Inference about the plastic behavior of materials from experimental data

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Overview

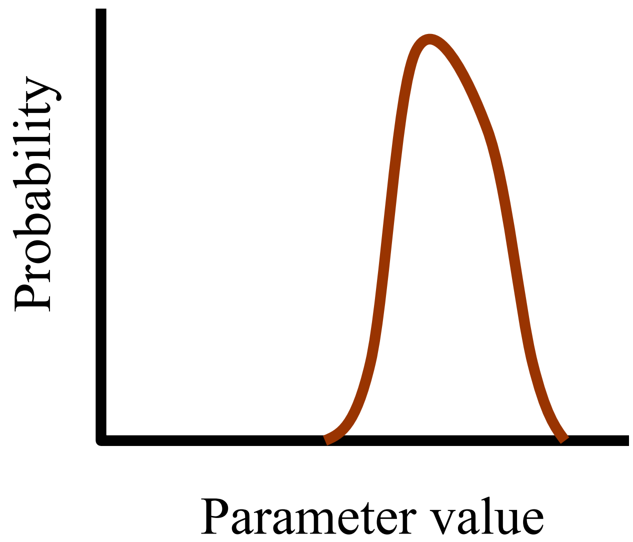
- Understanding physics simulations codes
  - ▸ employ hierarchy of experiments, from basic to fully integrated
  - ▸ role of Bayesian analysis - improve knowledge of models with each new experiment
- Analysis of experimental data to infer parameters of Preston-Tonks-Wallace plasticity model for tantalum
  - ▸ characterize uncertainties in measurement data
  - ▸ estimate PTW parameters and their uncertainties
  - ▸ demonstrate importance of including correlations

Bayesian analysis in context of physics simulations

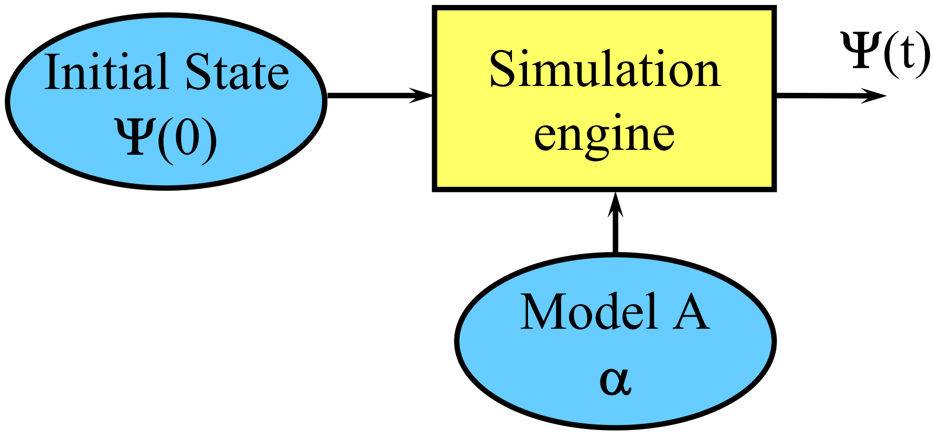
- Goal - describe uncertainties in simulations
  - physics submodels
  - experimental (set up and boundary) conditions
  - calculations (grid size, …)
- Use best knowledge of physics processes
  - rely on expertise of physics modelers and experimental data
- Bayesian foundation
  - focus is as much on uncertainties in parameters as on their best value
  - use of prior knowledge, e.g., previous experiments and expert judgement
  - 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

