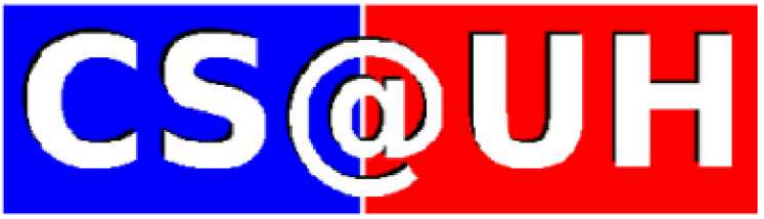

On Optimized Extrapolation Method for Elliptic Problems with Large Coefficient Variation

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Abstract

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Index Terms

Partial Differential Equations, Least Square Method, Richardson extrapolation, Optimization Method, a Posteriori Error Estimate.

I. Introduction and Motivation

We consider the elliptic problem

$$div(\rho \nabla u(x)) = f(x),\ x \in \Omega \subset \mathbb{R}^2,\ u = g\ on\ \partial\Omega, \tag{1}$$

with $\rho(x) > \epsilon, x \in \Omega,\ \epsilon > 0$. Ω is a polygonal domain.

We assume that the elliptic problem is well posed and has a unique smooth solution. We consider a finite volume approximation of (1) on a Cartesian mesh with square cells of size h. We use centered finite volume cells with a classical second order scheme. We denote symbolically the corresponding linear system

$$A_h U_h = F_h. \tag{2}$$

The goal of this paper is to present an optimization framework for extrapolation methods to construct improved numerical approximation of (1) from a set of two or three coarse grid approximations and provide a posteriori error estimates. While a posteriori error estimates is well understood for problems having smooth solutions [1], [26], [32], we address here the solution verification of elliptic problems when multi-scales or singularities are present. Let us first define our application.

We are first interested in situations where the coefficient ρ exhibits large variations throughout the domain Ω. This is a common problem for many applications. A typical example is the pressure solver in a two-phase flow problem with large ratio of the density of the two fluids.

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For example, bubbles of air rising in a liquid may have a density several orders of magnitude smaller than the density of the liquid itself. The inverse situation corresponds to drops of liquid falling in air [7], [8].

A second example is the pressure solves for flow in porous media through multi-layered materials with large permeability ratio between each layers. A third example is the problem of heat transfer in an heterogeneous material that has large ratio in the thermal conductivity between each component.

To simplify, we will consider test cases with the domain Ω being partitioned into two subsets $\Omega_1 \bigcup \Omega_2$, such that

$$||\rho||_{2,\Omega_1} \sim 1, \text{ and } ||\rho||_{2,\Omega_2} \sim \tau.$$

We assume either $\tau << 1$ or alternatively $\tau >> 1$. The more extreme is the ratio τ, the larger is the conditioning number of A_h, the more difficult it is to have an efficient numerical procedure as well as a good numerical approximation of the solution.

We are second interested in situation where the source term $f(x)$ is a collection of dipoles. This is typically the situation, for example, in the pressure equation in the immersed boundary method of Peskin [25]. While the Peskin's method is a very elegant technique for the simulation of fluid structure interaction and widely used in biological situations, it is well known that the accuracy of the method is not very high. A posteriori error estimator are then needed as a safe guard in the computation.

From the applied mathematics point of view, a posteriori estimates have been around for many years [1], [32]. Most rigorous 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 problems has been introduced by Sarrate et al [29]. A posteriori finite-element free constant output bounds can be constructed for the incompressible Navier Stokes equation [20]. While these methods have the advantage of being rigorous, they are not easy to adapt to finite volume approximations widely employed in fluid flow and heat transfer computation. They have also their own limitation on problem with stiff coefficients, singular sources or multi-scales.

On the other hand Richardson Extrapolation (RE) is a common practice in computational fluid dynamic and used extensively as an error indicator [26]. This tool is widely used because it is simple to implement, it uses the fact that one always compute several solutions on several meshes for a CFD application, and it does not require any detailed knowledge of the computer code used to generate the solution. While RE is a simple, elegant and general mathematical idea that works on approximations that have uniform convergence properties described by a Taylor expansion, its use on multi-scale problems is questionable. In Computational Fluid Dynamics (CFD) [3], [4], [17], [22], [23], [26], [27], [28], [31] the applicability of RE 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 parameter dependent [12], [31]. Boundary layers corresponding to large Reynolds number impact dramatically the convergence rate of the numerical methods and makes the assumption on a uniform asymptotic rate of convergence invalid.

This paper focuses on an optimized extrapolation technique to improve the numerical accuracy of the solution that is a generalization of RE. This improved solution might be used either to provide an error estimate on the coarse grid solution or to construct an initial guess for the iterative solver in a cascade of computations with finer and finer grids.

To cope with the limitations of RE, we have introduced recently [10], [12] the so-called Least Square Extrapolation method (LSE) that is based on the idea of finding automatically the order of convergence of a method as the solution of a minimization problem on the L_2

norm of the residual. From a practical point of view, we have shown that LSE is more robust than RE with several multiple-scale problems. We have benchmarked our method with a two dimensional turning point problem [24] exhibiting a sharp transition layer, the incompressible cavity flow problem with a sliding wall, and the back step incompressible flow problem with substantial Reynolds number. The implementation of the LSE method is fairly easy and its numerical procedure inexpensive.

In this paper, we pursue the research initiated in [10], [12] to elliptic problems with coefficients having large variations as described above or singular source terms such as a set of dipoles. In this context we will present a general optimization framework for the unknown weight coefficients of the extrapolation formula that can be set for various objective functions or norms. We will demonstrate in our numerical experiments that our method lead to robust a posteriori error estimates using different error norms.

The plan of this paper is as follows. In Section 2, we describe the general concept of an optimized extrapolation method and its application to error estimates. In Section 3, we present the numerical procedure to construct the extrapolation and the error estimate. In Section 4, we discuss the numerical results for the elliptic problem (1). Section 5 is our conclusion and perspective for future work.

II. THE OPTIMIZED EXTRAPOLATION METHOD

Let us first describe the general concept of the method.

A. Presentation of the method

Let G_1 and G_2 be two regular Cartesian meshes used to build two finite volume approximations of the elliptic problem (1). Let us denote h_1 and h_2 the size of the square cells for both meshes, and U_1 and U_2 to be the two corresponding approximations of the continuous solution $u \in (E, ||\ ||)$. We assume the convergence of these approximations, that is

$$U_1,\ U_2 \to u \text{ in } (\mathrm{E}, ||\ ||) \text{ as } \mathrm{h}_1,\ \mathrm{h}_2 \to 0.$$

A consistent linear extrapolation formula should have the form

$$\alpha U_1 + (1-\alpha)U_2,$$

where α is a weight function. In classical RE the α function is a constant. In our optimized extrapolation method α is a space dependent function. If U_1 and U_2 are in a finite element space $(E_h, ||\ ||)$, α must be such that the linear combination is still in $(E_h, ||\ ||)$.

We formulate the following optimization problem for the unknown function α:

$$P_\alpha\text{: Find } \alpha \in \Lambda(\Omega)\ \subset\ L_\infty \text{ such that } G(\alpha\, U_1\ +\ (1-\alpha)\, U_2) \text{ is minimum in } (E_h, ||\ ||),$$

where G is an objective function to be defined. The Optimized Extrapolated Solution (OES) is then $V_e = \alpha\, U_1\ +\ (1-\alpha)\, U_2$.

