ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

Solution Verification based on Grid Refinement Studies and Power Series Expansions

L. Eça (TU-Lisbon, IST)
M. Hoekstra (MARIN)

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

Contents

1. Motivation

- CFD simulations require the assessment of their numerical uncertainty to establish their credibility
- Most of the existing methods for uncertainty estimation require data in the so-called ``asymptotic range”
- This often means levels of grid refinement beyond those normally used in practical applications

ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

1. Motivation

- Uncertainty estimation for practical calculations as to deal with several difficulties:
  - Grids not sufficiently refined to attain the ``asymptotic range”
  - Scatter in the data originated by lack of geometric similarity, switches in the turbulence models, post-processing...
- Develop a reliable procedure for uncertainty estimation of practical calculations

2. Proposed procedure

- Power series expansions applied to data obtained from grid refinement studies
- Contributions of round-off and iterative errors are assumed to be negligible when compared to the discretization error
- Definition of the typical cell size, h_i, discussed at the ASME V&V 2012 Conference

ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

2. Proposed procedure

- Error estimation

$$\varepsilon_\phi \cong \delta_{RE} = \phi_i - \phi_o = \alpha h_i^p$$

δ_{RE} Estimated error of variable ϕ (integral or local)

ϕ_i Solution of variable ϕ in grid i

ϕ_o Estimated exact solution of ϕ

α Grid related constant

h_i Typical cell size

p Observed order of grid convergence

2. Proposed procedure

- Alternative expansions for error estimation

$$\delta_1 = \phi_i - \phi_o = \alpha h_i$$

$$\delta_2 = \phi_i - \phi_o = \alpha h_i^2$$

$$\delta_{12} = \phi_i - \phi_o = \alpha_1 h_i + \alpha_2 h_i^2$$

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

2. Proposed procedure

- All error estimators are solved in the least-squares sense

$$S_{RE}(\phi_o, \alpha, p) = \sqrt{\sum_{i=1}^{n_g} \left(\phi_i - \left(\phi_o + \alpha h_i^p\right)\right)^2}, \qquad \frac{\partial S_{RE}}{\partial \phi_o} = 0, \frac{\partial S_{RE}}{\partial \alpha} = 0, \frac{\partial S_{RE}}{\partial p} = 0$$

$$S_1(\phi_o, \alpha) = \sqrt{\sum_{i=1}^{n_g} (\phi_i - (\phi_o + \alpha h_i))^2}, \qquad \frac{\partial S_1}{\partial \phi_o} = 0, \frac{\partial S_1}{\partial \alpha} = 0$$

$$S_2(\phi_o, \alpha) = \sqrt{\sum_{i=1}^{n_g} \left(\phi_i - \left(\phi_o + \alpha h_i^2\right)\right)^2}, \qquad \frac{\partial S_2}{\partial \phi_o} = 0, \frac{\partial S_2}{\partial \alpha} = 0$$

$$S_{12}(\phi_o, \alpha) = \sqrt{\sum_{i=1}^{n_g} \left(\phi_i - \left(\phi_o + \alpha_1 h_i + \alpha_2 h_i^2\right)\right)^2}, \quad \frac{\partial S_{12}}{\partial \phi_o} = 0, \frac{\partial S_{12}}{\partial \alpha_1} = 0, \frac{\partial S_{12}}{\partial \alpha_2} = 0$$

2. Proposed procedure

- Observed order of grid convergence *p* and standard deviations σ of the fits are used to select error estimator

$$\sigma_{RE} = \sqrt{\frac{\sum_{i=1}^{n_g}\left(\phi_i - \left(\phi_o + \alpha h_i^p\right)\right)^2}{\left(n_g - 3\right)}}, \quad \sigma_1 = \sqrt{\frac{\sum_{i=1}^{n_g}\left(\phi_i - \left(\phi_o + \alpha h_i\right)\right)^2}{\left(n_g - 2\right)}}$$

$$\sigma_2 = \sqrt{\frac{\sum_{i=1}^{n_g}\left(\phi_i - \left(\phi_o + \alpha h_i^2\right)\right)^2}{\left(n_g - 2\right)}}, \quad \sigma_{12} = \sqrt{\frac{\sum_{i=1}^{n_g}\left(\phi_i - \left(\phi_o + \alpha_1 h_i + \alpha_2 h_i^2\right)\right)^2}{\left(n_g - 3\right)}}$$

