An Evaluation of Verification Procedures

September 20, 2004

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1 Introduction

In this study variations of Richardson Extrapolation are investigated as a contribution to the establishment of reliable procedures for verification of numerical CFD simulations. Taylor expansions with fixed exponents up to three terms and a single-term power series expansion with unknown exponent are tested, and these procedures are also applied as least square roots approach.
The evaluated forms of Richardson Extrapolation are the ones supposed by Eça and Hoekstra [1],[2]. In the following I will use their termininology to name these evaluation procedures.

- Method p: One-term Taylor series expansion with

$$\phi_0 \quad = \quad \phi_i - \alpha \cdot h_i^p \tag{1}$$

  where ϕ_0 is the extrapolated solution. p is the estimated order of convergence, and α is an unknown parameter. i denotes the index of the grid, where h_i is the characteristic grid size and ϕ_i is the variable to be extrapolated.

- Method t1: One-term Taylor series expansion with fixed exponent.

$$\phi_0 \quad = \quad \phi_i - \alpha \cdot h_i^{p_{min}} \tag{2}$$

  p_{min} is set equal to the lowest order of accuracy of the discretization scheme.

- Method t2: Two-term Taylor series expansion with p_{min} and $p_{min} + 1$.

- Method t3: Three-term Taylor series expansion using p_{min}, $p_{min} + 1$ and $p_{min} + 2$.

The fixed exponent methods and their least square root approaches have a straightforward implementation. Method p can be solved using a false position method and its least square root approach was solved by an iterative Gauss-Newton method.

The evaluation procedures were applied to an analytical function with artificial scatter in order to observe their behaviour in a statistical way.

2 An attempt to evaluate the influence of scatter

The least square root approaches were introduced in order to deal with scatter shown in the data. In this section artificially produced scattered data is presented to apply the evaluation procedures on it. Following considerations were made to formulate the conditions this data had to fulfill:

- The function shall simulate a grid refinement study in the asymptotic range. Therefore, it shall be representable by an equation as in the classical sense of a Richardon Extrapolation. In the absence of scatter it shall have an analytical solution that can be found by all the applied methods.

- The scatter has to be represented by an error function with a defined range of scatter.

- The scatter shall be zero as the grid independent solution is reached and the range of scatter shall grow as the grid spacing gets coarser.

2.1 Construction of the artificially scattered function

A data set was produced by taking $\phi_{(h)} = \phi_0 + a \cdot h^p$ and adding an errorfunction $s_{(h)}$ to it:

$$\phi_{(h)} \quad = \quad \phi_0 + a \cdot h^p + s_{(h)} \tag{3}$$

The parameters ϕ_0, a and p were chosen as follows:

ϕ_0	1.0
p	2.0
a	0.5

The errorfunction was constructed as a random function with a Gaussian Distribution of the error $s_{(h)}$ over $\phi_{(h)}$. This was done by adding a finite number of cosine functions with a random phase and a certain amplitude:

$$s_{(h)} = \sum_{i=0}^{N} \sqrt{2S_{(h,\omega_i)}\Delta\omega_i} \cdot \cos(\omega_i\ t + \epsilon_i) \tag{4}$$

with

$$S_{(h,\omega)} = \frac{c}{\omega^5} \cdot e^{(-1.25\frac{\omega_m^4}{\omega^4})} \tag{5}$$

This error function is similiar to the mathematical representation of a one-dimensional seaway spectrum (Johnswap spectrum) [3]. Now c is to be determined. The aim is to assure that the error $s_{(h)}$ lies within a certain range:

$$P(|\frac{s_{(h)}}{\phi_{(h)}}| \leq 0.001 \cdot \phi_{(h)}\ h^2) = 0.997 \tag{6}$$

