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42. Error Estimation, Multilevel Method and Robust Extrapolation in the Numerical Solution of PDEs

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1. Introduction and Motivation. Richardson extrapolation (**RE**) is a simple, elegant and general mathematical idea that works for numerical quadrature with the *Romberg* method or ODE integrations that have smooth enough solution with the *Bulirsch-Stoer* method. Its use in Computational Fluid Dynamics (**CFD**) raises the following questions [3] [4] [5]:

- Does all mathematical hypotheses needed by RE are fulfilled by the numerical approximation ?

- Are the (3D) meshes fine enough to satisfy accurately the a priori convergence estimates that are only asymptotic relations in nature?

- What to do, if the order of convergence of a CFD code is space dependent and eventually solution dependent?

- Can we afford three grid levels with a coarse grid solution that has a satisfactory level of accuracy, to be used in RE?

Our objective is to use any PDE or CFD solvers, independent of their inner working algorithm and procedures, provided that they can offer the information including the residual of the numerical approximation, stability estimates, and varying grid resolutions and numerical solutions, to accomplish the following goals:

- *Automatic estimate* of the order of convergence in space,

- Using three different grid solutions (not necessarily with uniformly increasing mesh resolution), *obtain a solution with improved accuracy*

The extrapolation procedure is simple to implement and can be incorporated into any computer code without requiring detailed knowledge of the source code. Its arithmetic cost should be negligible compare to a direct computation of the fine grid solution. Finally the procedure should overall enhance the accuracy and trust of a CFD application in the context of code verification.

In this paper, we pursue the research presented in [2] as follows. We first summarize basic properties of Richardson extrapolation method and evaluate its application to CFD. Then we provide elementary approximation theory for least square extrapolation applied to grid functions. Further, we generalise this technique to PDEs, and provide some numerical results for a turning point problem. For a detailed version of this work with results on steady incompressible Navier Stokes flows, we refer to [7].

2. Basic Properties of Richardson Extrapolation and Computational Implications.

2.1. Asymptotic expansion for continuous function in a normed vector space . Let E be a normed linear space, $||\ ||$ its norm, $v \in E$, $p > 0$, and $h \in (0, h_0)$. $u^i \in E$, $i = 1..3$ have the following asymptotic expansion,

$$u^i \ = \ v + C(\frac{h}{2^{i-1}})^p + \delta,$$

with C positive constant independent of h, and $||\delta|| = o(h^p)$.

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For known p, RE formula,

$$v_r^i = \frac{2^p\ u^{i+1} - u^i}{2^p - 1},\ i = 1, 2$$

provides improved convergence:

$$||v - v_r^i|| = o(h^p).$$

2.2. Numerical approximation for discrete functions defined on a mesh. Let E_i be a family of normed linear space, associated with a mesh $M_{h/2^{i-1}}$. We suppose a set of equations,

$$U^i\ =\ v + C_i(\frac{h}{2^{i-1}})^p + \delta_i,$$

with $C_i = (1+\epsilon_i)C$, and $\epsilon_i = o(1)$. δ_i is a model for the h independent numerical perturbation induced by consistency errors and/or arithmetic error. The Richardson extrapolate

$$V_r^2 = \frac{2^p\ U^3 - U^2}{2^p - 1},$$

has then for error in E_1,

$$v - V_r^2 = \frac{1}{2^p - 1}((\delta_2\ -\ 2^p\delta_3) + C\ (\epsilon_2 - \epsilon_3)(\frac{h}{2})^p).$$

The numerical perturbation is amplified by a factor $\frac{2^p+1}{2^p-1}$. For applications in (complex) CFD calculation, the asymptotic order of convergence is not well established and one uses:

$$p \sim \log_2 \frac{||u^1 - u^2||}{||u^2 - u^3||} \tag{2.1}$$

If one considers $\{u^i\}$ as a set of *real numbers* instead of a set of functions in $(E, ||\ ||)$, combining three ordered approximations gives the so-called Δ^2 Aitken formula,

$$v_r^2 \sim \frac{u^1u^3 - (u^2)^2}{u^1 - 2u^2 + u^3}.$$

But this formula has generally no rigorous basis in the corresponding space of approximation.

