Bayesian calibration and uncertainty quantification of computer models

Application to the simulation of astrophysical radiative shocks

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Outline

- model uncertainty formalism [Kennedy, O'Hagan 2001]

  reality = model (parameters β) + model discrepency $\varepsilon_{mod}(\theta)$

  Bayesian estimation of β,θ | data

- Description of the physical problem

  a plasma created by a laser beam hits an obstacle

  uncertainty on the collision time predicted by the model?

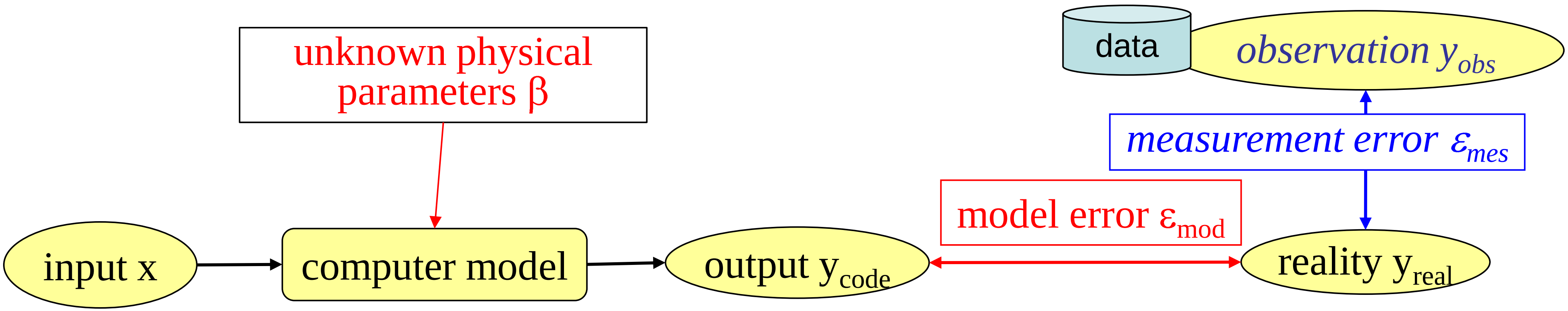
- Resolution

  We tune some parameters (without uncertainty) [Haan et al, 2009]

  reality = model(β) + $\varepsilon_{mod}(\theta)$ + numerical uncertainty ε_{num} [ASME 2010]

  the monotonic behaviour of the output is taken into account

Formalism for the quantification of uncertainties



KOH approach: Kennedy, O'Hagan, JRSS, 2001 – Higton et al, SIAM J. Sci. Comput., 2004

The 'universal' parameters of the physic model β* are unknown => β is a random vector

Even with β*, there is a discrepancy ε_{mod} between the model and the reality: ε_{mod} is an Gaussian process with hyper-parameters θ.

$y_{real}(x) = y_{code}(x,\beta^*) + \varepsilon_{mod}(x,\theta) \quad \forall x \in \mathbf{X} \subset R^d \quad (\mathbf{X}\text{: validity domain}), y \in R^q$

$y_{real}(x_i) = y_{obs,i} + \varepsilon_{mes}^{\ i} \ \ \forall x_i \in$ Data, ε_{mes} is a random vector

β and θ : random vectors with 'unknown' pdf

Bayesian framework

$$\begin{cases} y_{real}(x) = y_{code}(x,\beta^*) + \varepsilon_{mod}(x,\theta) \\ y_{real}(x_i) = y_{obs,i} + \varepsilon_{mes}^{i} \end{cases}$$

Bayes theorem:

$P_{post}(\beta, \theta \mid data) = P(data \mid \beta, \theta)\ .\ \pi(\beta, \theta) / L_{post}$

- $P(data \mid \beta, \theta)$ likelihood
- $\pi(\beta, \theta)$ prior probability
- $L_{post} = \int P(data \mid \beta, \theta).\pi(\beta, \theta)\, d\beta\, d\theta$ posterior (or total) likelihood

Resolution

- if θ fixed, y_{code} linear, π & ε_{mes} Gaussian, then β Gaussian (analytical expression)
  =>'plug-in' approach, with θ estimated by maximum likelihood or cross validation
  [Bachoc, Computational Statistics and Data Analysis, 2013]
- General case : Markov Chain Monte-Carlo
  => need to emulate the code with a metamodel

KOH framework

$y_{real}(x) = y_{code}(x,\beta^*) + \varepsilon_{mod}(x,\theta)$

$y_{code}(x,\beta) = \beta^T f_x + Z_x(\beta)$: kriging metamodel at each x (regression + GP)

$y_{obs,i} = \beta^T f_{xi} + Z_{xi}(\beta) + \varepsilon_{mod}(x_i,\theta) - \varepsilon_{mes}{}^i \ \forall x_i \in$ Data

Resolution

- for each experiment "x_i", construct the metamodel from N_i points $(\beta_j, y_{code}(x_i,\beta_j))$
- The likelihood $P(\text{data} \mid \beta, \theta)$ is then known
- MCMC resolution: $P_{post}(\beta, \theta \mid \text{data}) = P(\text{data} \mid \beta, \theta) \,.\, \pi(\beta, \theta) / L_{post}$
- We finally obtain the pdf of $y_{new},\beta,\theta|\text{data}$ for the prediction of a new experiment x_{new}

Extensions

- uncertainties on x (metrology, experimental setup...)
- tuning of "non-universal" parameters: Han, Santner, Rawlinson, Technometrics, 2009

$P_{post}(\beta, \varepsilon_{mod} \mid \text{data}, t) = P(\text{data} \mid \beta, \varepsilon_{mod}, t).\pi(\beta, \varepsilon_{mod}) / L_{post}(t)$

with $L_{post}(t) = \int P(\text{data} \mid \beta, \varepsilon_{mod}, t).\pi(\beta, \varepsilon_{mod})\, d\beta\, d\varepsilon_{mod}$ and $t = \text{argmax}\, L_{post}(t)$.

‘simple’ application of the KOH framework

Aim:

- comprehension of the method;
- (possible) difficulties

Experiments that are mainly 1D

- 1D code is sufficient => ‘quick’ simulations

Few unknown parameters

- MC resolution is sufficient

=> astrophysical POLAR experiments on the laser facility LULI

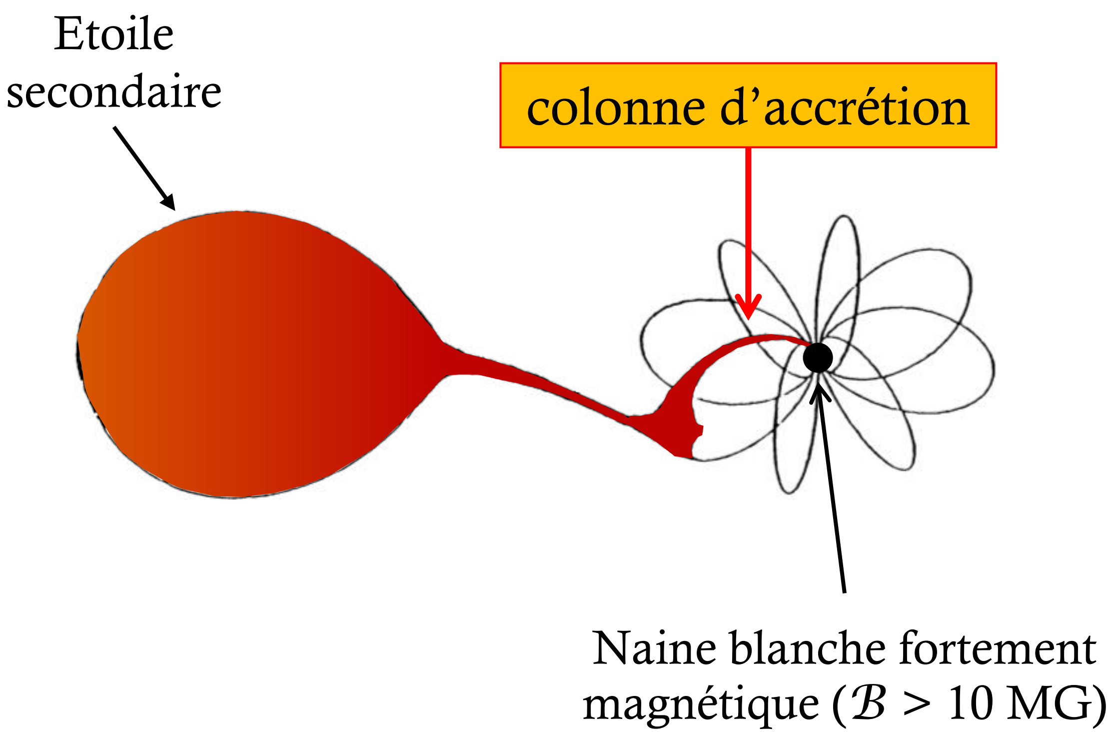
Accretion column in astrophysics

Polars are close binaries containing a magnetic white dwarf accreting material from a secondary star.

