A Least Square Extrapolation Method for the A Posteriori Error Estimate of CFD and Heat Transfer Problem

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ABSTRACT: 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 elliptic operators 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 on coarse grid solutions. 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 13^{th} international conference on domain decomposition and Garbey $\&$ Shyy JCP 2003] 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 an optimization framework facilitating multi-level extrapolation, improves accuracy and provides a posteriori error estimate. We will illustrate the method with incompressible Navier Stokes flow computations and present a new development of the method for unsteady heat transfer problems.

1 INTRODUCTION AND MOTIVATION

Richardson extrapolation (RE) has been extensively used in Computational Fluid Dynamics (CFD) (Hutton and Casey (2001), Oberkampf et al. (1995), Oberkampf and Trucano (2002), Roache (1998)) to produce aposteriori error estimates. Many variations of the RE method have been studied to approximate a fine grid solution instead of an asymptotic limit, works with non embedded grids (Roache (1998)), retrieve the convergence order of the method if it is an unknown (Roy et al. (2000)).

All these methods relies on the a priori existence of an asymptotic expansion of the error such as a Taylor formula, and make no direct use of the PDE formulation. As a consequence RE methods are extremely simple to implement.

But in practice, meshes might not be fine enough to satisfy accurately the a priori convergence estimates that are only asymptotic in nature. RE is then unreliable (W. Shyy andWu (2002)). Further RE extrapolation formula are fairly unstable and sensitive to noisy data (Garbey and Shyy (2003)).

On the other hand, a posteriori estimates in the framework of finite element analysis have been rigorously constructed (Ainsworth and Oden (2000),Verfurth (1996)). While most of the work has been limited to 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 (Machiels et al. (2000)). A posteriori Finite-Element free constant output bounds can be constructed for the incompressible Navier Stokes equation (Machiels et al. (2000)).

There is also a number of interesting papers on the a posteriori estimate of unsteady problems (Suli and Houston (1997), Machiels et al. (2000), Ainsworth and Oden (2000)). However, most often unsteady problems

$$\frac{\partial u}{\partial t} = N[u], \qquad (1)$$

are analyzed in their semi-discretized form

$$-dtN[u] + u = F, \quad (2)$$

where dt is the time step, to reuse the same a posteriori framework than for the steady problem.

We have recently proposed to embed the RE method into an optimization framework to cope with the limitation of RE while retaining the simplicity of RE's procedure. Our new method called Least Square Extrapolation (LSE) (Garbey (2002), Garbey and Shyy (2003), Garbey and Shyy (NA)) uses grid solutions that can be produced by any discretization. LSE sets the weights of the extrapolation formula as the solution of a minimization problem. 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 should 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 a very 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 (Garbey (2002), Garbey and Shyy (2003)) to generalize the method to parabolic problems. We use then LSE with coarse grid solutions that have different meshes in space *and* time. This method is therefore not a simple extension of our previous LSE method to the semi-discretized problem (2).

The plan of this paper is as follows. In Section 2, we first recall the general idea of the LSE method for steady problems. In Section 3, we discuss RE and LSE for unsteady problems. In Section 4 we present a benchmark problem in heat transfer and discuss the numerical results.

2 THE LSE METHOD

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: $v_h^1,\ v_h^2 \rightarrow u$ in E as h $\rightarrow 0$. 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 trigonometric polynomial functions of degree M. We have shown

Theorem (Garbey and Shyy (2003)): if $u,\ (v_h^i)_{i=1,\,2}\,, \in \ C^1(0,1)$, 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 $0(M^{-2}) \times 0(h^p)$ approximation of u.

In practice, we may have $v_h^1 - v_h^2 << u - v_h^2$, 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.

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 numerical approximation of the linear PDE

$L_h[U] = f_h, U \in (E_a^h, ||\ ||_a)$ 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

$$||U||_a \ \leq \ C\ h^s\ (||f_h||_b), \quad (3)$$

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 polator preserves the positivity of species. For steady problems, it is convenient to postprocess the interpolated functions $\tilde{U}^i$, by few steps of the relaxation scheme

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

with appropriate artificial time step δt. For elliptic problems, this may readily smooth out the interpolant.

Let $e_j, \; j = 1..m$ be 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.

• Interpolation of the coarse grid solution from $G_i, i = 1..3$ to M^0.

• 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.

• 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 nonlinear PDE problem is done via a Newton-like loop (Garbey and Shyy (2003)). The algorithm might be coded in a stand alone program independent of the main code application.

