Inference of material-model parameters from experimental data

Ken Hanson

CCS-2, Methods for Advanced Scientific Simulations
Los Alamos National Laboratory

This presentation available at
http://www.lanl.gov/home/kmh/

Overview

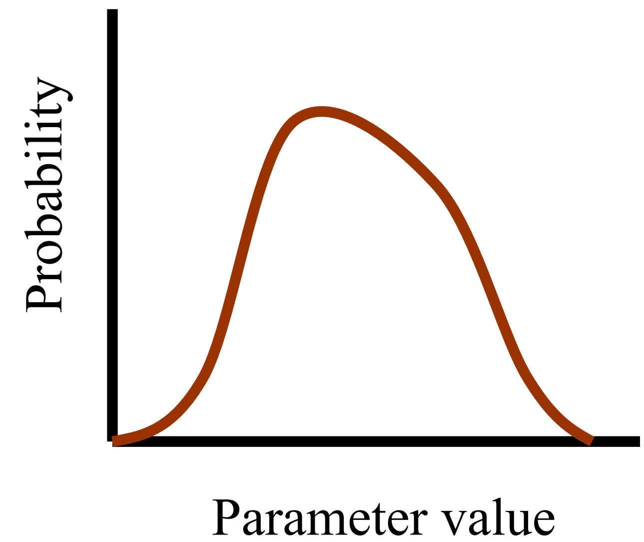
- Physics simulations codes
  - need to be understood on basis of experimental data
  - focus on physics submodels
- Bayesian analysis
  - uncertainty quantification (UQ) is central issue
  - each new experiment used to improve knowledge of models
- Analysis process
  - employ hierarchy of experiments, from basic to fully integrated
  - goal is to learn as much possible from all experiments
- Example of analysis process: material model evolution
  - material characterization experiments and Taylor impact test
  - role of systematic uncertainties
  - coping with inadequate model

Bayesian analysis in context of physics simulations

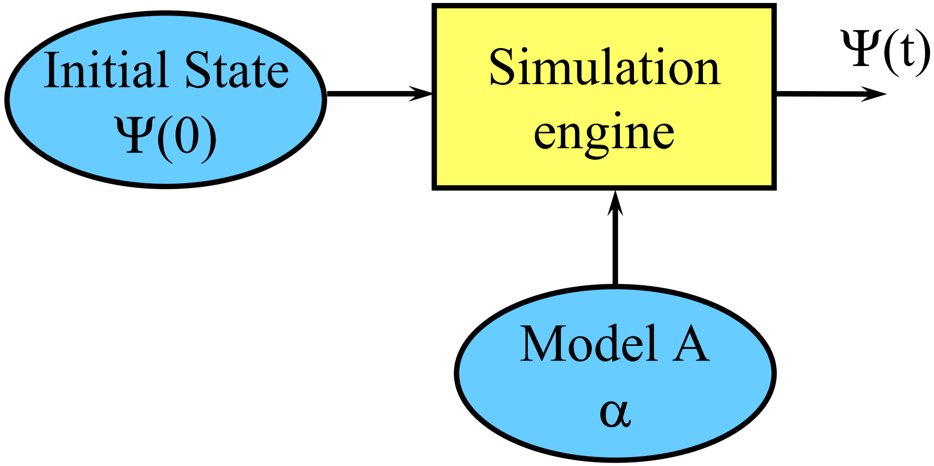
- Goal - describe uncertainties in simulations
  - physics submodels
  - experimental (set up and boundary) conditions
  - calculations (grid size, …)
- Use best knowledge of physics processes
  - rely on expertise of physics modelers and experimental data
- Bayesian foundation
  - focus is as much on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

Bayesian uncertainty analysis

- Uncertainties in parameters are characterized by probability density functions (pdf)
- Probability interpreted as quantitative measure of "degree of belief"
- Rules of classical probability theory apply
- Bayes law provides means to update knowledge about models as summarized in terms of uncertainty

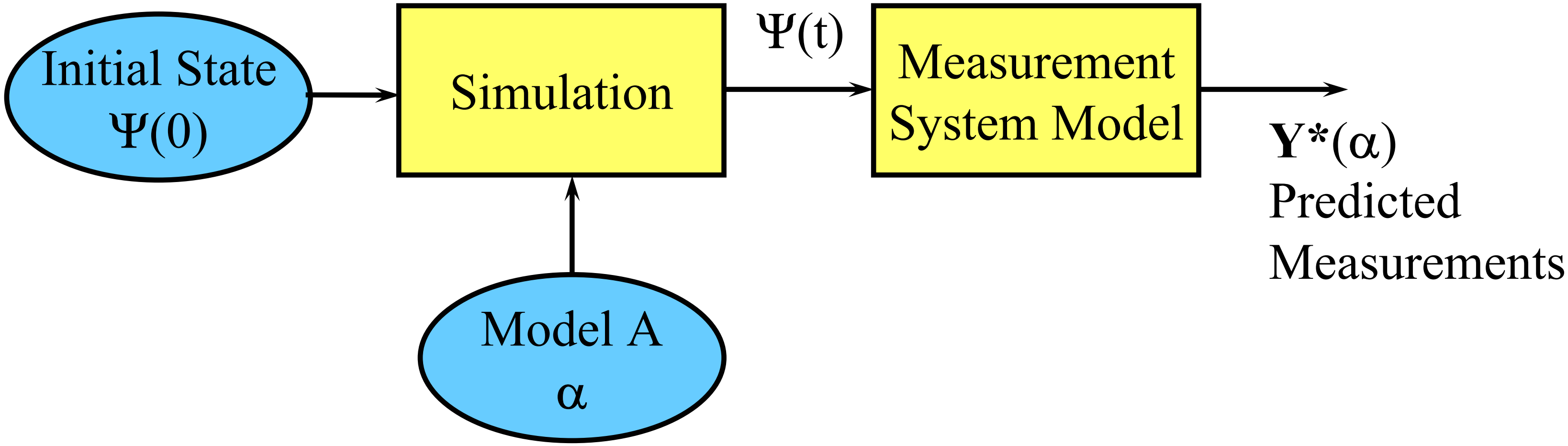


Schematic view of simulation code



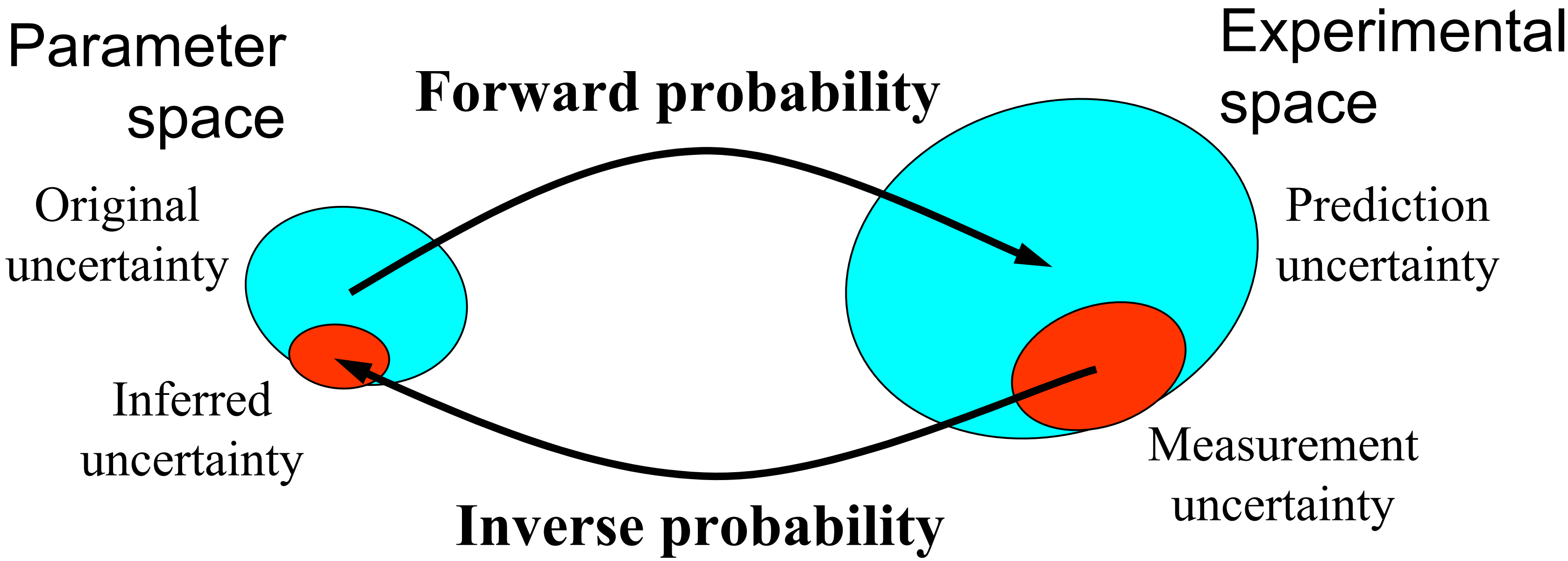
- Simulation code predicts state of time-evolving system
  $\Psi(t)$ = time-dependent state of system
- Requires as input
  - $\Psi(0)$ = initial state of system
  - description of physics behavior of each system component;
    e.g., physics model A with parameter vector α (e.g., constitutive relations)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

