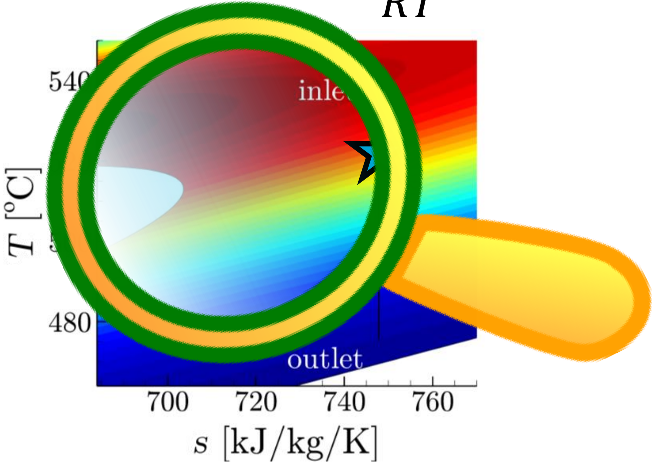
Towards the Validation of NICFD Codes

$$1 - Z = 1 - \frac{Pv}{RT}$$



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Matteo Pini

Delft University of Technology

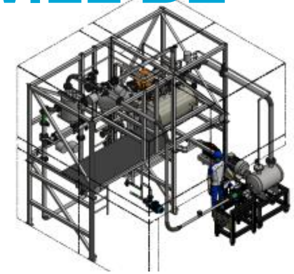
13-09-2017

Research Questions

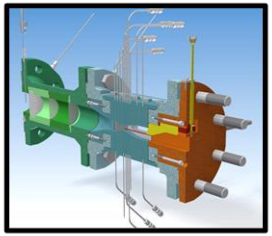
- How accurately can supersonic/transonic flows of dense organic vapors and supercritical fluids be predicted?

- Can CFD codes be **validated** against measurements in **non-ideal compressible flow regions**? How?

Deliverables
(HOW THE RESEARCH QUESTION WILL BE ANSWERED)



- ORCHID (**ORC H**ybrid **I**ntegrated **D**evice)



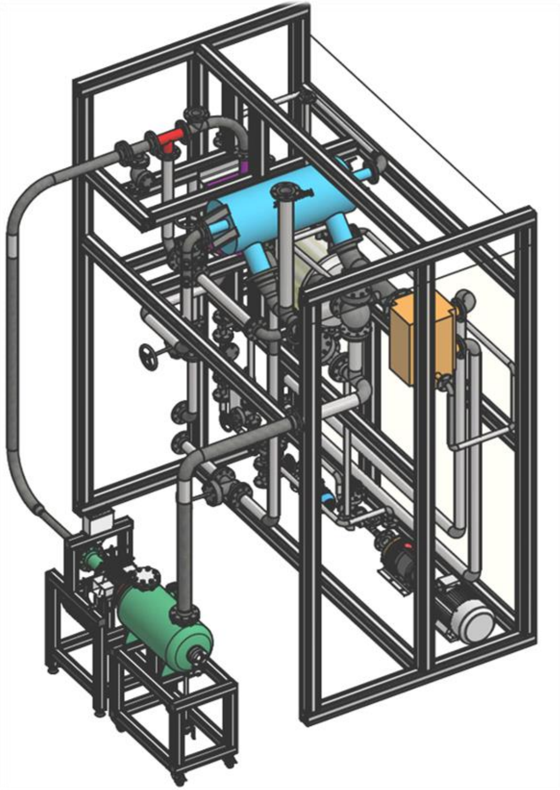
- Nozzle TS
- Validated in-house CFD code for non-conventional turbomachinery, and fundamentals of NICFD

- **Relevance:** Provide ORC turbine designers with **methods** and eventually data to validate NICFD codes (validate comp. submodels of SU2).

- **Originality:** Design of validation experiments (done exactly for NICFD)

General Overview

- The ORCHID
- SU2 for ORC Turb.
- Design of Experiments (DoE)
- Validation Method / Tools
- Feasibility Test
- Conclusions



The ORCHID

Local Measurements

),

city

PIV)

),

wave

n)

tics

vectors

Validation of SU2 for ORC Turbom.

COMPUTATIONAL SUBMODELS OF…

Turbulence

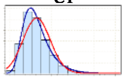
1 Eqn: Spalart–Allmaras
2 Eqn: SST
L&M Transitional

SU2
The Open-Source CFD Code

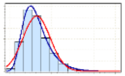
Transport Models

Sutherlands Law
Chungs Method
Method of corresponding states

P_{cr}



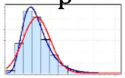
T_{cr}



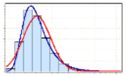
Eqn of State

PR, ideal gas, VW
LuT: iPRSV, RefProp

C_{p}



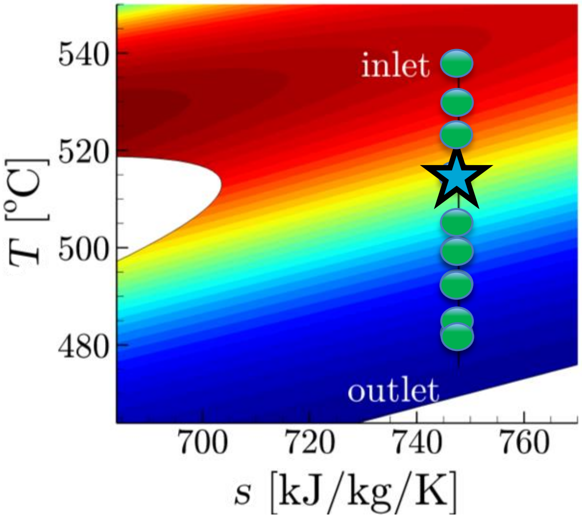
ω



Design of Experiments (1/2)

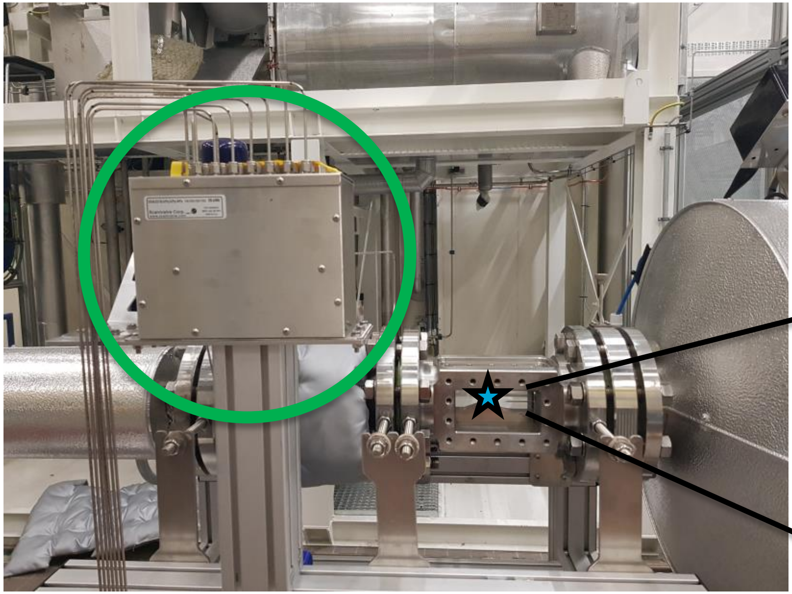
NOZZLE

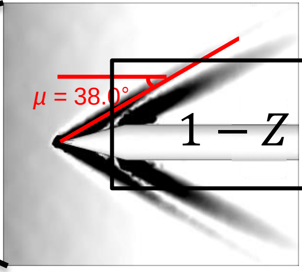
Phase 1: Flow Visualization and Conventional Techniques



Direct

Indirect



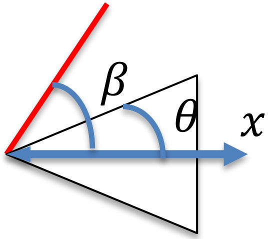


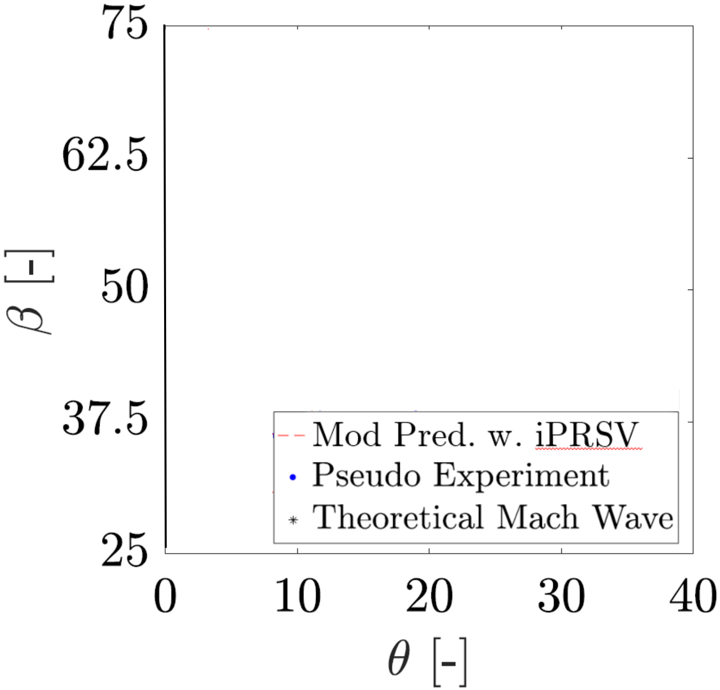
$$1 - Z = 1 - \frac{Pv}{RT}$$

$$M_{Tip} = \frac{1}{\sin \mu}$$

Design of Experiments (2/2)

