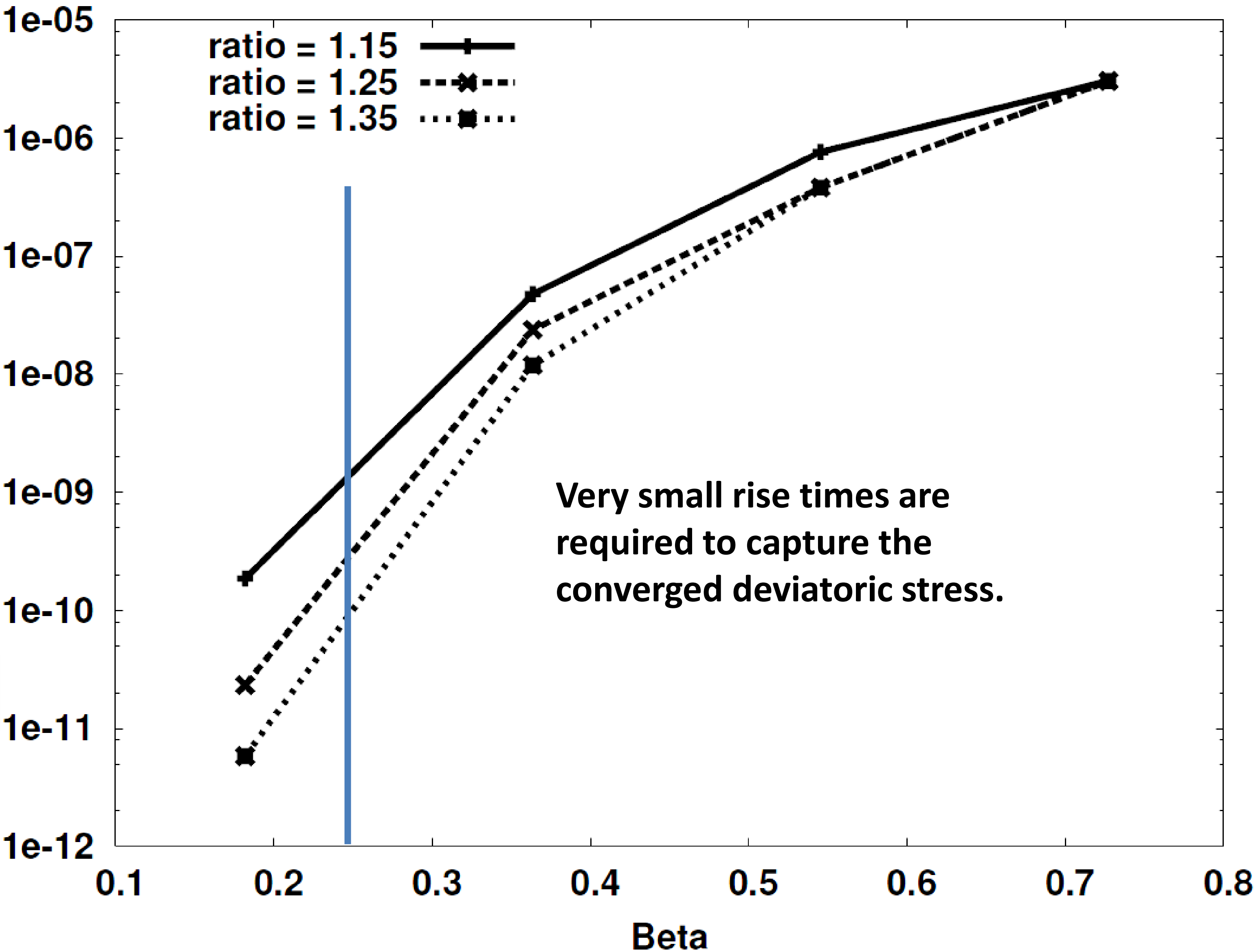

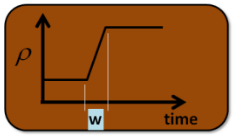

Very small rise times are required to capture the converged deviatoric stress.

