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High-precision room-temperature isotherm of Pt to over 400 GPa from ramp-compression experiments at the Z machine

Jean-Paul Davis and Justin L. Brown

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Session: Equation of State 1

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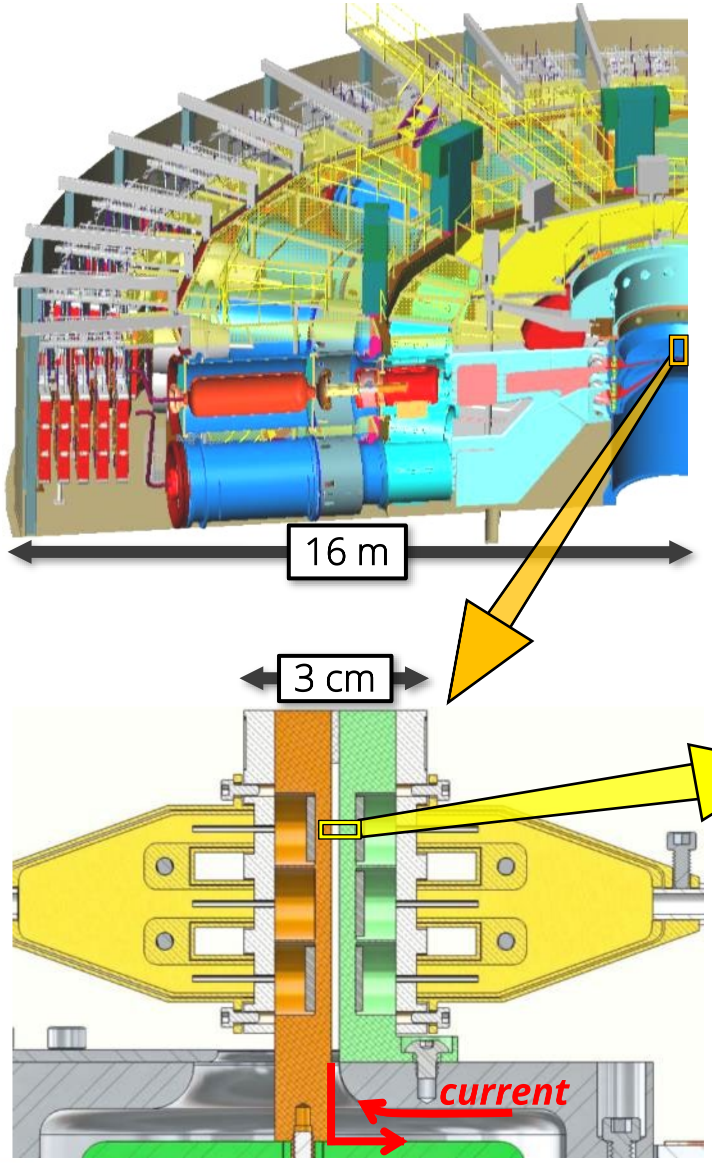
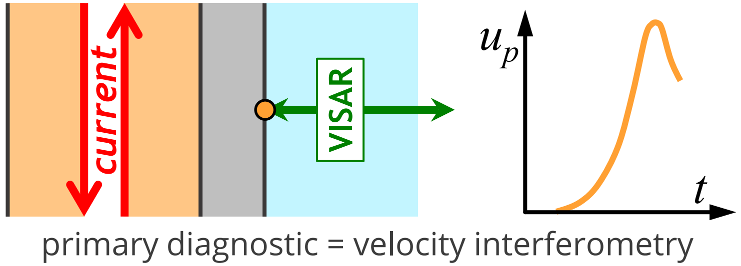
Stripline short-circuit loads on the Z pulsed-power machine can produce planar shockless compression of solids to 400+ GPa

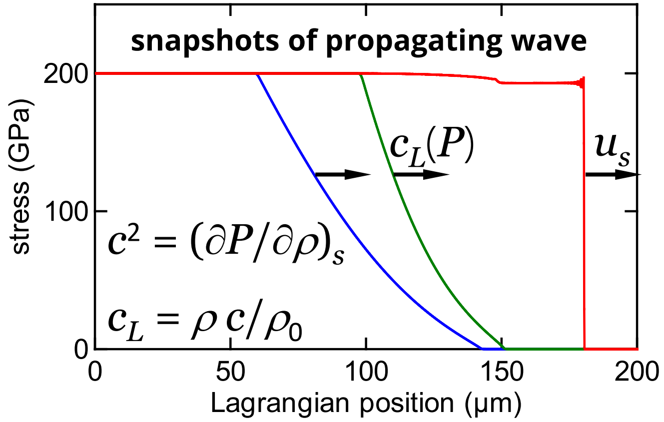
Magnetic drive propagates ramped stress wave into ambient material

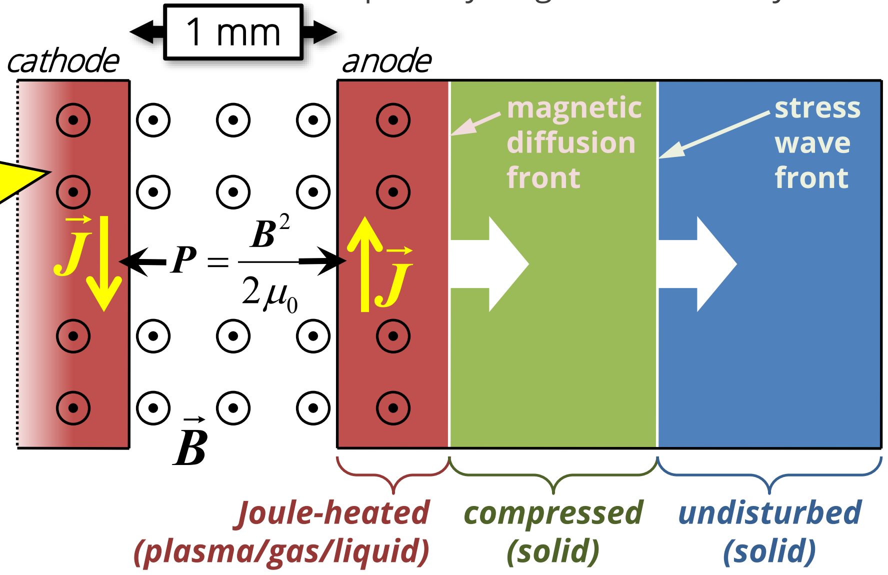
Material's compressibility deduced from velocimetry measurements

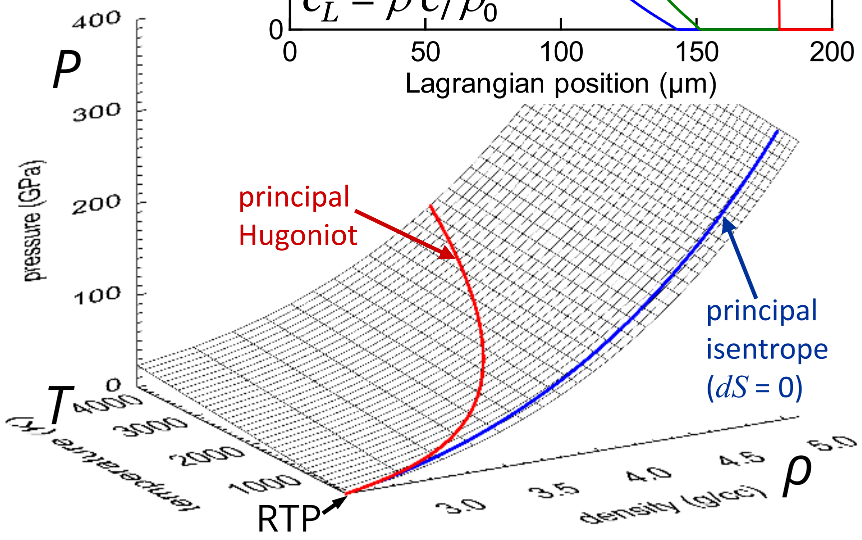
- Shockless compression along quasi-isentrope close to isotherm
- Accurate absolute measurement of pressure standards (*e.g.*, for DAC)



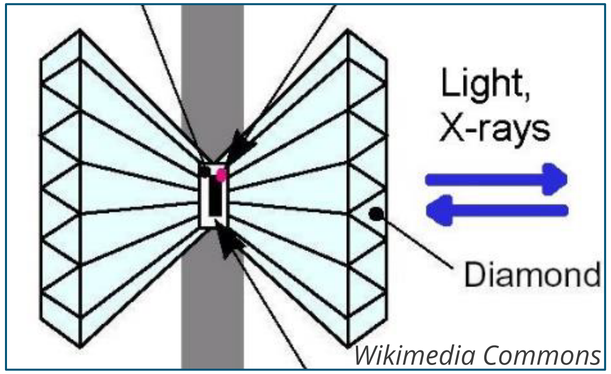








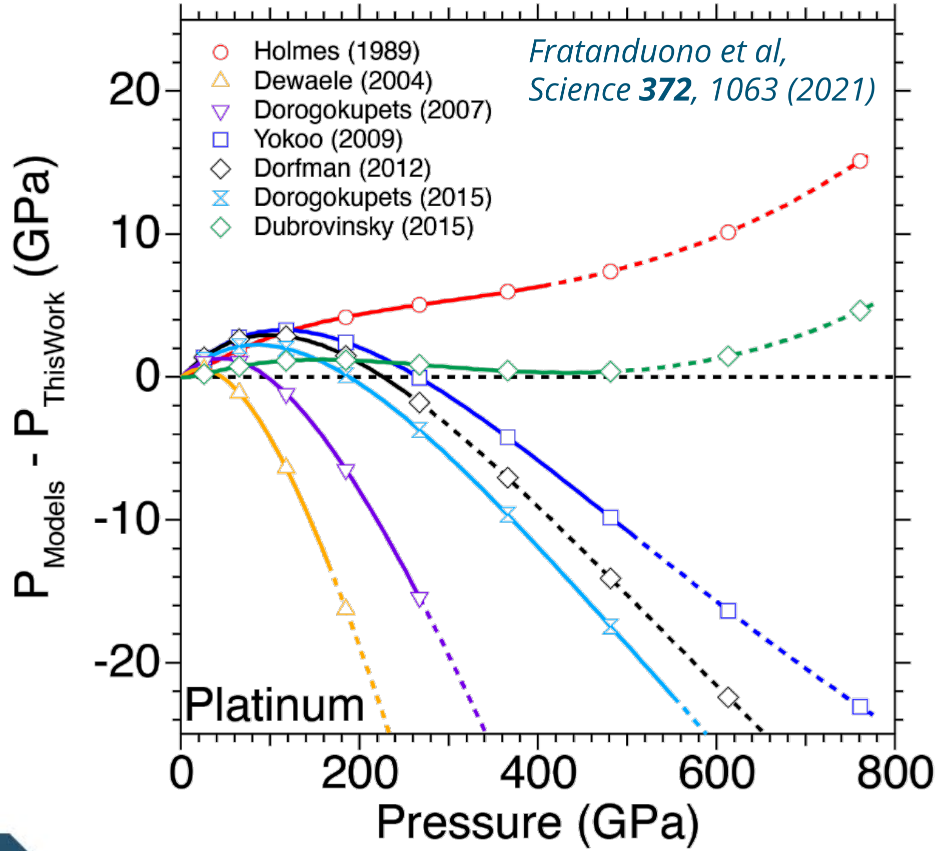
Platinum is a widely used pressure calibrant in DAC work

