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A least square extrapolation method for the *a posteriori* error estimate of the incompressible Navier Stokes problem

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SUMMARY

A posteriori error estimators are fundamental tools for providing confidence in the numerical computation of PDEs. To date, the main theories of *a posteriori* estimators have been developed largely in the finite element framework, for either linear elliptic operators or non-linear PDEs in the absence of disparate length scales. On the other hand, there is a strong interest in using grid refinement combined with Richardson extrapolation to produce CFD solutions with improved accuracy and, therefore, *a posteriori* error estimates. But in practice, the effective order of a numerical method often depends on space location and is not uniform, rendering the Richardson extrapolation method unreliable. We have recently introduced (Garbey, *13th International Conference on Domain Decomposition*, Barcelona, 2002; 379–386; Garbey and Shyy, *J. Comput. Phys*. 2003; **186**:1–23) a new method which estimates the order of convergence of a computation as the solution of a least square minimization problem on the residual. This method, called least square extrapolation, introduces a framework facilitating multi-level extrapolation, improves accuracy and provides *a posteriori* error estimate. This method can accommodate different grid arrangements. The goal of this paper is to investigate the power and limits of this method via incompressible Navier Stokes flow computations. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: partial differential equations; least square method; Richardson extrapolation; *a posteriori* error estimate

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

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(CFD) [1–9] is limited by the fact that meshes might not be fine enough to satisfy accurately the *a priori* convergence estimates that are only asymptotic in nature. Furthermore the order of convergence of a CFD code is often space dependent and eventually parameters, such as the Reynolds number, dependent.

To cope with these limitations of RE, we have introduced recently [10, 11] the so-called least square extrapolation method (LSE) that is based on the idea of finding automatically the order of a method as the solution of a least square minimization problem on the residual.

Our LSE method is based on the post-processing of data produced by existing PDE codes. The method has been described in detailed in Reference [11]. From a practical point of view, we have used a two dimensional turning point problem [12] exhibiting a sharp transition layer as well as a finite difference approximation of the cavity flow problem in $\omega - \psi$ formulation [13] to show that our method is more reliable than RE while the implementation is still fairly easy and the numerical procedure inexpensive.

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: (i) *a posteriori* estimates of PDEs that are more reliable and robust than straightforward Richardson extrapolation-based methods with low cost in additional CPU time, (ii) a solution with improved accuracy, (iii) arithmetic efficiency of the PDE multilevel solution procedure by providing a good starting point for iterative solvers [14], and (iv) a dynamic solution verification software.

From the applied mathematics point of view, *a posteriori* estimates have been around for many years [15, 16]. Most work has been done in the framework of finite element analysis on linear elliptic problems in order to drive adaptive mesh refinement. More recently a general framework for finite element a posteriori error control that can be applied to linear and non-linear elliptic problem has been introduced by Patera *et al.* [17]. *A posteriori* finite-element free constant output bounds can be constructed for the incompressible Navier Stokes equation [18]. We propose to use least square extrapolation to produce *a posteriori* estimate using grid solutions that can be produced by any discretization. This approach might be combined to existing *a posteriori* estimate when they are available, but is still applicable as a better alternative to straightforward RE when none such stability estimate is available.

The extrapolation procedure is simple to implement and can be incorporated into any computer codes without requiring detailed knowledge of the source code. Its arithmetic cost should be modest 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 solution verification.

In this paper, we pursue the research initiated in References [10, 11] to investigate the power and limit of the LSE for the incompressible Navier Stokes equation written in the $u - v - p$ formulation. This test case has a number of interesting features compared to the test case in the $\omega - \psi$ formulation already studied in Reference [11]. As a matter of fact, the $\omega - \psi$ formulation is essentially a fourth order problem with one unknown, i.e. the stream function ψ, while we will see that the LSE method applied to the $u - v - p$ formulation has to deal with coupled equations, i.e. the momentum equation, and search for an extrapolation solution constrained by the divergence free condition. Further, for problem with multiple scale, the relation ship between the residual and the numerical error can be fairly complex. In other words minimizing the residual via LSE does not guarantee that the error is minimized,

unless the space of search is close to the exact solution [19]. We will present in this paper a postprocessing procedure on our coarse grid solution that makes LSE numerically efficient.

The plan of this paper is as follows. In Section 2, we first summarize basic properties of RE and summarize the general idea of the LSE method for PDEs. In Section 3 we present in detail the algorithm for the incompressible Navier Stokes equation. In Section 4, we discuss the numerical results for the cavity flow problem. Section 5 is our conclusion and refer to ongoing research.

2. BASIC PROPERTIES OF RICHARDSON EXTRAPOLATION AND LEAST SQUARE EXTRAPOLATION

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:

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

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

For known p, RE formula,

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

provides improved convergence: $||v - v_r^i|| = o(h^p)$. An *a posteriori* error estimate on u^i is then

$$||u^i - v_r^i|| \tag{3}$$

In CFD practice, one applies RE to grid functions rather than to continuous functions. 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,

$$U^i = v + C_i\left(\frac{h}{2^{i-1}}\right)^p + \delta_i \tag{4}$$

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

$$V_r^2 = \frac{2^p\, U^3 - U^2}{2^p - 1} \tag{5}$$

defined on grid points of M_2 has then for error in E_2,

$$v - V_r^2 = \frac{1}{2^p - 1}\left((\delta_2 \ - \ 2^p\delta_3) + C\,(\varepsilon_2 - \varepsilon_3)\left(\frac{h}{2}\right)^p\right) \tag{6}$$

The numerical perturbation is amplified by a factor $(2^p+1)/(2^p-1)$. This RE gives then an *a posteriori* error estimate on U^i that is simply

$$||V_r^2 - U^i||, \quad i=1..3$$

RE can then be used also to approximate a finer grid solution, for example

$$U^4 \approx V_r^2 + C\left(\frac{h}{2^3}\right)^p \tag{7}$$

where C is obtained from the identity

$$U^3 = V_r^2 + C\left(\frac{h}{2^2}\right)^p \tag{8}$$

For applications in CFD calculation, the asymptotic order of convergence is in general not known or not closely satisfied on the computational grid. One may use the estimate:

$$p \sim \log_2 \frac{||u^1 - u^2||}{||u^2 - u^3||} \tag{9}$$

An entirely similar analysis can be applied to non-embedded refined grid solution U^i in a normed linear space E_i, associated with a mesh M_{h_i}, provided that one projects all grid functions to a fine grid M^0 with an interpolation procedure. However this interpolation should introduce an additional error term integrated in the δ_i term of (4) kept much less than the expected convergence accuracy h_i^p.