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Exact Radial Return

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The result was the Prandtl-Reuss model.

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - Gs_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

Exact Radial Return

In addition, they provided an analytical solution.

For the hardening case.

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - Gs_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

Exact Radial Return

Material Model with Hardening

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - Gs_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

In addition, they provided an analytical solution.

<u>For the hardening case.</u>

Analytical Solution over One Time Step

$$s_{ij}(t) = s_{ij}(t_o)\frac{Y(t)}{Y(0)}\frac{F(0)}{F(t)} + \frac{\sqrt{2}Y(t)}{IF(t)}\dot{e}_{ij}\int_{t_o}^{\alpha(t)} F(\alpha')d\alpha'$$

$$F(t) = A_o e^{\alpha t} + e^{-\alpha t}$$

$$A_o = \frac{\sqrt{2}\left(e_{kl}^n \cdot e_{kl}^n\right)Y + \left(s_{kl}^n \dot{e}_{kl}^n\right)}{\sqrt{2}\left(e_{kl}^n \cdot e_{kl}^n\right)Y - \left(s_{kl}^n \dot{e}_{kl}^n\right)}$$

$$\alpha = \sqrt{2}\int_0^t \frac{GI}{Y(t')}dt'$$

Exact Radial Return

Material Model with Hardening

$$\dot{s}_{ij} = 2G\dot{e}_{ij} + s_{ij}\frac{\dot{Y}}{Y} - Gs_{ij}\frac{s_{kl}\dot{e}_{kl}}{Y^2}$$

Other analytical solutions:

Yoder (1984)

Montmitonnet (1992)

Ristianmaa (1993)

Auricchio (1995)

Peric (1996)

Analytical Solution over One Time Step

$$s_{ij}(t) = s_{ij}(t_o)\frac{Y(t)}{Y(0)}\frac{F(0)}{F(t)} + \frac{\sqrt{2}Y(t)}{IF(t)}\dot{e}_{ij}\int_{t_o}^{\alpha(t)} F(\alpha')d\alpha'$$

