LA-UR-21-21087
Approved for public release; distribution is unlimited.

Title: Uncertainty Quantification for EoS and Porous Hugoniots

Author(s): Vander Wiel, Scott Alan
Dorn, Mary Frances

Intended for: Report

Issued: 2021-02-05

Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Uncertainty Quantification for EoS and Porous Hugoniots

Scott Vander Wiel
Mary Frances Dorn

3 February 2021

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Common Features Required of Statistical Methods

diverse data

– analyses combine data from varied sources

measurement uncertainties

– nested structure (observation within experiment)

– utilize reported uncertainties on observations

– inputs *and* outputs are measured with error

discrepancy

– observations may deviate from physical models

– discrepancies exceed measurement uncertainties

computationally-intensive physical models

– runs are resource-heavy

– calibration to observations can utilize a fast emulator

Calibration of EOS for Zr

Bayesian model calibration

- $\boldsymbol{\theta}$: unobservable parameters
- $\boldsymbol{Y}$: observations

Bayes Rule:

$$P(\boldsymbol{\theta}|\boldsymbol{Y}) = \frac{P(\boldsymbol{\theta}) * P(\boldsymbol{Y} \mid \boldsymbol{\theta})}{P(\boldsymbol{Y})}$$

- $P(\boldsymbol{\theta})$: Prior Distribution for $\boldsymbol{\theta}$
  - Diffuse priors to “let the data speak”
- $P(\boldsymbol{Y} \mid \boldsymbol{\theta})$: Likelihood of the observed data given a value for $\boldsymbol{\theta}$
  - This incorporates the physical model (EOS)
- $P(\boldsymbol{Y})$: Marginal likelihood of the data under the statistical model

- Explore the posterior using MCMC

Mie-Grüneisen-Debye EOS

- The physics model underlying the likelihood:

$$P_{total} = P_{300}\left(V; K_0, \frac{dK_0}{dP}, V_0\right) + P_{th}\left(V, T; \theta_0 \gamma_0, q\right)$$

$$P_{300} = \frac{3}{2} K_0 \left[\left(\frac{V_0}{V}\right)^{7/3} - \left(\frac{V_0}{V}\right)^{5/3}\right]\left[1 + \frac{3}{4}\left(\frac{dK_0}{dP} - 4\right)\left(\left(\frac{V_0}{V}\right)^{2/3} - 1\right)\right]$$

$$P_{th} = \frac{\gamma}{V}\left(U_T - U_{300}\right)$$

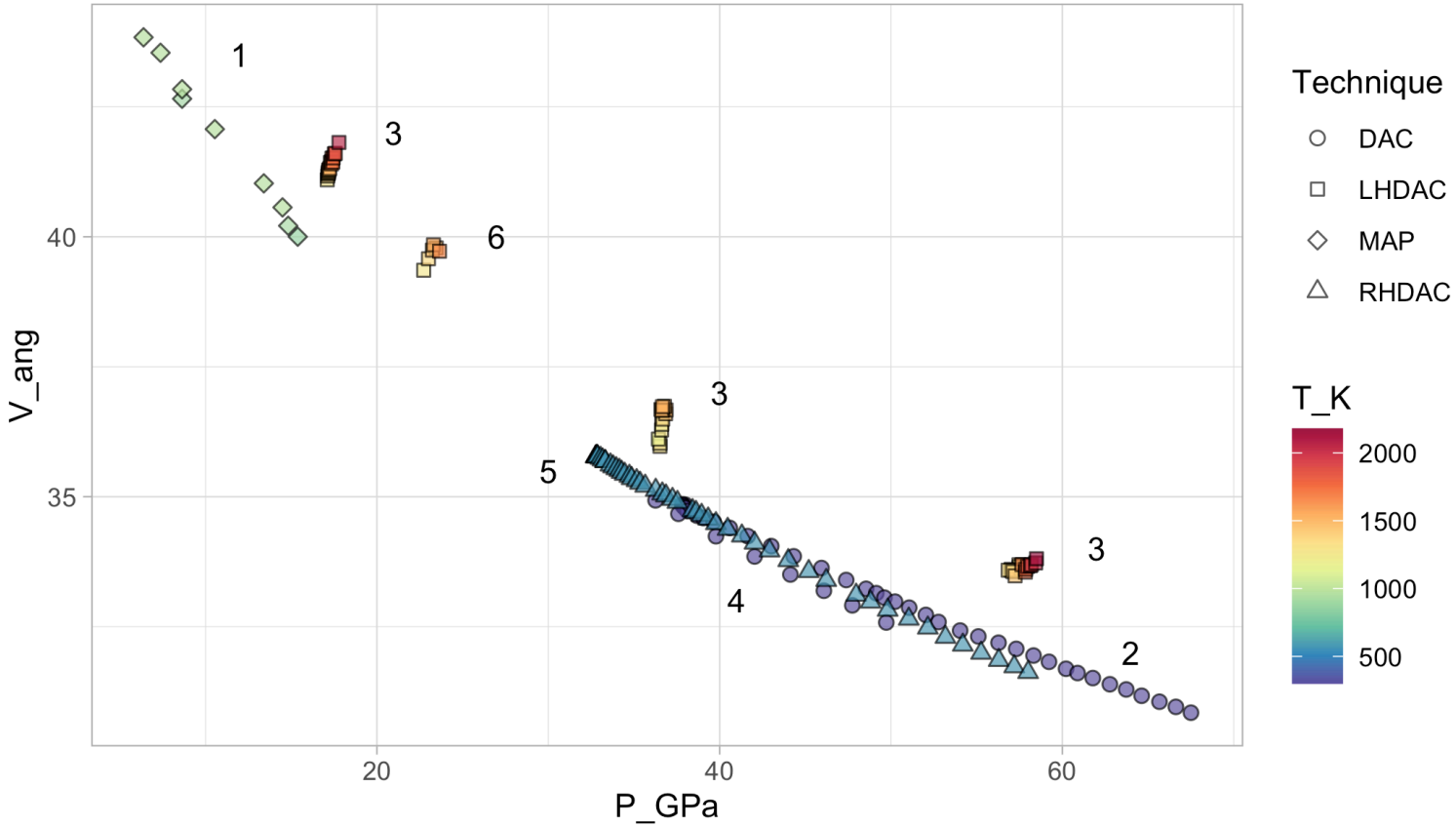
$$U_T = 9nR\left(\frac{\theta}{8} + T\left(\frac{T}{\theta}\right)^3 \int_0^{\theta/T} \frac{x^3}{e^x - 1} dx\right)$$