To illustrate the performance of this method, let us consider the velocity-pressure formulation of the square cavity problem in two space dimensions. The steady problem writes in $\Omega = (0,1)^2$,

$$N_1[u,v,p] = -\frac{1}{Re}\Delta u + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = 0, \; (x,y) \in \Omega \quad (4)$$

$$N_2[u,v,p] = -\frac{1}{Re}\Delta v + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = 0, \; (x,y) \in \Omega, \quad (5)$$

submitted to the constraint

$$Div(u,v) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \; (x,y) \in \Omega. \quad (6)$$

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

$$u(x,1) = g(x), \; x \in (0,1). \quad (7)$$

The grid functions (u_i, v_i, p_i) on G_i are computed with a standard finite differences code using a projection method and staggered grids (Peyret and Taylor (1985)). We have derived in (Garbey and Shyy (NA)) a LSE procedure that fullfill the divergence free constraint and performed significantly better than RE.

In Figure 1, 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 $N = 110$. In this particular example of the square cavity, we have $g(x) = -1$, and $Re = 400$. This test case is representative of the results obtained with our method. Let us notice that the first component u of the speed is singular at the corner, as well as the pressure. We refer to (Garbey and Shyy pear) for detailed explanations. We are going now to present a new development of the LSE method for unsteady problems.

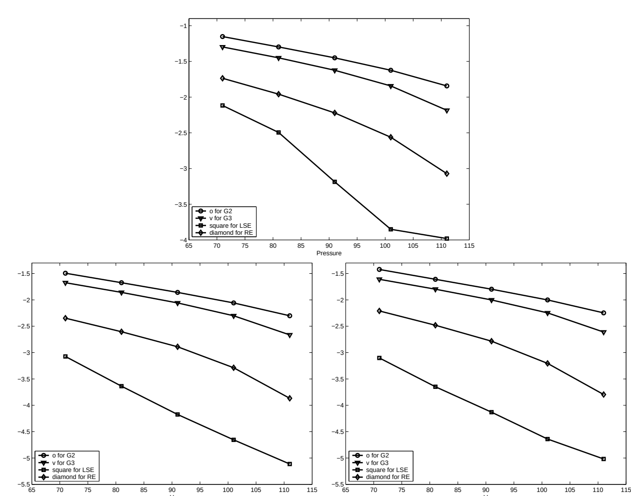

Figure 1. Comparison of LSE versus RE with varying accuracy for the coarse grid solution. G_1, G_2, G_3, are respectively $(N-20)^2$, $(N-10)^2$, N^2 grids. Horizontal axis gives the number of grid points N in each space direction for $G3$. Vertical axis gives the relative error in $l2$ norm, versus the 181×181 grid solution.

3 EXTRAPOLATION METHODS FOR PARABOLIC PROBLEMS

We will consider now the following parabolic problem

$$\frac{\partial u}{\partial t} = N[u], (x,t) \in \Omega \times (0,T), \quad (8)$$

$$u_{|\partial\Omega} = g(t),\ t \in (0,T), \quad (9)$$

$$u(x,0) = v(x),\ x \in \Omega. \quad (10)$$

where N is an elliptic operator. We will use the notation L instead of N if the operator is linear.

We assume that the parabolic problem is well posed and has a unique solution.

For the simplicity of the presentation, we will assume that the problem has one space dimension, i.e $\Omega = [0,1]$, and is discretized with a constant space step and time step. We will denote u the exact continuous solution and $U_{h,dt}$ its discrete approximation. Expression such as $U_{h,dt} - u$ stands for (x,t) restricted to the discretization grid of $\Omega \times (0,T)$.

In RE, one can ignore completely the origin of the problem and assume that the discrete solution as an asymptotic expansion as follows:

$$U_{h,dt} - u = C_1 h^p + C_2 dt^q + o(h^p) + o(dt^q), \quad (11)$$

where C_1 and C_2 are constant independent of the discretization parameters h and dt.

Once for all, we are going to assume that we work with four coarse grid solutions that are:

$$U_{H_1,dT}, U_{H_2,dT}, U_{H_1,dT/2}, U_{H_2,dT/2}. \quad (12)$$

For RE in space *and* time, we will assume that $H_2 = \frac{H_1}{2}$. We have then the following result :

Theorem 1 There exist a unique linear combination of the coarse grid solutions (12) with constant weights $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ such that

$$\alpha_1 U_{H_1,dT} + \alpha_2 U_{H_2,dT} + \alpha_3 U_{H_1,dT/2} + \alpha_4 U_{H_2,dT/2} - u = o(H^p) + o(dT^q), . \quad (13)$$

The $\alpha_i, i = 1..3$ are obtained explicitly.

