Determining PTW parameters from experimental data

Ken Hanson

CCS-2, Continuum Dynamics

Los Alamos National Laboratory

These slides and related work at
http://www.lanl.gov/home/kmh/

LA-UR-04-3574

Overview

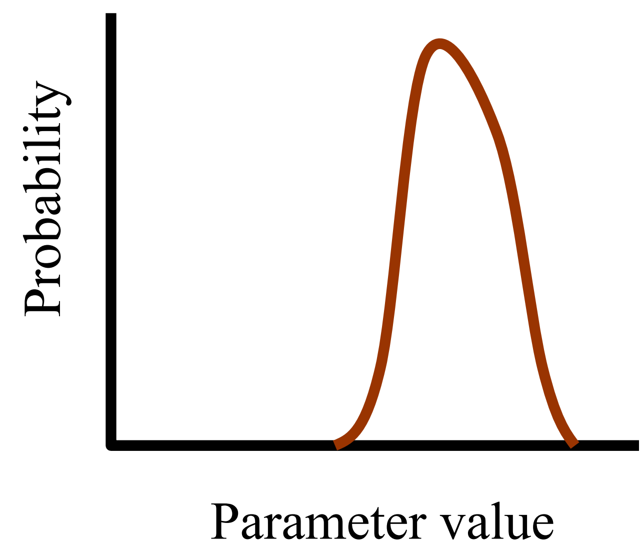
- Understanding physics simulations codes
  - employ hierarchy of experiments, from basic to fully integrated
  - role of Bayesian analysis - improve knowledge of models with each new experiment
- Statistical analysis – use of chi squared
  - treatment of systematic uncertainties
- Analysis of experimental data to infer parameters of Preston-Tonks-Wallace plasticity model for tantalum
  - characterize uncertainties in measurement data
  - estimate PTW parameters and their uncertainties
  - check model by drawing Monte Carlo samples from posterior distribution and comparing to data
  - demonstrate importance of including correlations

Bayesian analysis in context of physics simulations

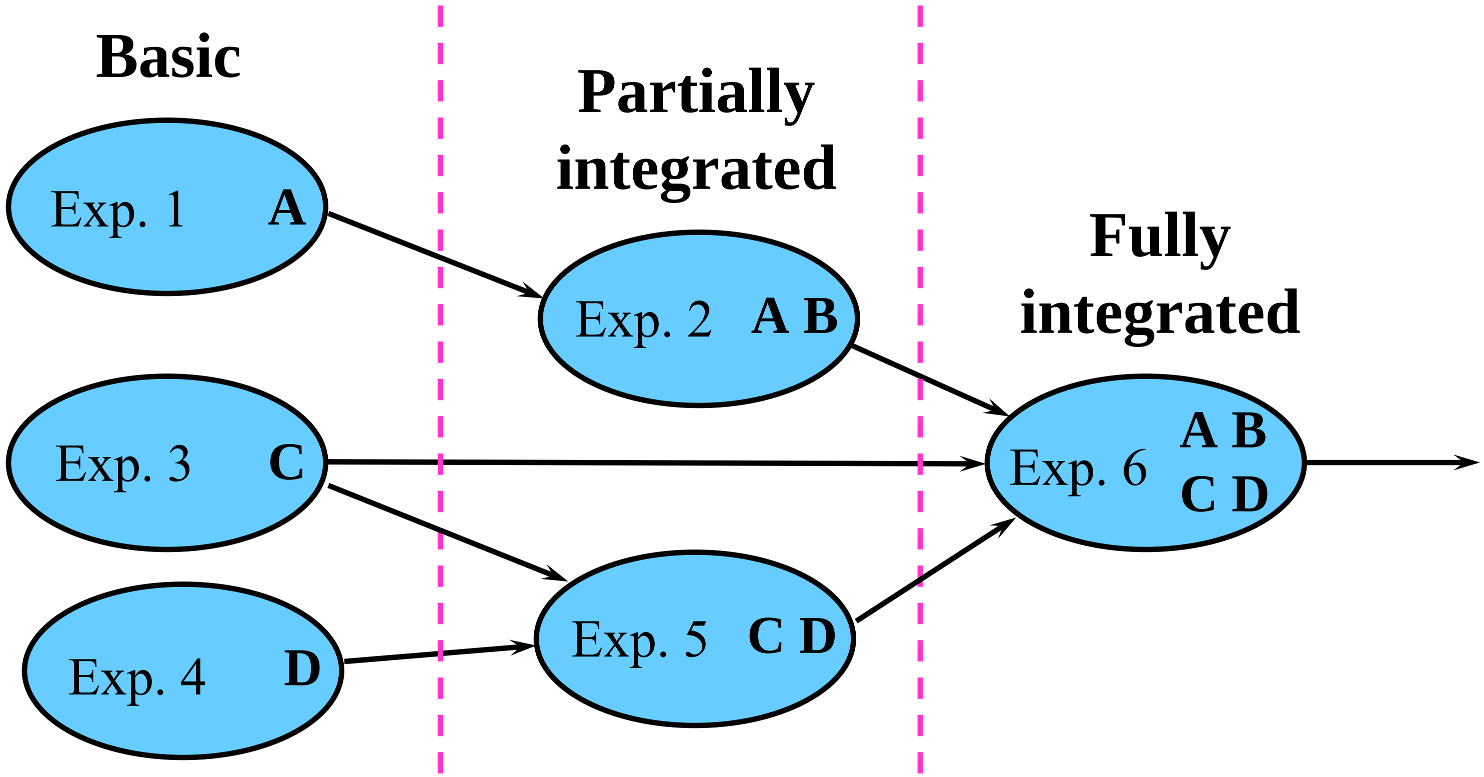
- Overall goal - describe uncertainties in simulations
  - physics submodels
  - experimental (set up and boundary) conditions
  - calculations (grid size, …)
- Use best knowledge of physics processes
  - rely on expertise of physics modelers and experimental data
- Bayesian foundation
  - focus is as much on uncertainties in parameters as on their best value
  - use of prior knowledge, e.g., previous experiments and expert judgment
  - model checking; does model agree with experimental data?

Bayesian uncertainty analysis

- Uncertainties in parameters are characterized by probability density functions (pdf)
- Probability interpreted as quantitative measure of "**degree of belief**"
- This interpretation sometimes called "subjective probability"
- Rules of classical probability theory apply



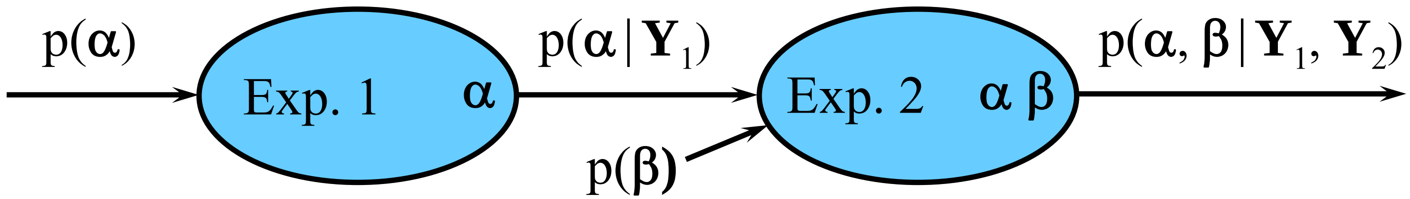
Analysis of hierarchy of experiments



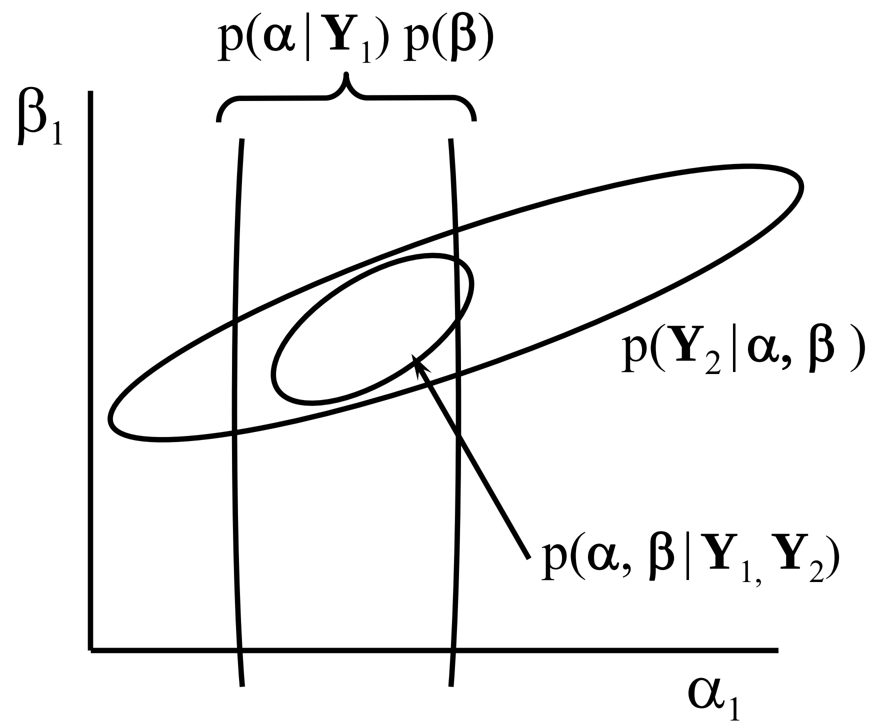
- Information flow in analysis of series of experiments
- Bayesian calibration –
  - analysis of each experiment updates model parameters (represented as A, B, C, etc.) and their uncertainties, consistent with previous analyses
  - information about models accumulates

Graphical probabilistic modeling

Propagate uncertainty through analyses of two experiments



- First experiment determines α, with uncertainties given by $p(\alpha|\mathbf{Y}_1)$
- Second experiment not only determines β but also refines knowledge of α by **Bayes law**
- Outcome is joint pdf in α and β, $p(\alpha, \beta|\mathbf{Y}_{1,} \mathbf{Y}_2)$ (correlations important!)

