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Quantifying uncertainty for multi-megabar ramp compression of Pt

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Session K01: Uncertainty Quantification and Propagation for EOS

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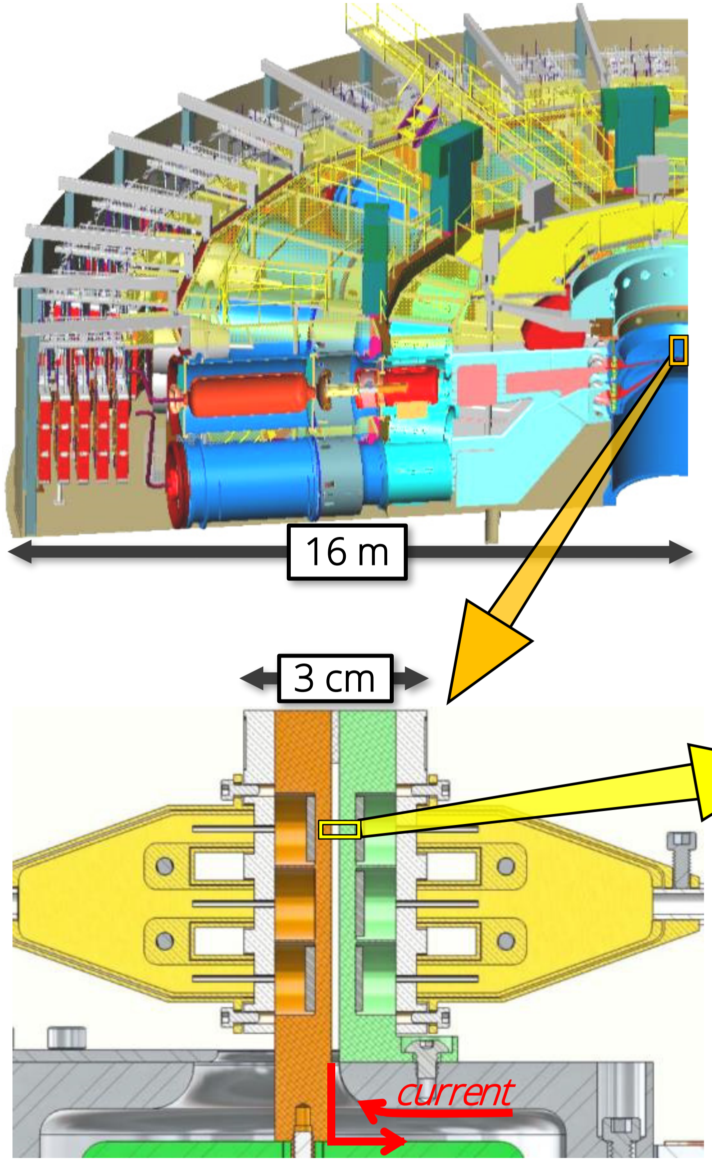
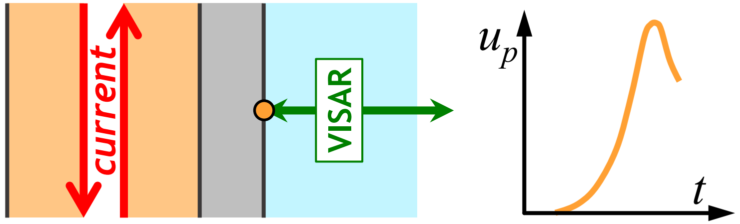
Stripline short-circuit loads on the Z pulsed-power machine can produce planar shockless compression of solids to 400+ GPa

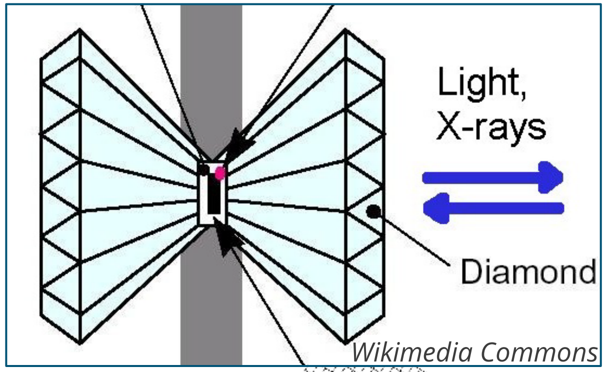
Magnetic drive propagates ramped stress wave into ambient material

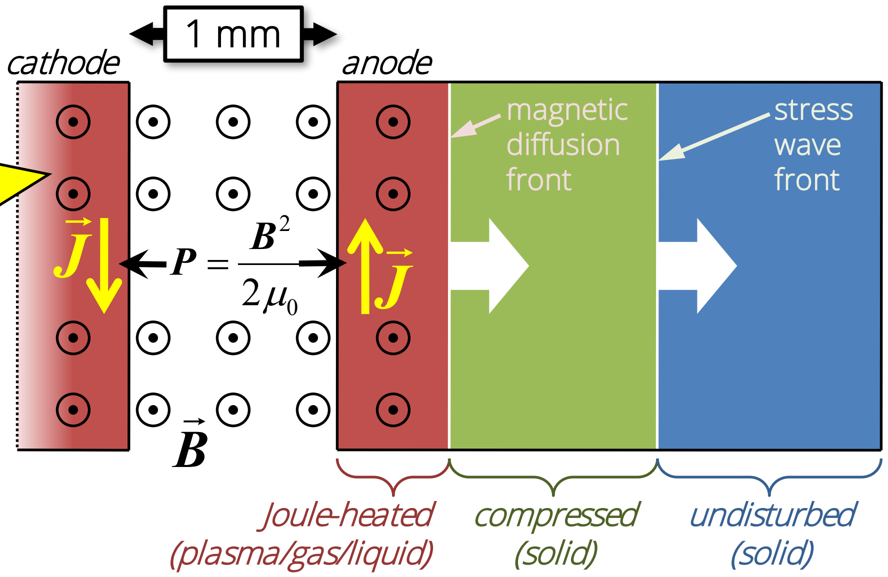
Material's compressibility deduced from velocimetry measurements