For computational efficiency, $\Lambda(\Omega)$ should be a finite vector space of very small dimension compared to the size of matrix A_h defined in (2). The objective function G can be any a posteriori existing error estimators, provided that it operates on the space of approximation $(E_h, ||\ ||)$.

In the most general situation, i.e, in the absence of the knowledge of any rigorous a posteriori estimator, we choose to minimize the consistency error for the numerical approximation of (1) on a fine mesh M^o of step h^0. The fine mesh M^0 should be set such that it captures all the scales of the continuous solution with accuracy required by the application. We have a priori $h^0\ <<\ h_1,\ h_2$. Let us emphasize that h_1 and h_2 do not have to be very different, and that

the ratio $\frac{h_1}{h_2}$ does not have to be an integer. Both coarse grid solutions U_1 and U_2 must be then interpolated onto M^0. We will denote $\tilde{U}_1$ and $\tilde{U}_2$ the corresponding grid functions. One needs second to get the approximation of the elliptic operator A_{h^0}. The objective function is then

$$G(U_h^0) = ||A_{h^0}\, U_{h^0} - F_{h^0}||, \tag{3}$$

where $U_h^0 = \alpha\, \tilde{U}_1 \; + \; (1-\alpha)\, \tilde{U}_2$.

The choice of the space $(E_{h^0}, \; || \; ||)$ and its norm should depend on the property of the solution. In LSE [12], [13] we chose the discrete L_2 norm on M^0. We will investigate here other possibilities such as the L_1 or the L_∞ norm.

One of the difficulties encountered with such a two-level extrapolation method is the so-called cancelation problem [12]. In practice there exists subsets of Ω where U_1 and U_2 are much closer to each other than what the expected order of accuracy based on local error analysis should provide. In such areas the sensitivity of the extrapolation to the variation of α is very weak and the problem is ill posed. These subsets should be treated as outliers of the optimization computation procedure. A potentially more robust optimization procedure consists of using three levels of grid solution. The optimization problem writes then

$$P_{\alpha,\beta}\textit{: Find } \alpha, \beta \in \Lambda(\Omega) \; \subset \; L_\infty \textit{ such that } G(\alpha\, U_1 \; + \; \beta\, U_2 \; + \; (1-\alpha-\beta)\, U_3) \textit{ is minimum in } (E_h, ||\;||),$$

where G is an objective function to be defined. The optimized extrapolated solution is then $V_e = \alpha\, U_1 \; + \; \beta\, U_2 \; + \; (1-\alpha-\beta)\, U_3$.

We notice that if all $U_j, \; j = 1..3$, coincide at the same space location there is either no local convergence or all solutions U_j are exact. In such a situation, one cannot expect improved local accuracy from any extrapolation technique. The robustness of the OES method should come from the fact that we do not suppose a priori any asymptotic formula on the convergence rate of the numerical method as opposed to RE.

Let us assume that the optimization problem P_α or $P_{\alpha,\beta}$ has been solved and that we have computed V_e either from the two levels or three levels method. We are going to discuss now its application to provide a posteriori error estimators.

B. Application to a posteriori estimates

Let us denote U_j to be one of the coarse grid approximations at our disposal. A global a posteriori estimate of the error $(U_j - u)$ may come in two different ways.

- First is the recovery method based on the idea that the optimized extrapolated solution is more accurate than the coarse grid solution: Let us denote $\tilde{U}_j$ the coarse grid solution projected onto the fine grid M^o via a suitable interpolation procedure. Let us assume that the extrapolated solution is decisively more accurate than that based on interpolation from the coarse grid solution, namely,

$$(V_e - u) << (\tilde{U}_j - u), \mathrm{in}\ (\mathrm{E_h}, ||\;||). \tag{4}$$

  Then $||V_e - \tilde{U}_2||$ is a good error indicator to assess the accuracy on G_2 solution. We have then

$$(\tilde{U}_j - V_e) \sim (\tilde{U}_j - u), \mathrm{in}\ (\mathrm{E_h}, ||\;||). \tag{5}$$

  We will show in our experiments that this method may give a good *lower* bound error estimates. But we do not know in general if the hypothesis (4) is correct. If G is chosen to be the residual on the fine grid, there is no guarantee that a smaller residual for V_e than for U_2 on the fine grid M^o will lead to a smaller error.

- Second is a global *upper* bound that follows from a stability estimate with the discrete operator. Let us assume that the objective function is the residual in the discrete norm $||\ ||$, namely (3). Let us denote U^0 to be the fine grid solution on M^0, and A_0 to be the corresponding linear operator. We have

$$||V_e - U^0||\ <\ \mu\, G(V_e),$$

where $\mu \geq ||(A_0)^{-1}||$.
We conclude then

$$||\tilde{U}_2 - U^0||\ <\ \mu\, G(V_e) + ||V_e - \tilde{U}_2||. \tag{6}$$

The procedure to derive an estimate for μ will be discussed later.

(6) is a good global a posteriori error estimator provided that

$$||U^0 - u||_2\ <<\ ||U^0 - \tilde{U}_2||_2. \tag{7}$$

One way to test this hypothesis (7) is to measure the sensitivity of the upper bound (6) with respect to the choice of the fine grid M^0. This is a feasible test because the fine grid solution is never computed in OES. Our verification procedure then checks that $||U^0 - U_2||_2$ increases toward an asymptotic limit as M^o gets finer.

We will now present in detail the solution procedure to obtain OES and a posteriori error estimates. We will assume that G is a linear operator.

III. Procedure to Construct the Optimized Extrapolation

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

- First, interpolation of the coarse grid solution from $G_j, j = 1..p$ to M^0. We have two coarse grids to interpolate for P_α, respectively three for $P_{(\alpha,\beta)}$.
- Second, evaluation of the objective function

$$G[e_i\ (\tilde{U}_j - \tilde{U}_{j+1})],\ i = 1..m,\ j = 1..p-1,\ \ and\ \ G[\tilde{U}_p]$$

on the fine grid M^0.
- Third, the solution of the optimization problem that has m unknowns for each weight coefficient α and β used in the extrapolation procedure.

In practice, we should keep m much lower than the number of grid points on any coarse grid used. If one chooses the discrete L_2 norm, the optimization problem can be solved easily and the arithmetic complexity of the overall procedure should be of order $Card(M^0)$. In the general case, the algorithm might be coded in a stand-alone program independent of the main numerical code.

Remark 1: This procedure can be generalized to non-linear elliptic problems via a Newton like loop [12], [13].

We will now discuss the first step of the algorithm.

A. Projection on the fine grid and postprocessing

To compute the objective function properly, the interpolation procedure should preserve the properties of the numerical solution.

For conservation laws, one may require that the interpolation operator should satisfy the same conservation properties. Other constraints related to physical realization can also be added. For example, for reacting flow problems, one can require that the interpolant preserves the positivity of species. One may use for example a transform of the unknown variable,

$$\Psi = \Phi(U),$$

such that the inverse map $\Phi^{-1}(\alpha\Psi_1 + (1-\alpha)\Psi_2)$ satisfies intrinsically the constraint.