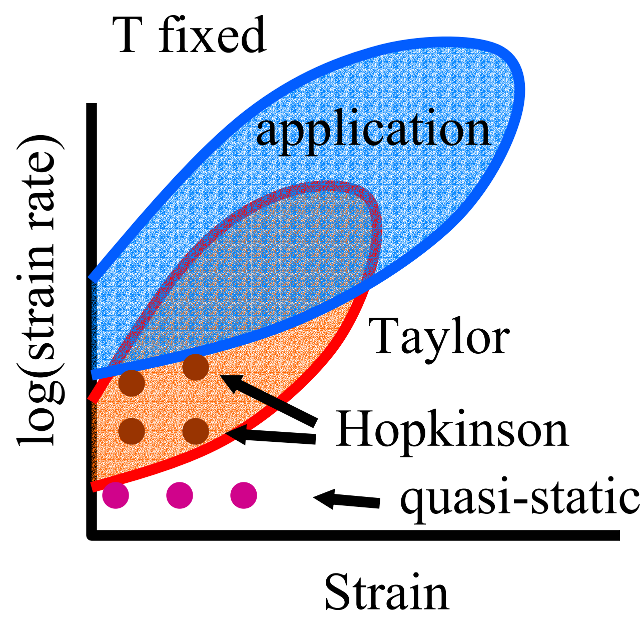


Uncertainty quantification for simulation codes

- Goal is to develop an uncertainty model for the simulation code by comparison to experimental measurements
  - ▸ determine and quantify sources of uncertainty
  - ▸ uncover potential inconsistencies of submodels with expts.
  - ▸ possibly introduce additional submodels, as required
- Recursive process
  - ▸ aim is to develop submodels that are consistent with all experiments (within uncertainties)
  - ▸ a hierarchy of experiments helps substantiate submodels over wide range of physical conditions
  - ▸ each experiment potentially advances our understanding

Hierarchy of experiments - plasticity

- Basic characterization experiments – measure stress-strain relationship at specific stain and strain rate
  - quasi-static – low strain rates
  - Hopkinson bar – medium strain rates
- Partially integrated expts. - Taylor test
  - covers range of strain rates
  - extends range of physical conditions
- Full integrated experiments
  - mimic application as much as possible
  - may involve extrapolation of operating range; introduces addition uncertainty
  - integrated expts. can help reduce model uncertainties in their operating range; may expose model deficiencies

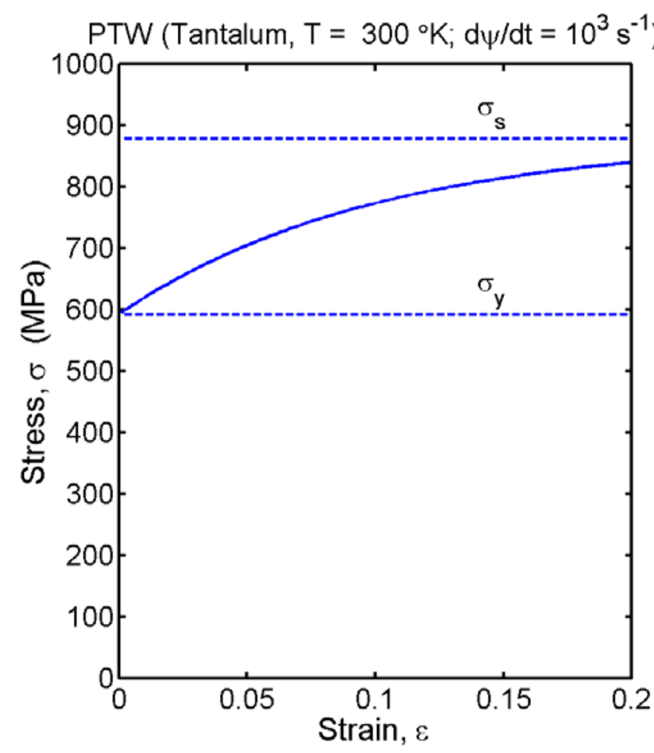


Determination of PTW parameters

- Goal is to assign plausible and defensible values to PTW parameters and their uncertainties
- Make use of data from quasi-static and Hopkinson-bar experiments (material-characterization experiments)
- Process:
  - estimate uncertainties in data based on statistical analysis and expertise of material scientists
  - translate experimental uncertainties into uncertainties in PTW parameters
  - seek feedback and guidance from experts; try to capture their beliefs in overall uncertainty analysis; build consensus

PTW model for plastic deformation

- Preston-Tonks-Wallace model describes plastic behavior of metals
  - provides stress σ (or s) as function of plastic strain ε_p for wide range of strain rate and temperature
  - nonlinear, analytic formulation
- 8 parameters (for low strain rates) plus material-specific constants
- PTW model based on dislocation mechanics model
  - does not include effects of anisotropy or material history



The model and parameter inference

- We write the model as

$$\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{x}, \boldsymbol{a})$$

  - where $\boldsymbol{y}$ is a vector of physical quantities, which is modeled as a function of the independent variables vector $\boldsymbol{x}$ and $\boldsymbol{a}$ represents the model parameters vector
- In inference, the aim is to determine:
  - the parameters $\boldsymbol{a}$ from a set of n measurements d_i of $\boldsymbol{y}$ under specified conditions x_i
  - **and** the uncertainties in the parameter values
- This process is called parameter inference, model fitting (or regression); however, uncertainty analysis is often not done, only parameters estimated

Inference – Bayes rule

- We wish to infer the parameters ***a*** of a model *M*, based on data ***d***
- Use Bayes rule, which gives the *posterior*:

$$p(\boldsymbol{a} \mid \boldsymbol{d}, M, I) \propto p(\boldsymbol{d} \mid \boldsymbol{a}, M, I)\ p(\boldsymbol{a} \mid M, I)$$

  - where *I* represents general information that we have about the situation
  - $p(\boldsymbol{d} \mid \boldsymbol{a}, M, I)$ is the *likelihood*, the probability of the observed data, given the parameters, model, and general info
  - $p(\boldsymbol{a} \mid M, I)$ is the *prior*, which represents what we know about the parameters exclusive of the data
- Note that inference requires specification of the prior

Likelihood analysis – chi squared

- When the errors in each measurement are Gaussian distributed and independent, likelihood is related to chi squared:
$$p(\boldsymbol{d} \mid \boldsymbol{a}) \propto \exp(-\tfrac{1}{2}\chi^2) = \exp\left\{ -\tfrac{1}{2} \sum_i \left[\frac{[d_i - y_i(\boldsymbol{a})]^2}{\sigma_i^2} \right] \right\}$$
- χ^2 is often approximately quadratic in the parameters $\boldsymbol{a}$
$$\chi^2(\boldsymbol{a}) = \tfrac{1}{2}\left(\boldsymbol{a} - \hat{\boldsymbol{a}}\right)^{\mathrm{T}} \boldsymbol{K} \left(\boldsymbol{a} - \hat{\boldsymbol{a}}\right) + \chi^2(\hat{\boldsymbol{a}})$$
  - where $\hat{\boldsymbol{a}}$ is the parameter vector at minimum χ^2 and K is the curvature matrix (aka the *Hessian*)
- The covariance matrix for the uncertainties in the estimated parameters is
$$\mathrm{cov}(\boldsymbol{a}) \equiv \left\langle (\boldsymbol{a} - \hat{\boldsymbol{a}})(\boldsymbol{a} - \hat{\boldsymbol{a}})^{\mathrm{T}} \right\rangle \equiv \boldsymbol{C} = 2\boldsymbol{K}^{-1}$$

Characterization of chi-squared

- Expand vector $\boldsymbol{y}$ around $\boldsymbol{y}^0$, and approximate:

$$y_i = y_i(x_i, \boldsymbol{a}) = y_i^0 + \sum_j \left.\frac{\partial y_i}{\partial a_j}\right|_{a^0} (a_j - a_j^0) + \cdots$$

- The derivative matrix is called the *Jacobian*, $\boldsymbol{J}$
- Estimated parameters $\hat{\boldsymbol{a}}$ minimize χ^2 (MAP estimate)
- As a function of $\boldsymbol{a}$, χ^2 is approximately quadratic in $\boldsymbol{a} - \hat{\boldsymbol{a}}$

$$\chi^2(\boldsymbol{a}) = \tfrac{1}{2}\left(\boldsymbol{a} - \hat{\boldsymbol{a}}\right)^{\mathrm{T}} \boldsymbol{K} \left(\boldsymbol{a} - \hat{\boldsymbol{a}}\right) + \chi^2(\hat{\boldsymbol{a}})$$