In other words, the error should go to zero as the grid spacing reaches zero. At $h_1 = 1.0$ the relative error should – with a probability of 0.997 – be smaller than $0.001\phi_{(h_1)}$. Speaking of a Gaussian Distribution with

$$\varphi_{(x,\sigma^2)} = \frac{1}{\sqrt{2\pi\sigma^2}}\ e^{(\frac{-x^2}{2\sigma^2})} \tag{7}$$

the standard deviation has to equal

$$\sigma_{(h)} = \frac{0.001 \cdot \phi_{(h)} \cdot h^2}{3} \tag{8}$$

to achieve this. (The error band grows with h^2, as one could assume, since we use $p = 2$) On the other hand there is a relation between the variance σ^2 and the spectrum of the amplitudes $S_{(\omega)}$ we can use to determine c:

$$\sigma^2_{(h)} = \int_0^\infty S_{(h,\omega)} d\omega \tag{9}$$

$$= c_{(h)} \int_0^\infty \omega^{-5}\, e^{(-1.25\frac{\omega_m^4}{\omega^4})} d\omega \tag{10}$$

$$= c_{(h)}\ \frac{1}{5\omega_m^4} \tag{11}$$

$$\Rightarrow \quad c_{(h)} = \sigma^2_{(h)} \cdot 5\omega_m^4 \tag{12}$$

The phases ϵ_i are chosen by random in the interval $[0\ ..\ 2\pi]$. Additionaly every frequency ω_i is chosen by random from the according interval $\Delta\omega$.
Now ω_m (which is the frequency where $S(h,\omega)$ has its maximum) is remaining the parameter to be freely chosen. In this study I set $\omega_m = 50$, so the characteristic amplitudes of the errorfunction have a period of $\Delta h = \frac{2\pi}{\omega_m} = 0.126$. Figure 1 shows two data sets superposed with errorfunctions that were generated in the manner described above. $\phi_{(h)}$ is made nondimensional by dividing with the exact solution ϕ_{exact}.
In figure 2 20 sets consisting of 5 data points are shown. The grid refinement ratio was set to $h_{i+1}/h_i = \sqrt{2}$. All data sets were obtained in the described manner and thus show an error in each "grid point" which is very weakly related to the error in every other point. Working with this data, we do not only know the exact solution, but we also have knowledge of the scatter.

2.2 Application of the evaluation procedures

For testing the evaluating procedures, $30,000$ sets of data points were produced, where each $10,000$ sets had the exact order $p_exact = 1.9, 2.0 and 2.1$, respectivly. Density functions for the sets of ϕ_{0_i} of each evaluating method, containing $10,000$ values, were generated. The evaluation procedures were applied with the minimum required grids, i.e. 5 grids for method t3 in the least square roots sense. Method p in the least square root sense

