Validation and Verification in compressible CFD

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Outline

1. Introduction
2. Verification. Editorial Policy for verification of one scientific journal
3. Numerical flow fields in the framework of a validation exercise
4. Drag estimation by experiment and calculation. Theory and one example
5. Conclusions

Verification and Validation in Computational Mechanics

- Verification and validation in quality management
    - Verification = checking the capabilities of a product w.r.t. its design specifications
    - Validation = checking the ability of a product to provide the service it has been built for
- Verification and Validation in Computational Fluid Dynamics
    - Verification = process of determining that a model implementation accurately represents the developers conceptual description of the model
    - Validation = process of determining the degree to which the model implementation is an accurate representation of the real world for the intended uses of the model
- Verification of numerical flowfields
- Checking numerical flowfields *in the framework* of a validation

Verification and Validation in Computational Mechanics

- Verification and validation in Computational Fluid Dynamics
    - Verification = process of determining that a model implementation accurately represents the developers conceptual description of the model Solving the equations right
    - Validation = process of determining the degree to which the model implementation is an accurate representation of the real world for the intended uses of the model Solving the right equations [surely too simple formula]
- Verification and Validation in Computational Mechanics
    - Verification = computational checks, error estimation, comparison to analytical solutions...
    - Validation = comparison of numerical solutions with experimental measurements
- Verification of numerical flowfields
- Checking numerical flowfields *in the framework* of a validation

Verification and Validation in Computational Mechanics

- General books / articles
  - P.J. Roache. Verification and validation in computational science and engineering. Hermosa publishers. Albuquerque. 1998.
  - P.J. Roache. Fundamentals of verification and validation. Hermosa publishers. Albuquerque. 2009.
- In fluid dynamics
  - P.J. Roache. Need for control of numerical accuracy. *J. of Spacecraft and Rockets.* Vol. 27(2) pp 98-102. 1990.
  - P.J. Roache. Quantification of uncertainty in Computational Fluid Dynamics. *Annu. Rev. Fluid. Mech.* Vol. 29 pp 123-160. 1997.
- Proceedings of the three Workshop(s) on CFD uncertainty & Proceedings of congress sessions organized by Luis Eça

Verification and Validation in Computational Mechanics

- Editorial policies of scientific journals, learned societies
  - AIAA Guide for the verification and validation of computational fluid dynamics simulations. AIAA Guide 077-1998.
  - ASME PTC V&V 10
  - ASME PTC V&V 20
  - Editorial policy of *Journal of Fluids Engineering, AIAA Journal, IJNMF, Journal of Heat Transfer*...
- About verification only
  - J.R. Roy. Review of code solution verification procedures for computational simulation. *J. of Computational Physics.* Vol. 205. pp 131–156. 2005.
  - J.R. Roy, A.J. Sinclair. On the generation of exact solutions for evaluating numerical schemes and estimating discretization error.*J. of Computational Physics.* Vol. 228. pp 1790–1802. 2009.

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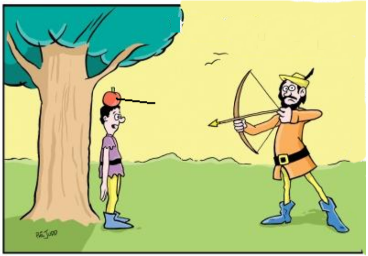
Journal Editorial Policies about verification

- *Journal of heat transfer* editorial policy statement on numerical accuracy (Vol. 116 pp 797–798)
    - The Journal of Heat Transfer will not accept for review or publication any manuscript reporting the numerical solution of a heat transfer problem that fails to establish adequately the accuracy of the computed results
    - All manuscripts [...] must contain [...]
        - a problem statement [...] to allow the reproduction of the results
        - a description of the solution technique employed [...]
        - the numerical solution must be supplemented with acceptable accuracy estimates for both the method employed and the results presented. A single calculation using a fixed discretization will not be acceptable since no error estimate can be possibly interfered from such a calculation

Journal Editorial Policies about verification

- A single calculation using a fixed discretization will not be acceptable since no error estimate can be interfered from such a calculation...
- Apparently good CFD