The matter is channelled to radial flow toward the magnetic pole.

Cropper M., Space Science Reviews **54** (1990)

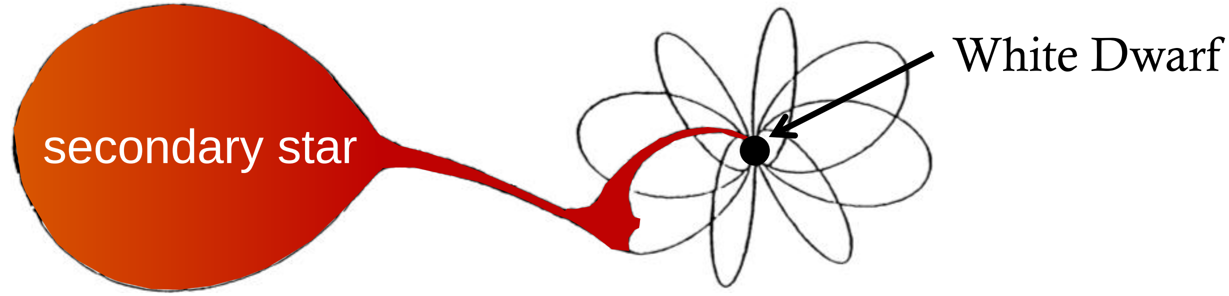
Wasner B., Cataclysmic variable stars (Cambridge Astrophysic Series,1995)



A radiative shock occurs in the accretion column

Wu, Space Sci. Rev. **93** (2000)
Cropper M. et al., PTRSA **360** (2002)
Drake R.P. Astropys.Spac. Sci. **298** (2005)

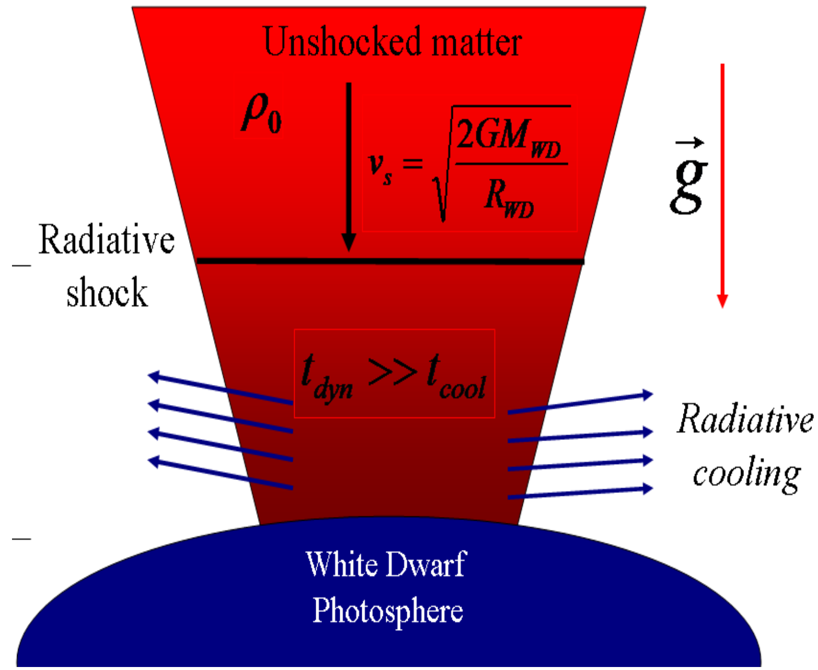
Michaut, ApSS 322, **77** (2009)



The falling matter hits the white dwarf surface at hypersonic velocity.

A reverse shock propagates through the accretion column.

Cooling processes in the shocked region slow down the shock.



This shock could be studied with computer models, but how to validate these models?

=> laboratory experiments

The radiative flow is characterized by dimensionless numbers reachable in laboratory with high-power laser facilities

dimensionless numbers

Fluid parameter	Astrophysics	LULI facility
shock length	100 km	0,5 mm
cooling time	1 sec	50 ns
accretion velocity [km/s]	100	80
Mach number	> 10	3
$R_{ps} = E_{int} / E_{rad}$	>> 1	2×10^4
$Bo_{ps} = F_{th} / F_{rad}$	>> 1	15
$\chi = t_{cool} / t_{hydro}$	<< 1	1

Falize E. et al. ApJ, 730, **96** (2011)

Scaling laws under the assumptions:

- optically thin medium, collisional shock, single temperature medium;
- curvature, Compton cooling, thermal conductivity, and gravitational field neglected.

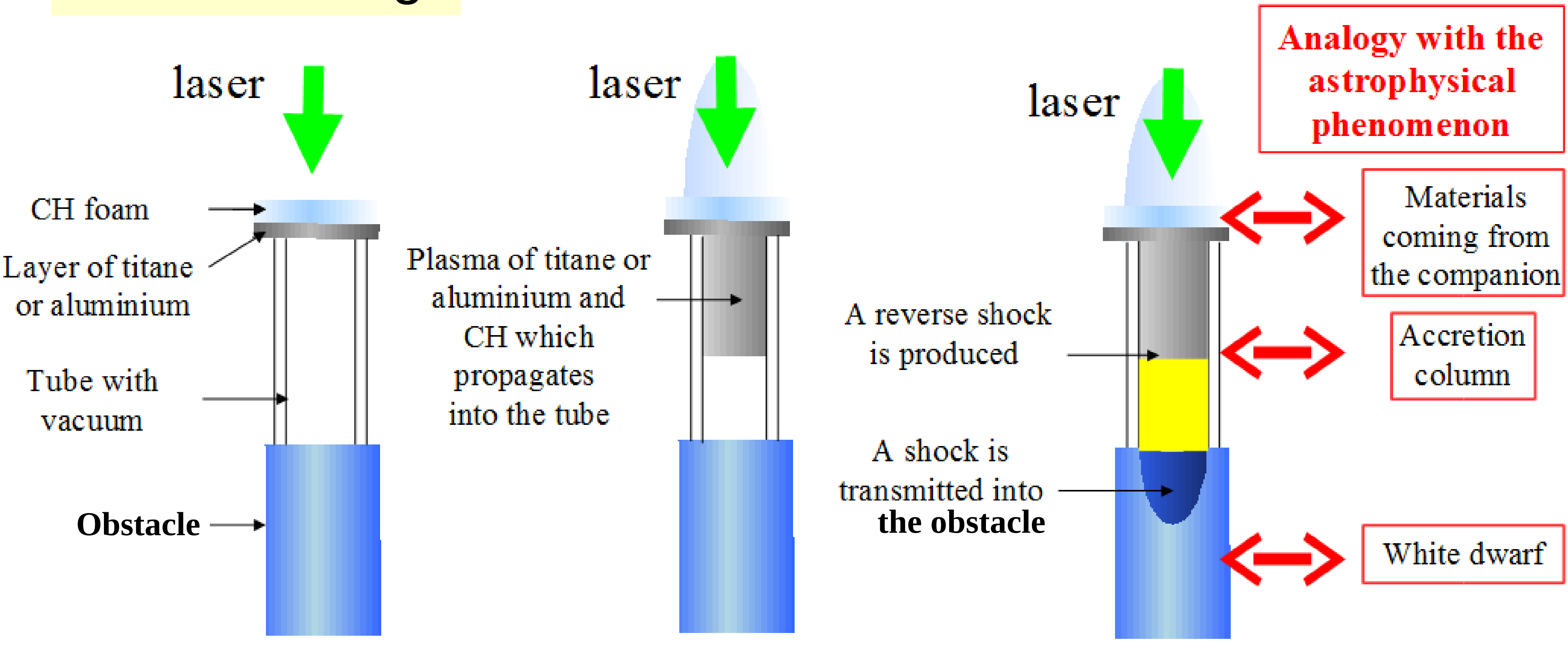
Kylafis N.D. & Lamb D.Q. , Astrophys ; J. Suppl. Ser. 48 (1982)
Falize E. et al. Astrophys. Space Science **322** (2009)

Experimental concept

A flow of plasma is created by the laser heating

The flow is collimated by a tube

The flow hits an obstacle to produce a reverse shock.