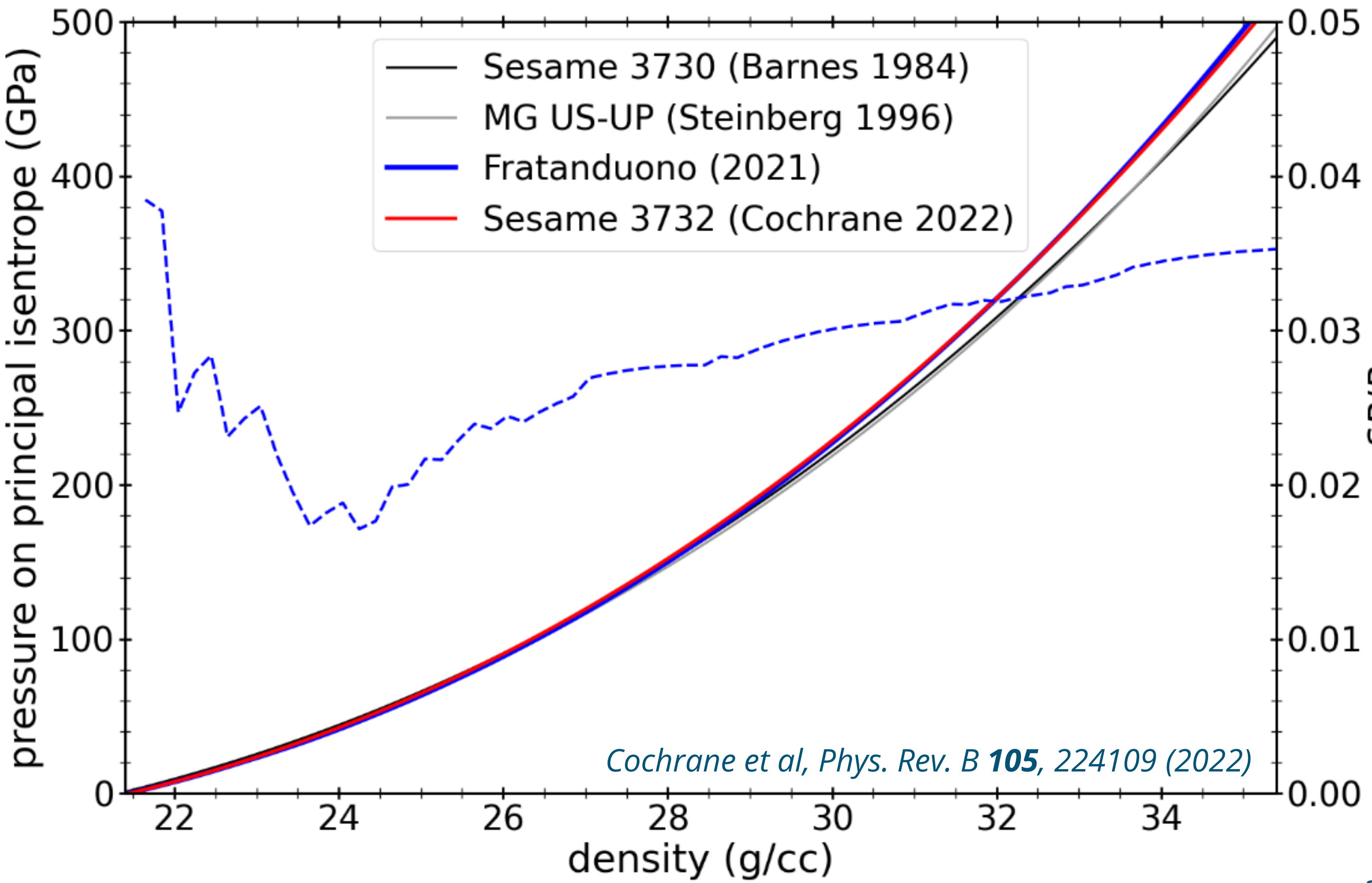


New DAC techniques to P > 300 GPa require precise calibration

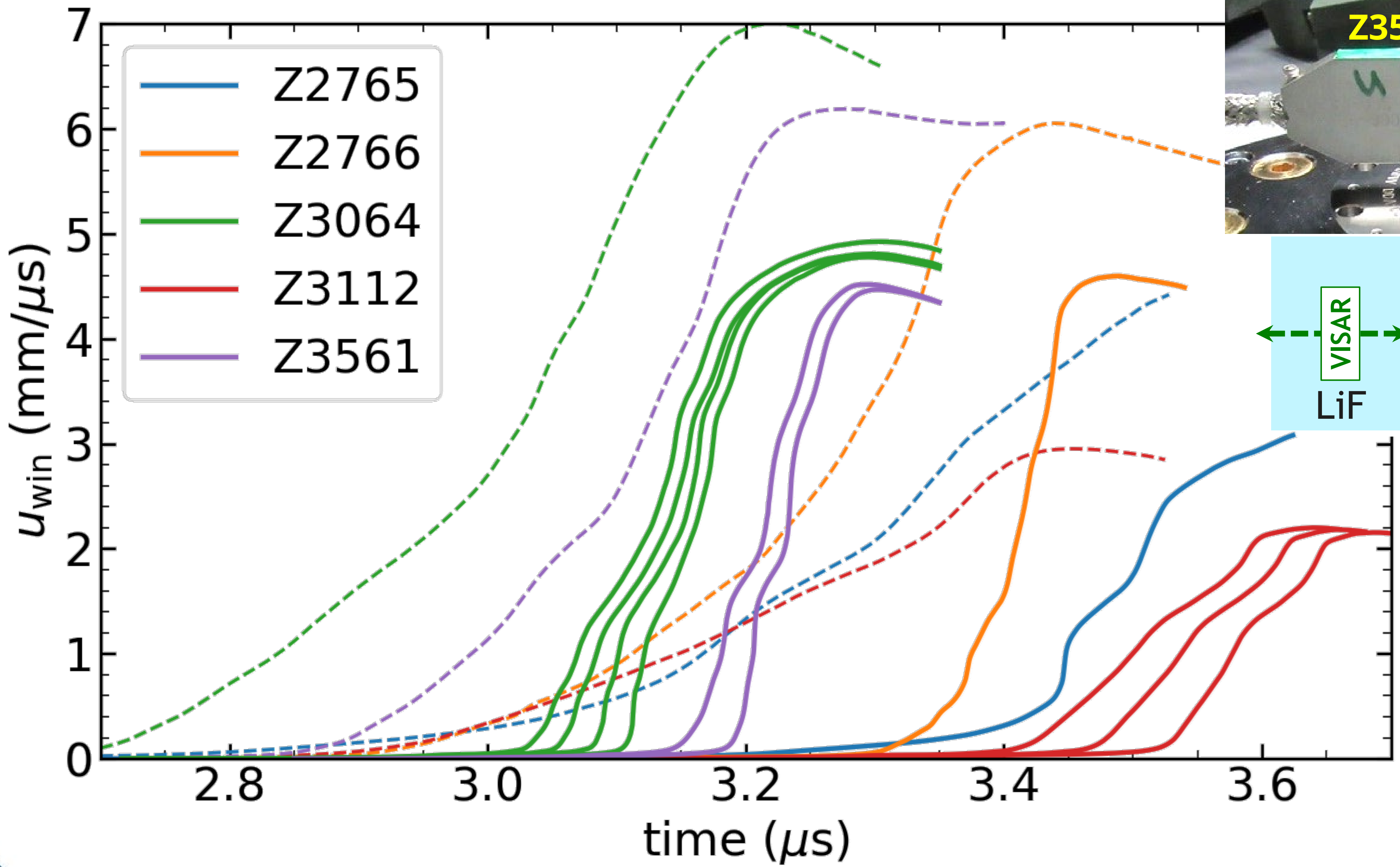
Extrapolated models differ 5-10%

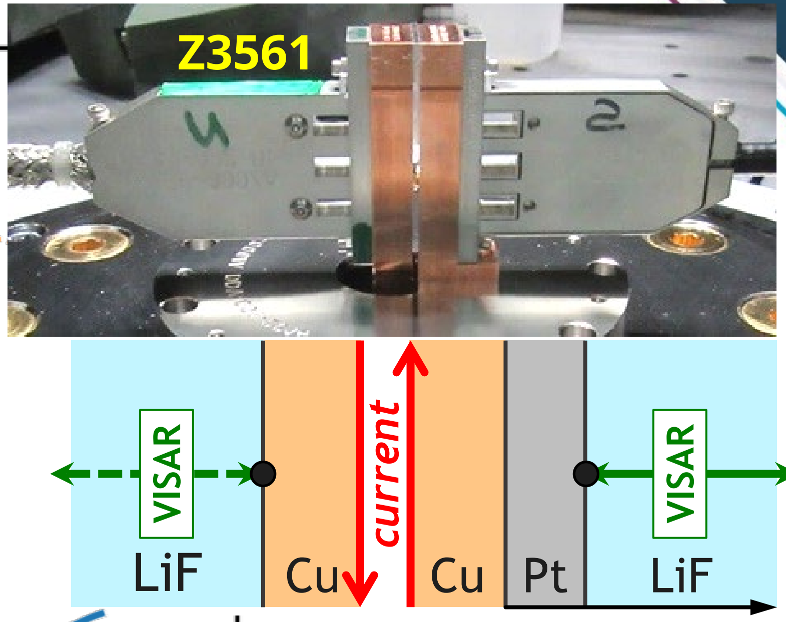
- recent NIF/Z ramp-compression result with uncertainty 3.5%
- included 3 Z measurements to ~400 GPa (NIF data to ~800 GPa)