Simulation code predicts measurements



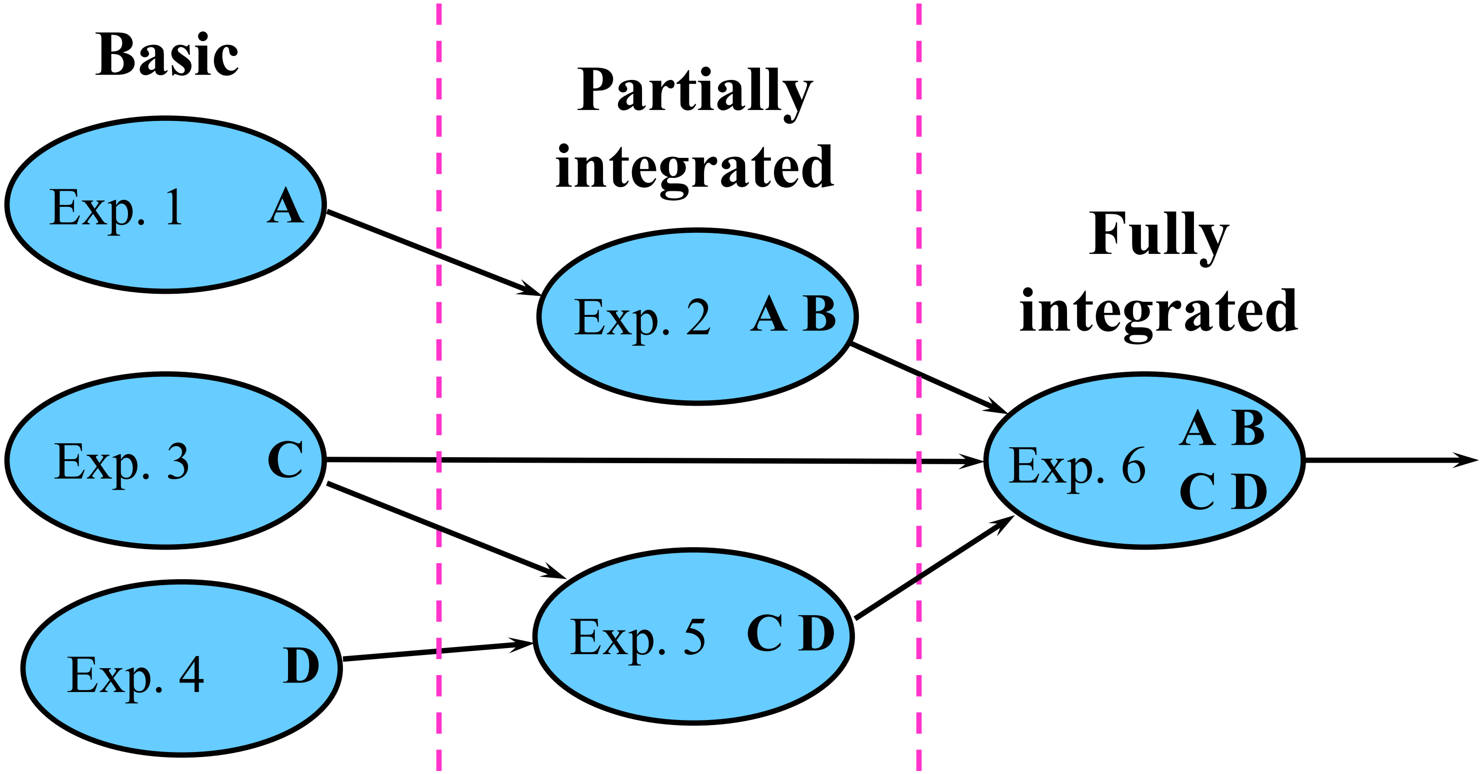
- Simulation code predicts state of time-evolving system
  - $\Psi(t)$ = time-dependent state of system
- Model of measurement system yields predicted measurements

Mapping between parameters and experiments



- Model inference
  - if uncertainties in measurements are smaller than prediction uncertainties that arise from parameter uncertainties, one may be able to use measurements to reduce uncertainties in parameters
  - requires that prediction uncertainties are dominated by uncertainties in parameters and not by those in experimental set up
  - **good experimental technique** important for **Bayesian calibration**

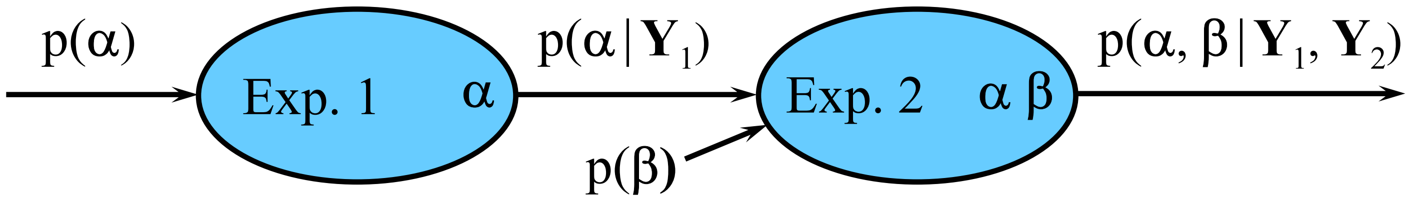
Analysis of hierarchy of experiments



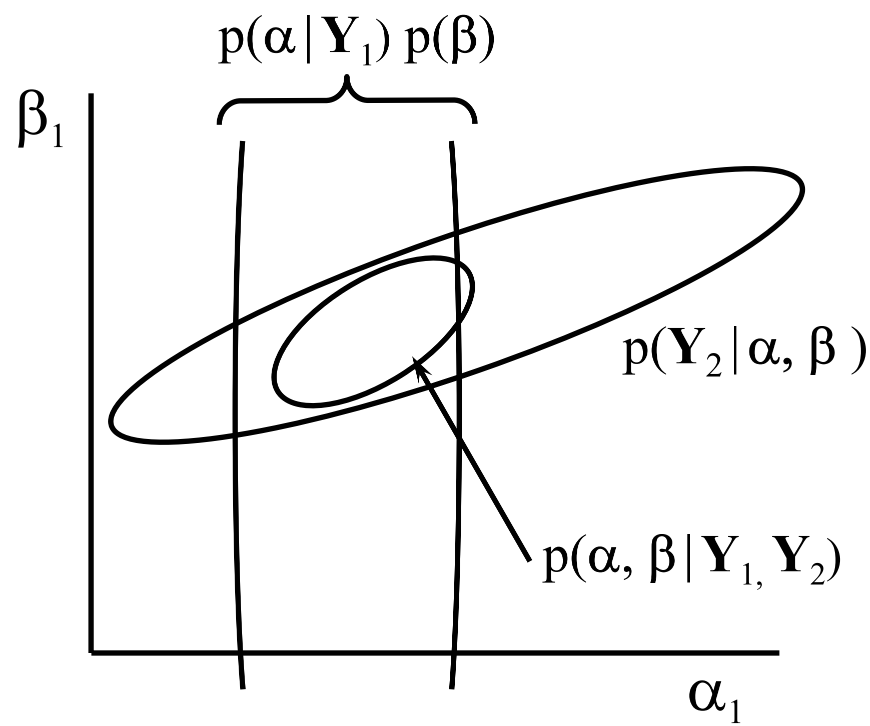
- Information flow in analysis of series of experiments
- Bayesian calibration –
  - analysis of each experiment updates model parameters and their uncertainties, consistent with previous analyses
  - information about models accumulates

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!)