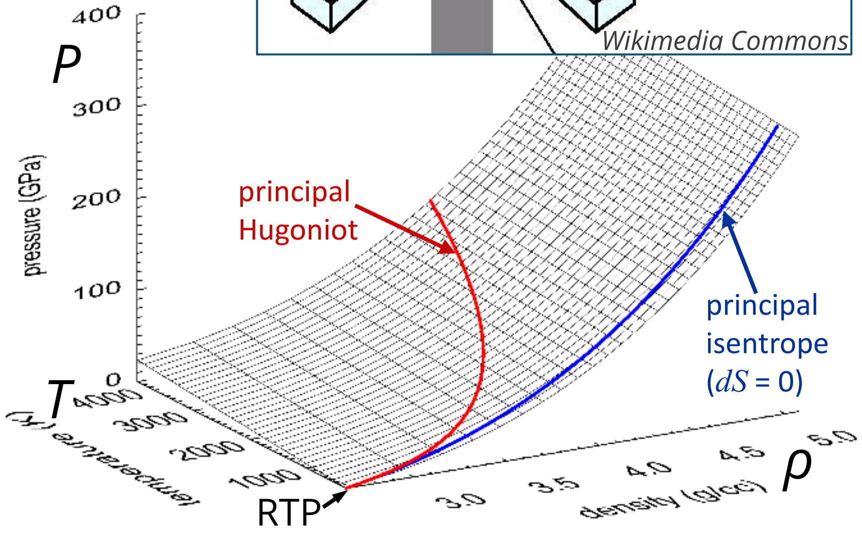
- Shockless compression along quasi-isentrope close to isotherm
- Accurate absolute measurement of pressure standards (*e.g.*, for DAC)



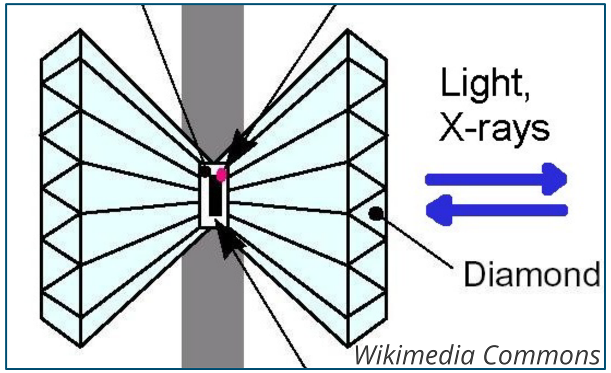








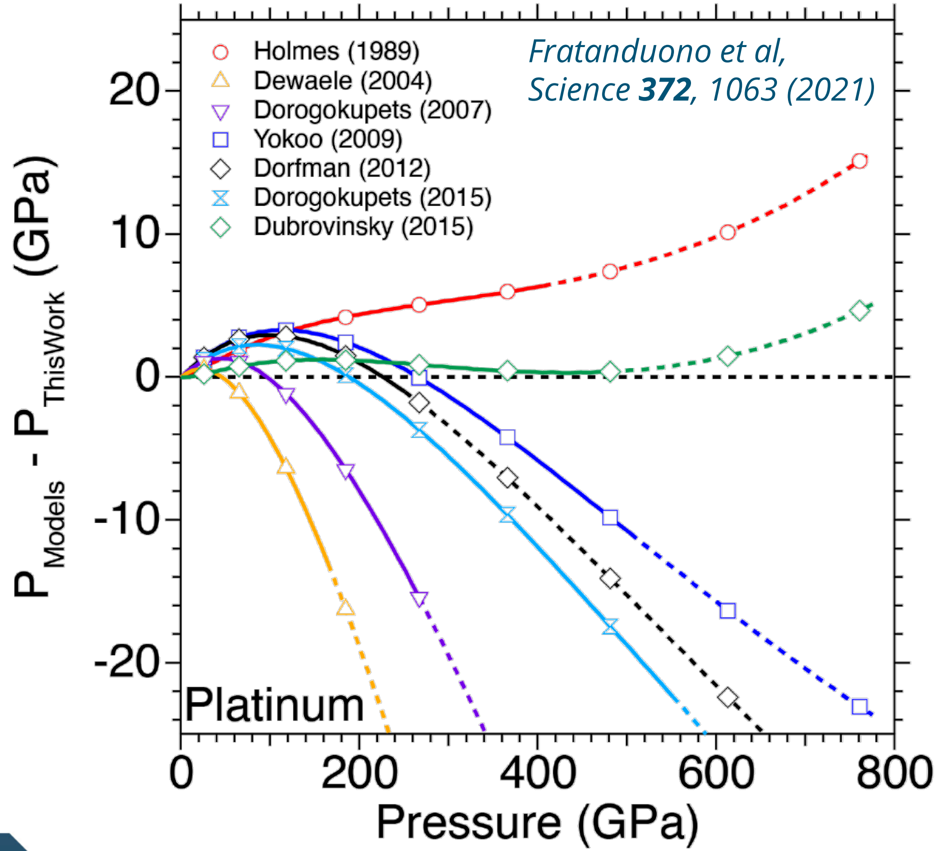
Platinum is a widely used pressure calibrant in DAC work