In practice, all pointwise RE extrapolation formulae, particularly (4), are sensitive to numerical perturbation. RE is a common tool for solution quality assessment in CFD. In our experience [9, 11], we have observed that RE can improve the order of accuracy, but not consistently. If the quality of the solution is poor then RE may provide worse approximations. These conclusions are reached based on extensive solution verification with two different Navier Stokes approximations for the steady state, 2-D laminar incompressible lid-driven square cavity flow with the Reynolds number (Re) in the range of 20–1000. Squared regular meshes using the $\omega - \psi$ formulation and finite difference (FD) [13] or the finite volume (FV) version of the $u - v - p$ formulation with centred cells [20] have been tested. Further experiments with turbulent flows on a back step has demonstrated the critical issue of multiscales [9].

In a recent stream of work of Eca *et al.* see References [2, 21] and its references, one can use a least square model of the error provided that enough grid solutions are computed. To be more specific most variant of RE suppose that the error is represented by an asymptotic expansion as follows:

$$e = v - u_i = \sum_{k=1..p} a_k \beta_k(h) + o(h_i^p) \tag{10}$$

in a normed space $(E_i, ||\ ||)$.

In RE procedure, one neglects the $o(h_i^p)$ residual and use the following identity pointwise:

$$e = v - u_i = \sum_{k=1..p} a_k \beta_k(h) \tag{11}$$

We observe that this pointwise equality not only neglects the higher order term $o(h_i^p)$ but also disregards the nature of the asymptotic expansion that is depending on the norm associated to E_i.

We have then two standard situations:

- If the basis function β are given, then one need $p+1$ grid solutions v_j to derive the unknown coefficients a_k, $k=1..p$ and the (approximated) true solution v.
- If the set of basis functions $\beta_k(h)$ is a one parameter family of functions, for example h_k^γ, with arbitrary exponent γ, one needs $2p+1$ grid solution to solve the error model, i.e. compute v, a_k, $k=1..p$, and γ_k, $k=1..n$, pointwise.

To cope with the fact that RE is very sensitive to noisy data, Eca *et al.* retrieve the error model with a least square fit instead of enforcing equalities. This procedure is indeed less sensitive to noisy data, but requires many more grid solutions than with the standard RE procedure.

We have developed a completely different technique to optimize RE. Our criterium to select the best extrapolate solution is to minimize an objective function such as the l^2 norm of the residual for the discrete solution on a very fine grid. This fine grid must be chosen to resolve the fine scale of the problem. We use no more than two or three coarse grids solution in our procedure. We do not try to compute directly an approximation of the exact solution either. We rather try to extract the best information from these two or three coarse grid solutions by reintroducing in the construction of the extrapolation formula, the discretization of the PDE, instead of assuming any kind of asymptotic model for the error.

Let us review briefly the LSE method for the numerical approximation of scalar function first.

Let $E=L_2(0,1)$, $u\in E$. Let v_h^1 and v_h^2 be two approximations of u in E:

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

A consistent linear extrapolation formula writes

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

In RE the α function is a constant. In the LSE method we formulate the following problem for the unknown function α that is in general a non-constant function.

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 $L_2(0,1)$.

Typically we choose for the space $\Lambda(0,1)$ a set of polynomial trigonometric functions of degree M, but this is not necessary. We have shown

Theorem (*Garbey and Shyy* [11])
if u, $v_h^i,\in C^1(0,1), i=1,\ 2$, *if* $1/(v_h^1-v_h^2)\ \in\ L_\infty(0,1)$ *and* $v_h^2-v_h^1=0(h^p)$ *then* $\alpha v_h^1+(1-\alpha)v_h^2$ *is an* $0(M^{-2})\times 0(h^p)$ *approximation of* u.

Special care must be done if $v_h^1-v_h^2 \ll u-v_h^2$, in some set of non-zero measure. These outliers should not affect globally the least square extrapolation and we impose α to be a bounded function independent of h. A potentially more robust approximation procedure consists of using 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 $L_2(0,1)$.

As a matter of fact, all v_h^j, $j=1..3$, may coincide at the same grid points only if there is no grid convergence locally. In such a situation, one cannot expect improved local accuracy from any extrapolation technique. The robustness of the LSE method comes from the fact that

the extrapolated solution does not deteriorate the accuracy of the coarse grid solution while it may not be the case for RE, especially when one uses (9).

In practice, we work with *grid functions* solution of discretized PDE problem. The idea is now to use the PDE in the RE process to find an improved solution on a given fine grid M^0.

Let us denote formally the linear PDE

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

and its numerical approximation,

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

parameterized by a mesh step h.

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

$$||U||_a \leqslant Ch^s\ (||f_h||_b) \tag{12}$$

with s real not necessarily positive.

Let G_i, $i = 1..3$, be three embedded grids that do not necessarily match, and their corresponding grid solutions U_i. Let M^0 be a regular grid that is finer than the grids G_i. Let $\tilde{U}_i$ be the coarse grid solutions interpolated on the fine grid M^0.

The main idea of the LSE method is to look for a consistent extrapolation formula based on the interpolated coarse grid solutions $\tilde{U}_i$ that minimizes the residual, resulting from $\tilde{U}_i$ on a grid M^0 that is fine enough to capture a good approximation of the continuous solution.

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 $(L_h[\alpha\tilde{U}^1 + (1-\alpha)\tilde{U}^2] - f_h)$ is minimum in $L_2(M^0)$.