$$\gamma = \gamma_0 \left(\frac{V}{V_0}\right)^q$$

$$\theta = \theta_0 \exp\left(\frac{\gamma_0 - \gamma}{q}\right)$$

→ 6 unknown parameters to be estimated

Experimental data



Experiment	Technique	Pressure Marker	Pressure Calibrant	Temperature (K)
1	MAP [8]	Boron epoxy	NaCl (Decker,1971)	873 - 975
2	DAC	He	Pt (Fei, 2007)	300
3	LHDAC	KBr	KBr (Fischer, 2012)	1171.5 - 2178.5
4	DAC	He	Pt (Fei, 2007)	300
5	RHDAC	Ne	Pt (Fei, 2007)	568 - 569
6	LHDAC	Ar	Ar (Jephcoat, 1998)	1258.5 - 1649.5

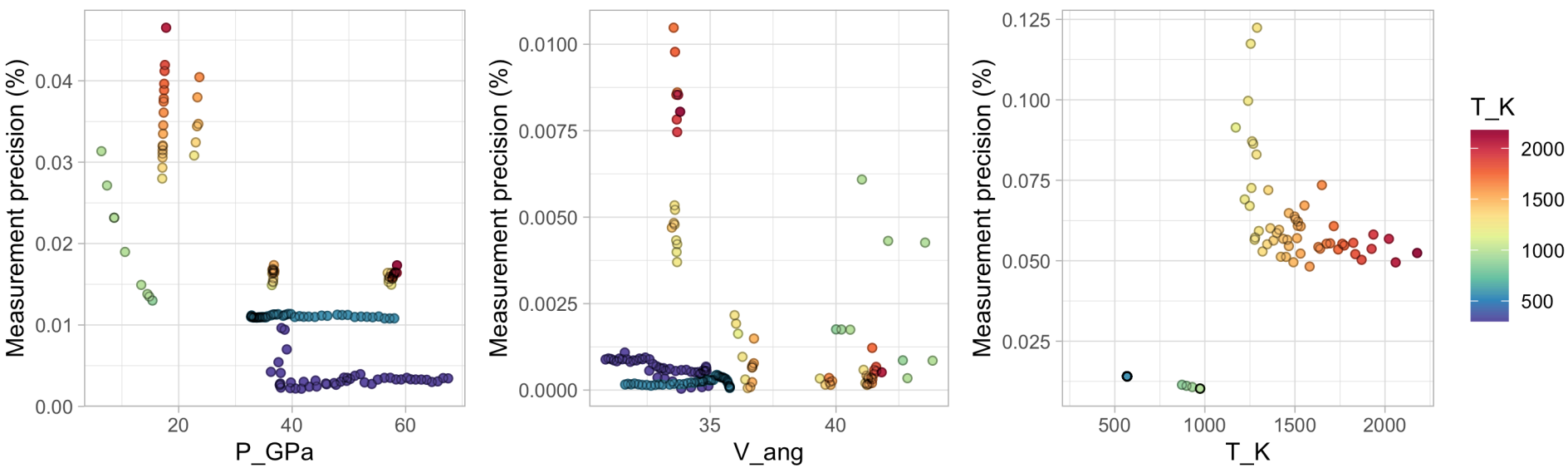
Errors in predictors and responses

- In addition to random observational error (precision of measurement), we have <u>structured uncertainties</u>

$$P_{ij} = P^*_{ij} + \delta^P_i + \epsilon^P_{ij}$$
$$V_{ij} = V^*_{ij} + \delta^V_i + \epsilon^V_{ij}$$
$$T_{ij} = T^*_{ij} + \delta^T_i + \epsilon^T_{ij}$$

i: experiment
j: observation

$$(\text{Observation} = \text{true value} + \text{experiment-specific offset} + \text{measurement error})$$



