

# Functional UNcertainty Constrained by Law and Experiment (F U.N.C.L.E.)

Andrew M. Fraser and Stephen A. Andrews, Los Alamos National Laboratory



## 2<sup>nd</sup> Order Approximation of Log Probability

Numerically find MAP estimate parameters of unknown function. For each experiment, estimate the Fisher information ( $\mathcal{I}_k$ ) and interpret it as how the  $k^{\text{th}}$  constrains the unknown function.

**Experiments**  $x = [x_0, \dots, x_n]$ , where  $x_k$  is data from the  $k^{\text{th}}$  experiment

**Likelihood**

$$p_l(x|\theta) = \prod_k p_l(x_k|\theta)$$

**Prior**

$$p_p(\theta)$$

**A posteriori distribution**

$$p(\theta|x) = \frac{p_l(x|\theta)p_p(\theta)}{\int p_l(x|\phi)p_p(\phi)d\phi}$$

**MAP** Maximum A posteriori Probability

$$\hat{\theta} \equiv \underset{\theta}{\operatorname{argmax}} p(\theta|x)$$

**Taylor series**

$$\begin{aligned} \log(p(\theta|x)) &= \log\left(\frac{p_l(x|\hat{\theta})p_p(\hat{\theta})}{\int p_l(x|\phi)p_p(\phi)d\phi}\right) \\ &+ \frac{1}{2}(\theta - \hat{\theta})^T \left( \frac{d^2 \log(p_l(x|\phi))}{d\phi^2} + \frac{d^2 \log(p_p(\phi))}{d\phi^2} \right)_{\phi=\hat{\theta}} (\theta - \hat{\theta}) \\ &+ R \\ &\equiv C + \frac{1}{2}(\theta - \hat{\theta})^T H (\theta - \hat{\theta}) + R \end{aligned}$$

**Gaussian approximation**

$$\begin{aligned} \theta|x &\sim \mathcal{N}(\hat{\theta}, \Sigma = H^{-1}) \\ p(\theta|x) &= \frac{1}{\sqrt{(2\pi)^{\dim|\Sigma|}}} \exp\left(-\frac{1}{2}(\theta - \hat{\theta})^T \Sigma^{-1} (\theta - \hat{\theta})\right) \end{aligned}$$

**Fisher information**  $\mathcal{I}_k \equiv -\mathbb{E}_{X_k} \left[ \left[ \frac{\partial^2}{\partial \theta^2} \log p(X_k; \theta) \right] \theta \right]$

## Bibliography

Andersen, M. and Vandenberghe, L.. "cvxopt Convex Optimization Package" <http://cvxopt.org>

Fickett, W. and Davis, W. C., 2000. "Detonation". University of California Press: Berkeley, CA.

"F.UNCLE: Functional Uncertainty Constrained by Law and Experiment". LA-CC-16-034, Los Alamos National Laboratory, [https://github.com/fraserphysics/F\\_UNCLE](https://github.com/fraserphysics/F_UNCLE)