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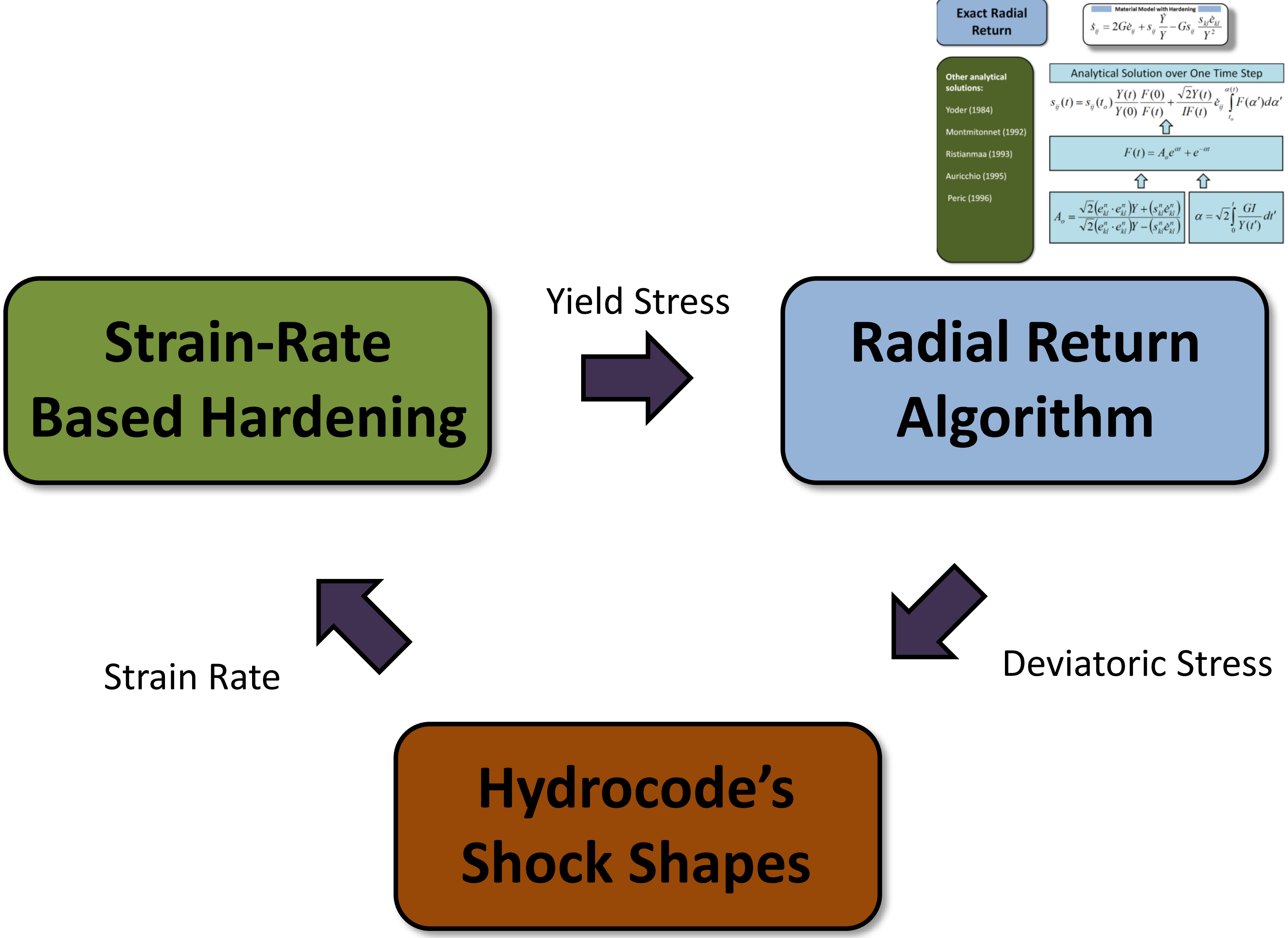
Exact Radial Return
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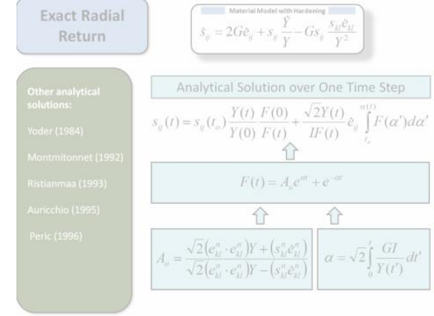
Strain-Rate Based Hardening
Yield Stress
Radial Return Algorithm
Deviatoric Stress
Strain Rate
Hydrocode's Shock Shapes



Strain-Rate Based Hardening

Yield Stress

Radial Return Algorithm

PTW

There are issues regarding how this ODE is integrated. The Radial Return interacts.

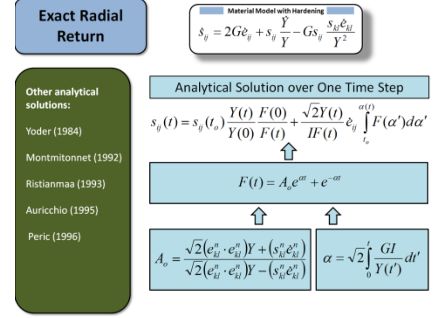
For overdriven (strong) shocks…

$$Y = G \cdot \left(\frac{\dot{e}}{\dot{\xi}} \right)^{\beta}$$

For weaker shocks…

$$\frac{dY}{d\varepsilon} = G\theta \frac{\exp\left[p \dfrac{\hat{\tau}_s - \hat{\tau}}{s_o - \hat{\tau}_y} \right] - 1}{\exp\left[p \dfrac{\hat{\tau}_s - \hat{\tau}_y}{s_o - \hat{\tau}_y} \right] - 1}$$