Falize E. et al. Astrophys. Space Science **336** (2011)

- **LULI: laser facility at Ecole Polytechnique, Palaiseau**
- **First POLAR campaign in 2009-10**
  - **preliminary experiments to demonstrate the feasibility**
  - **=> Uncertainty Quantification of computer model**
- *Second campaign in 2012 (diagnostics not fully available yet)*

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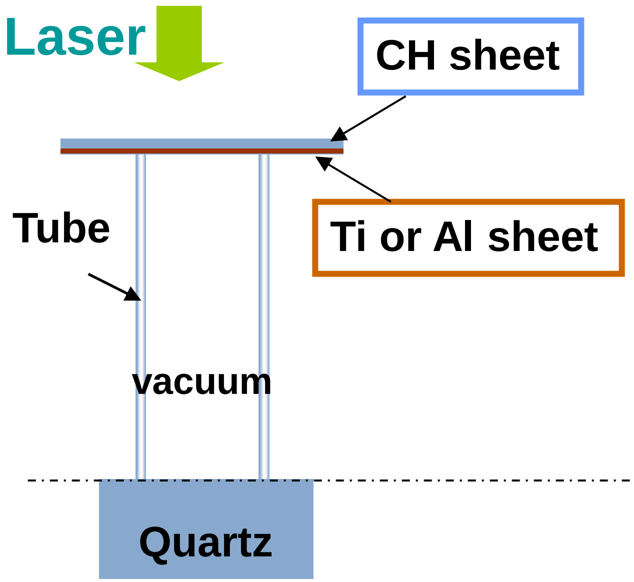
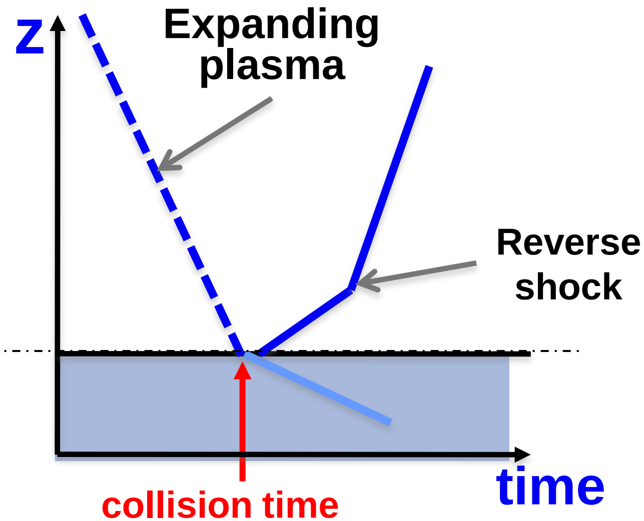
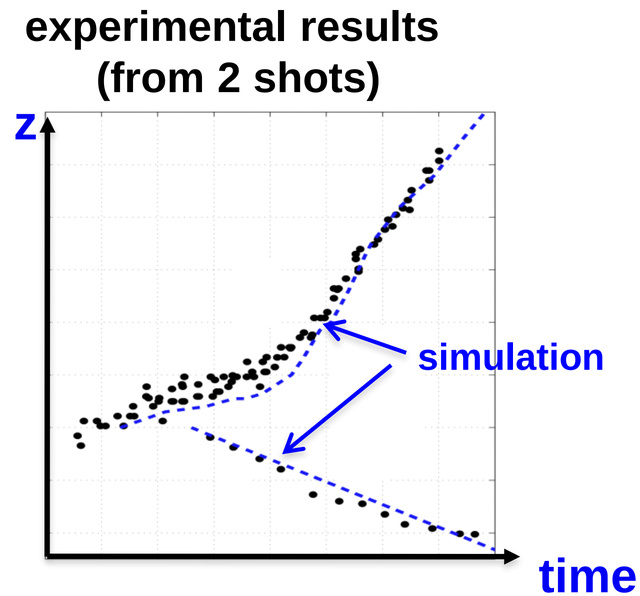
2009-2010 POLAR campaign on LULI facility: 8 experiments with collision time observations.

E. Falize et al. HEDP, **8** (2012)



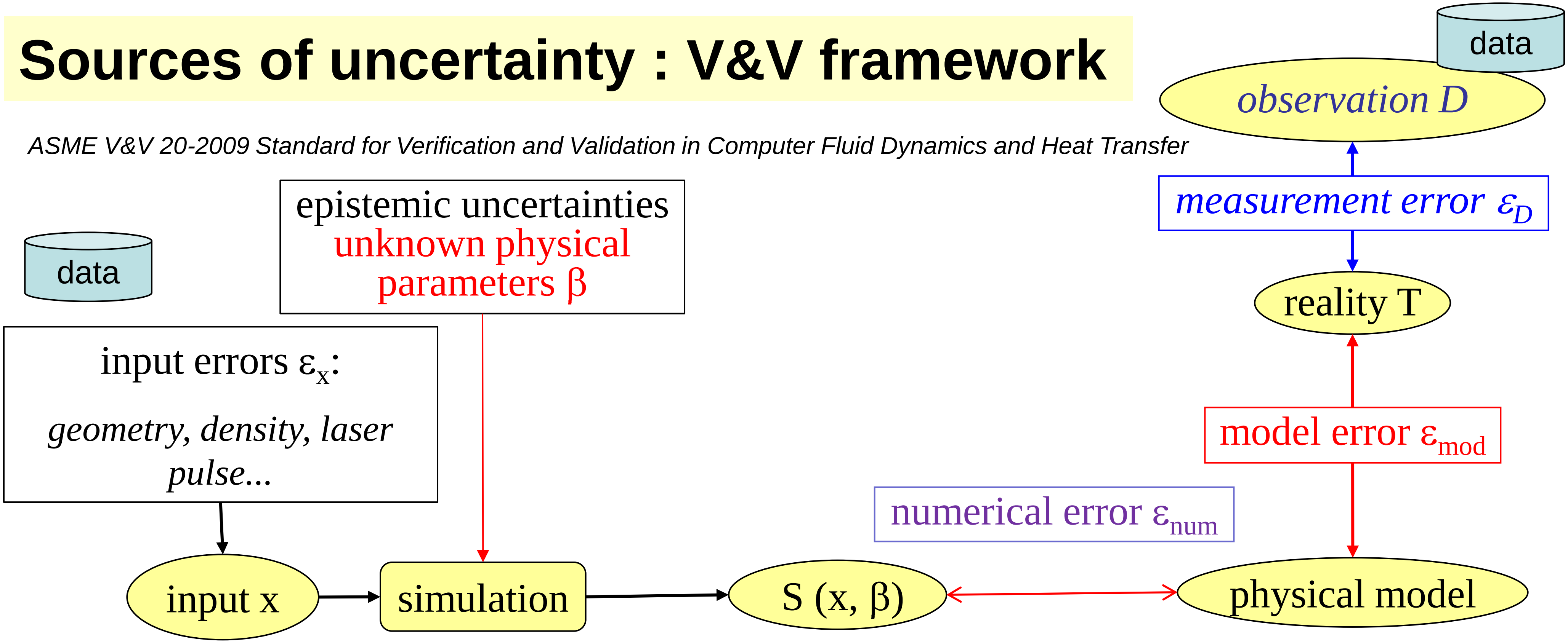




The aim of this study is to calibrate the simulation parameters from these 8 experiments and to quantify the uncertainty on the prediction of the collision time of a new experiment.

Sources of uncertainty : V&V framework

ASME V&V 20-2009 Standard for Verification and Validation in Computer Fluid Dynamics and Heat Transfer



Data: uncertainty on collision time measurement: $T = D + \varepsilon_D$

variations in hardware & laser drive: $x_T = x_D + \varepsilon_x$ for each exp^t.

Simulation:

$T(x) = S(x,\beta) + \varepsilon_{mod}(x) + \varepsilon_{num}(x)$;

uncertainty on input parameters β

model form uncertainty ε_{mod}

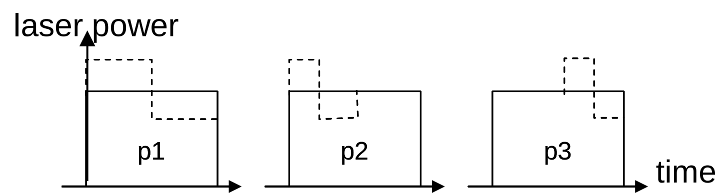
numerical uncertainties ε_{num}

Sequence of the study

- Reduction of the number of random parameters from a global sensitivity study (Morris method): 12 => 6
- Approximation of the code with a kriging metamodel for the 6 remaining random parameters
- Errors on x propagated on the metamodel => errors on y due to x unknown
- Numerical uncertainties obtained from a grid convergence study
- Resolution

13 unknown parameters

- 11 uncertain inputs x:
  - 5 target parameters: sheet densities & thicknesses (2 materials), tube length
  - 5 laser parameters: energy $E_{measured}$, duration and shape, measured outside the chamber window



  - laser transmission coefficient k_{Laser} from the outside chamber to the target