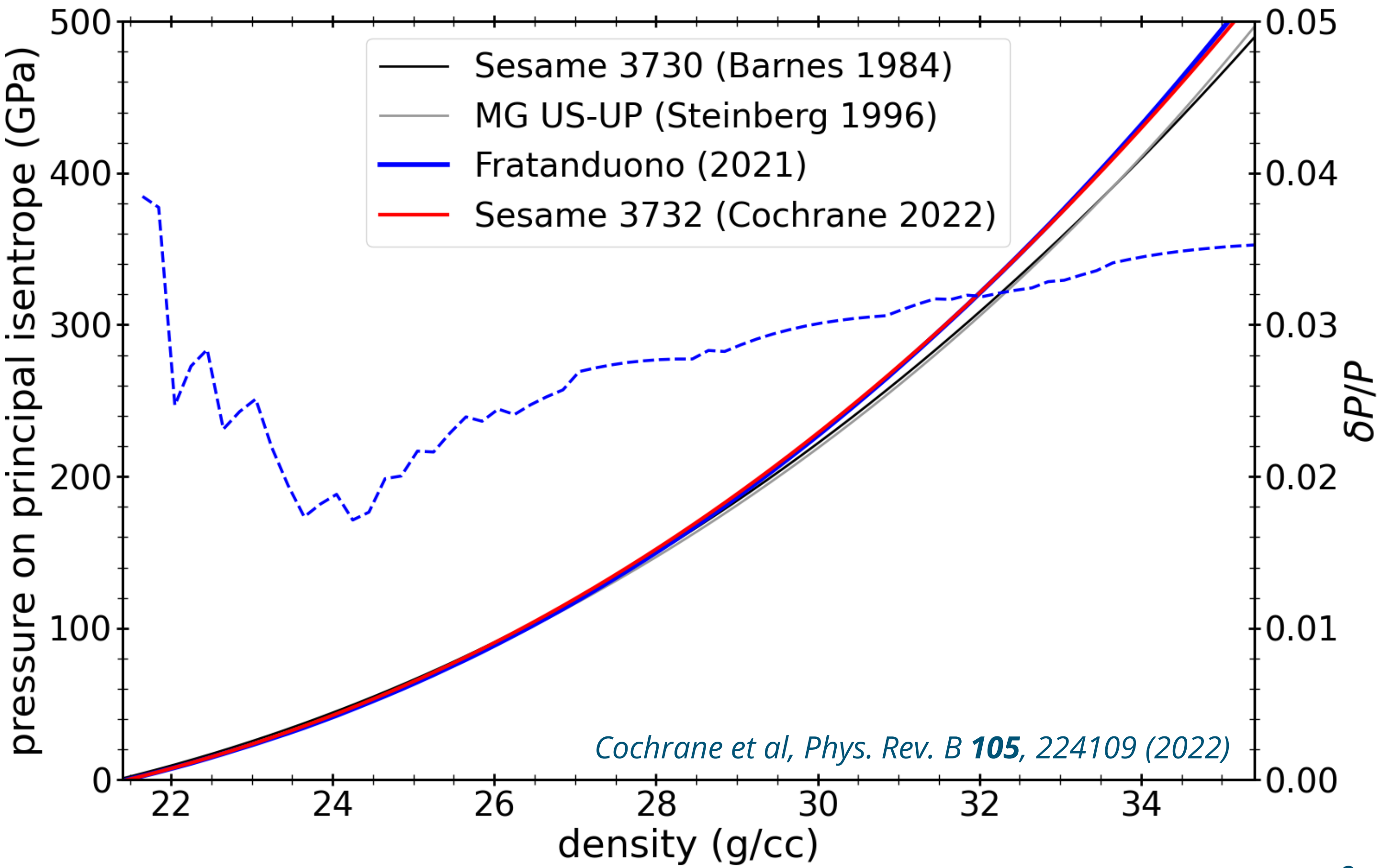


New DAC techniques to P > 300 GPa require precise calibration

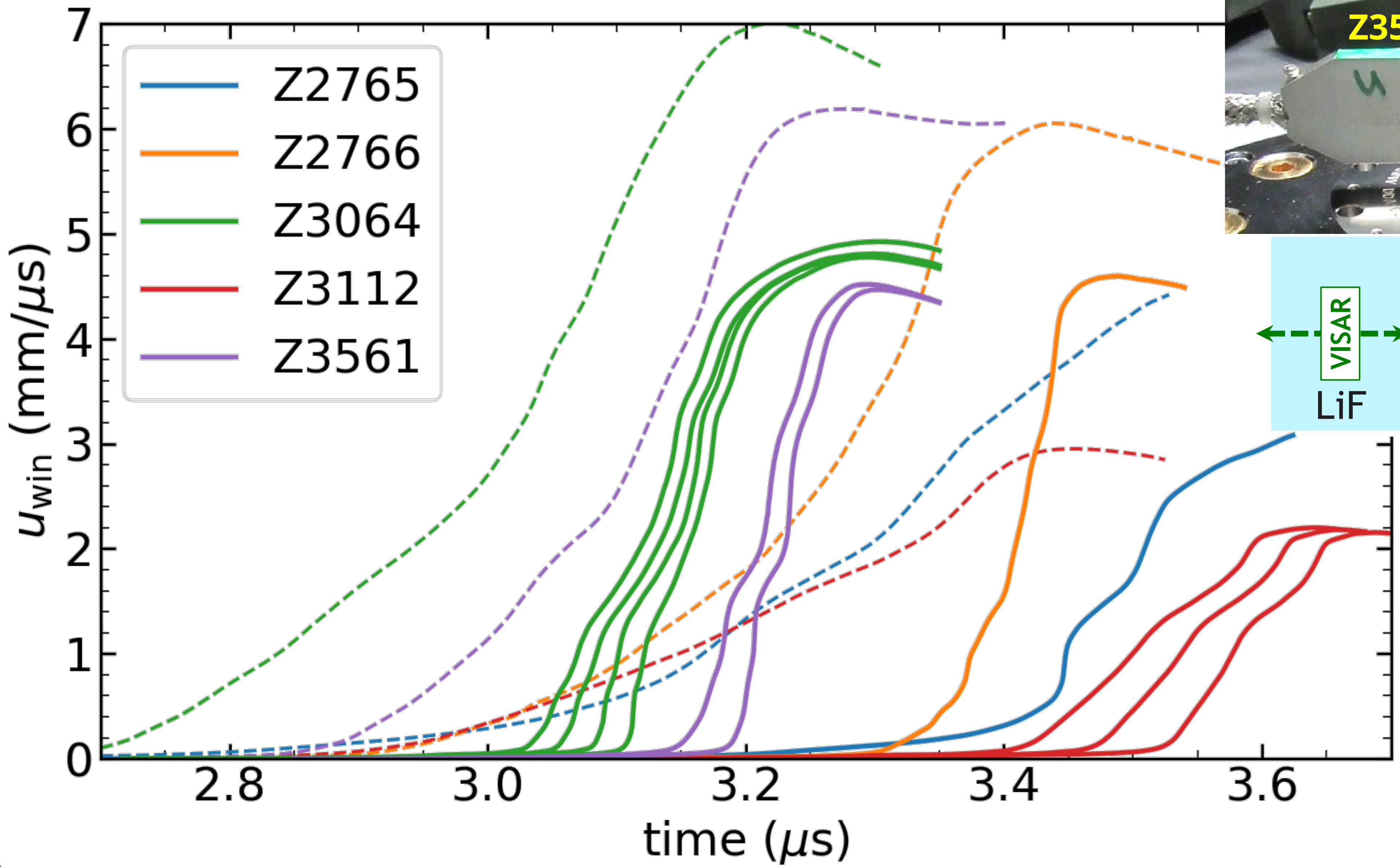
Extrapolated models differ 5-10%

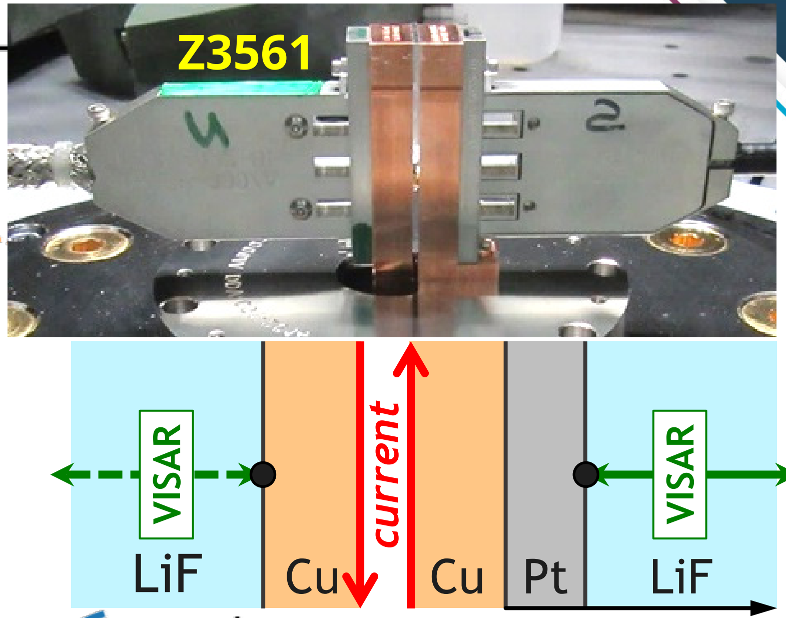
- recent NIF/Z ramp-compression result with uncertainty 3.5%
- included 3 Z measurements to ~400 GPa (NIF data to ~800 GPa)