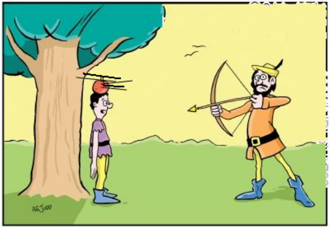


Journal Editorial Policies about verification

- A single calculation using a fixed discretization will not be acceptable since no error estimate can be interfered from such a calculation...
- One satisfactory calculation obtained by chance (one arrow in the apple, all the others in the boy = state variables change significantly with grid refinement, parameters...) or as part of a verified series of calculations (all the arrows close to the apple = no significant change going to finer grids, changing parameters...)
- Apparently good CFD

Journal Editorial Policies about verification

- A single calculation using a fixed discretization will not be acceptable since no error estimate can be interfered from such a calculation...
- One satisfactory calculation obtained by chance (one arrow in the apple, all the others in the boy) or as part of a verified series of calculations (all the arrows close to the apple)
- verified



not verified CFD

Journal Editorial Policies about verification

- Authors may use any appropriate method for the estimation of errors
    - 1/ comparison of numerical results with those from a sufficiently similar model problem available in the literature possessing a known exact or highly accurate approximate analytical solution
    - 2/ a precisely defined grid refinement or grid coarsening study. Marginal refinement showing a qualitative convergence trend is not acceptable. Other numerical parameters such as time step should also be varied
    - 3/ reasonable agreement with experimental data is not, in general, sufficient justification for acceptance of numerical results, especially when adjustable parameters are involved

Journal Editorial Policies about verification

- By implementation of this policy, it is intended to establish guideline requirements for the publication of numerical results and to enhance the quality of publications involving numerical solutions

- It is not our intend to effect a significant increase in the length of papers published in the journal or to impose excessive requirements we hope to elicit a good faith effort form authors

Verification versus Validation in fluid dynamics

- Verification of numerical flow fields
  - Mathematical / Computer Sciences
  - Clearly defined task...
  - ...nevertheless results (from Richardson's analysis) possibly difficult to understand
  - Can be defined in an abstract mathematical framework

- Checking numerical flowfields in the framework of a validation exercise
  - Computer Sciences & Mechanics
  - Involve terms of ...
    - Modeling error/uncertainty difficult to estimate
    - Experimental error/uncertainty difficult to control
  - Complex discussion (modeling error, experimental capability...)
  - In practice, difficult to do a general presentation

Code Verification versus Solution Verification

- Code verification (one mesh/one scheme)
    - computational verifications (single routine tests...)
    - checking physical basic properties (entropy, stagnation pressure, stagnation temperature/total enthalpy...)
    - checking flowfields w.r.t. known solution of continuous problem (incompresssible = Poiseuille flow, Lamb-Oseen flow, compressible = vortex advection, 1D shock tube – Cf E.F. Toro website)
    - manufactured solutions

- Solution verification (several meshes or several scheme orders)
    - checking mesh convergence (Richardson analysis, GCI...)
    - Specific checks for finite elements methods (interpolation *vs* discretization error)
    - Specific checks for high order methods (FE, DG methods...) Convergence with order of approximation

Code Verification versus Solution Verification

- Code verification *vs* solution verification
- Computer Science *vs* Computer Sciences & Maths
- Need for both
  - “Physical constant divided by two” not detected by solution verification
  - error for small increments specific formulas (MUSCL limiting function) may not be detected by code verification

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Validation in compressible Fluid Dynamics

- Hard to discuss in general (independly of the experimental device of the field)

- Theory of validation as described in ASME PTC V&V10, ASME PTC V&V20
- This theory does not include finite precision computations error. Added for consistency with the rest of the course

- Scalar output after simulation in continuum mechanics then aerodynamic force then lift as function of angle of attack

Validation in compressible Fluid Dynamics

- Concern about experimental errors older than counterpart for numerical error

- References for experimental error
    - Working group involving seven research centers started 1977
    - ISO Guide 1995. Guide to the expression of uncertainty in measurement. ISO, Geneva, Switzerland. (also known as G.U.M.)
    - Reference for U.S. National Institute of Science and Technology
    - Cited in ASME PTC 19.1-2005 “Test Uncertainty”