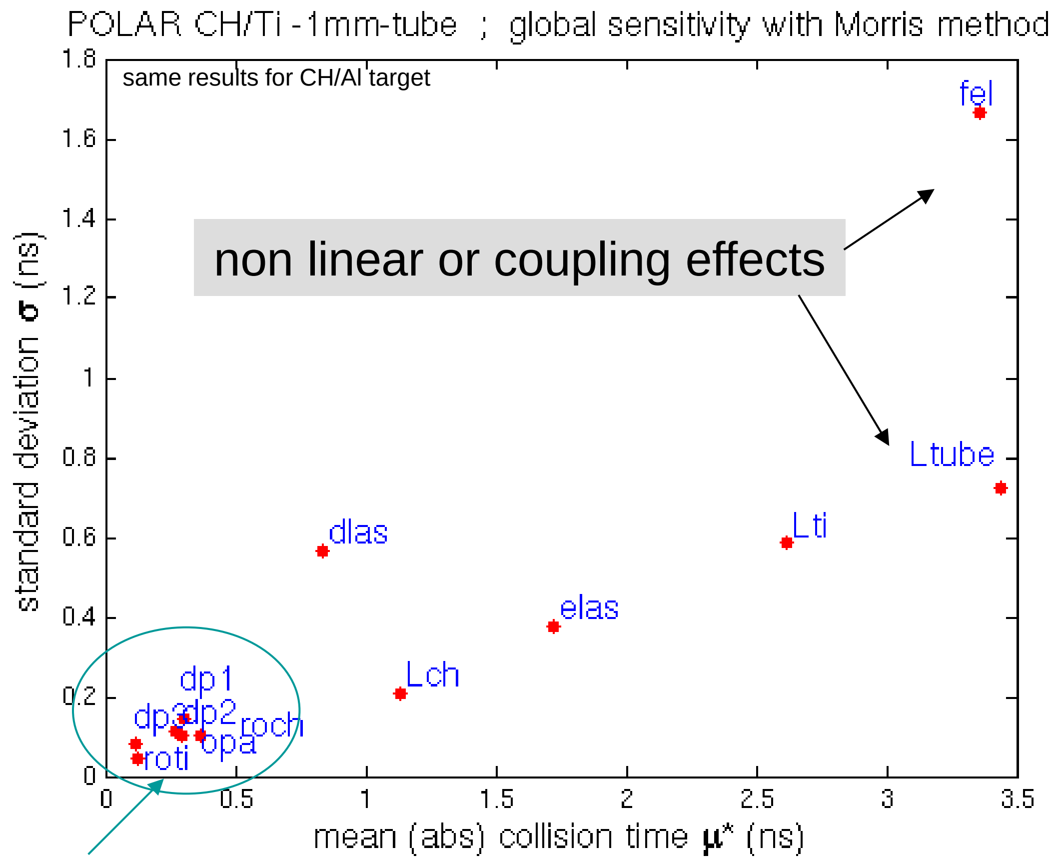
- 2 unknown physical parameters are:
  - the CH opacity scale factor x_{opa}
  - the electronic flux limiter f_{elec}.

As the code input is $E_{target} = K_{laser} * E_{measured}$,
we need only 12 variables to construct the emulator

A Global Sensitivity Analysis helps us to remove 6 factors among the 12

Morris method:

- 12 factors x_i, that is 13 differential simulations « One At a Time » OAT ;
- 32 trajectories OAT indexed by j.
- for each $\Delta x_{i,j}$, we obtain the collision time differential $\Delta y_{i,j}$.
- μ^* is the mean of $|\Delta y|$ and σ is the standard deviation of Δy.



6 factors are removed: ρ_{CH}, ρ_{pusher}, $p_{1/2/3}$, x_{opa}.

6 factors remain: L_{CH}, L_{pusher}, L_{tube}, E_L, d_L and f_{elec}.

Morris M., Technometrics 32 (1991)
Saltelli A. et al., Sensitivity Analysis, John Wiley and Sons, Chichester (2000).

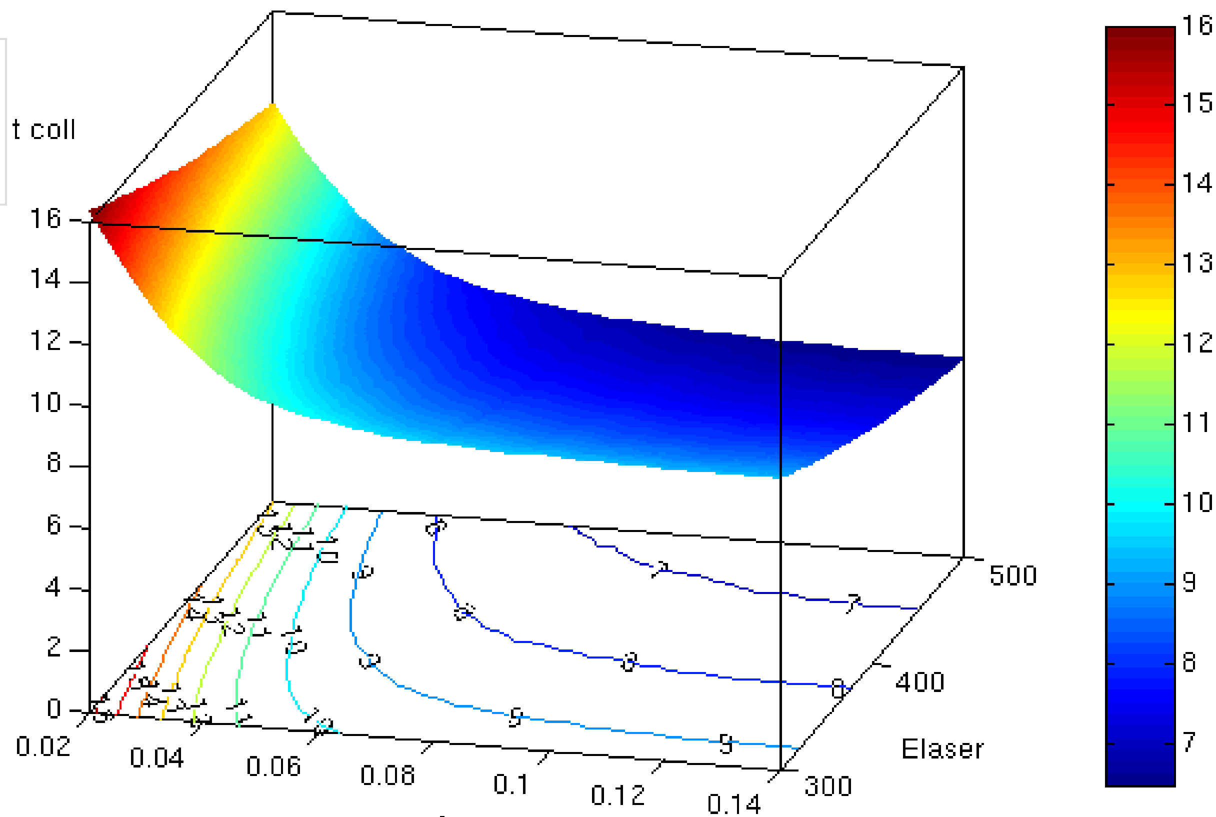
We have built a surrogate of the simulation outputs for each type of target

Kriging surrogates *. ~2000 points for each target, 2/3 to construct the surrogate & 1/3 to validate it.

*Lophaven, Nielsen, Søndergaard, IMM-REP-2002-13.

Surface response

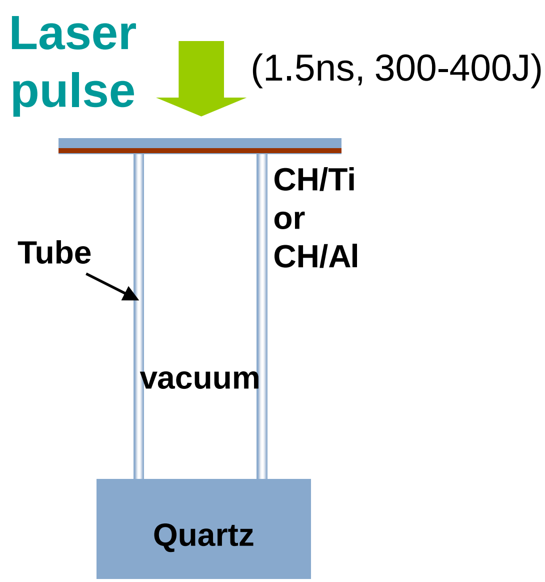
for nominal CH/Ti target

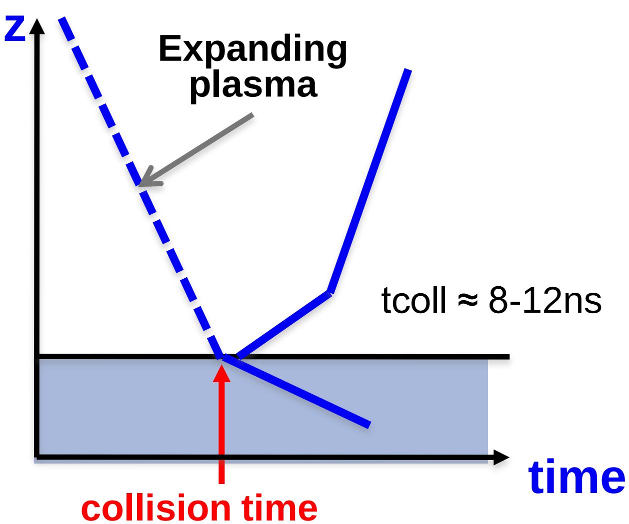


f_{elec}

The validation rmse (62ps) is negligible compared to data uncertainties.

