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– Error vs Uncertainty

• An error is defined as the difference between a given solution and its “true/exact” value. It has a sign and it requires the knowledge of the “truth”

• An uncertainty defines an interval that should contain the “true/exact” value with a certain degree of confidence. It is defined with a ±
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• Numerical Error:
  - Round-off error
  - Iterative error
  - Discretization error

• Three components of the numerical error behave differently with the increase of the number of degrees of freedom (grid refinement)
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• Round-off error:
  - Due to the finite precision of computers
  - Decreased by the use of double precision
  - May be dominant in ill-conditioned problems
  - It grows with the increase of the number of degrees of freedom (grid refinement)
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- Iterative error:
  - Non-linear equations (convection in momentum equations)
  - Decoupling of the equations (turbulence model solved for a given mean velocity field and momentum equations solved with a “known” eddy-viscosity)
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- Iterative error:
  - Discretization schemes with explicit corrections for the high-order terms
  - Solution of the systems of algebraic equations with iterative methods (Jacobi, Gauss-Seidel, Conjugate Gradients, GMRES, ...)

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• Iterative error:

  - In principle, it can be reduced to machine accuracy (if there are no problems with the round-off error)

  - The reduction of the iterative error becomes hardest with the increase of the number of degrees of freedom (grid refinement). Multigrid techniques may avoid problems with the size of the system of algebraic equations to solve
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• Iterative error:

  - It is important to define (know) the meaning of one iteration

  - Iterative error estimates based on differences or normalized residuals of the last iteration performed are not reliable

  - For iterative error estimates, the $L_\infty$ norm is a more appropriate choice than the $L_1$ and $L_2$ norms
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• Iterative error:

  - RANS (with eddy-viscosity model) calculation of the turbulent flow in a channel

  - Initial velocity field obtained from the specified profiles at the inlet

  - Solution converged to machine precision (10^{-14})
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• Iterative error:

  - Convergence criteria based on the maximum difference between consecutive iterations, \( e_t \)

  - Iterative error obtained from the difference to the solution converged to machine accuracy

  - Example of iterative errors for the horizontal velocity component, \( U^1 \)
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• Iterative error:

\[ e_I = 10^{-3} \]

\[ e_I = 10^{-5} \]

\[ e_I = 10^{-7} \]

• Largest iterative error is 2 orders of magnitude larger than \( e_I \).
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• Discretization error:
  
  - Consequence of the transformation of the continuum equation(s) into a system of algebraic equations
  
  - It may have a geometric component, which may even be the dominant contribution in domains bounded by surfaces with high curvature
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• Discretization error:

  - Usually, it is the main contribution to the numerical error
  - Can only be determined with the knowledge of the exact solution
  - Tends to diminish with the increase of the number of degrees of freedom (grid refinement)
  - Estimate of the discretization error may be obtained from grid refinement studies
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- Discretization error:
  - Glauert’s method for lifting line theory
  - Rectangular wing without twist and aspect ratio \( \Lambda=6 \)
  - Symmetric section (foil) with \( C'_l = 2\pi, \alpha = 2^\circ \)
  - Convergence of \( C_L \) and \( C_{Di} \) with the number of terms of the series, \( n \)

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• Discretization error:
  - In this example there is no iterative error
  - For series with more than 35 terms, the round-off error is no longer negligible
  - “Exact” solution obtained with 35 terms in the series
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- Discretization error:
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• Discretization error

- Assumed behaviour of the error

\[ e(\phi) = \phi - \phi_{exact} \equiv \alpha h_i^p \]

\begin{align*}
\phi & \quad \text{– Local or functional variable} \\
\phi_{exact} & \quad \text{– Exact solution} \\
\alpha & \quad \text{– Constant related to the error level} \\
h_i & \quad \text{– Typical dimension of the grid} \\
p & \quad \text{– Order of accuracy}
\end{align*}

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- Discretization error

\[ e(\phi) = \phi - \phi_{exact} \approx \alpha h_i^p \]

- Asymptotic region, i.e. all remaining (high-order) terms of the power series expansion are negligible

- Typical grid size, \( h_i \), may be troublesome to define. Geometrical similarity of the grids is required (Multi-block, unstructured grids)
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- Discretization error
  
  \[ e(\phi) = \phi - \phi_{\text{exact}} = \alpha h^p_i \]

- Minimum number of grids to obtain \( \alpha \) and \( \phi_{\text{exact}} \): 2.

