Assessing Uncertainties in Simulation Predictions

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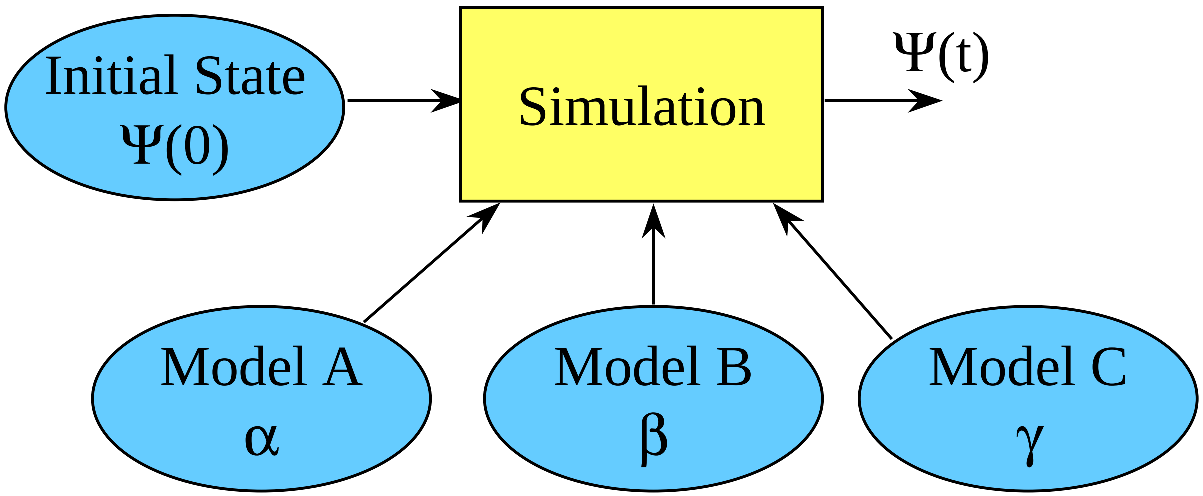
Simulation code



- Simulation code predicts state of time-evolving system
  - $\Psi(t)$ = time-dependent state of system
  - $\Psi(0)$ = initial state of system
- Many underlying models needed to simulate complex physical situation

Validation of Simulation Code

- Validation = experimentally demonstrate that simulation code satisfactorily predicts behavior of a specified aspect of the physical world
- Goal is to estimate and minimize uncertainties in predictions
- Simulation code depends on many basic models
- Validation experiments
  - basic experiments needed to validate basic models
  - integrated experiments to validate intermediate levels of combinations of basic models
  - fully integrated experiments to validate complete simulation package
- Need analysis methods to accumulate and quantitatively assess information about set of models for large number of experiments

Simulation Codes

- Used to predict time evolution of physical systems
- Based on
  - partial differential equations (PDEs)
    - fundamental physics
    - approximations
  - behavior of materials and interactions between them
    - domain of physical variables
- Examples
  - fluid dynamics; liquids, gases; ocean, atmosphere
  - hydrodynamics; solids under extreme pressures; high velocity impacts, explosives
  - electrodynamics; charged particles, magnetic fields; plasmas

Uncertainty Analysis

- Uncertainties in model parameters characterized by probability density function (pdf)
- Inference about models requires knowledge of uncertainties
  - e.g., needed for model revision
- New experiments may be designed to reduce uncertainties through sensitivity analysis
- Goal is to estimate and minimize uncertainties in predictions

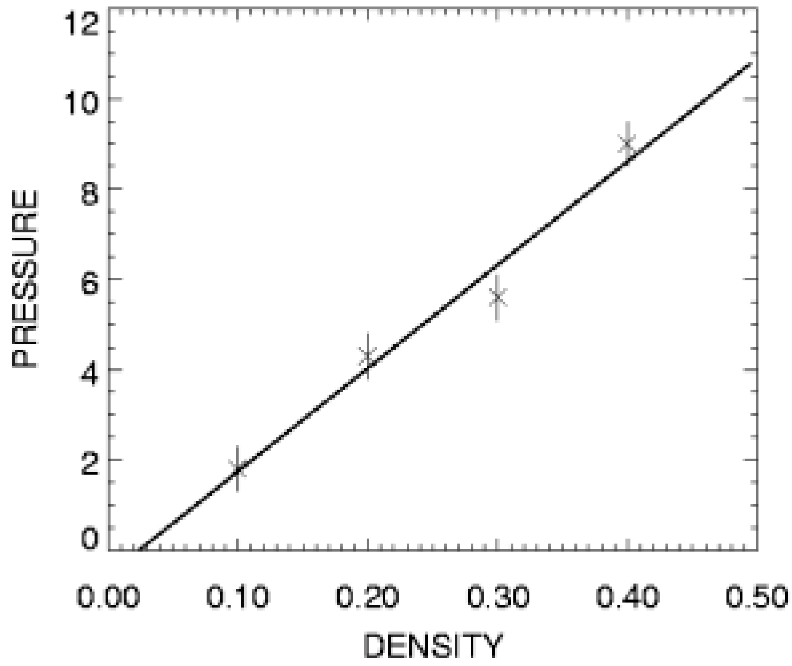
Uncertainty Analysis

- Based on complete characterization of uncertainties in experiments
  - incorporate "systematic" uncertainties
  - include uncertainties in experimental conditions
- Must handle correlations among uncertainties
- Combine results from many (all) experiments
  - reduce uncertainties in model parameters
  - require consistency of models with all experiments

Example of simple basic physics model

Isothermal dependence of gas pressure on density

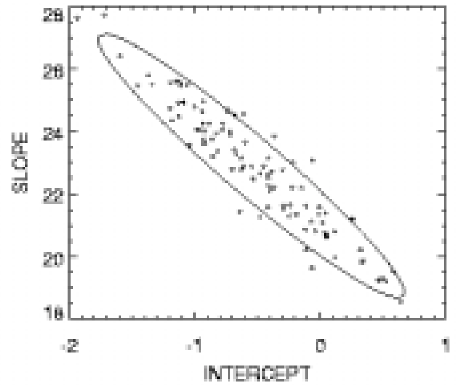
- Assume linear model to describe dependence (ideal gas)
- Determine two parameters, intercept and slope, by minimizing chi-squared based on four available measurements
- Use this linear model in simulation code where pressure of gas is needed and density is calculated