Huge experimental errors in this preliminary campaign





- **laser measurement errors:**

energy	U = 15%	*uncorrelated*
duration	U = 10%	*uncorrelated*
shape (modes 1-4)	U = 15%	*uncorrelated*

- **target characterization errors:**

sheet densities	U = 1 to 10%	*correlated*
sheet thicknesses	U = 10 to 20%	*correlated*
tube length	U = 20%	*uncorrelated*

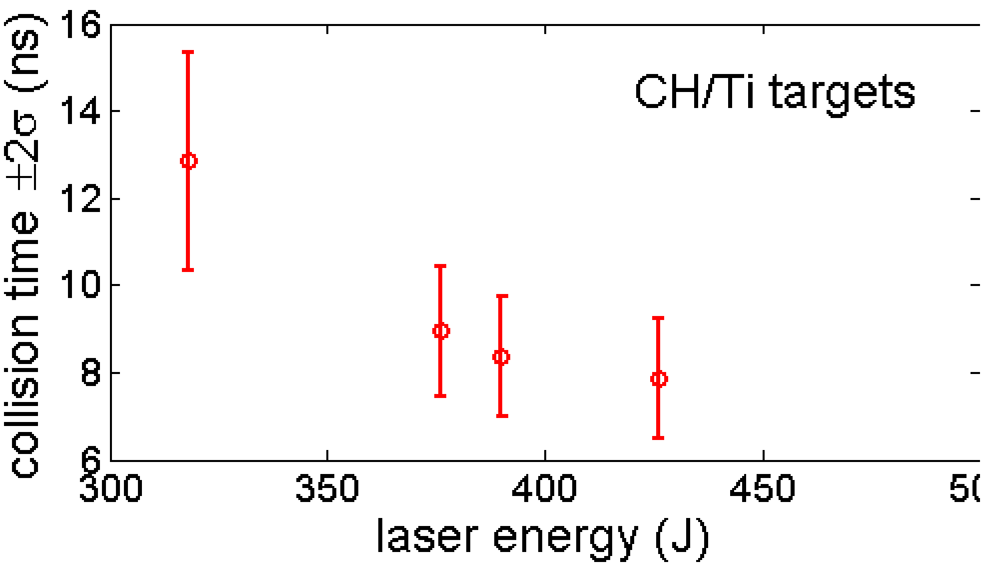
- **Collision time measurement errors:**

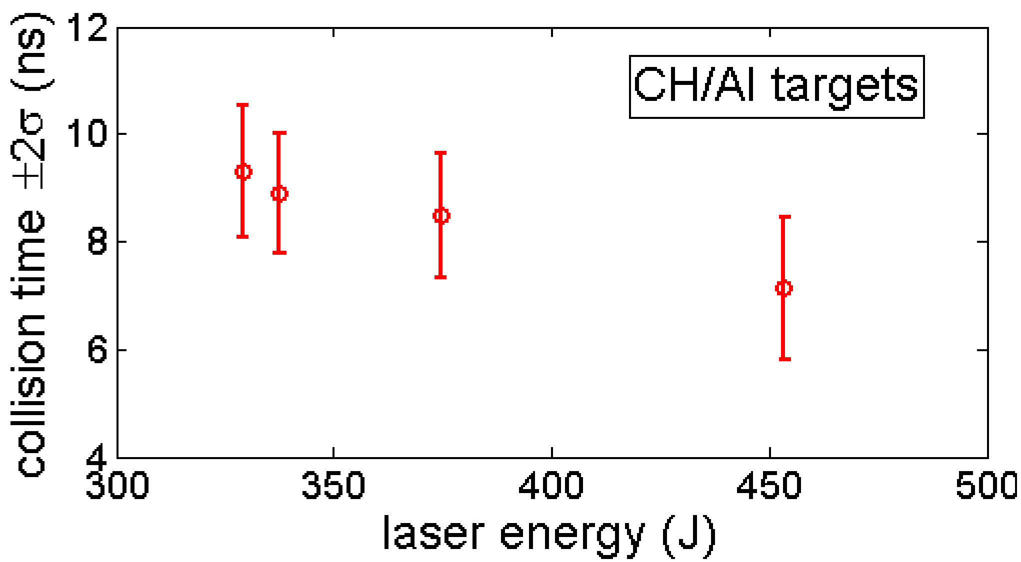
U = 250 ps (~2-3%) *uncorrelated*

Total data uncertainty is about U ≈ 3 ns.

Total uncertainty on collision time D (for a known input x) is obtained by propagating input uncertainties ε_x through the simulation with a Monte-Carlo method (Gaussian PDF with U=2σ).

Data uncertainties are huge ($\sigma_D \approx 1.5$ ns compared to observation time σ_{tcoll} = 0.25 ns) mainly due to poor target characterizations.





2 unknown parameters β : flux limiter & laser transmission

We use diffusion instead of transport for the thermal model, with an electronic flux limiter:

- geometric mean between f_{elec}* $F_{theoretical}$ and computed flux ∇T_e.

The laser energy is measured outside the chamber, not on the target:

- $E_{target} = E_{measured} * K_{laser}$
- K_{laser} comes from the non-perfect transmission into the last lenses.

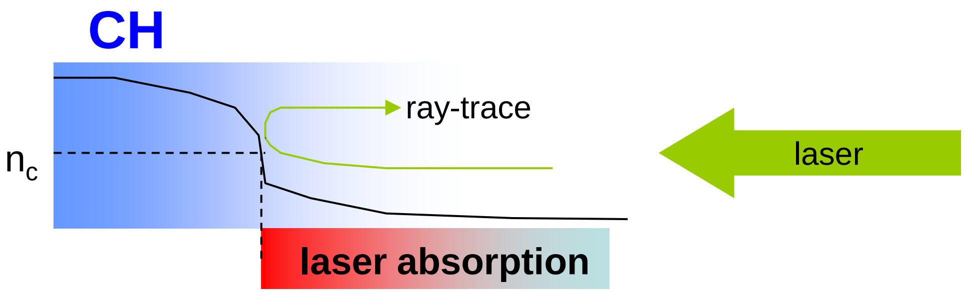
Initial statistical model: $T(x) = S(x,\beta) + \varepsilon_{mod}(x) + \varepsilon_{num}(x)$

For a given target, x is only the laser energy E.

The statistical model becomes:

$T(E) = S(K_{laser} * E,\ f_{elec}) + \varepsilon_{mod}(E) + \varepsilon_{num}(E)$

ε_{num} obtained from a grid convergence study



- The laser energy is absorbed along ray-traces until the critical density n_c.
- A part of the energy is deflected according to the density gradient at n_c.
- This gradient is very sharp, and needs a very fine mesh resolution.

E_{abs} errors are estimated with the GCI method on a simplified problem (only CH and X-ray diffusion scheme). The grid was halved 7 times (maximum reasonable run time). The convergence is very low: apparent order $p \ll 1$

$E_{abs}^{\text{converged mesh}} = E_{abs}^{\text{nominal mesh}} *(K_{num} + \eta_{num})$ with $\eta_{num} \sim \mathcal{N}(0,\sigma_{num})$.
This uncertainty is propagated on the model with a Taylor expansion.

final statistical model

$T(E) = S(K_{num} * K_{laser} * E, f_{elec}) + \varepsilon_{mod}(E, L_{cor}, \sigma_{mod}) + \partial S/\partial E * K_{laser} * E * \eta_{num}$

$T(E_D) = D(E_D) + \varepsilon_D(E_D)$ for the data points

Bayesian inference

We infer K_{Laser} & σ_{mod} from the data D and

we tune L_{cor} & f_{elec} in order to maximize the posterior likelihood

posterior $\propto$ likelihood * prior

$P_{post}(k_{Laser}, \sigma_{mod} \mid D, L_{cor}, f_{elec}) = P(D \mid k_{Laser}, \sigma_{mod}, L_{cor}, f_{elec}) * \pi(k_{Laser}, \sigma_{mod}) / L_{post}$

$(L_{cor}, f_{elec}) = \text{argmax } L_{post}$

Prior $\pi(k_L, \sigma) = \pi(k_L) . \pi(\sigma)$

$\pi(k_L)$ uniform on [0.6 ; 1]

Non-informative Jeffreys prior $\pi(\sigma)$ taking into account the observation errors

Robert C.P., The Bayesian Choice, Springer-Verlag, New York, (1994)

Jeffreys H., Proceeding of the Royal Society of London, Ser. A (1946)

Jeffreys prior for $X=(X_i)_{i=1,n}$ and $X_i \sim \mathcal{N}(0,\sigma^2+v_i)$:

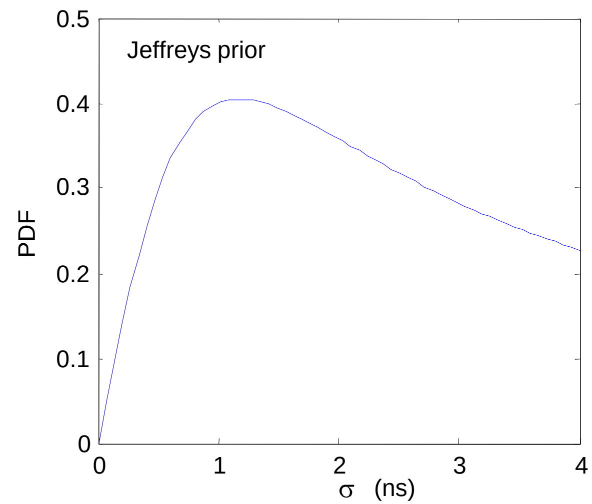
$$\pi(\beta,\sigma) = \sigma\left[\frac{1}{n}\sum_{i=1}^{n}\left(\sigma^2 + v_i\right)^{-2}\right]^{1/2}$$

For same observation errors $v_i=v$:

$$\pi(\beta,\sigma) = \frac{\sigma}{\left(\sigma^2 + v\right)}$$

v=0 gives the classical Jeffreys prior:

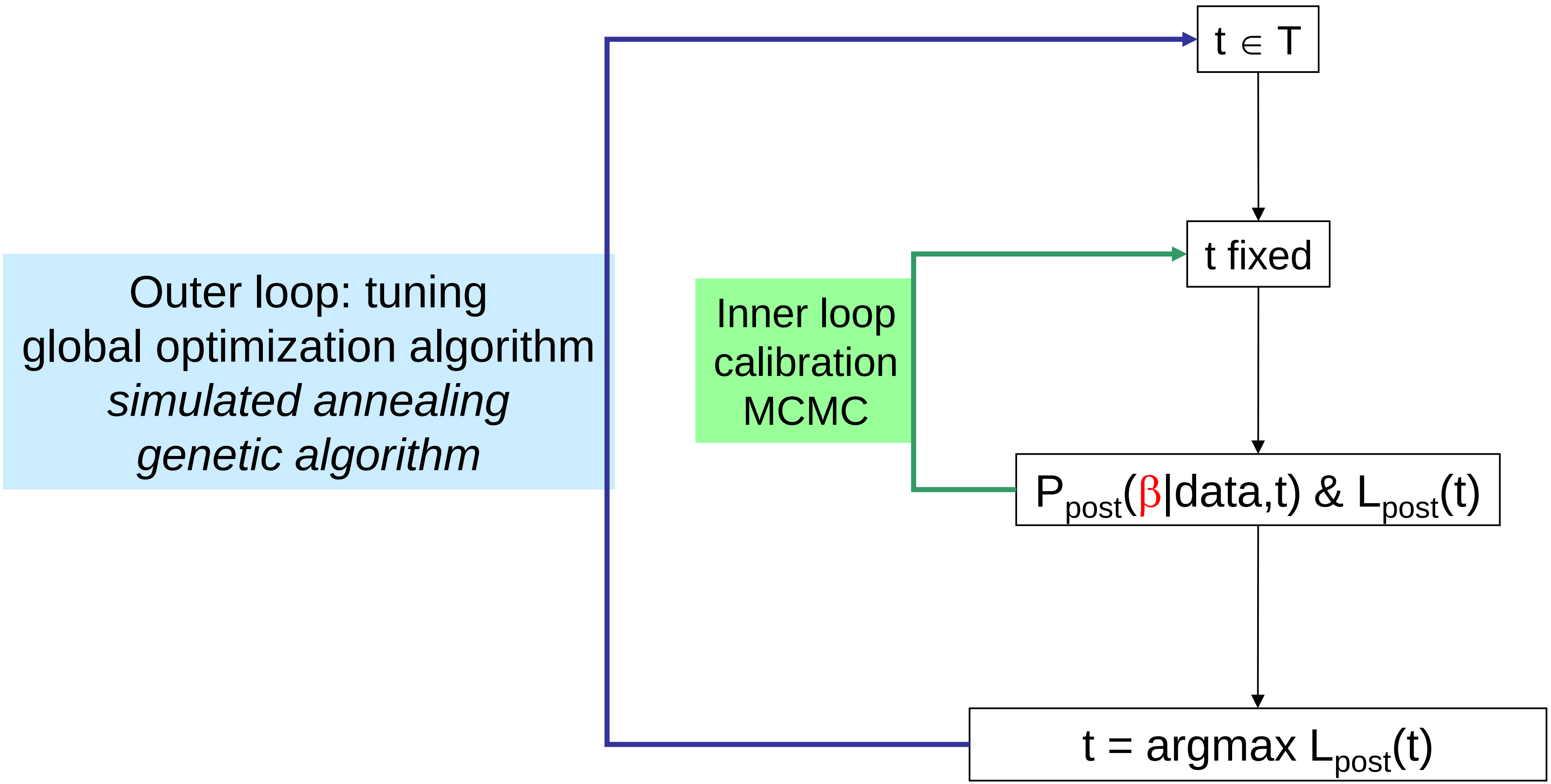
$$\pi(\beta,\sigma) = \frac{1}{\sigma}$$



Gaussian Process $\varepsilon_{mod}(x, L_{cor}, \sigma_{mod})$

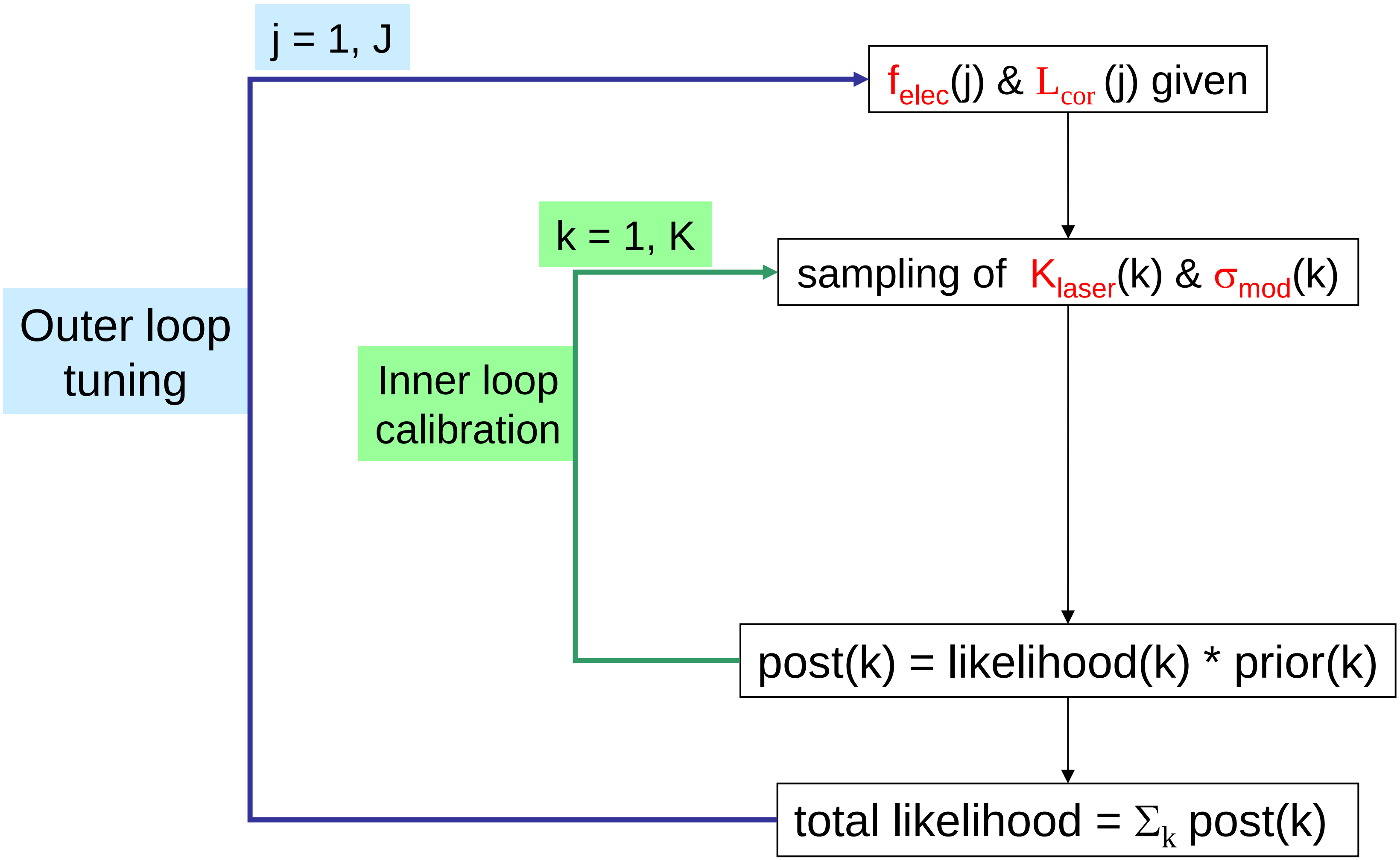
$\varepsilon_{mod}(x) \sim N(0,\sigma_{mod})$ and $<\varepsilon_{mod}(x),\varepsilon_{mod}(x')> = \exp -(x-x')^2/L_{cor}^2$ (Gaussian correlation)