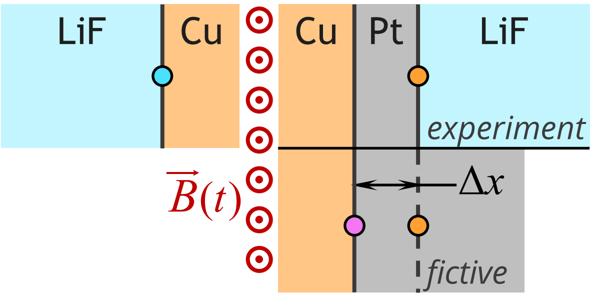
High-precision data are available from 11 single-sample measurements on Pt to peak stresses in the range 160-580 GPa

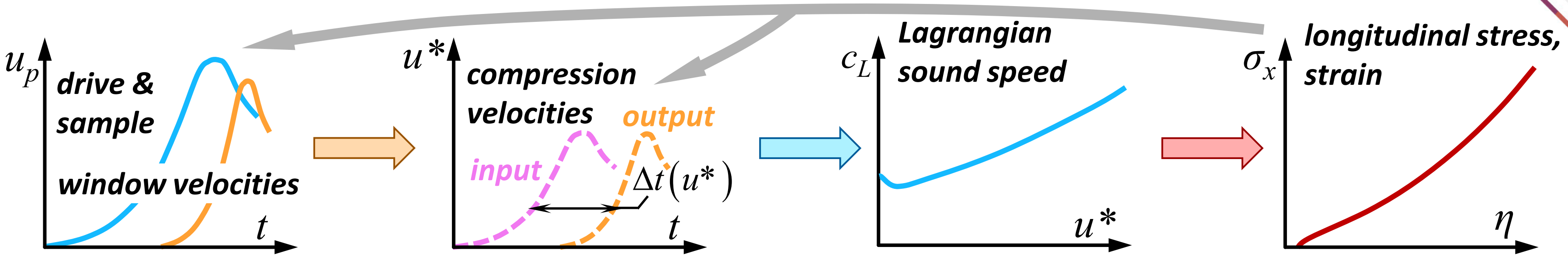




Davis and Brown, "Quantifying uncertainty in analysis of shockless dynamic compression experiments on platinum, Part 1: Inverse Lagrangian analysis," in preparation for submission to J. Appl. Phys. (2023)

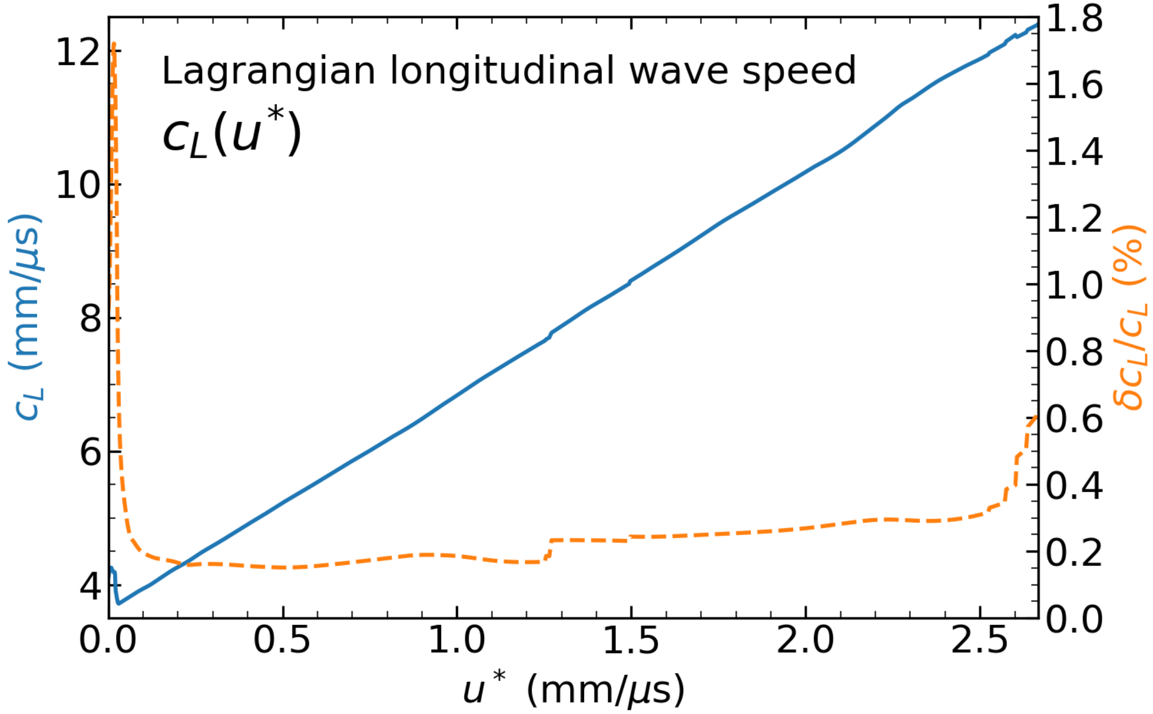
Inverse Lagrangian analysis (ILA) of these data gives weighted-mean longitudinal stress as function of strain with uncertainty

