Inference about simulation-code models from experimental data

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Summary

- 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

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"
- This interpretation sometimes referred to as "subjective probability"
- Rules of classical probability theory apply



Parameter value

Schematic view of simulation code



- Simulation code predicts state of time-evolving system $\Psi(t)$
- Requires as input
 - $\Psi(0) = \text{initial state of system}$
 - 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

Mapping between parameters and experiments



- Model inference
 - one may use measurements to reduce uncertainties in models and their parameters
 - good experimental technique and quantification of experimental uncertainties are critically important
 - simulation connects model parameters to experimental data

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

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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(α , $\beta | \mathbf{Y}_1, \mathbf{Y}_2$) (correlations important!)

 $p(\boldsymbol{\alpha} | \mathbf{Y}_1) p(\boldsymbol{\beta})$ β_1 $p(\mathbf{Y}_2 | \boldsymbol{\alpha}, \boldsymbol{\beta})$ $\mathbf{v} p(\boldsymbol{\alpha}, \boldsymbol{\beta} | \mathbf{Y}_1 | \mathbf{Y}_2)$ α_1

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



Strain

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 ($\alpha_5 \& \alpha_6$) 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: $p(d \mid a) \propto \exp(-\frac{1}{2}\chi^2) = \exp\left\{-\frac{1}{2}\sum_{i}\left[\frac{[d_i - y_i(a)]^2}{\sigma_i^2}\right]\right\}$
- χ^2 is quadratic in the parameters \dot{a}

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

- where \hat{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

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

The model and parameter inference

- We write the model as y = y(x, a)
 - where y is a physical quantity, which is modeled as a function of the independent variables vector x and a represents the model parameters vector
- In inference, the aim is to determine:
 - ► the parameters *a* from a set of *n* measurements *d_i* of *y* under specified conditions *x_i*
 - ▶ <u>and</u> the uncertainties in the parameter values
- This process is called parameter inference, model fitting (or regression) but often uncertainty analysis is not done, as in parameter estimation

Characterization of chi-squared

- Expand vector \boldsymbol{y} around \boldsymbol{y}^0 : $y_i = y_i(x_i, \boldsymbol{a}) = y_i^0 + \sum_j \frac{\partial y_i}{\partial a_j} \Big|_{a^0} (a_j - a_j^0) + \cdots$
- The derivative matrix is called the *Jacobian*, *J*
- Estimated parameters \hat{a} minimize χ^2 (MAP estimate)
- As a function of \boldsymbol{a}, χ^2 is quadratic in $\boldsymbol{a} \hat{\boldsymbol{a}}$ $\chi^2(\boldsymbol{a}) = \frac{1}{2} (\boldsymbol{a} - \hat{\boldsymbol{a}})^{\mathrm{T}} \boldsymbol{K} (\boldsymbol{a} - \hat{\boldsymbol{a}}) + \chi^2(\hat{\boldsymbol{a}})$

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▶ where *K* is the curvature matrix (aka the *Hessian*);

$$\begin{bmatrix} \mathbf{K} \end{bmatrix}_{jk} = \frac{\partial^2 \chi^2}{\partial a_j \partial a_k} \bigg|_{\hat{a}} = \mathbf{J} \mathbf{A} \mathbf{J}^{\mathrm{T}} \quad ; \quad \mathbf{A} = \operatorname{diag}(\sigma_1^{-2}, \sigma_2^{-2}, \sigma_3^{-2}, ...)$$

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

- 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 $p(d_k | a, I)$ is likelihood from *k*th data set

- Include Gaussian priors through Bayes theorem $p(a | d, I) \propto p(d | a, I) p(a | I)$
 - ► For a Gaussian prior on a parameter a $-\log p(a | d, I) = \varphi(a) = \frac{1}{2}\chi^2 + \frac{(a - \tilde{a})^2}{2\sigma_a^2}$

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

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 dev. ≈ 20 MPa at strain of 0.1
- Treat this variability as systematic uncertainty
- Represents an uncertainty in initial state



[†]data supplied by S-R Chen, MST-8

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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)

Fit ZA model to selected measurements

Analysis of quasi-static and Hopkinson bar measurements[†]

- dependent plasticity
- Parameters determined from Hopkinson bar measurements and quasistatic tests
- Full uncertainty analysis including systematic effects of offset of each data set (6 + 7 parms)
- \sim 30 iter., \sim 500 func. evals.
- Efficient sensitivities needed



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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
```

Minimum chi-squared fit yields estimated ZA parms. plus 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



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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



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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



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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 materialflow model
 - validating simulation code (including material model)





Taylor test simulations

- Simulate Taylor impact test
 - ► CASH Lagrangian code (X-7)
 - Zerilli-Armstrong model for ratedependent 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





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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.

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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

Predictions made with hydrocode CASH



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

[†]CASH code from Tom Dey, X-7

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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 ZA model

CASH simulations compared to experiment 0.6 0.55 (cm) 80.50 0.45 0.5 •••••••••••••••••••••••••••• 0.4 0.35 0.5 1.5 Λ 1 Axial Distance (cm) High-strength steel HSLA 100

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

[†]data supplied by Shuh-Rong Chen

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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 ($\chi^2 p$ value ≈ 0)

CASH simulations compared to experiment



Fit ZA model to Taylor data

- Compare stress-strain inferred ZA model from Taylor fit with data at 298°K, high strain rate
- Somewhat inconsistent with fit to material characterization data
- Conclude that ZA model may not account for both material characterization and Taylor experiments

ZA parm. determined from Taylor expt. compared to measured stress vs. strain



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 ~ 10^5 s⁻¹, strains up to 200% October 27, 2003 LACSI Workshop on Simulation-Driven Optimization 33

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

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