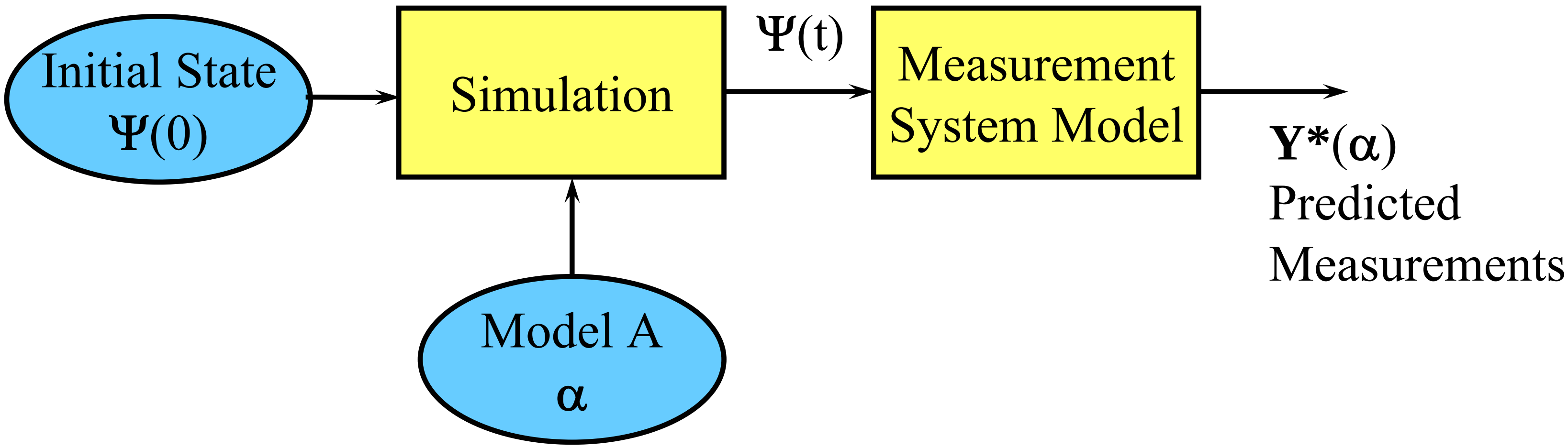


Schematic view of simulation code



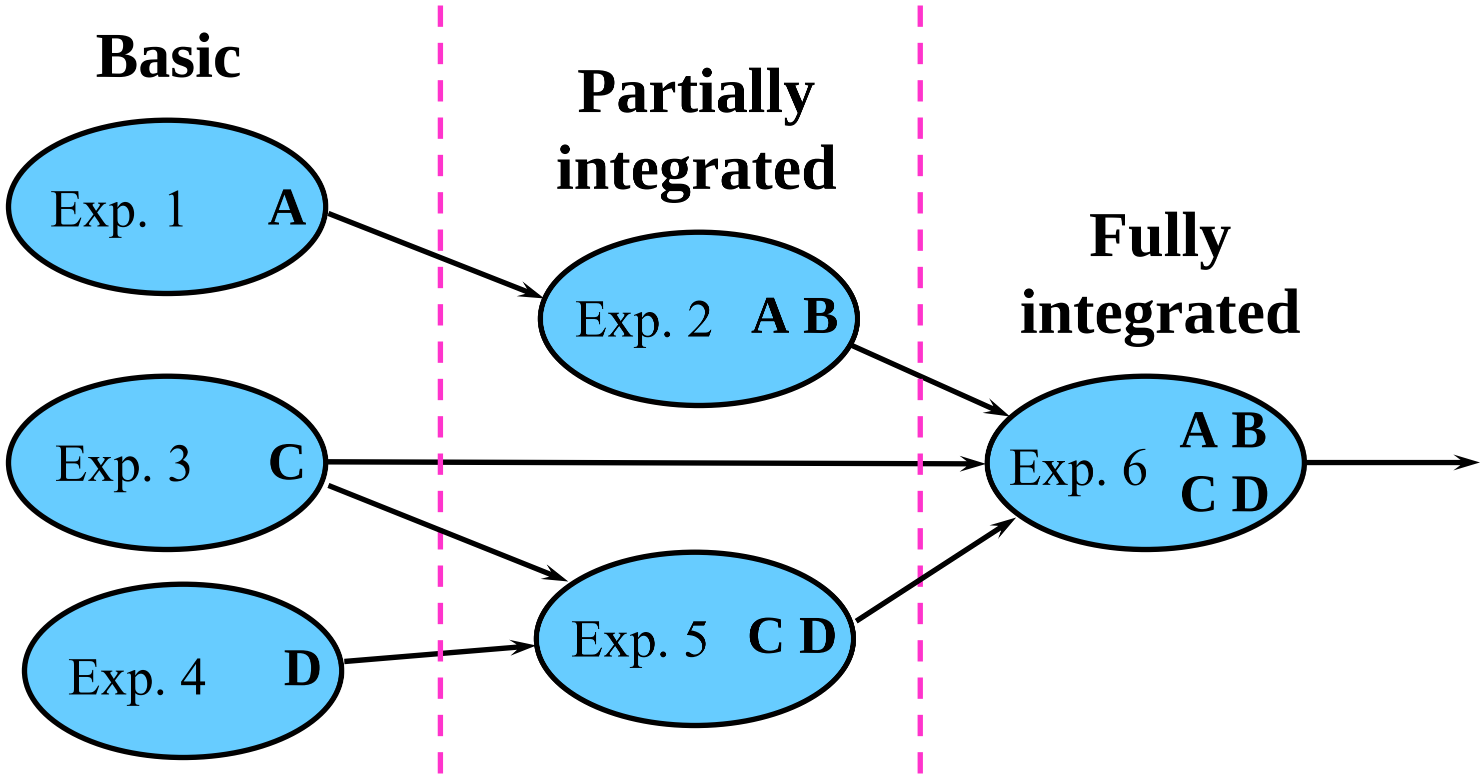
- Simulation code predicts state of time-evolving system $\Psi(t)$
- Requires as input
  - $\Psi(0)$ = initial state of system
  - description of physics behavior of each system component;
    e.g., physics model A with parameter vector α (e.g., constitutive relations)
- Simulation engine solves the dynamical equations (PDEs)
- Uncertainty in $\Psi(t)$ derive from uncertainties in $\Psi(0)$, A, α, and calculational errors

Simulation code predicts measurements



- Simulation code predicts state of time-evolving system
  $\Psi(t)$ = time-dependent state of system
- Model of measurement system yields predicted measurements
- Measurements provide insight about simulation models
- Comparison of experimental to predicted measurements forms basis for inference about simulation code and submodels

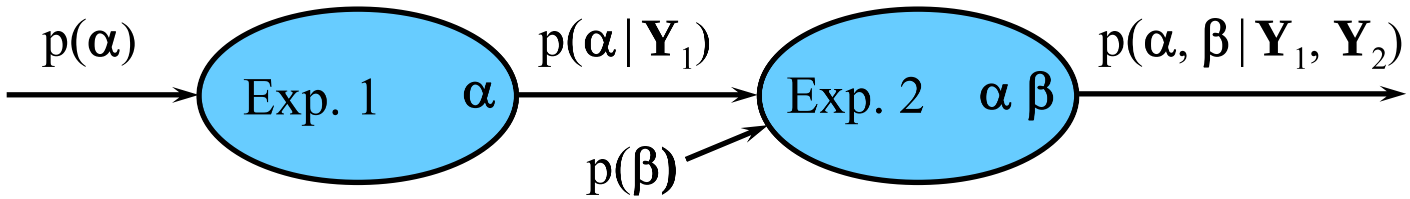
Analysis of hierarchy of experiments



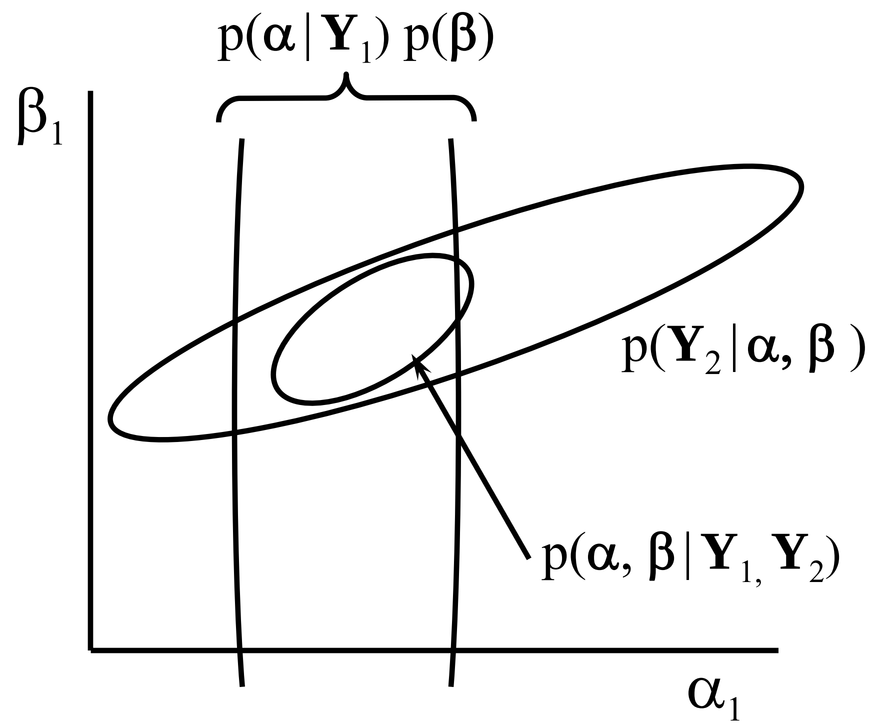
- Information flow in analysis of series of experiments
- Bayesian calibration –
  - analysis of each experiment updates model parameters (represented as A, B, C, etc.) and their uncertainties, consistent with previous analyses
  - information about models accumulates

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
- Outcome is joint pdf in α and β, $p(\alpha, \beta | \mathbf{Y}_{1,} \mathbf{Y}_2)$ (correlations important!)