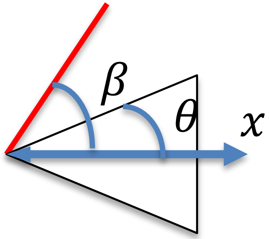
EXAMPLE RESULT: θ–β– M CURVE

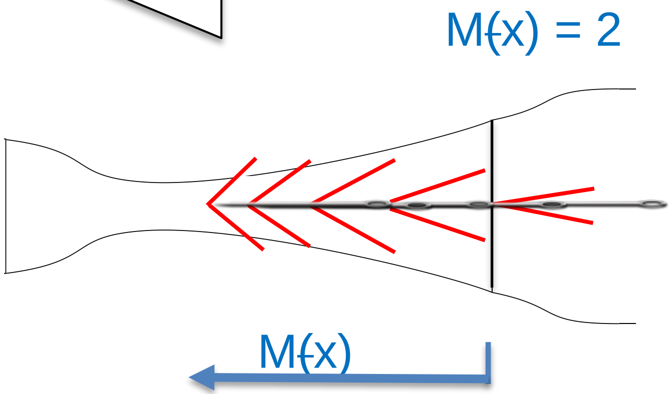




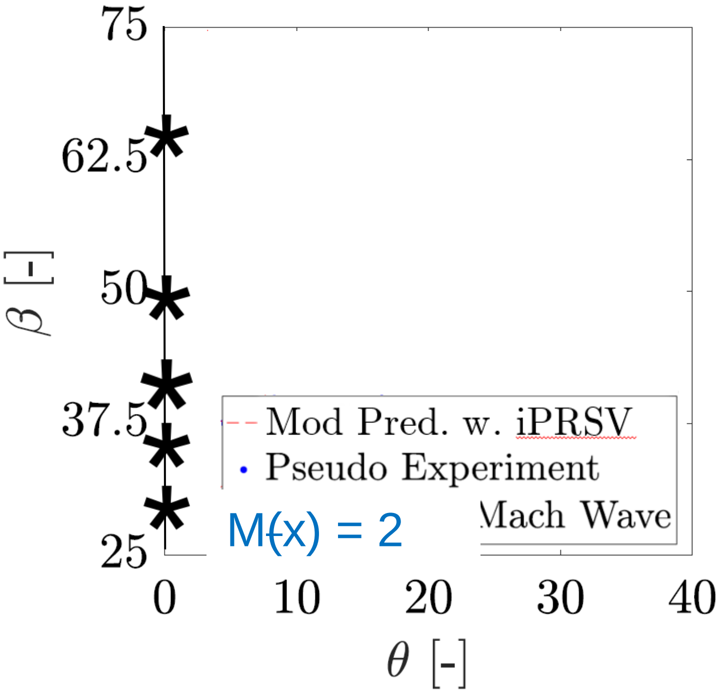
Design of Experiments (2/2)

EXAMPLE RESULT: θ–β– M CURVE



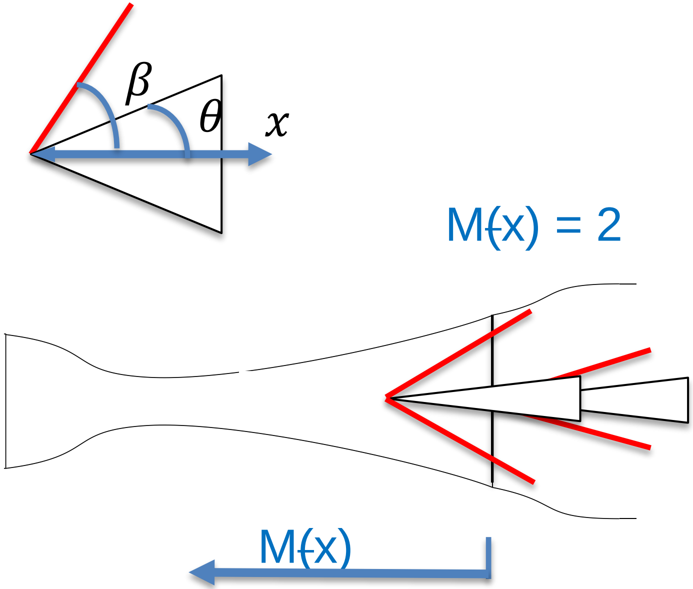


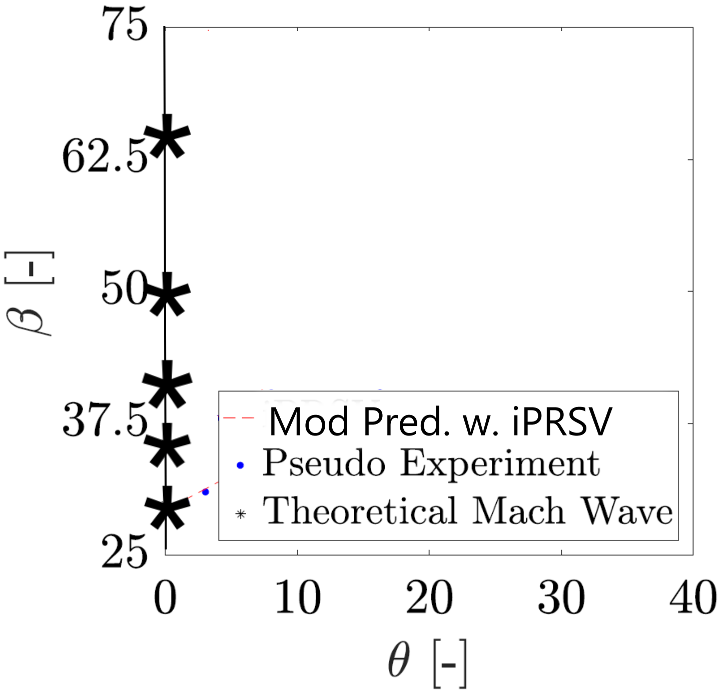
$$M_{Tip} = \frac{1}{\sin \mu}$$



Design of Experiments (2/2)

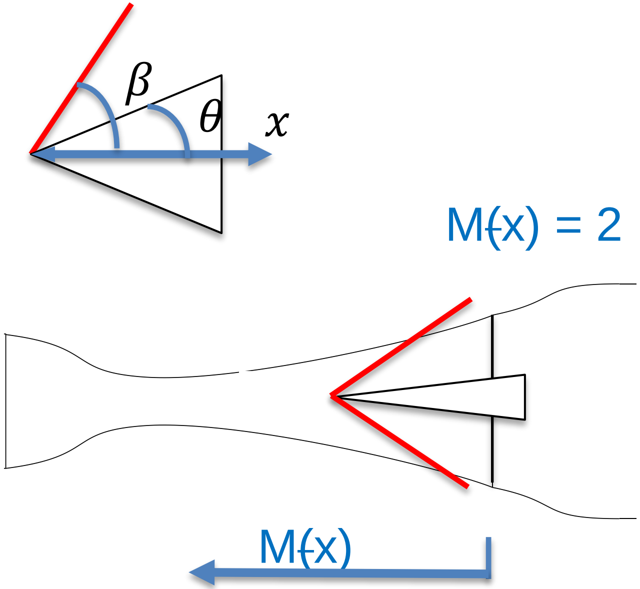
EXAMPLE RESULT: θ–β– M CURVE

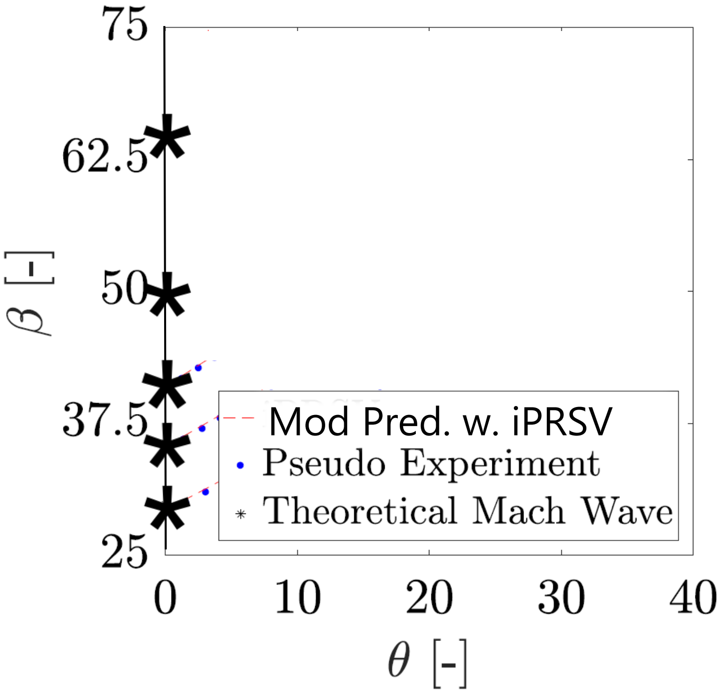




Design of Experiments (2/2)

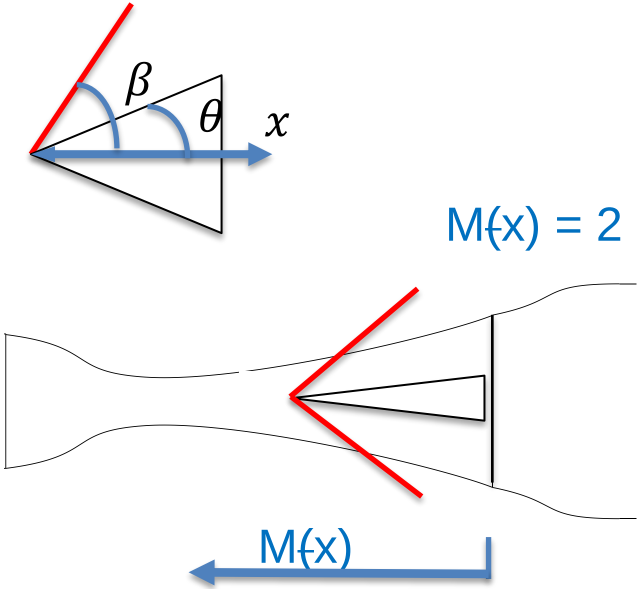
EXAMPLE RESULT: θ–β– M CURVE

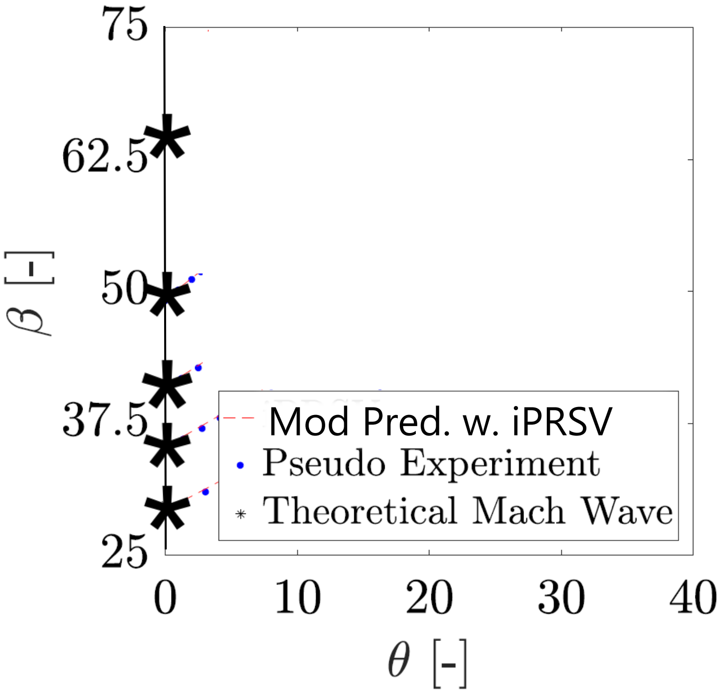




Design of Experiments (2/2)