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

2. Proposed procedure

- Alternative weighted fits also performed with

$$w_i = \frac{\frac{1}{h_i}}{\sum_{i=1}^{n_g}\frac{1}{h_i}}$$

that lead, for example, to

$$S_{RE}^w\left(\phi_o, \alpha, p\right) = \sqrt{\sum_{i=1}^{n_g} w_i\left(\phi_i - \left(\phi_o + \alpha h_i^p\right)\right)^2}$$

$$\sigma_{RE}^w = \sqrt{\frac{\sum_{i=1}^{n_g} n_g w_i\left(\phi_i - \left(\phi_o + \alpha h_i^p\right)\right)^2}{\left(n_g - 3\right)}}$$

2. Proposed procedure

- Monotonic convergence for $p>0$ or $p^w>0$

  - $0.5 \le p \le 2 \Rightarrow \varepsilon_\phi = \begin{cases} \delta_{RE} \Leftarrow \sigma_{RE} \le \sigma_{RE}^w \\ \delta_{RE}^w \Leftarrow \sigma_{RE} > \sigma_{RE}^w \end{cases}$

  - $p > 2 \Rightarrow \varepsilon_\phi = \delta$ of fit with $\sigma = \min(\sigma_1,\ \sigma_1^w,\ \sigma_2,\ \sigma_2^w)$

  - $p < 0.5 \Rightarrow \varepsilon_\phi = \delta$ of fit with $\sigma = \min(\sigma_1,\ \sigma_1^w,\ \sigma_2,\ \sigma_2^w\ \sigma_{12},\ \sigma_{12}^w)$

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

2. Proposed procedure

- Anomalous behaviour

  - $p<0$ and $p^w<0$ or impossible to determine

  - Error may be estimated from fits with fixed exponents

  - $\varepsilon_\phi = \delta$ of fit with $\sigma = \min(\sigma_1,\ \sigma_1^w,\ \sigma_2,\ \sigma_2^w\ \sigma_{12},\ \sigma_{12}^w)$

2. Proposed procedure

- Uncertainty estimation intends to satisfy

$$\phi_i - U_\phi \le \phi_{exact} \le \phi_i + U_\phi$$

95% of the times

- Quality of available data measured from

$$\Delta_\phi = \frac{(\phi_i)_{\max} - (\phi_i)_{\min}}{n_g - 1}$$

and σ of the selected fit for error estimation

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

2. Proposed procedure

- Uncertainty is obtained from the estimated error ε_ϕ and a safety factor F_s

$$U_\phi = F_s \varepsilon_\phi$$

- Definition of the safety factor F_s follows the G.C.I of P.J. Roache
  - Reliable error estimate, $F_s = 1.25 \Leftarrow \begin{cases} 0.5 \le p \le 2.1 \quad \wedge \sigma_{RE} < \Delta_o \\ 0.5 \le p^w \le 2.1 \wedge \sigma^w_{RE} < \Delta_o \end{cases}$
  - Otherwise, $F_s = 3$

2. Proposed procedure

- "Good" error estimation, $\sigma < \Delta_o$

$$U_\phi = F_s \varepsilon_\phi + \sigma + \left|\phi_i - \phi_{fit}\right|$$

- "Bad" error estimation, $\sigma \geq \Delta_o$

$$U_\phi = 3\frac{\sigma}{\Delta_o}\left(\varepsilon_\phi + \sigma + \left|\phi_i - \phi_{fit}\right|\right)$$

- For data without noise and monotonic convergence the method reduces to the G.C.I.

ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application

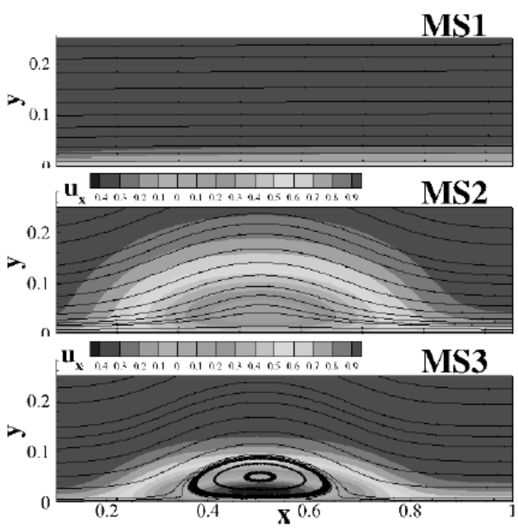
   1. Two-dimensional Manufactured Solutions that mimic a near-wall turbulent flow

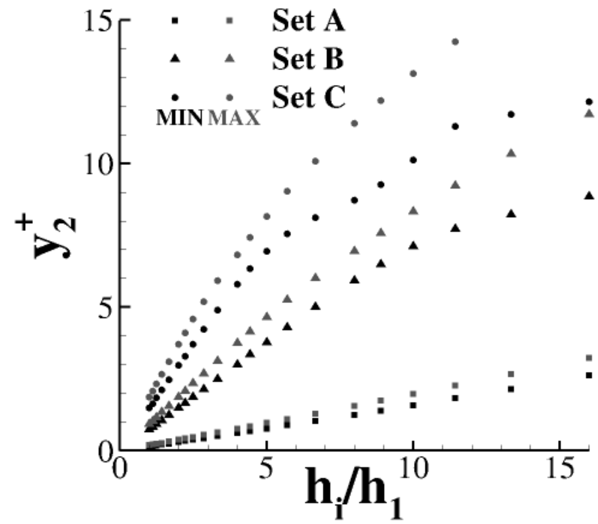
   2. Turbulent flow over a flat plate

   3. Flow over a backward facing step

   4. Flow around a tanker at model scale Reynolds number

3. Examples of application, 2-D MS's





ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, 2-D MS's

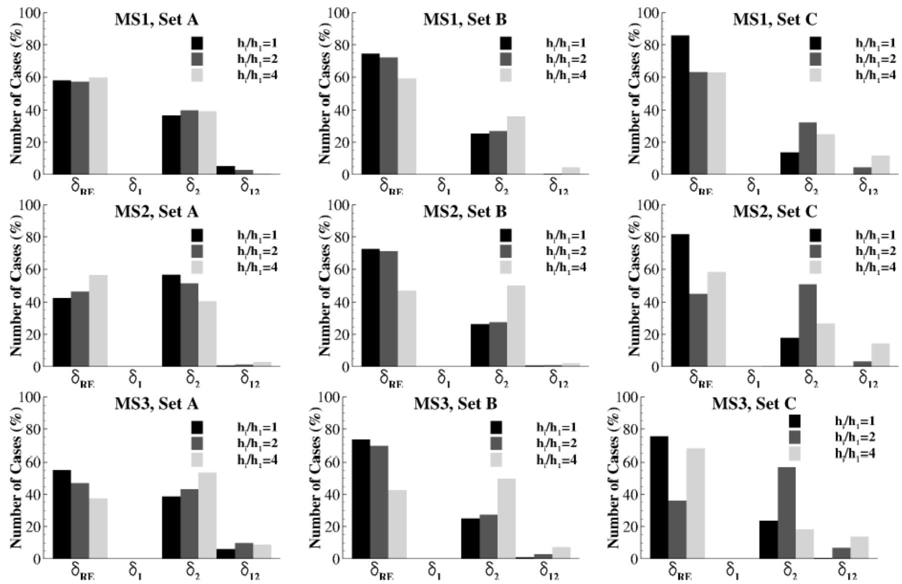
- Sets of 21 geometrically similar grids with different near-wall spacing
- Uncertainty of mean flow quantities estimated for three levels of grid refinement:

$$\frac{h_i}{h_1}=1\ (801\times 801),\ \frac{h_i}{h_1}=2\ (401\times 401),\ \frac{h_i}{h_1}=4\ (201\times 201)$$