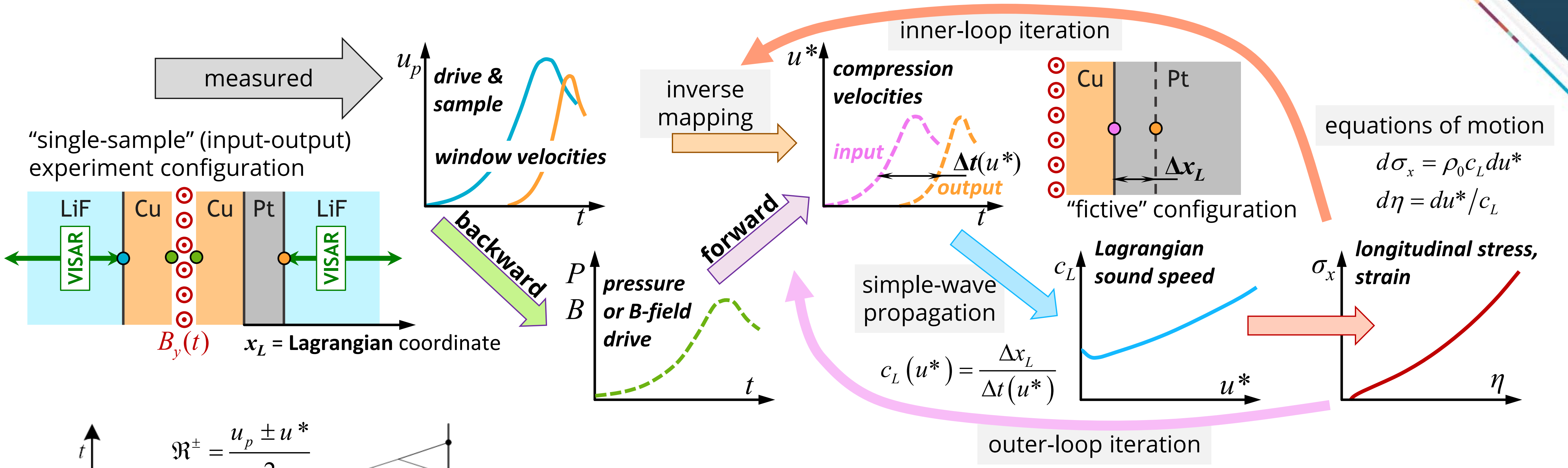
High-precision data are available from 11 single-sample measurements on Pt to peak stresses in the range 160-580 GPa

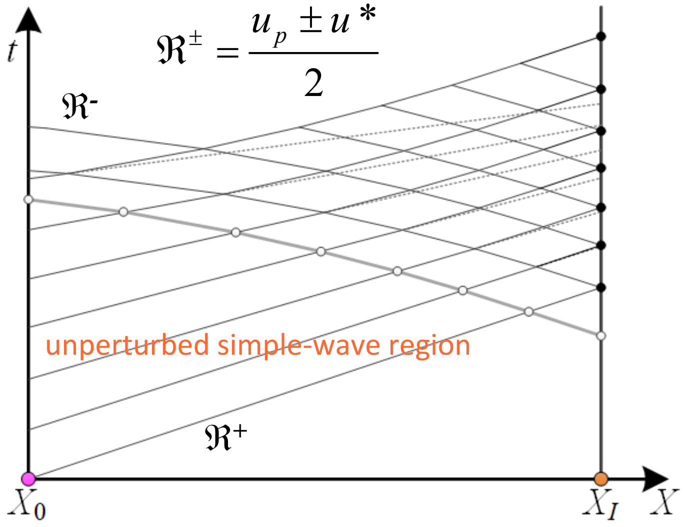




Davis and Brown, "Quantifying uncertainty in analysis of shockless dynamic compression experiments on platinum, Part 1: Inverse Lagrangian analysis," in preparation for submission to J. Appl. Phys. (2023)

Inverse Lagrangian analysis (ILA) extracts sample material's compressibility from shockless-compression velocimetry

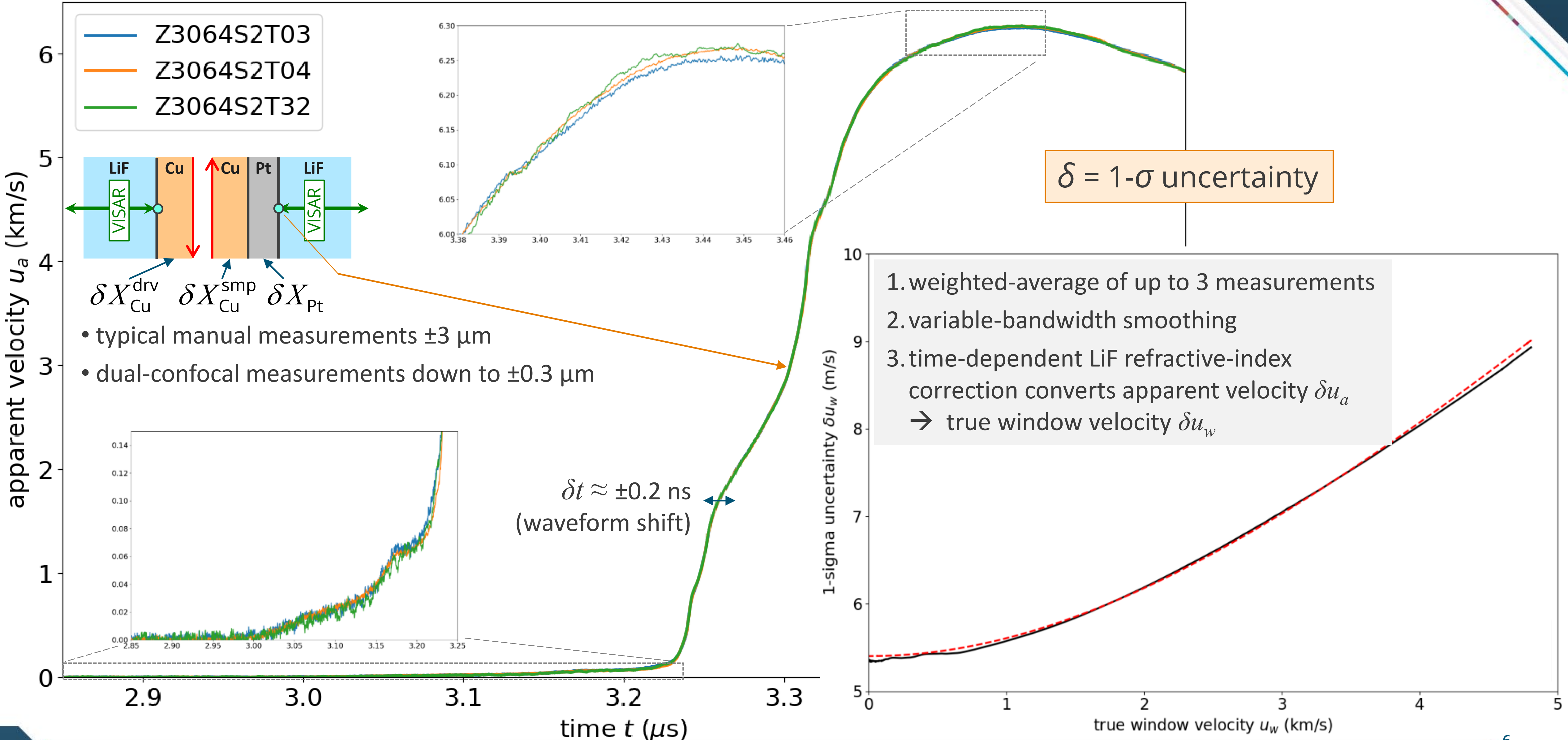




Inverse mapping = backward integration

- most developed approach uses characteristics net in t-x_L
- iterate to self-consistency with Lagrangian analysis of $u^*(t)$
  - the inner loop can be computed non-iteratively
- assumes single-valued material response $c_L(u^*)$, $\sigma_x(\eta)$

Experimental uncertainties consist of measurement uncertainties in velocity, time, and electrode/sample thicknesses