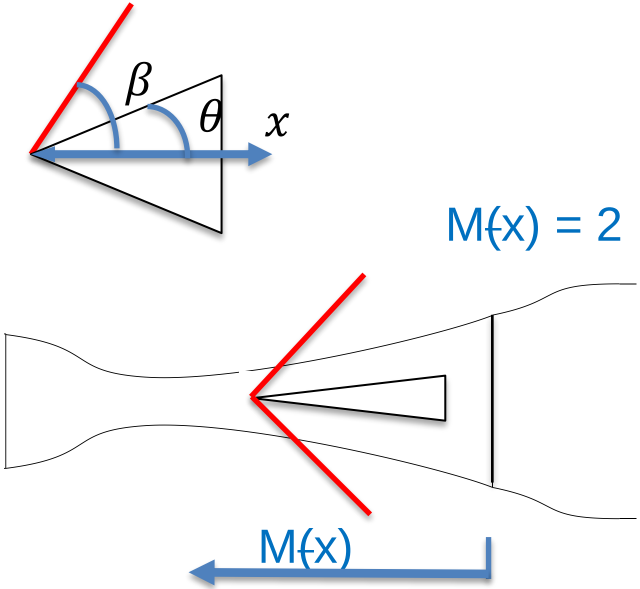
EXAMPLE RESULT: $\theta - \beta - M$ CURVE

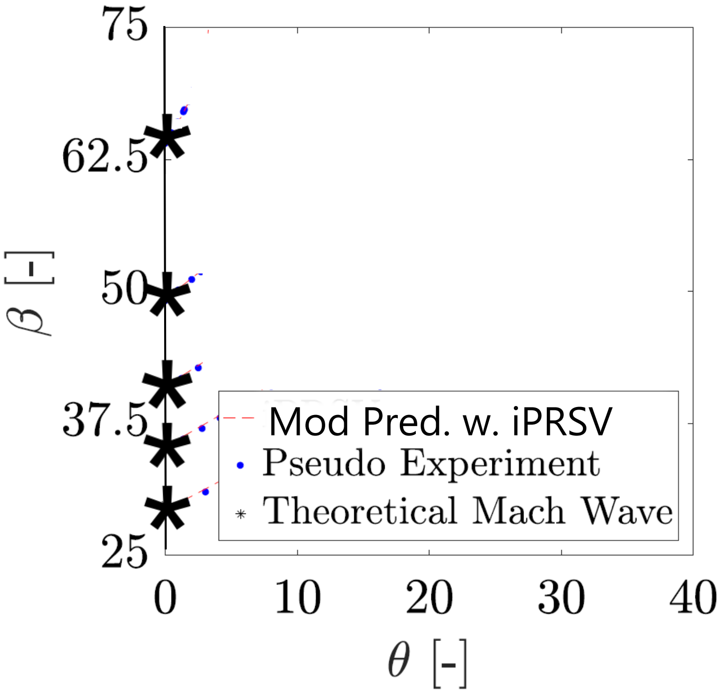




Design of Experiments (2/2)

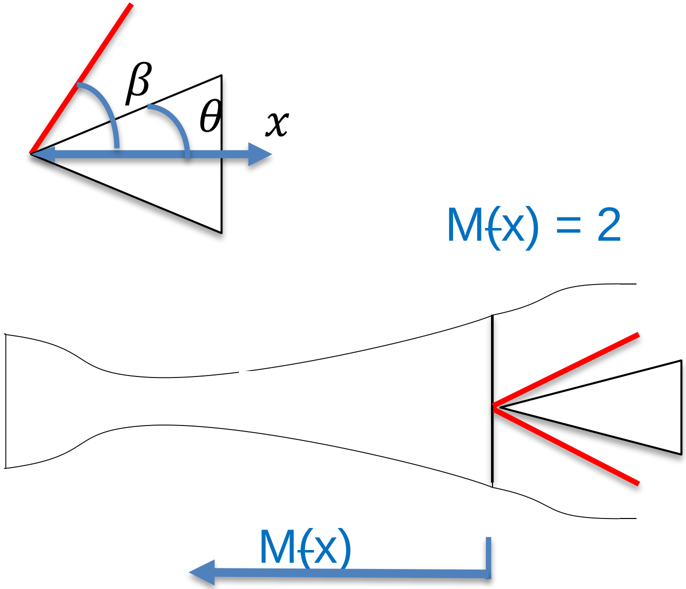
EXAMPLE RESULT: θ–β– M CURVE

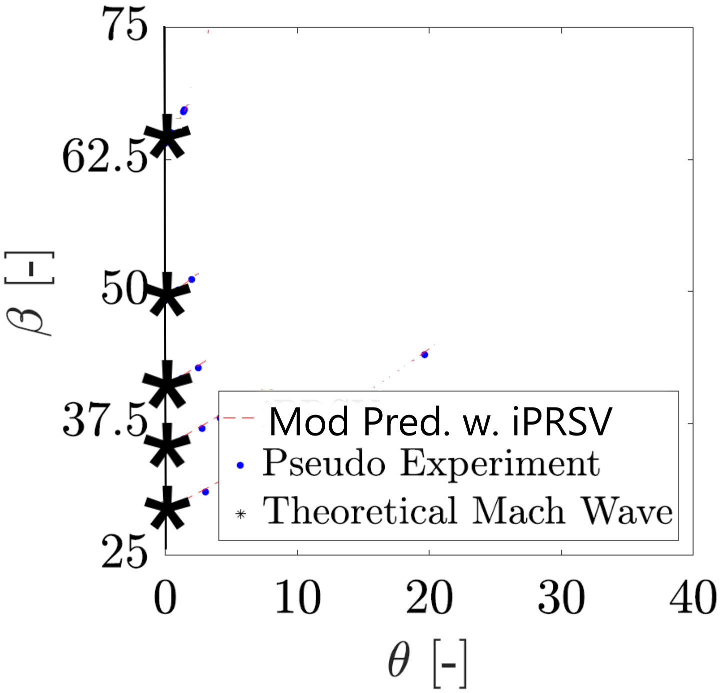




Design of Experiments (2/2)

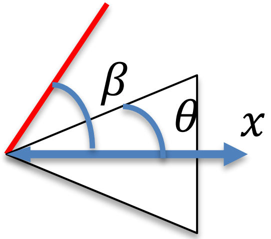
EXAMPLE RESULT: $\theta-\beta-M$ CURVE

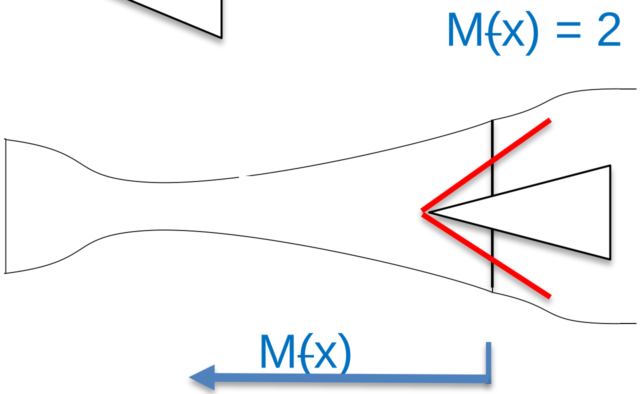


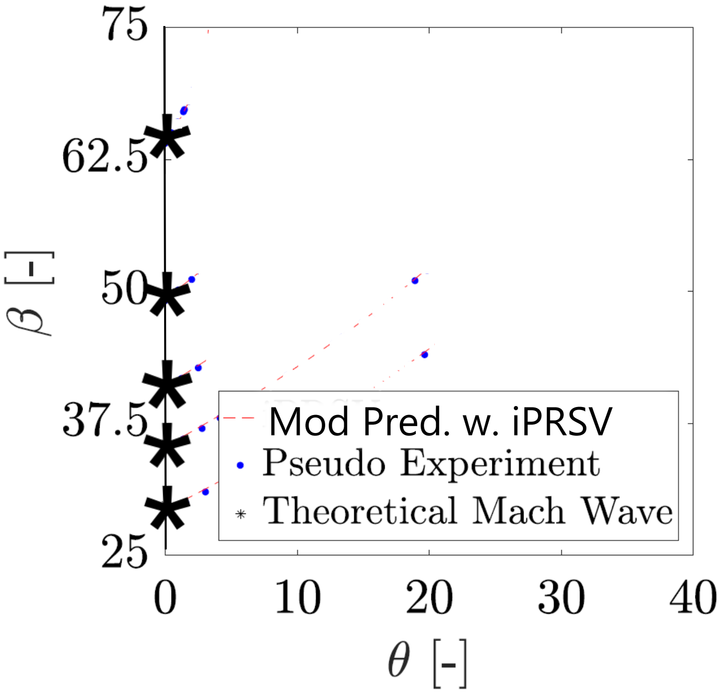


Design of Experiments (2/2)