Bayesian calibration for simulation codes

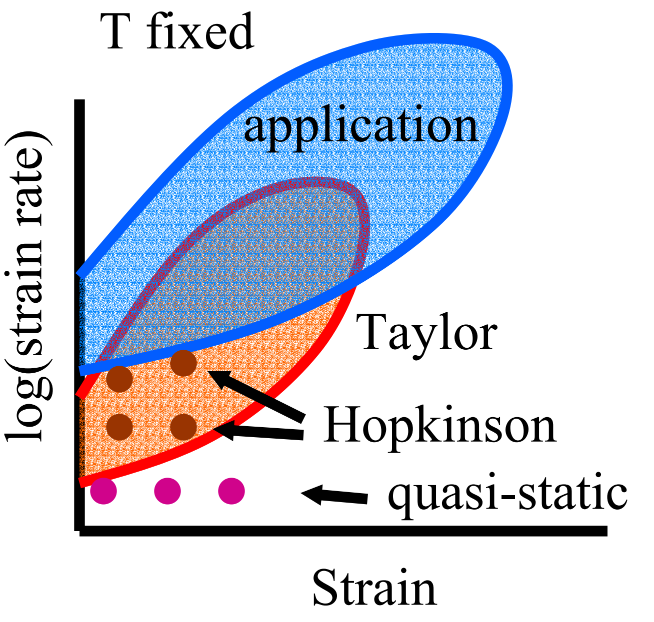
- Goal is to develop an uncertainty model for the simulation code by comparison to experimental measurements
  - determine and quantify sources of uncertainty
  - uncover potential inconsistencies of submodels with expts.
  - possibly introduce additional submodels, as required
- Recursive process
  - 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

Motivating example

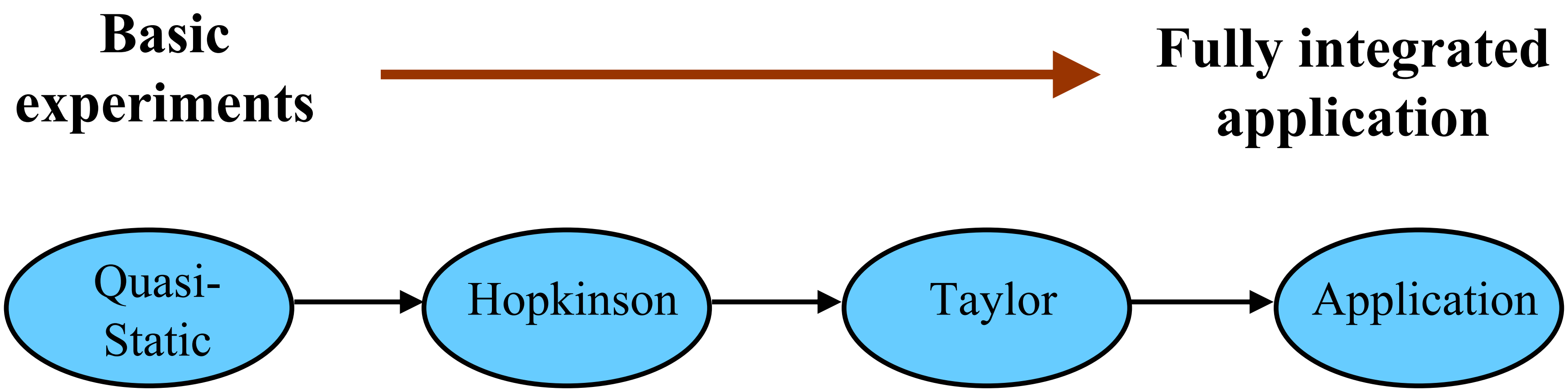
- Problem statement
  - design containment vessel using high-strength steel, HSLA 100
  - predict depth of vessel-wall penetration for specified shrapnel fragments at specified impact velocity
  - estimate uncertainty in this prediction to estimate safety factor
- Approach
  - determine what experiments are needed to characterize stress-strain relationship for plastic flow of metal
  - follow the uncertainty through the analysis of expt. data
  - variables to consider: temperature, strain rate, variability in material composition, processing, behavior

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 expts.
  - mimic application as much as possible
  - **projectile impacting plate**
  - may involve extrapolation of operating range; so introduces addition uncertainty
  - integrated expts. can help reduce model uncertainties



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

Stress-strain relation for plastic deformation

- Zerilli-Armstrong model describes strain rate- and temperature-dependent plasticity in terms of stress σ (or s) as function of plastic strain ε_p

$$\sigma = \alpha_1 + \alpha_5 \varepsilon_p^{\alpha_6} + \alpha_2 \exp\left[\left(-\alpha_3 + \alpha_4 \log \frac{\partial \varepsilon_p}{\partial t}\right) T\right]$$

- Six parameters -
  - 2 parameters (α_5 & α_6) specify dependence of stress on strain
  - 4 remaining parameters specify additive offset as function of temperature and strain rate
- Z-A formula based on dislocation mechanics model
  - may not hold for all materials or all experimental conditions

Likelihood analysis

- When the errors in each measurement are Gaussian distributed and independent, likelihood is related to chi squared:
$$p(\boldsymbol{d}\mid\boldsymbol{a}) \propto \exp(-\tfrac{1}{2}\chi^2) = \exp\left\{-\frac{1}{2}\sum_i \left[\frac{[d_i - y_i(a)]^2}{\sigma_i^2}\right]\right\}$$
- 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
$$\mathrm{cov}(\boldsymbol{a}) \equiv \left\langle(\boldsymbol{a}-\hat{\boldsymbol{a}})(\boldsymbol{a}-\hat{\boldsymbol{a}})^{\mathrm{T}}\right\rangle \equiv \boldsymbol{C} = 2\boldsymbol{K}^{-1}$$

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

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

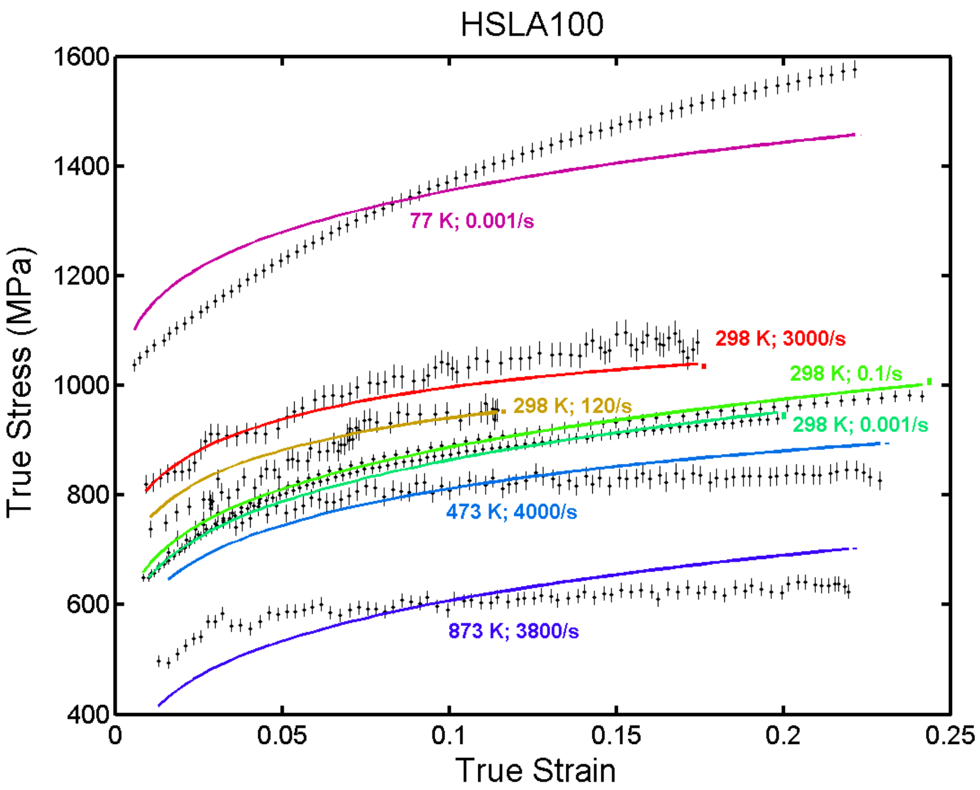
  - For a Gaussian prior on a parameter a

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

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

Fit ZA model to all data

- 7 data sets at various strain rates and temps
- Fit to all data above elastic region or after first bump in Hopkinson-bar data
- Model does not reproduce stress-strain curves at high and low temperatures
- Fit is far from expt. measurements for target conditions of room temp., high strain rate
- Uncertainties are highly correlated