From the numerical point of view,

$$p = \log_2 ||(1 - \gamma(p))\ \frac{U^1 - U^2 - (\delta_1 - \delta_2)}{U^2 - U^3 - (\delta_2 - \delta_3)}||,$$

where $\gamma(p) \sim \kappa(2^p\epsilon_1 - (2^p + 1)\epsilon_2 + \epsilon_3)$, and $\kappa = (2^p - 1)^{-1}$.

In practice,

$$p \approx \log_2 ||\frac{U^1 - U^2}{U^2 - U^3}||,\ in\ (E_1, ||\ ||)$$

The second order error term ϵ_2 on u_2 (respt ϵ_1 on u_1) has therefore $2^p + 1$ (respt 2^p) more impact on p calculation error than the second order error term ϵ_3 on u_3. Further, the "pointwise" extrapolation

$$v_r^2 = \frac{U^1U^3 - (U^2)^2}{U^1 - 2U^2 + U^3},\ \forall x \in M_1$$

that is routinely used in CFD is very sensitive to numerical perturbation.

The convergence order approximation and RE presented so far is a common tool for solution quality assessement in CFD. In our experience [5] [7], we have observed, for example, that for two different codes for the steady state, 2-D laminar incompressible lid-driven square cavity flow with the Reynolds number (**Re**) in the range of 20 to 1000 and squared regular

meshes using either $\omega - \psi$ formulation and FD approximation or $v - p$ formulation and FV approximation with centered cells, RE can improve the order of accuracy, but not consistently. If the quality of the grid solution is poor then RE may provide worse approximations.

Further, the theoretical bases of classical RE formula presented here, are not satisfied when the convergence order of the solution process is space dependent and solution dependent, which is rather common in CFD. We propose in this paper a method that seems to be more robust than RE, and that further can be used as a framework for aposteri estimates.

3. Least Square Extrapolation for Numerical Functions. Let $E = L_2(0,1)$, $u \in E$. Let v_h^1 and v_h^2 be two approximations of u in E:

$$v_h^1,\ v_h^2 \to u \ in\ E\ as\ h \to 0.$$

A consistent linear extrapolation formula formally written

$$\alpha v_h^1 + (1-\alpha) v_h^2 = u.$$

In p order RE the α function is a constant. We adopt here a more general point of view than RE. We formulate the following problem as a Least Square Extrapolation (**LSE**):

P_α: Find $\alpha \in \Lambda(0,1) \subset L_\infty$ such that $\alpha v_h^1 + (1-\alpha) v_h^2 - u$ is minimum in $L_2(0,1)$.

If $1/(v_h^1 - v_h^2)$ is in $L_\infty(0,1)$, we get an explicit solution for this problem. If $v_h^1 - v_h^2$ vanishes, we can approximate then v_h^i by a w_h^i function in $L_2(0,1)$ such that

$$w_h^i - u_h^i = O(h^q), q >> p,\ and\ 1/(w_h^1 - w_h^2) \in L_\infty(0,1).$$

where p is the expected order of convergence of v_h as $h \to 0$. We get then

$$\alpha = \frac{u - w_h^2}{w_h^1 - w_h^2},\ and\ \alpha \in L_2(0,1).$$

We have easily

Lemma 1: If $\alpha_M - \alpha = 0(M^{-1})$ as $M \to \infty$ and $v_h^1 - v_h^2 = 0(h^p)$ then

$$u \ = \ \alpha v_h^1 + (1-\alpha) v_h^2 + O(h^p) \ \times \ O(M^{-1}).$$

In the present work, we set $\Lambda(0,1)$ to be the space of α functions

$$\alpha = \alpha^0 + \alpha^1 \cos(x\pi) + \Sigma_{j=1..M} \alpha^j \sin((j-1)x\pi).$$

with $\alpha^j,\ j = 0..M$ reals. We can then show using [1]

Lemma 2: Let α be in $L_2(0,1)$. Let $x_j = \frac{j}{N}$ be a regular discretization of $(0,1)$. Let M be an integer such that $M << N$. There is a unique trigonometric polynomial

$$\alpha_M = \alpha^0 + \alpha^1 \cos(x\pi) + \Sigma_{j=1..M} \alpha^j \sin((j-1)x\pi)$$

that minimizes the discrete L_2 norm

$$\Sigma_{j=0..N} (\alpha(x_j) - \alpha_M(x_j))^2.$$

α_M converges to α in $L_2(0,1)$ as $M \to \infty$ while the ratio $\frac{M}{N}$ stays constant and less than one. If $\alpha \in C^1(0,1)$, the convergence $\alpha_M \to v$ is pointwise and of order M^{-1} in (0,1) and M^{-2} away from the end points.