- Check $F_e = U_\phi / e_\phi$ and the error estimate used to obtain the numerical uncertainty

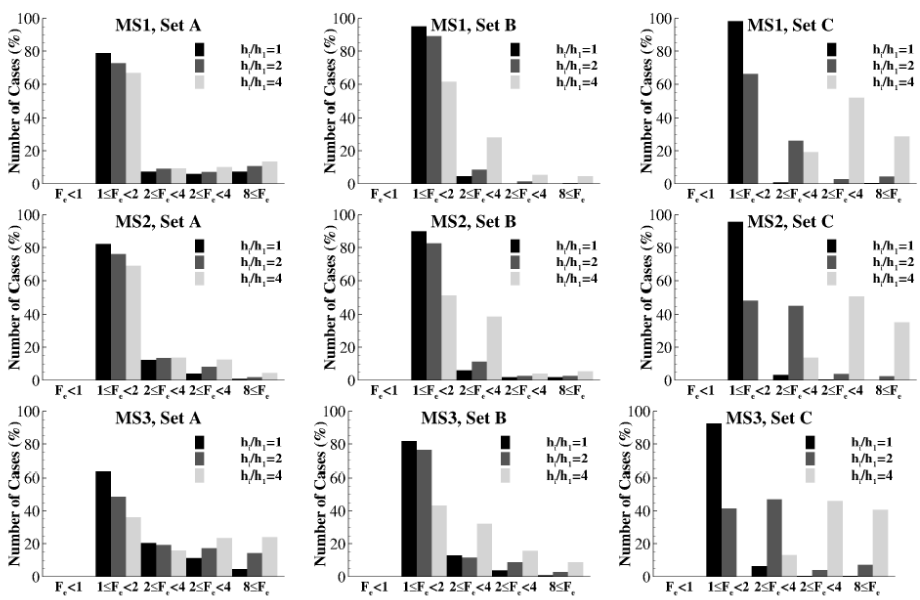
ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, 2-D MS's u_x



ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, 2-D MS's u_x $F_e = \frac{U_\phi}{e_\phi}$



3. Examples of application, Flat plate

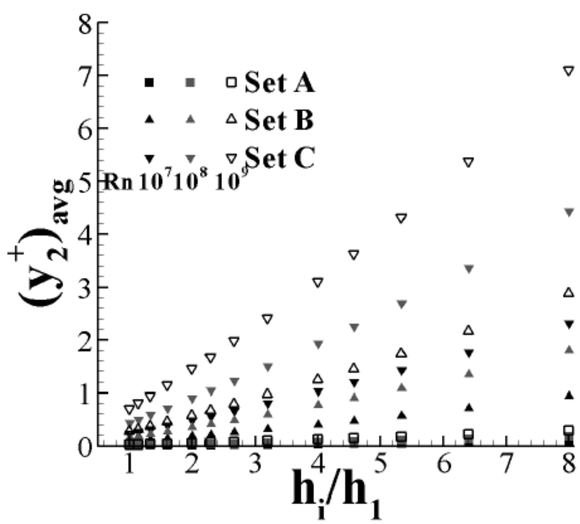
- Sets of 13 geometrically similar grids with different near-wall spacing for Reynolds numbers of 10^7, 10^8 and 10^9
- Spalart & Allmaras and SST *k*-ω turbulence models
- Uncertainty of mean flow, turbulence and integral quantities estimated for three levels of grid refinement:

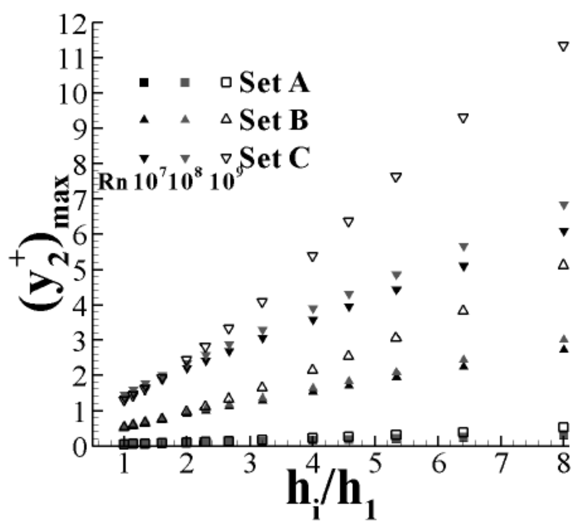
$$\frac{h_i}{h_1}=1\ (1537\times193),\ \frac{h_i}{h_1}=2\ (769\times97),\ \frac{h_i}{h_1}=4\ (385\times49)\ Rn=10^7$$

- Check overlap of error bars and the error estimate used to obtain the numerical uncertainty

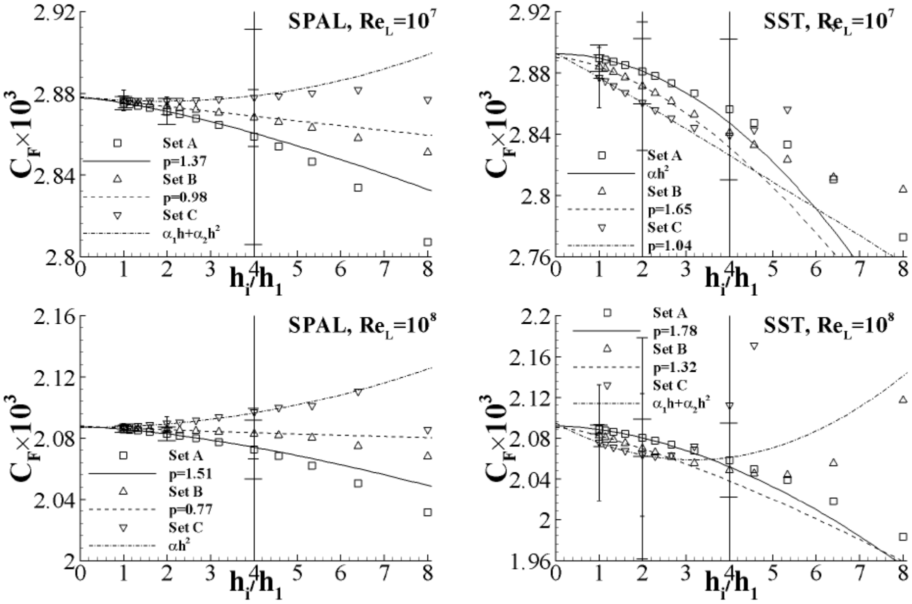
ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, Flat plate