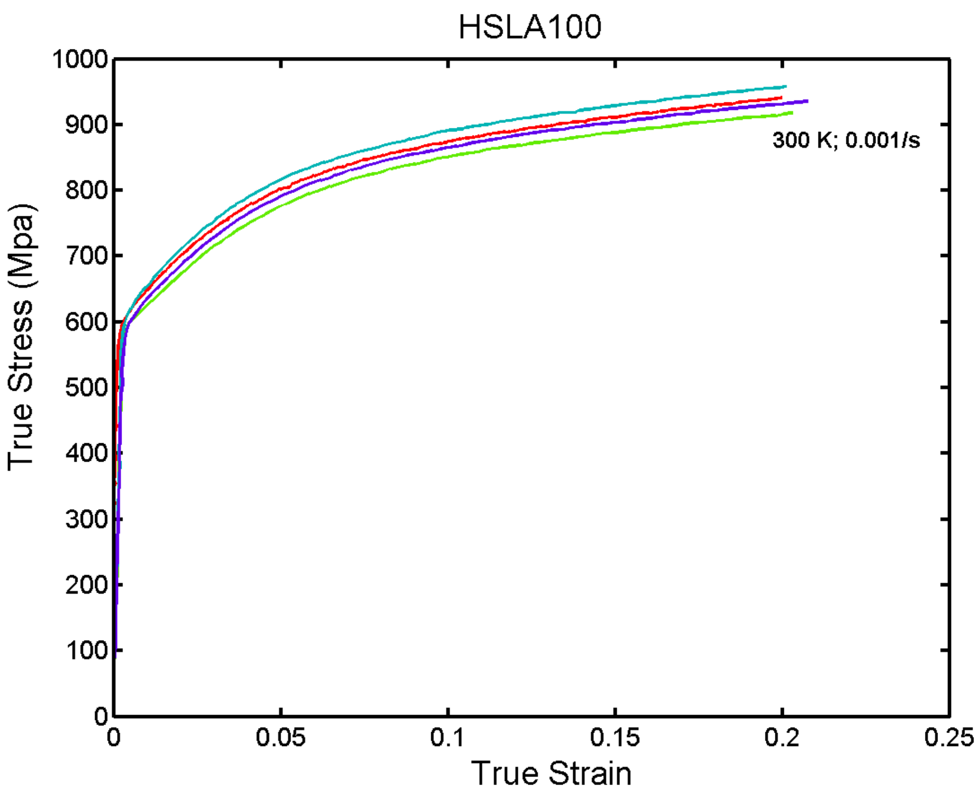


ZA curves include adiabatic heating effect for high strain rates

†data supplied by S-R Chen, MST-8

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 random positions in thick plate
- Sample-to-sample rms deviation is around 20 MPa at strain of 0.1
- Treat this variability as **systematic uncertainty**



†data supplied by S-R Chen, MST-8

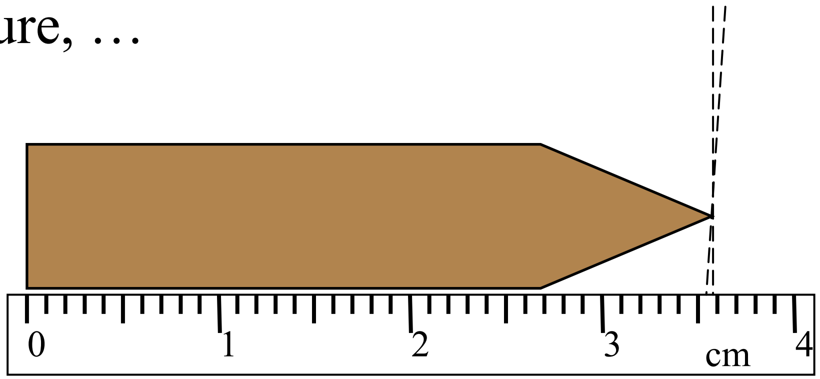
Types of uncertainties in measurements

- 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 each measurement 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



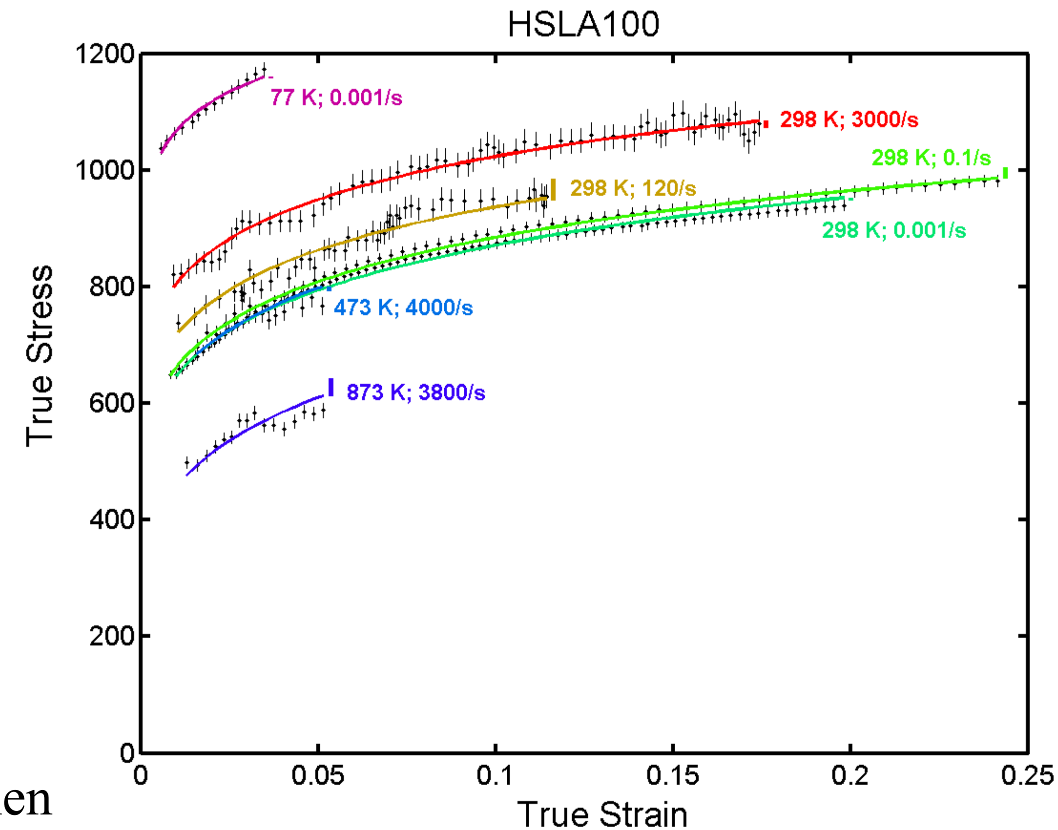
Fit ZA model to selected measurements

Analysis of quasi-static and Hopkinson bar measurements†

- Zerilli-Armstrong model for rate- and temperature-dependent plasticity

$$\sigma = \alpha_1 + \alpha_5 \varepsilon_p^{\alpha_6} + \alpha_2 \exp\left[\left(-\alpha_3 + \alpha_4 \log \frac{\partial \varepsilon_p}{\partial t}\right) T\right]$$

- Parameters determined from Hopkinson bar measurements and quasi-static tests
- Full uncertainty analysis – **including systematic effects** of offset of each data set (6 + 7 parms)



†data supplied by Shuh-Rong Chen

ZA parameters and their uncertainties

Parameters +/- rms error:

$\alpha 1 = 103 \pm 33$

$\alpha 2 = 954 \pm 63$

$\alpha 3 = 0.00408 \pm 0.00059$

$\alpha 4 = 0.000117 \pm 0.000029$

$\alpha 5 = 996 \pm 22$

$\alpha 6 = 0.247 \pm 0.021$

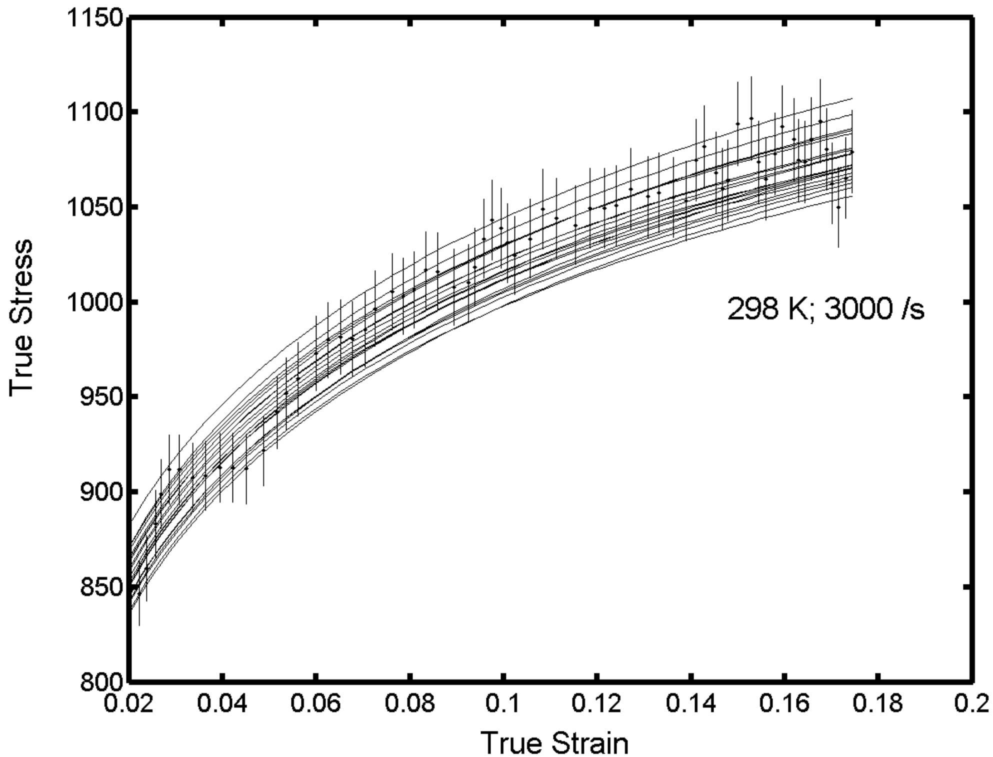
RMS errors, including correlation coefficients, which are crucially important!