PTW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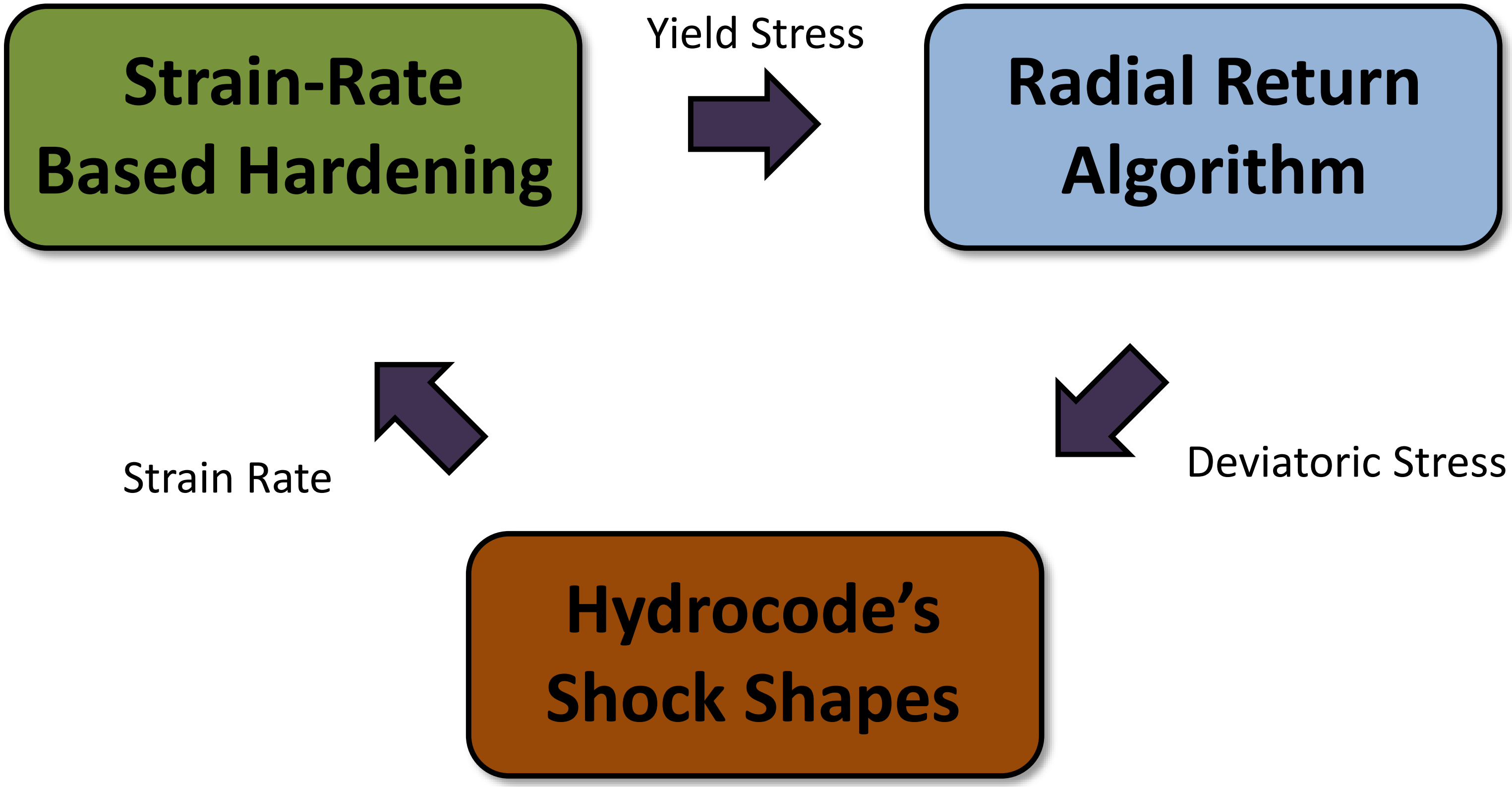