Validation in compressible Fluid Dynamics

Specific Flow

Exact geometry

M, Re, α

Ideal aerodynamic coefficient $\mathbf{C}_{\mathbf{ideal}}$

NB = aeroelastic shape, rough walls

Wind tunnel: Coefficient $\mathbf{C}_{\mathbf{expe}}$ no equal to $\mathbf{C}_{\mathbf{ideal}}$

Error term δ_{expe} split in

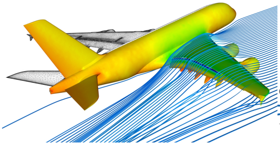
- δ_{cond} inability to reproduce flow conditions (+/- 0.001 on M)
- δ_{mes} limit of accuracy of measurement devices

NB= hopefully consistent geometry, no systematic bias in correction of wall/stick effects

Numerical Simulation(s): Coefficient $\mathbf{C}_{\mathbf{sim}}$ no equal to $\mathbf{C}_{\mathbf{ideal}}$

Error δ_{sim} split in

- δ_{model} RANS LES
- δ_{num} approximation error
- δ_{input} uncertainty on wall-roughness
- δ_{fp} finite precision floating point operations



Validation in compressible Fluid Dynamics

- Validation discussion according to ASME V&V 20 (PTC 61), reference for the three *Workshop(s) on CFD uncertainty analysis*
- Validation discussion analyses for sources of the difference

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

- Terminology (unfortunately, discussed)
  - Error δ_i : difference between a quantity measured/calculated and its value in the ideal flow
  - Uncertainty u_i : upper bound of absolute value of error δ_i
- Translation of "error" and "uncertainty" in French (by *"erreur"* and *"incertitude"*) does not sound intuitive at all
- Error δ_i in then split linearly into parts corresponding to its sources (assuming additivity of small independant contributions)

Validation in compressible Fluid Dynamics

- ASME V&V 20 terminology (used for the rest of the talk) (discussing outputs)
  - Error δ_i : difference between a quantity measured/calculated and its value in the ideal flow
  - Uncertainty u_i : upper bound of absolute value of error δ_i
- AIAA (AIAA-G-077-1998) terminology later completed by Oberkampf et al. (2003) Trucano et al. (2006) (discussing inputs)
  - Error : a recognizable deficiency in any phase or activity of the modeling (*) process that is not due to the lack of knowledge
  - Uncertainty : a potential deficiency in any phase or activity of the modeling process (*) that is due to the lack of knowledge
  - (*) modeling process in a very broad sense = defining relevant d.p.e., defining numerical scheme, coding...
  - Aleatory uncertainty = physical variability present in the system or its environment. Not strictly due to a lack of knowledge and cannot be reduced (typically turbulence...)
  - Reducible or epistemic uncertainty = potential deficiency that is due to a lack of knowledge (typically manufacturing tolerance...)

Validation in compressible Fluid Dynamics

- Discussion uses simple additive model of error terms

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

- Experimental part

$$\delta_{expe} = C_{expe} - C_{ideal}$$

$$\delta_{expe} = \delta_{mes} + \delta_{cond}$$

$$|\delta_{expe}| \leq |\delta_{mes}| + |\delta_{cond}| \leq u_{mes} + u_{cond} = u_{expe}$$

- Simulation part

$$\delta_{sim} = C_{sim} - C_{ideal}$$

$$\delta_{sim} = \delta_{num} + \delta_{fp} + \delta_{input} + \delta_{model}$$

$$|\delta_{sim}| \leq u_{num} + u_{fp} + u_{input} + u_{model} = u_{sim}$$

Validation in compressible Fluid Dynamics

- Discussion

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

$$\delta_{expe} = C_{expe} - C_{ideal} \qquad |\delta_{expe}| \leq u_{mes} + u_{cond} = u_{expe}$$

- “Content” of δ_{expe}
  - δ_{expe} due to limited capability of measurement devices plus disparity ideal *vs* experimental flow (inability to produce desired flow conditions)
- In practice, for a windtunnel
  - Walls/stick alter the flow w.r.t. free flight. Effect corrected for forces but not for local measurements
  - Walls/stick correction known to be good at low angles of attack
  - u_{expe} estimated by short and middle term repetition (assumption: no-systematic bias in aerodynamic flow conditions, wall/ stick correction...)