- It is not safe to use only two grids. There is no guarantee that the data is in the asymptotic range. Therefore, the order of accuracy, \( p \), is unknown.

- In non-linear problems, there is no guarantee that the theoretical order of accuracy is equal to the lowest order of all the discretization schemes adopted.

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• Discretization error

\[ e(\phi) = \phi - \phi_{exact} \equiv \alpha h_i^p \]

- Minimum number of grids to estimate \( \alpha, p \) and \( \phi_{exact} \): 3.

- In practical applications, the data may exhibit scatter (\( h_i \) definition, interpolations, integrations,...) Therefore, three grids do not guarantee a reliable estimate of \( \alpha, p \) and \( \phi_{exact} \)

- If more than three grids are available, \( \alpha, p \) and \( \phi_{exact} \) may be determined in the least squares sense
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• Discretization error

- Determination of the area of a cylindrical surface with a Gauss quadrature rule using 1 point per direction

> Two types of grids:

A. Equidistant points along the diameter, \( \Delta Z = \text{constant} \).

B. Equidistant points along the surface, \( \Delta \theta = \text{constant} \).
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- Discretization error
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- Discretization error
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Verification:

“Solve the equations right”

Validation:

“Solve the right equations”

Roache, 1998
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Verification and Validation in CFD Applications for Aerodynamics

• Verification includes two different activities:

  - Code Verification
    Guarantee that the computer code does not contain errors (bugs). Error evaluation that requires the knowledge of the exact solution

  - Solution/calculations Verification
    Estimate the numerical uncertainty for a numerical solution that has an unknown exact solution (Error estimation)
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Verification and Validation in CFD Applications for Aerodynamics

• Code Verification

  - In some practical applications, there are no exact solutions available. For example, the Reynolds-averaged Navier-Stokes equations supplemented by a turbulence model do not have any known exact solutions

  - The Method of Manufactured Solutions (MMS) is a viable alternative to perform Code Verification when analytical solutions are not available.
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- Method of Manufactured Solutions:

  1. Choose the calculation domain

  2. Choose the analytical solution for the dependent variables of the problem

  3. Substitute the chosen solution in the differential equations to determine source terms that guarantee that the selected exact solution satisfies the “new” system of differential equations
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• Method of Manufactured Solutions

  - The RANS equations do not form a closed system of equations

  - Any additional equations (turbulence model) should also be part of the manufactured solution

  - Numerical convergence properties may depend on the turbulence model equations
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- Method of Manufactured Solutions

  - Example for the one-equation model of Spalart & Allmaras

  - Manufactured solution includes the dependent variable of the turbulence model or alternatively the specification of the eddy-viscosity

  - Velocity field is similar to a zero pressure gradient boundary-layer

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- Method of Manufactured Solutions

MS Lisbon Workshop 2006

RMS error of $u_x$

Spalart & Allmaras one-equation model

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• Solution/Calculations Verification
  – Exact solution is not available
  – Numerical error estimation usually assumes that the discretization error is dominant (this requires an iterative error at least two orders of magnitude smaller)
  – Methods based on grid refinement studies are one of the alternatives for the estimation of the discretization error/uncertainty
  – Mathematical problem
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• Solution/Calculations Verification
  
  – Estimate the uncertainty, $U$, of a numerical solution of a flow quantity $\phi$ for which the exact solution is not known