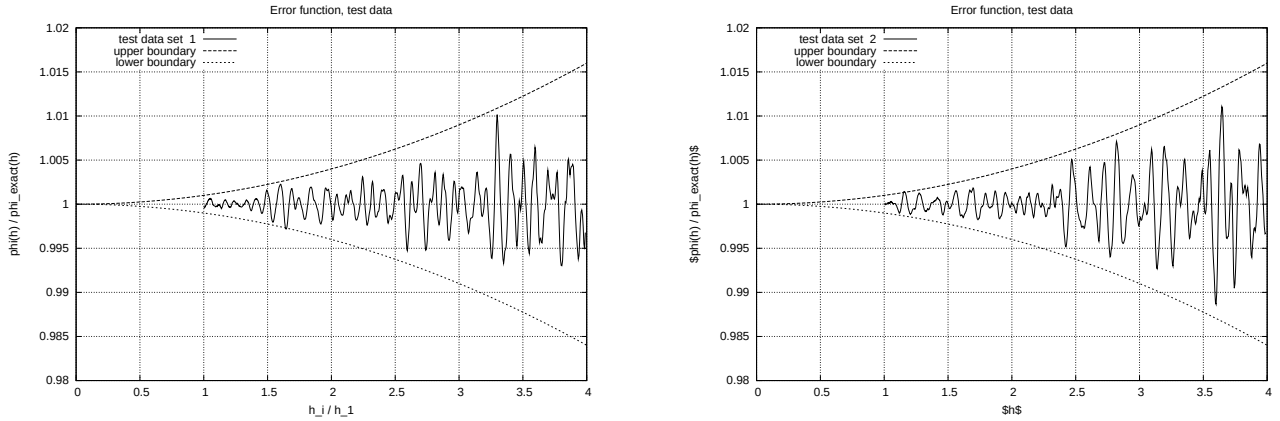

Figure 1: two errorfunctions as an example

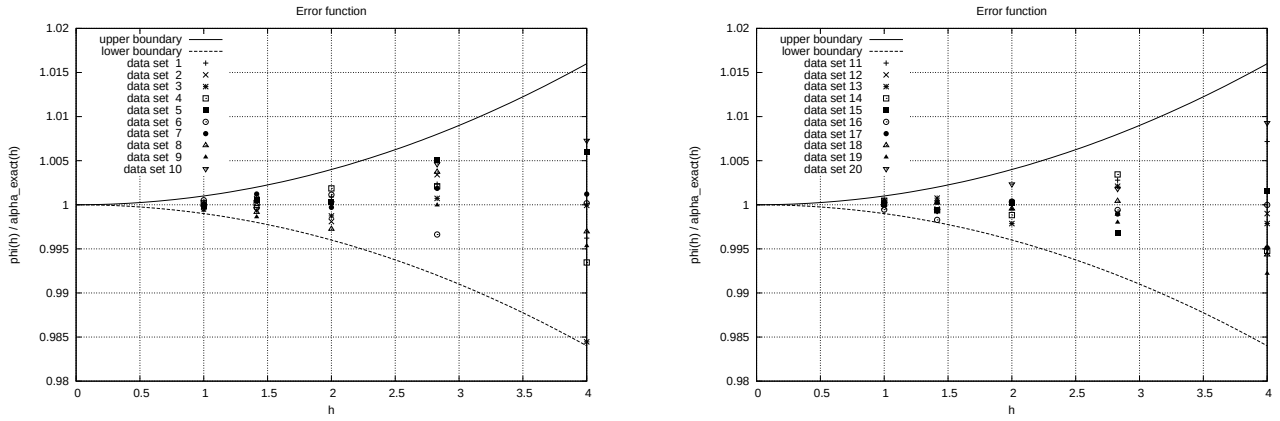

Figure 2: 20 data sets of five points with grid refinement ratio $\frac{h_{i+1}}{h_i} = \sqrt{2}$; here, only the error in each data point is shown

was also tested with 5 grids.
The results can be assumed to be gaussian density functions, as one would have expected. In table 2.2 the obtained averages μ_{fit} and standard deviations σ_{fit} are listed. μ_{fit} and σ_{fit} were calculated as

$$\mu_{fit} = \sum_{i=1}^{n} \phi_{0_i} \cdot \frac{1}{n} \tag{13}$$

$$\sigma_{fit} = \sqrt{\sum_{i=1}^{n} [\phi_{0_i} - \mu_{fit}]^2 \cdot \frac{1}{n}} \tag{14}$$

$$\tag{15}$$

The smaller σ_{fit}, the better can the inspected evaluation method be considered to be able to deal with this kind of scatter. In figures 4 to 6 the density functions are plotted. (For only $10,000$ extrapolated solutions were used in this exercise, the plots are not smooth. Anyway, they clearly tend to Gaussian Distributions and for a growing number of data they will obviously get smoother. In figure 3 the plot showing method t3 with $p_{min} = p_{exact}$ is compared to the Gauss function with corresponding μ and σ)

p		t1	t1 lsr	t2	t2 lsr	t3	t3 lsr	p	p lsr 4gr.	p lsr 5gr.
1.9	μ	1.0341	1.0499	1.0167	1.0245	1.0116	1.0169	1.0000	0.9999	0.9998
	σ	.164E-2	.207E-2	.429E-2	.526E-2	.900E-2	.110E-1	.754E-2	.948E-2	.169E-1
2.0	μ	1.0000	1.0000	1.0000	1.0000	1.0000	1.0001	0.9999	1.0000	0.9997
	σ	.166E-2	.218E-2	.441E-2	.561E-2	.940E-2	.121E-1	.694E-2	.901E-2	.171E-1
2.1	μ	0.9647	0.9459	0.9854	0.9776	0.9906	0.9857	0.9999	1.0000	0.9997
	σ	.167E-2	.227E-2	.451E-2	.597E-2	.973E-2	.131E-1	.638E-2	.858E-2	.170E-1

The most important observations can be summarized as followed:

- The least square roots approaches do in general produce results with a greater standard deviation σ_{fit}. For $p_{min} \neq p_{exact}$, the least square root approaches of the fixed exponent methods even show less accuracy in meeting the correct average, which should be $\mu_{exact} = \phi_{exact} = 1.0$.