EXAMPLE RESULT: θ–β– M CURVE

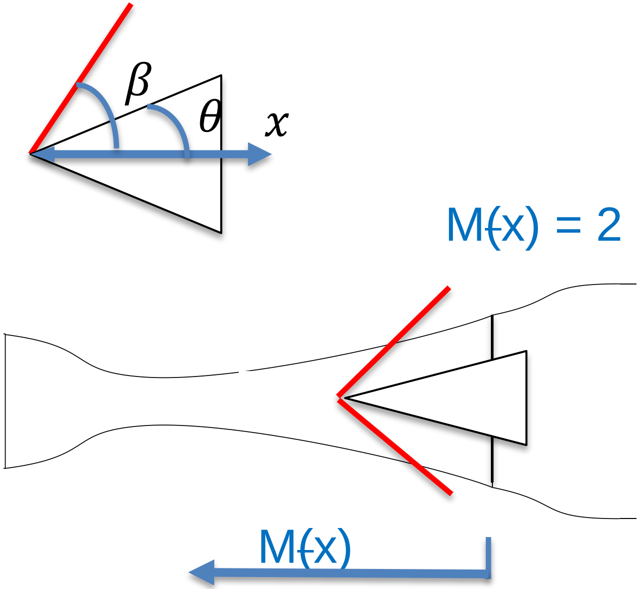


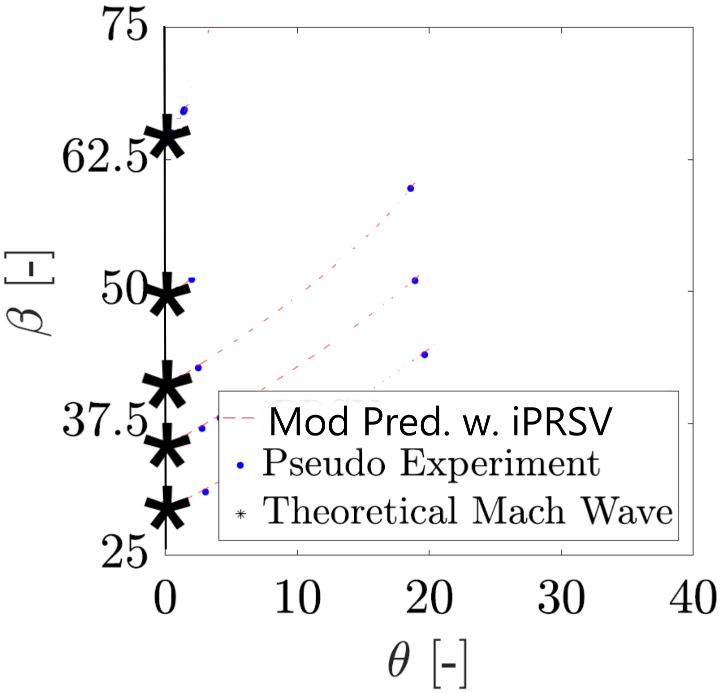




Design of Experiments (2/2)

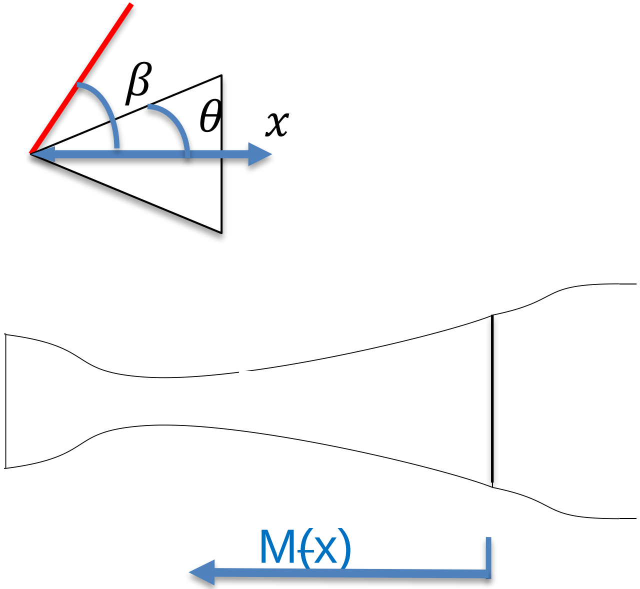
EXAMPLE RESULT: $\theta-\beta-M$ CURVE

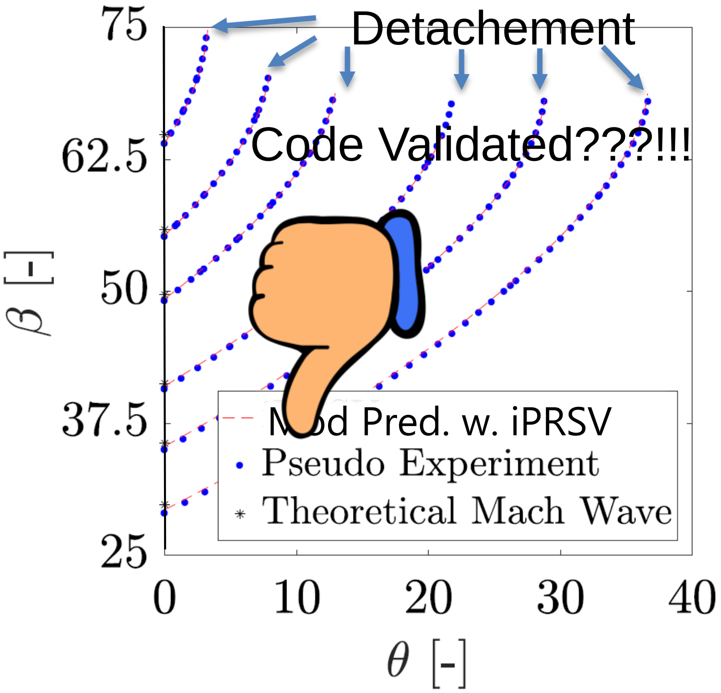




Design of Experiments (2/2)

EXAMPLE RESULT: θ–β– M CURVE



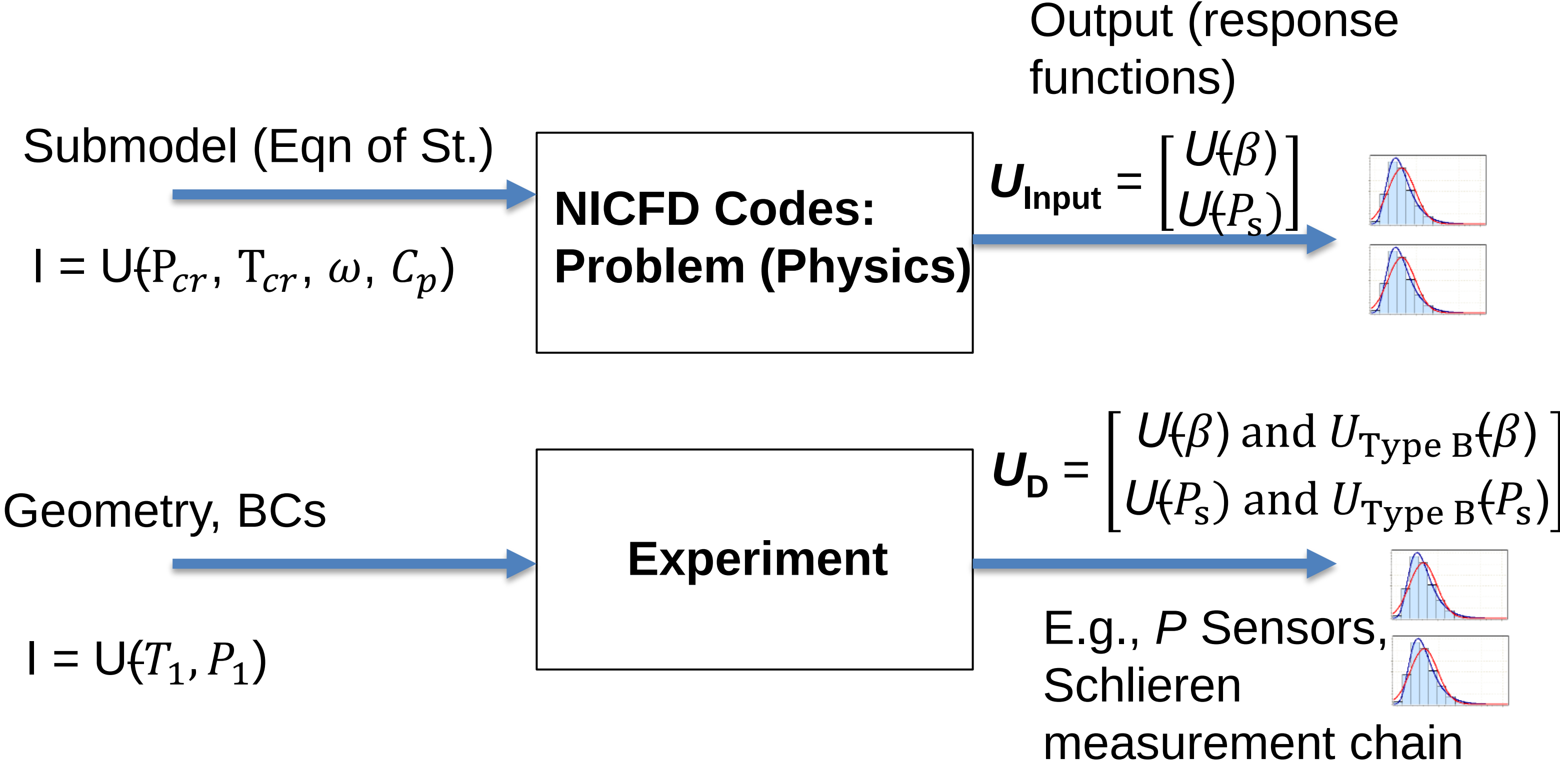


Detachement

Code Validated???!!!

V&V of a RANS code?

WHAT ABOUT possible uncertainties?



Output (response functions)

Submodel (Eqn of St.)