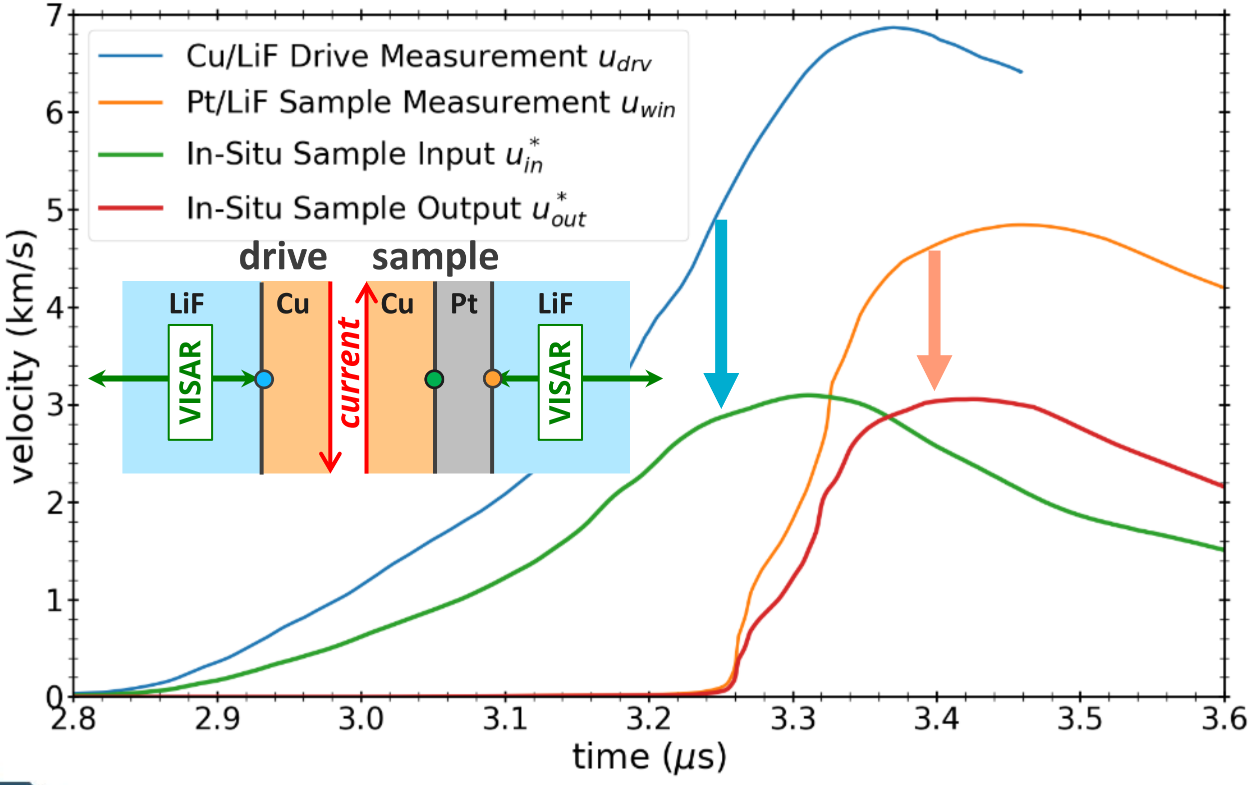


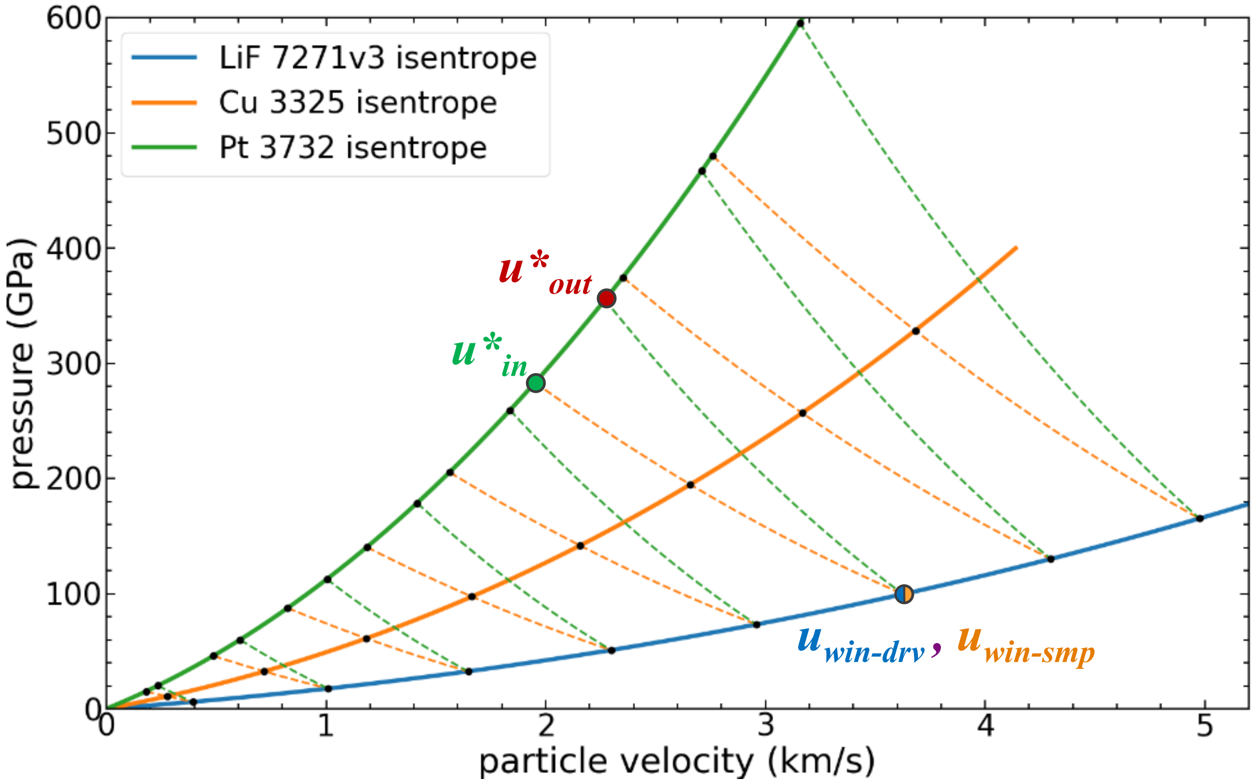
Velocity uncertainty maps to fictive configuration in σ_x-u_p plane

Propagate uncertainty from measured velocity to in-material compression velocity

- compute mapping in stress-velocity plane: known electrode/window EOS, result sample EOS
- δu transfers to/from δt by velocity-time derivative du/dt: relative $\delta u/u$ maps by change in shape

$$u^*(u_{win}) \rightarrow \delta u^* = \frac{\partial u^*}{\partial u_{win}} \delta u_{win}$$

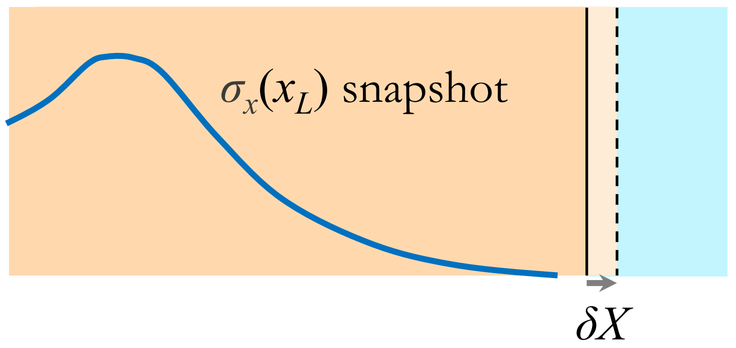




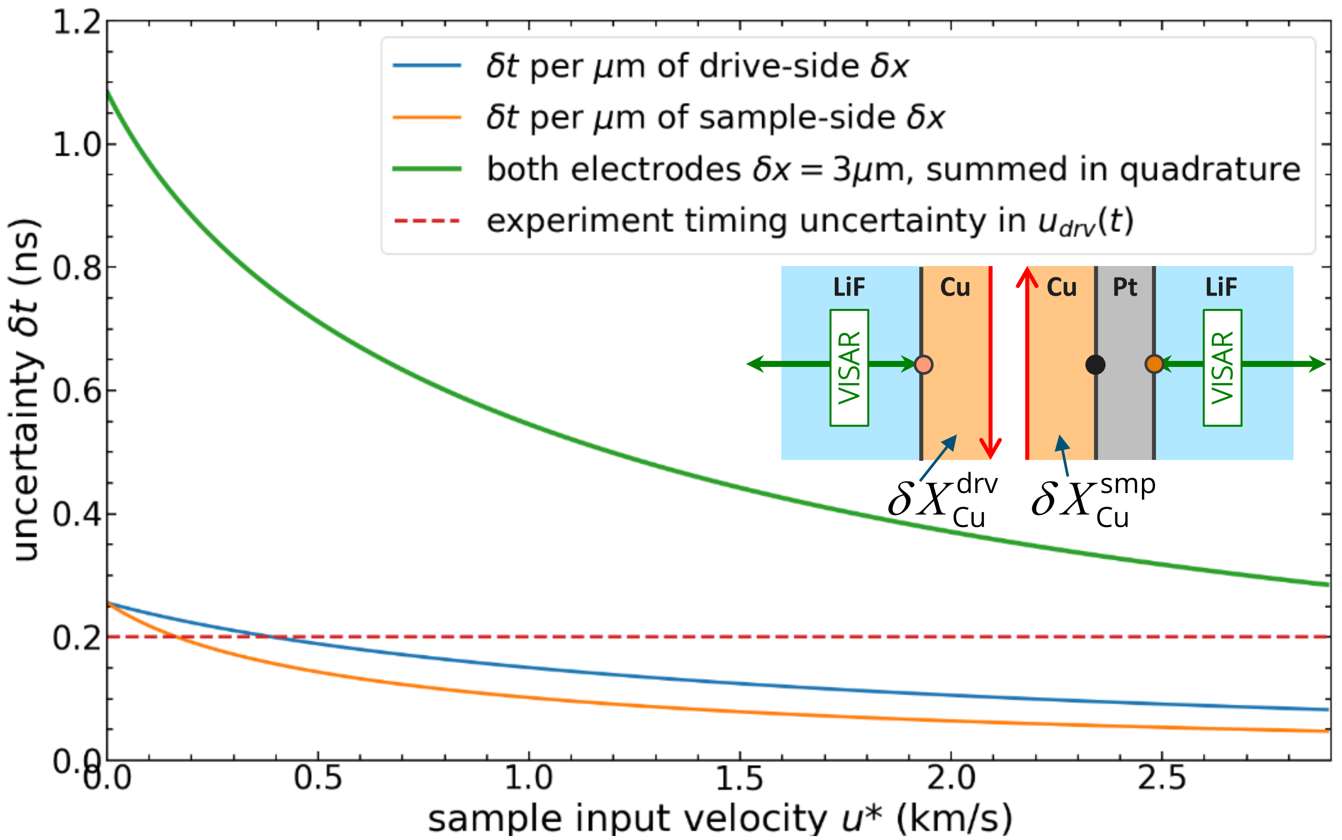
Electrode-thickness uncertainties map to velocity-dependent arrival-time uncertainty in sample-input velocity waveform

for small δX, interface-arrival time discrepancy given by electrode-material's Lagrangian sound speed at interface stress

- significantly increases time uncertainty of $u*_{in}$ waveform below ~1.5 km/s
- add $\delta t_{\delta X}(u*) \cdot (du*/dt)$ in quadrature to $\delta u*_{in}$ for input to Lagrangian analysis code



$$\delta t_{\delta X} = \sqrt{\left(\frac{\delta X_{\mathrm{Cu}}^{\mathrm{drv}}}{c_L\left(\sigma_x^{\mathrm{win}}\right)}\right)^2 + \left(\frac{\delta X_{\mathrm{Cu}}^{\mathrm{smp}}}{c_L\left(\sigma_x^{\mathrm{smp}}\right)}\right)^2}$$



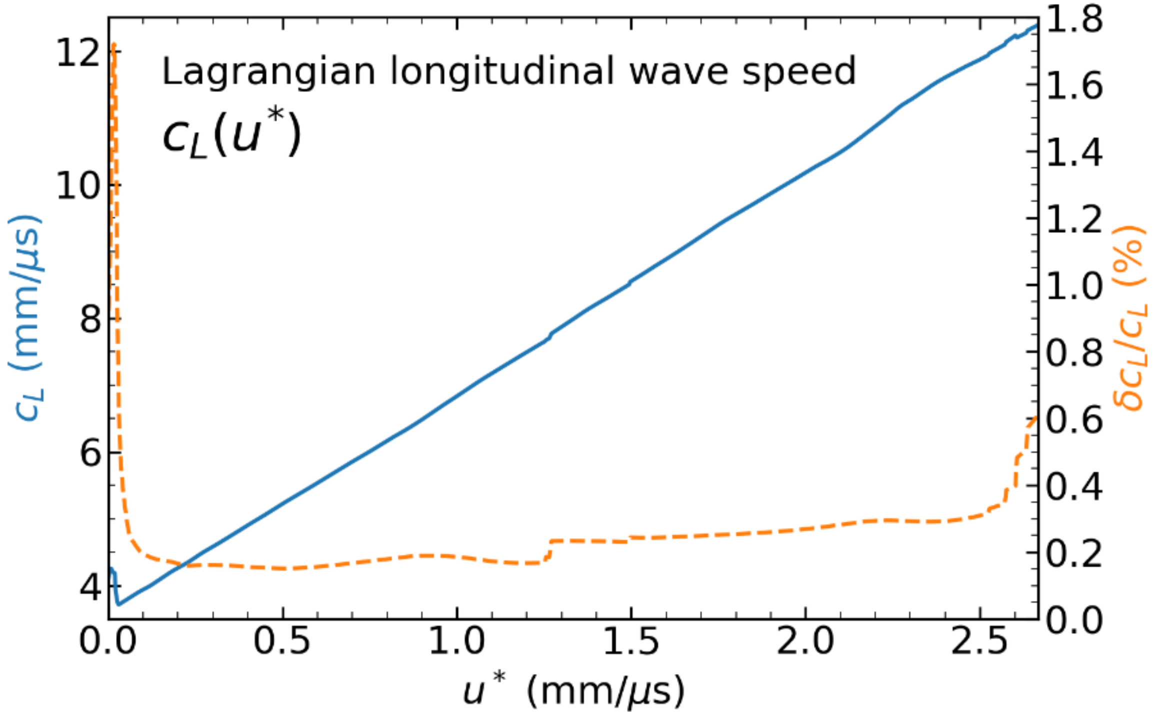
Take weighted average of 11 $c_L(u^*)$ & $\delta c_L(u^*)$, integrate to $\sigma_x(\eta)$ propagating δc_L and $\delta\rho_0$ to total $\delta\sigma_x(\eta)$ = 1% at σ_x = 450 GPa