Statistical model

- Likelihood
  - EOS constrains true relationship between P-V-T

$$P_{ij}^{*} \;=\; EOS(V_{ij}^{*}, T_{ij}^{*}; \boldsymbol{\theta})$$

  - Structured uncertainty

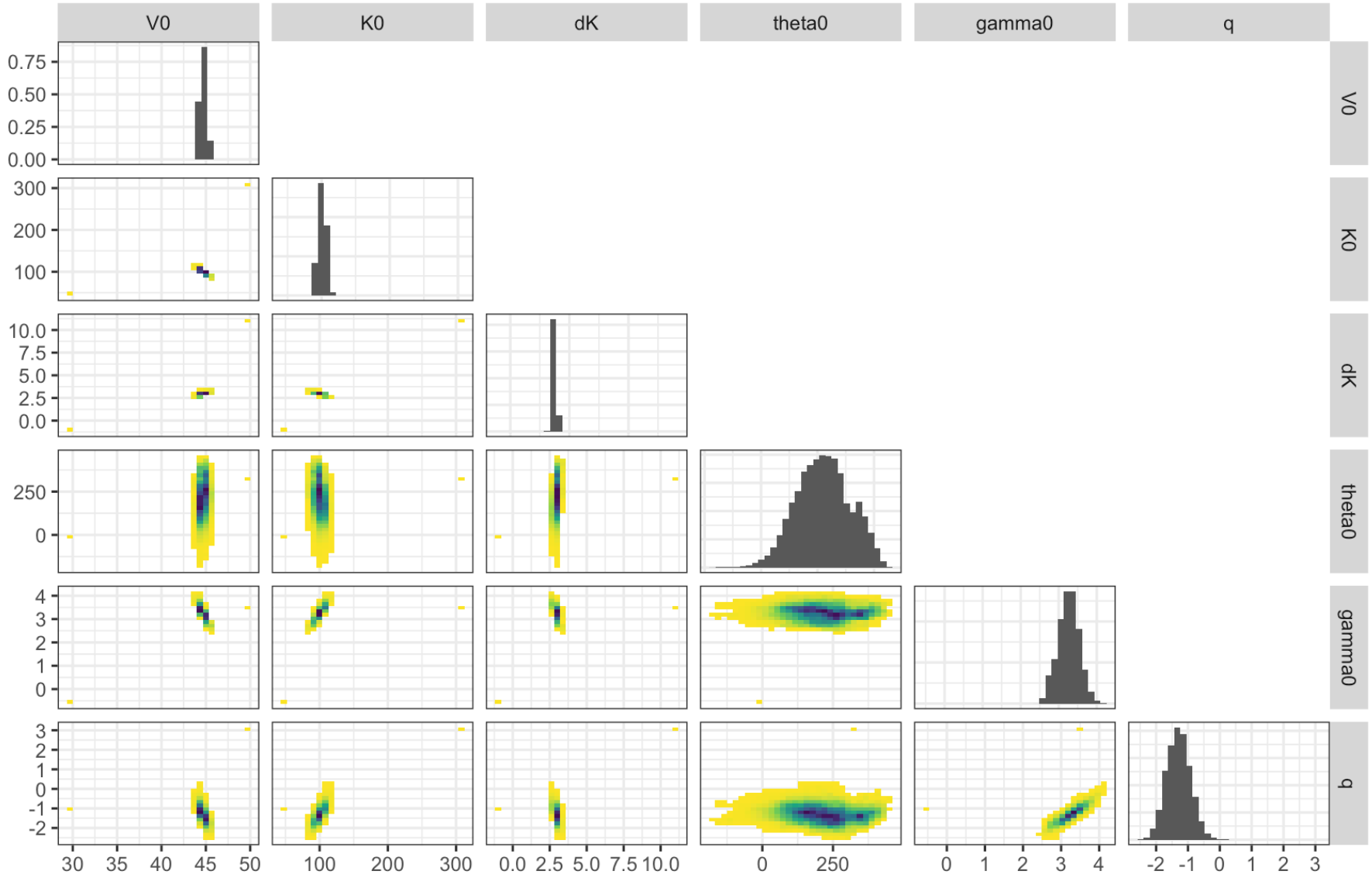
$$P_{ij} \sim N(P_{ij}^{*}, \tau_{P,i}^{2} + \sigma_{P}^{2})$$
$$V_{ij} \sim N(V_{ij}^{*}, \tau_{V,i}^{2} + \sigma_{V}^{2})$$
$$T_{ij} \sim N(T_{ij}^{*}, \tau_{T,i}^{2} + \sigma_{T}^{2})$$

- Priors
  - EOS parameters $\boldsymbol{\theta}$: $V_0, K_0, dK_0', \theta_0, \gamma_0, q$
  - Variance/uncertainty parameters:

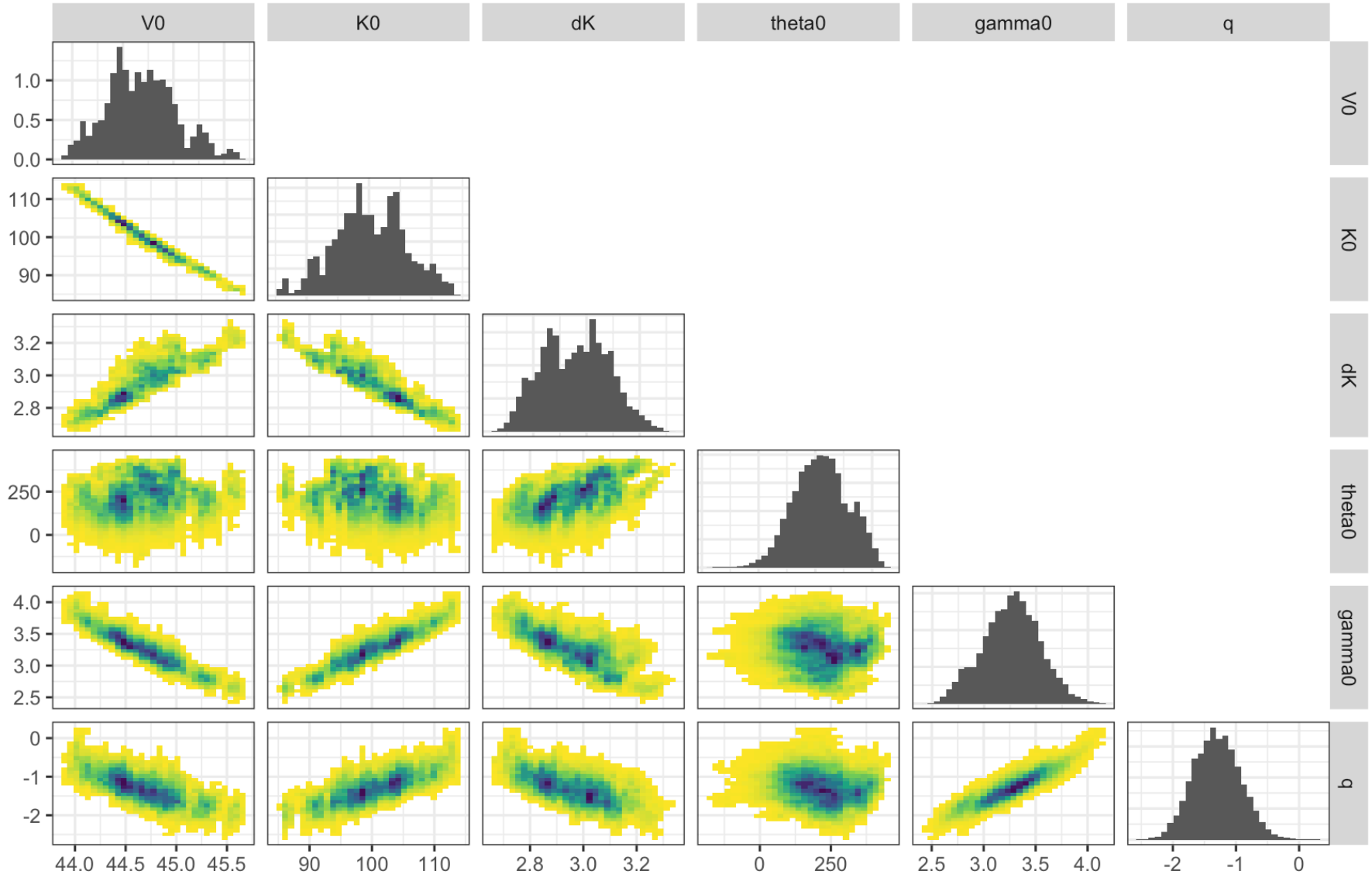
$$P_{ij}^{*}, \tau_{P,i}^{2}, \sigma_{P}^{2}, \qquad V_{ij}^{*}, \tau_{V,i}^{2}, \sigma_{V}^{2}, \qquad T_{ij}^{*}, \tau_{T,i}^{2}, \sigma_{T}^{2}$$