Validation in compressible Fluid Dynamics

- Discussion

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

$$\delta_{sim} = C_{sim} - C_{ideal} \qquad \delta_{sim} = \delta_{num} + \delta_{fp} + \delta_{input} + \delta_{model}$$

$$|\delta_{sim}| \leq u_{num} + u_{fp} + u_{input} + u_{model} = u_{sim}$$

- “Content” of δ_{sim}
  - approximation error δ_{num} u_{num}
    - u_{num} is estimated by mesh refinement
    - u_{num} should cancel at the limit of small step space sizes
    - u_{num} hence does not contain possible boundary definition error (to close far field boundary error for external aero)
  - finite precision algebra error δ_{fp} u_{fp}
    - u_{fp} is estimated through specific dedicated tools like CADNA
    - u_{fp} should cancel at the limit of long mantissa algebra

Validation in compressible Fluid Dynamics

- Discussion

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

$$\delta_{sim} = C_{sim} - C_{ideal} \qquad \delta_{sim} = \delta_{num} + \delta_{fp} + \delta_{input} + \delta_{model}$$

$$|\delta_{sim}| < u_{num} + u_{fp} + u_{input} + u_{model} = u_{sim}$$

- "Content" of δ_{sim}
  - δ_{model} u_{model} according to Fluid Dynamics model
    - (RANS) good for attached flows. Inaccurate for detached flows and transition
    - (DES) (LES) accurate except for phenomena at the scale of boundary layer
    - (DNS) no modeling error
  - δ_{input} u_{input} according to available information
    - Canceled if more information is obtained (accurate value for wall roughness involved in BC)
    - Estimated by uncertainty quantification if law for uncertain input parameter is available

Validation in compressible Fluid Dynamics

- Example of validation discussion : all uncertainty terms estimated but δ_{model}. δ_{expe} provided all in one by experimental guys

$$E = C_{sim} - C_{expe} = (C_{sim} - C_{ideal}) - (C_{expe} - C_{ideal}) = \delta_{sim} - \delta_{expe}$$

$$\delta_{sim} = \delta_{num} + \delta_{fp} + \delta_{input} + \delta_{model}$$

$$\delta_{model} = \delta_{sim} - \delta_{num} - \delta_{fp} - \delta_{input} = E + \delta_{expe} - \delta_{num} - \delta_{fp} - \delta_{input}$$

$$\delta_{model} - E = \delta_{expe} - \delta_{num} - \delta_{fp} - \delta_{input} = \delta_{expe} - \delta_{num} - \delta_{fp} - \delta_{input}$$

$$E - u_{expe} - u_{num} - u_{fp} - u_{input} \leq \delta_{model} \leq E + u_{expe} + u_{num} + u_{fp} + u_{input}$$

- Validation discussion : is last inequality possibly verified ?
- Principle for all validation discussion. Many other cases $u_{model} = 0$ – *strong model* – , $u_{input} = 0$ – *perfectly defined problem*...

Validation in compressible Fluid Dynamics

- Connection bewteen validation discussion and other topics
  - u_{num} grid convergence studies
  - u_{input} u_{cond} typically also assessed by (UQ) for robust design (more often calculating standard deviation evaluation maybe)
  - u_{fp} considered in control of needed numerical precision for (un)steady flow simulation
- Weakness of this theoretical framework: for (LES) and (DES) δ_{mod} is directly dependant of the mesh. How to distinguish a δ_{mod} and a δ_{num} ?

Validation in compressible Fluid Dynamics

Specific Flow

Exact geometry
M, Re, α
Ideal aerodynamic coefficient $\mathbf{C}_{\mathbf{ideal}}$

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Wind tunnel: Coefficient $\mathbf{C}_{\mathbf{expe}}$ no equal to $\mathbf{C}_{\mathbf{ideal}}$

Error term δ_{expe} split in

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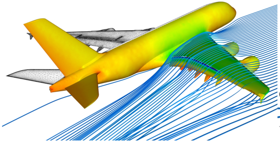


Validation in compressible Fluid Dynamics

Quite often more difference between abstract mechanical problem and experiment.
In particular too low Re in windtunnel

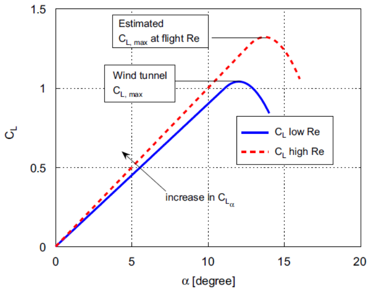


Fig. 22. Extrapolation of lift to free flight Reynolds number.