  - where $\boldsymbol{K}$ is the curvature matrix (aka the *Hessian*);

$$\left[\boldsymbol{K}\right]_{jk} = \left.\frac{\partial^2 \chi^2}{\partial a_j \partial a_k}\right|_{\hat{a}} \; ; \quad \boldsymbol{K} = \boldsymbol{J}\boldsymbol{\Lambda}\boldsymbol{J}^{\mathrm{T}} \; ; \quad \boldsymbol{\Lambda} = \mathrm{diag}(\sigma_1^{-2}, \sigma_2^{-2}, \sigma_3^{-2}, \ldots)$$

- Jacobian useful for finding min. χ^2, i.e., optimization

Advanced analysis

- Analysis of multiple data sets
  - to combine the data from multiple, independent data sets into a single analysis, the combined chi squared is

$$\chi^2_{all} = \sum_k \chi^2_k$$

  - where $p(\boldsymbol{d}_k \mid \boldsymbol{a}, I)$ is the likelihood from kth data set
- Include Gaussian priors through Bayes theorem

$$p(\boldsymbol{a} \mid \boldsymbol{d}, I) \propto p(\boldsymbol{d} \mid \boldsymbol{a}, I)\ p(\boldsymbol{a} \mid I)$$

  - for a Gaussian prior on a parameter a_j

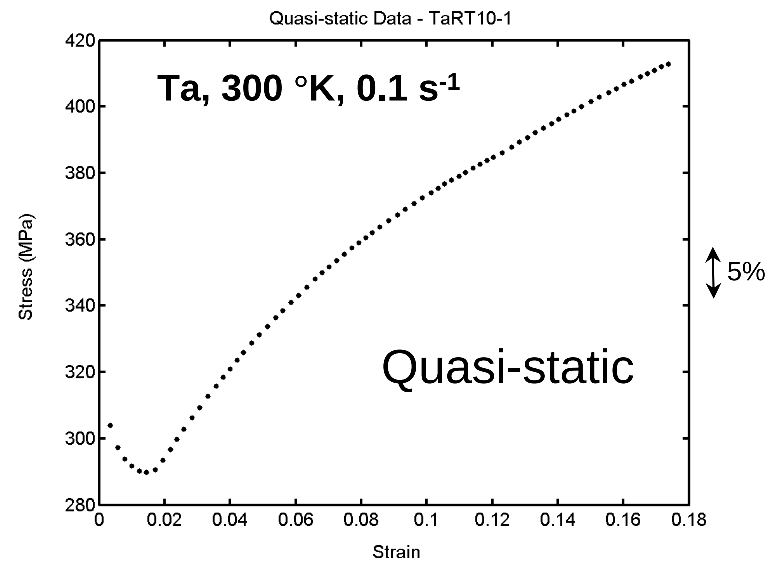
$$-\log p(\boldsymbol{a} \mid \boldsymbol{d}, I) = \varphi(\boldsymbol{a}) = \tfrac{1}{2}\chi^2 + \frac{\left(a_j - \tilde{a}_j\right)^2}{2\sigma_j^2}$$

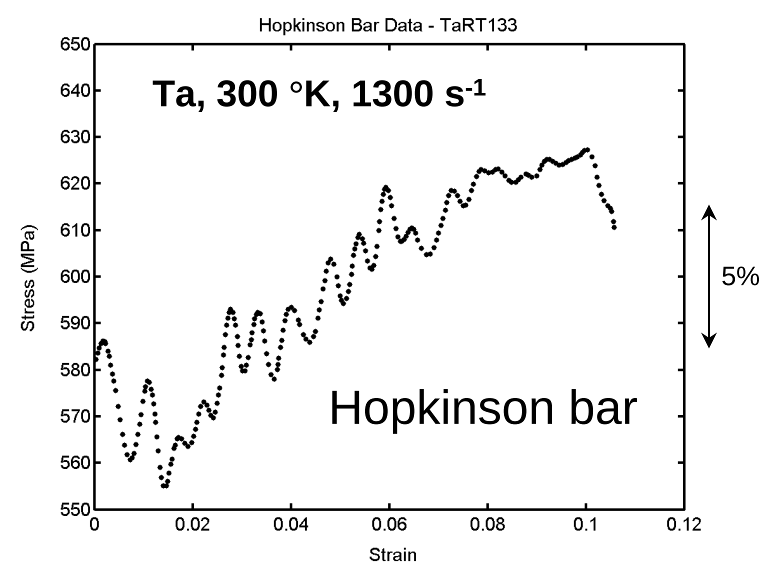
  - where $\tilde{a}_j$ is the default value for a_j and σ_j^2 is assumed variance

Material-characterization experiments

- Data from **quasi-static** compression experiments tend to be of high quality
  - rms 'noise' ≈ 0.1%
  - thin data set to limit undue influence in likelihood

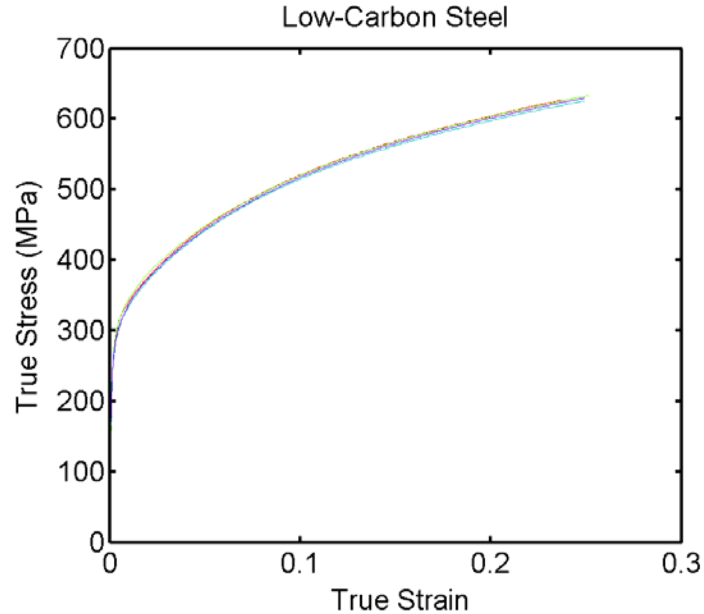
- Data from **Hopkinson-bar** experiments tend to be of medium quality
  - rms 'noise' ≈ 1%
- Observe artifacts in the data
  - arise from elastic-wave dispersion
  - need to account for these

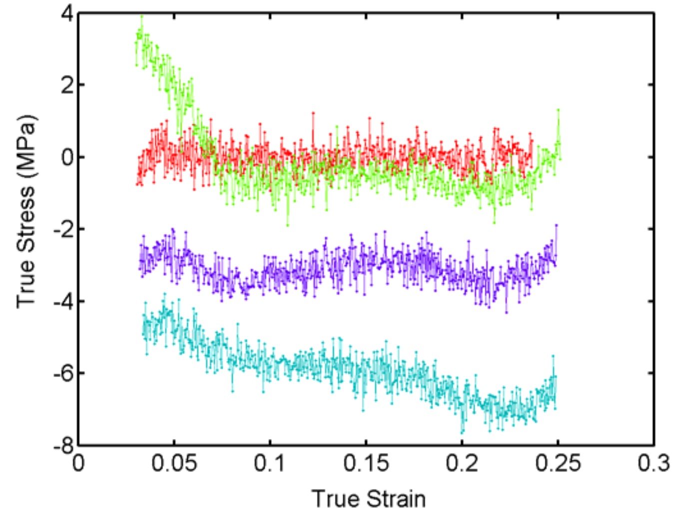




Repeatability of quasi-static experiments

- Low-carbon steel – has very consistent properties
- Figures show quasi-static measurements for four samples
- Data after subtracting smooth curve shown in bottom figure
- For each run:
  - rms dev. ≈ 0.2 MPa (0.04%)
  - random, independent "noise"
- From run-to-run:
  - rms dev. ≈ 3 MPa (0.6%)
- Sets lower limit on precision of quasi-static tests