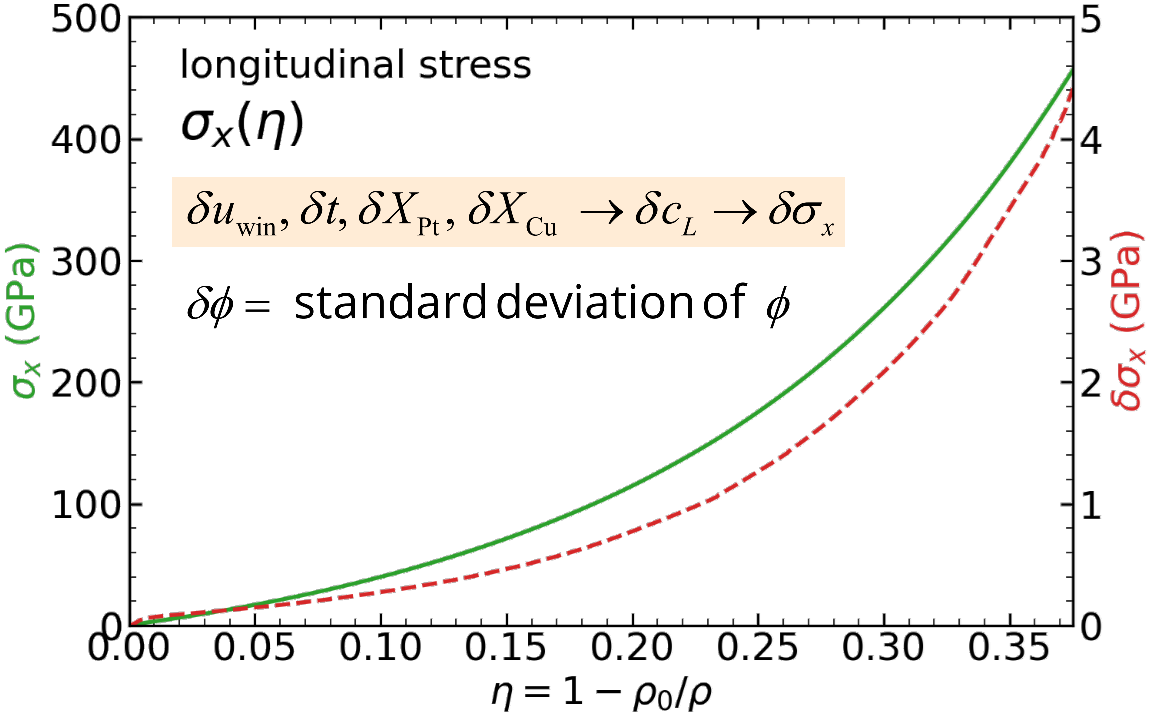




Davis, "Update on multi-megabar shockless compression at Sandia's Z machine (2022)," presented at APS March Meeting 2022

$c_L = \Delta x / \Delta t(u^*)$ $\quad \sigma_x = \rho_0 \int c_L(u^*)\, du^*$ $\quad \eta = \int \frac{du^*}{c_L(u^*)}$





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)

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 $\Gamma(\rho)$

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 …

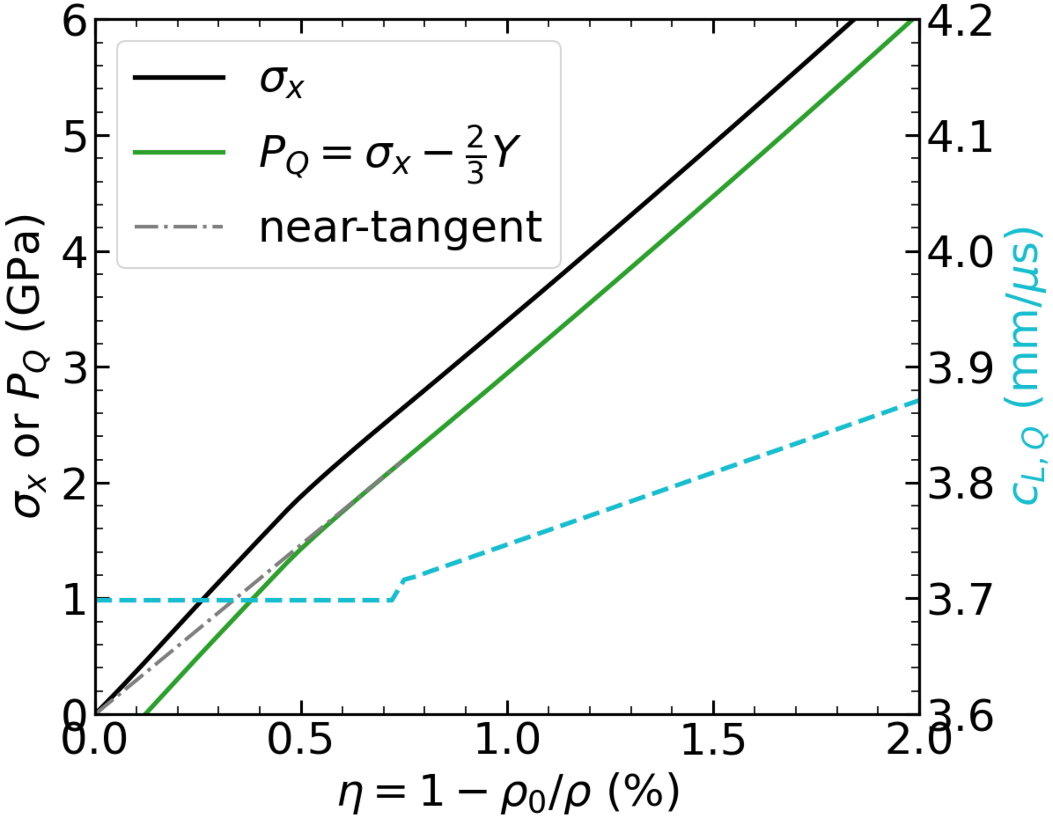
- Cannot avoid discontinuity in wave speed above elastic limit
- Does not match known elastic response at ambient

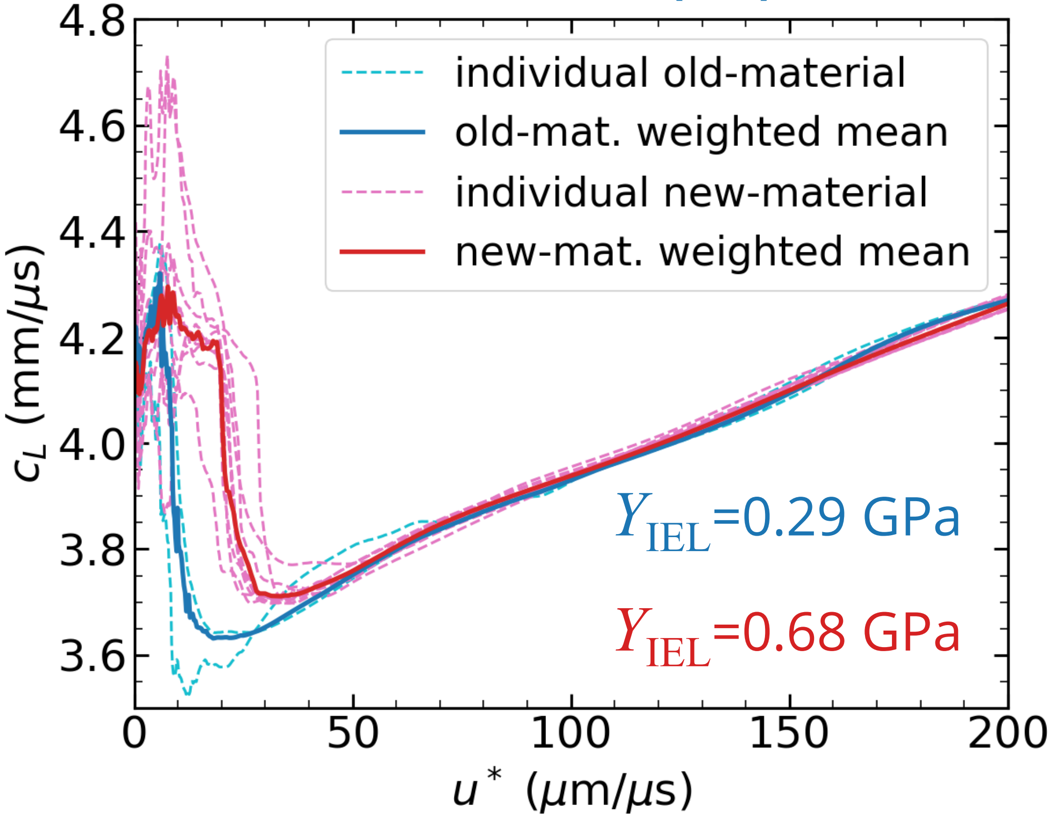
Initial yield stress depends strongly on microstructure