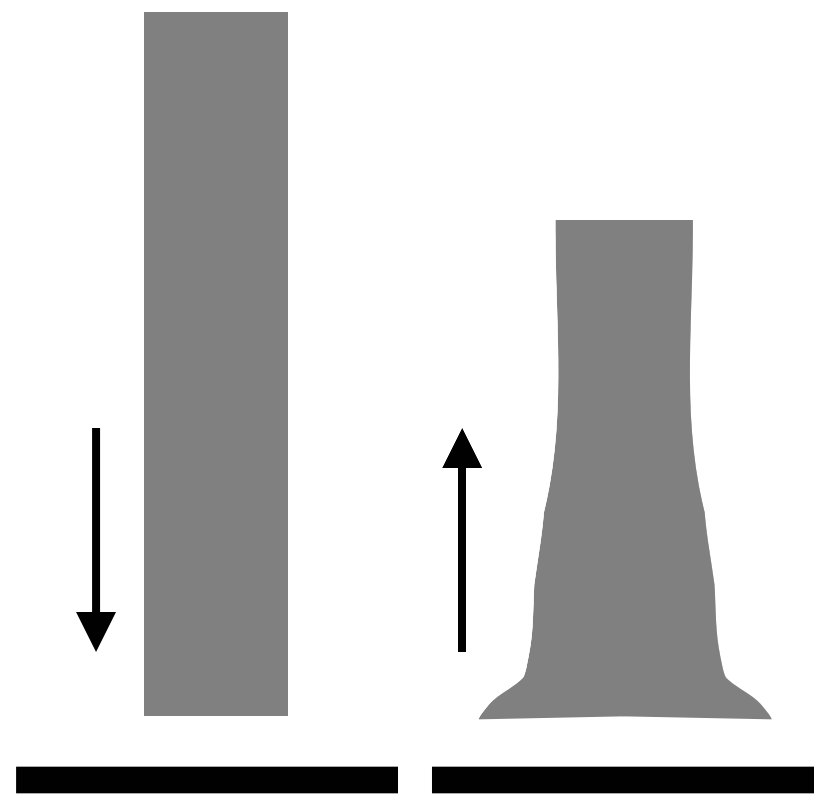


Uncertainty quantification for simulation codes

- 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

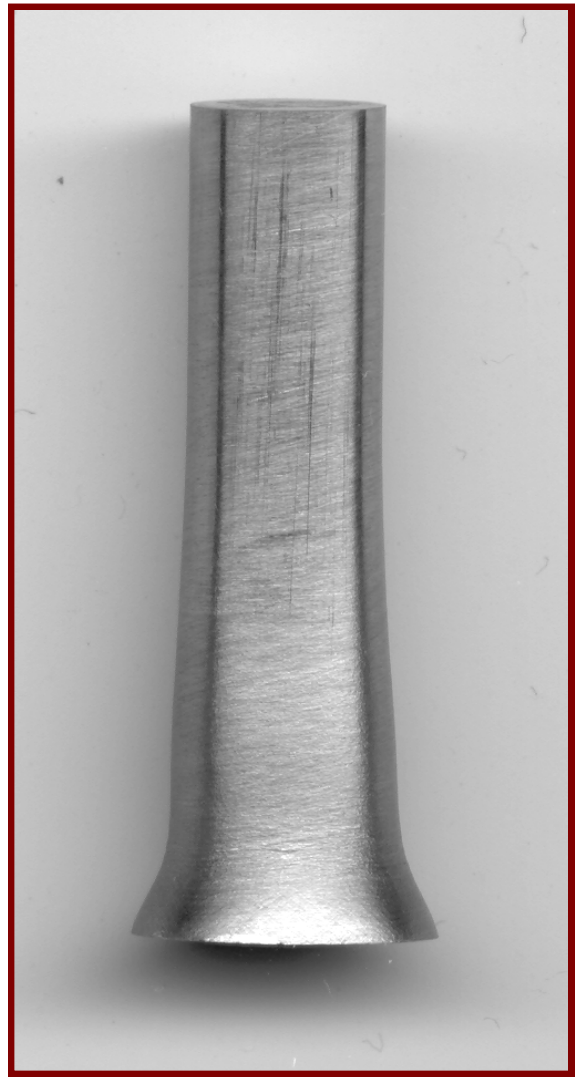
Taylor impact test

- Propel cylinder into rigid plate
- Measure profile of deformed cylinder
- Deformation depends on
  - cylinder dimensions
  - impact velocity
  - plastic flow behavior of material at high strain rate
- Useful for
  - validating simulation code (including material model)
  - improving knowledge of parameters in material-behavior model



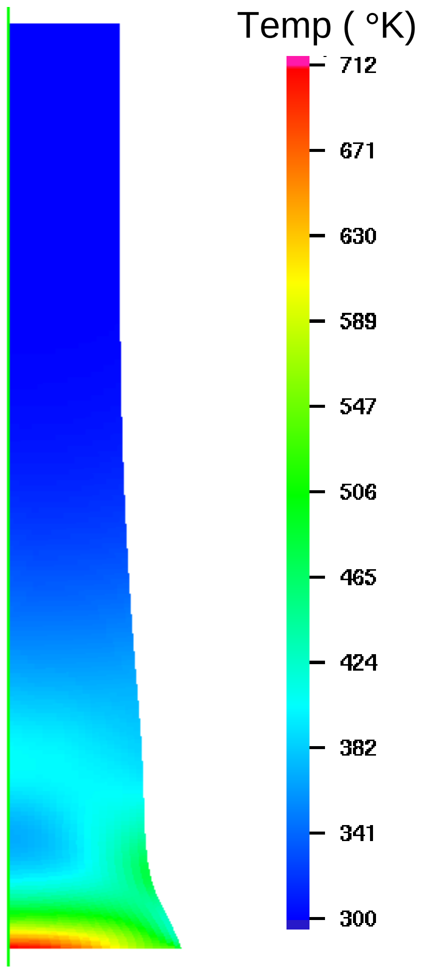
Taylor impact test experiment

- Taylor impact test specimen
  - high-strength steel, HSLA 100
  - room temperature, 298 °K
  - impact velocity = 245.7 m/s
  - dimensions, final/initial
    length 31.84 mm / 38 mm
    diameter 12.00 mm / 7.59 mm
  - experiment performed by MST-8