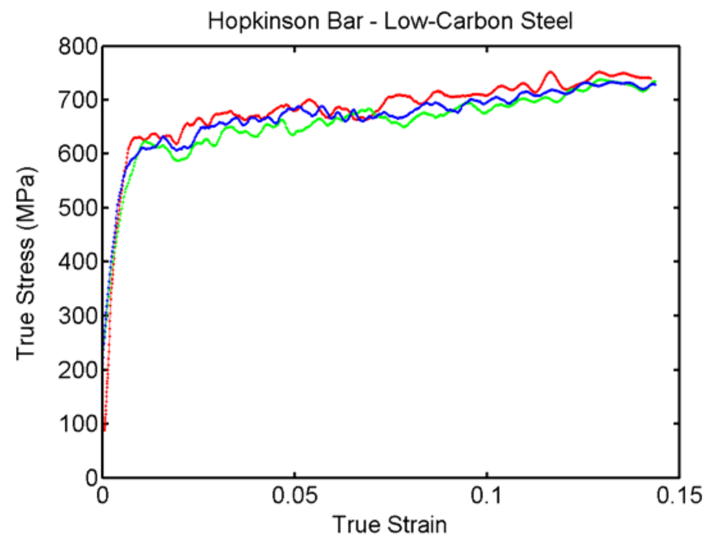


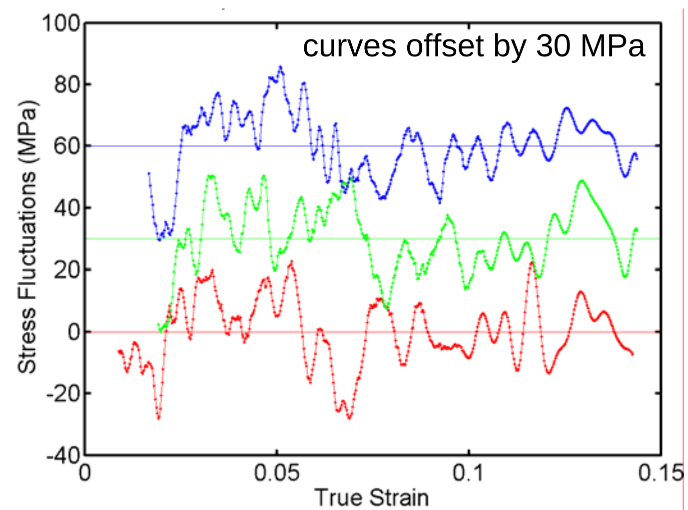


†data supplied by S-R Chen, MST-8

Repeatability of Hopkinson-bar experiments

- Figures show Hopkinson-bar measurements obtained with three low-carbon steel samples
  - observe fluctuations in measurements
  - produced by elastic waves reverberating in the sample
  - appear "random" in nature
- Data after subtracting smooth curve shown in bottom figure
- For each run:
  - rms dev. ≈ 12 MPa (1.8%)
  - highly correlated fluctuations
- Run-to-run variation is much smaller
- Treat fluctuations as a random process; characterize process for each run



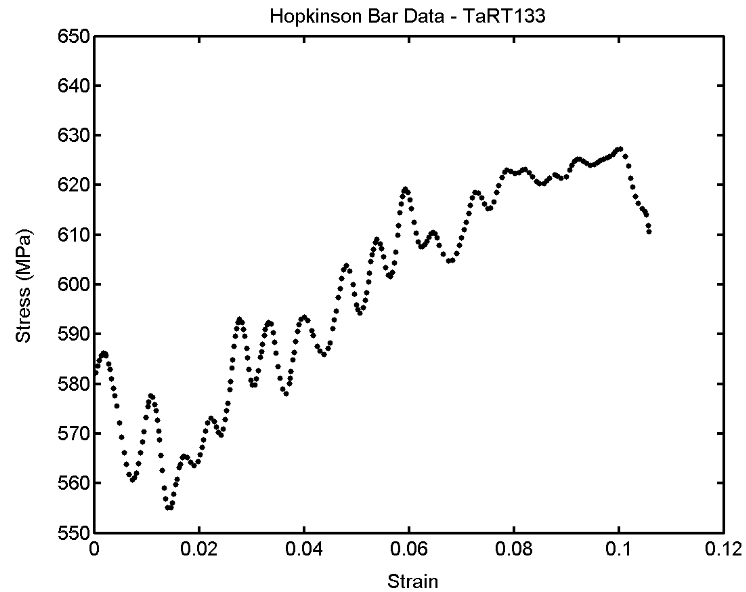


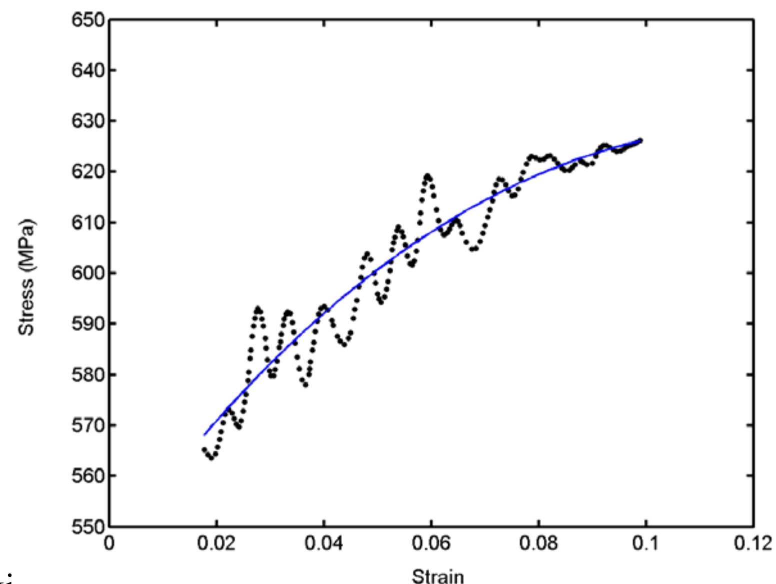
†data supplied by S-R Chen, MST-8

Hopkinson-bar measurements

- Hopkinson-bar data are degraded by fluctuations, caused by elastic wave dispersion
- Treat these fluctuations as coming from a random process with a high degree of correlation from point to point

- Analyze by subtracting low-order polynomial from data to get fluctuations from smooth dependence





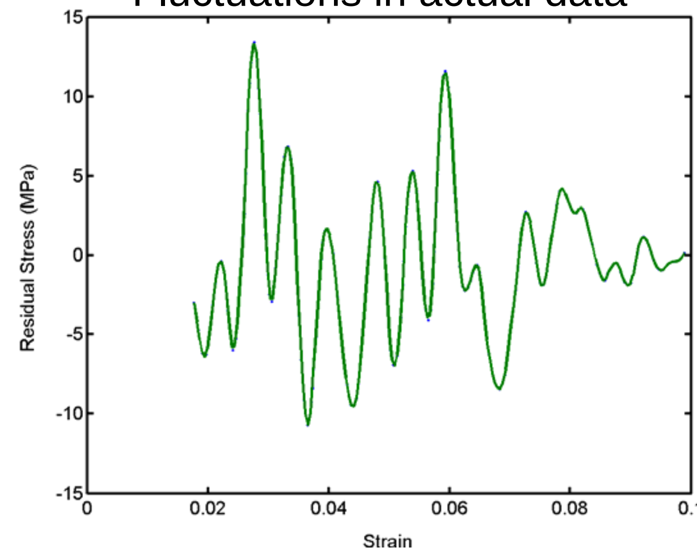
Hopkinson-bar measurements

- Treat Hop-bar fluctuations as a correlated Gaussian process; covariance given by

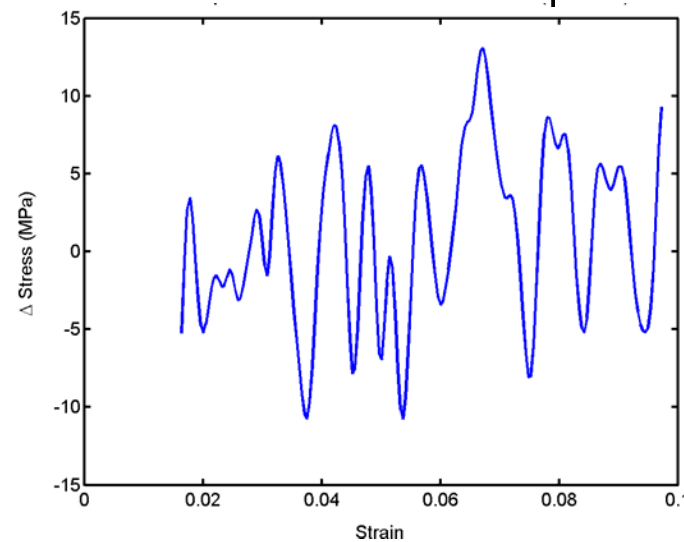
$$\mathrm{cov}(\boldsymbol{y}, \boldsymbol{y}') \propto \exp\left\{-\left[\frac{\boldsymbol{x}-\boldsymbol{x}'}{\lambda}\right]^{p}\right\}$$

  - where x is independent variable, strain
  - determine correlation length λ and exponent p from data
  - $p \cong 2$; $\lambda \cong 0.002$ (about 4 samples)
- Realization of random process shows behavior similar to data fluctuations
- Thin data set to avoid giving data undue weight in likelihood

Fluctuations in actual data



Realization from random process



Hopkinson-bar fluctuations

- Determine parameters of the Gaussian random process by minimizing the log-likelihood, given by