The three-level version is analogous to the two-level one. 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 and the regularity of the solution of the differential problem. For conservation laws, one may require that the interpolation operator satisfies the same conservation properties. For reacting flow 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

$$\frac{V^{k+1} - V^k}{\delta t} = L_h[V^k] - f_h, \quad V^0 = \tilde{U}^i \tag{13}$$

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

Let e_j, $j = 1..m$ be a set of basis function of $\Lambda(0, 1)$. The solution process of P_α and/or $P_{(\alpha,\beta)}$ can be decomposed into three consecutive steps.

- First, interpolation of the coarse grid solution from $G_i, i = 1..3$ to M^0.
- Second, evaluation of the residual $L_h[e_j\ (\tilde{U}^i - \tilde{U}^{i+1})]$, $j = 1..m$, and $L_h[\tilde{U}^3]$ on the fine grid M^0.
- Third, the solution of the linear least square problem that has m unknowns.

In practice, we keep m low by using a spectral representation of the unknown weight functions α and eventually β. The arithmetic complexity of the overall procedure is then still of order Card(M^0), i.e. it is linear. The application to non-linear PDE problem is done via a

Newton-like loop [11]. The algorithm might be coded in a stand alone program independent of the main code application.

We are going now to describe the algorithm for the incompressible Navier Stokes set of equations.

3. APPLICATION TO THE CAVITY FLOW PROBLEM

Let us consider the velocity–pressure formulation of the square cavity problem in two space dimensions. The steady problem writes in $\Omega = (0,1)^2$,

$$N_1[u,v,p] = -\frac{1}{Re}\Delta u + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = 0, \quad (x,y) \in \Omega \tag{14}$$

$$N_2[u,v,p] = -\frac{1}{Re}\Delta v + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = 0, \quad (x,y) \in \Omega \tag{15}$$

submitted to the constraint

$$\mathrm{Div}(u,v) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (x,y) \in \Omega \tag{16}$$

In this system of equations *Re* is the Reynolds number. Furthermore this set of equations is supplemented with the no-slip boundary conditions on the walls of the cavity. The flow speed is zero on all walls except on the sliding wall

$$u(x,1) = g(x), \quad x \in (0,1) \tag{17}$$

In applying the LSE method with $u-v-p$ formulation, we deal with three new difficulties that were not present in the Navier Stokes calculation of Reference [11].

- We have a system of coupled non-linear PDEs. The cavity flow problem with Ω_Ψ formulation is really a fourth order non-linear elliptic problem on Ψ only.
- The LSE on the velocity field should satisfy the divergence free constraint.
- Thanks to the discontinuity of the boundary condition on the velocity field at the corners, there is no valid pointwise model of the error that follows a standard Taylor expansion.

The grid functions (u_i, v_i, p_i) on G_i are computed with a standard FD code using a projection method and staggered grids [13].

Let us consider a set of three-grid solutions $(\tilde{u}_i, \tilde{v}_i, \tilde{p}_i)_{i=1..3}$ projected onto the fine grid M^0 via a high order smooth interpolation procedure. Let us denote N_1^0, N_2^0, Div^0 the corresponding discretized operator. For finite differences that we will consider from now on, M^0 is a staggered grid system, and the discretized operator are given by central second order finite differences.

The projected flow field $(\tilde{u}_i, \tilde{v}_i)$ does not satisfy *a priori* the divergence-free condition

$$\mathrm{Div}^0(\tilde{u}_i, \tilde{v}_i) = 0, \ (x,y) \in \Omega \tag{18}$$

In the unlikely case where (18) is satisfied, the extrapolated value of the flow field

$$\alpha(\tilde{u}_i, \tilde{v}_i) + (1-\alpha)(\tilde{u}_i, \tilde{v}_i), \quad i \neq j$$

will not be divergence-free anyway for the Div^0 operator, unless α is a constant.

We define then the following mapping $(u,v)\to\Psi\to(U,V)$, where

$$U=\frac{\partial\Psi}{\partial y},\quad V=-\frac{\partial\Psi}{\partial x},\quad (x,y)\in\Omega,\ \text{and}$$

$$\Delta\Psi=\frac{\partial u}{\partial y}-\frac{\partial v}{\partial x},\quad (x,y)\in\Omega,\ \Psi=0\ \text{on}\ \partial\Omega.$$

We define also its discrete analogue $(\tilde{u},\tilde{v})\ \to\ (\tilde{U},\tilde{V})$, in M^0.

Thanks to this mapping, we can retrieve from the grid function (u_i,v_i) in G_i a divergence free approximation $(\tilde{U}_i,\tilde{V}_i)$ in M^0. The least square extrapolation problem with two levels writes then

P_{α_1,α_2}: Find α_1 and $\alpha_2\in\Lambda(\Omega)\ \subset\ L_\infty(\Omega)$ such that

$$N^0[\alpha_1\,\tilde{\Psi}_1+(1-\alpha_1)\,\tilde{\Psi}_2,\alpha_2\,\tilde{p}_1+(1-\alpha_2)\tilde{p}_2]$$

is minimum in $L_2(M^0,M^0)$, with $N^0[\Psi,p]=(N_1^0[U,V,p],N_2^0[U,V,p])$.

Since this problem is non-linear, we use a Newton loop to construct a sequence of weight functions (α_1^n,α_2^n) that may converge to the solution. The iterative procedure starts from the finest coarse grid solution at our disposal. Convergence is not guaranteed and may depend on how close the initial guess is to the true M^0 grid solution. If (U^0,V^0,p^0) represents the current solution, the next iterate is found by applying the least square extrapolation procedure to the linear operator

$$L^0(U^0,V^0)[\Psi,p]=(L_1^0(U^0,V^0)[U,V,p],L_2^0(U^0,V^0)[U,V,p]) \tag{19}$$

with

$$\begin{aligned}L_1(U^0,V^0)[u,v,p]=&-\frac{1}{Re}\Delta u+U^0\frac{\partial u}{\partial x}+u\frac{\partial U^0}{\partial x}+V^0\frac{\partial u}{\partial y}+v\frac{\partial U^0}{\partial y}\\&+\frac{\partial p}{\partial x}-U^0\frac{\partial U^0}{\partial x}-V^0\frac{\partial U^0}{\partial y}\end{aligned}$$

$$\begin{aligned}L_2(U^0,V^0)[u,v,p]=&-\frac{1}{Re}\Delta v+U^0\frac{\partial v}{\partial x}+u\frac{\partial V^0}{\partial x}+V^0\frac{\partial v}{\partial y}+v\frac{\partial V^0}{\partial y}\\&+\frac{\partial p}{\partial y}-U^0\frac{\partial V^0}{\partial x}-V^0\frac{\partial V^0}{\partial y}\end{aligned}$$

A similar algorithm is derived for the three-level case.