- MCMC to explore the posterior

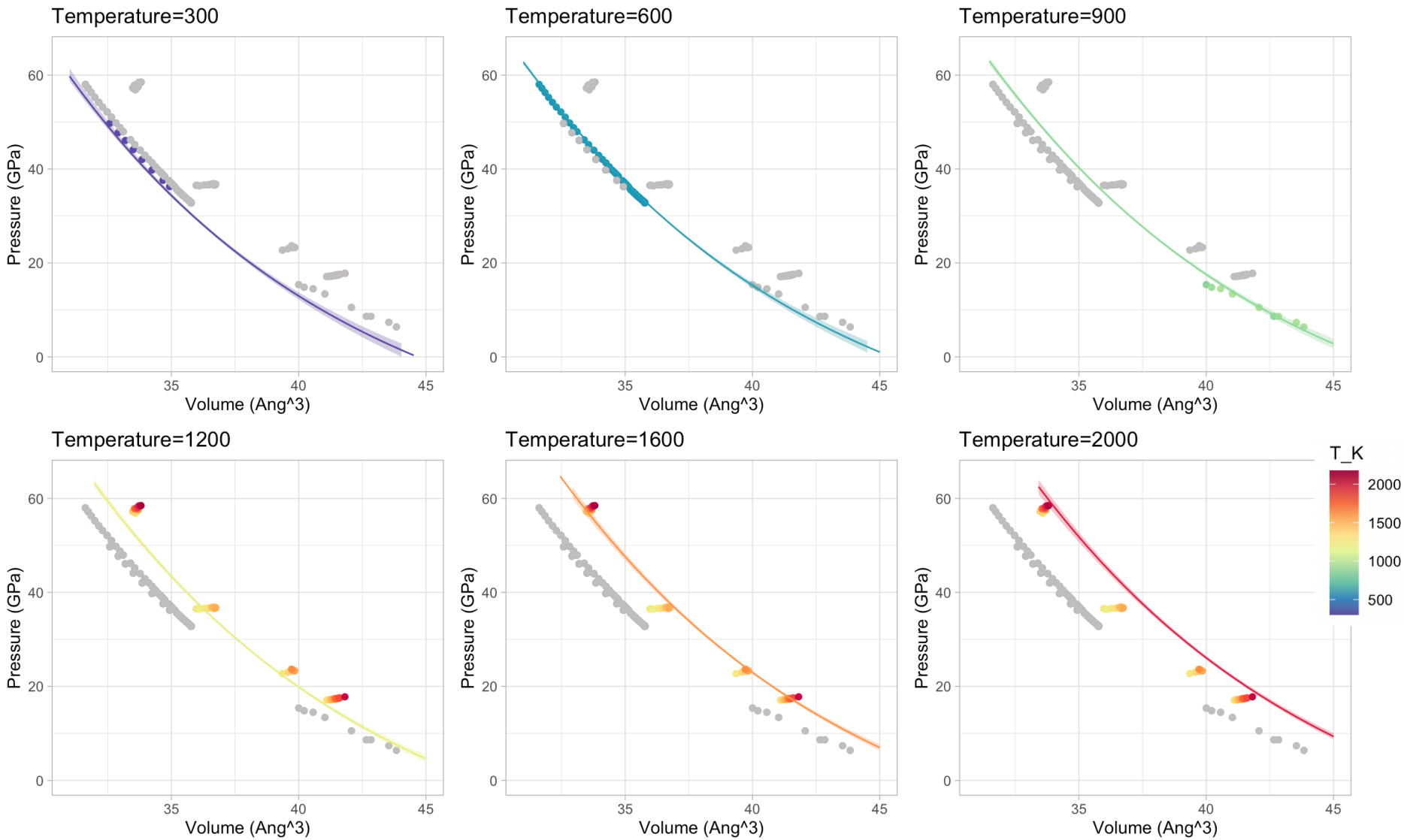
Posterior distribution of EOS parameters