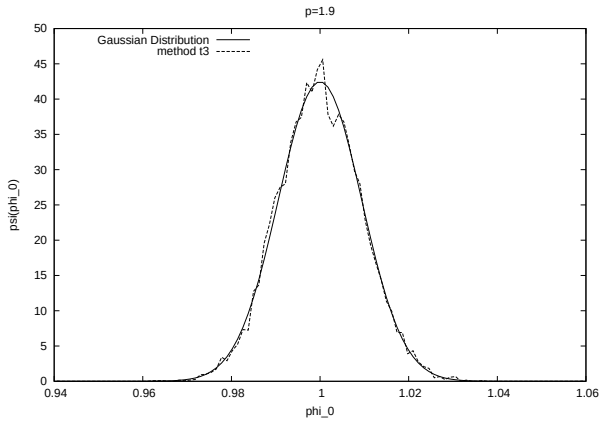

Figure 3: distribution resulted by method t3, compared to Gaussian Distribution with μ and σ obtained by equation 14 and 15

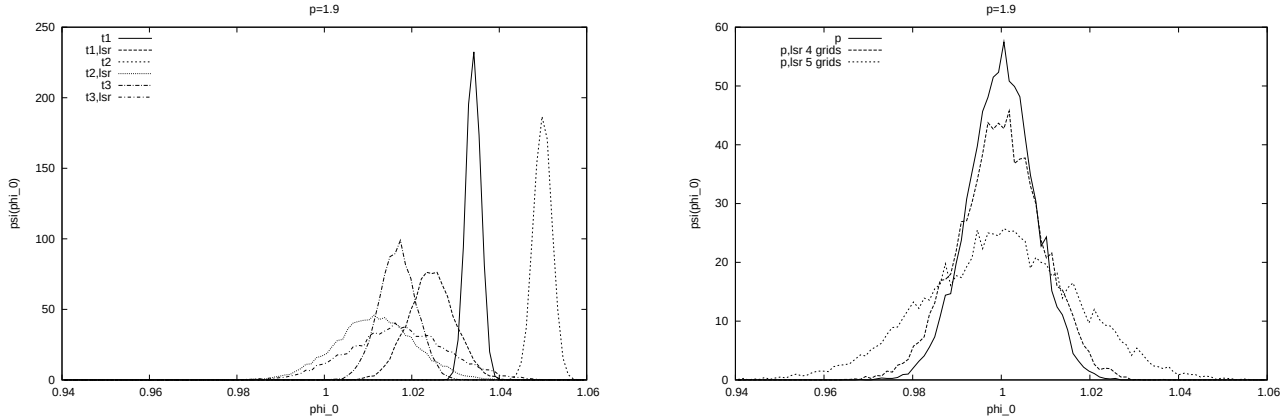

Figure 4: $p_{exact} = 1.9$; distribution function of ϕ_0 for fixed (left) and unknown (right) exponent methods

- With $p_{min} \neq p_{exact}$, the fixed exponent approaches using higher order terms obtain the more exact results than the methods t1 and t1 lsr. Although the former have greater σ_{fit}, μ_{fit} is calculated closer to the exact value. Nevertheless, all the fixed exponent methods do not turn out with $\mu_{fit} = \phi_{exact}$ unless $p_{min} = p_{exact}$.
- On the other hand, having $p_{min} = p_{exact}$, the results of the methods t1 and t1 lsr produce a smaller band of ϕ_0 than the methods t2 and t3 and their least square approaches.
- The fixed exponent methods seem to show a slightly growing standard deviation σ_{fit} as p_{exact} increases. The methods with unknown exponent exhibit a smaller standard deviation with increasing p_{exact} except for method p lsr using 5 grids.
- Using 5 grids (one more than the required minimum) for method p lsr does not improve the resulting standard deviation σ_{fit}, furthermore it leads to an even greater standard deviation of the resulting ϕ_0 than the standard deviation $\sigma_{(h_5)}$ which is the greatest occuring in the data.