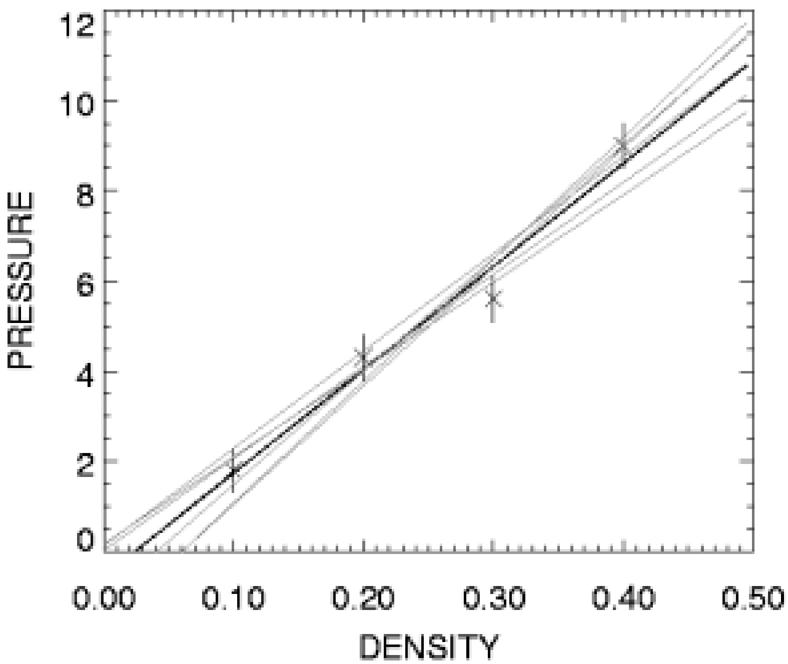


Example of simple basic physics model

Isothermal dependence of gas pressure on density

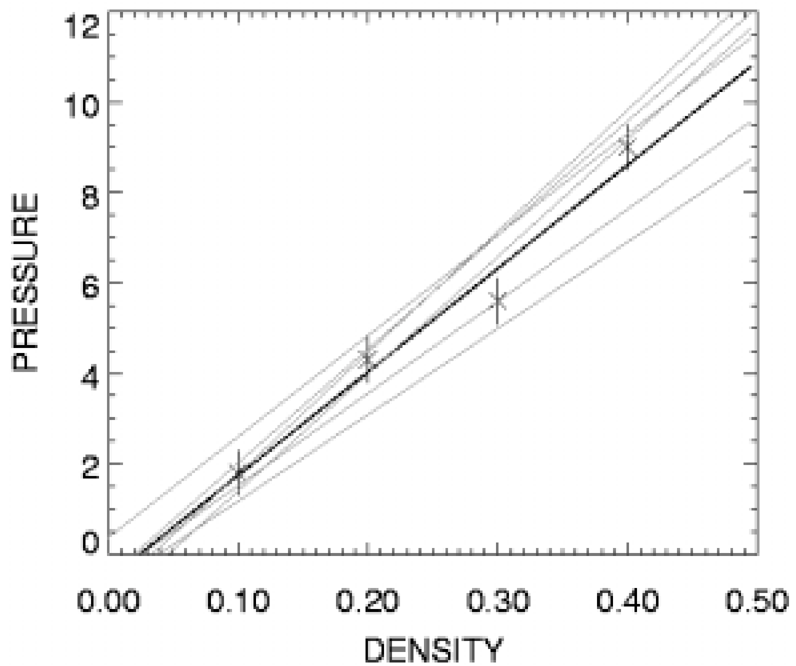
- Uncertainties in parameters, derived from uncertainties in measurements, given by Gaussian pdf in 2-D parameter space
  - correlations evidenced by tilt
  - points are random draws from pdf
- However, focus should be on implied uncertainties in dependence of pressure vs. density
  - light lines are plausible model realizations drawn from parameter pdf
  - characterize uncertainty in dependence





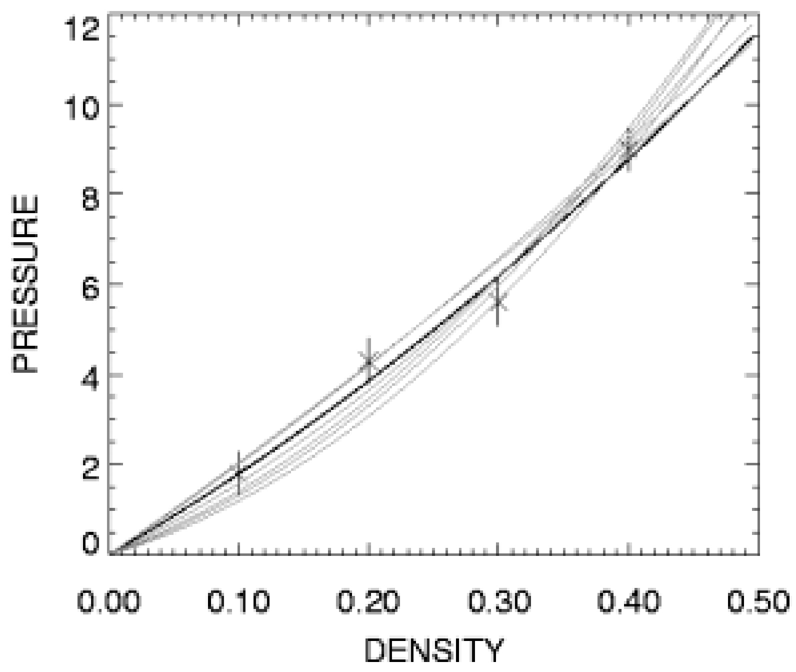
Example of simple basic physics model
Isothermal dependence of gas pressure on density

- Correlations in uncertainties are critically important
- Plot shows random samples from uncertainty in slope and intercept ignoring correlations
- Uncertainties in dependence of pressure vs. density far exceed uncertainties in measurements