Posterior distribution of EOS parameters



Parameter uncertainties in P-V-T space



Estimation of Hugoniots for Porous CeO_2

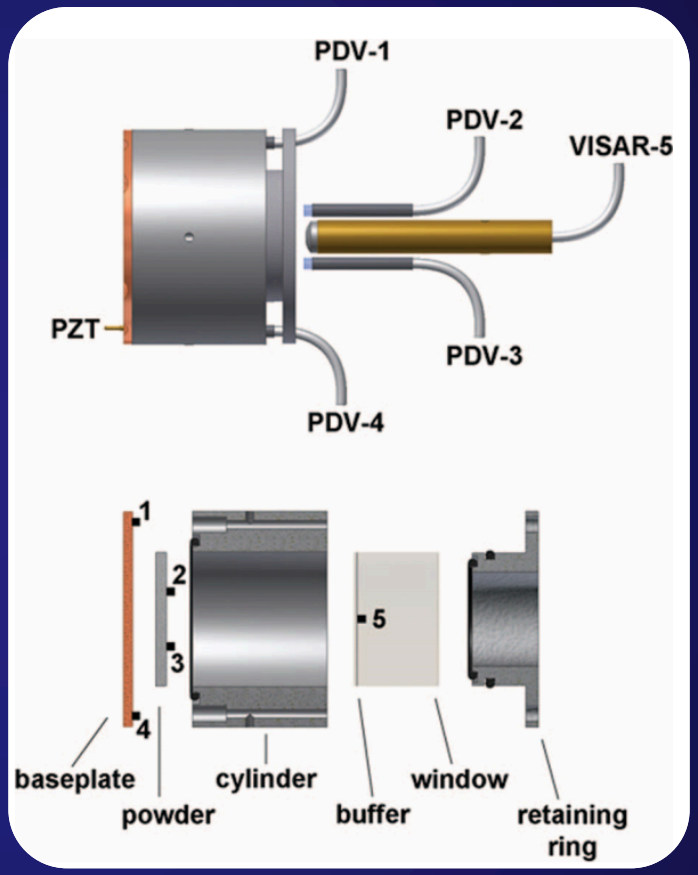
CeO_2 Shock Compression Experiments

An array of sensors is used to estimate

- ρ_0 initial density of powder sample
- f_0 initial density fraction $= \rho_0/\rho_{\max}$
- U_S speed of shock
- u_P speed of powder

Rankine-Hugoniot balance derives compressed state

- ρ final density
- P final pressure



$f_0 \approx 0.33, 0.44, 0.56, 0.63$

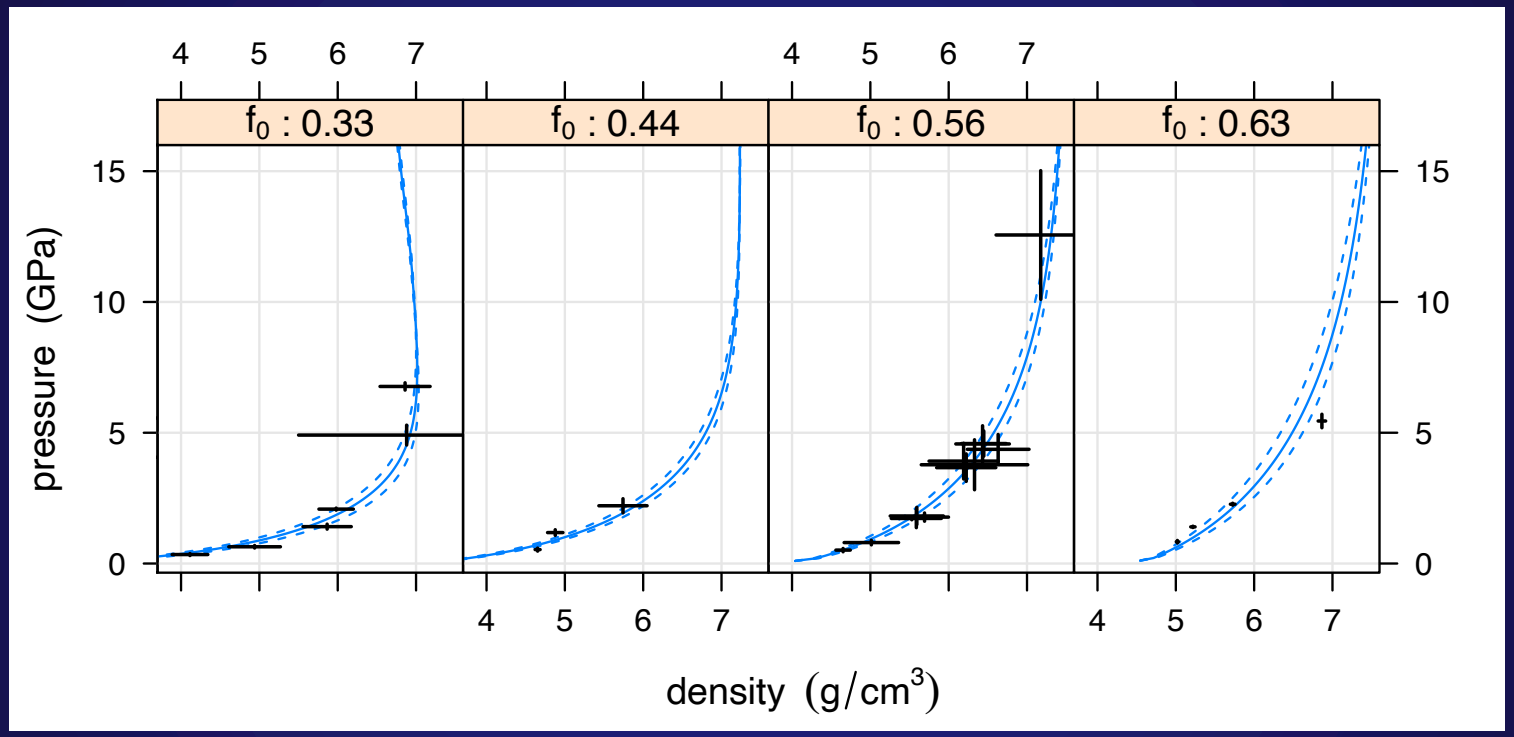
DA Fredenburg, DD Koller, PA Rigg, and RJ Scharff. High-fidelity Hugoniot analysis of porous materials. Review of Scientific Instruments, 84(1):013903, 2013.