For positivity, one may use a bijective map Φ from $\mathbb{R}^+$ to $\mathbb{R}$. For mass conservation, we used in [13] the standard stream function transform.

As discussed in [12] the interpolated solutions $\tilde{U}_i$ on the fine grid contains spurious high frequency components. Linear interpolation is much worse than spline interpolation from this point of view. This problem is amplified by the fact that the objective function usually requires the computation of the discrete derivatives of $\tilde{U}_j$.

This spurious frequency components of the interpolated solution are obviously carried on in all linear combination V_e. The computation of the objective function might then be polluted to the point where minimizing $G(U_h)$ does not guarantee any longer that one minimizes the numerical error.

One postprocessing procedure to overcome this difficulty is to filter out the artificial high frequency components of U_j that cannot be present on the coarse grid G_j. However for the elliptic problems (1) discretized by (2) on M^0, it is convenient to postprocess the interpolated functions $\tilde{U}_j$, by few steps of the artificial time stepping scheme

$$\frac{V^{n+1} - V^n}{\delta t} \;=\; A_0 V^{n+1} - F_{h_0},\; V^0 = \tilde{U}_j, \tag{8}$$

with appropriate artificial time step δt. This will readily smooth out the interpolant. We will discuss later a criterion to stop this smoothing relaxation (8).

We will also compare in our numerical experiments on (1) the numerical results obtained with linear interpolation and spline interpolation. Let us now discuss the choice of the objective function in OES.

B. Choice of the objective function

In principle, OES should be much cheaper than the computation of the fine grid solution U^0 on M^0. The easiest solution is to choose the objective function to be the residual computed in L_2 norm. This choice presents two essential advantages.

First, the optimization problem to be solved is a least square problem that is well understood, easy to solve, and easy to process with existing software libraries [2].

Second, we can easily estimate μ to asses the global error bounds in (6). We have

$$\mu = \frac{1}{|\lambda|},$$

where λ is the smallest eigenvalue in modulous of the matrix A_0. λ can be computed, for example, with few iterations of the inverse power method [14]. As a matter of fact, we expect to use μ with no better than a ten percent error margin. For very fine grid M^0, this procedure is still fairly expensive. We can alternatively make use of the numerical approximations of λ obtained with the coarse grid operators.

We found in our numerical experiments that λ converges with second order to its lower limit as the space discretization parameter $h \to 0$. We have then computed the sequences of λ for the coarse grid operators $A_{h_j},\; j = 2, 3$, and use a second order RE formula, namely,

$$\lambda = \frac{(h_2)^2\;\lambda_3 \;-\; (h_3)^2\;\lambda_2}{(h_2)^2 - (h_3)^2} \tag{9}$$

to predict μ for the fine grid operator A_0.

For problems with discontinuous solution the choice of the L_2 norm might not be best. We can devise an entirely similar approach using for example the L_1 norm. That choice might be more relevant for problems having a discontinuous solution. Unfortunately, the minimization of the residual in L_1 norm is a more difficult task because the objective function is non-differentiable.

We have used in this case the simplex search of Nelder and Mead [21] implemented in Matlab starting from the optimum solution obtained with the L_2 norm. The computation of an estimate of the L_1 norm $||A_0^{-1}||_1$ might be done with an iterative procedure as well. We refer to the papers of N J.Higham [15], [16] that presents the method. A well known procedure that implements this algorithm is available in LINPACK. We have chosen in our numerical experiment to apply RE to the sequence of estimates $||A_{h_j}^{-1}||_1,\ j = 1, 2, 3$, to get an estimate on μ. This computation is less expensive than to compute directly $||A_0^{-1}||_1$. For problem where one is interested in the maximum of the error, we can devise a similar OES using the L_∞ norm.

Finally, one can use standard finite element a posteriori estimators [1], [32] in place of the norm of the residual to define G. We will not discuss this approach in this paper, since we work with finite volume discretization for which, to our knowledge, such rigorous estimators for (1) are not available.

Remark 2: We emphasize that all fine scales that are not present in the two or three coarse grid solutions will *not* be computed properly by the OES V_e. OES tries at best to recover all the scales that are present in the provided coarse grid solutions.

Remark 3: In multiscale problems, the numerical error is often dominant in some small local area of the domain where the solution is stiff. One example is a boundary layer or a singularity at some corner of the domain. One criterion to choose the objective function G is to be able to capture such singularities. We refer to the literature in singular perturbation theory to give an extensive review of the choice of the norms to analyze boundary layer problems and its numerical solution - see for example [5], [11], [18].

Let us now discuss the representation of the weight function of $\Lambda(\Omega)$.

C. Representation of the weight functions

We look for a compact representation of the weight function that can capture the main feature of the convergence order of the method with very few coefficients. Let us assume for the time being that Ω is a square domain.

As presented in [12], one can use a trigonometric expansion of the weight functions α and β that is adapted to square domain. The space of unknown weight function is chosen to be the set of trigonometric polynomial functions

$$\alpha(x) = \sum_{i=1..m,\ j=1..m} \alpha_{i,j}\ e^i(x_1)\ e^j(x_2), \tag{10}$$

with $x = (x_1, x_2)$, $e^0 = 1$, $e^1 = cos(\pi x_{1/2})$ and $e^i = sin((i-2)\pi x_{1/2}),\ \text{for i} = 3..\text{m}.$

This set of trigonometric functions allows us to approximate at second order in L^2 norm any smooth non-periodic functions of $C^1[(0,1)^2]$, [9]. One additional advantage of this choice of approximation space for the weight function is that it allows us to easily interpret our numerical result in the frequency space.

We observe in practice that the higher order is the expansion (10), the more amplified are the spurious modes in the interpolated solution $\tilde{U}_i$. Postprocessing is then particularly important to stabilize the OES.

In this paper we have tested a second alternative that might be better suited to capture the local properties of the convergence rate. First, let us define $e_{i,j}$ to be the set of Q_1 basis function of the square domain Ω on the very coarse grid of $m \times m$ cells. $e_{i,j}$ is then one at the center of the cell of coordinates (i, j) and zero elsewhere. Second we transform $e_{i,j}$ into $\tilde{e}_{i,j}$ that is the interpolated function defined on the fine mesh M^o. Our second solution is then to look for the weight functions as follows:

$$\alpha(x) = \sum_{i=1..m,\ j=1..m} \alpha_{i,j}\ \tilde{e}_{i,j}(x_1, x_2), \tag{11}$$

Both representations of the weight coefficients will be compared in our numerical experiments.

In the general case, Ω is a polygonal domain that can be embedded, after appropriate rescaling, into a square $(0,1)^2$. Because no boundary conditions are imposed on the unknown weight functions of the OES, we can use exactly the same set of basis functions. However the OES problem depends only on the grid point of the interpolated solutions that are inside the domain Ω. With the representation given in (11), all coefficients of the basis function $\tilde{e}_{i,j}$ that are null identically inside Ω should be then removed from the OES formulation.

We have now described all the components of the solution procedure to build the OES and some global a posteriori error estimate.

We are going to show in the next section that the OES method provides robust a posteriori global error estimates for the elliptic problem (1) with stiff coefficient ρ.