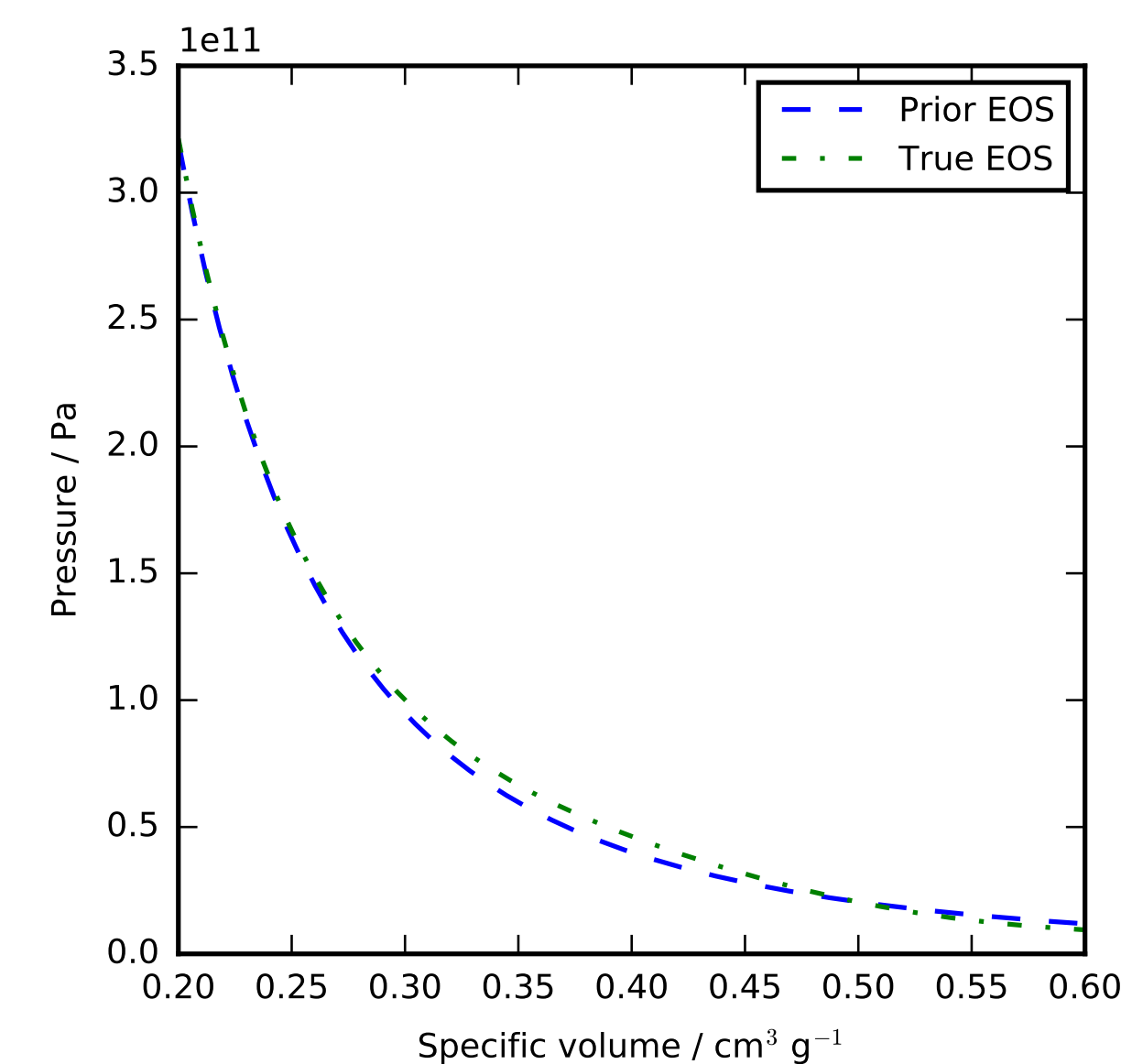
Hixson, R. S. et al., 2000. "Release isentropes of overdriven plastic-bonded explosive PBX-9501" *J. Applied Physics* **88** (11) pp. 6287-6293

Jones, E., Oliphant, E., Peterson, P., et al. "SciPy Open Source Scientific Tools for Python", 2001-, <http://www.scipy.org>

Pemberton et al. "Test Report for Equation of State Measurements of PBX-9501". LA-UR-11-04999, Los Alamos National Laboratory, Los Alamos, NM.