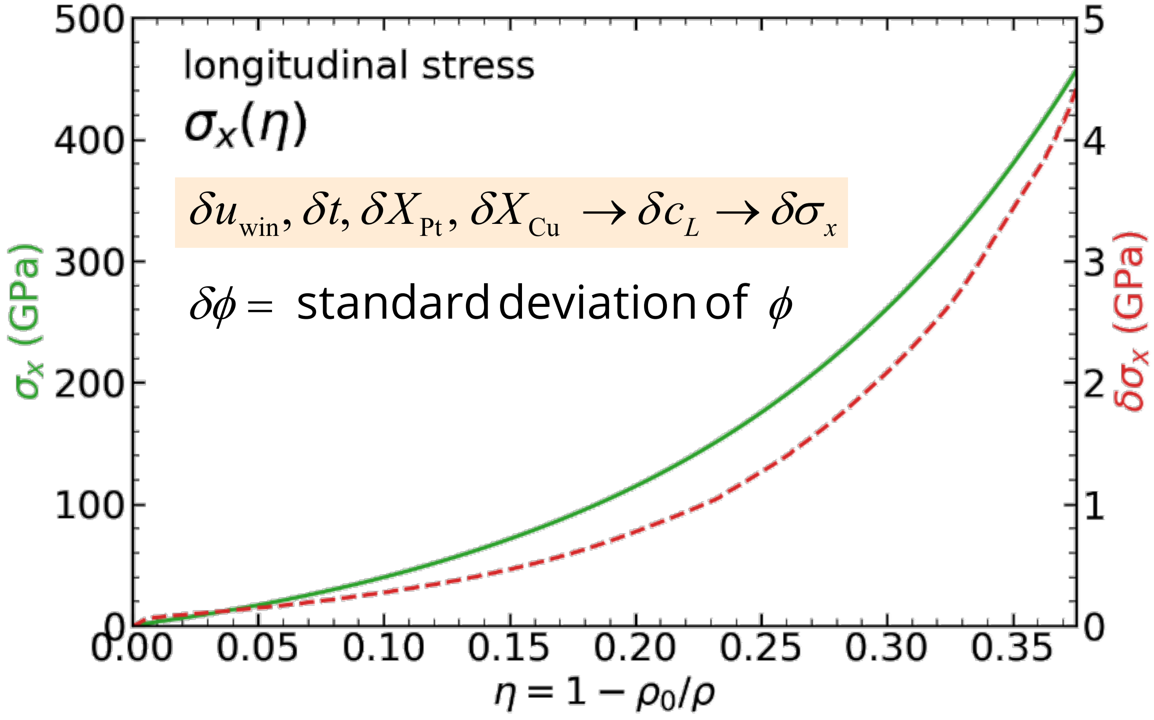
$$c_L(u^*) = \frac{X_{\mathrm{Pt}}}{\Delta t(u^*)}; \qquad \left(\frac{\delta c_L(u^*)}{c_L(u^*)}\right)^2 = \left(\frac{\delta X_{\mathrm{Pt}}}{X_{\mathrm{Pt}}}\right)^2 + \left(\frac{1}{\Delta t(u^*)}\right)^2 \left[2\left(\delta t_{\mathrm{exp}}\right)^2 + \left(\frac{\delta u^*_{\mathrm{in}}}{du^*_{\mathrm{in}}/dt}\right)^2 + \left(\frac{\delta u^*_{\mathrm{out}}}{du^*_{\mathrm{out}}/dt}\right)^2\right]$$

$$\delta\eta(u^*) \simeq \int \frac{\delta c_L}{c_L^2}\, du^*$$

include η-c_L covariance!

$$\delta\sigma_x^{\mathrm{TOT}}(\eta) \simeq \left[\left(\rho_0 \int \delta c_L\, du^*\right)^2 + \left(\frac{\delta\rho_0}{\rho_0}\sigma_x\right)^2\right]^{1/2} + \rho_0 c_L^2 \delta\eta$$





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Yield stress and thermal EOS models allow reduction of long. stress to pressures on quasi-isentrope, isentrope, and isotherm

Standard application of Von Mises yield criterion and Mie-Grüneisen EOS

Mie-Grüneisen EOS

$$P = P_{\text{ref}} + \frac{\rho_0 \Gamma \left(E - E_{\text{ref}}\right)}{1-\eta}$$

power-law Grüneisen parameter

$$\Gamma = \Gamma_0 \left(1-\eta\right)^q$$

Assume constant c_V and β = 0.9

Need functions $Y(P)$, $G(P)$, and $\Gamma(\eta)$

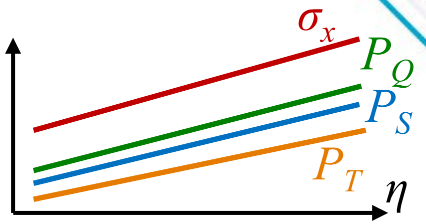
Iterate to self-consistent $P_Q \leftrightarrow Y$

Integrate ordinary diff. eqn. to get P_T

quasi-isentrope $P_Q = \sigma_x - \sigma' = \sigma_x - \frac{2}{3}Y$

isentrope $P_S = P_Q - \frac{\rho_0 \Gamma}{1-\eta} \beta \int dW_p$

isotherm $P_T = P_S - \frac{\Gamma}{1-\eta} \int \left(P_S - P_T - \frac{\rho_0^2 \Gamma c_V T}{1-\eta} \right) d\eta$



σ' deviatoric stress

Y yield stress

Γ Grüneisen parameter

β integral Taylor-Quinney coefficient

$dW_p = \frac{2}{3} \frac{Y}{\rho_0} \left(\frac{1}{1-\eta} - \frac{1}{2G} \frac{dY}{d\eta} \right) d\eta$ incremental plastic work

G shear modulus

c_V isochoric specific heat

Simply subtracting deviatoric stress to obtain quasi-isentrope pressure can introduce elastic-region errors, limiting accuracy

A straight line in u, ρ, or η from P_Q=0 …

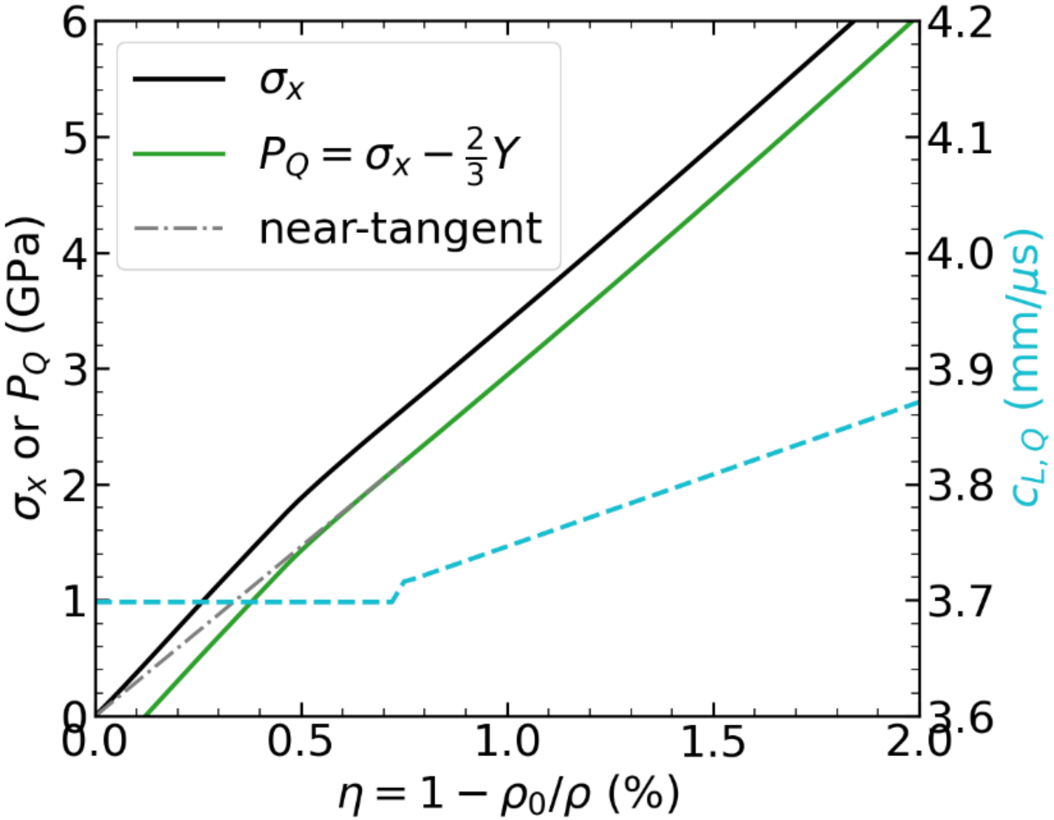
- Cannot avoid discontinuity in wave speed above elastic limit
- Does not match known elastic response at ambient

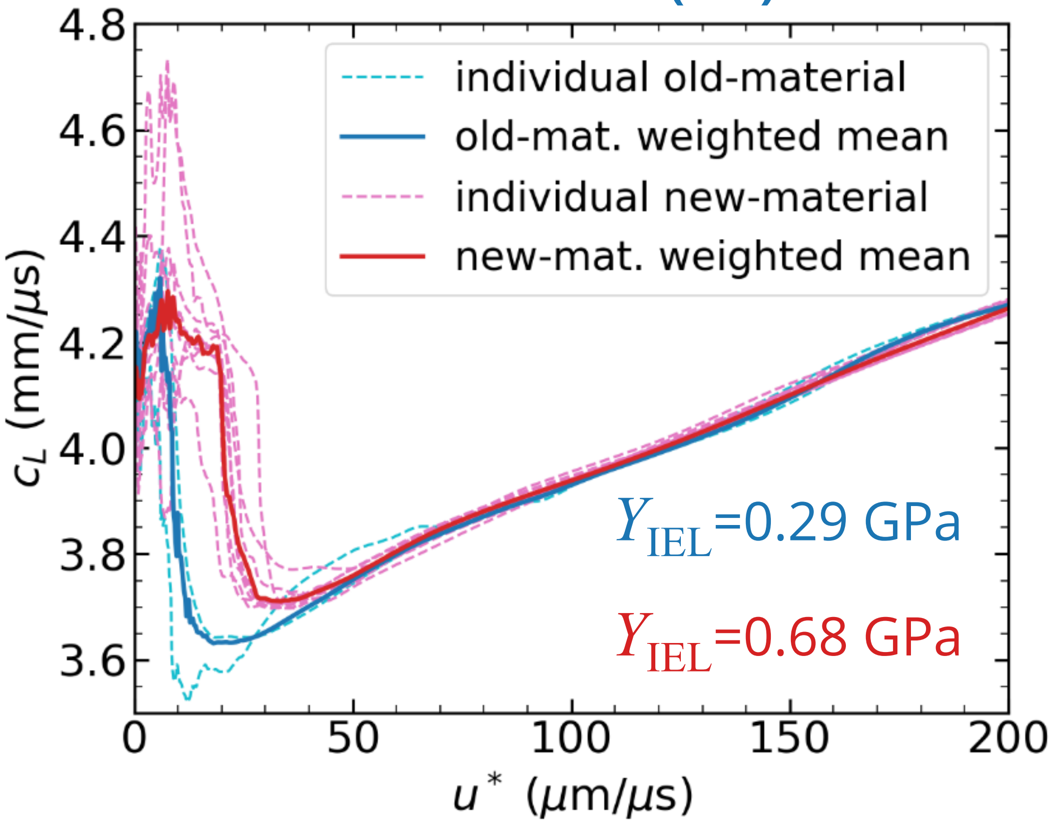
Initial yield stress depends strongly on microstructure