Further, the consistency of the extrapolation formula implies

$$\alpha_4 = 1 - \alpha_1 - \alpha_2 - \alpha_3.$$

One can use this result to approximate a fine grid solution $U_{h,dt}$. We have

Corollar 1 there is a unique linear combination of the coarse grid solutions (12) with constant weights $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ such that

$$-U_{h,dt} + C_1 h^p + C_2 dt^q + \alpha_1 U_{H_1,dT} + \alpha_2 U_{H_2,dT} + \alpha_3 U_{H_1,dT/2} + \alpha_4 U_{H_2,dT/2} = o(H^p) + o(dT^q).$$

The α_i are given in theorem 1 and the constants C_1 and C_2 can be computed explicitly.

Remark 1 one can notice that this asymptotic expansion is useful iff the expansion $C_1 h^p + C_2 dt^q$ is not negligible against the error term $o(H^p) + o(dT^q)$.

The stability analysis of this time-space RE formula can be analyzed using the following model

$$U_{h,dt} - u = C_1 h^p + C_2 dt^q + \delta, \quad (14)$$

where $C_1 = c_1 (1 + \epsilon_1)$ and $C_2 = c_2 (1 + \epsilon_2)$. c_1 and c_2 are constants and the parameters $\epsilon_i,\ i = 1,2$ stands for the higher order term in the expansion (11), and δ for the numerical error coming for example from the imperfect convergence of the iterative scheme used in implicit time stepping. This stability analysis shows the limit of validity of RE applied to noisy data.

Let us now describe the generalization of the LSE method for space-time problems. Let us denote $U^n_{h,dt}$ the solution given at time t^n by a one step time integration scheme

$$U^{n+1}_{h,dt} = G(U^n_{h,dt}). \quad (15)$$

First we introduce an interpolation operator in space I^h_H, that project the coarse grid solution at each time step on the fine grid in space for the same time step:

$$\tilde{U}^n_{H,dT} = I^h_H[U^n_{H,dT}].$$

Second we introduce an interpolation operator in time $\mathcal{I}^{dt}_{dT}$ that interpolates the coarse grid solution in time on the fine grid in time at the same physical location:

$$\tilde{U}_{H,dT} = \mathcal{I}^{dt}_{dT}[U_{H,dT}].$$

For simplicity of the presentation, we use the generic notation $\tilde{U}$ for all types of projection of U.

Let us assume once for all that $dt = dT/4$. The goal is to have a construction of the interpolation of the four coarse grid solutions on the fine grid (h, dt) using only the information in the time interval $(t^n, t^n + dT)$.

LSE in space time will combine then ten vectors

$$U_{H,dT}(t^n), U_{H,dT}(t^n + dT),$$
$$U_{H/2,dT}(t^n), U_{H/2,dT}(t^n + dT),$$
$$U_{H,dT/2}(t^n), U_{H,dT/2}(t^n + dT/2),$$
$$U_{H,dT/2}(t^n + dT), U_{H/2,dT/2}(t^n),$$
$$U_{H/2,dT/2}(t^n + dT/2), U_{H/2,dT/2}(t^n + dT).$$

From $U^n_{H,dT}$ and $U^{n+1}_{H,dT}$, one can get with linear interpolation $\tilde{U}_{H,dT}$ at time steps $t^n + j\ dt,\ j = 1..3$. This method is second order in time.

Thanks to the PDE (10), with $U^n_{H,dT},\ N[U^n_{H,dT}]$ and $U^{n+1}_{H,dT},\ N[U^{n+1}_{H,dT}]$, one can get a third order approximation in time with Hermite interpolation.

With $U^n_{H,dT/2}$ we have one more time steps to be used. One can use either cubic or Hermite interpolation that are third order in time.

Applying interpolation in time, followed by interpolation in space

$$\tilde{U}_{H,dT} = I^h_H[\mathcal{I}^{dt}_{dT}[U_{H,dT}]],$$

we build finally for each coarse time step $(t^n, t^n + dT)$ a projection of all four coarse grid solutions (12) on the fine grid of space step h and time step dt.

Formally, the LSE problem can be defined as

Problem Fine the three weight functions α_j, $j = 1..3$ such that the residual

$$\Sigma_{j=1..4}\alpha_j\, \tilde{U}^{n+1}_{h,dt} \;-\; G(\Sigma_{j=1..4}\alpha_j\, \tilde{U}^{n}_{h,dt}), \qquad (16)$$

is minimum in the discrete l^2 norm on the space time grid

$$\{ih\}_{i=1 \cdot N} \times \{t^n, t^n + dt, t^n + 2dt, t^n + 3dt, t^{n+1}\}$$

We recall that thanks to the consistency of the extrapolation method, we have $\alpha_4 = 1. - \Sigma_{j=1,3}\alpha_j$.

Because we compute the LSE for each coarse time step separately, we will assume that the weight functions are space dependent only. We will use the space of approximation for the weight function as in the steady case.

We are going now to present some numerical experiments with this method.