LA-UR-16-24568

## Unknown EOS function



**Pressure** unknown function,  $p(v)$

**Spline** Represent functions as cubic splines with fixed knot locations. Optimize over coefficients.

**Prior** Gaussian with mean coefficients,  $c_f[i]$ , fit to

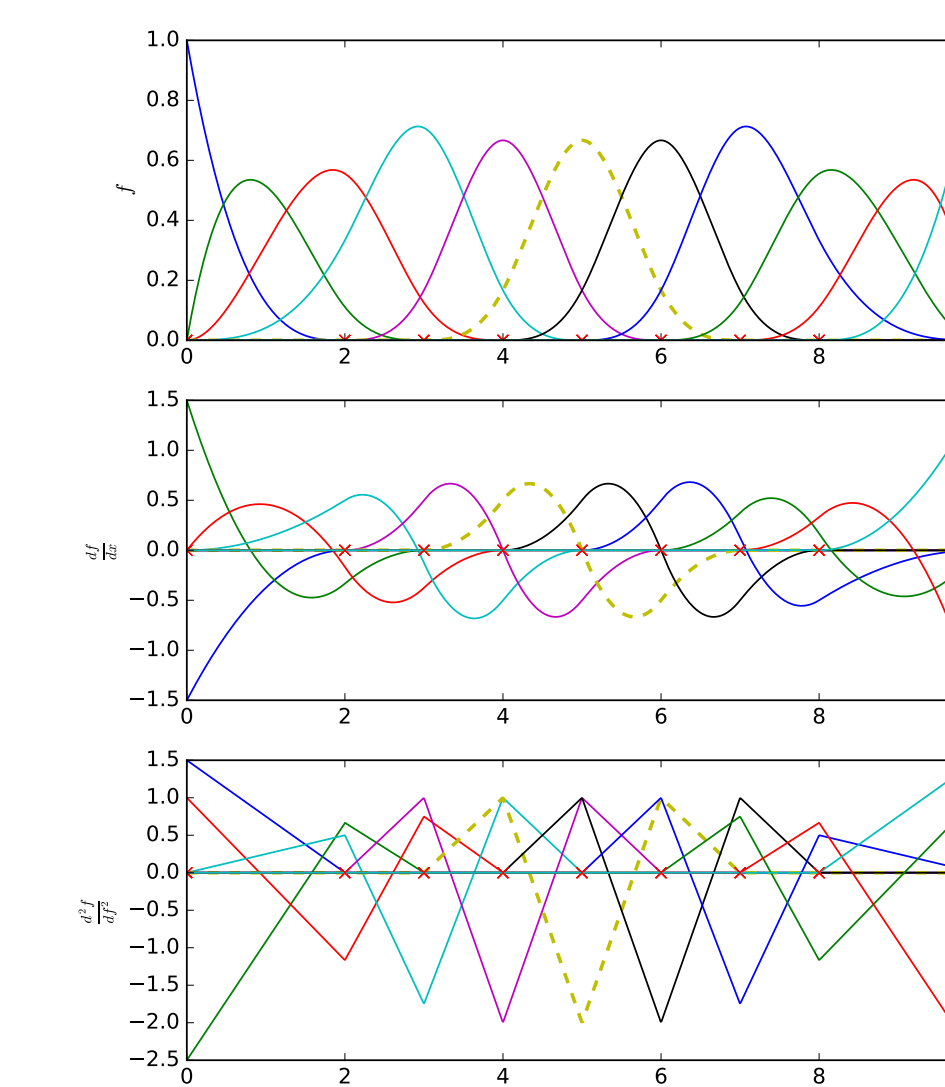
$$\tilde{f}(v) = \frac{F}{v^3}, \text{ where } F \leftrightarrow 2.56 \times 10^9 \text{ Pa at one cm}^3 \text{g}^{-1}$$