The space of unknown weight function is chosen as in Reference [11] to be the set of trigonometric polynomial functions

$$\alpha=\sum_{i=1..m,\,j=1..m}\alpha_{i,j}e^i\ e^j$$

with $e^1=1$, $e^2=\cos(\pi x)$ and $e^i=\sin((i-2)\pi x)$, for $i=3..m$.

This set of trigonometric functions allows us to approximate at second order in L^2 norm any smooth non-periodic functions of $C^1[(0,1)^2]$, [22]. The main advantage of this choice of

approximation space for the weight function is that it will allow us to easily interpret our numerical result in the frequency space.

However, for Navier Stokes computation with large Reynolds number, we are currently investigating the use of wavelets since the convergence order might be closely related to the multiscale properties of the solution.

We are going now to present our numerical experiments with the LSE method.

4. RESULTS AND DISCUSSION

To illustrate the numerical result, we restrict ourselves to the test case of the square cavity with a constant sliding wall velocity that is $g(x) = -1$, and a Reynolds number $Re = 400$. This test case is representative of the results obtained with our method. In particular, the first component u of the speed is singular at the corner, as well as the pressure. From this numerical experiment and many others we can draw the following conclusions:

The three-level extrapolation method is more robust and more accurate than the two-level extrapolation method. Figure 1 illustrates the cancelation phenomenon with two grid solutions 51×51 and 61×61. We plot in this picture the local minimum per vertical and/or horizontal lines of the difference between two coarse grid solutions projected on the fine grid. These minima are such that any *a priori* bounded weight coefficient α will have no influence on the extrapolated solution. The two-level extrapolated solution cannot therefore improve the accuracy of the solution. Further we cannot decide if the grid solutions are fully converged at these points or, on the contrary, if the numerical methods lack convergence locally, unless

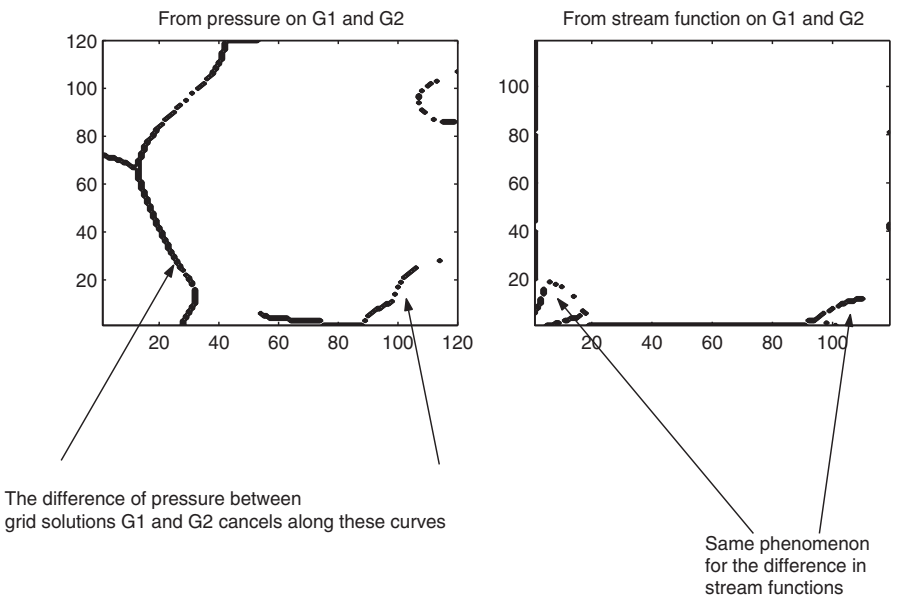

Figure 1. Location of some local minima of $\tilde{p}_2 - \tilde{p}_1$ on the left and $\tilde{\psi}_2 - \tilde{\psi}_1$ on the right where cancellation with the two level's LSE take places.

we use a very fine grid solution to compare. We have verified then that the RE formula based on three-level extrapolated solution with the computed convergence order as in (9) exhibits large local errors on the convergence order. Following the approach of Reference [1], one may select adaptively the points where RE has better chances to be valid. We are going to present the numerical experiments for LSE using three grids only.

In the following we will present a fair comparison between RE and LSE, i.e. we will compare RE and LSE to predict the same fine grid solution, instead of using RE to predict the continuous true solution. In each graph (2)–(6) the horizontal axis indicates the number of grid points N in each space direction for the fine grid M^0 used to evaluate the residual. The vertical axis gives in $\log_{10}$ scale the relative error in $L2$ norm's. Labels of curves are as follows: '$\circ$' for the grid solution G_2 solution, 'v' for the finest coarse grid solution G_3 solution, $\diamond$ for RE, $\square$ for LSE.

We recall that M^0 is the finer grid on which the extrapolation is conducted. Let us take M^0 to be a grid with a slightly smaller space step than G_3. RE as well as LSE predicts very accurately the solution on M^0. In Figure 2, the three coarse grid solutions are 51×51 for G1, 61×61 for G2, and 71×71 for G3. We see that as M^0 gets finer the LSE deteriorates, while the RE assuming second order improved.

In general LSE seems to be reliable to bounds from below the true error on G_3 by comparing the prediction on M^0 done by LSE and the coarse grid solution $G3$ interpolated on M^0. This seems to be a promising tool for routine solution verification. RE gives similar performance for this specific benchmark, and gives much better result than LSE for finer grid prediction.