3. Examples of application, Flat plate

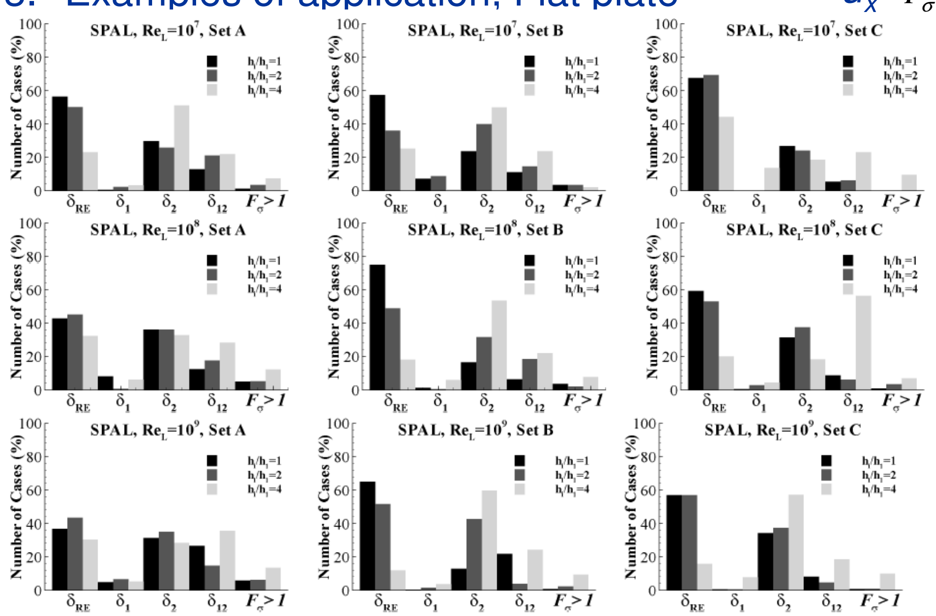


ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, Flat plate

u_x $\quad F_\sigma = \dfrac{\sigma}{\Delta_o}$

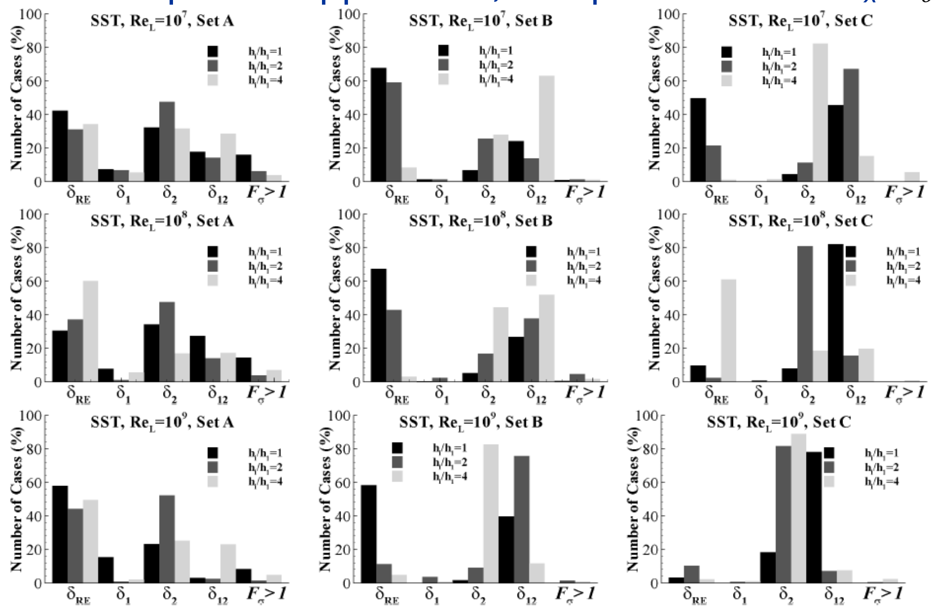
SPAL



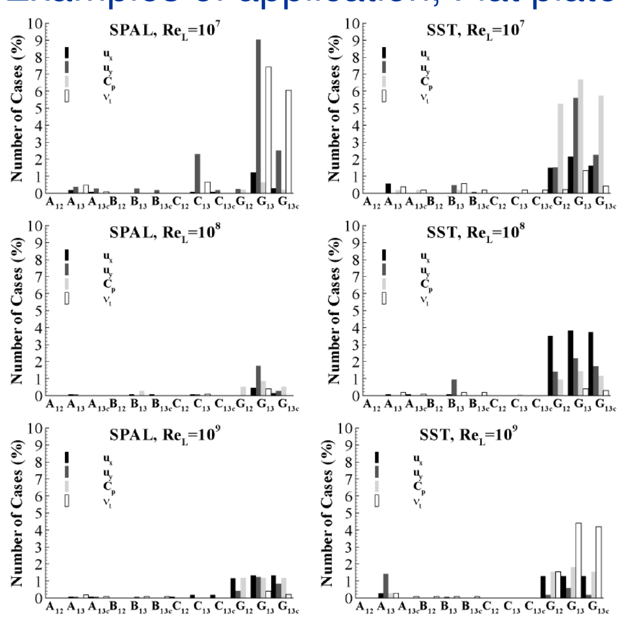
3. Examples of application, Flat plate

u_x $F_\sigma = \frac{\sigma}{\Delta_o}$

SST



3. Examples of application, Flat plate



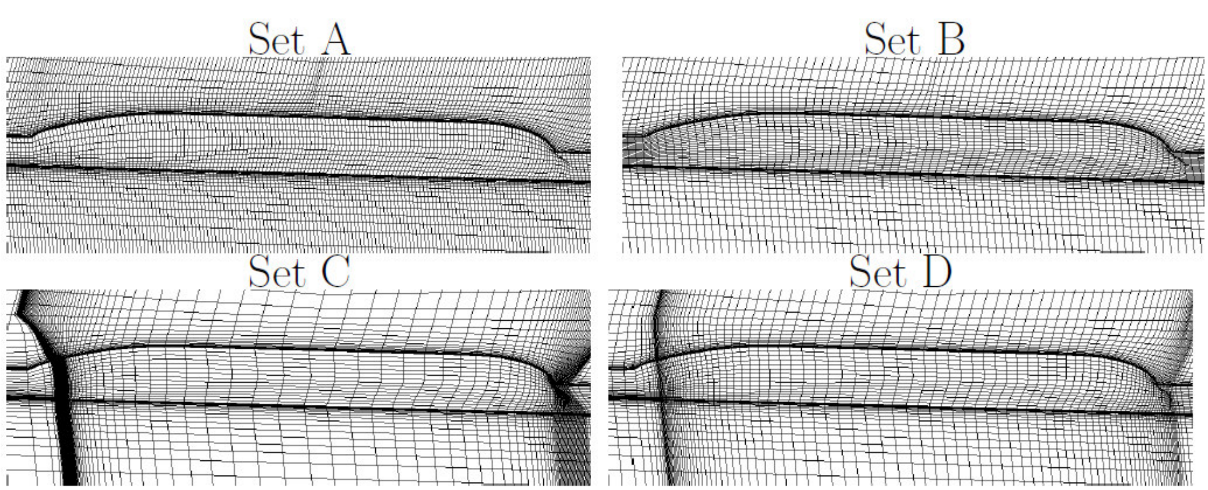
Inconsistent error bars (non overlapping)

3. Examples of application, Tanker $Rn = 4.6\times10^6$

- 4 sets of 6 nearly-geometrically similar grids with 0.9×10^6 to 8×10^6 cells covering a grid refinement ratio of 2
- SST k-ω turbulence model
- Uncertainty of mean and turbulence flow quantities at the propeller plane and resistance coefficients
- Check overlap of error bars and the error estimate used to obtain the numerical uncertainty