One explanation for the unexpected bad behaviour of the least square roots approaches is the growing relative error with increasing h. In this example the least square roots approaches are using one more data point than the simple approaches. Because of $h_{i+1}/h_i = \sqrt{(2)}$ and equation 8, the relative standard deviation at h_{i+1} is twice the relative standard deviation at h_i:

$$\frac{\sigma_{(h_{i+1})}}{\phi_{(h_{i+1})}} = \frac{0.001 \cdot \phi_{(h_{i+1})} \cdot h_{i+1}^2}{3 \cdot \phi_{(h_{i+1})}} \tag{16}$$

$$= \frac{0.001 \cdot 2 \cdot h_i^2}{3} \tag{17}$$

$$= \frac{\sigma_{(h_i)}}{\phi_{(h_i)}} \tag{18}$$

$$\tag{19}$$

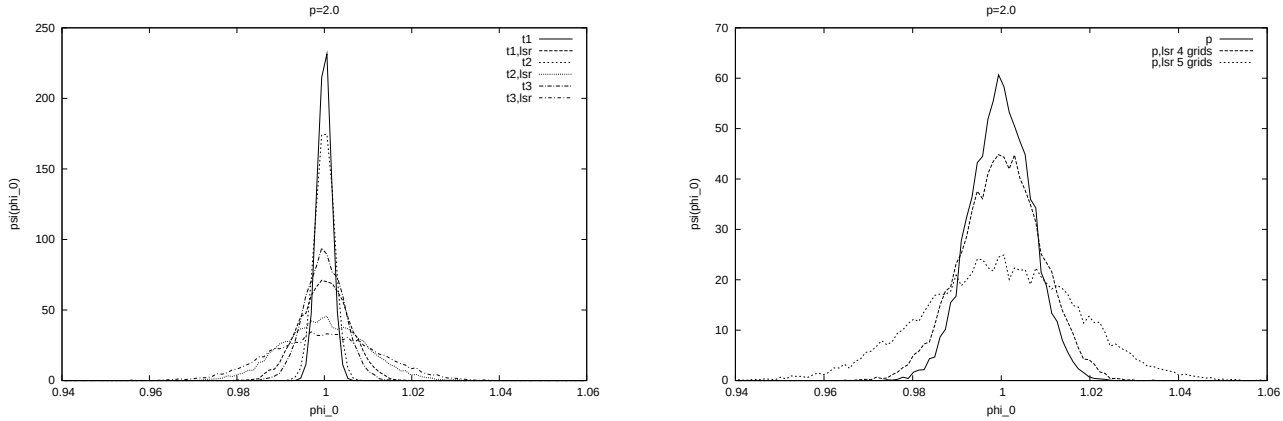

Figure 5: $p_{exact} = 2.0$; distribution function of ϕ_0 for fixed (left) and unknown (right) exponent methods

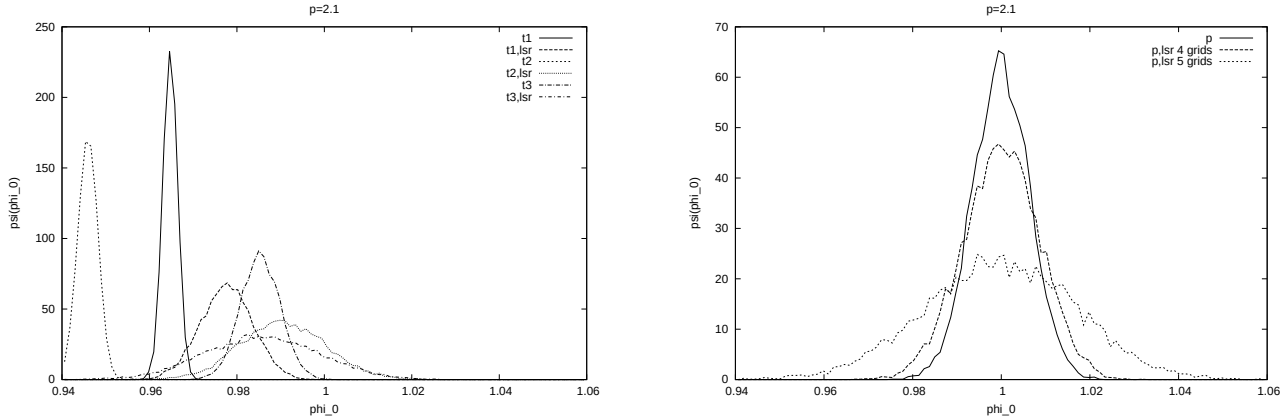

Figure 6: $p_{exact} = 2.1$; distribution function of ϕ_0 for fixed (left) and unknown (right) exponent methods