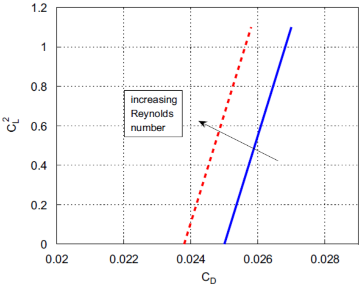


Fig. 14. A typical Reynolds number trend on a $C_D - C_L^2$ polar.

Validation in compressible Fluid Dynamics

Quite often more difference between abstract mechanical problem and experiment

- $CL(\alpha)$ for an aircraft
    - Half-model in widtunnel (flows w/o sideslip). Influence of the peniche...
    - High α (RANS) known to poorly predict stall...
    - Aeroelasticity. Is the shape of the model, as deformed in the wind-tunnel, right ?...
    - Stick-model junction causes lack of corresponding contribution to forces / moments...
    - Inability to get high enough Re in windtunnel for large aircrafts...
- Merging more dissimilar data
    - Flight tests / Wind-tunnel (right and too low RE) / Calculations
    - Wind tunnel full mesh and simulation (since 2005), free flight simulation, wind tunnel test $\Longrightarrow$ no more outer-boundary, wall, stick... errors. Better understanding of free flight simulation *vs* windtunnel tests experiments
    - Unfortunaltey windtunnel walls have holes and slits to lower difference with free-flight... Extremely tough for numerical simulation

Outline

Reference precisions for WT aerodynamics coefficients

- Reference precisions requested by aircraft manufacturers (clients) for WT tests.
- Unchanged since 80ies (AGARD 1982, 1988)

	absolute values		increments	
	confidence interval ($\pm 2\sigma$)	std (σ)	confidence interval ($\pm 2\sigma$)	std (σ)
C_L	$\pm 1 \cdot 10^{-2}$ (*lift-count*)	$0.5 \cdot 10^{-2}$	$\pm 0.5 \cdot 10^{-2}$	$0.25 \cdot 10^{-2}$
C_D	$\pm 1 \cdot 10^{-4}$ (*drag-count*)	$0.5 \cdot 10^{-4}$	$\pm 0.5 \cdot 10^{-4}$	$0.25 \cdot 10^{-4}$
C_m	$\pm 1 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$	$\pm 0.5 \cdot 10^{-3}$	$0.25 \cdot 10^{-3}$

- Do we attain this precision? Let us look at the drag coefficient estimation in WTs and CFD...

WT precision - (σ)

- *Drag Prediction Workshop 2001*
- 35 WT experiments from 3 different WTs have been compared

	std (σ)		
	Test F4	w.r.t. Ref ?	
C_L	$0.24 \cdot 10^{-2}$	✓	$[< 0.5 \cdot 10^{-2}]$
C_D	$4 \cdot 10^{-4}$	×	$[> 0.5 \cdot 10^{-4}]$
C_m	$5 \cdot 10^{-3}$	×	$[> 0.5 \cdot 10^{-3}]$

- Even experimental results do not attain the desired precision.