CeO_2 Shock Compression Data

Shot	target density fraction, f_0	initial density g/cm^3		density g/cm^3		pressure GPa	
		ρ_{0i}	$(\delta\rho_0)_i$	ρ_i	$(\delta\rho)_i$	P_i	$(\delta P/P)_i$
1906	0.330	2.433	0.037	4.114	0.114	0.343	0.055
1903	0.330	2.396	0.012	4.939	0.165	0.641	0.037
1908	0.330	2.400	0.026	5.865	0.154	1.410	0.034
1S-1587	0.330	2.320	0.010	5.980	0.110	2.080	0.010
2S-855	0.330	2.330	0.010	6.880	0.690	4.910	0.039
2S-853	0.330	2.380	0.010	6.860	0.160	6.770	0.010
2004	0.440	3.142	0.058	4.652	0.016	0.532	0.055
1907	0.440	3.225	0.043	4.877	0.049	1.184	0.046
2006	0.440	3.140	0.046	5.742	0.154	2.208	0.061
56-11-26	0.560	4.023	0.114	4.652	0.046	0.513	0.062
56-11-20	0.560	4.039	0.252	5.013	0.174	0.801	0.055
1701	0.560	4.045	0.020	5.529	0.030	1.729	0.016
56-12-01	0.560	4.028	0.070	5.587	0.160	1.724	0.103
56-11-27	0.560	4.052	0.178	5.692	0.153	1.775	0.045
56-11-19	0.560	4.023	0.138	5.593	0.170	1.817	0.091
56-11-55	0.560	4.020	0.143	6.224	0.189	3.666	0.072
56-11-56	0.560	4.033	0.150	6.191	0.221	3.915	0.087
56-12-13	0.560	4.010	0.186	6.330	0.340	3.776	0.127
56-12-06	0.560	4.044	0.114	6.632	0.197	4.366	0.065
1S-1523	0.560	4.055	0.066	6.433	0.171	4.572	0.076
1S-1525	0.560	4.012	0.090	6.448	0.143	4.587	0.053
1S-1523	0.560	4.031	0.079	7.175	0.285	12.560	0.098
1801	0.630	4.551	0.025	5.020	0.007	0.834	0.029
1703	0.630	4.472	0.011	5.218	0.014	1.402	0.009
1702	0.630	4.515	0.010	5.726	0.015	2.268	0.008
1811	0.630	4.558	0.018	6.865	0.024	5.449	0.024

Uncertainties (δs) derived from error propagation.

CeO_2 Shock Data
(Hugoniot estimation to be described)



Notice:

- substantial measurement errors in both ρ and P
- some observations miss curves beyond measurement precision

Menikoff-Kober Hugoniot for a Powder

Inputs to the "$P-\alpha$" model

- **EoS of CeO_2**: latest from Sesame
- **Crush curve**: void fraction vs. PV of particles

P_C = characteristic pressure (exponential decay rate)

`MatHugoniot.py`: Ted Carney's Python program calculates

$P(\rho)$ = porous Hugoniot curve

dependent on f_0 and P_C

We link P_C to f_0 and fit to shock data, with uncertainty.

Statistical Model Assumptions

yellow indicates unknowns

- **Unknown `true` state $(\bar{f}_{0i}, \bar{\rho}_i, \bar{P}_i)$ lies exactly on Hugoniot**
- $P_C = \exp(\beta_0 + \beta_1 \bar{f}_{0i})$
- **Observations are normal (N) or log-normal (LN) centered on true states**

$$f_{0i} \sim \mathbf{N}[\bar{f}_{0i}, U_i], \qquad U_i = \delta_{f0i}^2 + \sigma_{f0}^2$$
$$\rho_i \sim \mathbf{N}[\bar{\rho}_i, V_i], \qquad V_i = \delta_{\rho i}^2 + \sigma_{\rho}^2$$
$$P_i \sim \mathbf{LN}[\bar{P}_i, W_i], \qquad W_i = \delta_{Pi}^2 + \sigma_{P}^2$$

  - δs are given uncertainties
  - σs are extra uncertainties needed to fit observations
- **Bayesian formulation**
  - diffuse priors on unknowns
  - Markov Chain Monte Carlo explores

$$\text{posterior} \propto \text{prior} \times \text{likelihood}$$

Measurement Error Likelihood

Given i-th observation

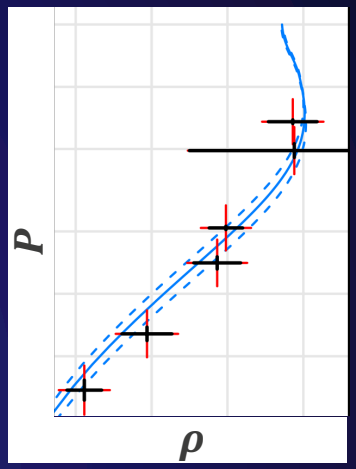
$$(\, f_{0i}, \rho_i, P_i \,)$$

and parameters

$$\boldsymbol{\theta} = (\, \bar{f}_{0i},\ P_C,\ \ U_i, V_i, W_i \,)$$

the likelihood contribution is

$$L_i(\boldsymbol{\theta}) = \phi_{\mathrm{N}}\left(\rho_i; \bar{f}_{0i}, U_i\right) \times \oint_{H(P_C, \bar{f}_{0i})} \phi_{\mathrm{N}}(\rho_i; \bar{\rho}_i, V_i)\ \phi_{\mathrm{LN}}(P_i; \bar{P}_i, W_i)\ \underline{d(\bar{\rho}_i, \bar{P}_i)}$$



Uncertainty in $\bar{\rho}_i$ <u>*and*</u> $\bar{P}_i$

Likelihood of $\boldsymbol{\theta}$ must integrate normal densities (ϕ_{N}) along the Hugoniot curve (H).