and variance

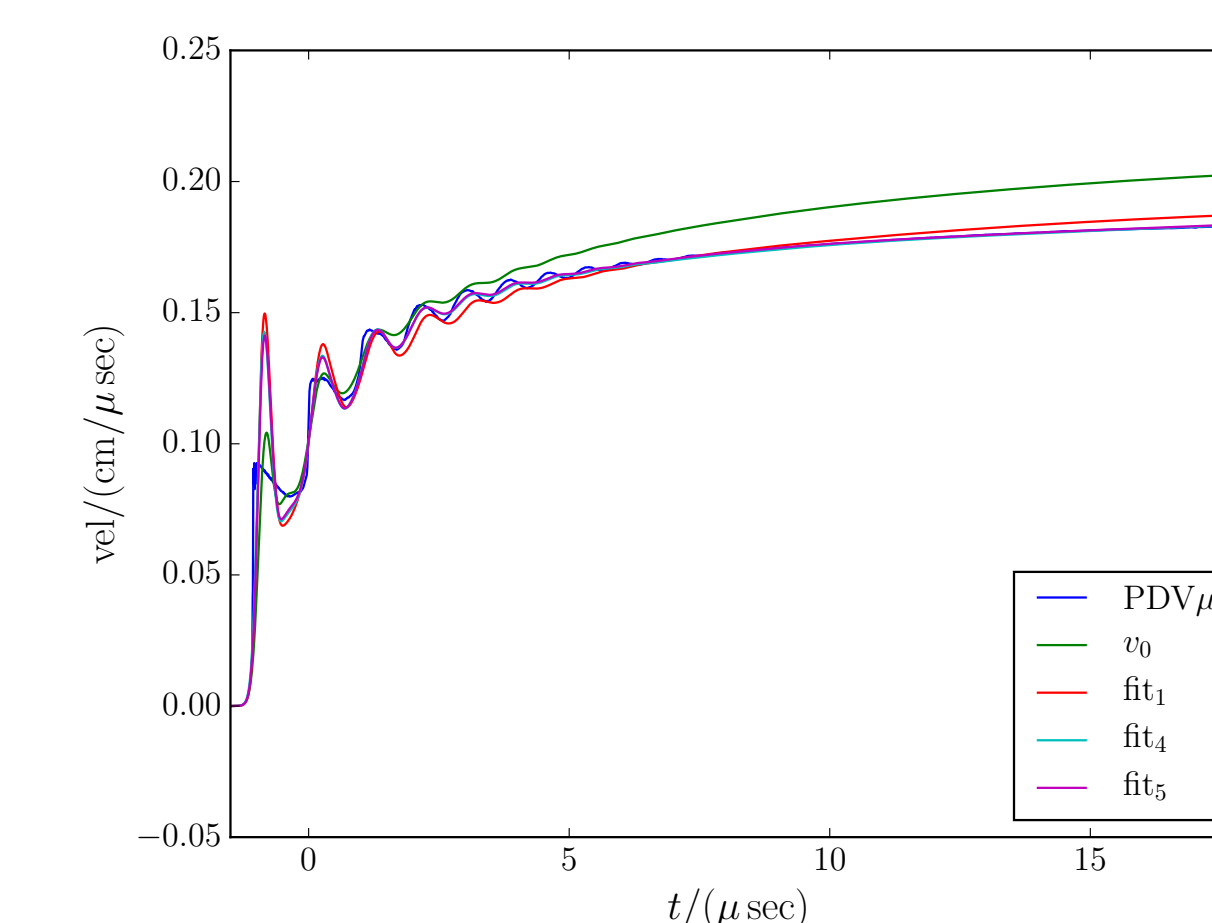
$$\sigma^2[i] = (0.05 \cdot c_f[i])^2$$