Correlation coefficients

	α1	α2	α3	α4	α5	α6
α1	1	-0.083	0.372	0.207	-0.488	0.267
α2	-0.083	1	0.344	0.311	0.082	0.130
α3	0.372	0.344	1	0.802	0.453	-0.621
α4	0.207	0.311	0.802	1	0.271	-0.466
α5	-0.488	0.082	0.453	0.271	1	-0.860
α6	0.267	0.130	-0.621	-0.466	-0.860	1

Monte Carlo sampling of ZA uncertainty

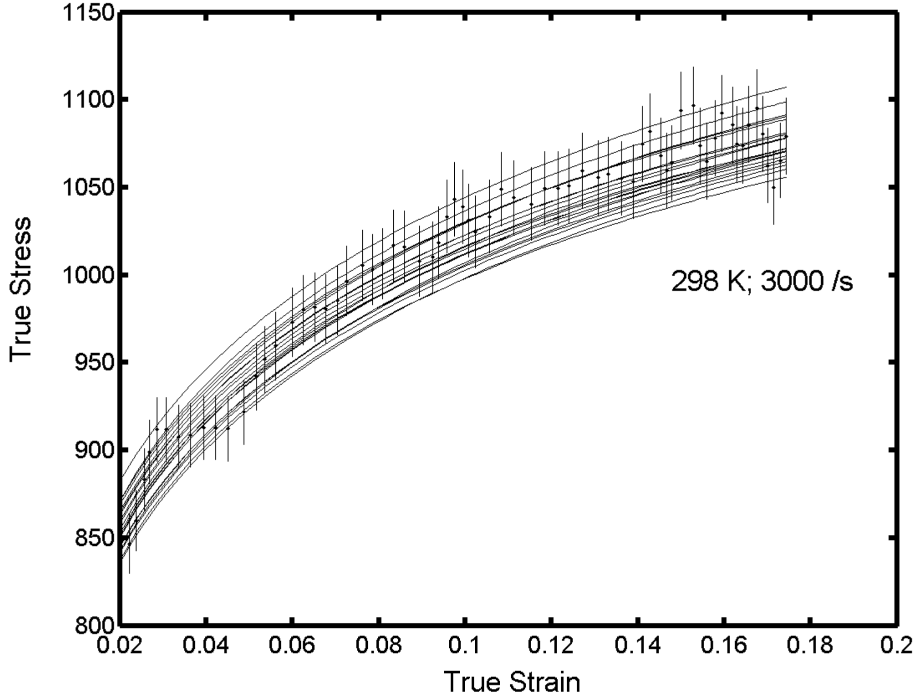
- Use Monte Carlo technique to draw random samples from uncertainty distribution for Zerilli-Armstrong parameters
- Display stress-strain curve for each parameter set
- Conclude fit faithfully represents data and their errors at 298°K