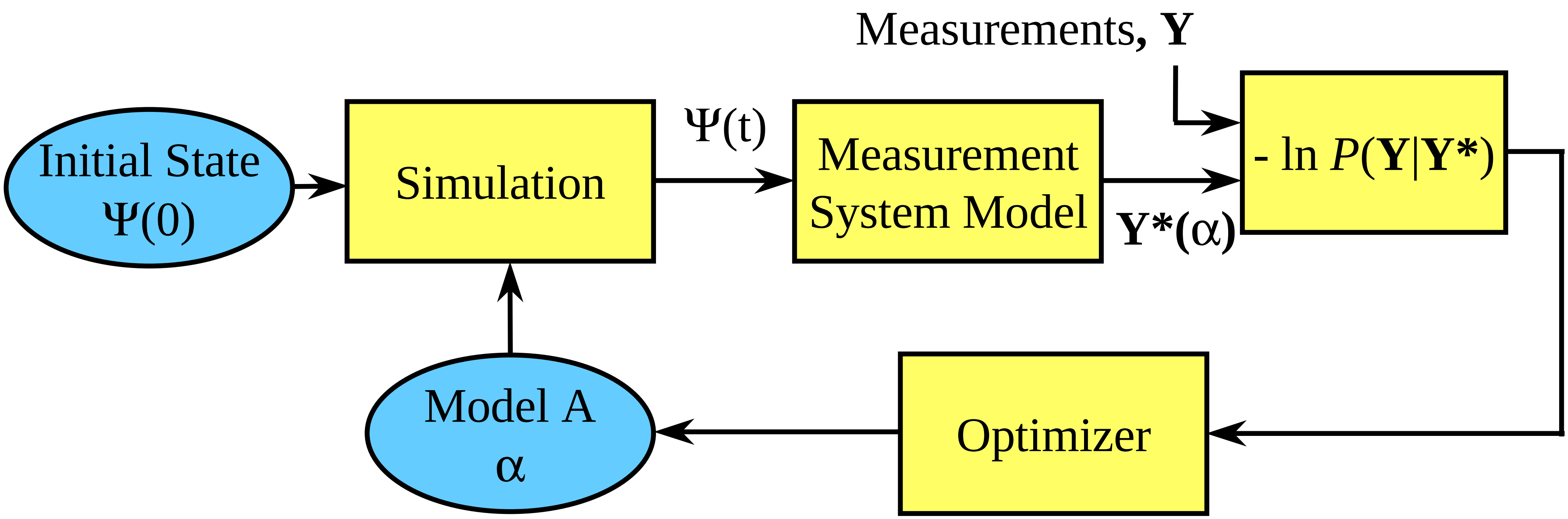


Example of simple basic physics model
Isothermal dependence of gas pressure on density

- Suspected departure from linearity might be handled by using quadratic for model
  - curve constrained to go through origin
- Comparison with previous linear model demonstrates increased uncertainties in model outside of density measurement range
- Conclusion: desirable to conduct basic physics experiments over full operating range of physical variables used by simulation code; extrapolation increases uncertainty

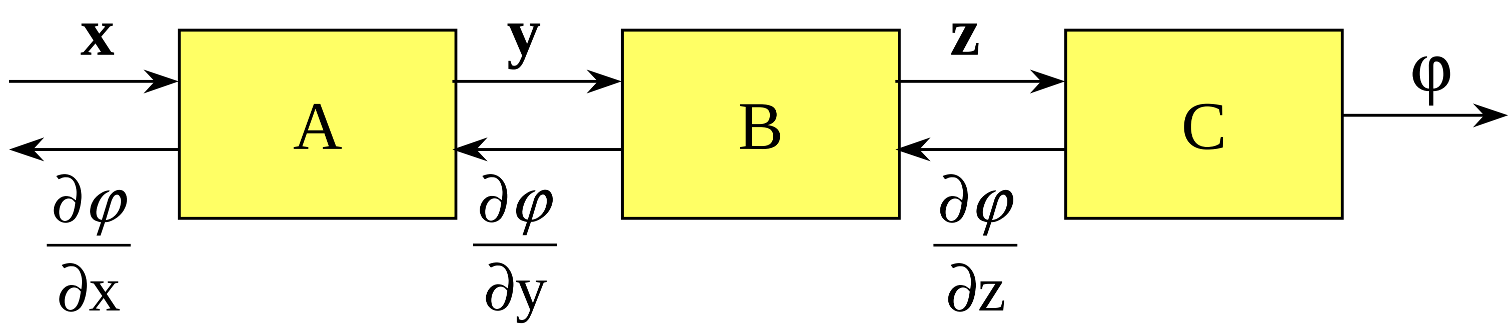


Parameter estimation - maximum likelihood



- Measurement system model calculates measurements that experiment would obtain for the simulated state of the physical system $\Psi(t)$
- Match to data summarized by minus-log-likelihood, $-\ln P(\mathbf{Y}|\mathbf{Y}^*\} = {}^1/_2\, \chi^2$
- Optimizer adjusts parameters (vector α) to minimize $-\ln P(\mathbf{Y}|\mathbf{Y}^*(\alpha)\}$

Adjoint Differentiation of Forward Calculation



- Data-flow diagram shows sequence of transformations A, B, C that convert data structure **x** to **y** to **z** and then scalar φ.
- Derivatives of φ with respect to **x** are efficiently calculated in the reverse (adjoint) direction.
- CPU time to compute **all** derivatives comparable to forward calculation
- One may need to keep intermediate data structures to evaluate derivatives
- Code based: logic of adjoint code derivable from forward code

Analysis of single experiment

- Likelihood
  - p(**Y** | **Y***) = probability of measurements **Y** given the values **Y*** predicted by experiment simulation. (NB: **Y*** depends on α)
- The pdf describing uncertainties in model parameter vector α, called posterior:
  - $p(\alpha \,|\mathbf{Y}) \propto p(\mathbf{Y} \mid \mathbf{Y}^*)\, p(\alpha)$ (Bayes law)
  - p(α) is prior; summarizes previous knowledge of α
  - "best" parameters estimated by maximizing p(α |**Y**) (called MAP solution)
  - uncertainties in α are fully characterized by p(α |**Y**)