As we could see in the behaviour of the least square root approach of method p with 5 grids, even bad data at a coarse grid can affect the curve fitting at $h \to 0$.
Eça and Hoekstra introduced U_s as a contribution to the uncertainty which takes into account the possible existence of scatter in the data and is calculated for the least square root approaches. U_s was defined as

$$U_s = \sqrt{\frac{\sum_{i=1}^{n_g}(\phi_i - (\phi_0 + \sum_{j=1}^{n_j} \alpha_j h_i^{p_j}))^2}{n_g - n_u}} \tag{20}$$

$$\tag{21}$$

In table 2.2 the average U_s of the calculations are compared to the standard deviation of the curve fits at $h = 0$.

p		t1 lsr	t2 lsr	t3 lsr	p lsr 4gr.	p lsr 5gr.
1.9	U_s	.849E-2	.251E-2	.251E-2	.197E-2	.605E-2
	σ	.207E-2	.526E-2	.110E-1	.948E-2	.169E-1
2.0	U_s	.122E-2	.181E-2	.257E-2	.203E-2	.650E-2
	σ	.218E-2	.561E-2	.121E-1	.901E-2	.171E-1
2.1	U_s	.101E-1	.263E-2	.283E-2	.209E-2	.693E-2
	σ	.227E-2	.597E-2	.131E-1	.858E-2	.170E-1

The U_s of the fixed exponent method t1 lsr give a quite good estimation of the uncertainty produced by the scatter, but only in case $p_{min} \neq p_{exact}$. The other evaluation procedures have a great discrepancy between the predicted uncertainty U_s and the actual deviation caused by scatter. Method t3 lsr gives the poorest results.

2.3 Variation of the Standard Deviation

To get an impression of the influence of a growing relative standard deviation on the obtained ϕ_0, σ at h first was reduced to:

$$\sigma_{(h)} = \frac{0.001 \cdot \phi_{(h)}}{3} \tag{22}$$

As a result, the standard deviations at ϕ_0 decrease, and now the least square root approaches provide smaller bands of extrapolated solutions at $h = 0$ than their according standard approaches do. (See table 2.3) Method t1 lsr is able to achieve $\sigma_{fit} \leq \sigma_{(h)}$. There are no significant changes in the averages μ_{fit} compared to the former variant of scatter. The uncertainty of the fit calulated by the least square root approaches is also listed. Here, the U_s are greater than σ_{fit} in general. Here U_s can be regarded being conservative except for method p lsr with 4 grids, where U_s is smaller than σ_{fit}. Method t1 lsr obtains very good results.

p		t1	t1 lsr	t2	t2 lsr	t3	t3 lsr	p	p lsr 4gr.	p lsr 5gr.
1.9	μ	1.0341	1.0500	1.0167	1.0246	1.0114	1.0171	0.9999	1.0002	1.0000
	σ	.120E-2	.776E-3	.238E-2	.135E-2	.395E-2	.208E-2	.379E-2	.211E-2	.170E-2
	U_s		.853E-2		.257E-2		.259E-2		.202E-2	.612E-2
2.0	μ	1.0000	1.0000	1.0000	1.0001	0.9999	1.0002	0.9999	1.0002	1.0000
	σ	.120E-2	.783E-3	.241E-2	.138E-2	.403E-2	.218E-2	.349E-2	.198E-2	.168E-2
	U_s		.122E-2		.182E-2		.256E-2		.204E-2	.648E-2
2.1	μ	0.9647	0.9459	0.9853	0.9777	0.9904	0.9857	0.9999	1.0002	1.0000
	σ	.121E-2	.801E-3	.244E-2	.143E-2	.410E-2	.229E-2	.322E-2	.188E-2	.167E-2
	U_s		.101E-1		.264E-2		.282E-2		.209E-2	.691E-2

Additionally table 2.3 presents the results for a linear shape of $\sigma_{(h)}$. As one would expect, the σ_{fit} of the evaluation preocedures are smaller as for the first introduced kind of scatter and greater than the σ_{fit} obtained with a constant relative standard deviation. Only method p lsr with 5 girds and method t1 lsr with $p_{min} \neq p_{exact}$ obtain a U_s that is greater than σ_{fit}.