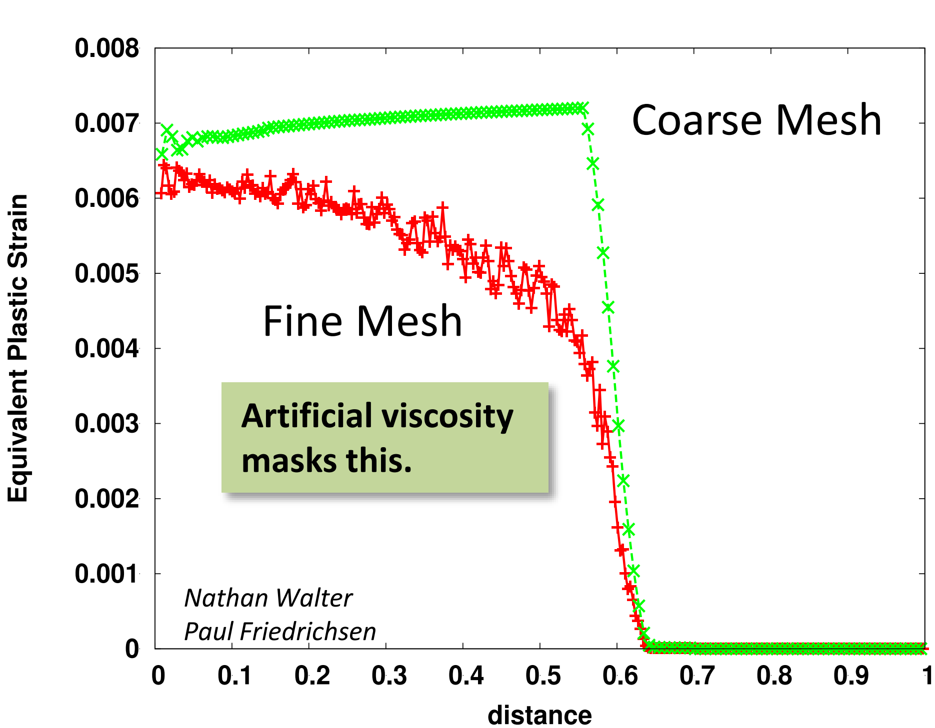
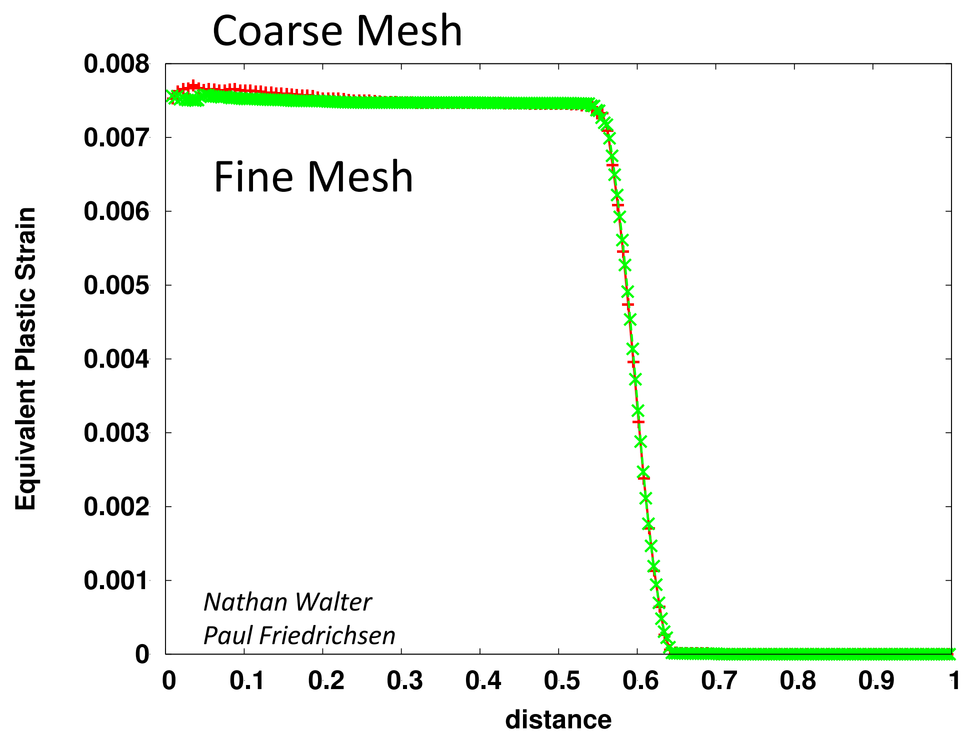