**Constraints** Enforced by CVXOPT, (Not consistent with prior)

- Positive
- Monotonic
- Convex

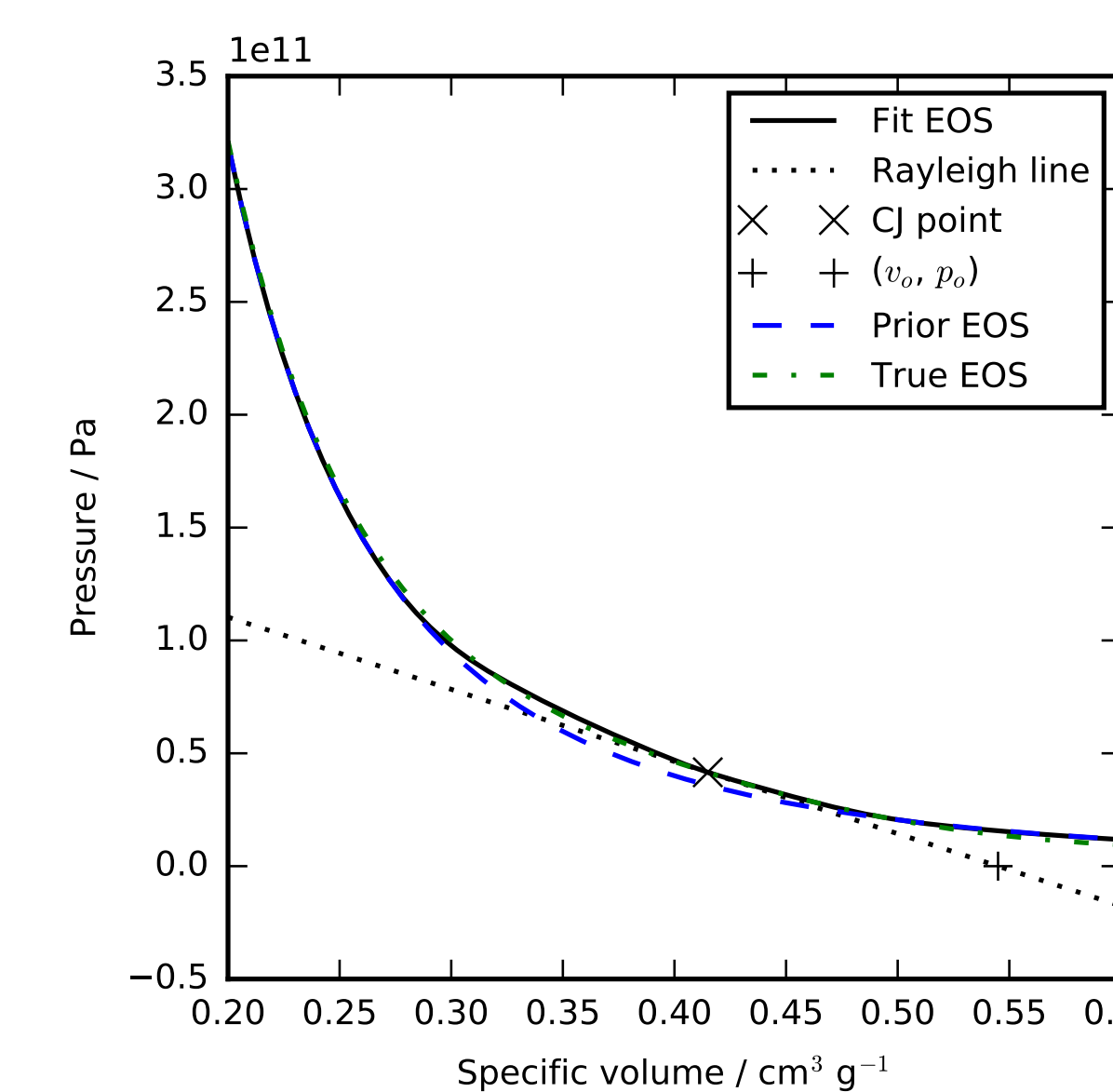
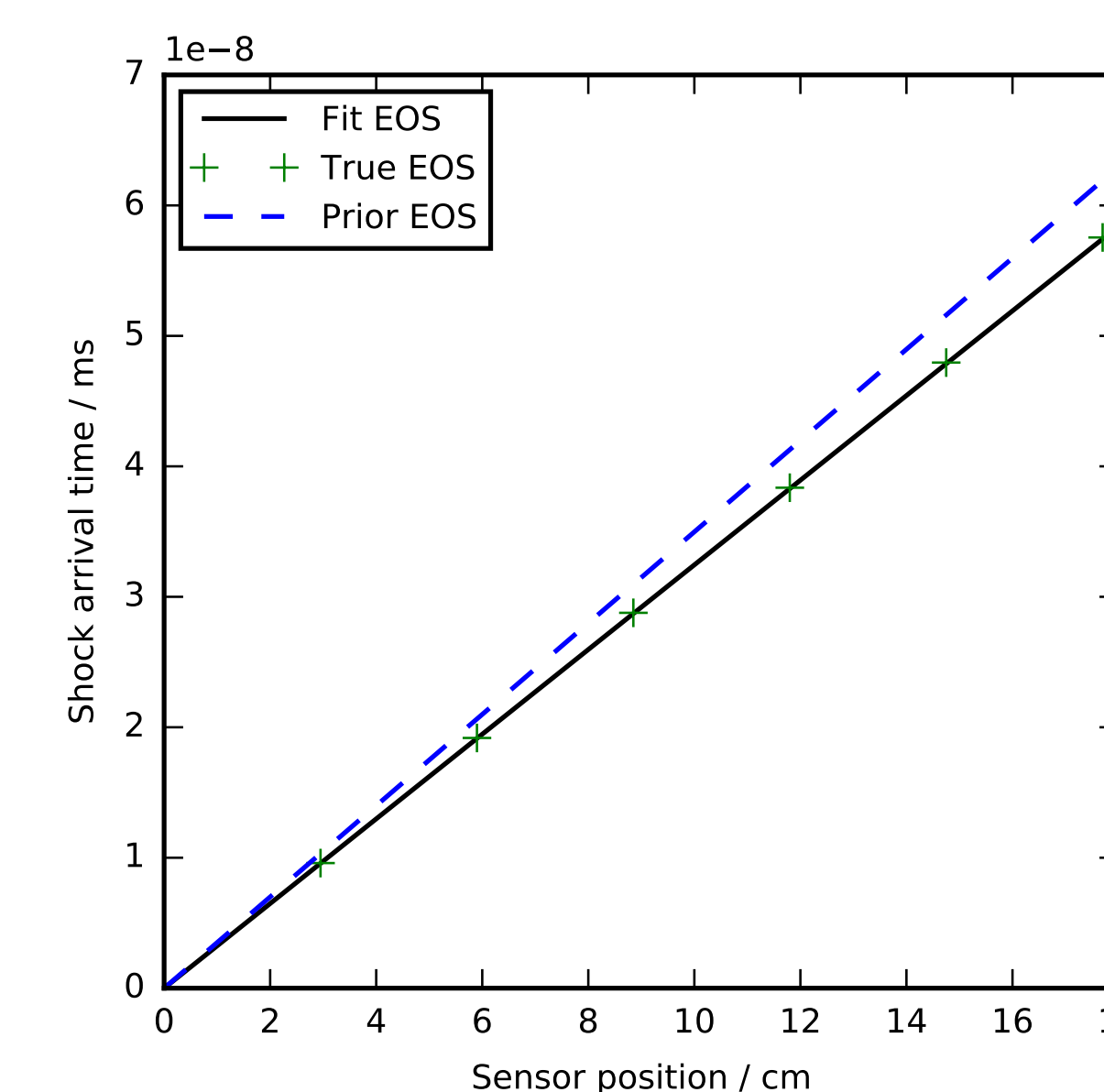
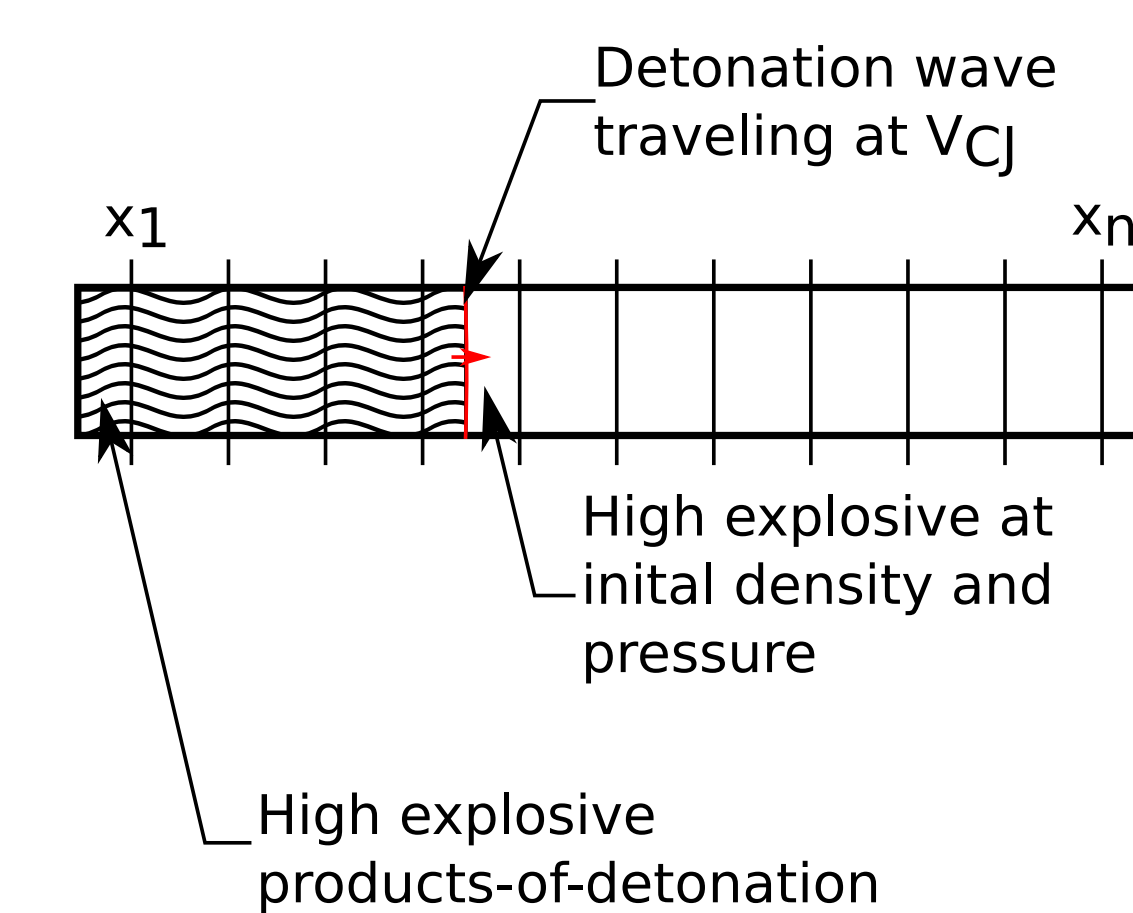