We observe a numerical locking of the LSE method to predict solution when the grid M^0 gets significantly finer than G_3. In other words increasing the number of Fourier modes m to approximate the weight function provides little improvement on the minimum of the residual. Further, the optimal weight function does not correspond necessarily to the minimum of the residual. This phenomenon has been clearly demonstrated in Reference [19], where LSE was restricted to the search for constant α values with two grid levels only. In this specific case, the best weight coefficient that minimizes the residual in the least square sense, can give poorer result than the RE method assuming second order of convergence. Figure 3 illustrates the poor performance of the LSE method with three grid levels and $m = 4$ Fourier modes in each space direction to approximate the weight function. In this figure, we have compared the solution with the 121×121 grid solution declared as the true solution, while the LSE uses a fine grid M^0 with growing size from 81×81 to 121×121. The three coarse grids solution are still 51×51 for G1, 61×61 for G2, and 71×71 for G3.

We propose the following explanation of this phenomenon: we observe that the coarse grid solution interpolated on a fine grid M^0 has high spurious wave number terms brought by the interpolation procedure. We know that the high wave number components of the coarse grid solution relative to the coarse grid itself are inaccurate. The interpolation procedure combined with the weight function expansion worsen the phenomenon. These high wave numbers components are amplified in the computation of the residual for a non-linear stiff problem as the cavity flow with large Reynolds number. The LSE method minimizes therefore the L^2 norm of a residual polluted by high wave number components. To get the minimum of this residual does not guarantee therefore that the error on the low wave number component of the solution is minimum. This phenomenon is not visible when LSE is used to predict the solution on a near by G_3 finer grid, because the gap in frequency between G_3 and M^0 is small.

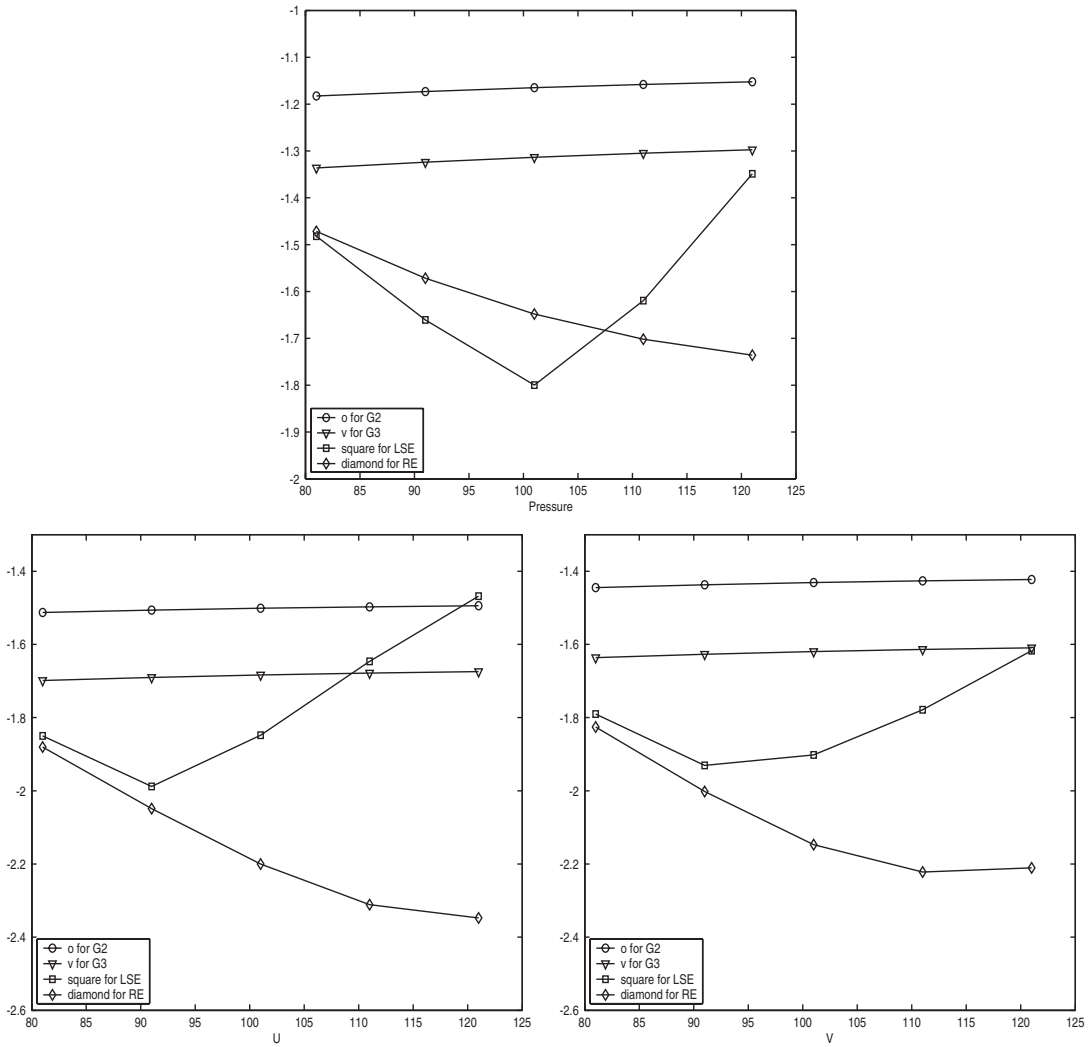

Figure 2. Performance of LSE (without postprocessing of the residual) to predict the solution on the grid 121×121. The coarse grid solution G_1, G_2, G_3, are, respectively, 51×51, 61×61, 71×71.