Helpful to use logarithms of probabilities

- In terms of log-probability, Bayes law becomes:

$$- \ln p(\alpha \mid \mathbf{Y}) = - \ln p(\mathbf{Y} \mid \alpha) - \ln p(\alpha) + \text{constant}$$

- Parameters are estimated by minimizing $- \ln p(\alpha \mid \mathbf{Y})$
- Gaussian approximation of probability:

$$- \ln p(\alpha) = \phi = \phi_0 + (\alpha - \alpha_0)^T \mathbf{K} (\alpha - \alpha_0) ,$$

  where $\mathbf{K}$ is the curvature or second derivative matrix of ϕ (aka Hessian) and α_0 is the position of the minimum in ϕ
- Covariance matrix is inverse of $\mathbf{K}$: $\mathbf{C} = \mathbf{K}^{-1}$
- Likelihood for Gaussian measurement uncertainties is

$$-\ln P(\mathbf{Y} \mid \mathbf{Y^*}\} = {}^1\!/_2\, \chi^2 = \Sigma \{(y_i - y^*_i)/(2\, \sigma_i)\}^2$$

Gaussian probabilities

- Bayes law:

  $$- \ln p(\alpha \,|\mathbf{Y}) = - \ln p(\mathbf{Y}|\alpha) - \ln p(\alpha) + \text{constant}$$

- For Gaussians

  $$- \ln p(\alpha \,|\, \mathbf{Y}) = \phi = \phi_0 + (\alpha - \alpha_0)^T \mathbf{K_0} (\alpha - \alpha_0) =$$

  $$(\alpha - \alpha_\mathbf{L})^T \mathbf{K_L} (\alpha - \alpha_\mathbf{L}) + (\alpha - \alpha_\mathbf{P})^T \mathbf{K_P} (\alpha - \alpha_\mathbf{P}) + \text{const.},$$

  where subscripts L & P refer to likelihood & prior

- Covariance matrix of posterior is:

  $$\mathbf{C_0} = \mathbf{K_0}^{-1} = [\mathbf{K_L} + \mathbf{K_P}]^{-1}$$

- Estimated parameters are:

  $$\alpha_0 = \mathbf{K_0}^{-1} [\alpha_\mathbf{L} \mathbf{K_L} + \alpha_\mathbf{P} \mathbf{K_P}]$$

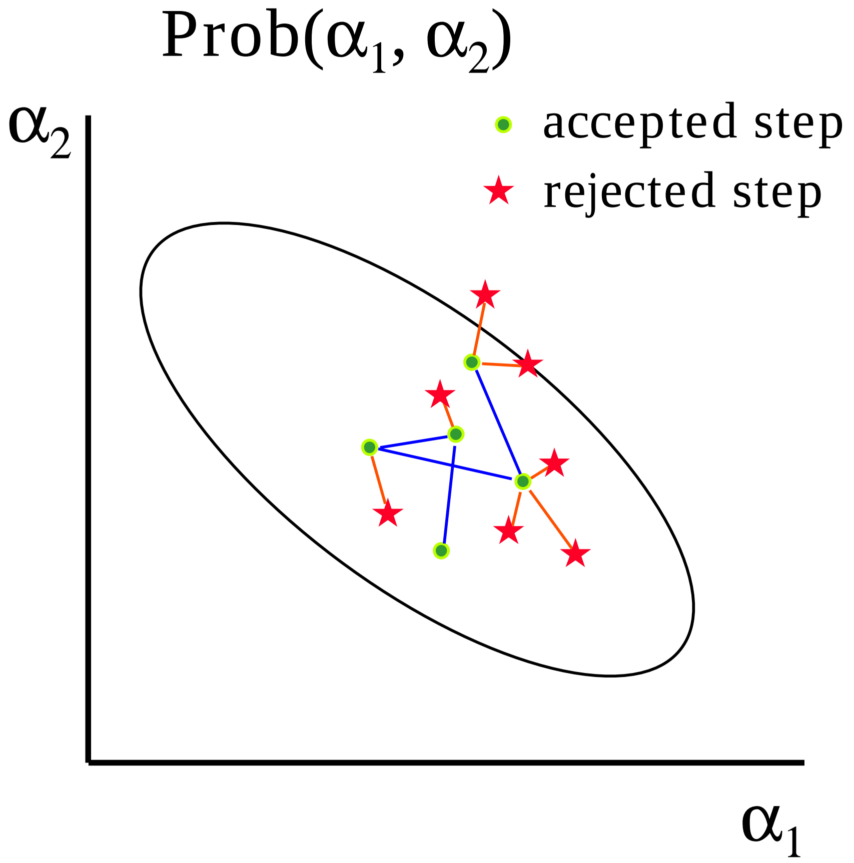
Parameter uncertainties via MCMC

- Posterior $p(\alpha \mid \mathbf{Y})$ provides full uncertainty distribution
- Markov Chain Monte Carlo (MCMC) algorithm generates a random sequence of parameters that sample $p(\alpha \mid \mathbf{Y})$
  - results in plausible set of parameters $\{\alpha\}$
  - representative of uncertainties
  - second moments of parameters can be used to estimate covariance matrix **C**
- MCMC advantages
  - can be applied to any pdf, not just Gaussians
  - automatic marginalization over nuisance variables
- MCMC disadvantage
  - potentially calculationally demanding