IV. Results and Discussion for the $div(\rho\nabla)$ Operator

We are going to consider seven test cases based on the homogeneous Dirichlet problem

$$div(\rho\nabla u(x)) = f(x),\ x \in \Omega \subset \mathbb{R}^2,\ u = 0 \text{ on } \partial\Omega, \tag{12}$$

with a smooth right hand side function:

$$f(x) = \exp\left(-2\ (x_1(i) - 0.5)^2\ -\ 2\ (x_2(j) - 0.5)^2\right). \tag{13}$$

The first test case T_1 used as a basic reference is the Poisson problem into the square $(0,1)^2$. All other test cases correspond to different distribution of the ρ function and/or different geometry of the domain.

Let us define D_1 (respectively D_2) the disc of center $C = (0.38, 0.48)$ ($C = (0.64, 0.74)$) and radius $R = 0.15$. The coefficient ρ is as follows

$$\rho(x,y) = 1\ +\ 0.5\ (\tau - 1)\ \left(1. + \tanh(-100\ (dist((x,y),C) - R))\right),\ x \in \Omega, \tag{14}$$

where $dist((x,y),C)$ is the distance from the point of coordinates (x,y) to the center C of the disc. ρ is close to τ inside the disc of center C and radius R, and 1 outside.

For the five first test cases $T_i,\ i = 1..5$, Ω is the unit square. The test cases T_6 and T_7 correspond to an L-shape domain $(0,1)^2 \setminus (0,0.5)^2$. The last test case T_8 is for a Poisson problem with a circle of dipoles source terms. This test case will be used to analyze the impact of the choice of the norm in the error estimate. Figures 1 to 4 show respectively the solution on the fine grid M^0 for the test cases $T_i,\ i = 2,\ 6,\ 7,\ 8$.

The test cases $T_i,\ i = 1..7$, are designed to be representative of the pressure equation for a two-phase flow problem. The disc $D_{1/2}$ is the analogue of a bubble of circular shape that has the relative density τ with its medium. Small τ are for bubble of gas immersed in liquid. Large τ can be interpreted as a liquid drop immersed in air.

We see in Figure 1 that small τ gives a high pressure pick in the disc. Large τ in Figures 2 and 3, induces a plateau in the pressure that matches the disc contours. In test case $T6$ the disc D_1 intersects the wall, and the plateau matches the zero boundary condition. In test case $T7$ the disc D_2 stays inside the L shape domain, and we have a strong interaction between the "bubble" and the singularity of the solution at the entry corner.

With homogeneous Dirichlet boundary conditions, complex geometry does not play a significant role for small τ values. As a matter of fact, it can be observed that for small τ the solution of the elliptic problem is of order τ outside the disc D.

We have done a fairly large number of experiments with various grid resolutions for $G_i,\ i = 1..3$ as well as M^0. We focus this experimental section on the discussion of

- the postprocessing of the interpolated solution, i.e., the number of time steps in the relaxation procedure (8),

- the impact of the parameter τ,
- the choice of the interpolant: linear versus spline,
- the choice of the basis function for $\Lambda(\Omega)$, i.e., Fourier versus interpolated $Q1$,
- the choice of the norm L_2 versus L_1 in the objective function

$$G(U_h) = ||A_h\, U_h - F_h||.$$

All the codes have been written in Matlab. In all the graphics representing the performance of our method for these seven test cases, we have chosen for convenience and comparison purposes to fix the parameters of the method as follows.

- We solve each test case with a direct solver on the Cartesian grid of the same space step h_i in both space directions. For the coarse grid G_1, (respectively G_2 and G_3) we have $h_1 = 1/14$ (respectively $h_2 = 1/20$ and $h_3 = 1/26$).
  This coarse grid does not resolves the sharp transition of the density function ρ defined in (14). ρ appears to be almost a step function on these coarse grids.
- The fine grid solution M^0 is chosen to be a grid of step $1/128$. To verify the quality of this fine grid solution we use as a benchmark solution the grid M^∞ of space step $1/256$.
- The coarse grid solutions are interpolated on M^0 either by the bilinear interpolation or by the cubic spline procedure of Matlab.
- These interpolated solutions are post-processed with the time integration of the heat equation

$$\frac{\partial u}{\partial t} = div(\rho \nabla u(x)) - f(x),\ x \in \Omega \subset \mathbb{R}^2,\ u = 0 \text{ on } \partial\Omega. \tag{15}$$

  on the interval of time length of order 10^{-2}. To this end, we use time steps of order $\delta t = 10^{-3}$ in a first order implicit Euler scheme. Typically each time step requires two iterates of a biconjugate gradient method (BICGSTAB) with an incomplete LU pre-conditioner.
  The fine grid solution M^o is not resolved by this scheme by all means. We will see that the quality of the OES improves dramatically with this relaxation procedure.

In Figures 5 to 7, we use the following conventions. The left graph gives an error estimate based on the recovery method (4), while the right graph gives an upper bounds of the error based on the global estimate (6). The graph in the middle shows the residual obtained in the norm of choice for the OES method.

To check the accuracy of the error prediction, we have computed the M^o fine grid solution. The curves labeled with '*' gives the error $||\tilde{U}_3 - U^0||$.

To check the accuracy of the M^0 solution, the curve with 'v' labels gives the error of the M^0 solution versus the ground true solution M^∞, that is $||U^0 - U^\infty||$ on M^0.

We will compare systematically the OES with the two-level methods using the coarse grid solution U_2 and U_3, with the three-level methods based on all three coarse grid solutions. The influence of the time stepping used to postprocess all three projected solutions $\tilde{U}_j,\ j = 1..3$, is demonstrated by representing on the horizontal axis of each graph the time variable of the postprocessing (15).

The dashed curved '- -' in the left and right graphs are the Aitken acceleration of the sequences of error prediction versus the time step based on the three-level method. By construction, this Aitken acceleration does improve the convergence of the numerical approximation *only* if the sequence of error prediction has linear rate of convergence. Oscillation of the sequence of number generated by the Aitken process detect the lack of linear convergence, or possibly occurs when the accelerated sequence is close to convergence within computer arithmetic accuracy.

We will now analyze the result that we obtained in our numerical experiments. Let us report first on the result with the LSE method for all the test cases.

A. L_2 norm

All estimates here used the discrete L_2 norm and the trigonometric expansion (10) of α and β. Let us discuss the influence of the relaxation procedure (8).

1) Discussion on the postprocessing method: Both the recovery method and upper bound estimate (6) are providing accurate estimates for the Poisson problem in a square. This is the minimum that we should expect from a new method, since a basic second order Richardson extrapolation gives already satisfactory results. One notices, however, that four time steps are needed to reach good accuracy in the prediction, and that the spline interpolant gives slightly better results than the bilinear interpolant. Further, for this Poisson problem there is no advantage to using a three-level extrapolation versus a two level-method. For the Laplace operator, one can easily derive a priori how many time steps are required to damp the artificial frequency components of the interpolated solution that were not present in the coarse grid solution.