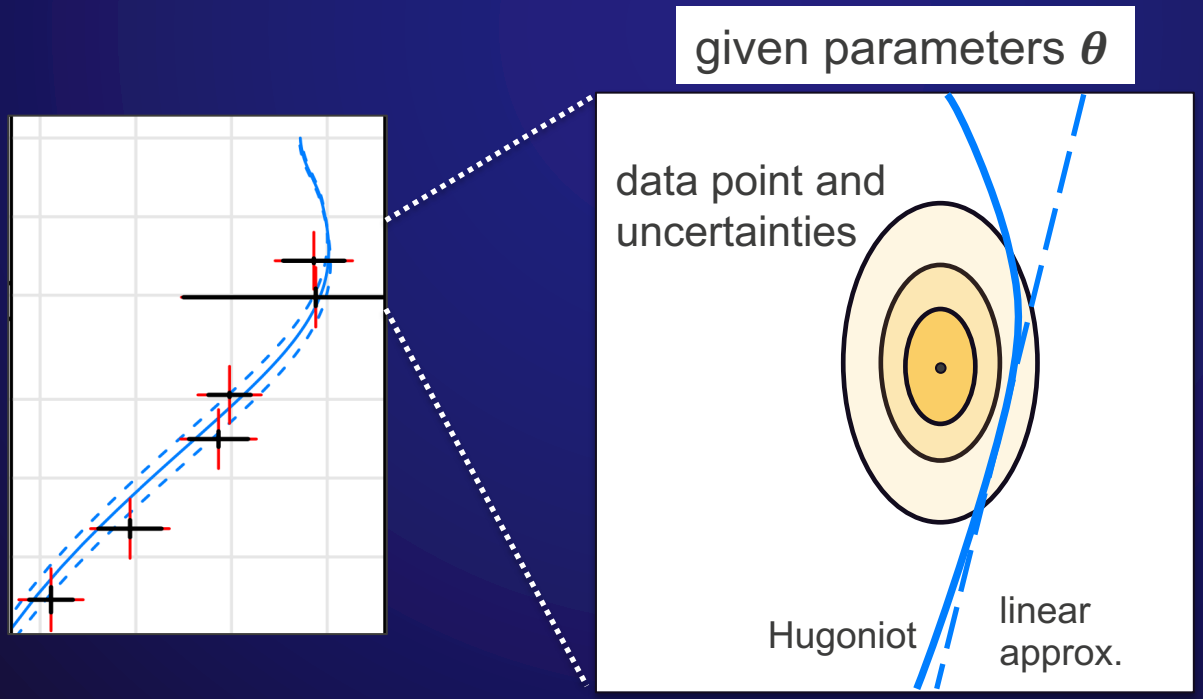
Not closed form. ☹

Local Likelihood Approximation

Approximate the Hugoniot as linear in the neighborhood of the data point

Line integral simplifies to a conditional normal density.