We have now a solution to the approximation problem P_α or its modified analog if we have possibly to modify locally the v_h^i function at neighborhood of points where $v_h^1 - v_h^2$ cancels.

From Lemma 1 and Lemma 2, we have

Theorem: if $u,\ v_h^i, \in\ C^1(0,1), i=1,\ 2$, if $\frac{1}{v_h^1-v_h^2}\ \in\ L_\infty(0,1)$ and $v_h^2-v_h^1=0(h^p)$ then $\alpha v_h^1+(1-\alpha)v_h^2$ is an $0(M^{-1})\times 0(h^p)$ approximation of u.

Special care must be done if $v_h^1-v_h^2 << u-v_h^2$, in some set of non zero measure Ω_S.

These outliers points should not affect globally the least square extrapolation as long as we impose that α be a bounded function independently of h. Further, a more robust approximation procedure consists to use three levels of grid solution as follows:

$P_{\alpha,\beta}$: *Find* $\alpha,\beta\in\Lambda(0,1)$ *such that* $\alpha v_h^1+\beta v_h^2+(1-\alpha-\beta)v_h^3-u$ *is minimum in* $L_2(0,1)$.

Existence of the solution (α,β) is established if one can partition $(0,1)$ into two overlapping subset $\Omega_1\bigcup\Omega_2=(0,1)$ of nonzero measure intersection, such that $1/(v_h^1-v_h^3)$ is in $L_\infty(\Omega_1)$ and $1/(v_h^2-v_h^3)$ is in $L_\infty(\Omega_2)$. But uniqueness is no longer guaranteed. We can use a Singular Value Decomposition method (**SVD**) then, to account for the fact that the linear system can be both over determined and under determined. But SVD requires many more arithmetic operations than a direct solve of the normal set of equations when $M << N$. In practice, if $v_h^1-v_h^3 << u-v_h^3$ and $v_h^2-v_h^3 << u-v_h^3$ in some set of non zero measure then there is no local convergence of our sequence of functions. We want to make sure that these outlier points do not affect the quality of the least square solution at points where convergence is achieved.

In practice, we work with *grid functions* solution of discretized PDE problem. In contrast to classical RE, where all grid solutions are projected onto a common coarse grid, our solution procedure consists of interpolating all data on a very fine grid denoted M^0 via a high order interpolant $\tilde{U}_i=I_i[U_i]$. We want then to get our best fitted extrapolation formula on the fine grid itself as follows.

P_α: *Find* $\alpha\in\Lambda(0,1)\ \subset\ L_\infty$ *such that* $\alpha\tilde{U}^1+(1-\alpha)\tilde{U}^2-U$ *is minimum in* $L_2(M^0)$.

The three-level extrapolation problem is analogous.

We have checked the numerical accuracy and sensitivity to perturbation of LSE on numerical function examples that possess different type of asymptotic behavior and different degree of smoothness. In all cases our least square extrapolation method seems to give improved accuracy and robustness. In particular our least square extrapolation is definitively an improvement on fixed order RE when the solution has a hybrid order of convergence that is first order in some subset of the domain and second order elsewhere.

The extension to multidimensional problem with rectangular grid that are tensorial products of one-dimensional regular grids is straightforward. The generalization to body fitted meshes generated by PDEs [6], is easy since the Fourier expansion technique is insensitive to change of variables as long as they are smooth transformations. However generalisation to FE approximation with unstructured grid will require obviously a different space of approximation for the weight functions α and β.

4. Least Square Extrapolation for PDEs and Computational Algorithm.

The idea is now to use the PDE in the RE process to find an improved solution on the fine grid.

Let us denote formally the linear PDE

$$L[u]=f,\ \textit{with}\ u\in(E_a,||\ ||_a)\ \textit{and}\ f\in(E_b,||\ ||_b),$$

and its numerical approximation,

$$L_h[U]=f_h,\ \ \textit{with}\ U\in(E_a^h,||\ ||_a)\ \textit{and}\ f_h\in(E_b^h,||\ ||_b),$$

parameterized by a mesh step h.