Objective:

$$\phi - U(\phi) \leq \phi_{\text{exact}} \leq \phi + U(\phi)$$

with a confidence level of 95%

$$U(\phi) = F_s e(\phi)$$

$F_s \rightarrow$ Safety factor

$e(\phi) \rightarrow$ Error estimate
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• Solution/Calculations Verification

\[ e(\phi_i) = \phi_i - \phi_o = \delta_{RE} = \alpha \cdot h_i^p \]

\( \phi_i \rightarrow \text{Numerical solution of a local or functional variable} \)

\( \phi_o \rightarrow \text{Estimate of the exact solution} \)

\( \delta_{RE} \rightarrow \text{Estimate of the error} \)

\( \alpha_j \rightarrow \text{Constant related to the error level} \)

\( h_i \rightarrow \text{Typical cell size} \)

\( p_j \rightarrow \text{Observed order of accuracy} \)

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• Solution/Calculations Verification
  - At least 3 grids are required to determine $\phi_o$, $\alpha$, $p$

\[
\phi_1 - \phi_o = \delta_{RE} = \frac{\phi_2 - \phi_1}{(h_2/h_1)^p - 1}
\]

\[
\frac{\phi_3 - \phi_2}{\phi_2 - \phi_1} \left( \frac{h_2}{h_1} \right)^p \left( \frac{h_3/h_2}{h_2/h_1} \right)^p - 1 = 0
\]
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• Solution/Calculations Verification

  - Apparent convergence or divergence for a grid triplet with \( h_2/h_1 = h_3/h_2 \)!

Convergence ratio: \( R = \frac{\phi_2 - \phi_1}{\phi_3 - \phi_2} \)

- \( 0 < R < 1 \) → Monotonic Convergence
- \( -1 < R < 0 \) → Oscillatory Convergence
- \( R > 1 \) → Monotonic Divergence
- \( R < -1 \) → Oscillatory Divergence
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• Solution/Calculations Verification

• Example for the turbulent flow over a flat plate

  - Time-averaged RANS equations with eddy-viscosity $k-\omega$ two equation models

  - Convergence of the friction resistance coefficient of the plate with the grid refinement. Estimate of the numerical uncertainty for two levels of grid refinement:

    \[ h_1 \leftrightarrow 1537 \times 193, \ h_i/h_1=2 \leftrightarrow 769 \times 97. \]
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- Solution/Calculations Verification

\[ \text{Re}_L = 10^7 \]
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• Solution/Calculations Verification

Re_L = 10^8

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- Solution/Calculations Verification

\[ \text{Re}_L = 10^9 \]

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• Validation
  – Estimate of the modeling error by comparison to experimental data
  – Validation method proposed recently by the ASME:
    > Comparison error obtained from the difference between the numerical solution and the experimental result, $|E|$
    > Validation uncertainty, $U_{val}$, that combines numerical uncertainty, experimental uncertainty and input parameters uncertainty (boundary conditions, Reynolds number...)

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• Validation

\[ |E| > U_{val} \]

- Modeling error is probably similar to \(|E|\). Therefore, there is information about the need to improve or not the model

\[ |E| < U_{val} \]

- Modeling error smaller than the noise originated by the numerical, experimental and input parameters uncertainty.
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- Validation

- Flow at the propeller plane of a tanker at model scale

- Comparison of axial velocity

- RANS equations with an eddy-viscosity model

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• Validation

Experimental

Numerical

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• Validation

Usual Comparison
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- Validation

![Graph showing experimental uncertainty and validation results.](image)
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- Validation

![Graph showing experimental and SST results with error bars and a legend for experimental and SST data.]

Introdução of numerical uncertainty
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• Validation

\[
E = |S - D| \\
U_{val} = (U_{num}^2 + U_D^2)^{1/2}
\]

Comparison of validation error with validation uncertainty
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• What we want to avoid!