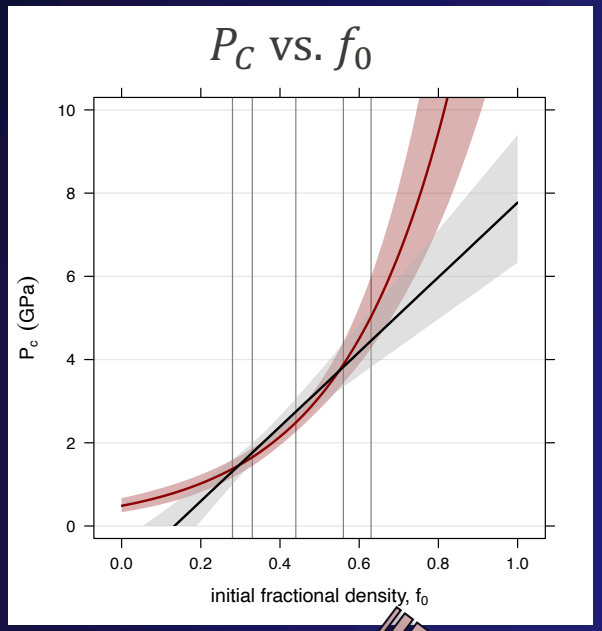
Closed form. ☺



Local approx. at each data point and each $\boldsymbol{\theta}$ explored by MCMC

saves bookoo compute time

Statistical fit with 95% bands

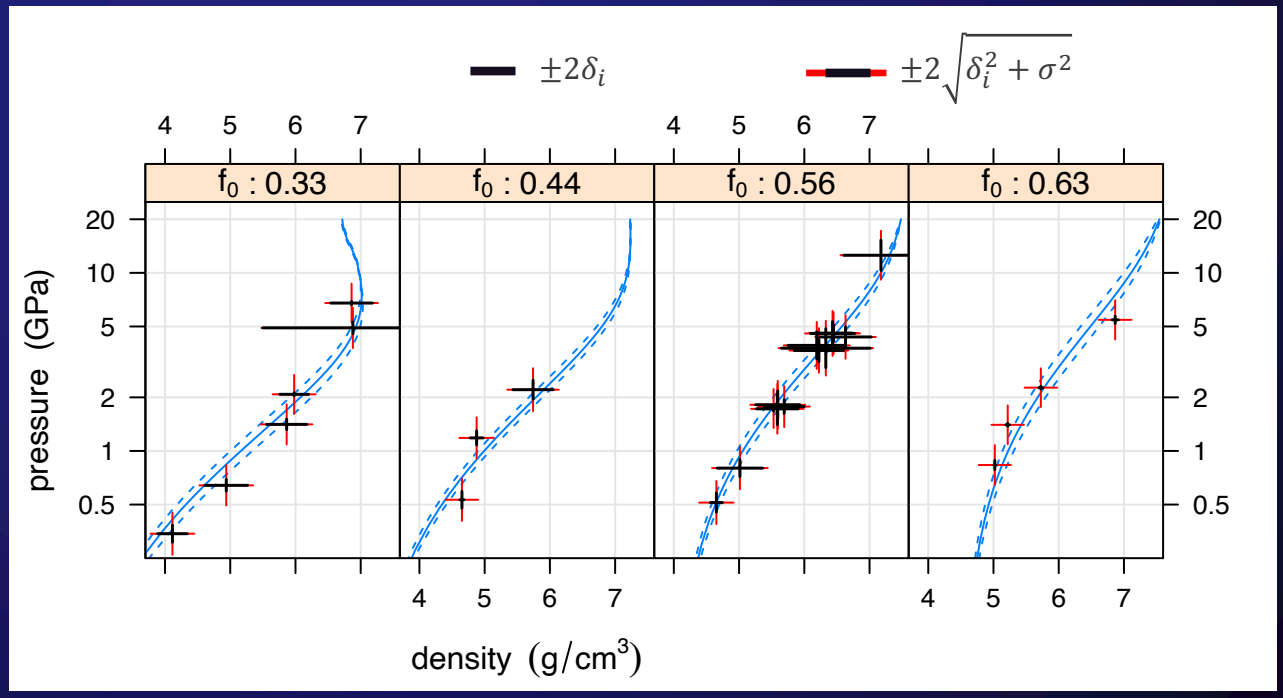


two assumed forms

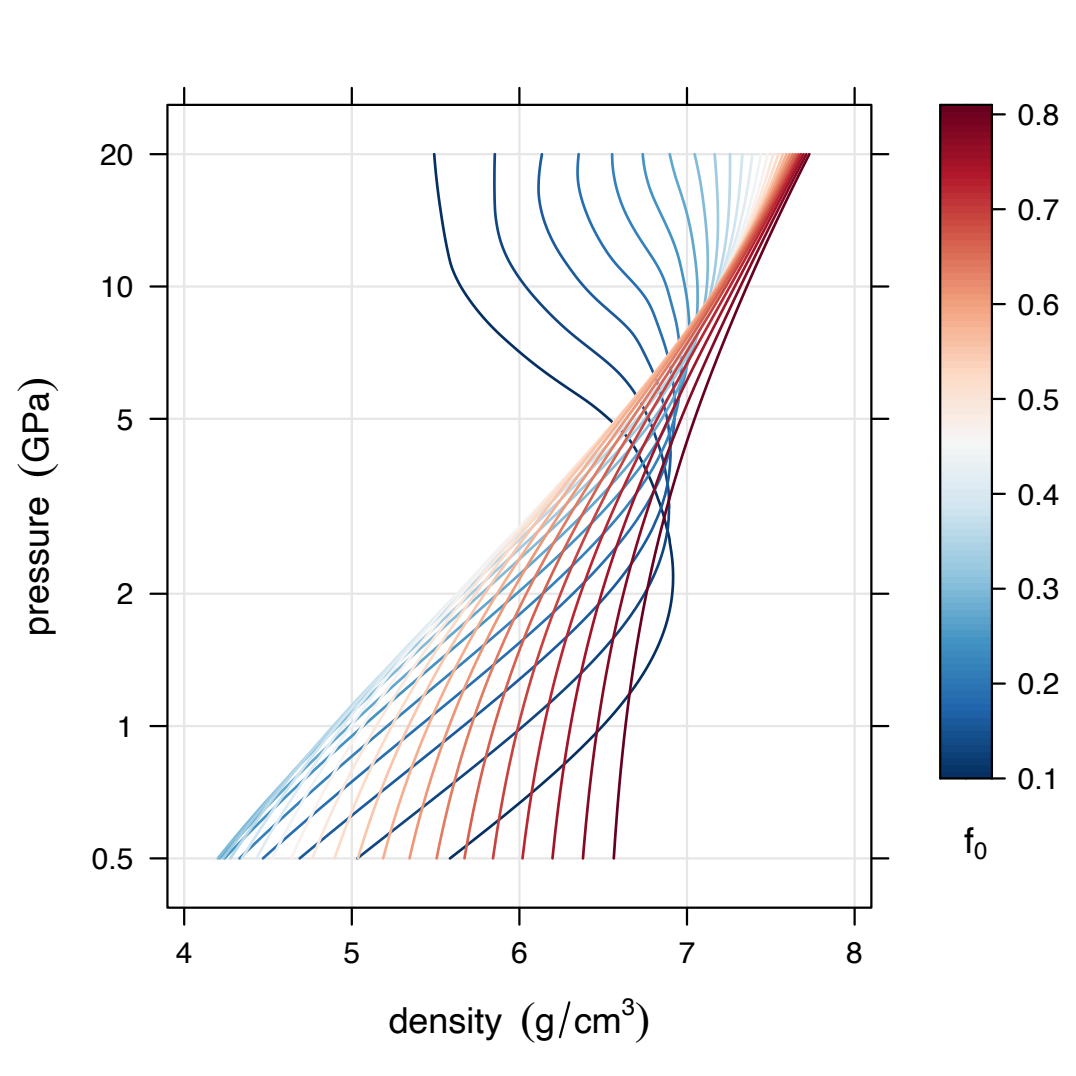
uncertainty bands derive from fit to data

exponential form

propagate uncertainty



Fitted Hugoniots vs. f_0 (uncertainties not shown)



Future Extensions

Incorporate additional uncertainties

- Flexible form of P_C vs. f_0
- EoS
- MK $\boldsymbol{P-\alpha}$ is imperfect

Propagate Hugoniot uncertainties through shock-physics applications

Summary of Analysis Features

diverse data

– combined analysis

measurement uncertainties

– nested structure

– errors on inputs *and* outputs

discrepancy

– beyond measurement precision

– imperfect physical models

computationally-intensive physical models

– can utilize fast emulators