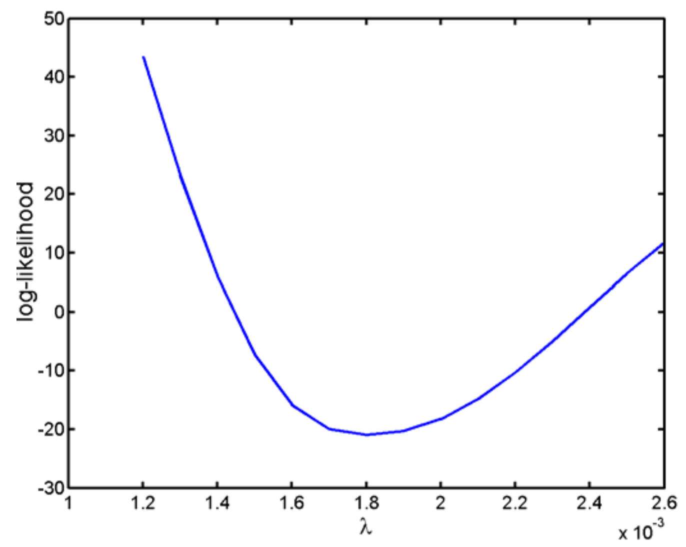
$$-\ln\left(p(\lambda \mid p, \boldsymbol{y}(\boldsymbol{x}))\right) =$$

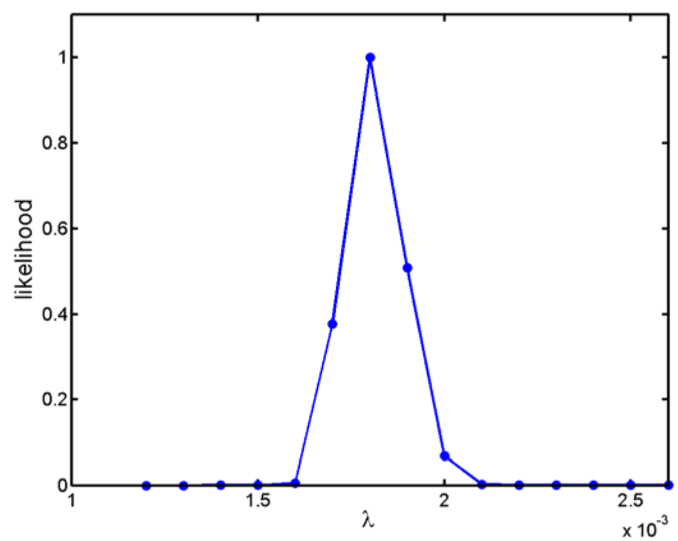
$$\tfrac{1}{2}\left(\boldsymbol{y}-\boldsymbol{y}'\right)^{\mathrm{T}}\boldsymbol{C}^{-1}\left(\boldsymbol{y}-\boldsymbol{y}'\right)+\tfrac{1}{2}\ln(\det(\boldsymbol{C}))$$

where $\boldsymbol{C}$ is a function of p and λ

$$\mathrm{cov}(\boldsymbol{y},\boldsymbol{y}') \propto \exp\left\{-\left[\frac{\boldsymbol{x}-\boldsymbol{x}'}{\lambda}\right]^{p}\right\}$$

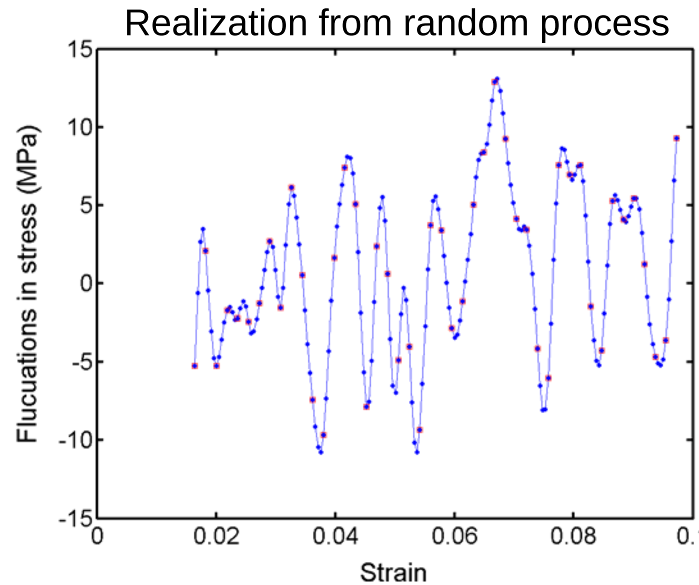
  - where x is independent variable (strain)
  - minimum at $\lambda \cong 0.0018 \pm 0.0002$ (about 4 samples) for fixed $p = 2$
  - similar analysis determines $p = 2$

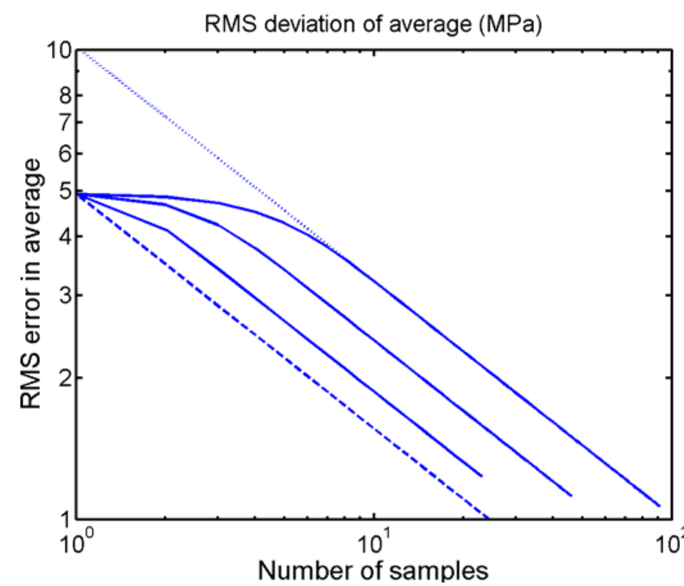




Hopkinson-bar measurements

- Figure shows all data from Gaussian random process and thinned subset of points (red), taking every fourth point
- Figure at lower right shows uncertainty in average of *n* samples:
  - dashed line is for uncorrelated noise
  - solids lines for actual correlated noise (far right), and for data thinned by factor of two and four
- Effect of thinning data is to make samples less correlated; which is more appropriate when using standard expression for chi-squared

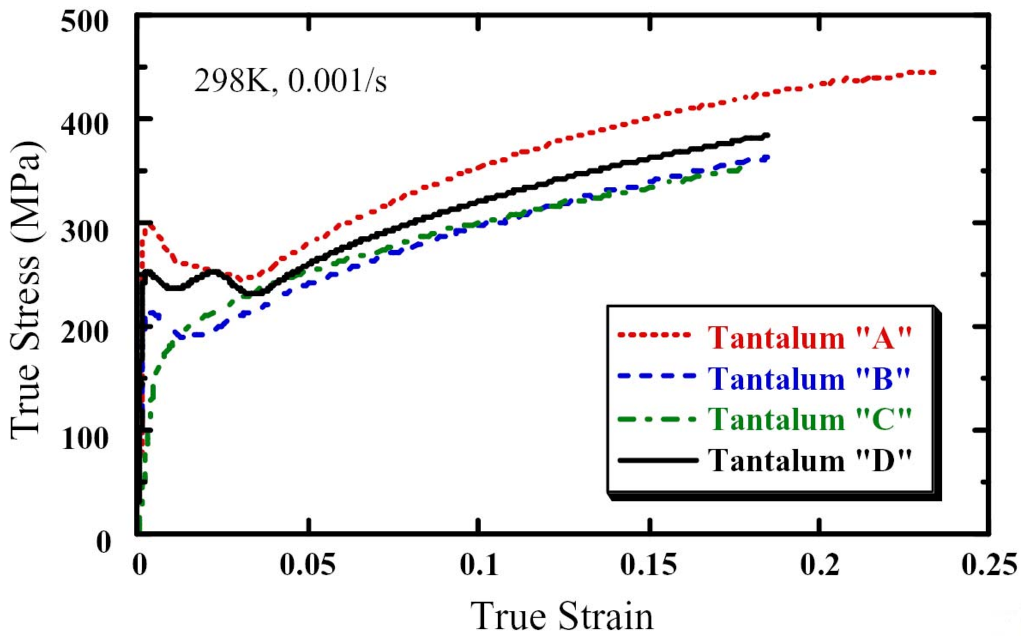




Repeated experiments for tantalum

- Repeated experiments
  - stability of measurements
  - indication of random component of error
  - may or may not indicate systematic error
- Figure shows curves obtained from four samples taken from different lots
- Sample-to-sample rms dev. ≈ 8%
- Treat this variability as a **systematic uncertainty** common to each tantalum specimen/data set

repeated quasi-static expts



†data supplied by S-R Chen, MST-8

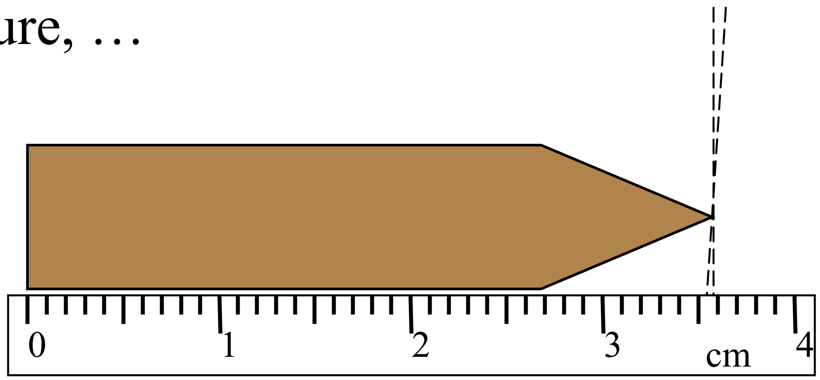
Types of uncertainties in measurements

- Two major types of errors
  - random error – different for each measurement
    - in repeated measurements, get different answer each time
    - often assumed to be statistically independent, but often aren't
  - systematic error – same for all measurements within a group
    - component of measurements that remains unchanged
    - for example, caused by error in calibration or zeroing
- Nomenclature varies
  - physics – random error and systematic error
  - statistics – random and bias
  - metrology standards (NIST, ASME, ISO) – random and systematic uncertainties (now)