I = U$(\mathrm{P}_{cr}, \mathrm{T}_{cr}, \omega, C_p)$

NICFD Codes: Problem (Physics)

$\boldsymbol{U}_{\mathbf{Input}} = \begin{bmatrix} U(\beta) \\ U(P_s) \end{bmatrix}$

Geometry, BCs

I = U(T_1, P_1)

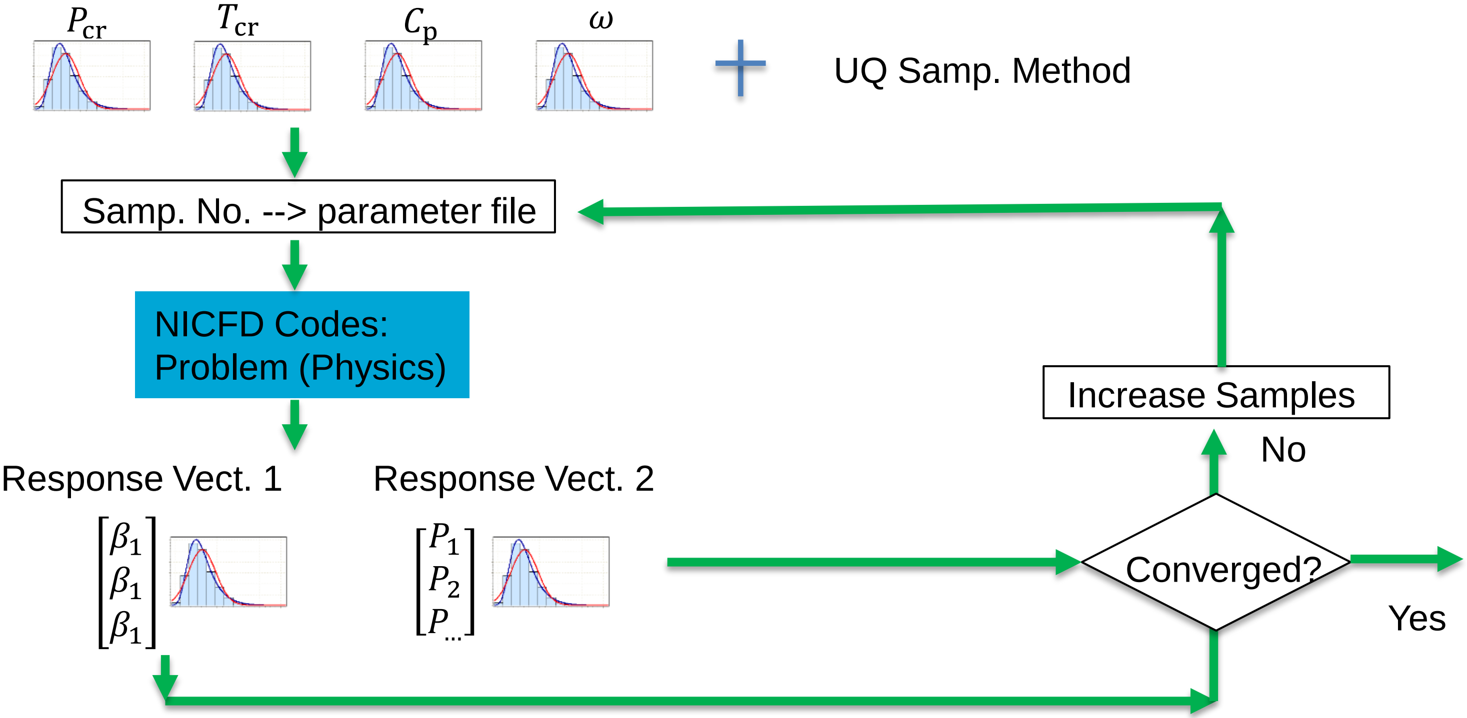
Experiment

$\boldsymbol{U}_{\mathbf{D}} = \begin{bmatrix} U(\beta) \text{ and } U_{\text{Type B}}(\beta) \\ U(P_s) \text{ and } U_{\text{Type B}}(P_s) \end{bmatrix}$

E.g., *P* Sensors, Schlieren measurement chain

UQ Infrastructure for validation (1/2)

Generic Method



P_{cr} T_{cr} C_{p} ω + UQ Samp. Method

Samp. No. --> parameter file

NICFD Codes:
Problem (Physics)

Response Vect. 1

$$\begin{bmatrix} \beta_1 \\ \beta_1 \\ \beta_1 \end{bmatrix}$$

Response Vect. 2

$$\begin{bmatrix} P_1 \\ P_2 \\ P_{\dots} \end{bmatrix}$$

Converged?

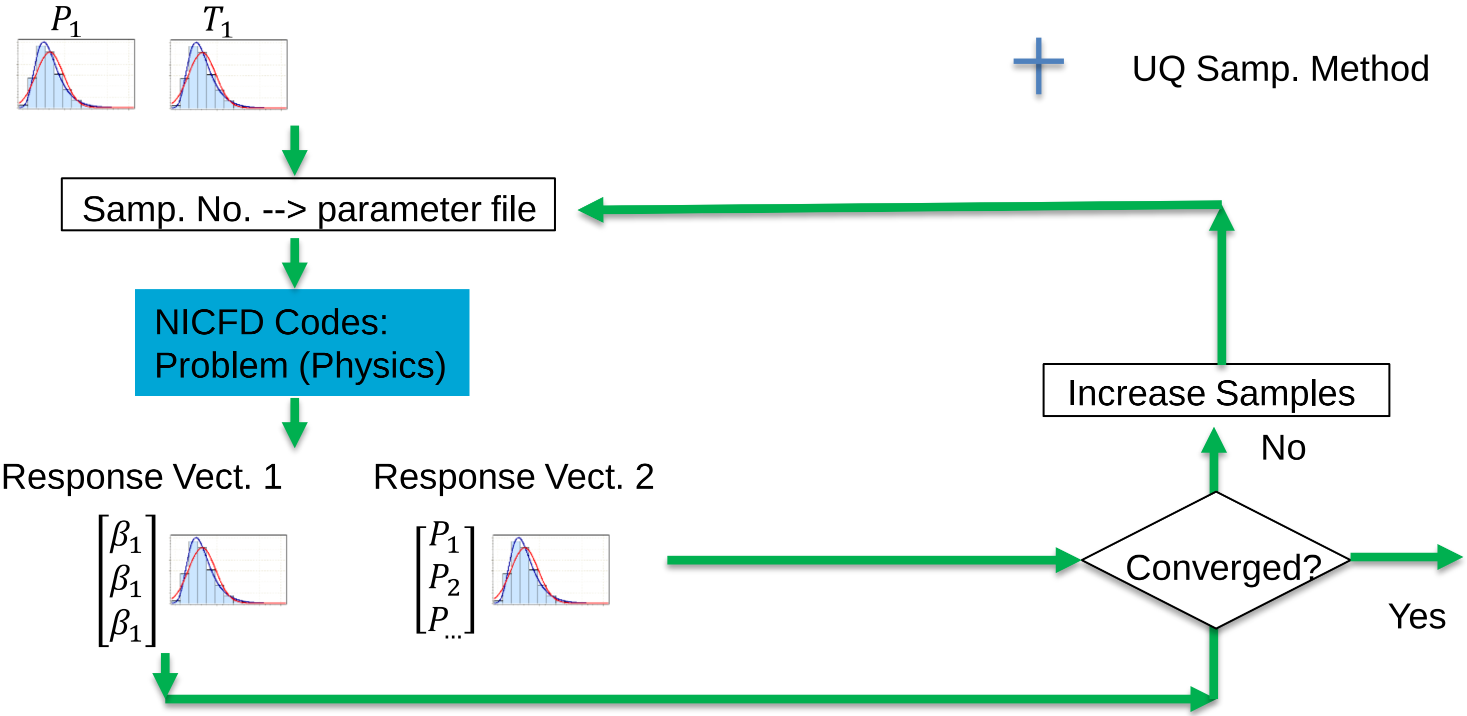
No

Increase Samples

Yes

UQ Infrastructure for validation (1/2)

Generic Method for Pseudo Experiment



P_1 T_1

+ UQ Samp. Method

Samp. No. --> parameter file

NICFD Codes:
Problem (Physics)

Response Vect. 1

$$\begin{bmatrix}\beta_1\\ \beta_1\\ \beta_1\end{bmatrix}$$

Response Vect. 2

$$\begin{bmatrix}P_1\\ P_2\\ P_{...}\end{bmatrix}$$

Converged?

No

Increase Samples

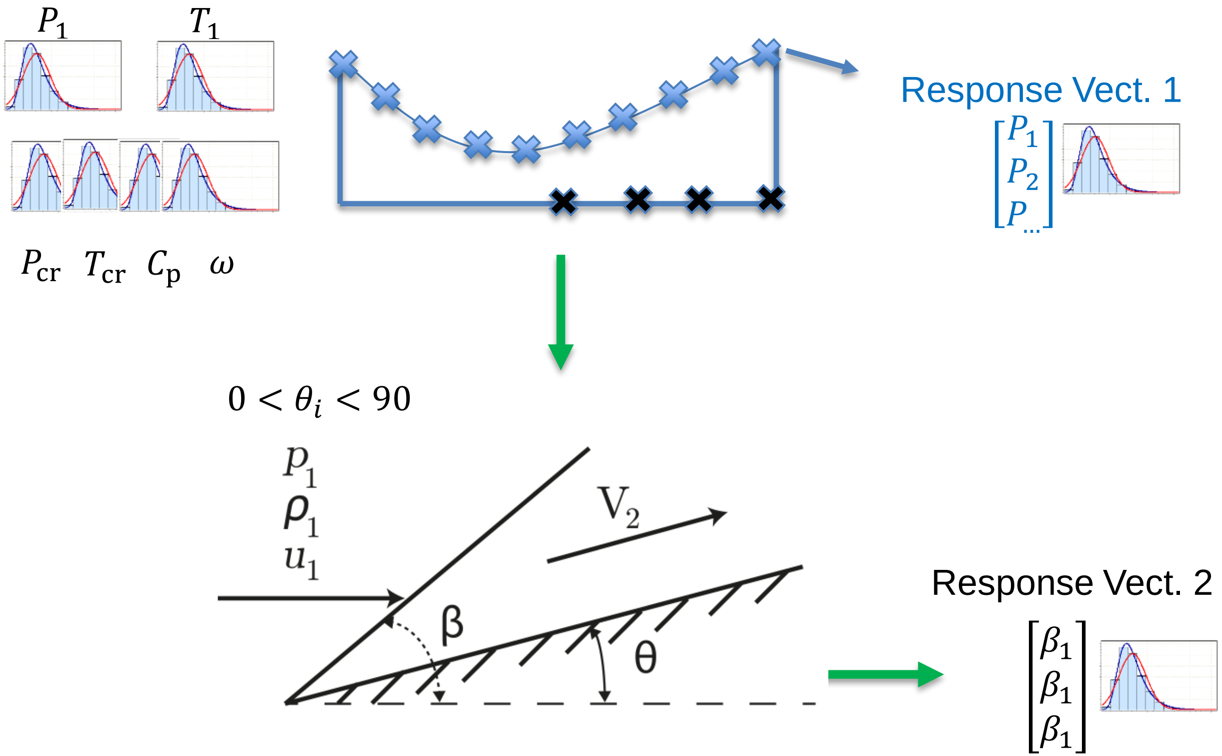
Yes

UQ Infrastructure for validation (2/2)