Taylor test simulations

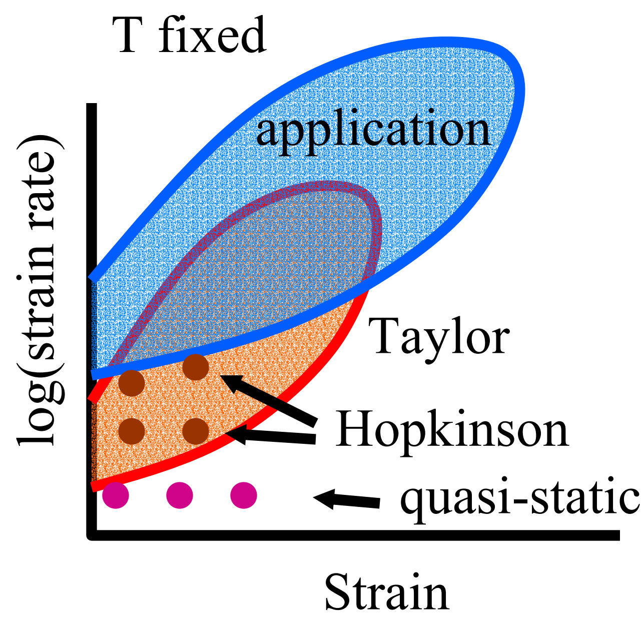
- Simulation of Taylor impact test
  - cylinder: high-strength steel, HSLA100,
    15-mm dia, 38-mm long,
    room temperature
  - impact velocity = 247 m/s
  - CASH - Lagrangian code (X-7)
  - Zerilli-Armstrong model for rate-dependent strength and plasticity
  - ignore anisotropy, fracture effects
- Effective total strain exceeds 100%
- Temperature rises more than 400 °C



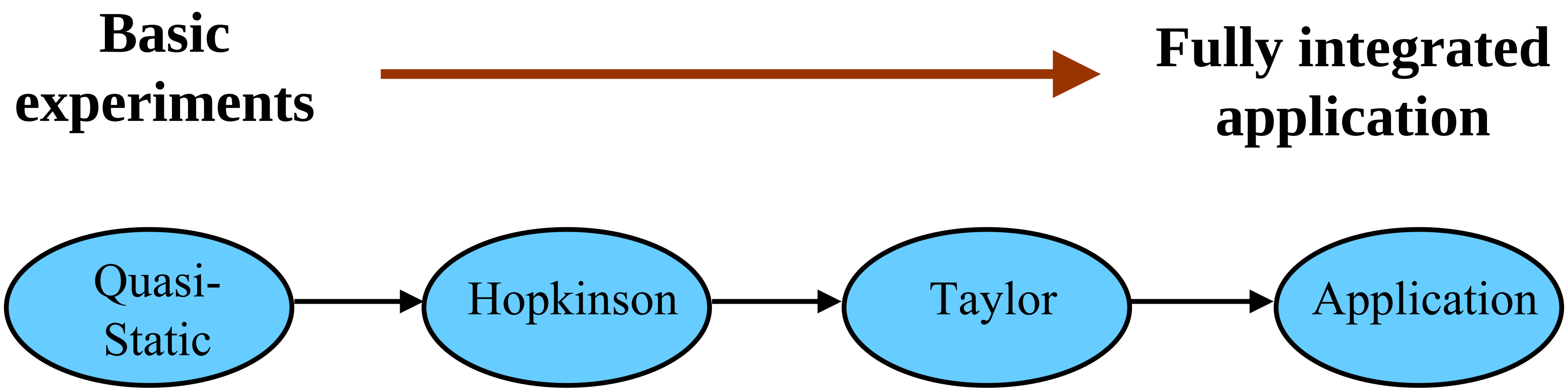
HSLA 100
247 m/s, 298°K

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



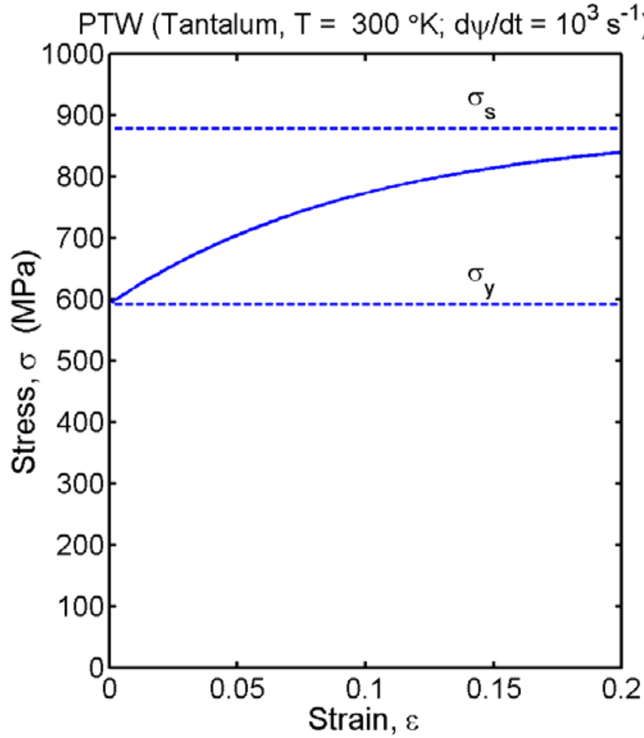
Analysis of hierarchy of experiments



- Series of experiments to determine plastic behavior of a metal
- Information flow shown for analysis sequence
- Bayesian calibration –
  - analysis of each experiment updates model parameters and their uncertainties, consistent with previous experiments
  - information about models accumulates throughout process

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
- 7 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

Likelihood analysis

- 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 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

$$\operatorname{cov}(\boldsymbol{a}) \equiv \left\langle (\boldsymbol{a} - \hat{\boldsymbol{a}})(\boldsymbol{a} - \hat{\boldsymbol{a}})^{\mathrm{T}} \right\rangle \equiv \boldsymbol{C} = 2\boldsymbol{K}^{-1}$$