To validate our heuristic analysis, we postprocess each coarse grid solution with the NS code on the fine grid. We use explicit time stepping with dt constraint by the CFL condition as well as the explicit treatment of the diffusion term. Ten time steps does not allow the NS to converge on M^0 by all means, but relax efficiently the high frequency components of the projected coarse grids due to the interpolation. We further apply a least square low mode approximation of the computation of each residual computed in the LSE method. LSE is therefore now computing the weight functions that minimize the *low mode approximation* of the residual. In other words high frequency components are completely filtered out, and the

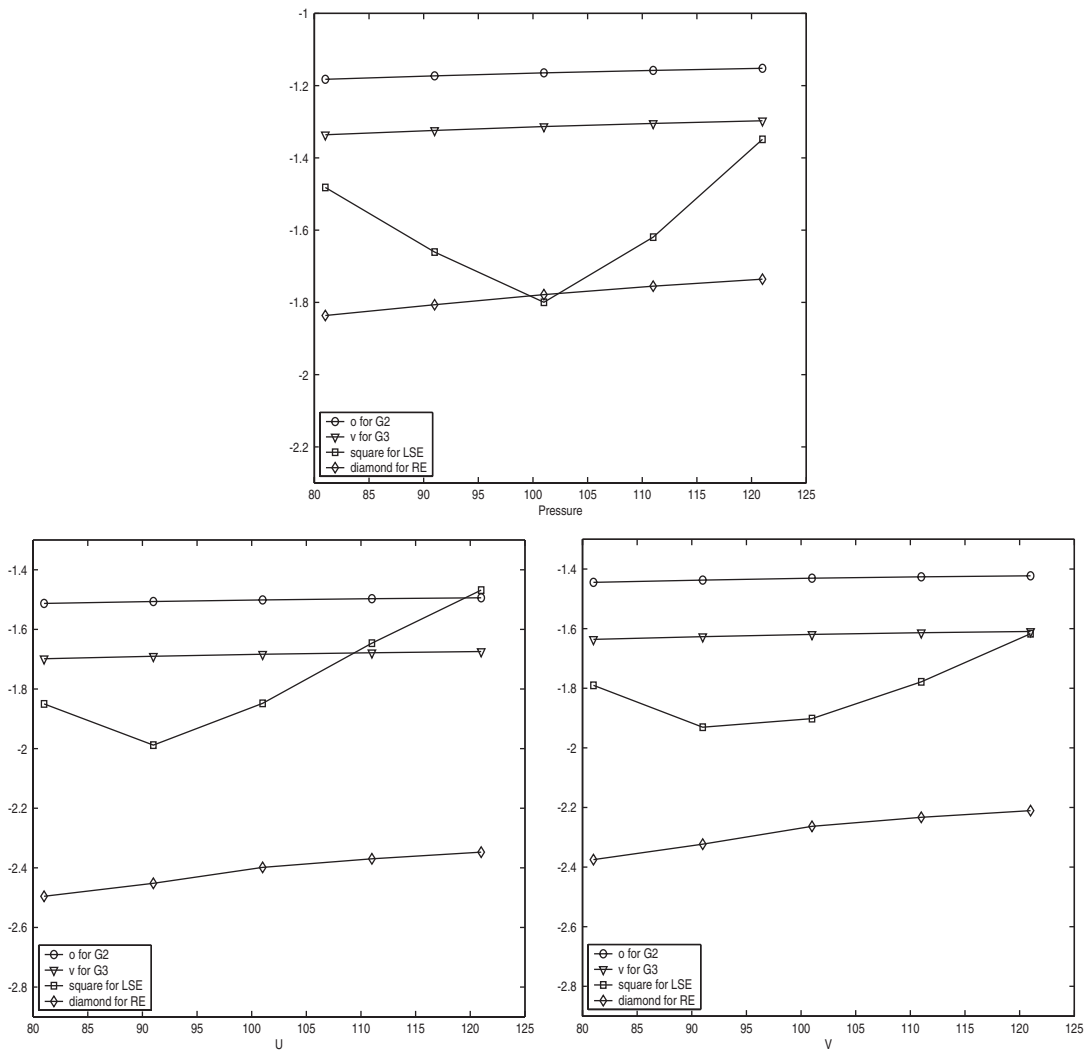

Figure 3. Performance of LSE to predict the M^0 grid solution with the same notation and computation as in Figure 2.

effect of the singularity at the corner in the computation of the residual is somehow weakly weighted.

The same test case as the one illustrated in Figure 3 has been used. Figure 4 shows that keeping a 8 Fourier modes in each space direction for the residual approximation, improves significantly the result. This result is fairly insensitive to the number of NS iterates on the fine grid, once the spurious oscillations introduced by the interpolation of the coarse grids are damped out on M^0. We checked for example that to take 100 NS iterates instead of 10 improve the accuracy of LSE marginally only.