- Isentrope pressure P_S should **not** depend on yield stress

isentropic elastic limit Y_{IEL}

Z2765 & Z2766 used different (old) material





To avoid these issues, compute quasi-isentrope & isentrope reductions in wave speed instead of stress/pressure

Lagrangian wave speeds $c_L = \sqrt{\frac{1}{\rho_0}\frac{d\sigma_x}{d\eta}}$, $c_{L,Q} = \sqrt{\frac{1}{\rho_0}\frac{dP_Q}{d\eta}}$, $c_{L,S} = \sqrt{\frac{1}{\rho_0}\frac{dP_S}{d\eta}} = \frac{\rho}{\rho_0}\sqrt{\left(\frac{\partial P}{\partial \rho}\right)_S}$ (sound speed)

$$\sigma_x = P_Q + \frac{2}{3}Y \quad \rightarrow \quad \frac{d\sigma_x}{du^*} = \frac{dP_Q}{d\eta}\frac{d\eta}{du^*}\left(1+\frac{2}{3}\frac{dY}{dP_Q}\right)$$

$$u^* = \int c_L d\eta \quad \neq \quad u_Q \quad \neq \quad u_S$$

$$c_{L,Q}^2 = c_L^2\left(1+\frac{2}{3}\frac{dY}{dP_Q}\right)^{-1}$$

$$u_Q = \int c_{L,Q} d\eta \qquad P_Q = \rho_0 \int c_{L,Q} du_Q = \rho_0 \int c_{L,Q}^2 d\eta$$

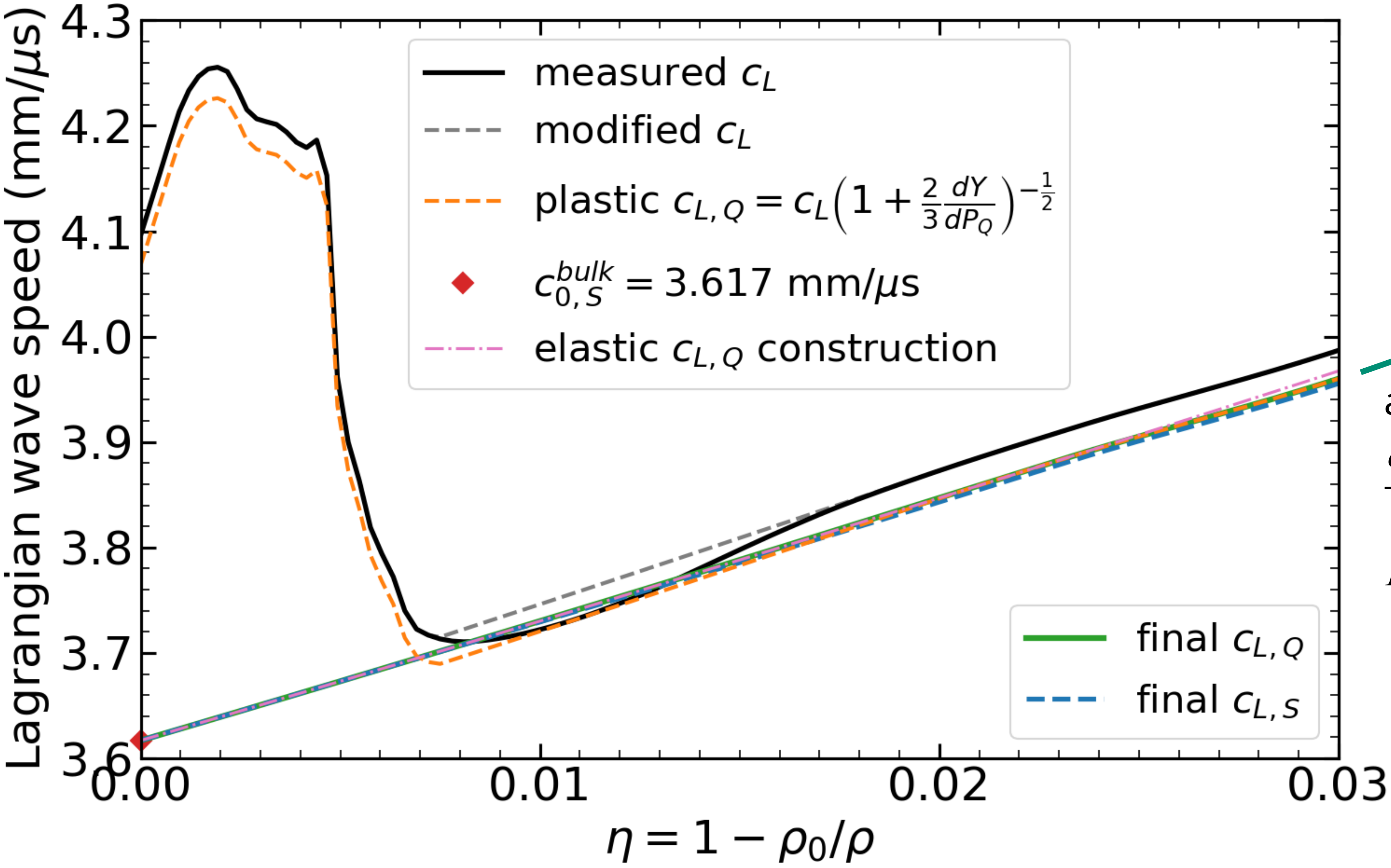
$$c_{L,S}^2 = c_{L,Q}^2 - \beta\Gamma_0 (1-\eta)^{q-1}\left(\frac{dW_p}{d\eta} - \frac{q-1}{1-\eta}W_p\right)$$

$$u_S = \int c_{L,S} d\eta \qquad P_S = \rho_0 \int c_{L,S} du_S = \rho_0 \int c_{L,S}^2 d\eta$$

$$dW_p = \frac{2}{3}\frac{Y}{\rho_0}\left(\frac{1}{1-\eta} - \frac{1}{2G}\frac{dY}{d\eta}\right)d\eta$$

velocity material would have under shockless "bulk" compression wave (as if for strengthless, inviscid fluid)

Interpolating bulk wave speed between known ambient value and plastic region gives smooth pressure curve



at $\eta = 0.375$:

$$\frac{c_{L,Q} - c_{L,S}}{c_{L,S}} = 0.33\%$$

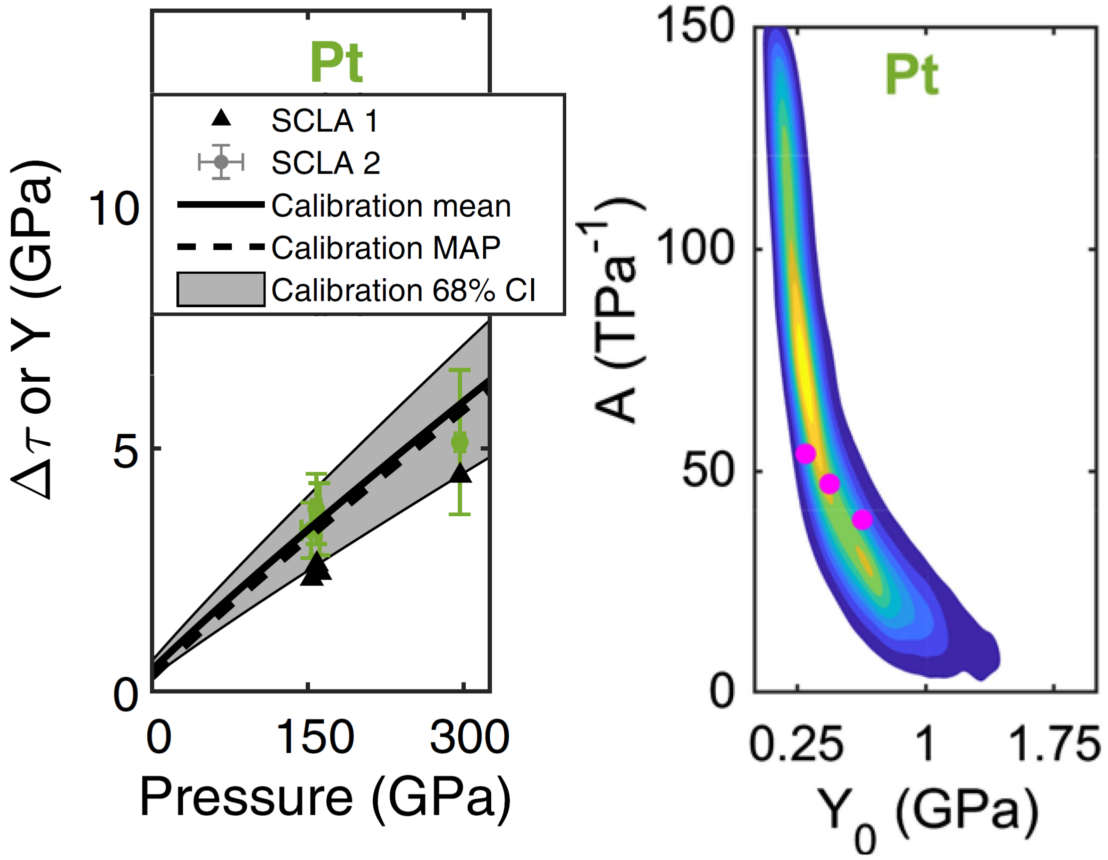
$$P_Q - P_S = 2.16 \text{ GPa}$$

Monte-Carlo UQ analysis of the reduction procedure requires statistical models for 10 input parameters

	distribution	$\mu, s^{1/2}$	units
Y_0	$p([Y_0, A] \| D)$	**0.29, N/A**	**GPa**
A	$p([Y_0, A] \| D)$	**72, N/A**	**TPa $^{-1}$**
Γ_0	$N([\mu_{\ln\Gamma_0}, \mu_q], \Sigma)$	0.971, 0.118	
q	$N([\mu_{\ln\Gamma_0}, \mu_q], \Sigma)$	0.94, 0.411	
β	$B(6.4, 1.6)$	0.90; [0.66, 0.93]	
ρ_0	$N(\mu_{\rho_0}, s_{\rho_0})$	21.421, 0.043	g/cm^3
$c_{0,S}$	$N(\mu_{c_{0,S}}, s_{c_{0,S}})$	3.617, 0.055	mm/μs
G_0	$N(\mu_{G_0}, s_{G_0})$	63.7, 3.6	GPa
c_V	$N(\mu_{c_V}, s_{c_V})$	130.2, 0.4	J/(kg·K)
T_0	$N(\mu_{T_0}, s_{T_0})$	300, 3	K