We suppose that we have a priori a stability estimate for these norms

$$||U||_a \ \leq \ C\ h^s\ (||f_h||_b), \tag{4.1}$$

with s real not necessarily positive. We will look for consistant extrapolation formula that minimize the residual.

Let us restrict for simplicity to a two-point boundary value problems in $(0,1)$. Our least square extrapolation is now defined as follows:

P_α: Find $\alpha \in \Lambda(0,1) \ \subset \ L_\infty$ such that $\alpha L_h[\tilde{U}^1] + (1-\alpha)L_h[\tilde{U}^2] - f_h$ is minimum in $L_2(M^0)$.

The three levels version is analogue. To focus on the practical use of this method, we should make the following observations. It is essential that the interpolation operator gives a smooth interpolant depending on the order of the differential operator. For conservation laws, one may require that the interpolation operator satisfies the same conservation properties. For chemical problems, one may require that the interpolant preserves the positivity of species. For elliptic problems, it is convenient to postprocess the interpolated functions $\tilde{U}^i$, by few steps of the relaxation scheme

$$\frac{V^{k+1} - Vk}{\delta t} \ = \ L_h[V^k] - f_h,\ V^0 = \tilde{U}^i,$$

with appropriate artificial time step δt. This will readily smooth out the interpolant.

Let $G_i,\ i = 1..3$, be three embedded grids that does not necessary match and their companion grid solutions U_i. Let M^0 be a regular grid that is finer than the grids G_i. The solution process of P_α and/or $P_{(\alpha,\beta)}$ can be decomposed into three consecutive steps.

- First, interpolation from $G_i, i = 1..3$ to M^0. We choose interpolation tools that have a number of arithmetic operations proportional to $Card(M^0)$, i.e. the number of grid points of M^0.
- Second, the evaluation of the residual on the fine grid M^0, that has the same asymptotic order of arithmetic operations.
- Third the solution of the linear least squares problem with M unknowns.

If we keep M of the same order as $Card(M^0)^{1/3}$, and use a standard direct solver for symmetric system to solve the normal set of equations, the arithmetic complexity of the overall procedure is still of order $Card(M^0)$, i.e., it is linear.

The application to nonlinear PDE problem is done via a Newton-like loop [7]. The algorithm is coded in an independent program from the main code application.

We choose a Fourier expansion for each weight function α and β, that has M terms with $M \approx Card(M^0)^{1/3}$, to keep a linear cost for the complete procedure when the direct solution of the normal set of equations is giving a good result. An SVD, if needed, will lead however to more intense computation.

Let us now illustrate the numerical efficiency and robustness of our method with a 2D Turning Point Problem:

$$\epsilon\ \Delta u + a(x,y)\frac{\partial u}{\partial x} = 0,\ x \in (0,\pi)^2,$$

with Dirichlet boundary conditions of opposite signs at $x = 0$ and $x = \pi$, and homogeneous Neumann at $y = 0/\pi$. We take

$$a(x,y) = x - (\frac{\pi}{2} + 0.3(y - \frac{\pi}{2})).$$

We have then a transition layer (**TL**) of ϵ order thickness centered on the curve $a(x, y) = 0$, which is not parallel to the x or y axis.

The application code uses second order central FD of the diffusion term and first order upwinding for the convection term with either direct sparse LU linear or GMRES solver. There are no spurious oscillations because of the discrete maximum principle.

Figures 4.1 and 5.2 report on the accuracy of the two-level and three-level least squares extrapolation versus RE assuming either first or second order convergence. The errors are given in L_∞ norm. The curve with hexagram signs gives an accurate estimation of the discrete solution error between the exact grid solution on the fine grid M^0 of size $N \times N$, versus the exact continuous solution of the turning point problem. Let G_I be square grids of size $N_i \times N_i$.

The number of Fourier modes in the approximation of the weight α, β is 4 in each space direction. We observe that for both cases $\epsilon = 0.1$ and $\epsilon = 0.01$ in Figure 4.1 and 5.2, R1 gives better results than R2. This is an indication of the fact that the transition layer is not under-resolved. We observe in Figure 4.1 with $\epsilon = 0.1$, and modest base grid sizes, namely, $N_1 = 17,\ N_2 = 23,\ N_3 = 29$, meaning that we have on average only one or two grid points in the transition layer for the G3 solution, our least squares is as accurate as the fine grid solution. This is still true when the Richardson extrapolation fails for $N \geq 70$. The least squares extrapolation also gives satisfactory results in Figure 5.2, where $\epsilon = 0.01,\ N_1 = 39,\ N_2 = 49,\ N_3 = 59$, but R1 predicts the grid solution on M^0 with an error less than or equal to the error with the exact continuous solution for $N \leq 110$. In all cases LS2 is more accurate than LS1, especially for large N values. In these experiments, LS1 and LS2 predict the fine grid solution with an error less than the fine grid approximation of the exact solution for N as large as 150: we gain therefore more than one order of convergence. Similar results on the lid-driven cavity flow confirm the capabilities of our method [7].