Let us write algebraically

$$(Id - \delta t\ A_0)\ \tilde{U}^{n+1} = \tilde{U}^n - \delta t\ F_h^0,$$

to be the time stepping (8) applied to each interpolated coarse grid solution $\tilde{U}_j, j = 1, 2, 3$. A_0 is symmetric definite negative and we can order its eigenvalues λ_k as follows

$$0 > \lambda_1 > \lambda_2 ..... > \lambda_m.$$

$m = (N_o)^2$ is the number of grid points on the fine Cartesian grid M^0. Let us denote $v_k,\ k = 1..N$ the corresponding orthonormal eigenvectors of A_o.
The matrix $B = (Id - \delta t\ A_0)^{-1}$ has for eigenvalues μ_k with $\mu_k = (1 - \delta t \lambda_k)^{-1}$. The eigenvalues of B are ordered as follows $0 < \mu_m < \mu_{m-1} ..... < \mu_1 < 1$.
Let us express $\tilde{U}_j^n$ in the orthonormal eigenvector basis v_k, with

$$\tilde{U}_j^n\ =\ \sum_{k=1..m} \tilde{U}_{j,k}^n\ v_k.$$

The following high frequency component of the solution

$$\sum_{k=m_j+1..m} \tilde{U}_{j,k}^n\ v_k,$$

is an artifact of the interpolation procedure. It leads to the following error term that is part of the residual R^{n+1}

$$\sum_{k=m_j+1..m} \lambda_k\ \tilde{U}_{j,k}^n\ v_k.$$

Let us assume that we expect a priori an error on $\tilde{U}_j,\ j = 1..3$, much larger than the tolerance number tol in L_2 norm.
The high frequency component of the residual due to the interpolation process will decay as

$$\sum_{k=m_j+1..N} \mu_k^q \lambda_k\ \tilde{U}_{j,k}^n\ v_k,$$

after q time steps. q should be chosen such that

$$\left(\sum_{k=m_j+1..N} (\mu_k^q \lambda_k)^2 \right)^{\frac{1}{2}}\ <\ tol. \tag{16}$$

A practical bound on q can be derived from (16) and the analytical formula on the eigenvalue of the discrete Laplacian operator. The same analysis is not straightforward for stiff problem

with arbitrary ρ function in (12). As a matter of fact the operator A_o is still definite negative but no longer symmetric.

We use then the following heuristic argument. We know that for q large enough, the decay of the numerical error $E^n = \tilde{U}^n - U_o$ satisfies the asymptotic estimate

$$E^n \sim C^t \mu_1^q. \tag{17}$$

Similarly the residual satisfies

$$R^n \sim C^t \lambda_1 \mu_1^q \tag{18}$$

Once the spurious high frequency components of the error due to the interpolation process have been damped enough, the error *and* the residual decay at the same linear rate μ_1. Further the larger is the number of time steps, the more accurate is this convergence rate. This is the essence of the power method [14] to compute μ_1. We look then for a stop criterion that estimates how close the sequence is to its asymptotic rate of convergence.

Our criterion to stop the iteration is to compute the discrete second order derivative in time of $\log_{10} ||R^n||_2$ that is

$$R_{tt}^n = \frac{\log_{10}(||R^{n+1}||_2) - 2\log_{10}(||R^n||_2) + \log_{10}(||R^{n-1}||_2)}{(\delta t)^2}, \tag{19}$$

and insure that this number is below some a priori tolerance values.

We are going to show that our heuristic stop convergence criterion is also consistent with the use of the Aitken acceleration on our sequence of upper error bounds

$$\mu \, ||A_0 V_e^n - F||_2 + ||V_e - \tilde{U}_2||_2, \tag{20}$$

where V_e is the LES based on $\tilde{U}_j^n, \ j = 1, 2, 3$.
Let us denote r_n the sequence of numbers

$$r_n = \mu \, ||A_0 V_e^n - F||_2.$$

The sequence r_n has also a linear rate of convergence at the speed μ_1.
The Aitken acceleration procedure that we apply to our upper-bound estimate (20) writes

$$s_n = ||V_e - \tilde{U}_2||_2 + \frac{r_n \, r_{n+2} \ - \ r_{n+1}^2}{r_{n+2} \ - \ 2 \, r_{n+1} \ + \ r_n}. \tag{21}$$

Let us rewrite r_n as follows

$$r_{n+1} - r_\infty = (\mu_1 + \delta_n) \, (r_n - r_\infty). \tag{22}$$

We have $\delta_n \to 0$, as $n \to \infty$. We get

$$s_n - s_\infty = (r_n - r_\infty) \frac{(\mu_1 + \delta_{n+1}) \, (\mu_1 + \delta_n) \ - \ (\mu_1 + \delta_n)^2}{(\mu_1 + \delta_{n+1}) \, (\mu_1 + \delta_n) \ - \ 2 \, (\mu_1 + \delta_n)^2 \ + 1}. \tag{23}$$

We have then

$$s_n - s_\infty \sim (r_n - r_\infty) \frac{\mu_1}{(\mu_1 - 1)^2} (\delta_{n+1} - \delta_n). \tag{24}$$

In the meantime

$$||R^n||_2 \approx r_n,$$

and therefore

$$R^{n+1} - R^\infty \approx (\mu_1 + \delta_n) \, (R^n - R^\infty). \tag{25}$$

Using this estimate (25) in (19), we have

$$R_{tt}^n \approx (\delta_{n+1} - \delta_n). \tag{26}$$

To insure that R_{tt}^n is small is then a good stop criterion for the Aitken acceleration because of (24). This Aitken acceleration will systematically be applied to enhance the upper bounds (20).

We are going now to study the impact of the τ scale on the results obtained with the LSE method.

2) Impact of τ on the LSE result: In Figures 5 to 7, we present the results with spline interpolation using $m = 4$ in the trigonometric expansion of α, β. Let us consider the test cases T_2 to T_7. In all these test cases, we have checked that the second order RE improves the solution accuracy, but not consistently. The corresponding error estimate based on the recovery method is then unreliable. Because of the effect of the discrete operator on the interpolation, the upper bound error based on the computation of the residual is far too crude.

The LSE method always gives better results than RE with very few time steps to postprocess the coarse grid solution on the fine grid. For these stiff problems, the three-level method gives consistently better results than the two-level method.

In most of the cases the recovery method may give an acceptable estimate from below of the error after very few time steps as shown in Figures 5 and 6. The test case T_7 in Figure 7 is an exception. It can be checked in this test case that the code is not converging well, because $||U^0 - U^\infty||$ is not much smaller than $||U_3 - U^0||$.

The Aitken acceleration of the sequence of estimates based on the recovery method may sharpen this estimate, but not consistently. There is no obvious reason for which $||V_e - \tilde{U}_3||$ should converge linearly. In all these test cases, the failures of the Aitken acceleration might be easily detected from the existence of oscillations.

In all test cases, the upper bound (6) overestimates the error by a factor five to ten at most provided that we process the time integration of the solution with few time steps for an interval of time of size $2\ 10^{-2}$.

The Aitken acceleration of this time sequence of estimate provides a faster improvement of the upper bound for large τ than for small τ. This is consistent with the fact that the time stepping converges faster to the linear rate of convergence for large τ than for small τ. In the test case $T7$ we do have a strong oscillation of the Aitken acceleration of the upper bounds sequence. We conjecture that this is a good indicator of the bad convergence properties of the code due to the reentry corner in this specific situation.

We found in all test cases the LSE method is robust provided that the relaxation scheme (8) is used to post-process the interpolated coarse grid solutions.

Let us now discuss the advantage of spline interpolation versus bilinear interpolation.