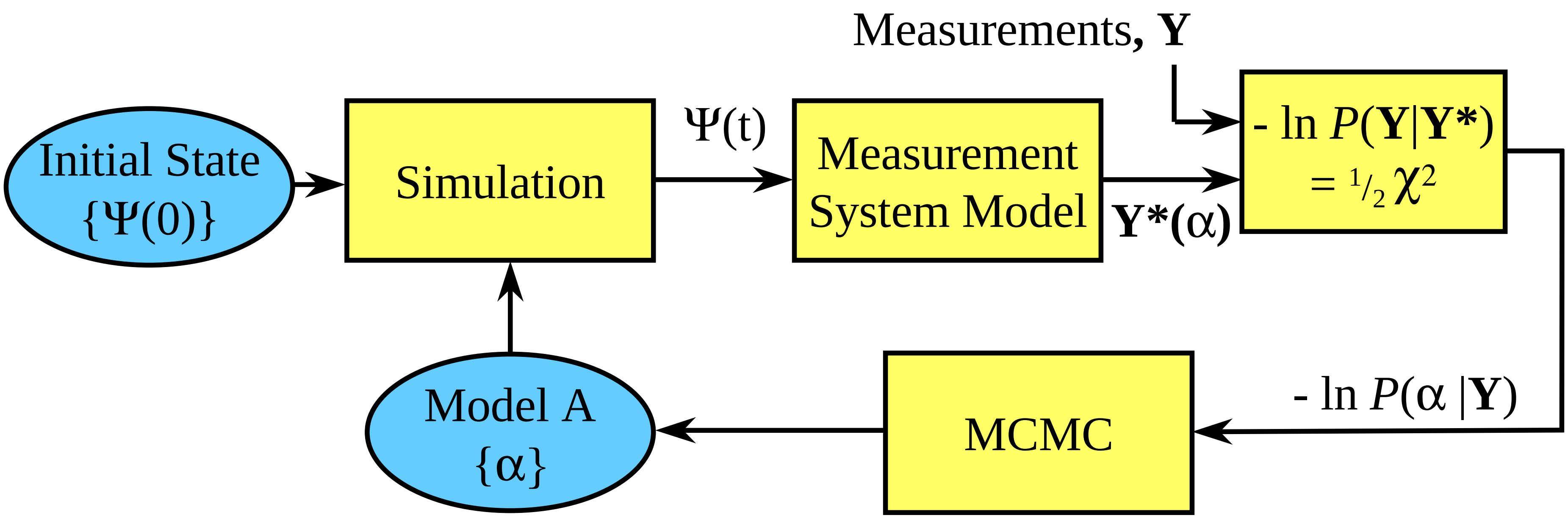
Markov Chain Monte Carlo

Generates sequence of random samples from a target probability density function

- Metropolis algorithm:
  - draw trial step from symmetric pdf, i.e., $T(\Delta\alpha) = T(-\Delta\alpha)$
  - accept or reject trial step
  - simple and generally applicable
  - relies only on calculation of target pdf for any α
  - works well for many parameters



Parameter uncertainties via MCMC

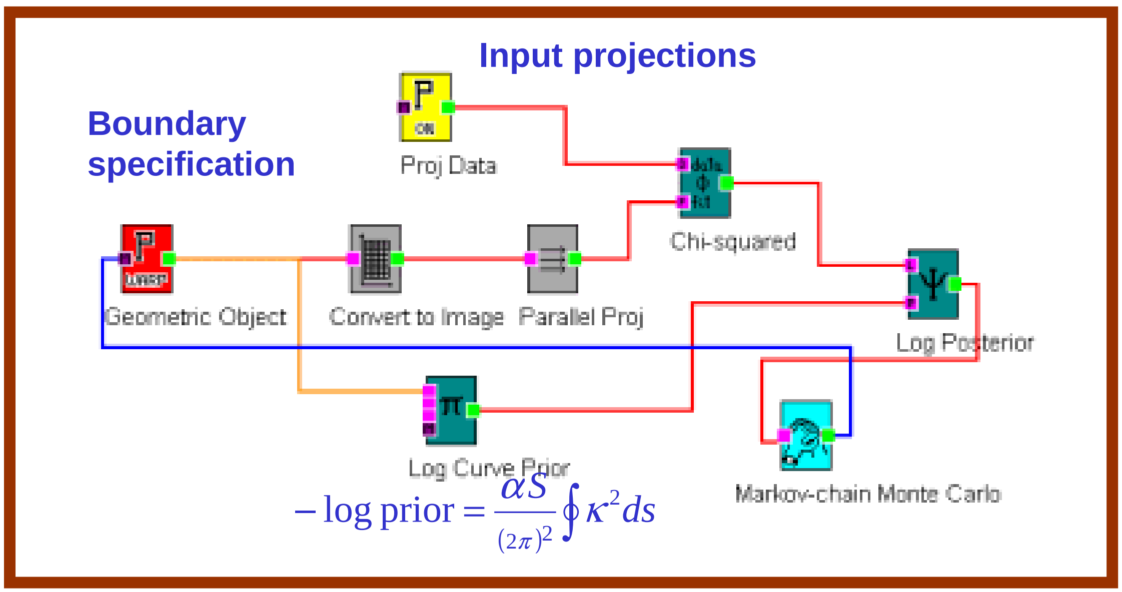


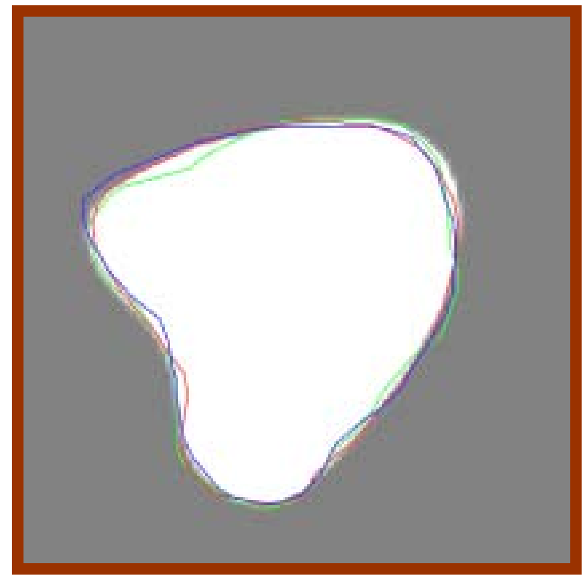
- Markov Chain Monte Carlo (MCMC) algorithm generates a sequence of parameter vectors that randomly sample posterior probability of parameters for given data **Y,** $P(\alpha | \mathbf{Y})$
- This sequence $\{\alpha\}$ represents a plausible set of parameters
- Must include uncertainty in initial state of system, $\{\Psi(0)\}$

Uncertainty analysis with Bayes Inference Engine
Example of reconstruction from just two radiographs

- Reconstruction problem solved with Bayes Inference Engine (BIE) using deformable boundary model
- MCMC generates set of plausible solutions, which characterize uncertainty in boundary localization