- 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)

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

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

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

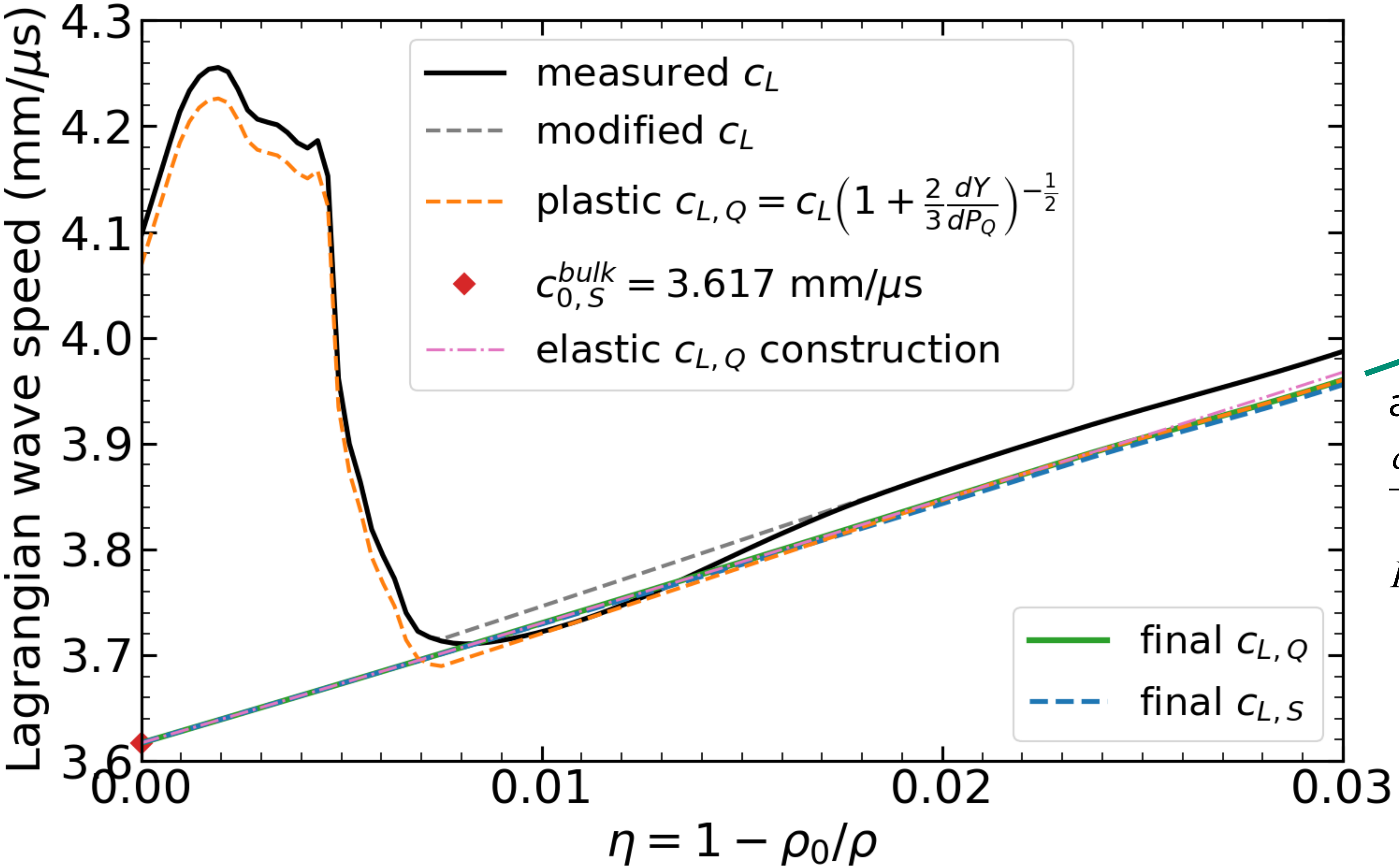
$$u_Q = \int c_{L,Q} d\eta \qquad P_Q = \rho_0 \int c_{L,Q} du_Q = \rho_0 \int c_{L,Q}^2 d\eta$$

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

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

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

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



at $\eta = 0.375$:

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

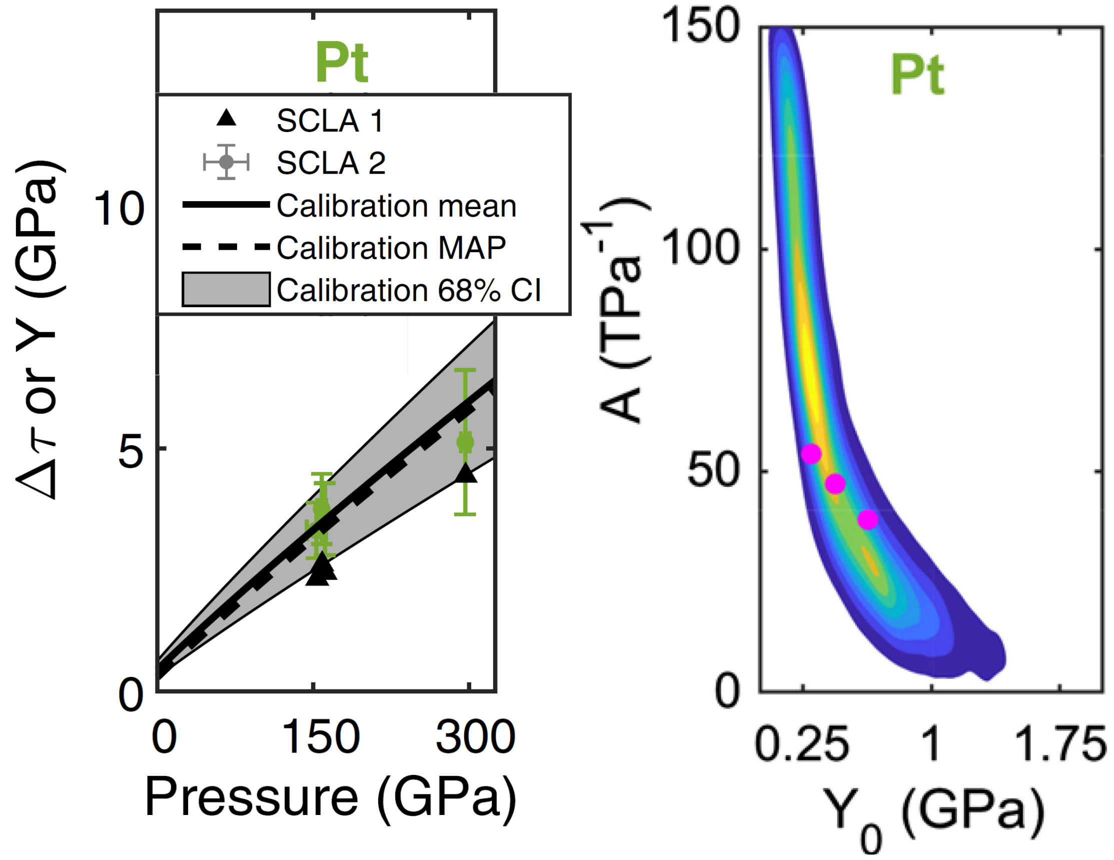
$$P_Q - P_S = 2.16\text{ GPa}$$

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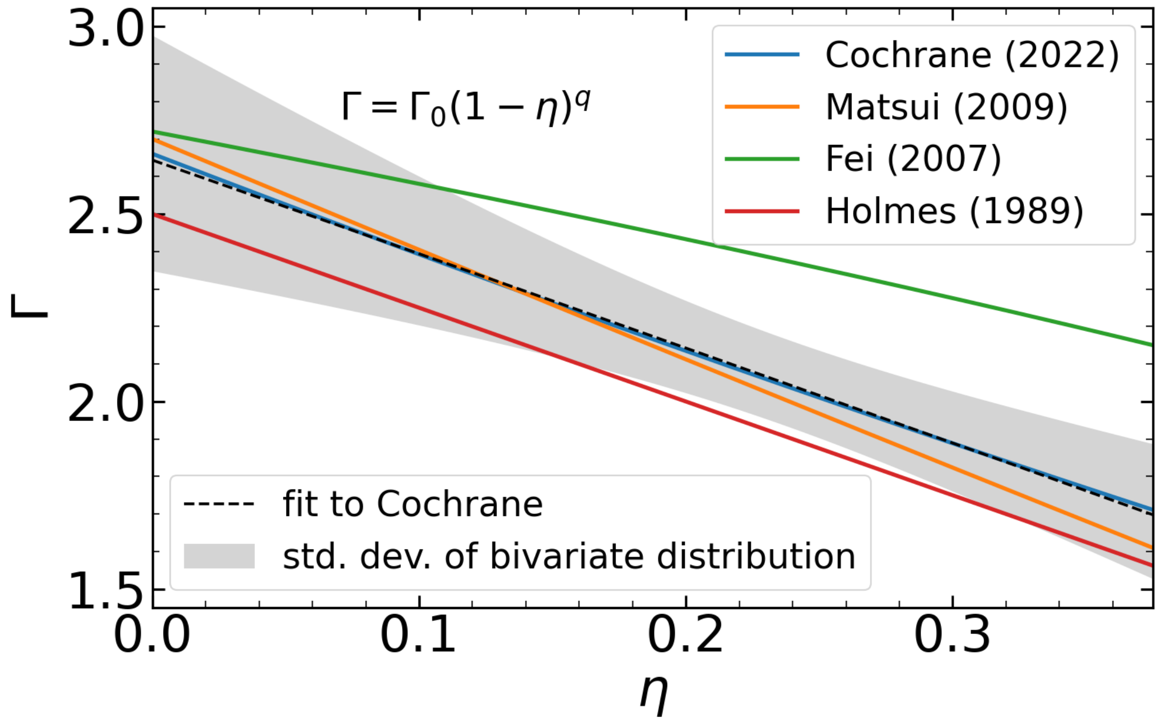
mean: fit to Cochrane et al (2022)