5. Conclusions and Discussions. We have studied a new extrapolation method for PDEs that is more robust and accurate than RE applied to numerical solutions with inexact or varying convergence order. Our method provides a better tool to establish a posteriori estimate than Richardson extrapolation when the convergence order of a CFD code is space dependent. However there are still many open questions. To cite some but a few, we still need to establish a criterion to relax the constraint on the accuracy of the coarse grid data for efficient least squares extrapolation. Further, from the application point of view, it might be interesting to test the robustness of our least squares extrapolation method to elliptic problems with general geometry domains via fictitious domain technique.

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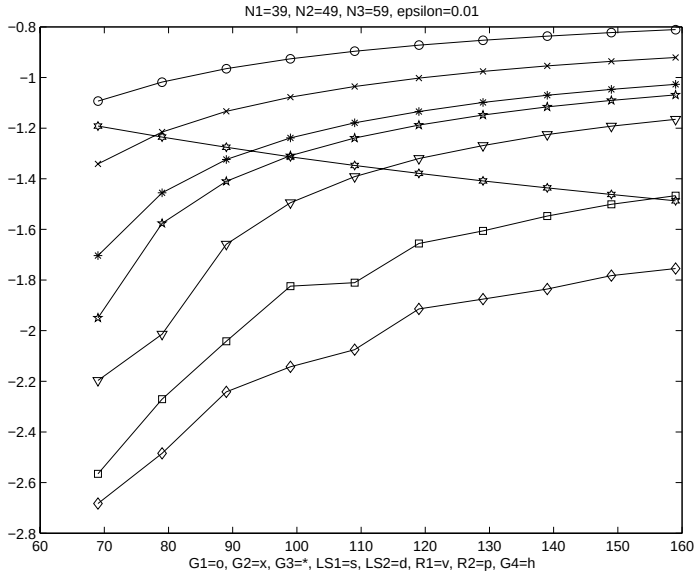

Figure 5.1: x axis is for the number of grid points N in each space direction for the fine grid M^0. y axis gives in log_{10} scale the errors in maximum norm. Labels of curves are as follows: 'o' for G_1 solution, 'x' for G_2 solution, '*' for G_3 solution, $\star$ for R2, 'v' for R1, *square* for LS1, $\diamond$ for LS2.

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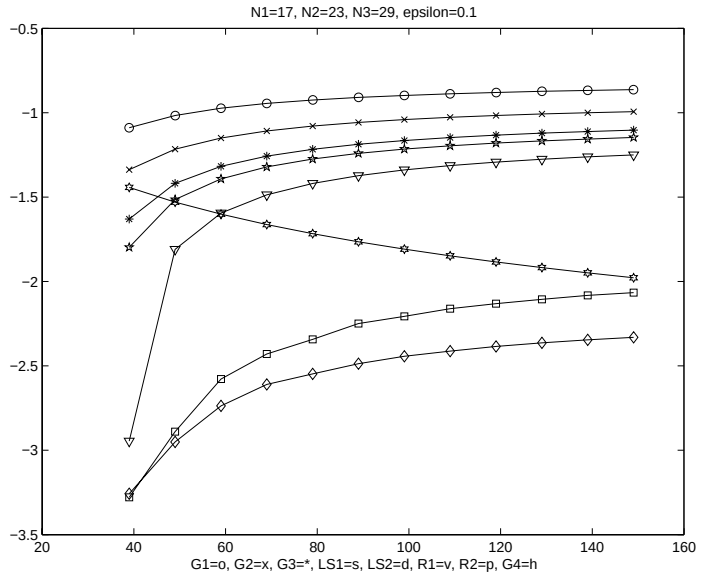

Figure 5.2: Same labels as in Figure 5.1.