Strain-Rate Based Hardening
Yield Stress
Radial Return Algorithm
Deviatoric Stress
Hydrocode's Shock Shapes
Strain Rate

FLAG - Prior:

Poor PTW Integration + Std. Radial Return + No Iterations = Spatially Non-Convergent





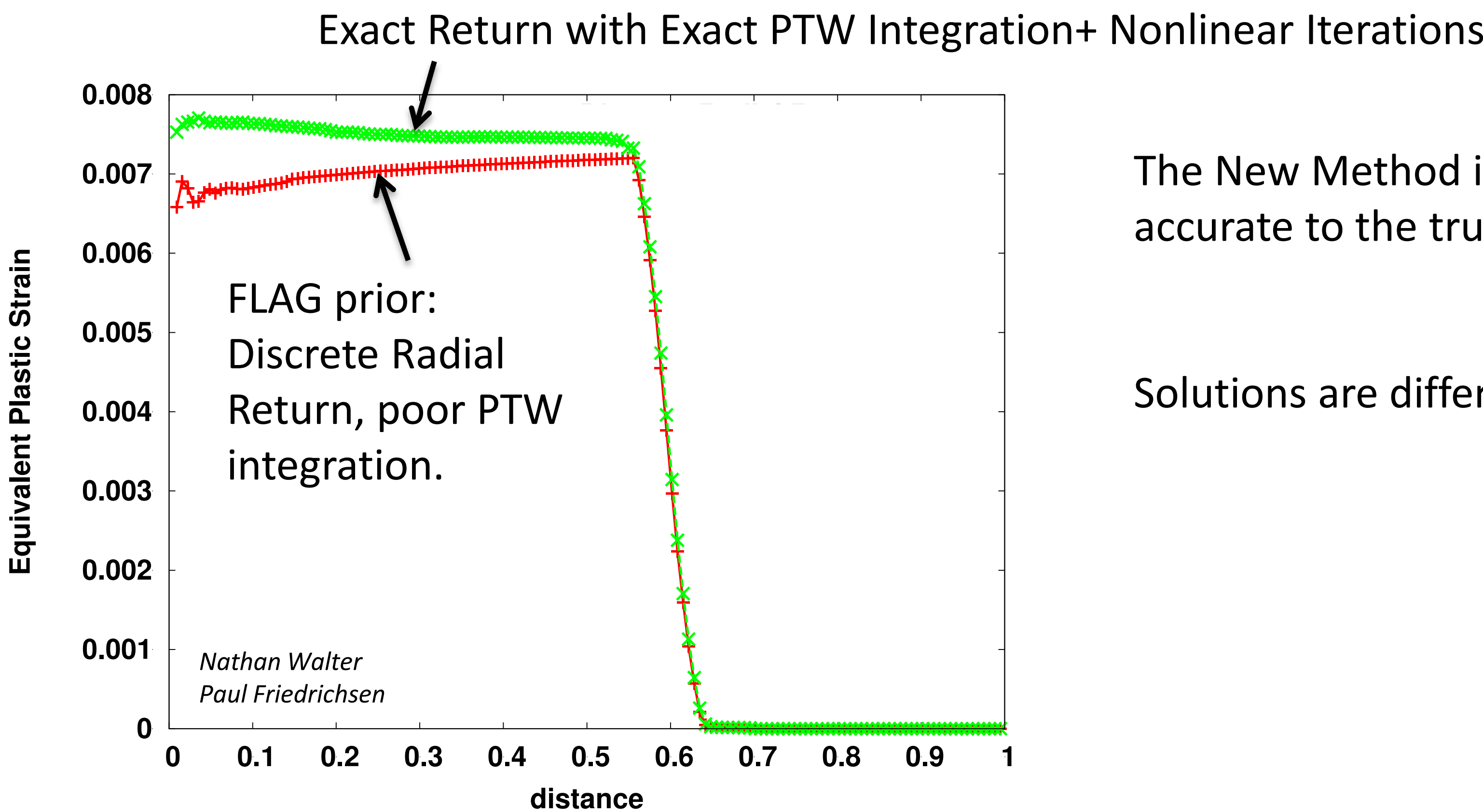
Discrete Radial Return with no iterations