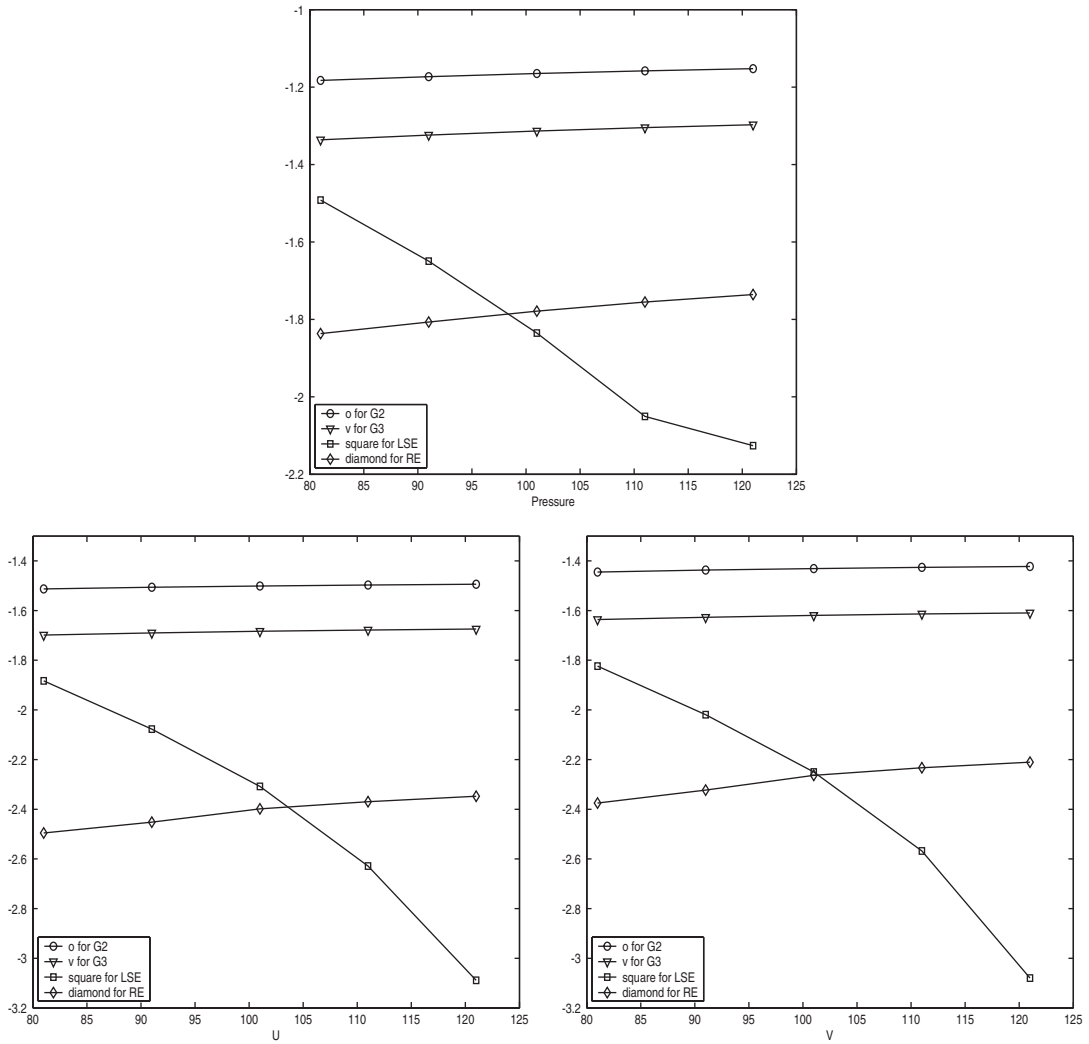

Figure 4. Performance of LSE to predict the M^0 grid solution with the same notation and computation as in Figure 2 but with postprocessing of the coarse grid solution and the residual to filter out the high waves components.

The same result can be reproduced with higher accuracy for finer meshes as in Figure 5. In this last case the declared true solution is for the grid 181×181 and the three coarse grid solutions are 101×101, 111×111 and 121×121 grids. It demonstrates some practical convergence of the LSE method with very good error estimate on the solution. Further LSE gives the best performance to predict the grid solution on M^0 when the coarse grid solution are projected on the same M^0. However, how good should be the coarse grid solution is still an open issue.

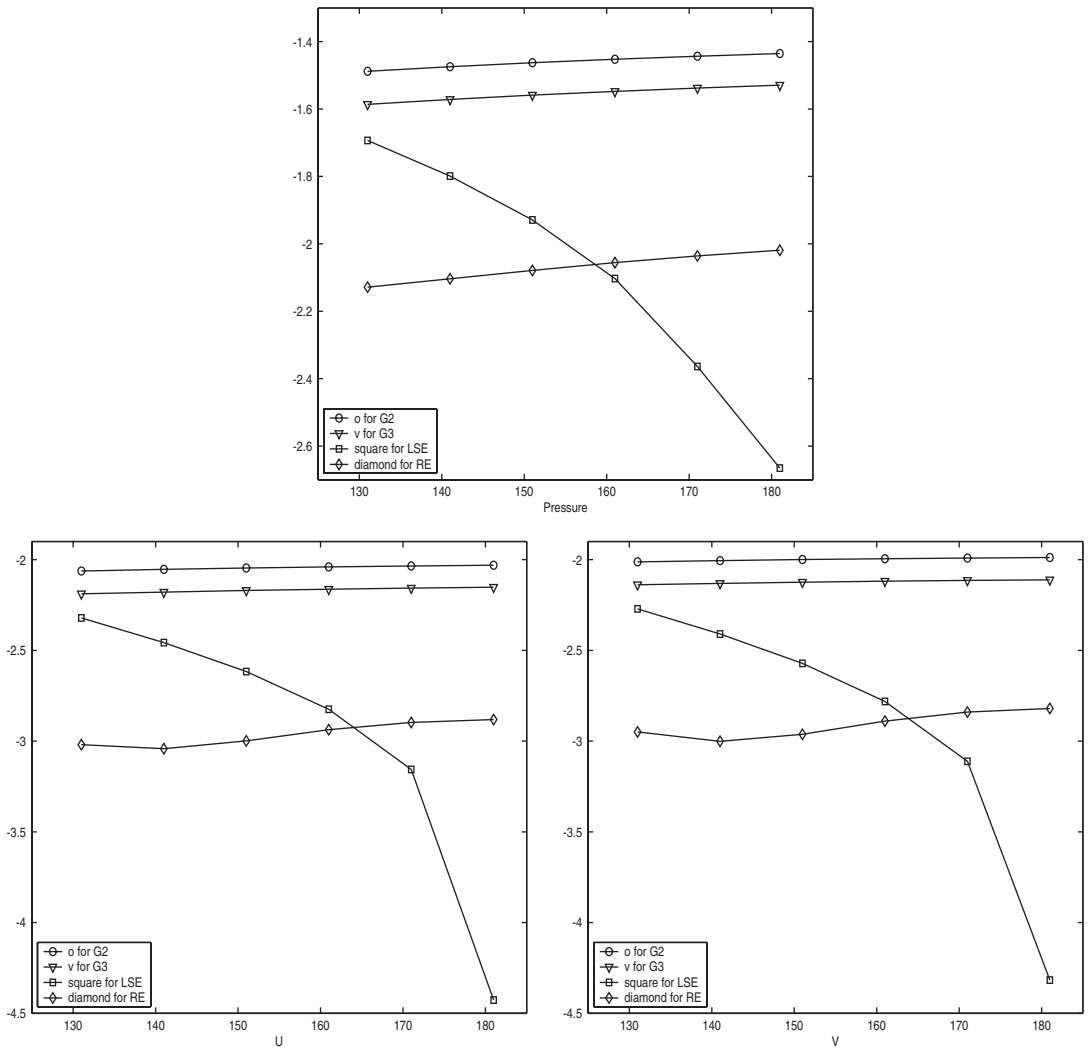

Figure 5. Performance of LSE, with postprocessing of the residual, to predict the solution on the grid 181×181. The coarse grid solution G_1, G_2, G_3, are, respectively, 101×101, 111×111, 121×121.