Algorithm: double loop for calibrating β and tuning t



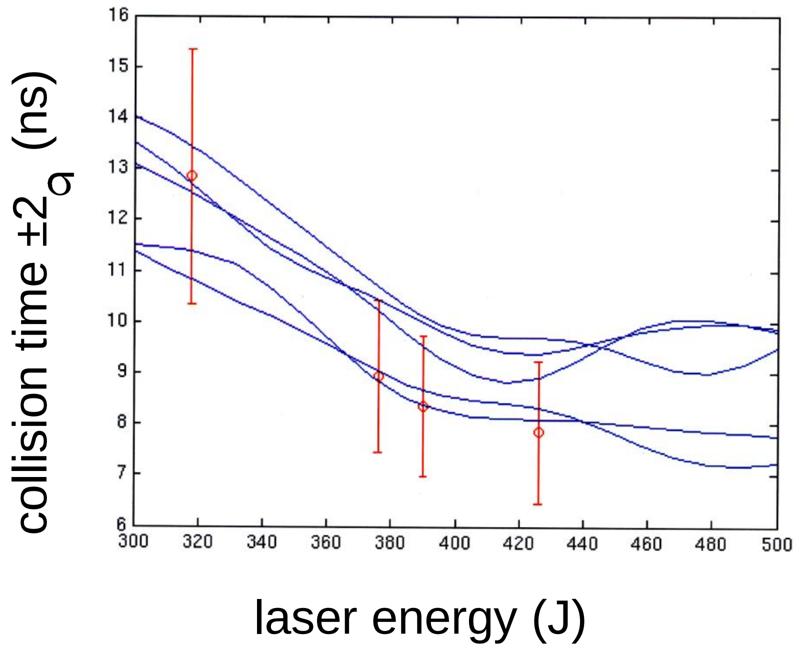
here β is a 2D vector (=> MC) and t is 2D also => ‘scanning’ of T

Calibration of (K_{laser}, σ_{mod}) and tuning of (f_{elec},L_{cor})

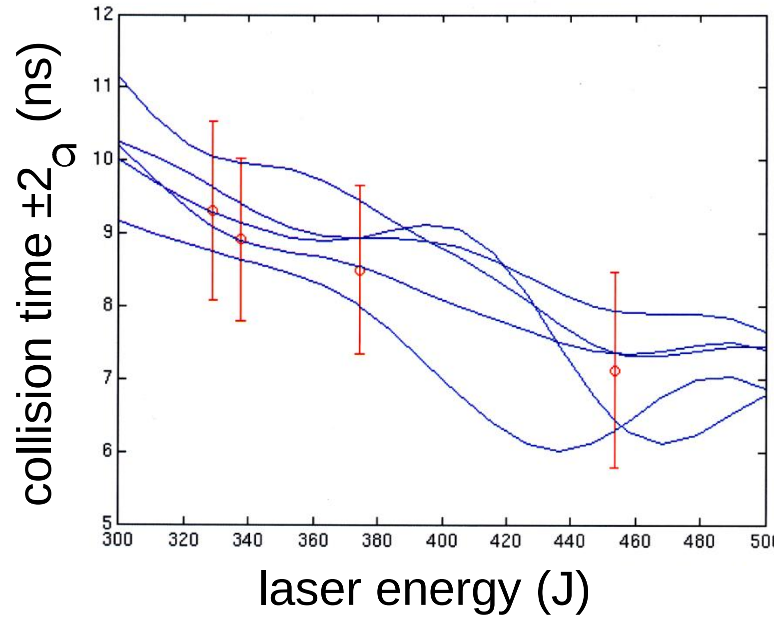


Predictive uncertainty on collision time: non monotonic behavior of $t_{coll} = F(E)$!

CH/Titanium targets



CH/Aluminum targets



Only 5 realizations plotted, L_{cor} = 50J

Taking into account monotonic behavior in kriging surrogate:

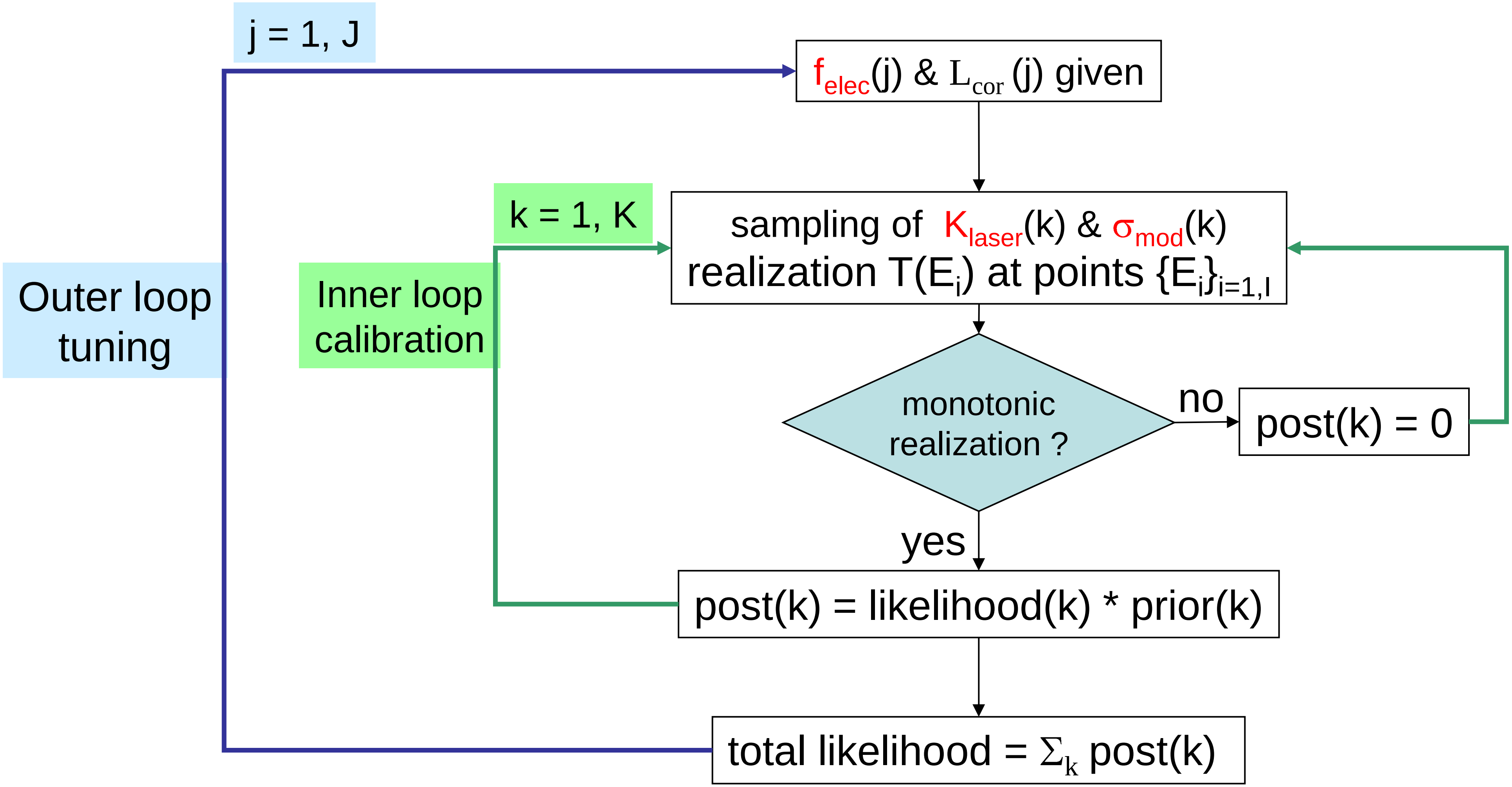
[Kleijnen, van Beers, 2001] bootstrap

[Da Veiga, Marrel, 2012] truncated normal laws

in both papers, the likelihood is not consistent with monotonicity

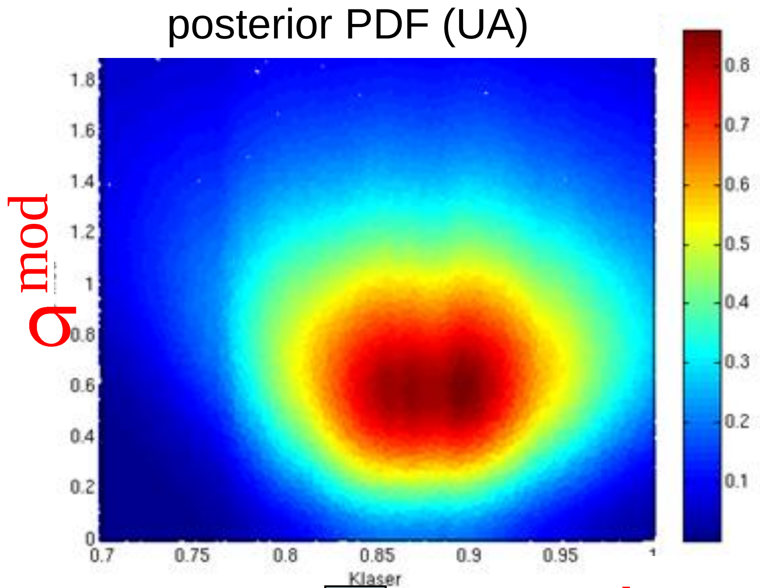
likelihood=0 if realizations y_m at E_m are non monotonic => Ppost (y_m, β | data, y_m monotonic)