p		t1	t1 lsr	t2	t2 lsr	t3	t3 lsr	p	p lsr 4gr.	p lsr 5gr.
1.9	μ	1.0340	1.0500	1.0166	1.0246	1.0113	1.0170	0.9998	1.0001	0.9999
	σ	.135E-2	.118E-2	.306E-2	.247E-2	.564E-2	.443E-2	.512E-2	.417E-2	.506E-2
	U_s		.849E-2		.253E-2		.253E-2		.199E-2	.602E-2
2.0	μ	1.0000	1.0000	1.0000	1.0001	0.9998	1.0002	0.9999	1.0002	0.9999
	σ	.136E-2	.120E-2	.312E-2	.259E-2	.579E-2	.474E-2	.470E-2	.395E-2	.499E-2
	U_s		.122E-2		.181E-2		.256E-2		.202E-2	.652E-2
2.1	μ	0.9647	0.9459	0.9853	0.9777	0.9904	0.9858	0.9999	1.0002	0.9999
	σ	.138E-2	.124E-2	.317E-2	.273E-2	.595E-2	.507E-2	.433E-2	.377E-2	.497E-2
	U_s		.101E-1		.257E-2		.279E-2		.208E-2	.695E-2

2.4 Weighted least square root curve fitting

Returning to the initial calculation, it can be assumed that the wider spreading results of the least square root methods are due to the growing scatter when h is increased.
To solve this problem, one could apply the least square root regression with a weighting of the data by the according standard deviation. This was tested for four data sets by performing method p in the standard way and the least square root sense, where the latter was applied both in the earlier described way and with a data weighting (figures 7 and 8). The outcoming was not very encouraging, as the weighting of the the data turned out to be not a real improvement of the estimated solution. In the first two cases, data weighting improved the outcome of the least square root approach but was farer away from the exact solution at $h = 0$ than the simple method p. The examples in figure 8 show that data weighting can even detoriate the results of the least square root approach. On the other hand, for these four tests, the weighted fit never came up with the worst outcome of this three approaches. The timeframe for this work did not allow to have a closer look at this task and to statistically evaluate the data weighting method, but it would be interesting to do this in the future.

3 Conclusions

Using the scattered test function, we had the advantage of knowing the the exact "converging order". This implies on the other hand that the fixed order methods were able to produce more correct estimates of ϕ_0 than they would under realistic conditions where the order of convergence can only be estimated.
On the other hand, the methods with unknown exponent exhibited problems with a growing error as a result of scatter increasing with the characteristic grid size. As their advantage, they still obtained a quite good estimate of the order of cenvergence. Figure 9 presents the calculated p obtained with the unknown exponent methods applied to the data sets with $\sigma_{(h)} = 0.001 \cdot \phi_{(h)} \cdot h^2$, where they performed worst.