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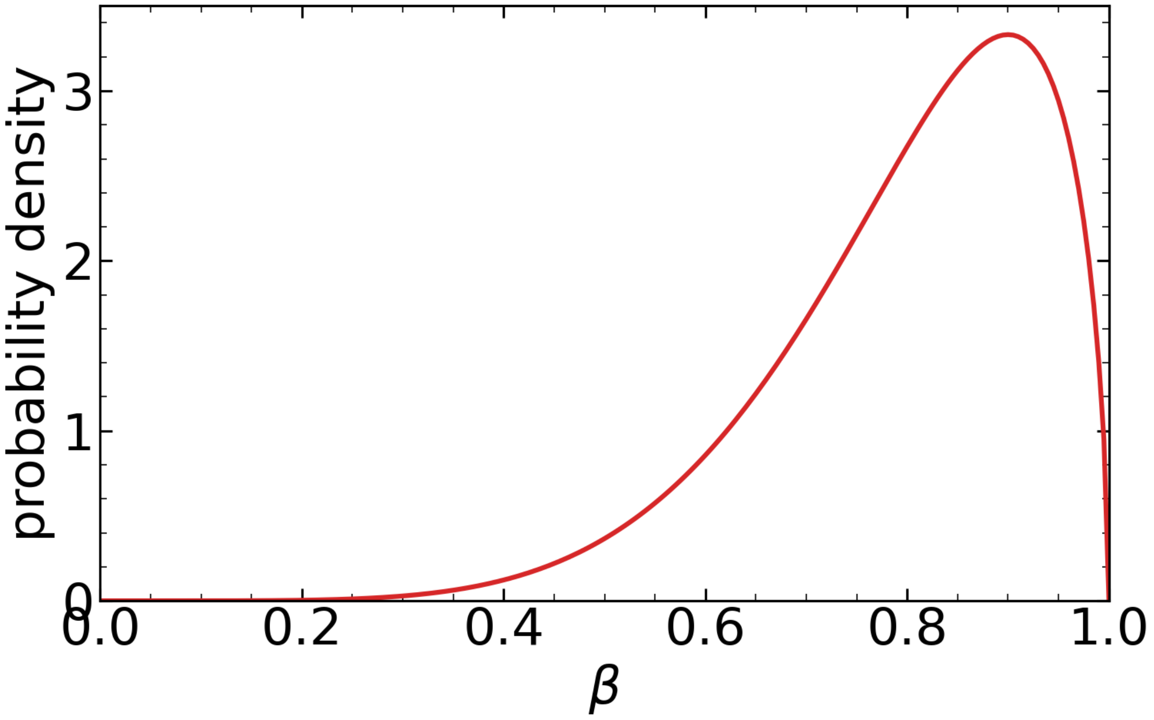
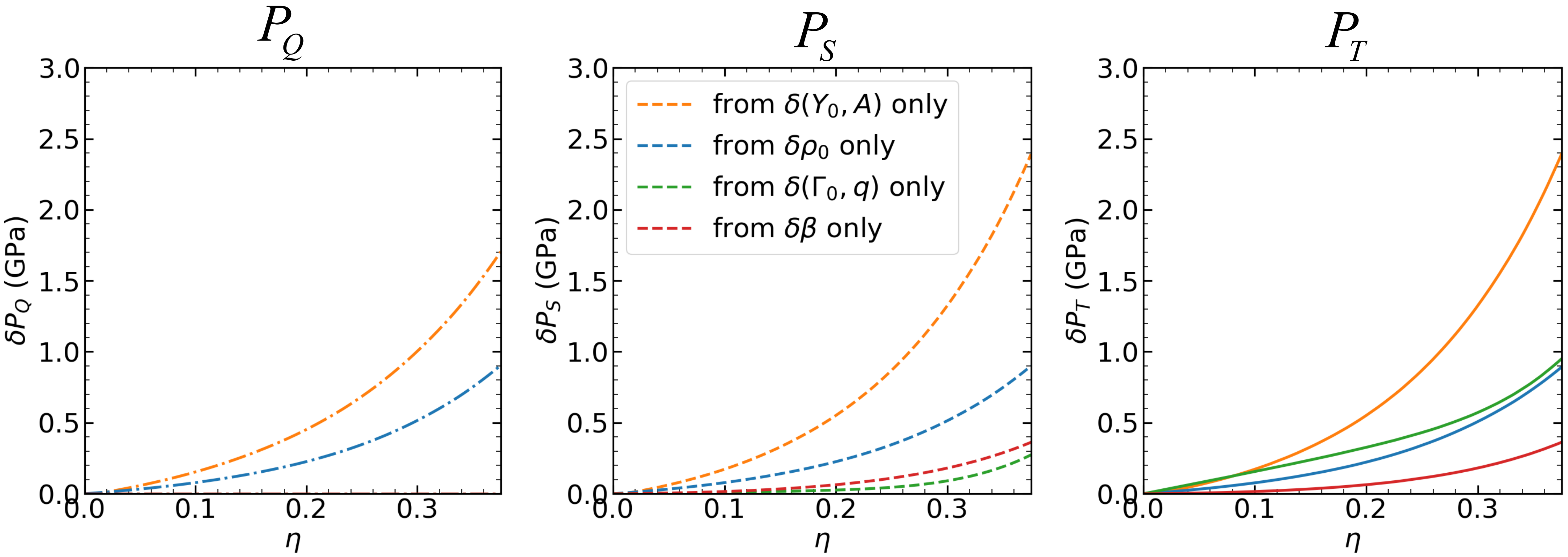
mode = 0.9; 68.3% CI = [0.66, 0.93]
95.4% CI = [0.48, 0.98]



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

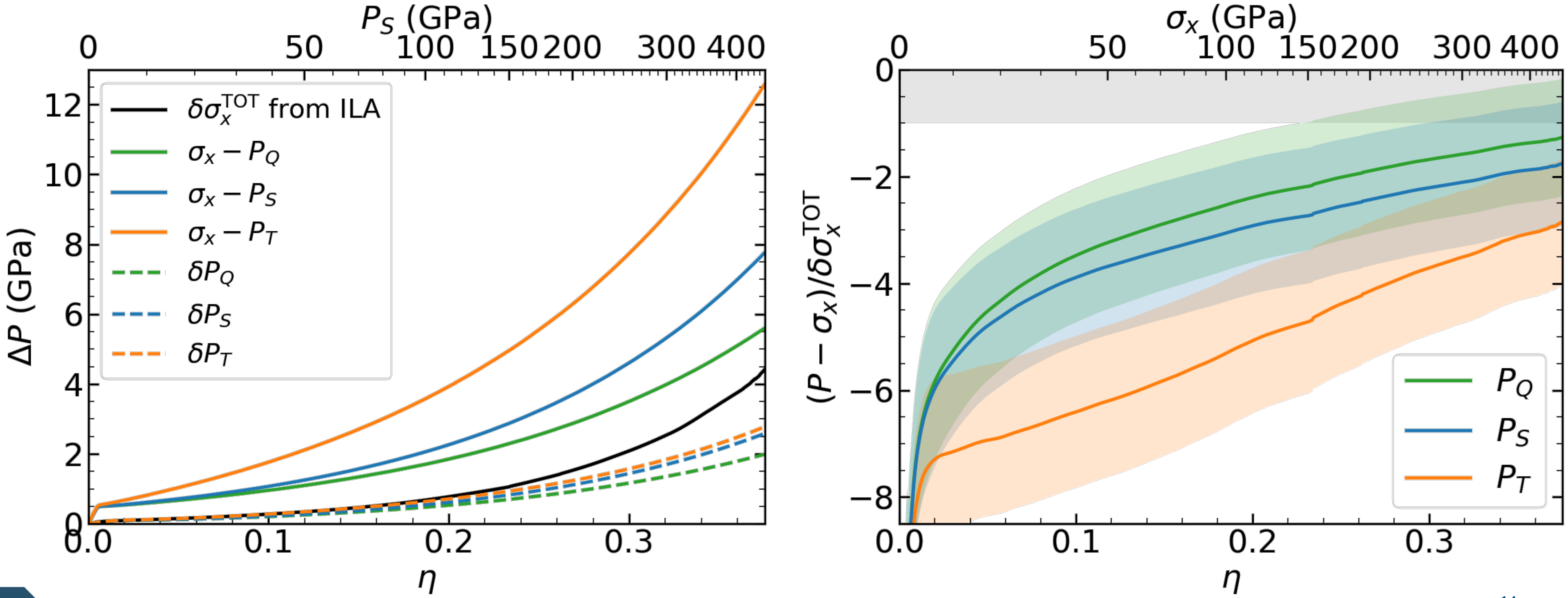
- Screening Monte Carlo (MC) converged by 100,000 samples
- Non-normal distributions described by average median-centered 68.3% confidence interval (CI)



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.



Conclusion

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

Improved procedure for reduction to pressures on quasi-isentrope, isentrope, isotherm
- work in wave speeds instead of stress and pressure
- 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
- in descending order of importance, parameters of measurable effect are those for strength, initial density, Grüneisen parameter, and Taylor-Quinney coefficient
- ambient bulk sound speed, shear modulus, heat capacity, and temperature are inconsequential
- non-normal distribution described well by averaged median-centered confidence intervals
- Reduction to isotherm P_T is correction of ~3 $\delta\sigma_x$ at ~450 GPa, resulting in δP_T around 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 should inflate uncertainty there (1.2% from ILA might really be 1.5%)

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)