simplified Steinberg-Guinan yield

$$Y = Y_0\left[1 + AP_Q(1-\eta)^{1/3}\right], \quad G = G_0\frac{Y}{Y_0}$$



Brown et al, J. Dynamic Behavior of Materials ***7****, 196-206 (2021)*

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$\boldsymbol{\Gamma_0}$	$\boldsymbol{N([\mu_{\ln\Gamma_0}, \mu_q], \Sigma)}$	**0.971, 0.118**	***R*=0.882**
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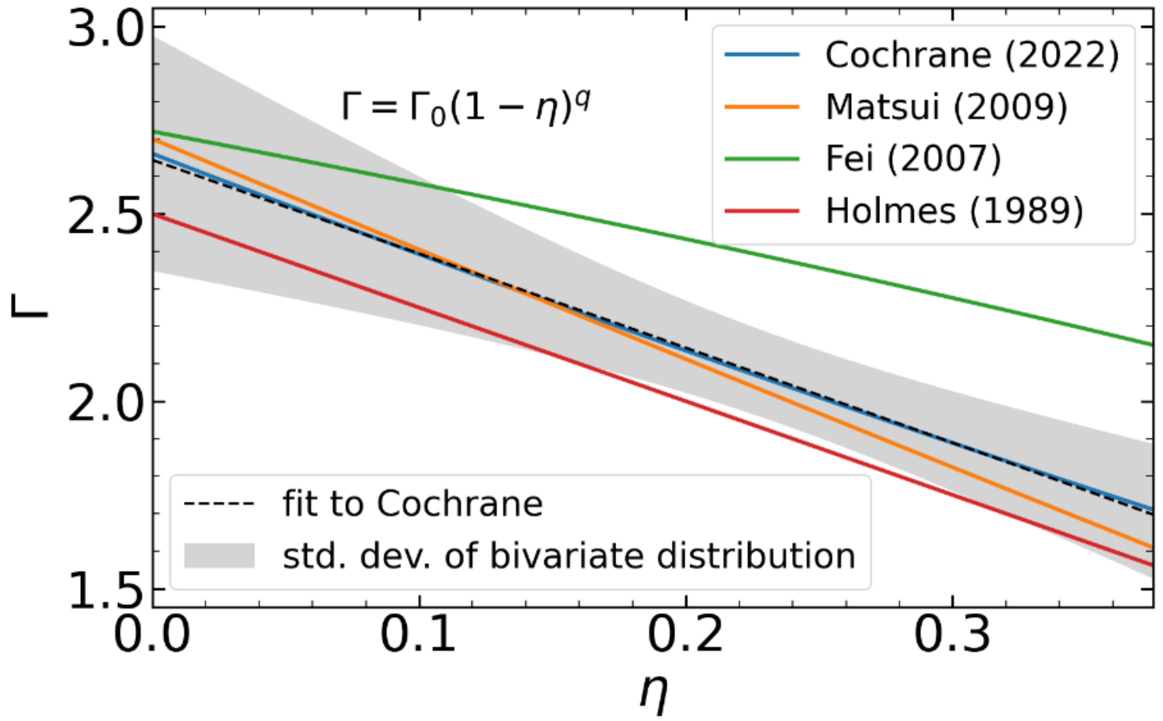
mean: fit to Cochrane et al (2022)

std. dev: fit $\Delta\ln\Gamma = \Delta\ln\Gamma_0 + \Delta q\ln(1-\eta)$

where $\Delta\Gamma = \Gamma_{\text{Matsui, Fei, or Holmes}} - \Gamma_{\text{Cochrane}}$



Cochrane et al, Phys. Rev. B ***105****, 224109 (2022)*

Matsui et al, J. Appl. Phys. ***105****, 013505 (2009)*

Fei et al, Proc. Nation. Acad. Sci. ***104****, 9182-9186 (2007)*

Holmes et al, J. Appl. Phys. ***66****, 2962-2967 (1989)*

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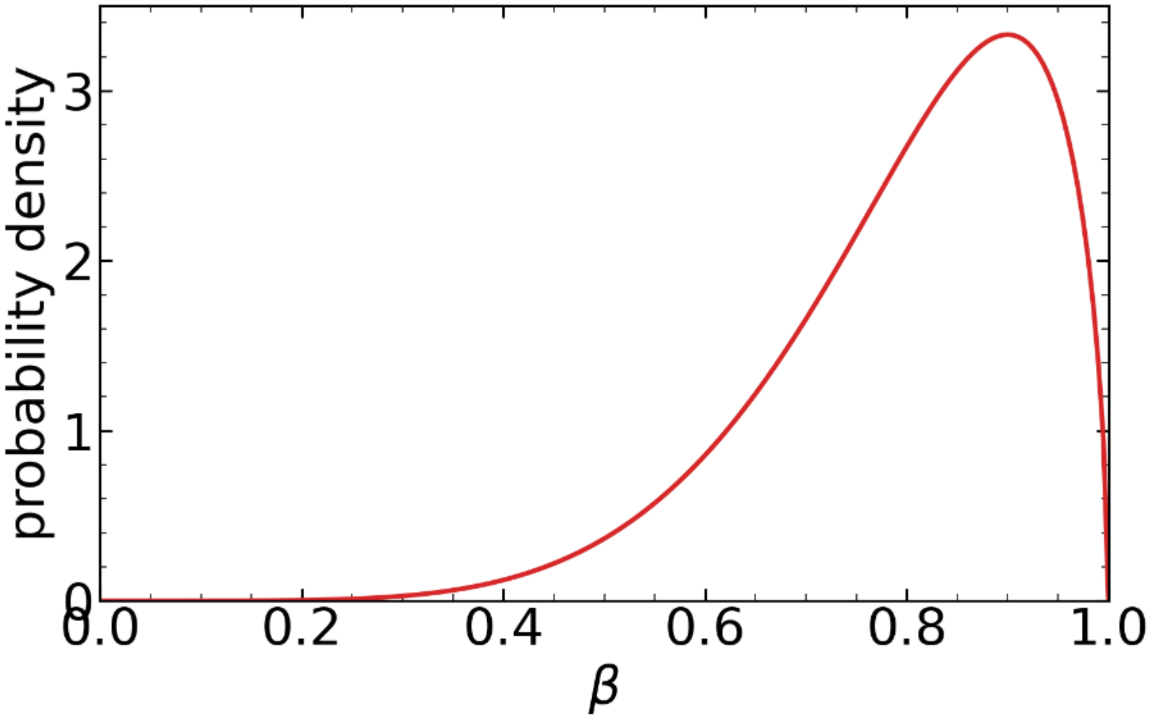
T_0	$N(\mu_{T_0}, s_{T_0})$	300, 3	K

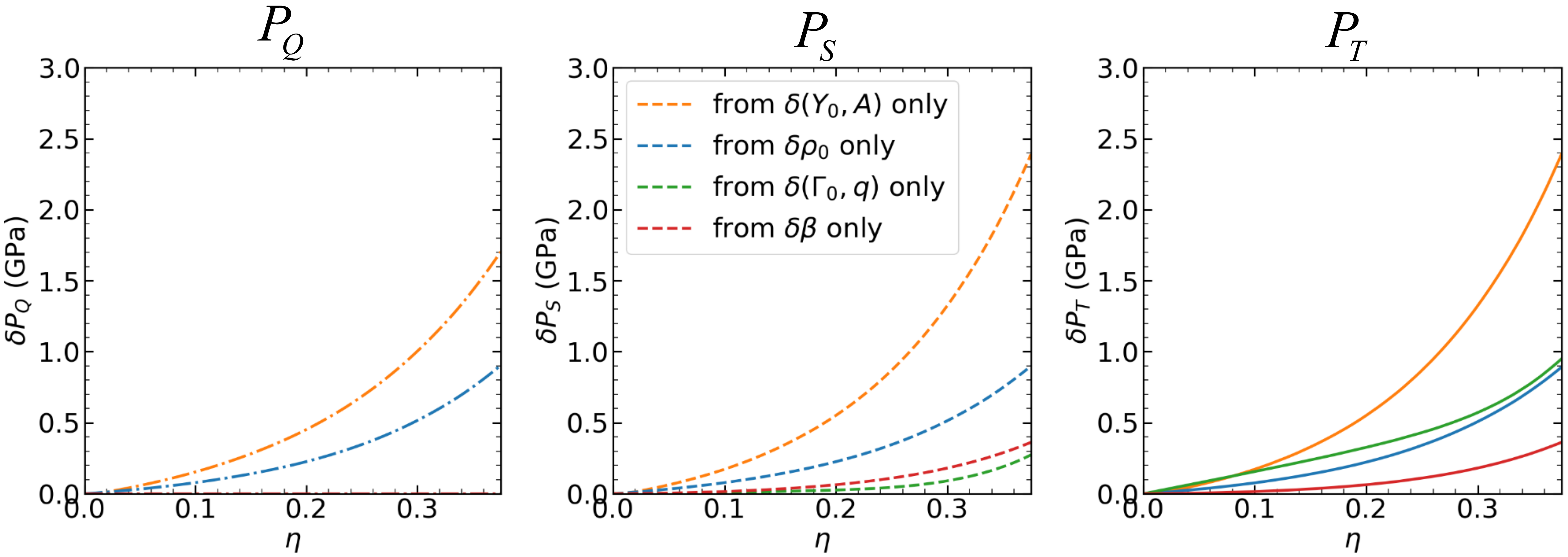
mode = 0.9; 68.3% CI = [0.66, 0.93]
95.4% CI = [0.48, 0.98]



Remaining 5 parameters = independent univariate normal distributions

Obtain rough estimate of sensitivities by "screening" for effect of one univariate or bivariate parameter distribution at a time