Characterization of chi-squared

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

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

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

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

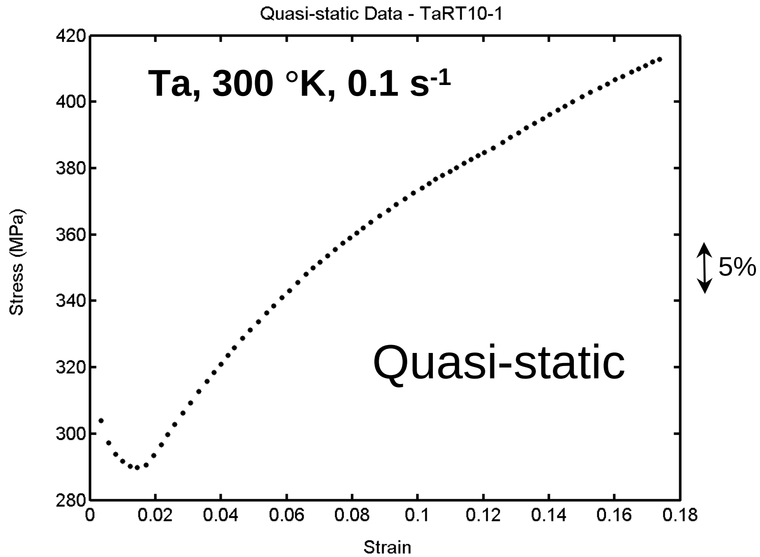
  - For a Gaussian prior on a parameter $\boldsymbol{a}$

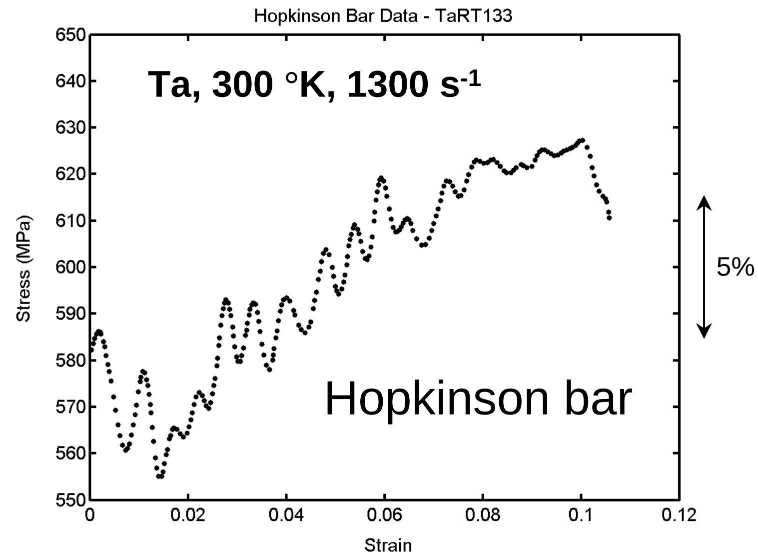
$$-\log p(\boldsymbol{a} \,|\, \boldsymbol{d}, I) = \varphi(\boldsymbol{a}) = \tfrac{1}{2}\chi^2 + \frac{(\boldsymbol{a} - \tilde{\boldsymbol{a}})^2}{2\sigma_{\boldsymbol{a}}^2}$$

  - where $\tilde{\boldsymbol{a}}$ is the default value for $\boldsymbol{a}$ and σ_a^2 is assumed variance

Material-characterization experiments

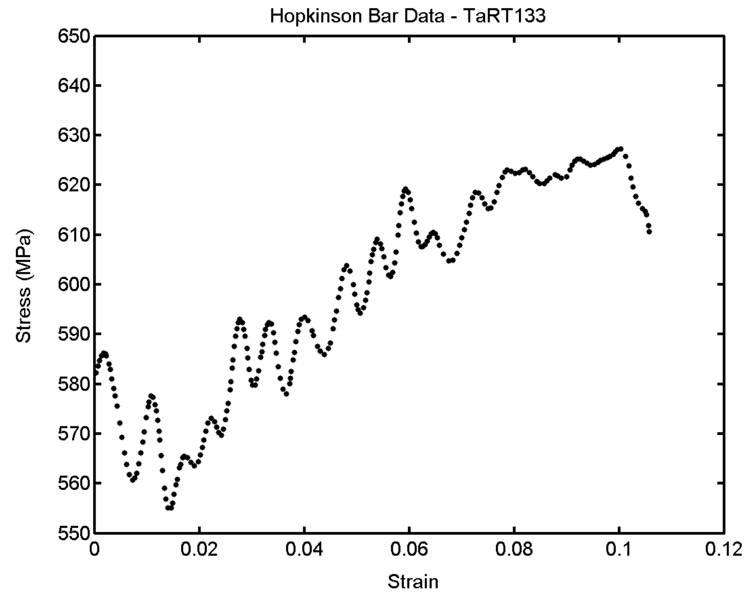
- Data from **quasi-static** compression experiments tend to be of high quality
  - rms ‘noise’ ≈ 0.1%
  - thin data set to limit undue influence in likelihood
- Data from **Hopkinson-bar** experiments tend to be of medium quality
  - rms ‘noise’ ≈ 1%
- Observe artifacts in the data
  - arise from reflected shocks
  - need to account for these

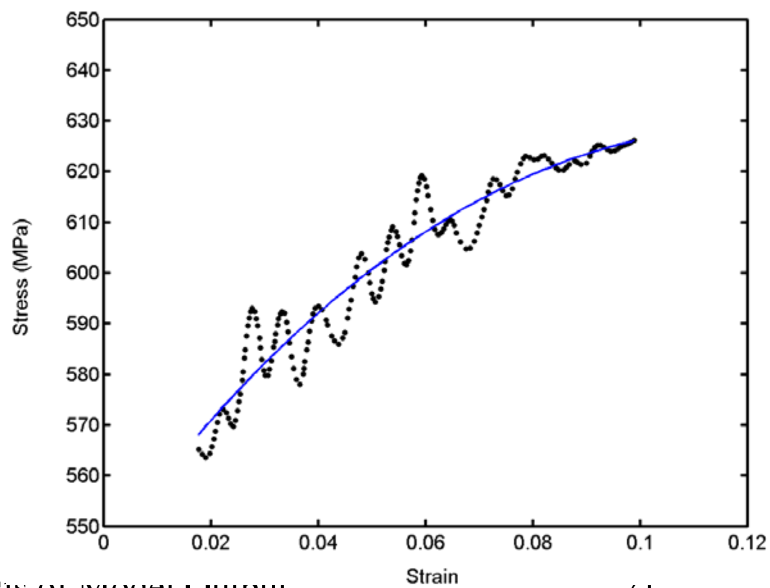




Hopkinson bar measurements

- Hopkinson-bar data are degraded by oscillations, caused by reflected shocks and bar oscillations
- Treat these fluctuations as a random process with a high degree of correlation from point to point
- Subtract low-order polynomial from data to get fluctuations from smooth dependence