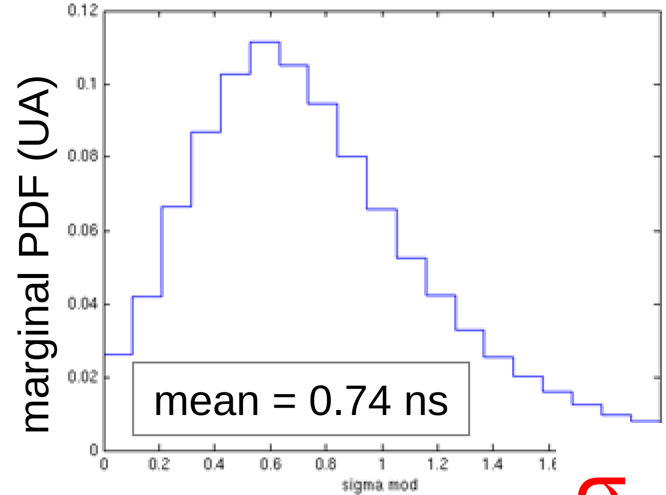
Algorithm: double loop & monotonic realizations

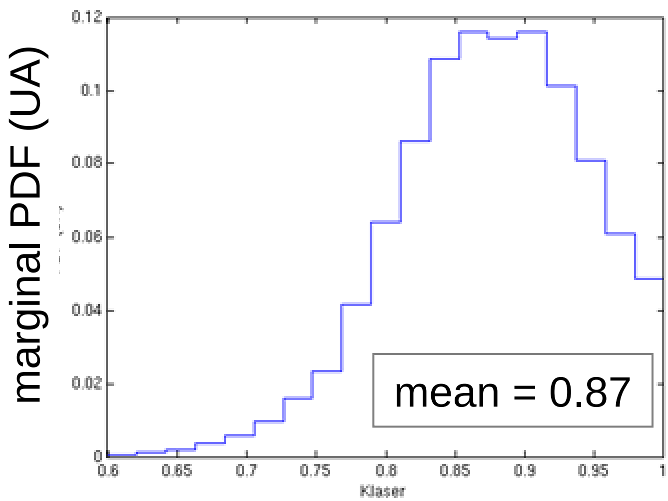


$$T(E) = S(K_{num}*K_{laser}*E,\ f_{elec}) + \varepsilon_{mod}(E) + \partial S/\partial E*K_{laser}*E*\varepsilon_{num}$$

Posterior probability $P_{post}(k_{Laser}, \sigma_{mod})$





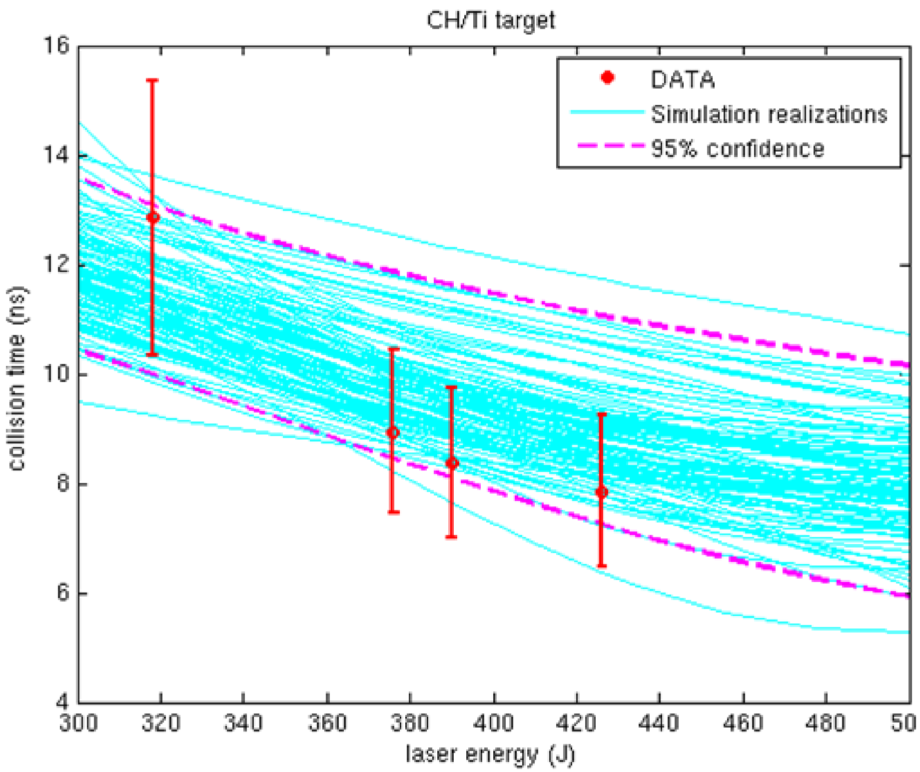


The tuning parameters that maximize the posterior likelihood are:

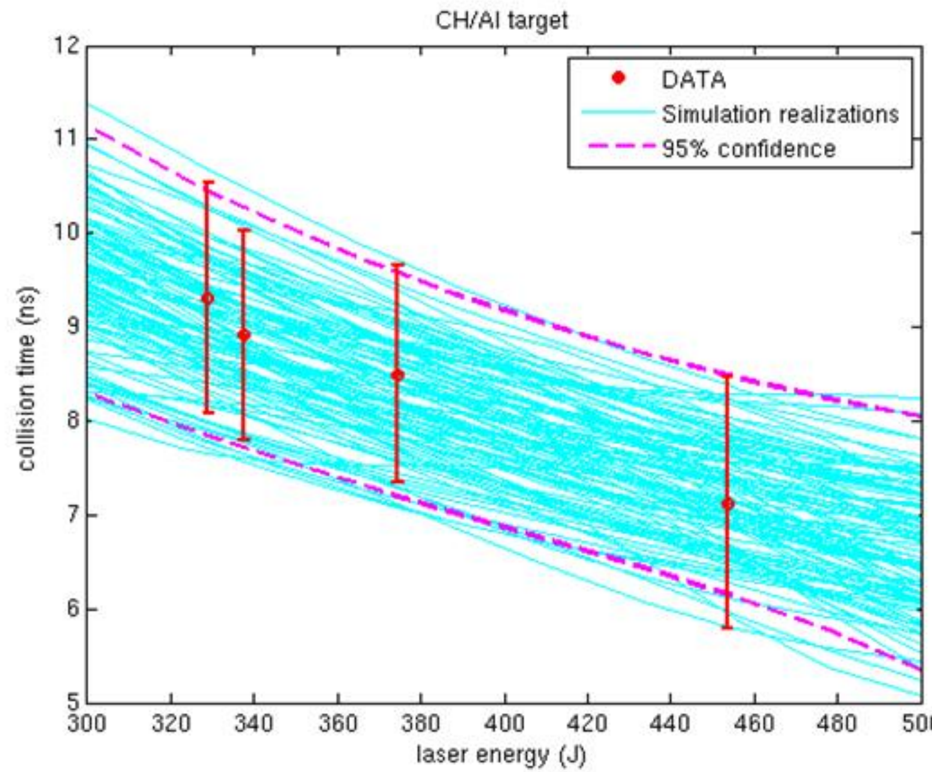
- f_{elec} = 0.096
- L_{cor} = 150 J

Predictive uncertainty on collision time

CH/Titanium targets



CH/Aluminum targets



Only 100 monotonic realizations plotted

Summary

- The KOH framework [2001] was applied to a real *1D*-problem.

- Another source of uncertainty is the numerical errors [ASME 2009]

- 2 tuned parameters and 2 calibrated ones [Han 2009]

- Likelihood with monotonic behavior of the output as a function of E

N.B. The numerical resolution is possible here due to the very low dimension.

Future work

- multi-fidelity codes (i.e. different grids) with multi-fidelity kriging emulator [Le Gratiet & Garnier, 2012, submitted to International Journal of Uncertainty Quantification].