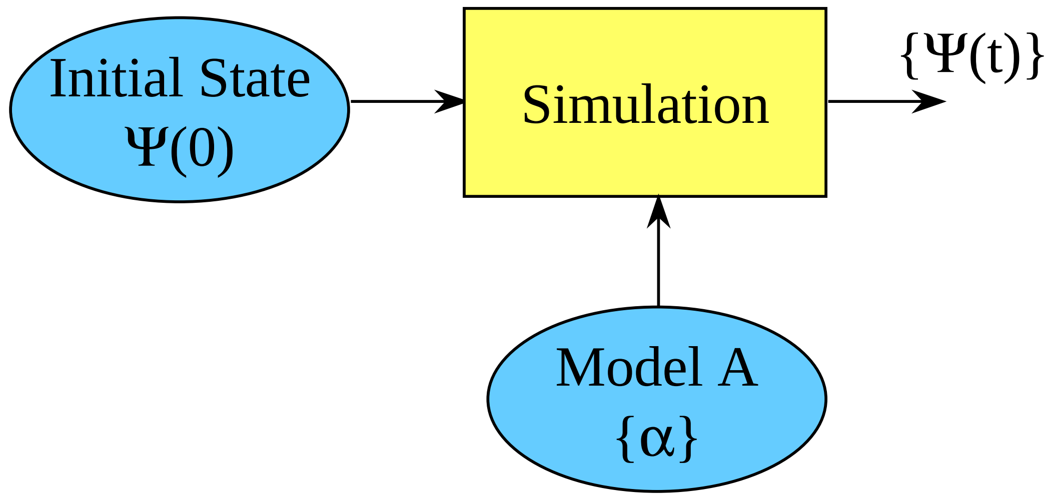
Data flow diagram in BIE





Reconstruction with several plausible boundaries

Simulation of plausible outcomes - characterizes uncertainty in prediction

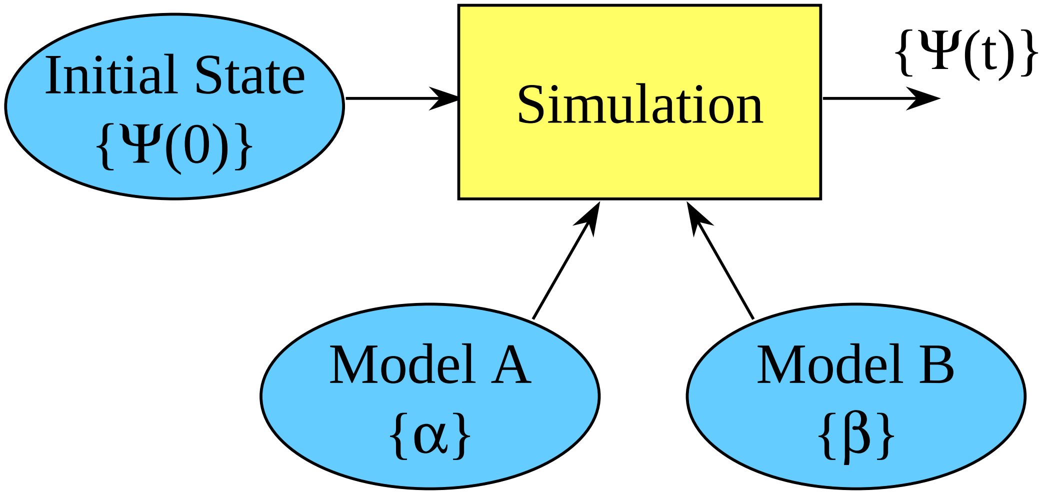


- Simulation code predicts plausible results for known uncertainties in parameters
  - $\{\Psi(t)\}$ = plausible sets of dynamic state of system
  - $\{\alpha\}$ = plausible sets of parameter vector α

Uncertainty in predictions

- Estimate by propagating through simulation code a set of parameter samples drawn from joint posterior distribution of all parameters describing constituent physics models
- Assumptions about simulation code:
  – appropriate physics models included; can be checked using carefully designed experiments (validation issue)
  – numerically accurate (verification issue)
- Other stochastic effects in simulation may be included
  – variability in densities
  – chaotic behavior

Plausible outcomes for many models



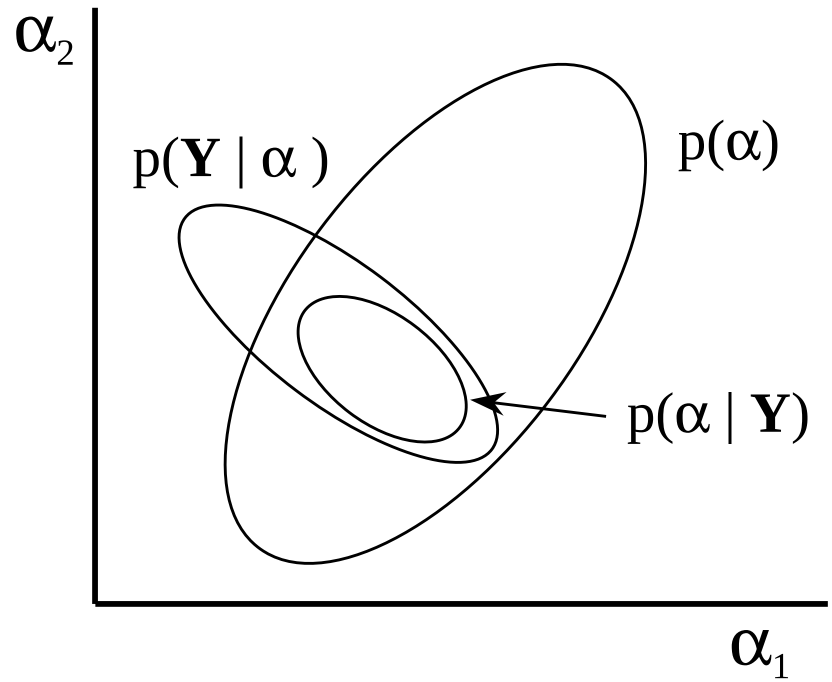
- Integrated simulation code predicts plausible results for known uncertainties in initial conditions and material models
  - $\{\Psi(t)\}$ = plausible sets of dynamic state of system
  - $\{\Psi(0)\}$ = plausible sets of initial state of system
  - $\{\alpha\}$ = plausible sets of parameter vector α for material A
  - $\{\beta\}$ = plausible sets of parameter vector β for material B