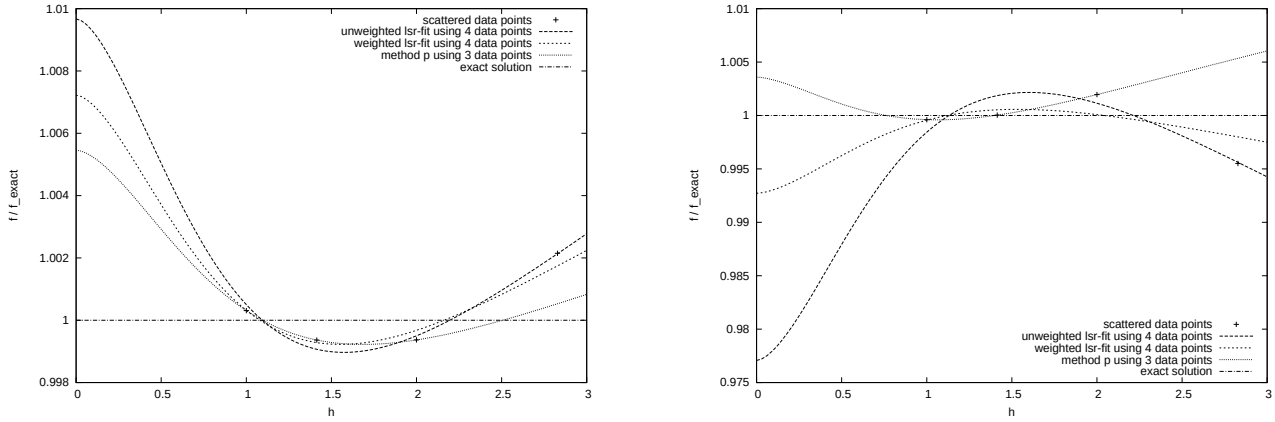

Figure 7: fitted curves obtained by method p, p lsr and weighted lsr

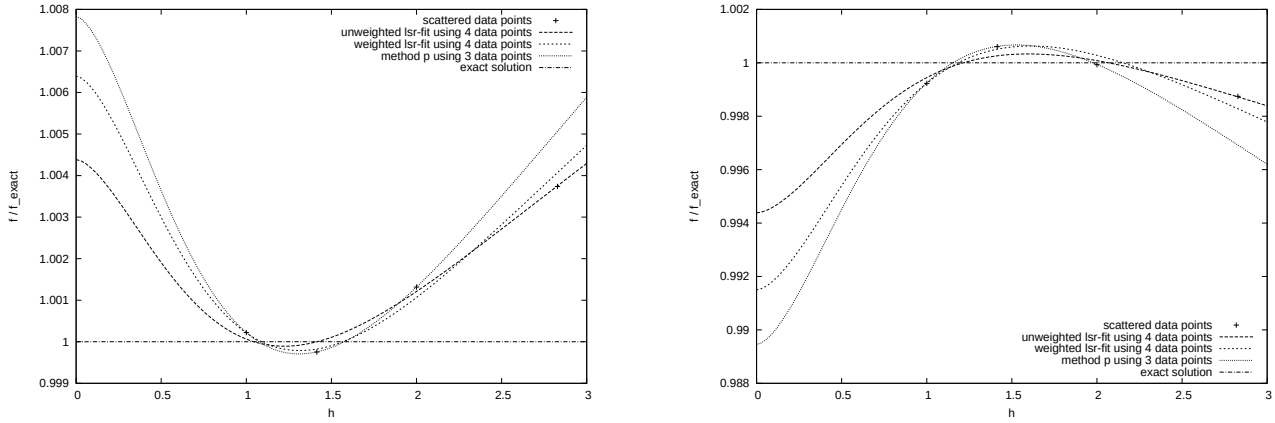

Figure 8: fitted curves obtained by method p, p lsr and weighted lsr

It might be necessary to have knowledge of the behaviour of the scatter occuring in a grid refinement study to handle it. Assuming that there might be still scatter existing alltough the grid study is performed in the asymptotic range, the use of a method using unknown exponents might have disadvantages, at least this is the result this exercise suggests in case the scatter is increasing with the grid spacing. One could think of combining both kinds of Richardson Extrapolation. Method p or its least square root derivates could be applied for estimating the order of convergence and this could be used as the input for a fixed exponent method using only the finest grids.

References

[1] L. Eça and M. Hoekstra. An evaluation of verification procedures for cfd applications. 2002.

[2] L. Eça and M. Hoekstra. An example of uncertainty estimation in the calculation of a 2-d turbulent flow. 2003.

[3] H. Söding. Bewegungen und belastungen der schiffe im seegang. Vorlesungsmanuskript 18, 1982.

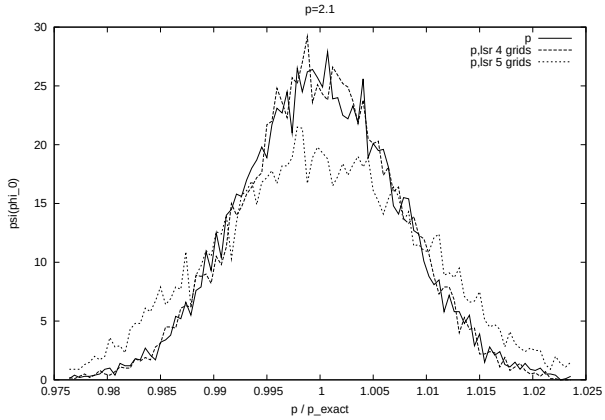

Figure 9: Distribution function of the estimated p by unknown exponent methods for $\sigma_{(h)}/\phi_{(h)}$ growing with h^2