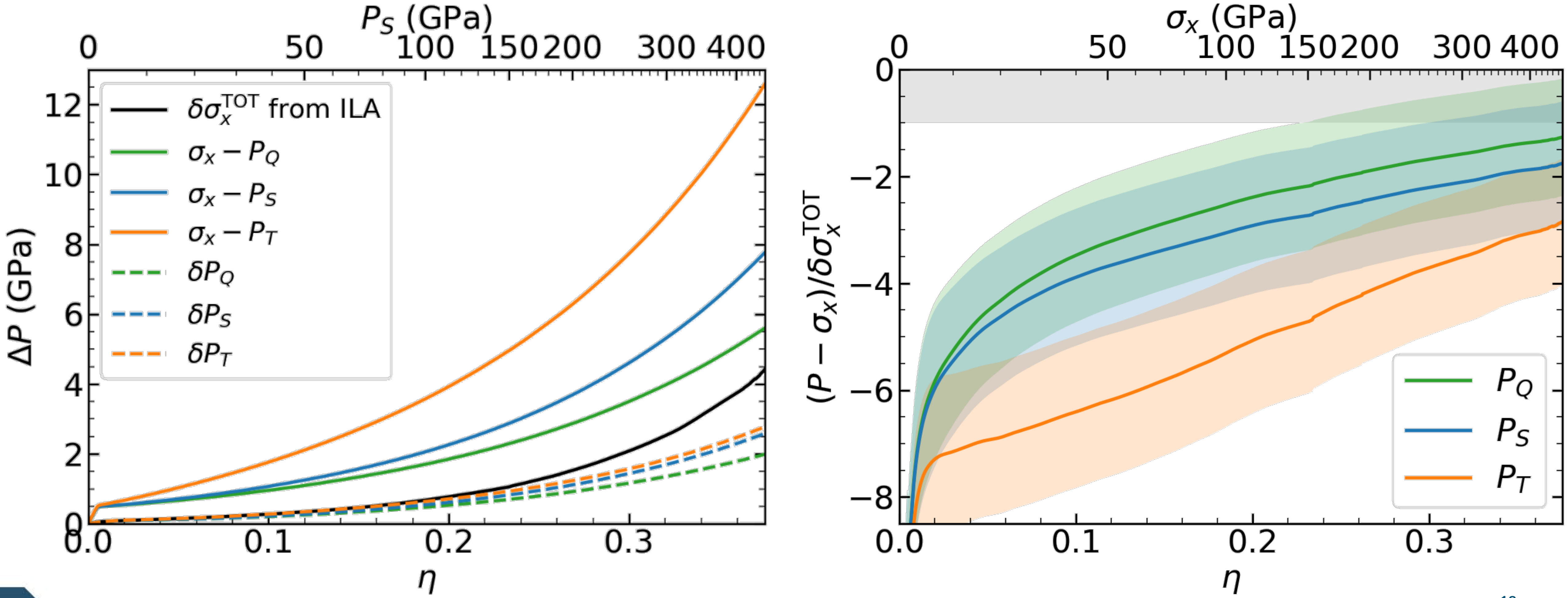
- Screening Monte Carlo (MC) converged by 100,000 samples
- Non-normal distributions described by average median-centered 68.3% confidence interval (CI)



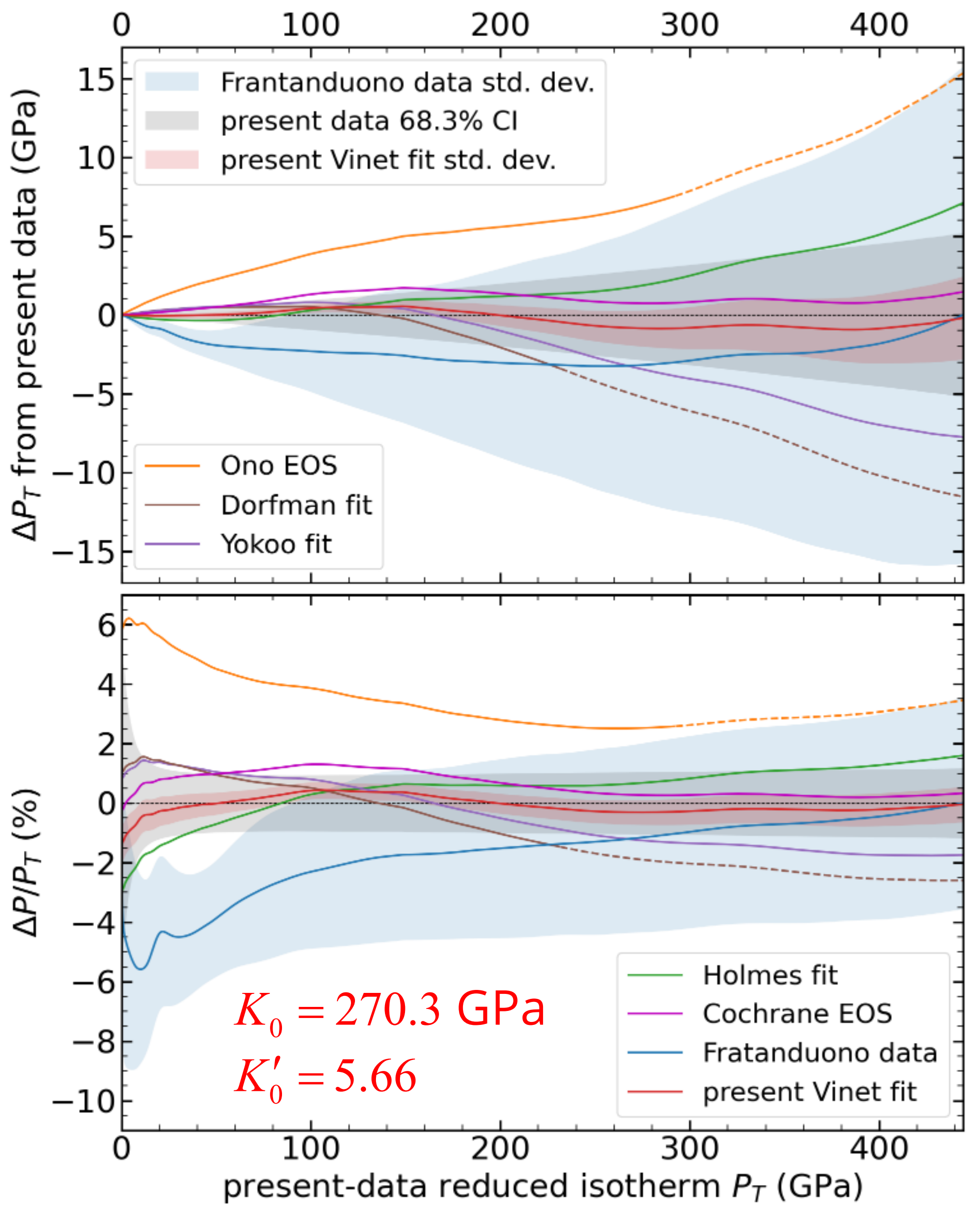
None of the remaining 4 parameters surpassed 0.1-GPa effect

Uncertainty contributed by reduction procedure quantified by 500,000-sample Monte Carlo added in quadrature to total $\delta\sigma_x$

- Non-normal distributions again described by average median-centered 68.3% confidence interval (CI)
- Two views of reduction corrections and CI: (left) absolute, before adding to total $\delta\sigma_x$ std. dev., and (right) in units of $\delta\sigma_x$, after adding to total $\delta\sigma_x$ std. dev.

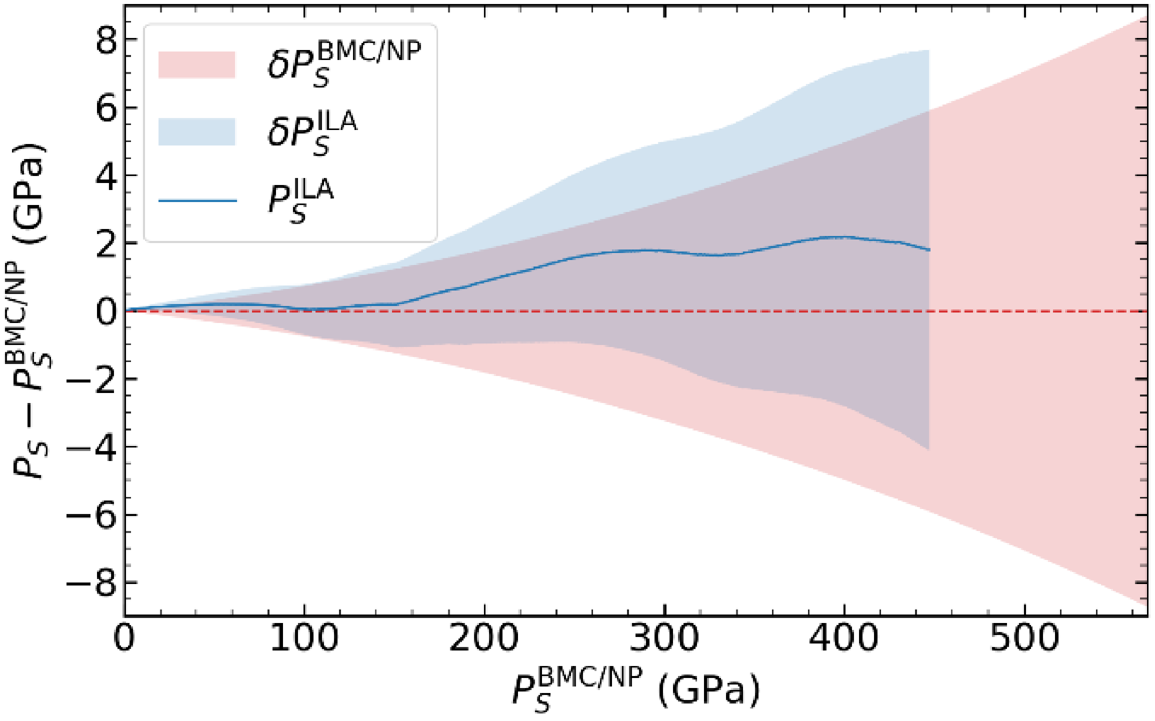


Determined absolute P(η) isotherm of Pt to unprecedented precision of ±1.2% at 444 GPa



Bayesian model calibration of same data set

- non-parametric isentrope model = 5-knot PCHIP spline in Eulerian sound speed $c_E(\eta)$
- increases δP by ~15% (correctly accounts for decreased sensitivity at higher pressures)
- extends result to peak loading of P_S ~ 570 GPa



Brown et al, "Quantifying uncertainty in analysis of shockless dynamic compression experiments on platinum, Part 2: Bayesian model calibration," in preparation for submission to J. Appl. Phys. (2023)

Conclusions

Rigorous propagation of experimental uncertainties to total $\delta\sigma_x(\eta)$

- about 1% at ~450 GPa from weighted averaging of 11 high-precision Z measurements on Pt

Reduction to pressures on quasi-isentrope, isentrope, isotherm computed in wave speeds

- interpolate across elastic-plastic transition from known ambient bulk $c_{0,S}$ to plastic-flow $c_{L,Q}$
- P_Q depends only on yield-stress derivative dY/dP, not initial yield stress Y_{IEL}
- P_S depends also on absolute $Y(P)$ but with nearly inconsequential sensitivity

Monte Carlo analysis quantifies reduction procedure contribution to uncertainty

- Reduction to isotherm P_T is correction of ~3 $\delta\sigma_x$ at ~450 GPa, resulting in δP_T just under 1.2%

UQ does not yet include uncertainty in Cu and LiF material models used in ILA

Bayesian model calibration (BMC) suggests decreased sensitivity at highest pressures inflates uncertainty there (1.14% from ILA but 1.32% from BMC)

Important differences between ILA and BMC