Finally, it should be noticed that as the *coarse grid* solutions get finer, the LSE accuracy is always significantly better than the RE prediction. This is shown in Figure 6 where LSE is computed with simultaneous increasing resolution of the coarse grid solutions $(N-20)^2$ for $G1$, $(N-10)^2$ for $G2$ and N^2 for $G3$, for $N=70$ up to 110.

Finally it can be observed on this test case that the flow speed is discontinuous at the two corners of the sliding wall. This singular behaviour of the pressure and the velocity components

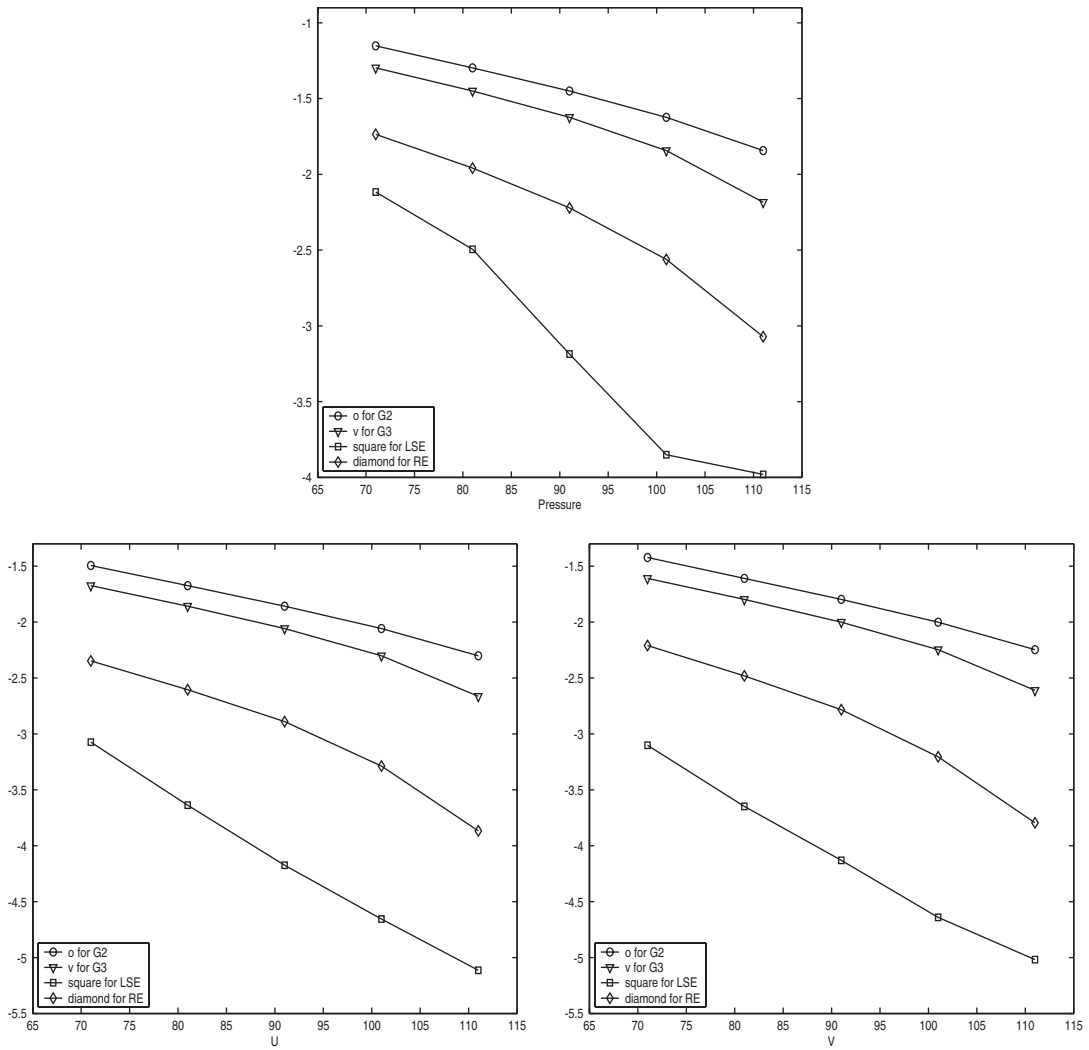

Figure 6. Comparison of LSE versus RE with varying accuracy for the coarse grid solution. G_1, G_2, G_3, are, respectively $(N-20)^2$, $(N-10)^2$, N^2 grids. Horizontal axis gives the number of grid points N in each space direction for $G3$.

at these corner points leads to locally low order accuracy of the numerical solution [9]. This impacts the efficiency of the RE indeed. We obtain then better *a posteriori* estimate with LSE than with RE, thanks to the postprocessing of the coarse grid solution.

It is not yet clear if a wavelet representation of the weight function α and β, will better approximate sharp variation of the convergence order at the corner and give a significantly better result for the singular case obtain with $g(x) = -1$. We have also observed that spline interpolation of the coarse grid solution on M^0 smears out the singularity at the corner and

might be also one of the barriers for recovering accurate solution in the L_2 norm with very coarse grids. This is currently the subject of further investigations.

5. CONCLUSIONS

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* error estimate than RE when the convergence order of a CFD code is space dependent. However there are still many open questions concerning mainly how fine should be the coarse grid solution to provide accurate *a posteriori* error estimate. We are currently investigating the use of wavelet approximation instead of regular trigonometric polynomial to track the multiscale properties of the solution reflected in sharp variation of the convergence order.

Further let us mention that there are many variants of the least square method [23]. We have so far considered the most straightforward method with an unreliable estimator. We may therefore need to find an optimal weight to the Least square, and eventually use better methods such as the generalized least square or non-linear least square method.

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