3) On the choice of the interpolant: In principle spline interpolation preserves the smoothness of the solution and should give better results than linear interpolation with LSE. On the contrary if the solution is very stiff, the spline interpolant smooths out the interpolated solution where it should exhibit a sharp front. The result should then be worse than linear interpolation with LSE. This is exactly what we have observed for the numerical error after very few time steps. However, thanks to the relaxation process the difference between both solutions after five time steps is completely marginal. We should rather use then bilinear interpolation that is easier to implement in more complicated geometry. Let us discuss now the choice of the representation of the weight function.

4) On the choice of the basis function to represent the weight function: We have also tested the impact of the choice of the basis function to represent the unknown weight coefficients α and β. The general observation is that the accuracy of the LES prediction increases when one increases the value of m from one to few units, typically four. The gain obtained in

further increasing m becomes then marginal in the Fourier case (10). On the contrary our numerical simulation with m up to 12 shows slightly better convergence using (11). However the postprocessing procedure may make this improvement marginal after few time steps. We speculate that the main contribution of the error with stiff problem is so dominant in some local area that even the coarser grid solution is good enough outside the region of stiffness. In other words the weight coefficient has very little influence on the quality of the LES outside the region of stiffness. The LES method can then capture the main component of the error with local or non local basis functions as well . This hypothesis should be revised indeed when the coarse grid solutions are computed with locally refined meshes. Let us further notice that the representation (11) gives less unknowns to compute for complex shape domains than with (10). We will now compare the LSE method with OES using L_1 norm and L_∞ norm.

B. Discussion on the choice of the norm

In Figure 8, we compare the error estimate based on the recovery method obtained with the L_1 , (curved with '-' lines) and the L_2 norm (curved with continuous line), for the test case T_5. Curves labeled with $\square$ and o correspond to the two level methods and three level methods. Except in this test case T_5 reported here, we did not found any significant advantages to using the L_1 norm instead of the L_2 norm for the objective function. The recovery method gives similar results for all other test cases with the L_1 and the L_2 norm.

In particular our conclusion on the impact of τ, the choice of the interpolant and the basis function to represent the weight function is identical to our previous conclusion with LSE.

Further, the simplex search of the Nelder and Mead minimization procedure is obviously much more time consuming than the least square method and generally less accurate at convergence. The Aitken acceleration of the upper bound estimate is therefore not very effective. Figure 9 gives a representative example of our result. While a more efficient optimization procedure to construct OES might be used, we have also noticed that the upper bound obtained with the L_1 norm is much coarser than in the L_2 norm case for all test cases. This is a major draw back of the method.

There is however a significant interest to use the L_1 norm for solution of PDE problems exhibiting discontinuities. Let us consider then the following test case denoted T_8:

$$\Delta u = div(\vec{a}\ \delta^{\Gamma}(x,y),\ (x,y) \in (-1,1)^2,\ u_{|\partial\Omega} = 0, \tag{27}$$

where Γ is a circle of center 0 and radius $\frac{1}{2}$.

This test case is designed to represent the pressure solve in the Peskin method [25] when the membrane is the circle Γ. The force is distributed along the membrane with a set of discrete dirac delta function. These force terms have the direction of the radius of the circle. We choose then $\vec{a}$ to be the vector of components $(2\pi x, 2\pi y)$. These force terms leads to a distribution of dipoles in the pressure equation. Let δ_h be the discrete approximation of the dirac delta function based on the piecewise cubic function given in [6] with a support of radius two space step h. The discrete representation of Γ uses M points. To insure that the space steps between these grid points is of order h we take $M = 6N$ with $N = 2/h$. The source term in (27) writes then

$$\delta^{\Gamma}(x,y) = \frac{1}{M}\sum_{i=1}^{i=M} \delta_h\left(x - 0.5\cos\left(\frac{2(i-1)\pi}{M}\right)\right)\ \delta_h\left(y - 0.5\sin\left(\frac{2(i-1)\pi}{M}\right)\right).$$

The solution of (27) on the fine grid is given in Figure 4. One can notice the severe oscillation of the solution at the Γ location. Figure 10 shows respectively our results using successively the L_2, L_1 and L_∞ norm and linear interpolation for the coarse grid projection on M^0.

Spline interpolation gives less accurate results as one can expect from the discontinuity of the solution.

One can notice that there is almost no advantage to use the three-level solution instead of the the two-level solution. We conjecture that $\tilde{U}_2 - \tilde{U}_3$ and $\tilde{U}_1 - \tilde{U}_3$ have similar random behavior in the vicinity of Γ. There is then no advantage to use $\tilde{U}_1$ in the three-level method.

The two upper bounds of the error in L_2 and L_∞ norm are accurate after five time steps. The L_1 error estimate is more accurate than in the previous test cases. Although the error in L_∞ norm is very large, the L_∞ error estimate gives a good prediction of the error that comes from the inaccuracy in the interface location. There is therefore no real advantage to use the L_1 norm versus the L_2 norm. Further, the L_∞ norm gives interesting complementary information to the L_2 norm estimate, on how inaccurate the solution can be near the circle of discontinuity. We present in the next section our general conclusion of this study.

V. Conclusions

In this paper we have extended the LSE method to a general optimization framework that allows one to use arbitrary norms and/or objective functions. We concentrate our work on giving a posteriori estimates. We have presented a rigorous upper bound error estimator technique to predict very fine grid solutions. We have used an acceleration technique to sharpen this error estimate and/or detect failures of convergence. We have applied the method to a multi-scale elliptic problem and a Poisson problem with a singular source term to demonstrate the robustness of the OES method . The overall concept of our method is simple and easy to implement with off the shelf component software.

Our experimental results motivate further numerical analysis studies. There should be many interesting ways of expanding this method, and deriving rigorous constructions.

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Figures

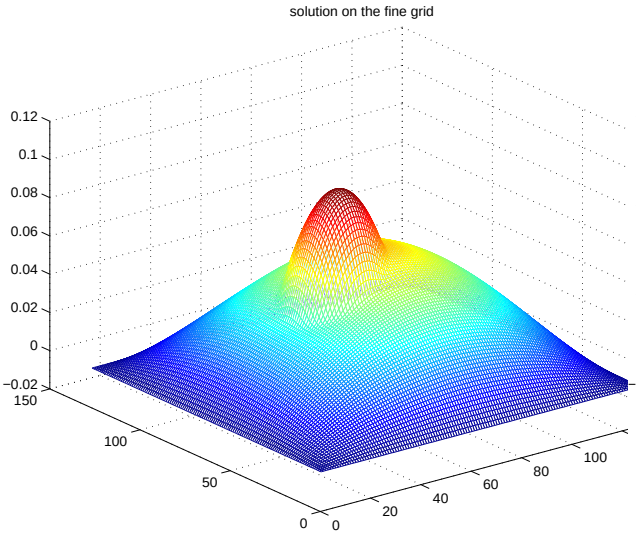

Fig. 1. Solution of T_2 with $\rho \approx 0.1$ in the disc D_1.