Types of uncertainties in measurements

- Simple example – measurement of length of a pencil
  - ▸ random error
    - interpolation between ruler tick marks
  - ▸ systematic error
    - accuracy of ruler's calibration; manufacturing defect, temperature, …
- Parallax in measurements
  - ▸ reading depends on how person lines up pencil tip
  - ▸ random or systematic error?

    depends on whether measurements always made by same person in the same way or made by different people



Incorporating systematic effects (1)

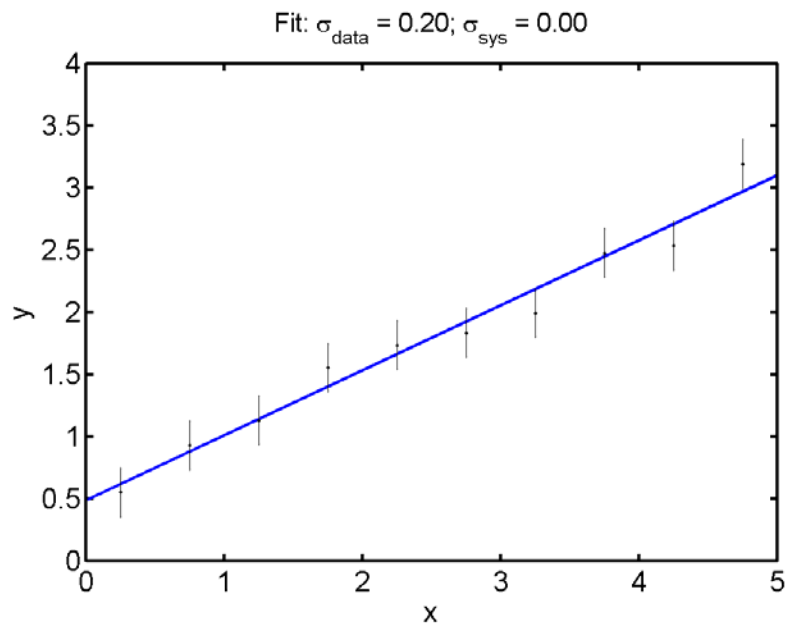
- Fit straight line

  $y = a + b\,x$

  to measurements of y, m_i
- Figure shows fit to10 data points, each with $\sigma_i = 0.2$
- "Best" fit by minimizing χ^2:

$$\chi^2_{\text{data}} = \sum_{i} \left(\frac{y_i - m_i}{\sigma_i} \right)^2$$

- Assumptions
  - measurements are independent
  - standard errors in are known (σ_i)
  - no systematic effects



Fit straight line to data

Incorporating systematic effects (2)

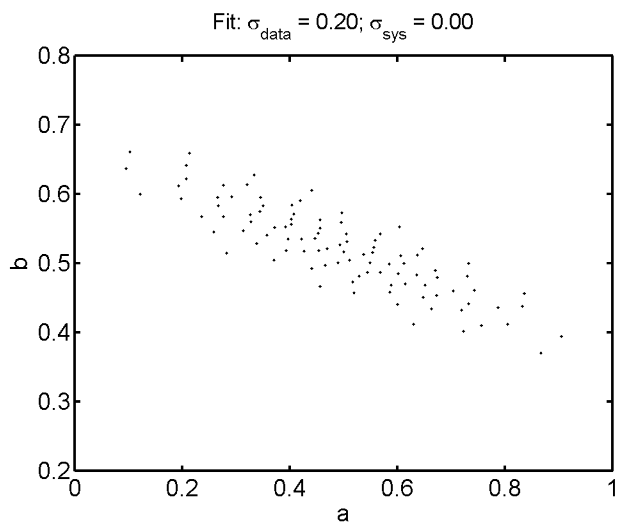
- Uncertainties in the parameters ***a*** can be determined from the curvature matrix of χ^2

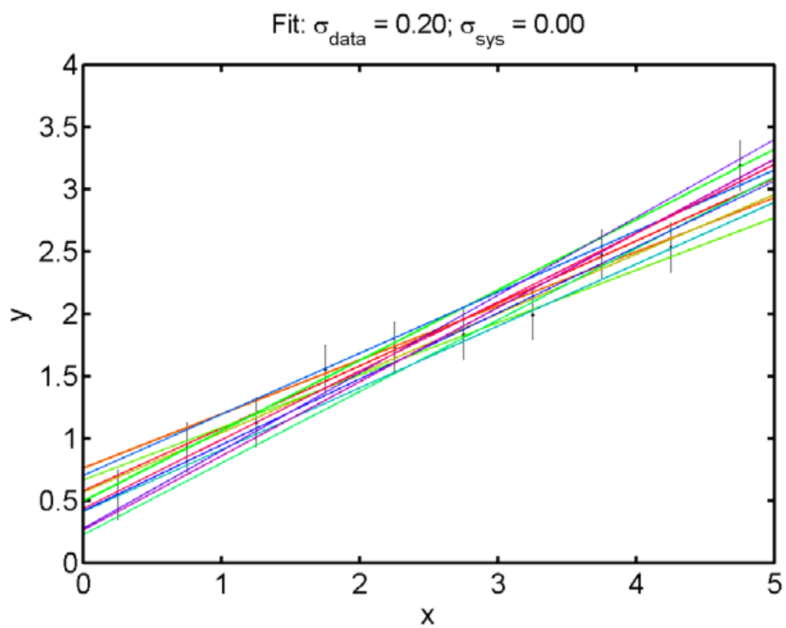
$$[\boldsymbol{K}]_{jk} = \left.\frac{\partial^2 \chi^2}{\partial a_j \partial a_k}\right|_{\hat{a}}$$

- The covariance matrix is

$$\boldsymbol{C} = 2\boldsymbol{K}^{-1}$$

- Upper figure shows quasi-random samples from (Gaussian) posterior, which gives parameter uncertainties
- Lower figure shows straight lines for 12 quasi-random samples, compared to the original data
  - variability ~ uncertainty



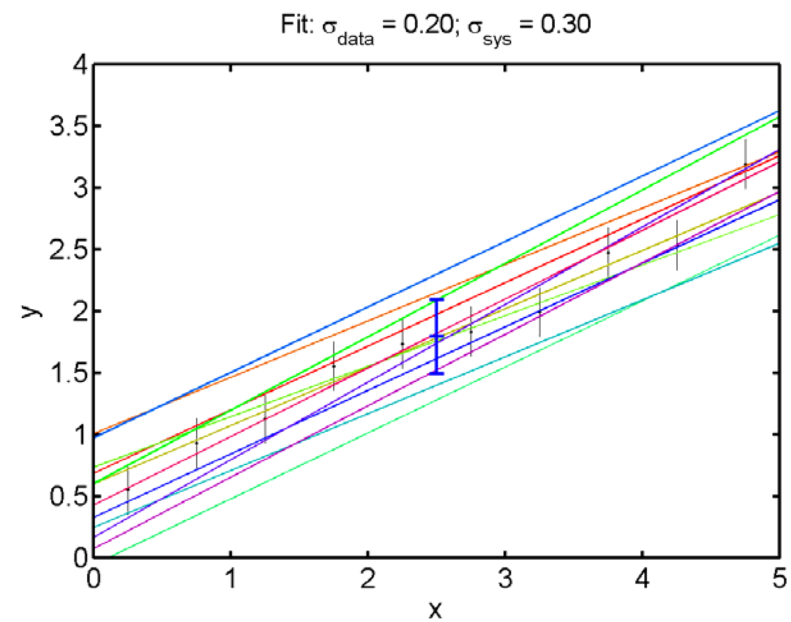


Incorporating systematic effects (3)

- Suppose all the data are uncertain to within an addition offset Δ, with a known uncertainty $\sigma_\Delta = 0.3$
- Include this systematic effect by writing χ^2 as

$$\chi^2 = \sum_i \left(\frac{y_i - m_i - \Delta}{\sigma_i} \right)^2 + \left(\frac{\Delta}{\sigma_\Delta} \right)^2$$