CFD precision - (σ)

- Long-term objective:
  replace WT experiments with CFD simulations $\Rightarrow$ CFD simulations should aim to obtain the *same* reference precision given previously
  (D. Mavriplis, *Aerodynamic Drag Prediction Using Unstructured Mesh solvers*, 2003)

	std (σ)		
	GARTEUR AG05 (1988)	GARTEUR AG39 (2007)	w.r.t. Ref ?
C_D	$10 \cdot 10^{-4}$	$5 \cdot 10^{-4}$	× $[> 0.5 \cdot 10^{-4}]$

- GARTEUR AG05: fully potential and Euler - GARTEUR AG39: RANS
- **In 20 years the standard deviation has been just halved.**

WT & CFD precision - (μ)

- Gap between the mean of the computed values and the experimental ones
- Configuration: fuselage-wing A/C

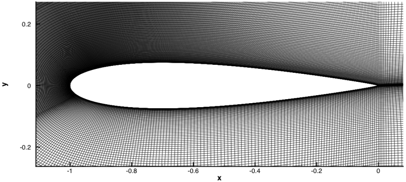
	$\Delta[\mu_{CFD} - \mu_{WT}]$			
	DPW-1 (2001)	DPW-2 (2003)	GARTEUR AG39 (2007)	w.r.t. Ref ?
C_L	-	-	$-0.7 \cdot 10^{-2}$	✓ $[< 1 \cdot 10^{-2}]$
C_D	$+7 \cdot 10^{-4}$	$-3 \cdot 10^{-4}$	$-7 \cdot 10^{-4}$	✗ $[> 1 \cdot 10^{-4}]$
C_m	$-29 \cdot 10^{-3}$	$-17 \cdot 10^{-3}$	$+9 \cdot 10^{-3}$	✗ $[> 1 \cdot 10^{-3}]$

- The objective precision is not reached even fixing laminar/turbulent transition.
- A computation is a numerical simulation. But even a WT test is a simulation. Using CFD simulation to validate WT test has no less meaning than using WT test to validate CFD solution (Destarac *et al.*, *RANS Validation for transonic Wing-Body*, 2007)

Example: 2D turbulent flow about airfoil NACA0015

- 2D NACA0015
- RANS + Spalart-Allmaras turbulence closure (SA) or Kok $k-\omega$ model (KW)
- ONERA Finite Volume structured *elsA* code
- Computations at nominal input values, *i.e.* no uncertainties on the input values
- $M_\infty = 0.291,\ Re = 1.9 \cdot 10^6,\ \alpha = 5^\circ$

Figure: Mesh M1



- Meshes
  - M1 = $\mathcal{O}(0.1\text{M})$ points
  - M3 = $\mathcal{O}(0.4\text{M})$ points
  - M5 = $\mathcal{O}(1.7\text{M})$ points

Example: 2D turbulent flow about airfoil NACA0015

Experimental values: $C_L = 0.53$, $C_D = 0.0086$

		C_L			C_D		
		SA *sp*	SA *dp*	KW *dp*	SA *sp*	SA *dp*	KW *dp*
↑	**M1**	0.5282	0.5282	0.5196	0.013195	0.013195	0.012142
δ_{num}	**M3**	0.5270	0.5270	0.5161	0.012639	0.012639	0.012372
↓	**M5**	0.5263	0.5262	0.5148	0.012549	0.012537	0.012691
		$\leftarrow \delta_{fp} \rightarrow$			$\leftarrow \delta_{fp} \rightarrow$		
			$\leftarrow \delta_{model} \rightarrow$			$\leftarrow \delta_{model} \rightarrow$	

M3	$R_\rho = 10^{-2}$	$R_\rho = 10^{-3}$	$R_\rho = 10^{-4}$	...	$R_\rho = 10^{-9}$
C_L	0.522872	0.527097	0.527060	...	0.527055
C_D	0.012850	0.012646	0.012639	...	0.012639
		$\leftarrow \delta_{conv} \rightarrow$			

Conclusions

- **Both CFD and WT simulations need to be improved to attain the desired precision.**
- *"If your computation predicts drag with an error of 2 to 5 drag counts, it is a good computation; if the prediction is perfect, something must be wrong with the computation; if the error is of 20 drag counts, something may be wrong with the experiment."*

  Destarac, *Far-Field/Near-Field drag balance and applications of drag extraction in CFD*, VKI, 2003

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Conclusions

- Validation in fluid dynamics is a broad topic involving several complex terms contributing to the experimental/ computational gap
- For a 2D (RANS) flow about an airfoil all types of error (convergence, model, finite precision) were checked
- Articles with assessment of numerical and modeling error plus influence of uncertain parameters = probably the future of applied numerical studies for aeronautics
- Data assimilation will probably change the way we consider validation exercises