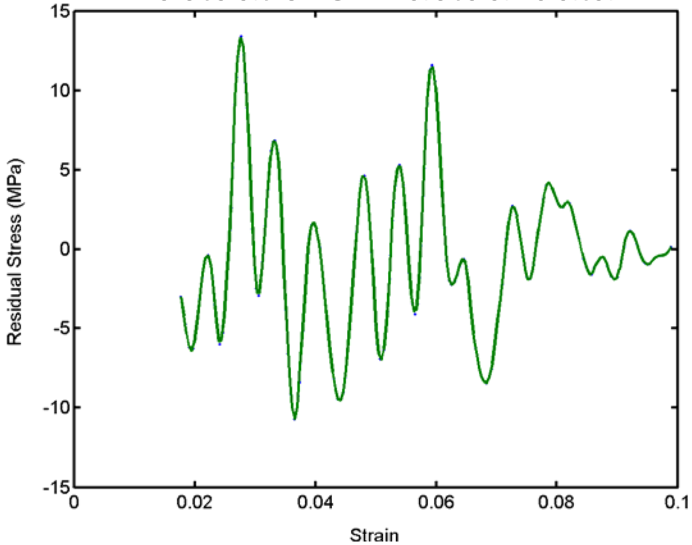
Hopkinson bar measurements

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

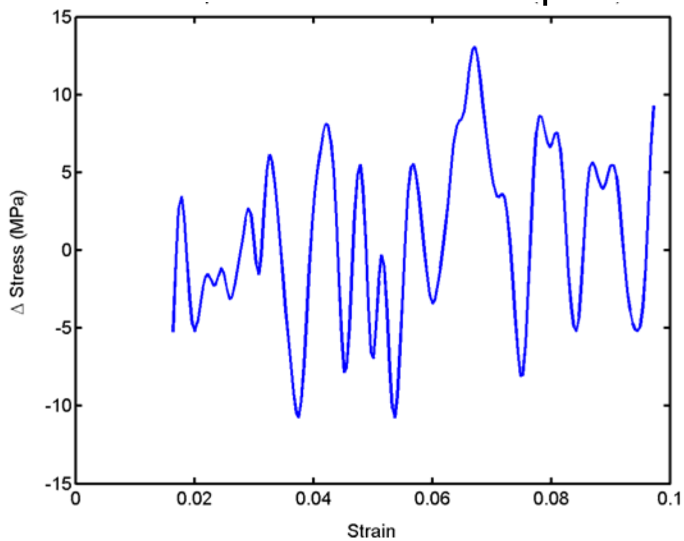
$$\mathrm{cov}(\boldsymbol{y}, \boldsymbol{y}') \propto \exp\left\{-\left[\frac{\boldsymbol{x}-\boldsymbol{x}'}{\lambda}\right]^{p}\right\}$$

  - 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

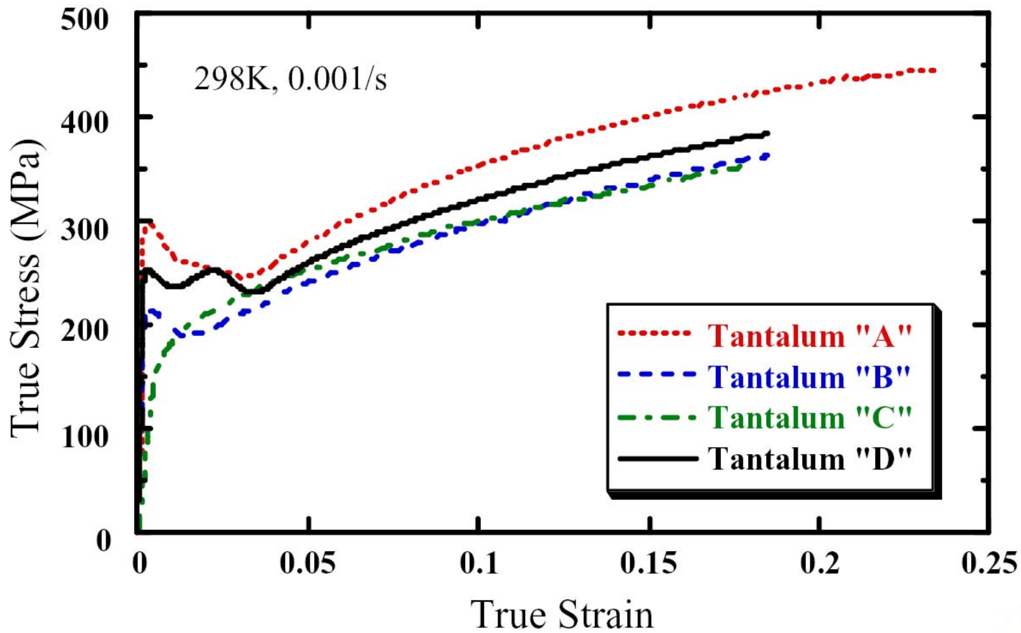


Realization from random process



Repeated experiments

- Repeated experiments
  - stability of apparatus
  - 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 specimen
- Represents an uncertainty in initial state



†data supplied by S-R Chen, MST-8

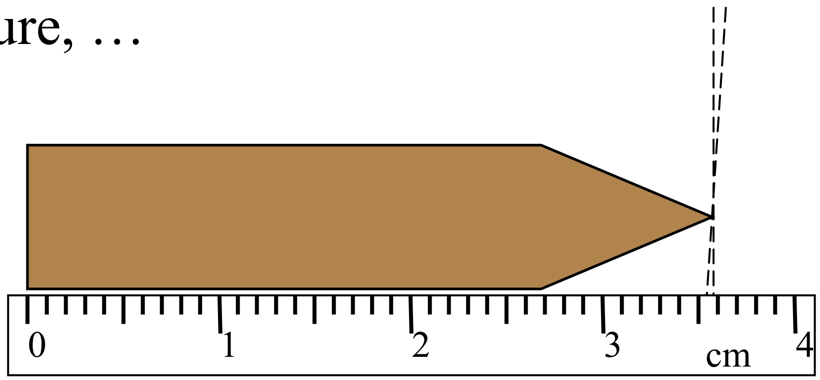
Types of uncertainties in measurements

- 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?