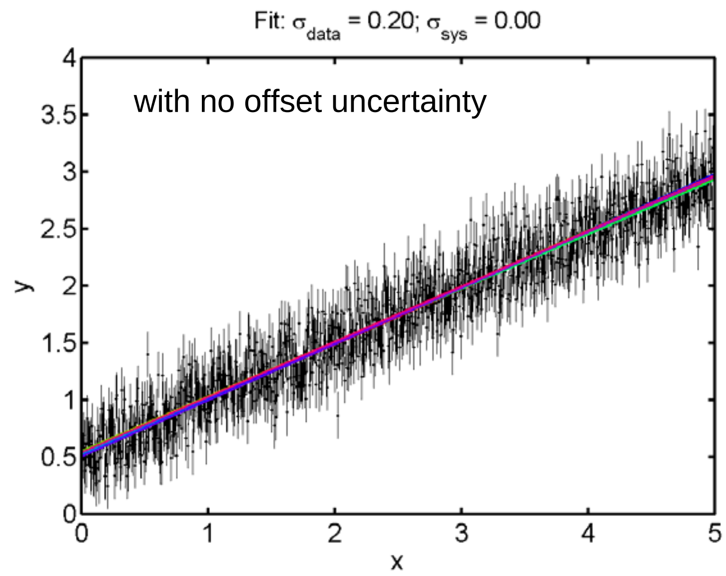
- Follow standard procedure
  - minimize χ^2 to estimate parameters a, b, and Δ
  - estimate covariance matrix by inverting curvature matrix (including all variables)
- Random samples from posterior, shown in figure, exhibit the expected increase in uncertainty about the inferred line

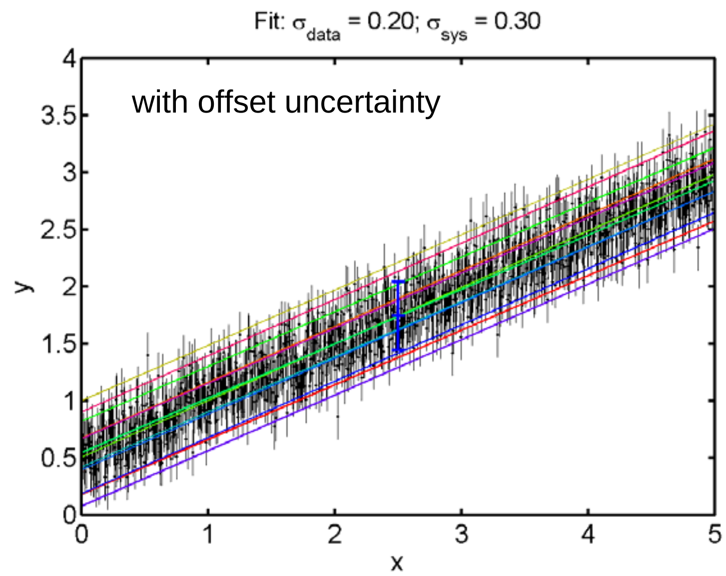


Error bar in middle of plot shows uncertainty in offset of all points

Incorporating systematic effects (4)

- Repeat previous exercise for 1000 data points with and without systematic uncertainty
- Plots show random samples from posterior
- With no offset uncertainty
  - the effect of data averaging is to reduce uncertainties in line parameters by factor of 10 [$= \sqrt{1000/10}$]
- With offset uncertainty ($\sigma_\Delta = 0.3$)
  - slope of lines has same uncertainty as above
  - offset of lines is subject to uncertainty in systematic offset
- Systematic uncertainties impose lower limit on inference

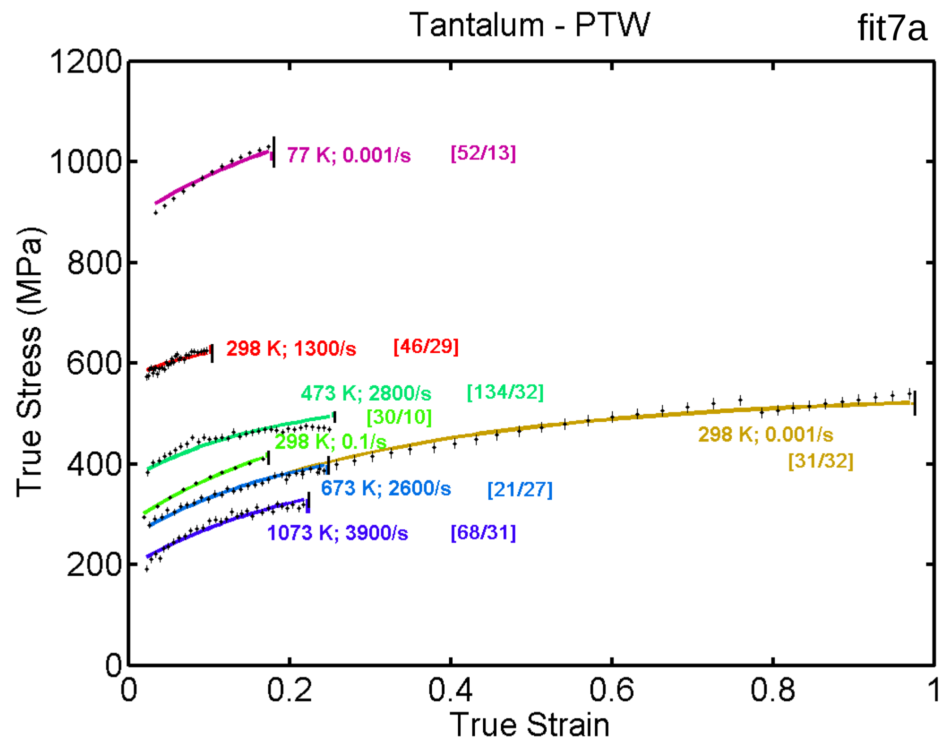




Fit PTW model to measurements

Preliminary fit (7a) to quasi-static and Hopkinson bar meas.

- Assuming for random standard errors
  - quasi-static: 0.5% (simple)
  - quasi-static: 2% (reloaded)
  - Hop-bar: 1% to 2.4%
- Include 3% systematic uncertainty in offset of each data set (7 + 7 parms)
- χ^2/DOF = 383/174 data; largest discrepancy for 473 K (pulls down slope)



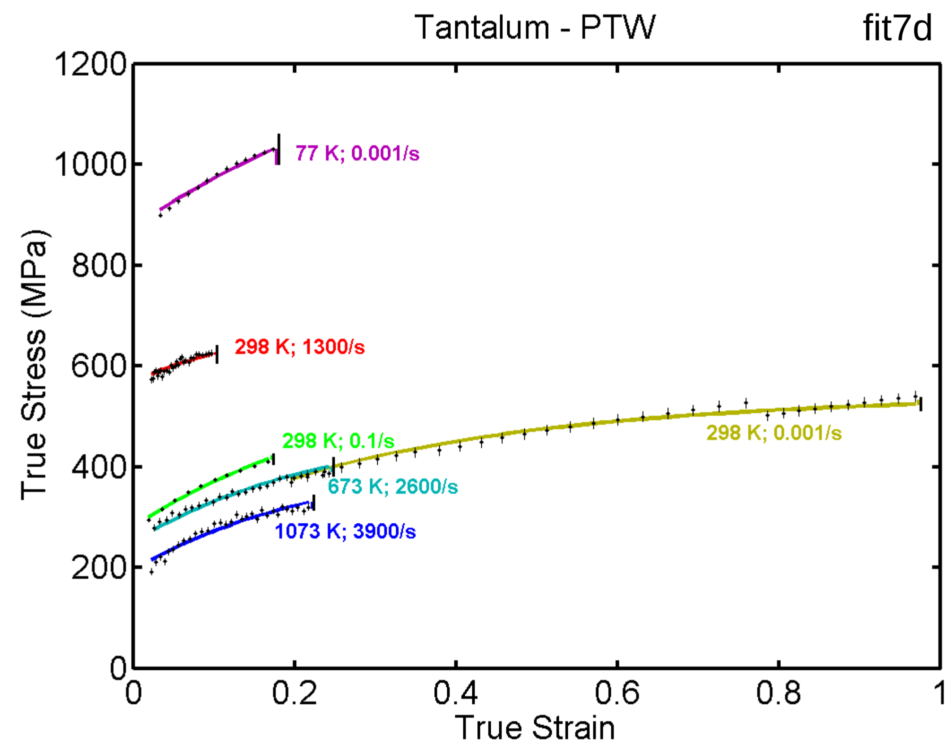
PTW curves include adiabatic heating effect for high strain rates

†data supplied by S-R Chen, MST-8

Fit PTW model to measurements

Final fit (7d) to quasi-static and Hopkinson bar measurements

- Assuming for random standard errors
  - quasi-static: 0.5%
  - quasi-static: 2% (reloaded)
  - Hop-bar: 1% to 2.4%
- Include 3% systematic uncertainty in offset of each data set (6 + 7 parms)
- ~ 4 iter., ~ 65 func. evals.
- χ^2/DOF = 214/142 data; largest discrepancy for 298 K, 0.1/s data set



PTW curves include adiabatic heating effect for high strain rates

†data supplied by S-R Chen, MST-8

PTW parameters and their uncertainties

Parameters +/- rms error:

$\theta = 0.0080 \pm 0.0004$
$\kappa = 0.68 \pm 0.06$
$-\ln(\gamma) = 11.5 \pm 0.8$
$y_0 = 0.0092 \pm 0.0005$
$y_\infty = 0.00147 \pm 0.00011$
$s_0 = 0.0176 \pm 0.0032$
$s_\infty = 0.00358 \pm 0.00018$

Minimum chi-squared fit yields estimated PTW parms. and rms errors, as well as correlation coefficients, which are crucially important!