4 NUMERICAL RESULTS AND CONCLUSION

For our numerical simulation, we have chosen the thermal wave problem (Ropp, Shadid, and Ober 2004),

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + 8\, T^2\,(1 - T). \qquad (17)$$

We refer to (Ropp, Shadid, and Ober 2004) for the notation and values of the parameters.

The coarse grid solution used in the numerical solution correspond to the discretization (H, dT), $(H/2, dT)$, $(H, dT/2)$, $(H/2, dT/2)$. We will denote these coarse grids $(H/i, dT/j)$ $G_{i,j}$, $i = 1,2$ $j = 1,2$. The fine grid G^* used in LSE corresponds to $(H/4, dT/4)$. The projected coarse grid solutions are denoted now $\tilde{U}_{i,j}$, $i \in \{1,2\}$, $j \in \{1,2\}$.

We have restricted ourselves in this preliminary work to the constant coefficient case. We do not take advantage of the full potential of LSE therefore. This is an important remark because our benchmark problem exhibits a traveling wave with a relatively sharp front. The traveling wave speed is of order one.

We have studied the performance of LSE for an individual time step. We have also experimented the stability of the time integration scheme using RE or LSE to predict an improved numerical solution at the end of each time step. For time stepping we have used fully implicit scheme with first oder backward Euler or Crank-Nicholson.

We use the unconstrained minimization subroutine of matlab, to compare results with different choices of the norm, i.e either discrete l^2 norm or maximum norm. We have three unknown coefficients and start the search from the set of RE coefficients.

We have the following preliminary conclusions:

- RE does not work on the fine grid G^*, but may work well on the coarse grid $G_{1,1}$ at time steps kdT, where dT is the coarse time step. The main reason is that RE is too unstable to perturbation introduced by linear interpolation in time.
- One requires few SSOR smoothing of $\tilde{U}_{i,j}$ on G^* solutions to have LSE performing better than the fine grid solution $\tilde{U}_{2,2}$. SSOR is not used to resolve the fine grid problem by far. SSOR removes nicely the high frequency components of the projected coarse grid solutions.
- Let us use for RE formula the expression in theorem 1 that is an approximation of the exact solution. LSE is designed to approximate the fine grid solution on G^*. One can have LSE better than RE for G^* and in the same time LSE worst than RE as an approximation of the exact solution.
- The higher the order of the scheme, and/or the finer the discretization, the more iterates of SSOR we need. The optimal number of SSOR iterates has not yet been determined.
- LSE gives best results for under resolve solutions with lower order scheme. Under resolve solutions have large time steps and space steps, as well as Newton iterations that cannot reach complete convergence.
- Smaller residual on G^* does not lead to smaller errors. The lack of monotonicity in the stability estimate results in poor performance of LSE. This problem is as in the steady case, the result of the spurious high frequency components of the projected fine grid solutions. The postprocessing step with SSOR is then essential to recover the monotonicity of the error as a function of the residual.
- Filtering the residual and/or the solution in space, as we did in the steady case, might be beneficial for large time step.

Let us illustrate these preliminary conclusions with few numerical results.

Figure 2 shows that with plain LSE, to minimize the residual does not necessary result in minimizing the error. The diamonds are for the result with LSE, and the crosses are for RE. Each of the points of the cloud of point is for a different combination of weight function. We have plotted roughly several hundred of them. We see a large discrepancy between the l^2 and the l^∞ results.

Figure 3 shows the result for Backward Euler. The vertical axis shows the l^2 error versus the exact analytical solution of (17). The horizontal axis is for the time. The grid is very coarse in space, and RE is not accurate. LSE predict fairly well the fine grid solution. We have similar results for Crank Nicholson.

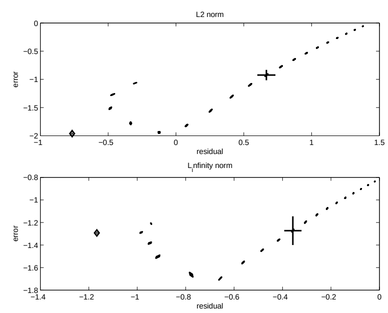

Figure 2. Error versus residual in a given norm.

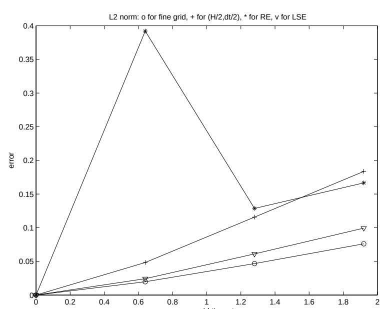

Figure 3. Backward Euler with fairly coarse grids.

These preliminary results are rather encouraging and are currently generalized to unsteady problems with multiscales.

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