Applied to pressures and shockwaves

1st Step

2nd Step



Response Vect. 1

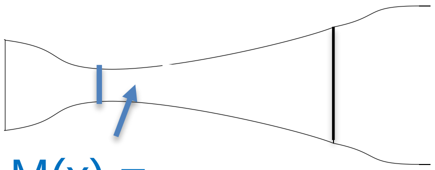
$$\begin{bmatrix} P_1 \\ P_2 \\ P_{\dots} \end{bmatrix}$$

Response Vect. 2

$$\begin{bmatrix} \beta_1 \\ \beta_1 \\ \beta_1 \end{bmatrix}$$

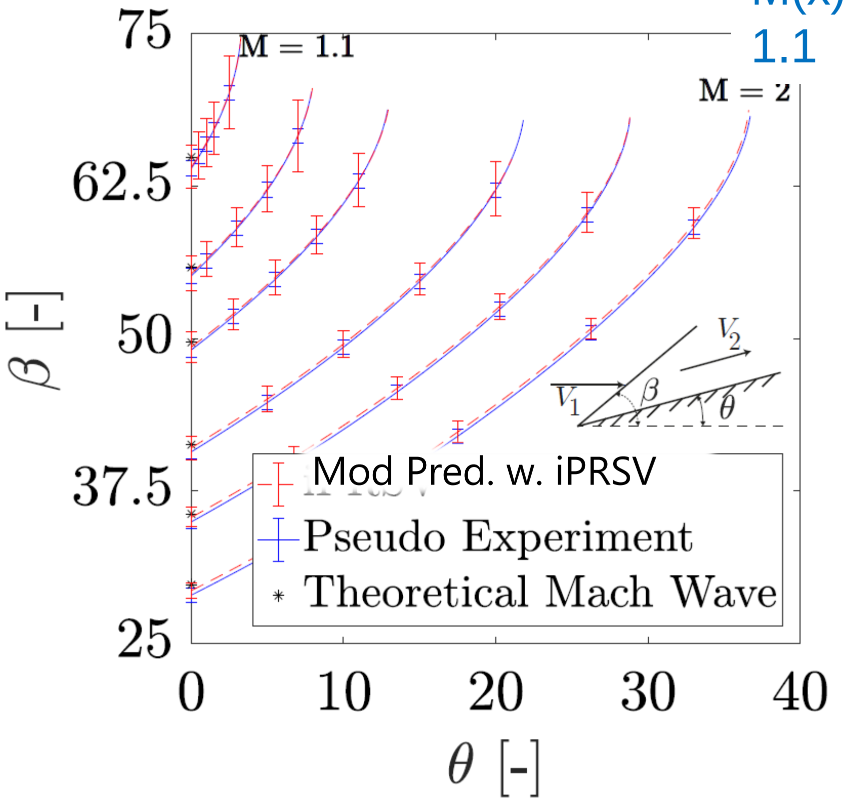
Result

θ β M with uncertainties!



M(x) = 1.1

M(x) = 2

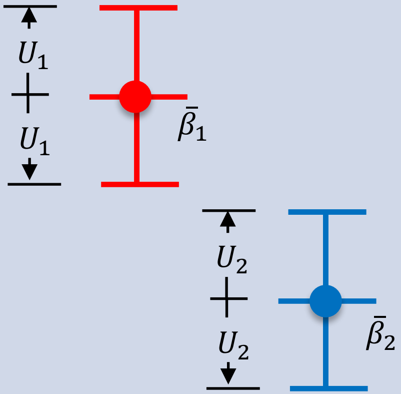
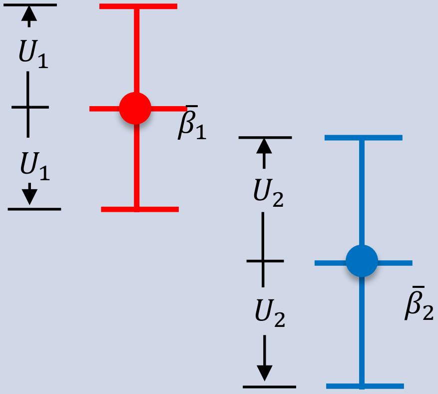
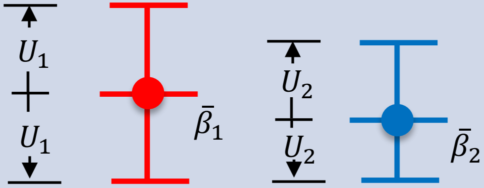


Result

θ β M with uncertainties!

Simulation

Experiment

Case 1: No Overlap	Case 2: Partial Overlap	Case 3: Complete Overlap
		

$$\boldsymbol{E} = \boldsymbol{S} - \boldsymbol{D} \ \& \ \boldsymbol{U_{val}} = \sqrt{\cancel{\boldsymbol{U_\phi^2}} + \boldsymbol{U_{input}^2} + \boldsymbol{U_D^2}}$$

Conditions:

$|\boldsymbol{E}| \gg U_{\mathrm{val}}$ or $|\boldsymbol{E}| < U_{\mathrm{val}}$

Concluding Remarks

- The **experiment** is **well designed** for validating the equation of state computational sub-model.

- ORCHID is almost ready for hot commissioning!

- Now the real experiments!

Thanks

Appendix

E and U

Let

$$\boldsymbol{E} \pm \boldsymbol{U}_{\mathbf{val}}$$

$$\boldsymbol{S} - \boldsymbol{D} \pm \boldsymbol{U}_{\mathbf{val}}$$

define an interval within which the modelling error δ_{model} resides. $\boldsymbol{\delta_{model}} \subseteq [\boldsymbol{E} - \boldsymbol{U_{val}}, \boldsymbol{E} + \boldsymbol{U_{val}}]$

Where S is the calculated result originating from the mean values of all the samples. D is the mean experimental result.

$$\bar{S} = \frac{1}{n} \sum_{i=1}^{n} S_i$$

Appendix

E and U

The validation uncertainty $\boldsymbol{U}_{\mathbf{val}}$ is an estimate of the standard deviation of the parent population of the combination of errors $\left(\boldsymbol{\delta}_{\mathbf{num}}+\boldsymbol{\delta}_{\mathbf{input}}-\boldsymbol{\delta}_{\mathbf{D}}\right)$.

$$u_{input}^{2}=\frac{1}{n-1}\sum_{i=1}^{n}(S_i-\bar{S})^2$$

Appendix

E and U

$$(\boldsymbol{\delta}_{\mathbf{num}} + \boldsymbol{\delta}_{\mathbf{input}} - \boldsymbol{\delta}_{\mathbf{D}}) \pm \boldsymbol{U}_{\mathbf{val}}$$

By making an assumption on the distribution of the parent population of the errors $(\boldsymbol{\delta}_{\mathbf{num}} + \boldsymbol{\delta}_{\mathbf{input}} - \boldsymbol{\delta}_{\mathbf{D}})$, an interval can be estimated within which δ_{model} falls with a specified confidence level.

Appendix
DEFINITIONS

Uncertainty: the uncertainty U associated with a measured quantity or a predicted quantity defines the ±U interval about that quantity within which we expect the true (but unknown) value of that quantity to lie 95 times out of 100.

Error: Once the true value of a measurand has been defined, the errors associated with estimating the true value must be identified. Uncertainties are estimates to quantify the limits of these errors.

Appendix
DEFINITIONS

Measurement Uncertainties: Instead of categorizing uncertainties as either bias (systematic) or precision (random), the various *U* are divided into **type A** standard uncertainties and **type B** standard uncertainties.

Appendix

DEFINITIONS

Validation Uncertainty: is defined as the combination of the uncertainties in the experimental data and the portion of the uncertainties in the CFD prediction that can be estimated. The choice of the required level of U_v is associated with the degree of risk deemed acceptable in a program.

V&V of a RANS code?

Different Procedures

Commonly Adopted

Simple graphical comparisons between numerical predictions and experimental data → Almost no uncertainty bands

Rigorous Procedures:

ASME V&V-20 committee or AIAA standards: W. Oberkampf, P.J. Roache, L. Eca

Two dominant stages:

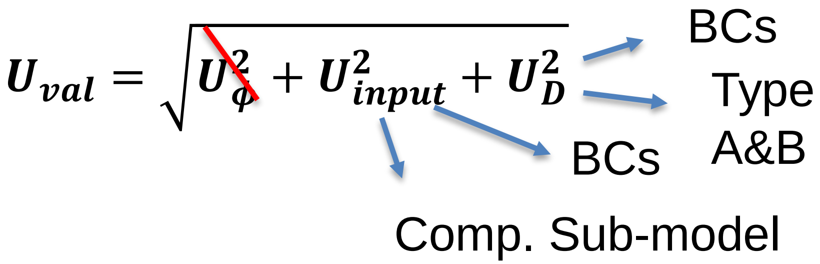
1. **Verification** split into two steps: **Code and Solution Verification**
2. Validation uses knowledge from verification phase and metrics

V&V of a RANS code?