Correlation coefficients

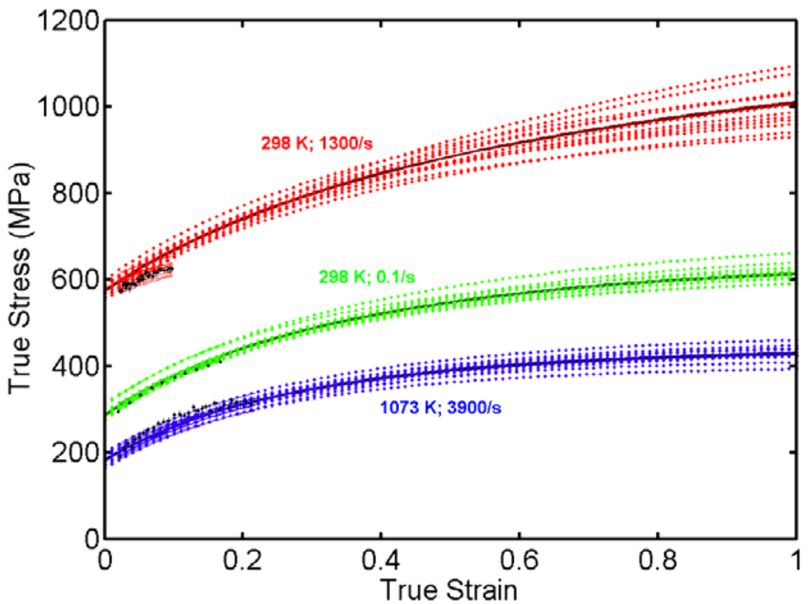
	θ	κ	$-\ln(\gamma)$	y_0	y_∞	s_0	s_∞
θ	1	-0.180	-0.108	-0.113	-0.283	-0.817	0.211
κ	-0.180	1	0.716	0.596	0.644	0.292	0.580
$-\ln(\gamma)$	-0.108	0.716	1	0.046	0.111	0.105	0.171
y_0	-0.113	0.596	0.046	1	0.502	0.282	0.477
y_∞	-0.283	0.644	0.111	0.502	1	0.350	0.640
s_0	-0.817	0.292	0.105	0.282	0.350	1	-0.278
s_∞	0.211	0.580	0.171	0.477	0.640	-0.278	1

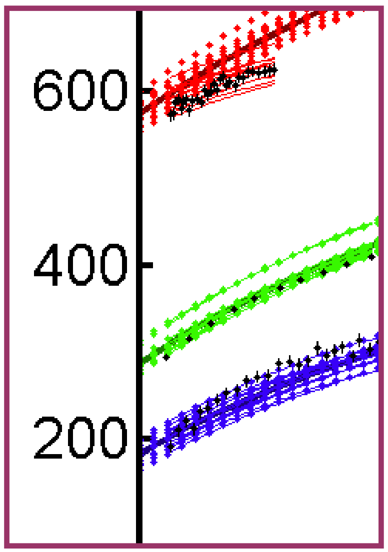
Fixed parms:

$p = 4$
$y_1 = 0.012$
$y_2 = 0.4$
$\beta = 0.23$
$\alpha_p = 0.48$
$G_0 = 722$ MPa
$T_{melt} = 3290$ ºK
$\rho = 16.6$ g/cm^2

Monte Carlo sampling of PTW uncertainty

- Use Monte Carlo technique to draw random samples from complete uncertainty distribution for PTW parameters
- Display stress-strain curve for each parameter set (at three specimen conditions)
- Conclude that fit faithfully represents data and their errors
- This procedure confirms the analysis and model (model checking)



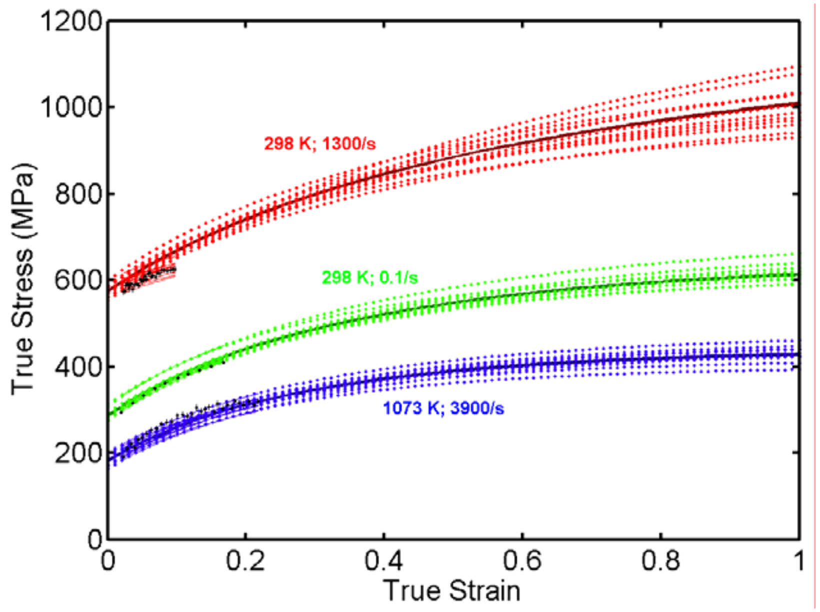


Blow up of data region

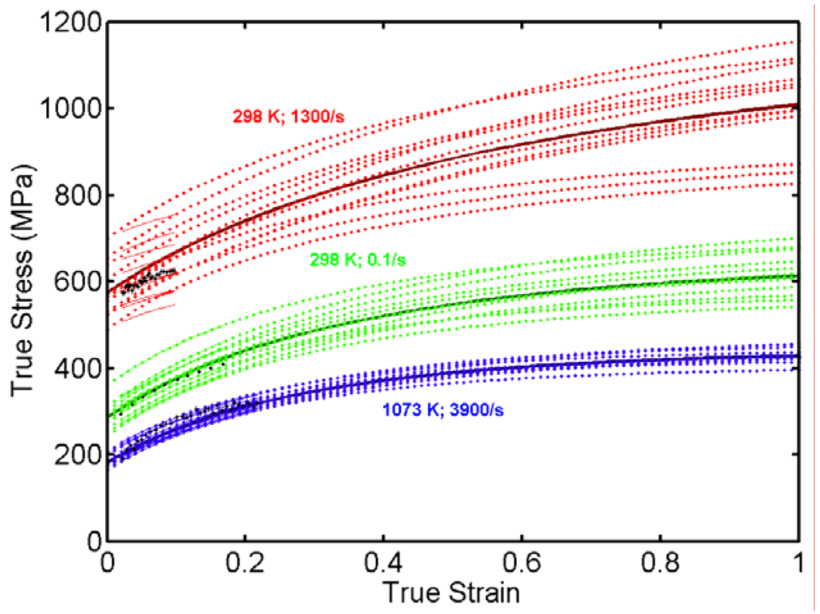
Importance of including correlations

- Monte Carlo draws from uncertainty distribution, done **correctly** with full covariance matrix (left) and **incorrectly** by neglecting off-diagonal terms in covariance matrix (right)

MC with correlations



MC without correlations



Future work: Taylor impact experiment

- Next step in plan to validate PTW model is to proceed to next level of hierarchy of experiments
- Analyze data from Taylor impact experiments
  - need to use simulation code
  - use posterior distribution from foregoing analysis as prior
  - determine posterior distribution for Taylor data
  - check consistency with Taylor data
  - check consistency with prior
  - resolve discrepancies or cope with model deficiencies
- Then proceed to analysis of more complex experiments, which extend the operating range, e.g., flyer -impact experiments

Acknowledgments

Many people have contributed:

- Material scientists: Shuh-Rong Chen, Rusty Gray, Paul Maudlin, Frank Addessio, Tom Mason, Jim Hammerberg, Dave Tonks, George Rinker, Tom Dey
- Physicists: Patrick Talou, Toshihiko Kawano, Gerry Hale, Ralph Nelson, John Hopson
- Engineers: Francois Hemez, Ed Rodriguez, Tom Duffy
- Statisticians: Dave Higdon, Mike McKay, Kathy Campbell, Rick Picard

and others whom I may have forgotten to mention

Bibliography

- "Introduction to PTW," K. M. Hanson, *LA-UR-04-0305* (2004)
- "Inference about the plastic behavior of materials from experimental data," K. M. Hanson, *Proc. Sensitivity Analysis of Model Output Conf.* (2004)
- "A framework for assessing confidence in simulation codes," K. M. Hanson and F. M. Hemez, *Experimental Techniques* **25**, pp. 50-55 (2001); application of uncertainty quantification to simulation codes with Taylor test as example
- "A framework for assessing uncertainties in simulation predictions," K. M. Hanson, *Physica D* **133**, pp. 179-188 (2000); an integrated approach to determining uncertainties in physics modules and their effect on predictions
- "Inversion based on complex simulations," K. M. Hanson, *Maximum Entropy and Bayesian Methods*, pp. 121-135 (Kluwer Academic, 1998); describes adjoint differentiation and its usefulness in simulation physics

These and related papers available at http://www.lanl.gov/home/kmh/