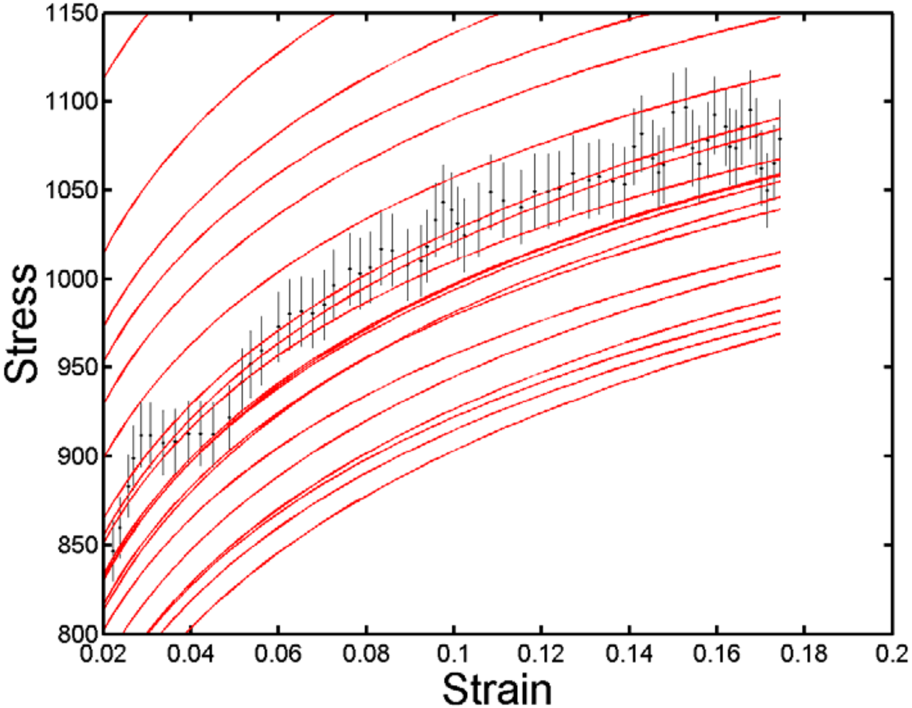
Importance of including correlations

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

MC with correlations

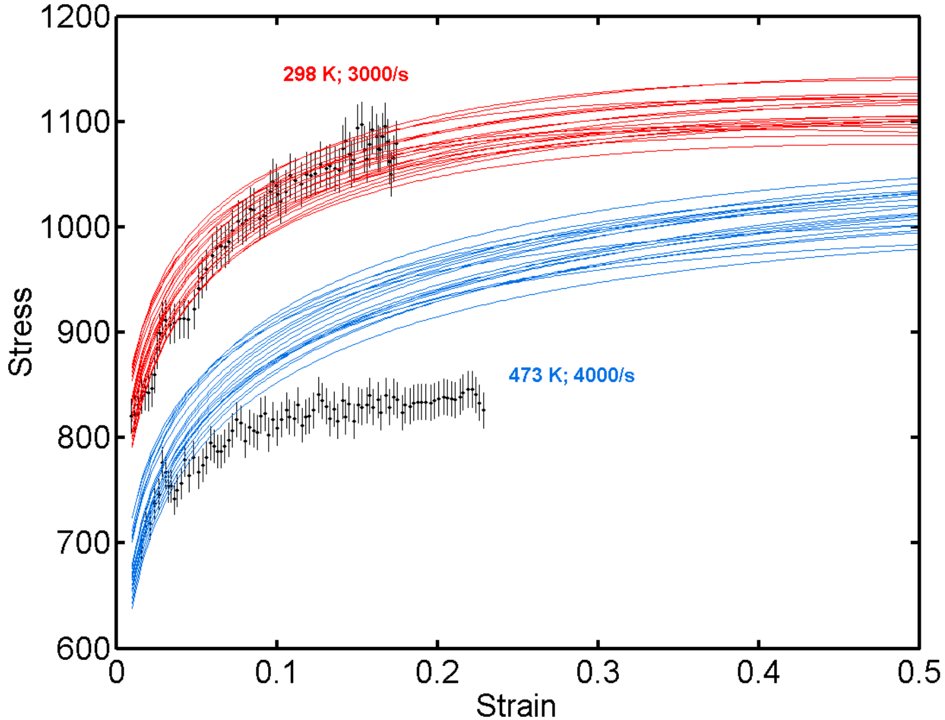


MC without correlations



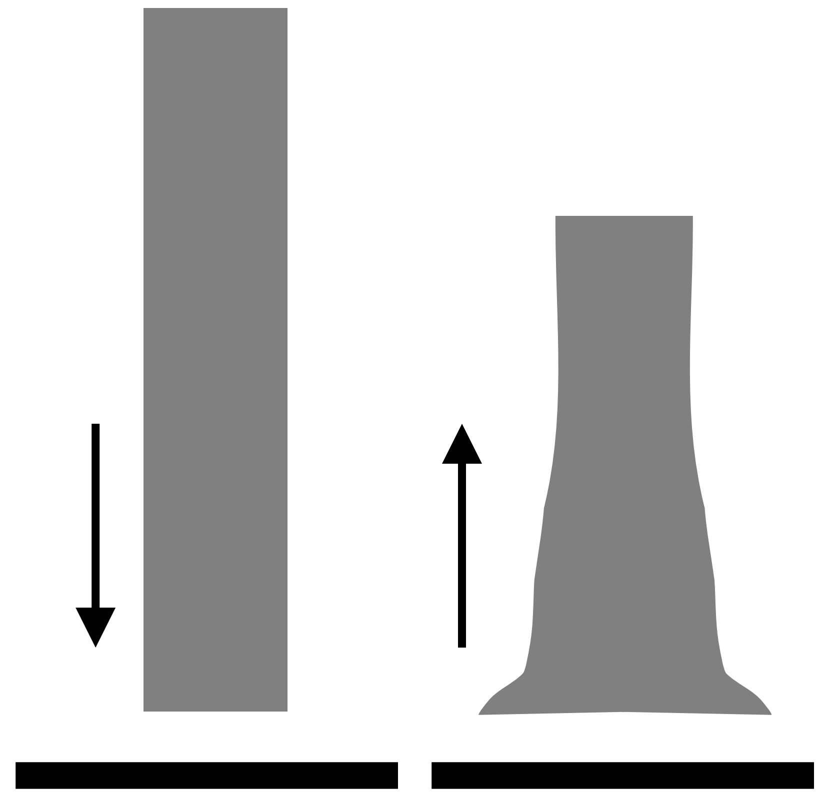
Monte Carlo sampling of ZA uncertainty

- Use Monte Carlo to draw random samples from uncertainty distribution for ZA parameters optimized for 298° K
- Show behavior at two temps and out to strain of 50%
- Does not match 473°K data, >10% error above 20% strain



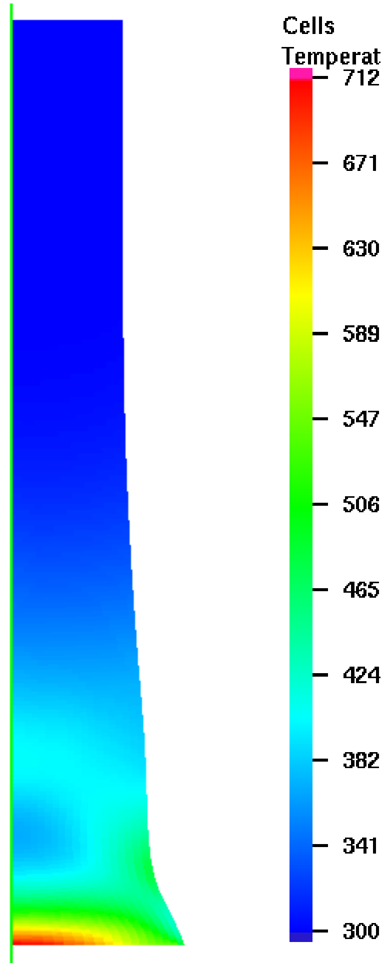
Taylor impact test

- 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
  - determining parameters in material-flow model
  - validating simulation code (including material model)



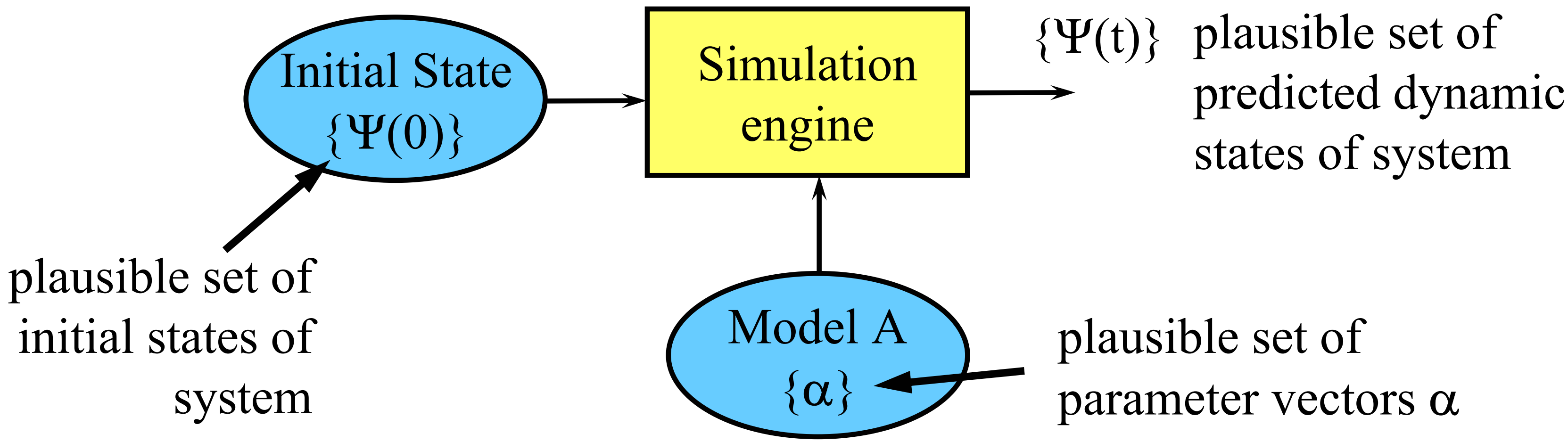
Taylor test simulations

- Simulate Taylor impact test
  - CASH - Lagrangian code (X-7)
  - Zerilli-Armstrong model for rate-dependent strength and plasticity
  - ignore anisotropy, fracture effects
  - cylinder: high-strength steel, HSLA100
    15-mm dia, 38-mm long
  - impact velocity = 247 m/s
- Effective total strain exceeds 100%
- Temperatures rise above 700° K



HSLA 100
247 m/s, 298°K

Plausible simulation predictions (forward)



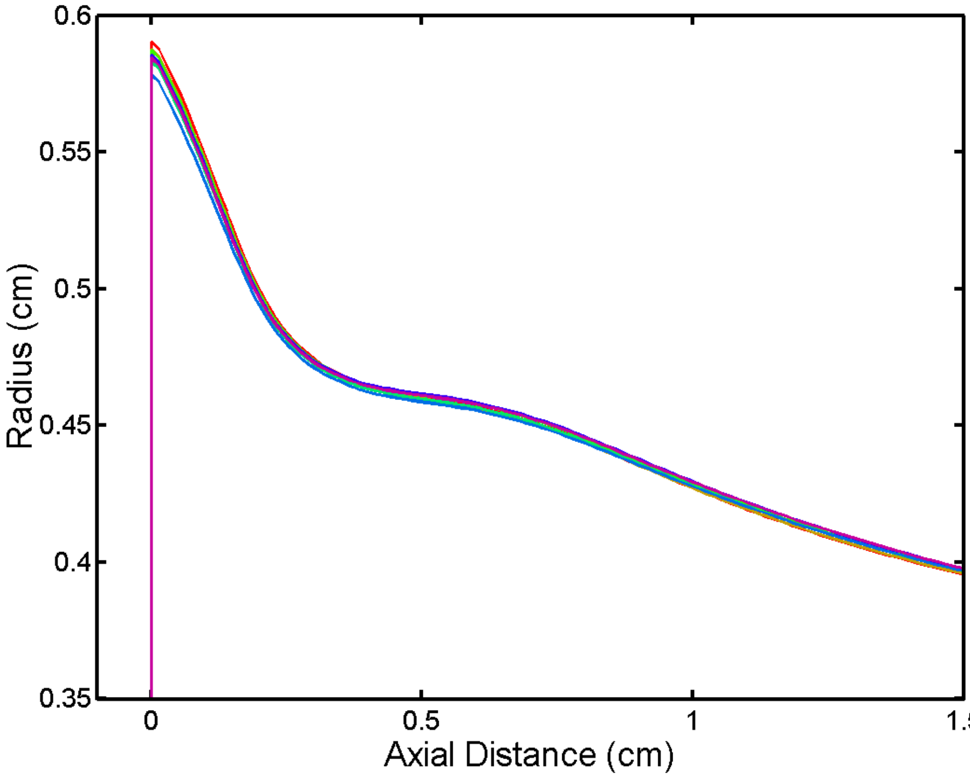
- Generate plausible predictions for known uncertainties in parameters and initial conditions
- Monte Carlo method
  - run simulation code for each random draw from pdf for α, $p(\alpha \,|\, .)$, and initial state, $p(\Psi(0) \,|\, .)$
  - simulation outputs represent plausible set of predictions, $\{\Psi(t)\}$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