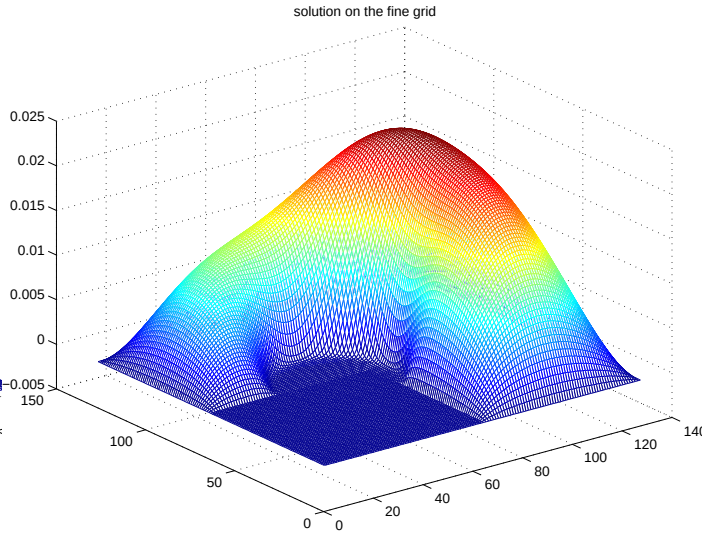

Fig. 2. Solution of T_6 with $\rho \approx 100$ in the disc D_1.

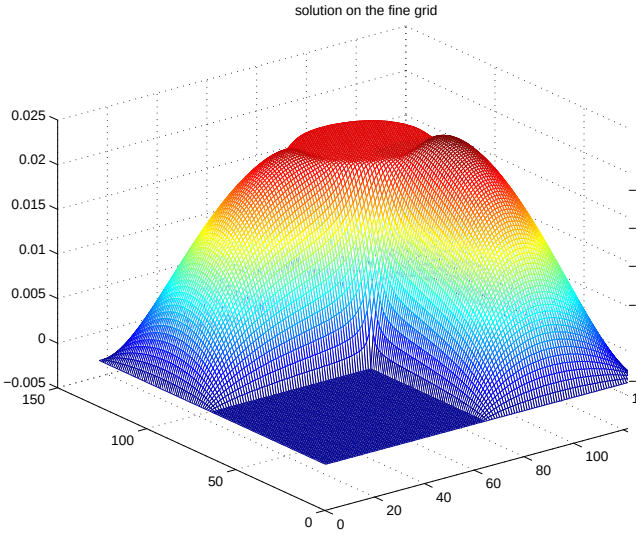

Fig. 3. Solution of T_7 with $\rho \approx 100$ in the disc D_2.

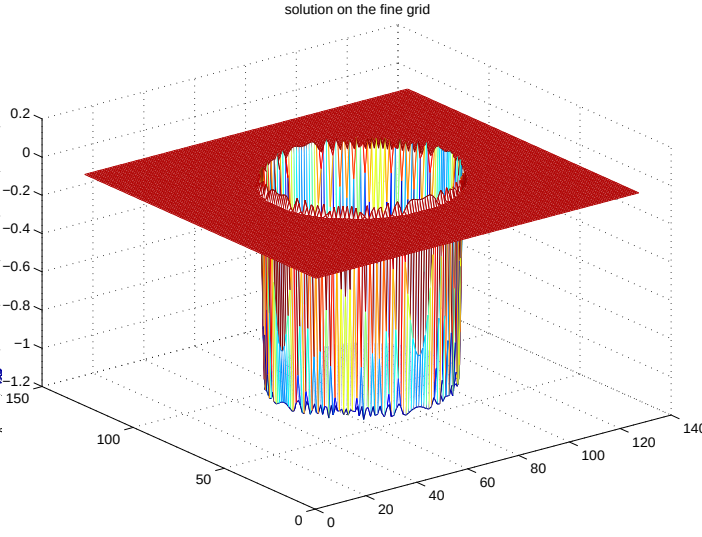

Fig. 4. Solution of the Poisson Problem with a circle of dipoles source terms.

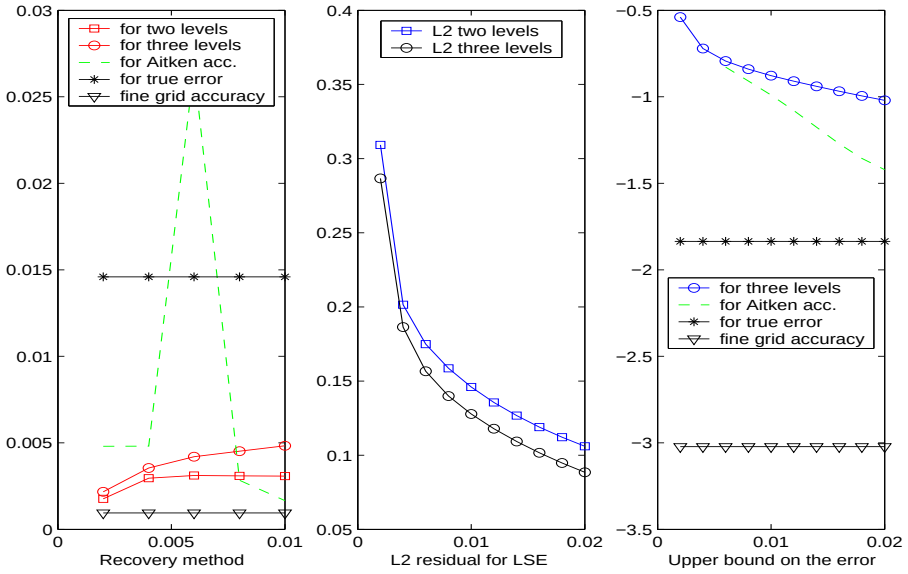

Fig. 5. Error estimates with T_3. $\tau = 0.01$.

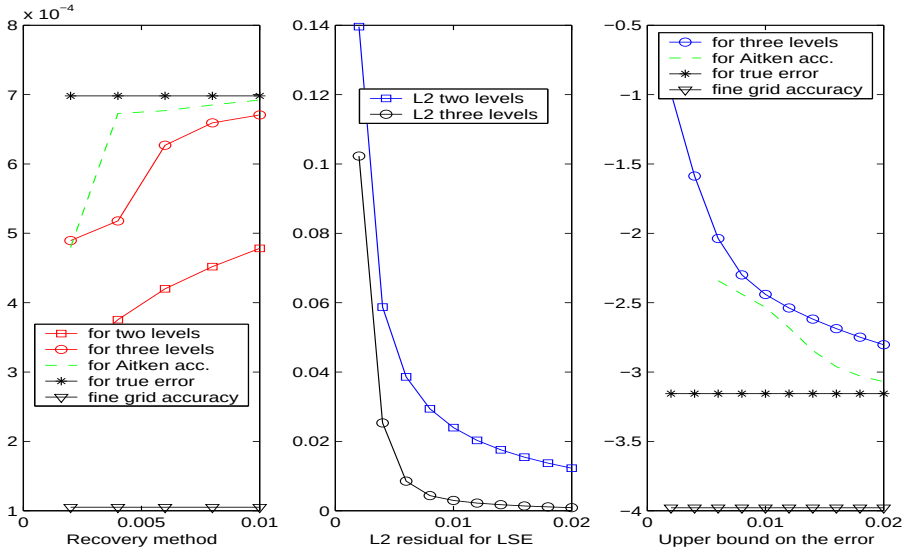

Fig. 6. Error estimates with T_6. $\tau = 100$.