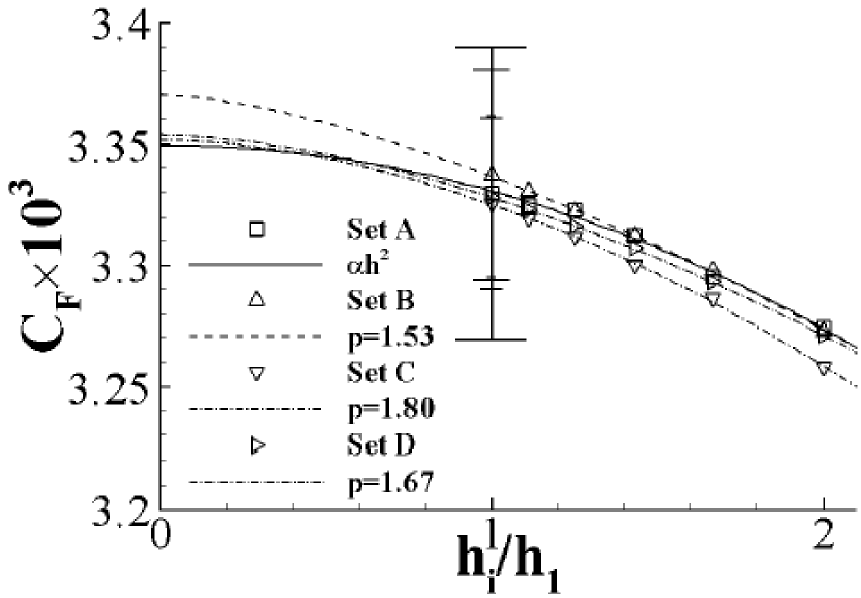
ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, Tanker $Rn = 4.6\times10^6$



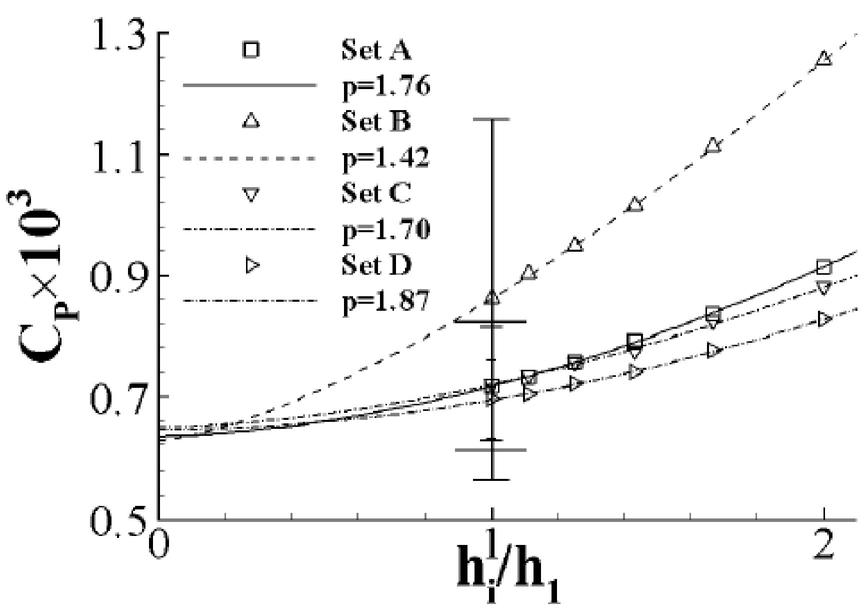
ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, Tanker $Rn = 4.6\times10^{6}$



ASME 2013 MAY 22–24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

3. Examples of application, Tanker $Rn = 4.6\times10^{6}$



4. Final Remarks

- We presented a procedure for the estimation of the numerical uncertainty of any integral or local flow quantity based on grid refinement studies
- The uncertainty is based on an error estimation multiplied by a safety factor
- The error is estimated with power series expansions as a function of the typical cell size, which are fitted to the data in the least squares sense

ASME 2013 MAY 22-24, 2013 • LAS VEGAS, NEVADA
VERIFICATION AND VALIDATION SYMPOSIUM

4. Final Remarks

- Several alternative formulations are involved, including weighted and non-weighted fits of expressions with different exponents in the leading term of the series
- The selection of the best error estimate is based on the standard deviation of the fits
- For well-behaved data sets, i.e. monotonic convergence with the expected observed order of accuracy and no scatter in the data, the method reduces to the well known Grid Convergence Index