Monte Carlo example - Taylor test

- Use MC technique to propagate uncertainties through deterministic simulation code
  - draw values of seven parameters from correlated Gaussian pdf
  - run CASH code for each set of parameters
- Figure shows range of variation in predicted cylinder shape implied by uncertainties in ZA parameters from previous fit

†CASH code from Tom Dey, X-7

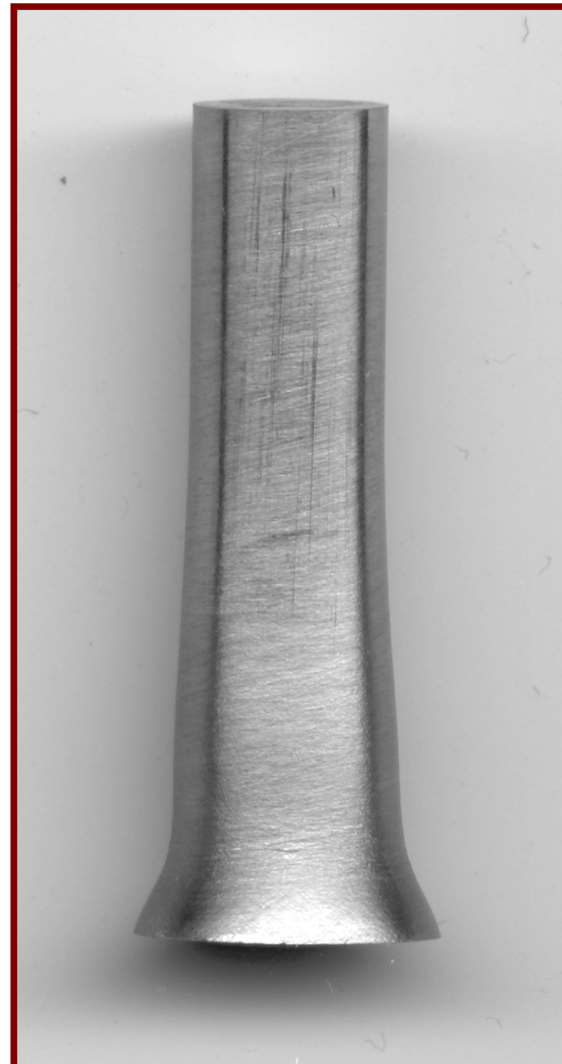
Predictions made with hydrocode CASH



High-strength steel HSLA 100
246 m/s impact velocity, 298°K

Taylor 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

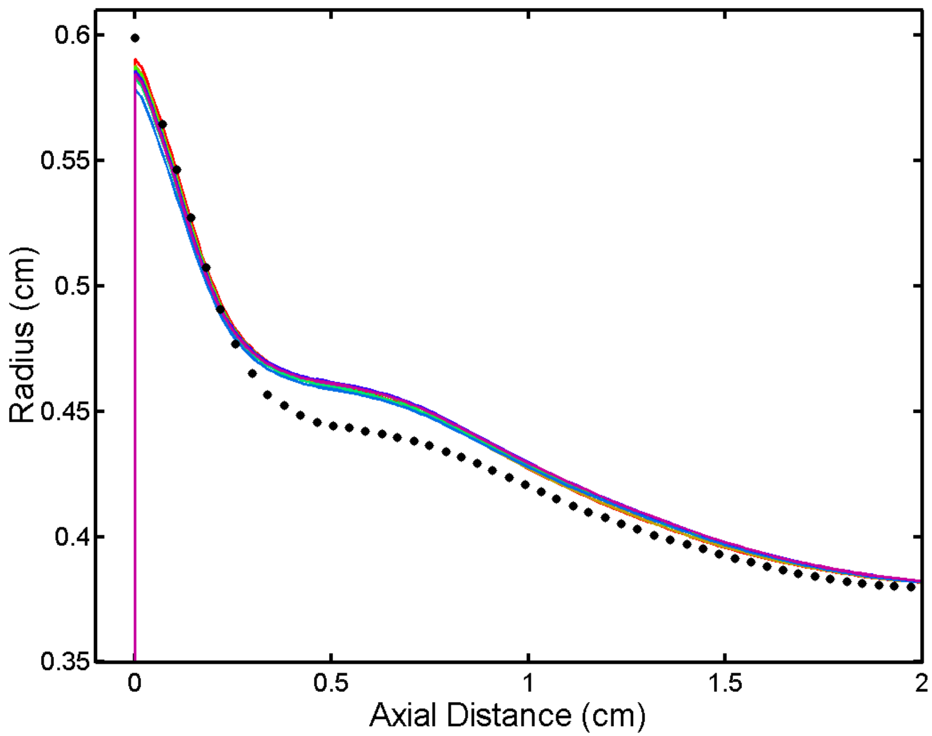


Compare simulation with experiment

- Compare CASH predictions of radial profile with data from MST-8 experiment
- Moderate (~10%) disagreement in radius increase in bulge region
- Simulation indicates temp greater than 400°K here
- Discrepancy may be caused by failure of

†data supplied by Shuh-Rong Chen

CASH simulations compared to experiment

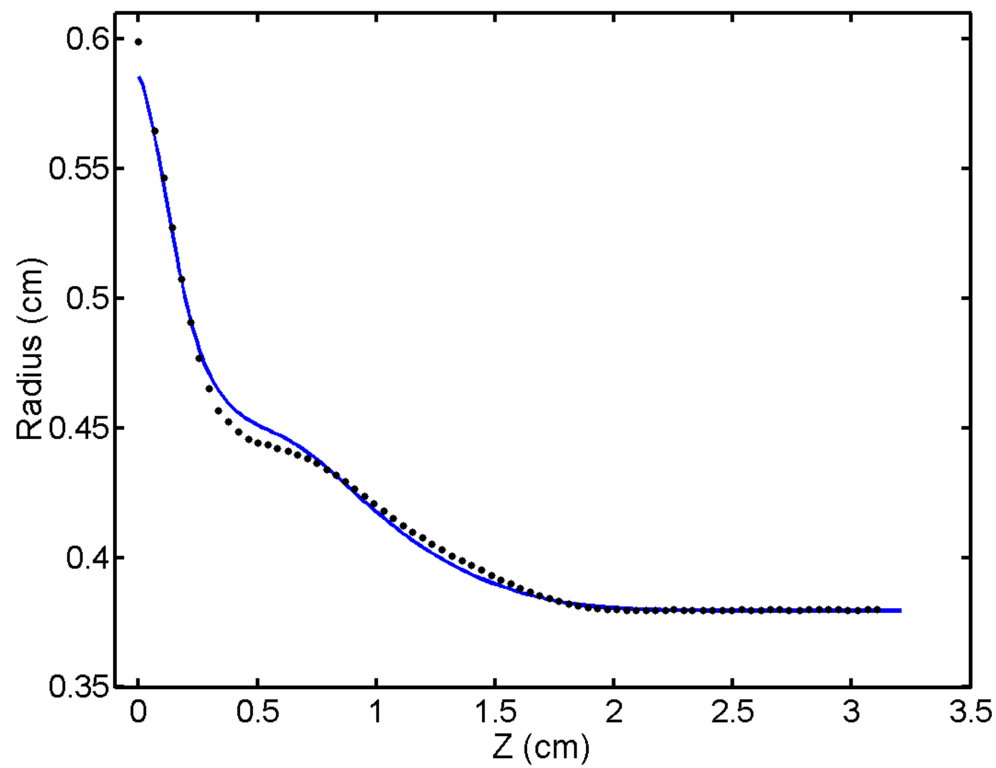


High-strength steel HSLA 100
246 m/s impact velocity, 298°K

Fit ZA model to Taylor data

- ZA model parameters can be fit to Taylor data in same way as they were to basic material characterization data
- Results of previous analysis used as prior in this analysis
- Discrepancies reduced, but requires large shift of parameters, inconsistent with prior (χ^2 p value ≈ 0)