Cubic spline basis functions with first and second derivatives.



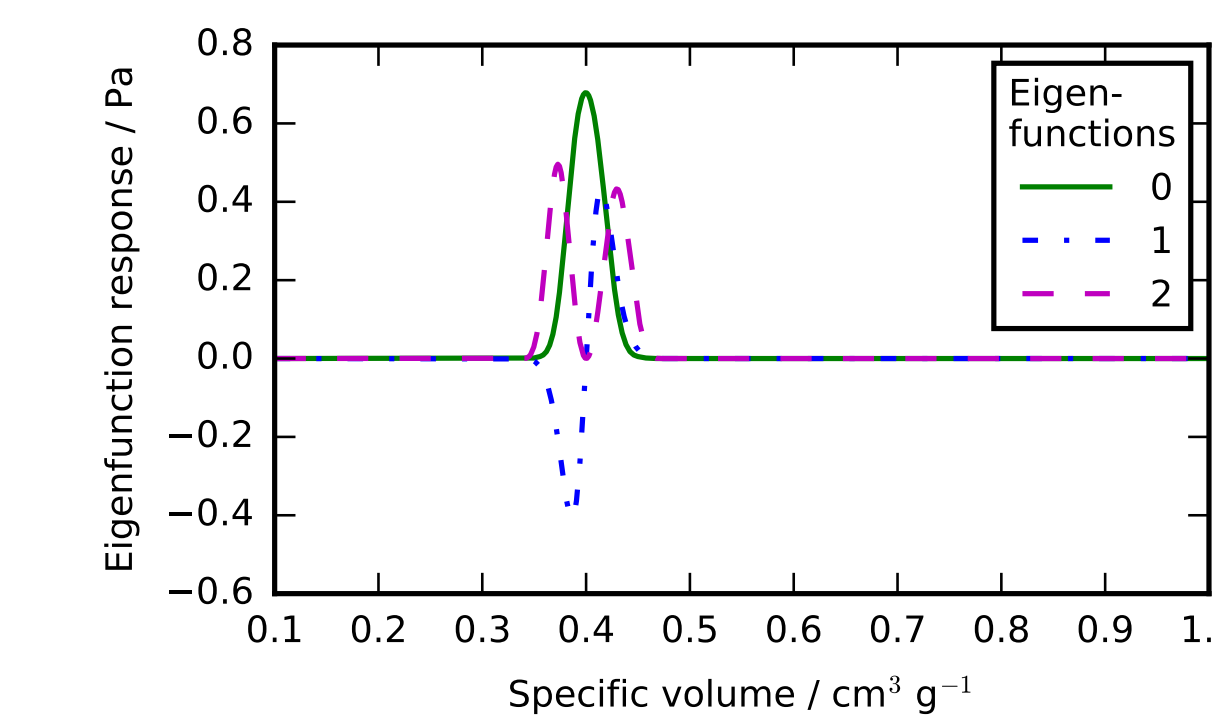
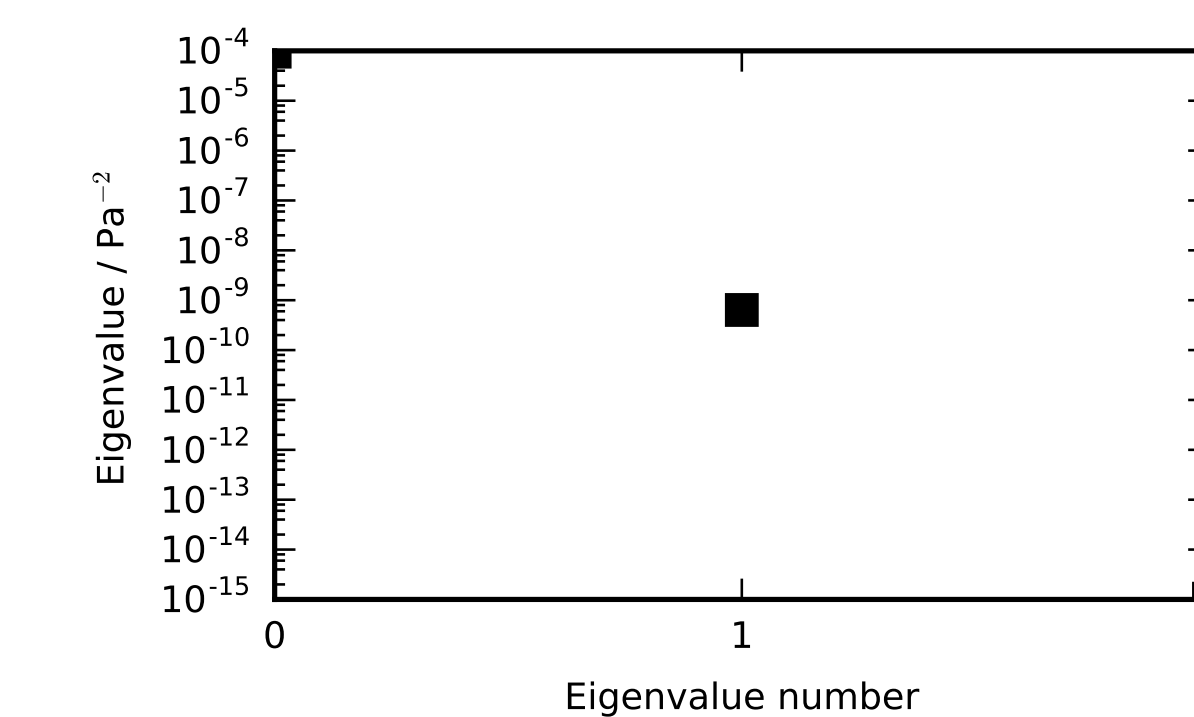
Photon Doppler velocimetry (PDV) data and sequence of fits to experiments on PBX-9501.