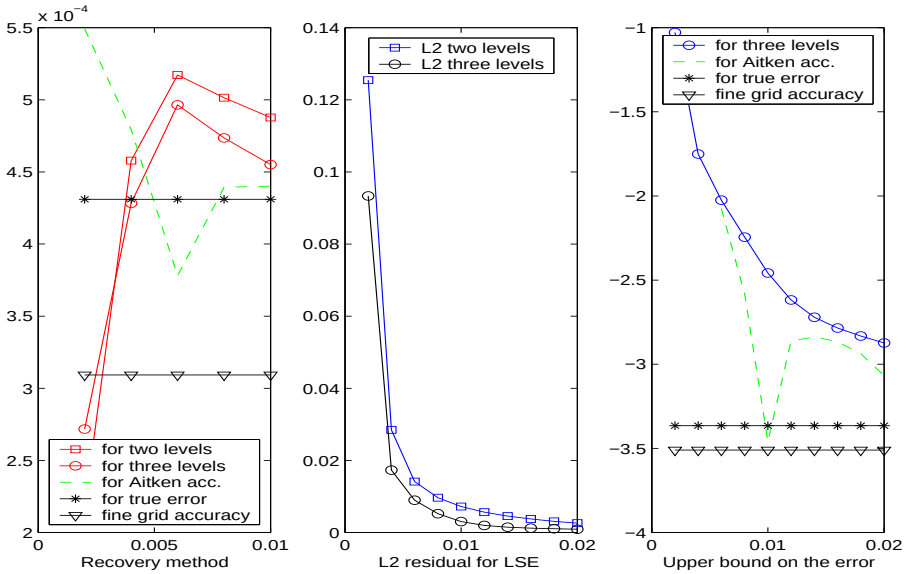

Fig. 7. Error estimates with T_7. $\tau = 100$.

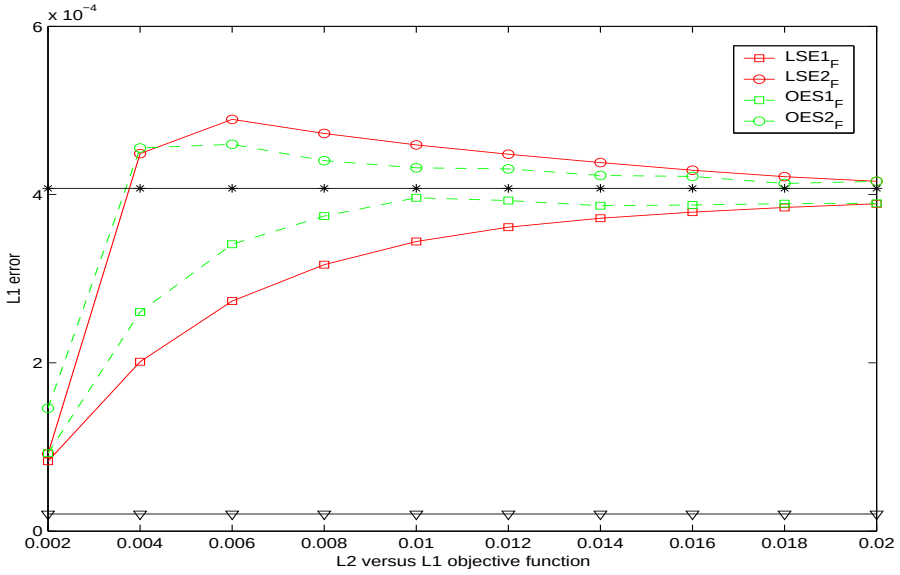

Fig. 8. Error estimates in L_1 norm with T_5, i.e $\tau = 100$, based on linear interpolation and the recovery method.

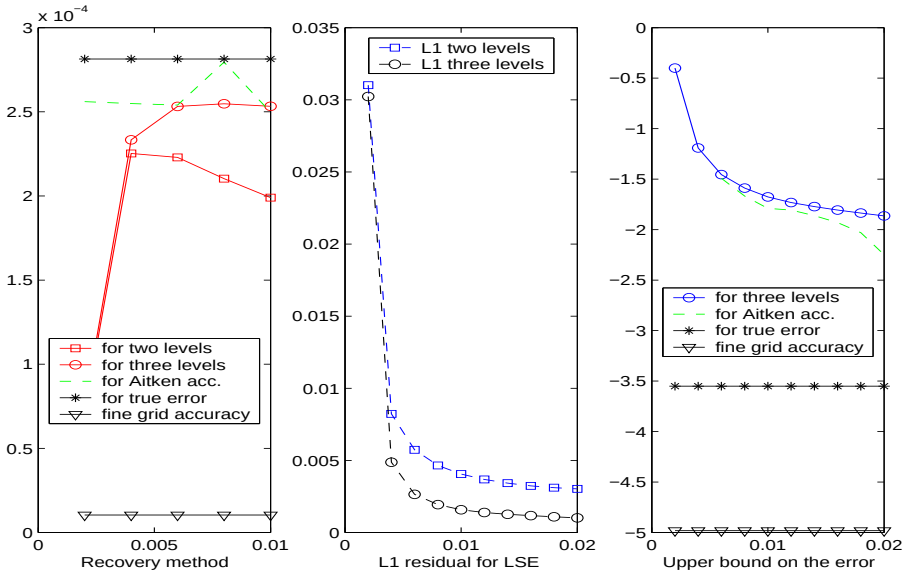

Fig. 9. Upper error bounds in L_1 norm with T_4, i.e $\tau = 10$, based on linear interpolation.

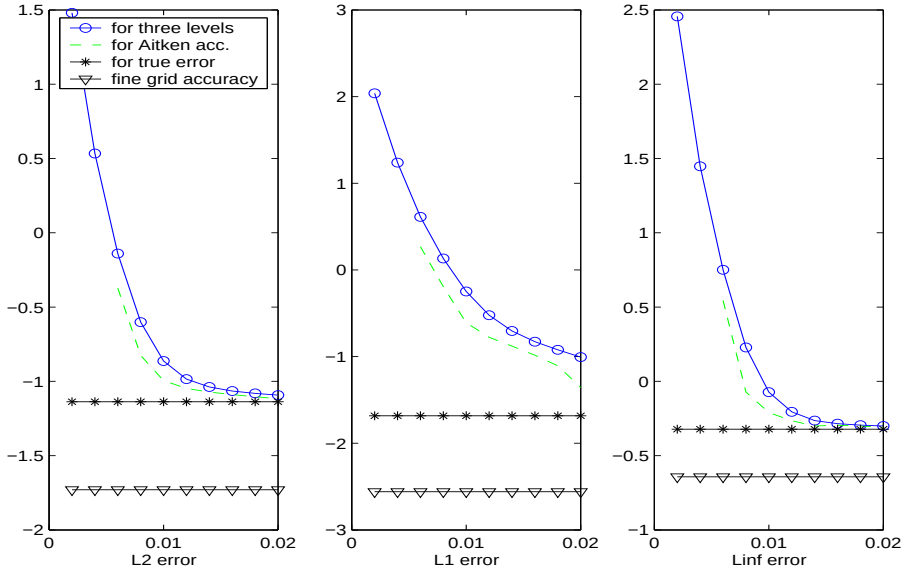

Fig. 10. Upper bound on the error with L_2, L_1, and L_∞ norm with T_8 based on linear interpolation.