CASH simulations compared to experiment

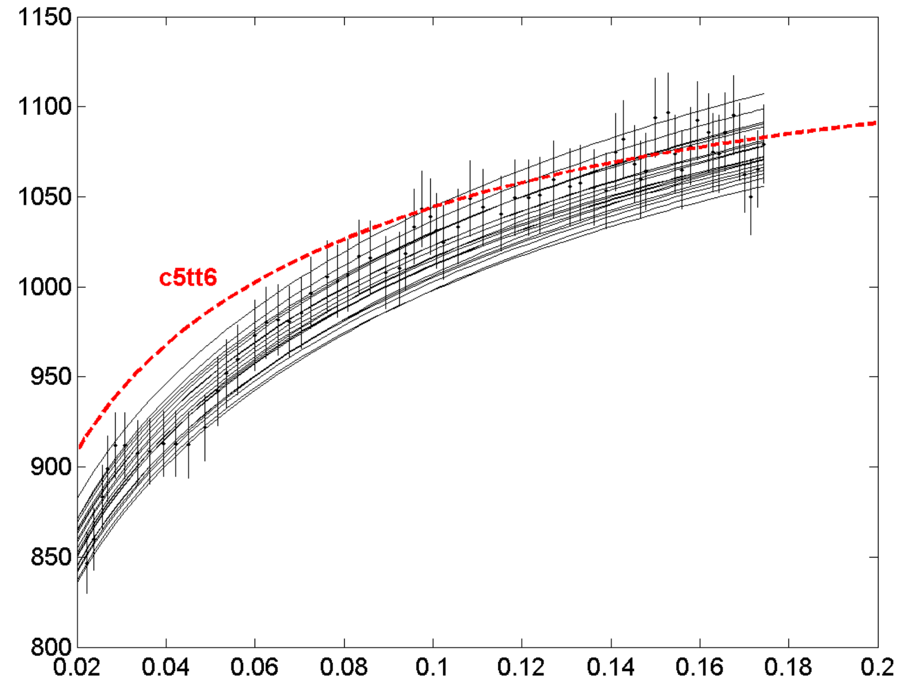


Fitted impact velocity = 235 m/s

Fit ZA model to Taylor data

- Compare stress-strain inferred ZA model from Taylor fit with data at 298°K, high strain rate
- Inconsistent with first fit to material character- ization data
- Conclude that ZA model does not account for both material characterization and Taylor experiments

CASH simulations compared to experiment

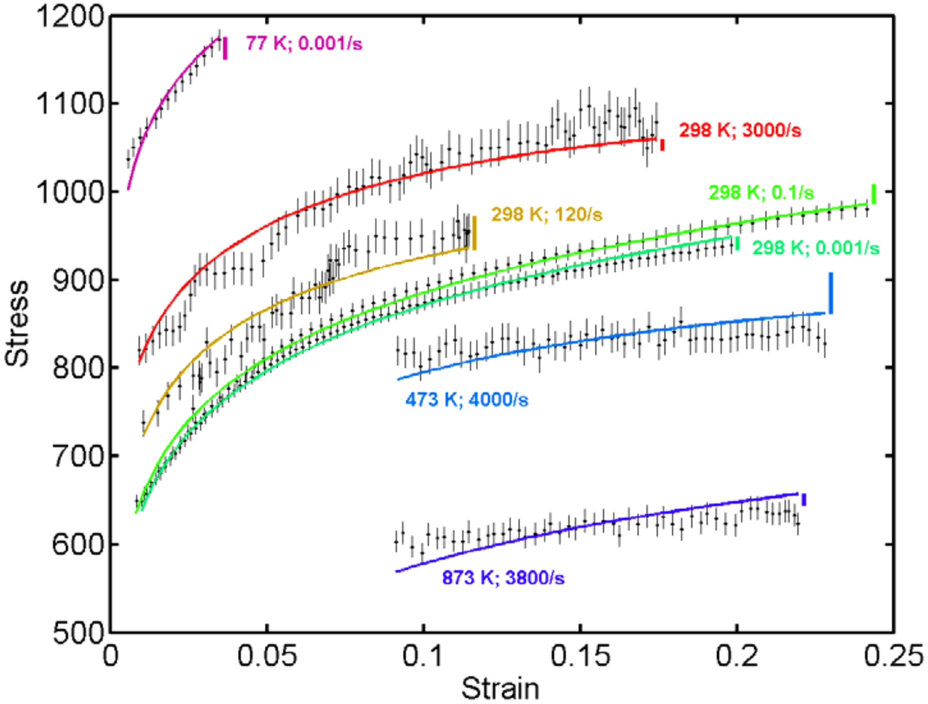


High-strength steel HSLA 100
246 m/s impact velocity, 298°K

Fit including high-strain, high-temp data

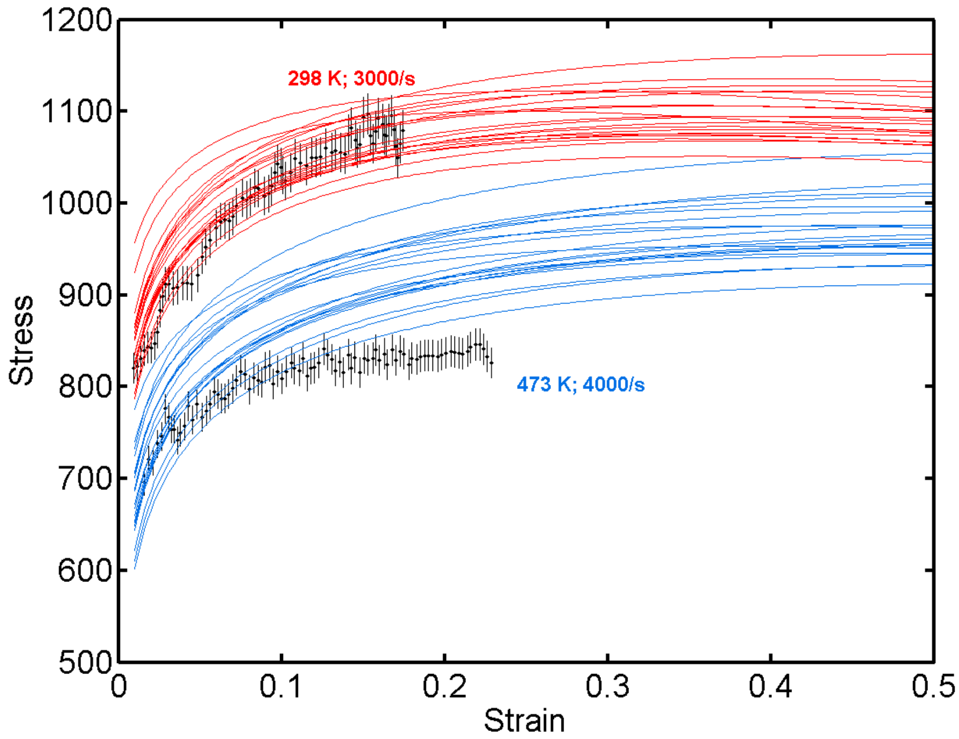
Analysis of quasi-static and Hopkinson bar measurements†

- Change ZA fit to include high-strain data at high temps
- Observe that stress vs. strain curves are too flat at 298°K and not flat enough at high temps
- Conclude that ZA model can not accommodate varying temperature dependence of strain hardening effect



Monte Carlo sampling of ZA uncertainty

- Draw Monte Carlo samples from uncertainty distribution for Zerilli-Armstrong parameters for fits to high-strain data
- Conclude that ZA fit optimized for high-strain behavior at high temps can not match both 298°K and 473°K stress-strain data



Caveats

- Verification of CASH code for Taylor test simulation
  - convergence study confirms 0.2 mm x 0.2mm grid is OK
  - other calculational details – artificial viscosity, etc.
- Validation of other submodels
  - other submodels required in simulation need to be validated, e.g., EOS, elastic response, etc., although these seem OK
- Check experimental data
  - experiments done by experienced staff, so probably OK
  - worth repeating some experiments; under more severe conditions
- Consider operating conditions
  - Hopkinson bar expt – strain rates $< 10^4\ s^{-1}$, strains < 25%
  - Taylor impact test – strain rates $\sim 10^5\ s^{-1}$, strains up to 200%

Possible approaches to cope with bad model

- Use better model to model plastic behavior
  - perhaps most preferable approach
  - however, sometimes not possible because of lack of resources; simulation code may not handle new model
- Bayesian calibration (Kennedy and O'Hagan)
  - build model of discrepancy between model and data
  - however, may not be able to incorporate into simulation code
  - if not physics based, may result in unphysical behavior
- Increase uncertainties in model parameters
  - to encompass mismatch between model and relevant data
  - include extra uncertainty to account for bad model
  - systematic uncertainty, so may not be reduced thru many meas.

Conclusions

- Zerilli-Armstrong model does not account for plastic behavior of HSLA 100 under the operating conditions of these experiments to better than ~10%
- Full uncertainty analysis in model fitting useful for
  - capturing the implications of uncertainties in data
  - predicting uncertainties in simulations
  - determining when model is inadequate to describe sequence of experiments
- Regarding uncertainties, one needs to
  - include correlations between uncertainties in each parameter
  - keep track sources of uncertainty
  - respect difference between random and systematic errors

Bibliography

- "Uncertainty quantification of simulation codes based on experimental data," K. M. Hanson and F. M. Hemez, *Proc. AIAA Aerospace Conf.* (2003)
- "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
- "Uncertainty assessment for reconstructions based on deformable models," K. M. Hanson et al., *Int. J. Imaging Syst. Technol.* **8**, pp. 506-512 (1997); use of MCMC to sample posterior

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