## Rate Stick Experiment

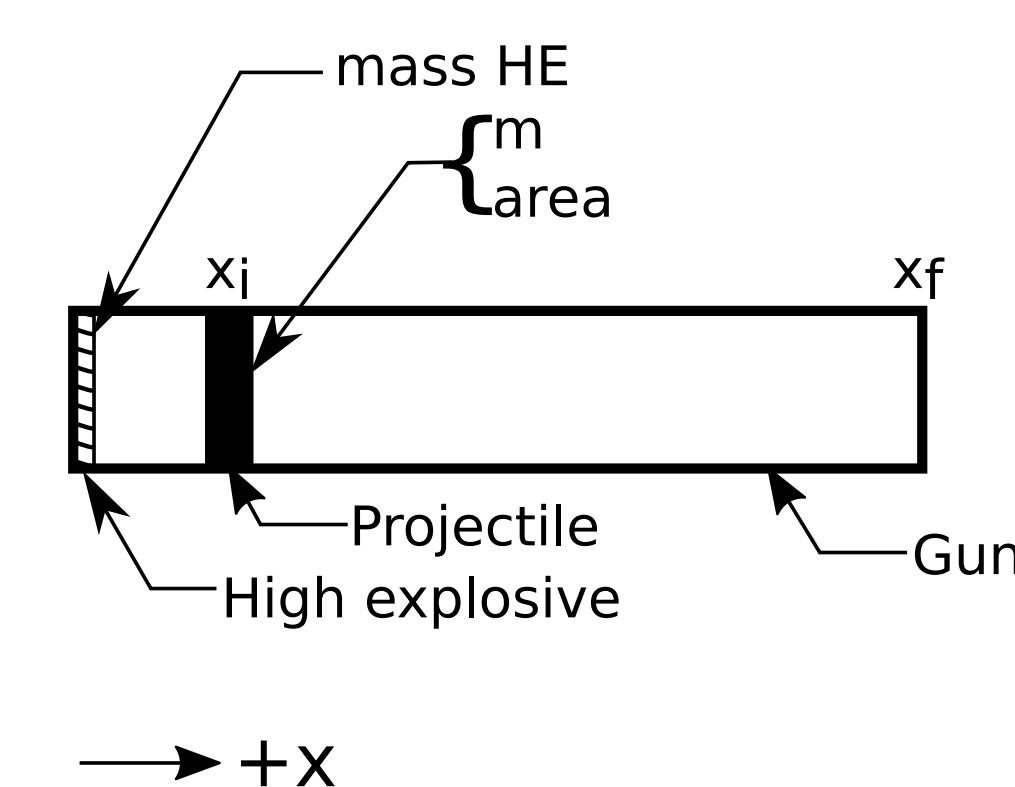


Detonation velocity from Chapman Jouguet conditions:

- Rayleigh line through  $(v_0, p_0)$  and tangent to EOS defines  $(v_{CJ}, p_{CJ})$
- Velocity  $V_{CJ} = v_0 \sqrt{\frac{p_{CJ} - p_0}{v_0 - v_{CJ}}}$



## Gun Experiment



$$\begin{aligned} F &= m \cdot a \\ p(v) \cdot A &= m \cdot \frac{d^2}{dt^2} x \\ p\left(\frac{A \cdot x}{m_{H.E.}}\right) \frac{A}{m} &= \frac{d^2}{dt^2} x \\ \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} &\equiv \begin{bmatrix} x \\ \frac{dx}{dt} \end{bmatrix} \equiv \begin{bmatrix} x \\ V \end{bmatrix} \\ \frac{dz}{dt} &= \begin{bmatrix} z_2 \\ p(A \cdot z_1) \frac{A}{m} \end{bmatrix} \end{aligned}$$

- Sample times  $\mathbf{t} = [0, \Delta t, 2\Delta t, \dots, N\Delta t]$
- `scipy.integrate.odeint`  $\rightarrow [V_0, V_1, \dots, V_N]$
- `scipy.interpolate.UnivariateSpline`  $\rightarrow V(t)$