Analytical Solution with Iterations

Analytical solution is convergent in spatial refinement

No artificial viscosity needed

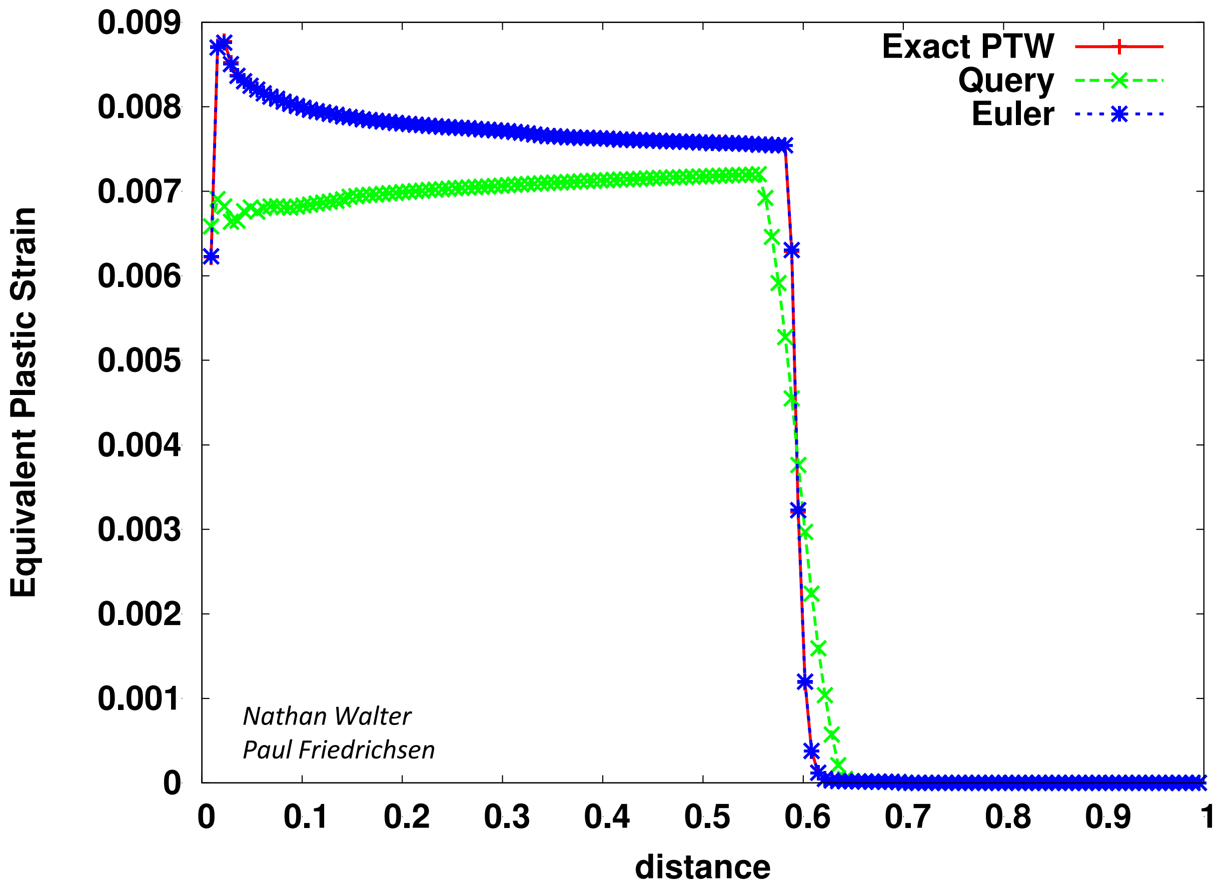
The Prandtl-Reuss Analytical Solution with the PTW Analytical Solution and Nonlinear Iterations



The New Method is more accurate to the true solution.