Analysis of many experiments involving several models

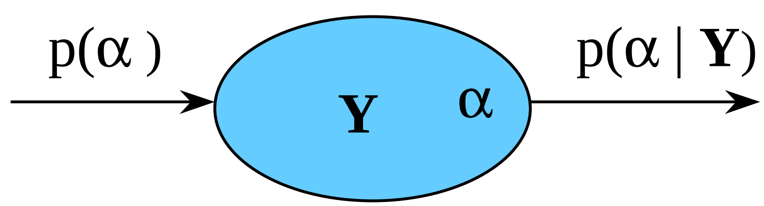
- Complications
  - complexity of handling large number of analyses
  - logic and dependencies are difficult to follow
  - need for global analysis
  - correlations between uncertainties in parameters for various are induced by analyses dependent on several models
- A comprehensive methodology is needed

Graphical probabilistic modeling

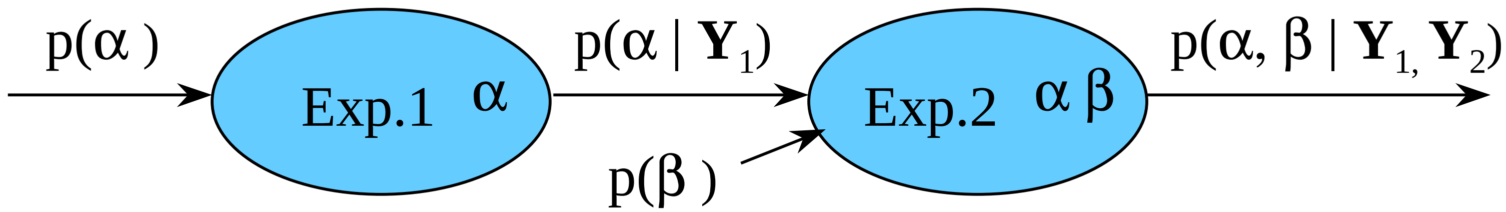
- Analysis of experimental data **Y** improves on prior knowledge about parameter vector α
- Bayes law
  p(α | **Y**) ~ p(**Y** | α) p(α)
  (posterior ~ likelihood x prior)



- Use bubble to represent effect of analysis based on data **Y**
- In terms of logs: - ln p(α |**Y**) =
  - ln p(**Y**|α) - ln p(α) + constant



Graphical probabilistic modeling



Output of second bubble:

$$p(\alpha, \beta \mid \mathbf{Y}_1, \mathbf{Y}_2) \sim p(\mathbf{Y}_1, \mathbf{Y}_2 \mid \alpha, \beta)\, p(\alpha, \beta)$$ (Bayes law)

$$\sim p(\mathbf{Y}_2 \mid \alpha, \beta)\, p(\beta)\, p(\alpha \mid \mathbf{Y}_1)$$

(likelihood 2 x prior(β) x posterior 1)

$$\sim p(\mathbf{Y}_2 \mid \alpha, \beta)\, p(\beta)\, p(\mathbf{Y}_1 \mid \alpha)\, p(\alpha)$$

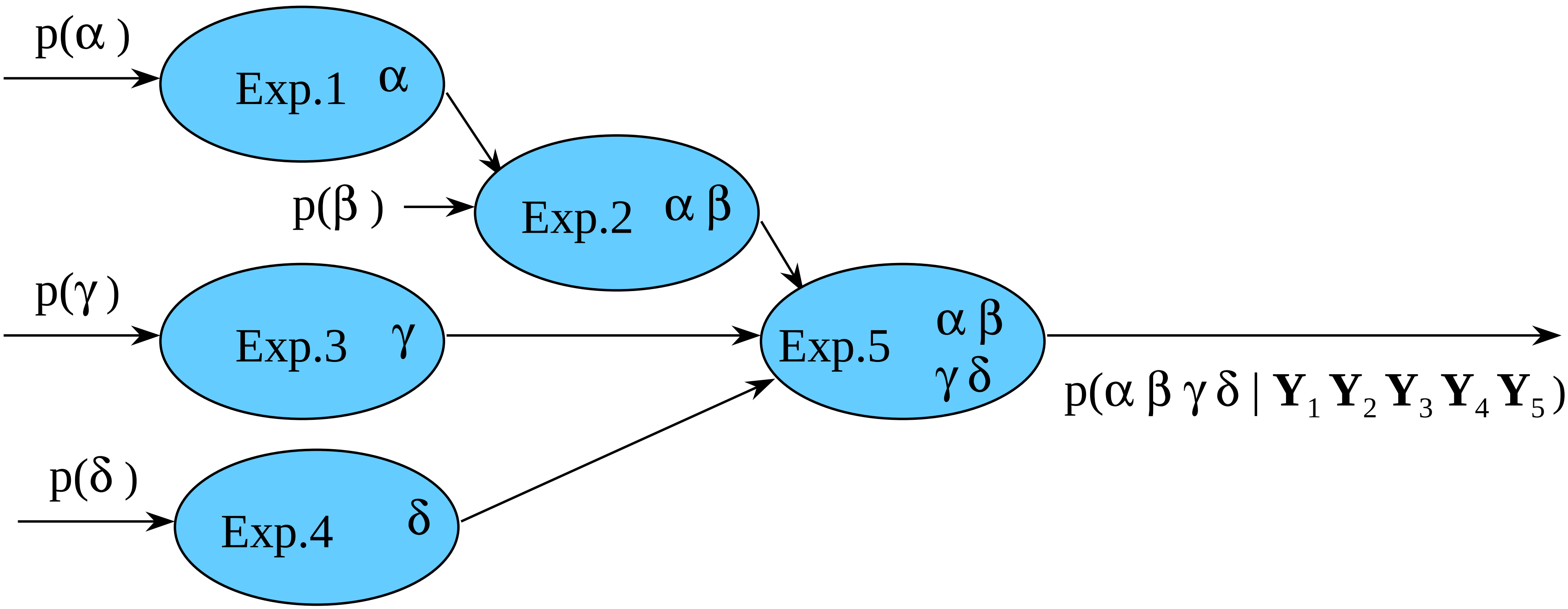
(likelihood 2 x prior(β) x likelihood 1 x prior(α))