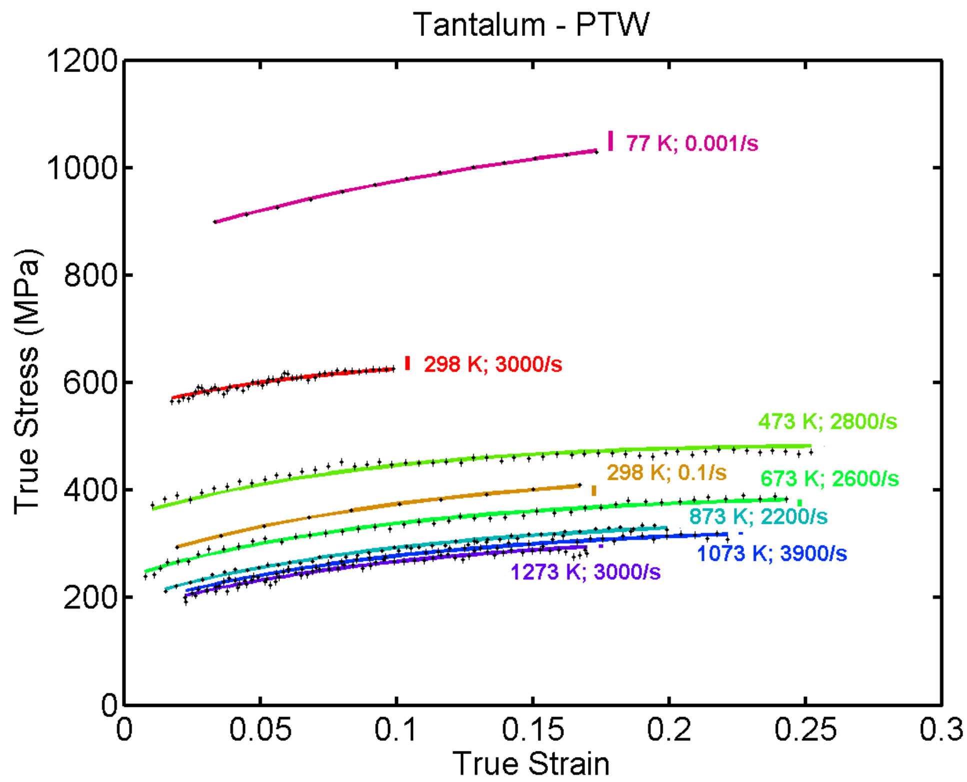
    depends on whether measurements always made by same person in the same way or made by different people



Fit PTW model to measurements

Analysis of quasi-static and Hopkinson bar measurements†

- PTW model for rate- and temperature-dependent plasticity
- Parameters estimated from Hopkinson bar measurements and quasi-static tests
- Full uncertainty analysis – **include 3% systematic uncertainty** in offset of each data set (8 + 7 parms)
- ~ 6 iter., ~ 100 func. evals.



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:

$y_0 = 0.0123 \pm 0.0006$

$y_\infty = 0.00164 \pm 0.00004$

$s_0 = 0.0164 \pm 0.0007$

$s_\infty = 0.00308 \pm 0.00005$

$\kappa = 0.91 \pm 0.08$

$\gamma = (2.4 \pm 2.0)\times 10^{-6}$

$\theta = 0.0145 \pm 0.0002$

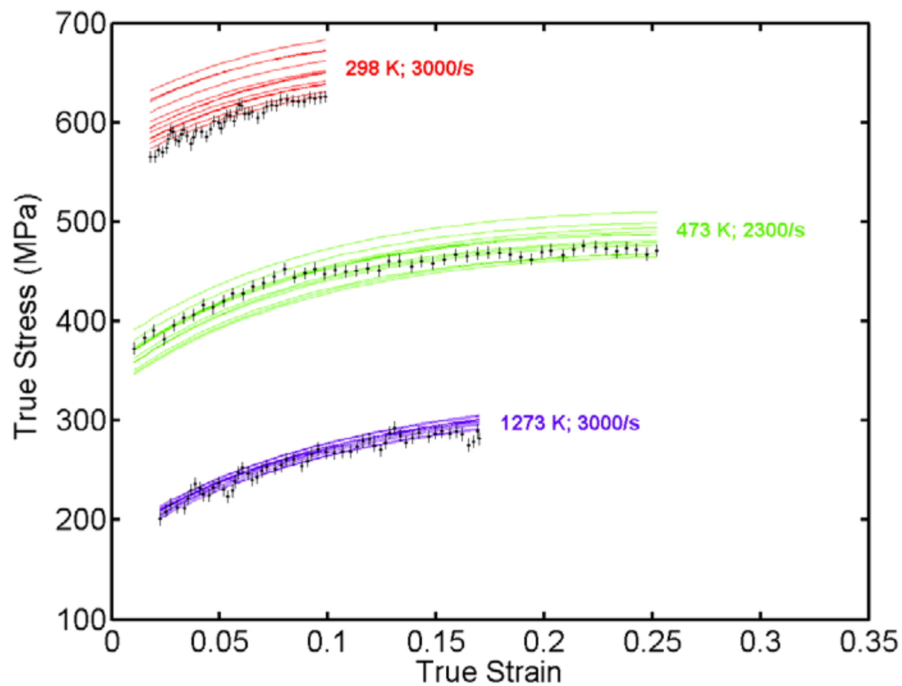
Minimum chi-squared fit yields estimated PTW parms. and rms errors, including correlation coefficients, which are crucially important!