Validation

Requires comparisons with experimental data (physical models) and it involves numerical, experimental and parameter uncertainties.

The validation uncertainty, U_{val}



$$U_{val} = \sqrt{\cancel{U_{\varphi}^2} + U_{input}^2 + U_D^2}$$

BCs

Type A&B

BCs

Comp. Sub-model

The validation comparison discrepancy, E

$$E = S - D$$

Appendix

DEFINITIONS (Verification)

Purely a mathematical exercise consisting of two parts:

- **Code verification**, intending to demonstrate by error evaluation the correctness of the code that contains the algorithm to solve a given mathematical model.
- **Solution verification**, attempting to estimate the error/uncertainty of a given numerical solution, for which, in general, the exact solution is unknown.

Step sometimes
separated from the
validation process

numerical error → the round-off error, iterative error and the discretization error.

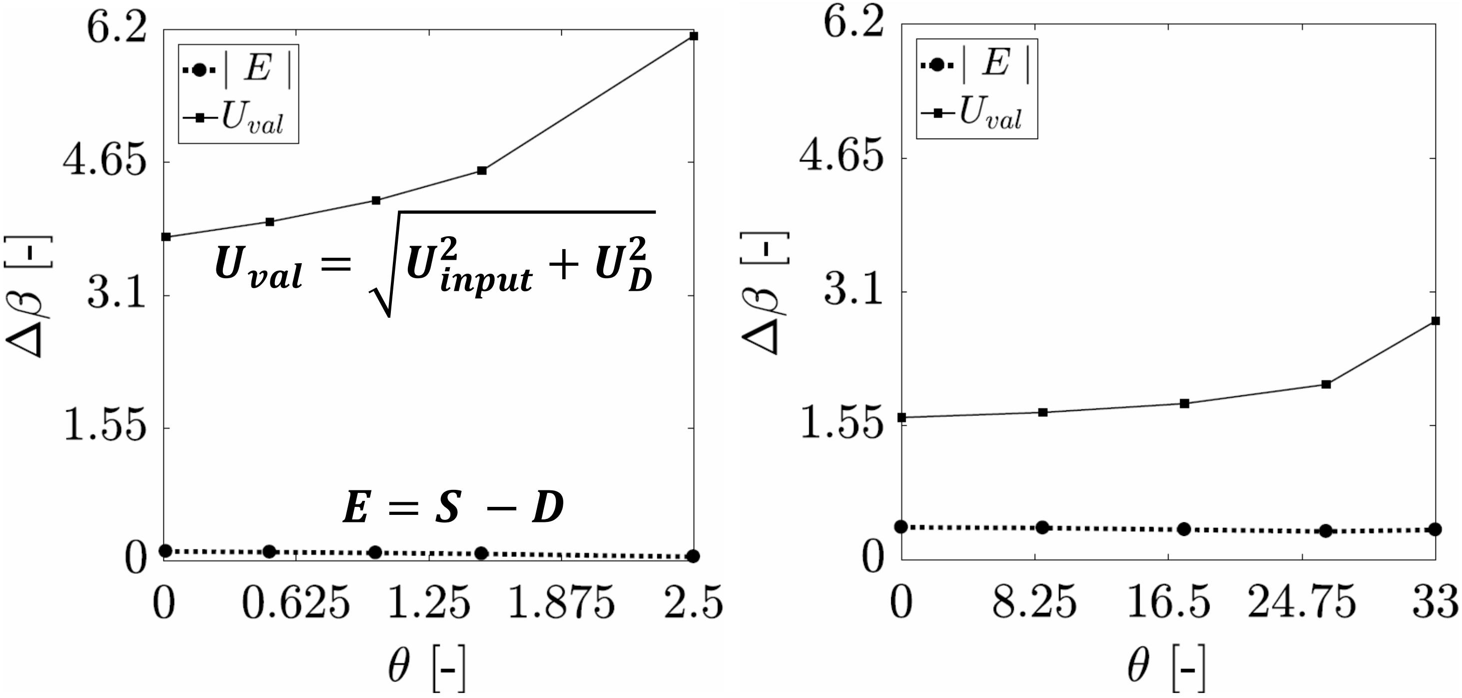
Appendix
DEFINITIONS (Validation)

Outcome of exercise is determined from comparison with $|E|$ with U_{val}.

- If $|E| >> U_{val}$ then comparison error is dominated by the modelling error: Model must be improved
- For $|E| < U_{val}$, model is within the "noise level" imposed by the numerical, experimental and parameter uncertainties. It can mean two things:
    1. if E is small, the model and its solution are validated against the given experiment;
    2. Or numerical solution and/or the experiment should be improved before conclusions made about the adequacy of the mathematical model.

Result

θ β M with metrics



$$U_{val} = \sqrt{U_{input}^2 + U_D^2}$$

$$E = S - D$$

Appendix

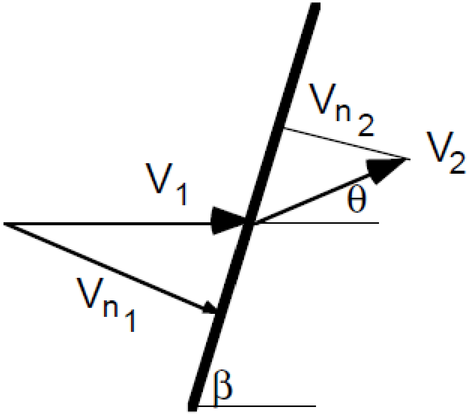
Jump Conditions: Steady OSW (1/5)

(1) $$\rho_1 V_{n1} = \rho_2 V_{n2},$$

(2) $$\rho_1 V_{n1}^2 + p_1 = \rho_2 V_{n2}^2 + p_2,$$

(3) $$h_1 + \frac{V_{n1}^2}{2} = h_2 + \frac{V_{n2}^2}{2},$$

(4) $$V_{t_1} = \mathrm{V}_{\mathrm{t}_2}$$



Appendix

Jump Conditions: Steady OSW (2/5)

- Using trigonometry and the jump condition expressing continuity of tangential velocity, e.g., Eqn 4 → can relate the normal velocity before and after the shock.

$$\frac{\tan(\beta-\theta)}{\tan(\beta)}=\frac{V_{n_2}}{V_{n_1}} \tag{5}$$

- We know V_{n2}/V_{n1} by the solution of Eqn. 1 – 3 along with a state eqn.

Appendix

Jump Conditions: Steady OSW (3/5)

- Cannot get a closed form expression for the β, θ, M_1 as is possible with perfect gases. From the continuity of tangential velocity (Eqn 5) and rewriting the jump in normal velocity in terms of a density jump (Eqn 1), e.g., $V_{n2}/V_{n1} = \rho_1/\rho_2 = \nu$ can solve for β

$$\tan(\beta) = \frac{(1-\nu) \pm \left[(1-\nu)^2 - 4\nu\tan^2\theta\right]^{\frac{1}{2}}}{2\nu\tan\theta} \qquad (6)$$

- Using an iterative procedure one can determine ν and solve for β

Appendix

Jump Conditions: Steady OSW (4/5)

- Step 1: Starting with V_1, p_1, ρ_1, and θ calculate $h_1 = h(p_1, \rho_1)$ from an eqn of state.
- Step 2: Guess a value of $\nu = \rho_1/\rho_2$. Then $\rho_2 = \rho_1/\nu$.
- Step 3: From Eqn. 6 solve for β corresponding to this value of ν. Then $V_{n_1} = V_1 \sin\beta$.
- Step 4: From Eqn. $1-3$, $V_{n_2} = V_{n_1}\nu$, $p_2 = p_1 V_{n_1}^2(1-\nu)$ and $h_2 = h_1 + \frac{V_{n_1}^2}{2}(1-\nu^2)$.
- Step 5: From the eqn of state we can also determine the enthalpy, $\tilde{h}_2 = (p_2, \rho_2)$

Appendix

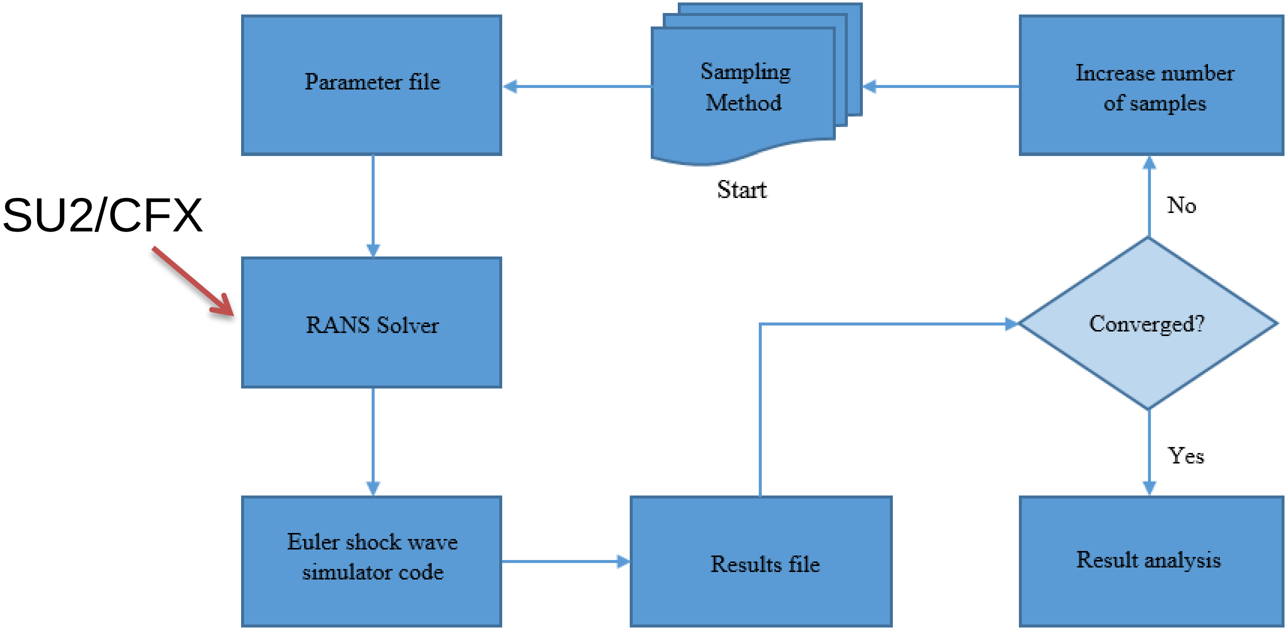
Jump Conditions: Steady OSW (5/5)

- Step 6: Does $\tilde{h}_2 = h_2$? If not, use a root-finding procedure such as a bracketing or a secant method to modify the value of ν and continue from step 3.