Solutions are different.

Forward Euler Method for PTW also Works



The figure shows that the exact PTW equation, when implemented correctly, is identical to Euler integration.

This is good verification for the Exact PTW equation and of Euler's method for the hardening rule.

Different Combinations Were Tested

Test Case	Exact Return	Discrete Radial Return	Nonlinear Iterations	PTW: Query	PTW: Euler	PTW: Exact	Spatially Convergent	Viscosity effects	Notes
1		X		X			No	Drastically effects solution. Viscosity smears solution, masks inaccuracies and nonconvergence	Solutions are very inaccurate
2		X			X		Yes	Viscosity smears the solution, wall heating is smeared	Large wall heating present in solution
3	X		X	X			Yes	Minimal effect, solution smears but not by a lot	Solution is closer to test case 2 solution, but still not exactly the same
4	X		X		X		Yes	Minimal effects, solution wall heating is smeared	Solution is very similar to test case 2
5	X					X	Yes	Minimal effects, solution wall heating is smeared	Solution is identical to test case 2. No nonlinear iterations was implemented in combination with PTW:Exact

Nathan Walter and Paul Friedrichsen

Conclusions

Analytical integration of Prandtl-Reuss eliminates spatial non-convergence and reduces impact of artificial viscosity.

Artificial viscosity masks non-convergence and hardening rule errors

Analytical integration of Prandtl-Reuss reduces impact of no iterations.

Final Comments

Summary and Conclusions

Singular Shocks input into PTW: What would it mean?

The hydrocode's radial return algorithm regularizes the singularity in the limit.

Hydrocode's relatively wide shocks: How do they impact PTW?

Hydrocode's typical rise times are not small enough to approximate the limiting value.

Positive outcomes for hydrocodes

Analytical radial return:
(1) Improves stability in FLAG.
(2) Reduces the impact of artificial viscosity.
(3) Opens the opportunity to use shock locators with the singular solution.

Acknowledgements

Funding: Diane Vaughn and Mark Schraad

Collaborators: Len Margolin, Ted Carney, Tom Canfield.

Students: Nathan Walter and Paul Friedrichsen – implementation of exact return in FLAG and producing results.

Los Alamos National Laboratory's

Computational Physics Summer Workshop

Research in teams of two.

Under LANL mentor(s).

35 hours of lectures.

Students from across the US compete to participate.

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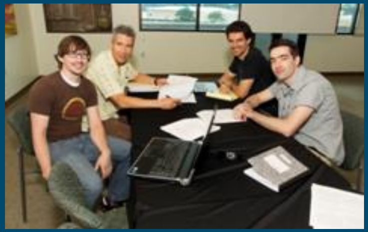

This year's geographic and academic diversity.

People whom we've never met before.

5th Anniversary

Five Years, 104 Students from across the US.

65%	Extended their relationships beyond the workshop
65%	Were expanded relationships to other staff
69%	Published work from the workshop
48%	Workshop research appears in thesis/dissertation

"The workshop was the best thing that could have happened to me academically. My experiences there have completely changed the course of where I want my career to go and what I want to do with my life. I am incredibly grateful that I got to be a part of it."
Jenifer Lilieholm, 2014

"The workshop allowed me to make connections with lab scientists and help me choose a dissertation project which was modern, academically interesting and scientifically useful to the computational physics community."
Cori Hendon, 2011

CompPhysWorkshop.LANL.gov

Applications due in January

Thank You