Correlation coefficients

	y_0	y_∞	s_0	s_∞	κ	γ	θ
y_0	1	0.186	0.988	0.400	0.687	-0.464	-0.182
y_∞	0.186	1	0.208	0.913	0.142	0.022	-0.140
s_0	0.988	0.208	1	0.432	0.713	-0.496	-0.299
s_∞	0.400	0.913	0.432	1	0.443	-0.263	-0.257
κ	0.687	0.142	0.713	0.443	1	-0.935	-0.119
γ	-0.464	0.022	-0.496	-0.263	-0.935	1	0.087
θ	-0.182	-0.140	-0.299	-0.257	-0.119	0.087	1

Monte Carlo sampling of PTW uncertainty

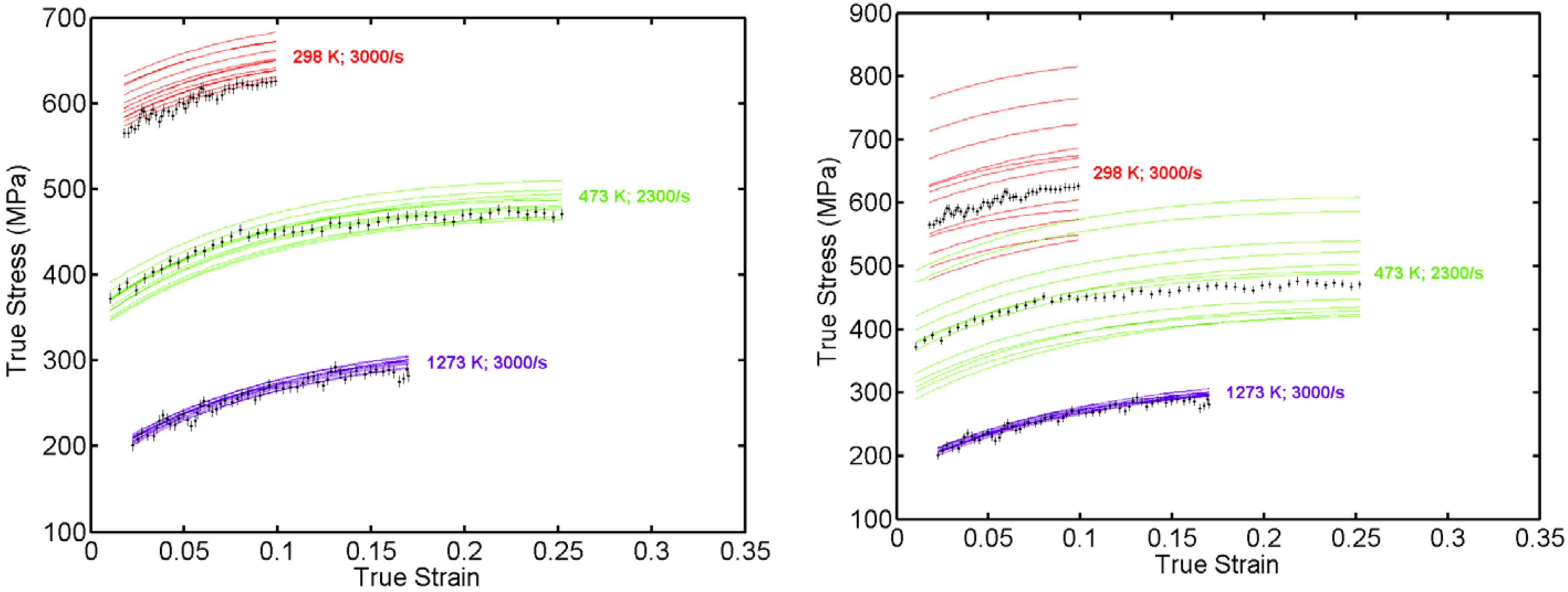
- Use Monte Carlo technique - draw random samples from complete uncertainty distribution for PTW parameters
- Display stress-strain curve for each parameter set (at three temps)
- Conclude that fit faithfully represents data and their errors
- This procedure confirms the analysis and model



Importance of including correlations

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

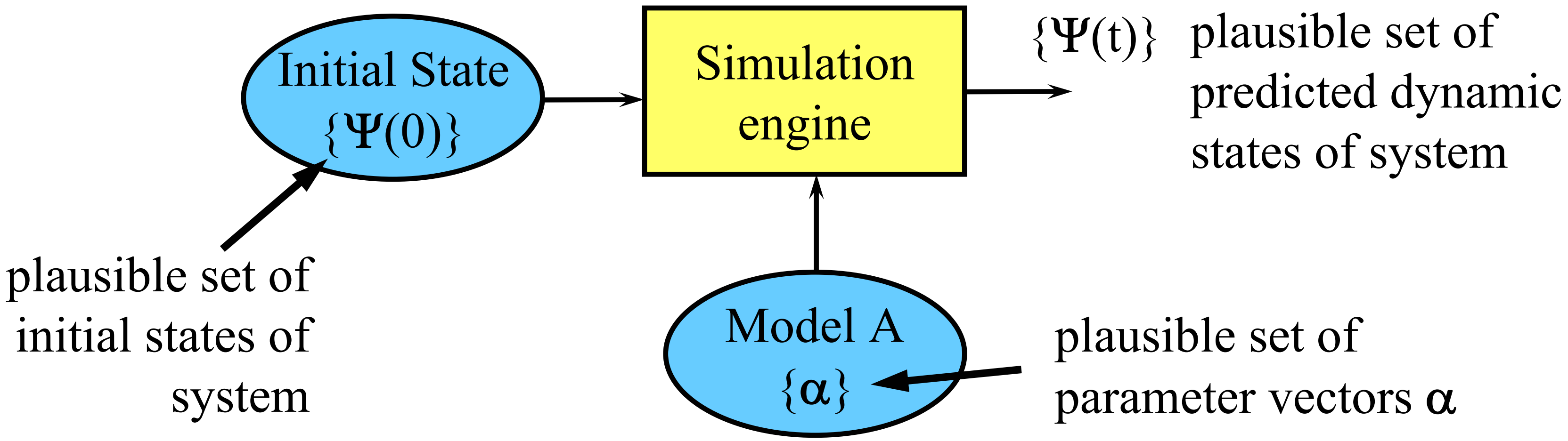
MC with correlations | MC without correlations



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

Plausible simulation predictions (forward)



- Generate plausible predictions for known uncertainties in parameters and initial conditions
- Monte Carlo method
  - run simulation code for each random draw from pdf for α, $p(\alpha\,|\,.)$, and initial state, $p(\Psi(0)\,|\,.)$
  - simulation outputs represent plausible set of predictions, $\{\Psi(t)\}$
  - advanced sampling methods useful to reduce number of calcs needed
    - Latin Hypercube, Centroidal Voronoi Tessellations, etc.

Summary

- Physics simulations codes
  - employ hierarchy of experiments, from basic to fully integrated
  - role of Bayesian analysis - improve knowledge of models with each new experiment
- 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
  - demonstrate importance of including correlations

Bibliography

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- "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
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