After convergence, with the given values of V_1, p_1, ρ_1, θ and the converged value of ν, we can compute β, V_{n_1}, V_{n_2}, p_2, and h_2. Then $V_2 = \frac{V_{n_2}}{\sin(\beta-\theta)}$

Appendix

Model Workflow



Appendix

Commissioning Plan

- Functional Hardware tests (21/09/2017)
- Control System FAT (28/09/2017)
- Hot Commissioning (25/10/2017)
- Experimental Campaigns (10/10/2017)

Appendix

Type A and Type B uncertainties

- Type A: resulting from smulation

- Type B: Systematic

Appendix

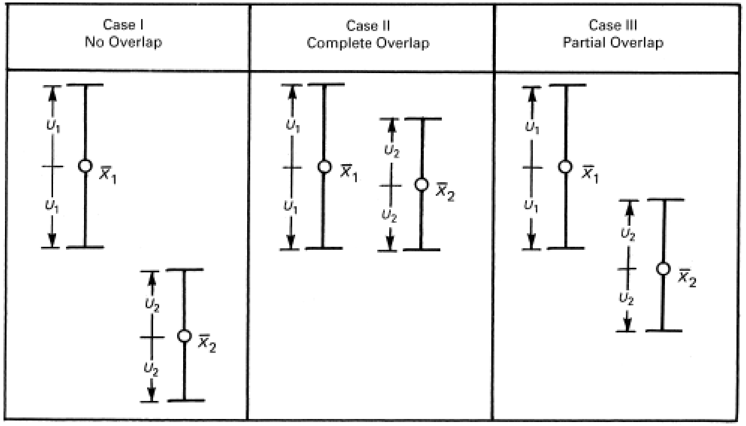
Validation Metrics

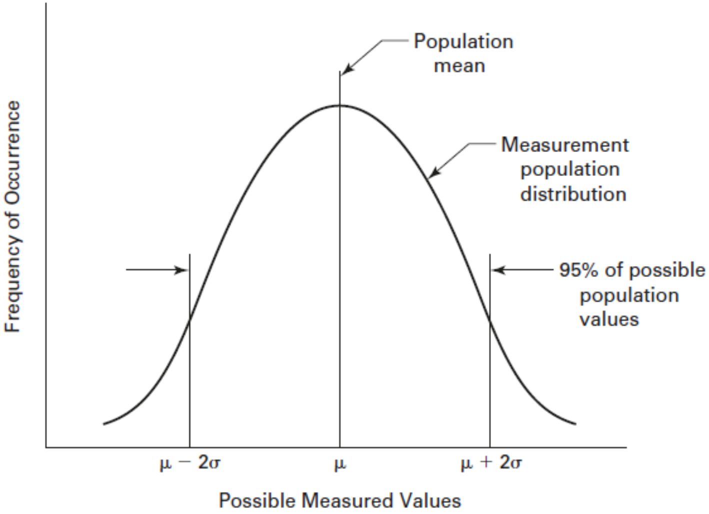
Validation uncertainty *Uv is* the combination of all uncertainties that we know how to estimate.

E defined as the difference between the experimental data set value the value produced by the simulation

Appendix

Validation Metrics





Appendix

Total Uncertainty

The expanded uncertainty, $U_{\tilde{x}}$ for a 95% level of confidence and large degrees of freedom, is

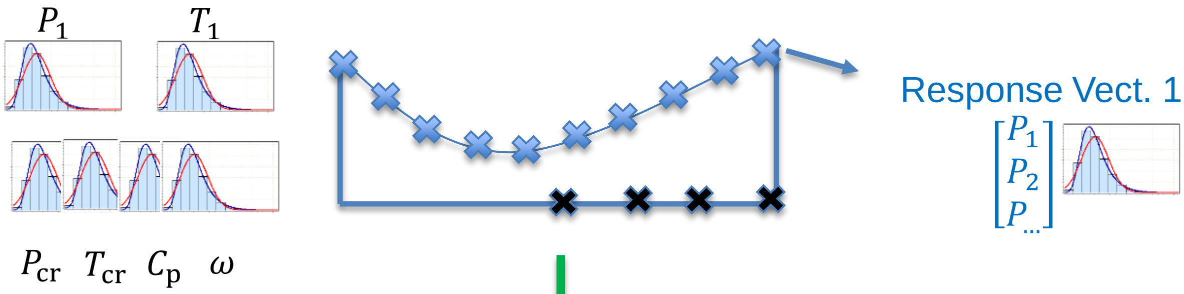
$$U_{\tilde{x}} = 2u_{\tilde{x}} = 2\sqrt{(b_{\tilde{x}})^2 + (s_{\tilde{x}})^2}$$

- Assume that the systematic standard uncertainties of the measured parameters are all independent of each other.

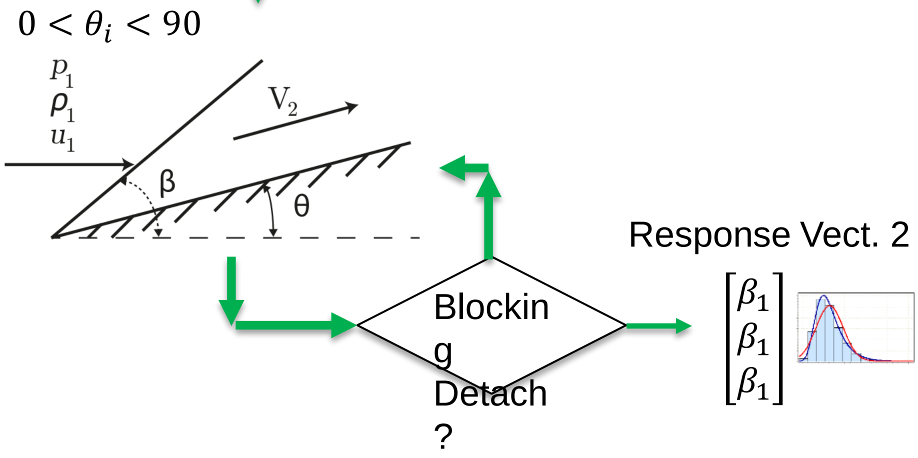
UQ Infrastructure for validation (2/2)

Applied to pressures and shockwaves

1st Step



2nd Step

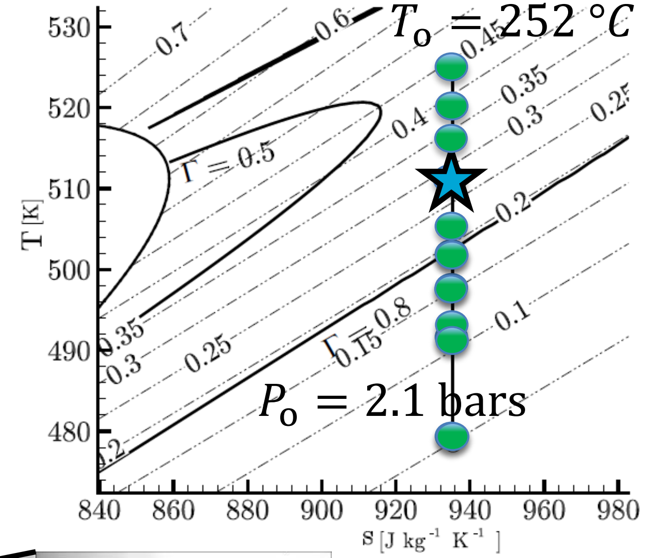


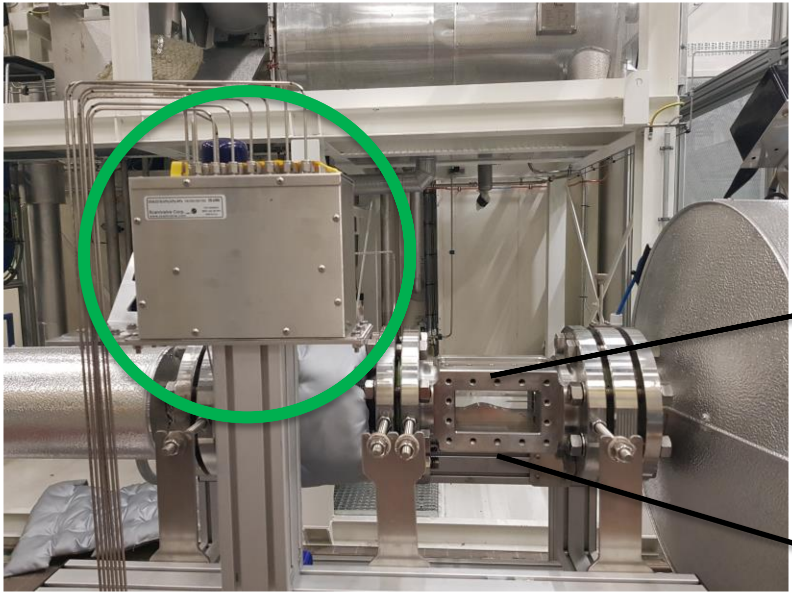
Design of Experiments (1/2)

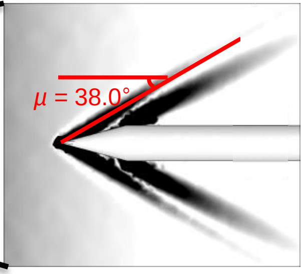
NOZZLE

Phase 1: Flow Visualization and Conventional Techniques

$P_o = 18.4$ bars







$$M_{Tip} = \frac{1}{\sin \mu}$$