Summary: Action of bubble is to multiply input pdfs on left by likelihood from experiment to get output joint pdf

Graphical probabilistic modeling

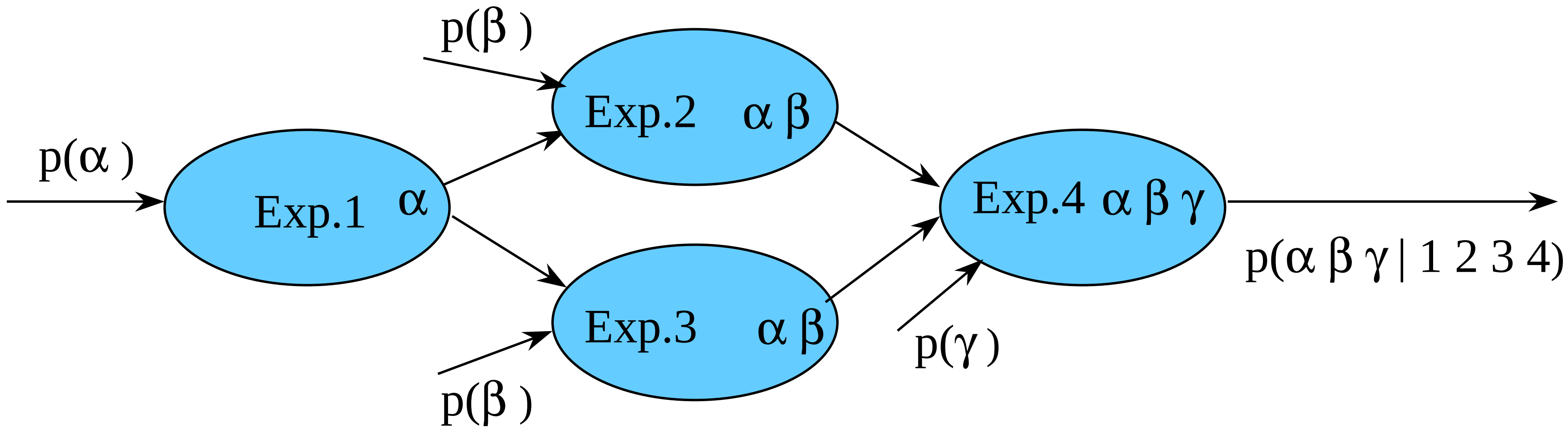
- Useful for complete analysis of many experiments related to several models
  - displays logic
  - explicitly shows dependencies
  - sociological and organizational tool when many modelers and experimenters are involved
- Result is full joint probability for all parameters based on every experiment
  - uncertainties in all parameters, including their correlations, which is crucially important

Example of analysis of several experiments



Output is full joint probability for all parameters based on all experiments

Need to avoid double counting

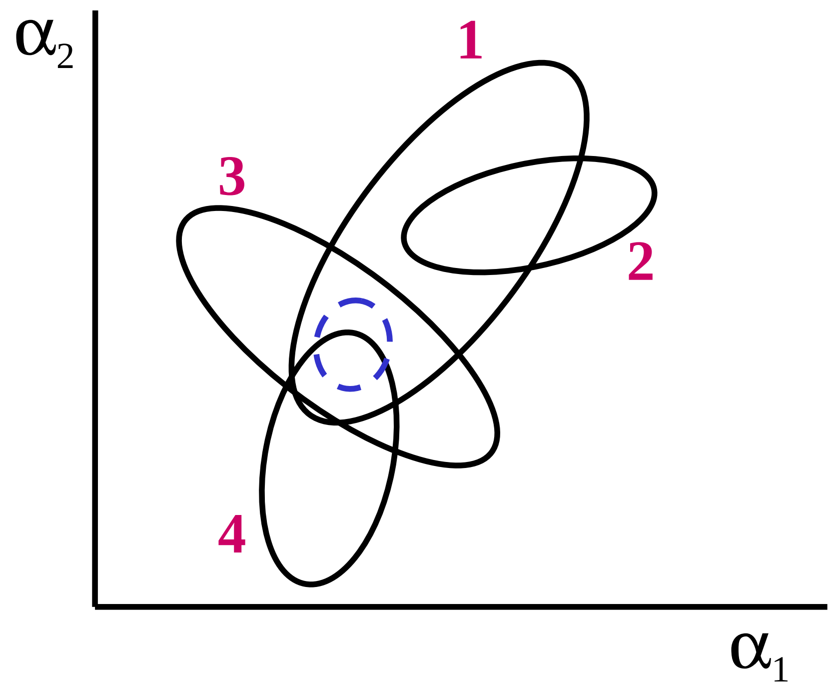


Output of analyses of both Exps. 2 and 3 make use of output of Expt. 1 and prior on β. This repetition must be avoided in overall posterior calculation through dependency analysis:

$$- \ln p(\alpha\, \beta\, \gamma \mid 1\ 2\ 3\ 4) = - \ln p(1 \mid \alpha) - \ln p(\alpha) - \ln p(2 \mid \alpha\, \beta) - \ln p(\beta)$$
$$- \ln p(3 \mid \alpha\, \beta) - \ln p(4 \mid \alpha\, \beta\, \gamma) - \ln p(\gamma) + \text{constant}$$

Model checking

- Model checking is a necessary part of any analysis: check model against all experimental data
- Thus, need to check consistency of full posterior wrt each of its contributions, for example
  - likelihoods from Exps. 1 and 2 are consistent with each other
  - however, Exp. 2 is inconsistent with posterior (dashed) from other exps.
  - inconsistency must be resolved in terms of correction to model and/or experimental interpretation



Summary

- A methodology has been presented to cope with combining experimental results from many experiments relevant to several basic physics models in the context of a simulation code
  - suggest using a graphical representation of a probabilistic model
- Many challenges remain
  - correlations in experimental uncertainties
  - systematic experimental uncertainties
  - detection and resolution of inconsistencies between experiments and simulation code
  - normalization of likelihoods of different types
- More on WWW- http://home.lanl.gov/kmh