Toward a General Solution Verification Method for Complex PDE problem with Hands off Coding

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The goal of this paper is to present a versatile framework for the solution verification of complex partial differential equation problems. Our goal is to produce an a posteriori error estimate *with no internal knowledge* of the simulation code that computes the solution. Our method decomposes into an optimization procedure that reconstruct the best consistent solution from two or three coarse grid solutions and a perturbation technique that estimates the conditioning number of the problem. Because this procedure is cumbersome and may involve hundred of uncoupled small computations, we use distributed computing to compute the a posteriori error bound.

I. Introduction and Motivation

This paper addresses the challenge of solution verification and accuracy assessment for computing complex Partial Differential Equation (PDE) model. Our main target applications are bio-heat transfer and blood flow simulation problems. However our long term goal is to provide a postprocessing package that can be attached to any existing numerical simulation package, for example widely used commercial codes such as ADINA, Ansys, Fluent, Star-CD etc... and provide an a posteriori error estimate to their simulation. Important design decision are based on simulation done with these softwares. Unfortunately we know that to verify a numerical solution and provide a quantitative assessment on the numerical accuracy of the solution is extremely difficult.

The problem of accuracy assessment is a necessary step that comes after the code verification step and before the code validation step to complete the global task of providing a reliable virtual experiment tool.[51, 52]

Our major goal in this paper is to pursue our work on the design of a new method that offer a general framework to do solution verification efficiently. The standard approach in applied mathematics to handle the problem of solution verification is to work on the approximation theory of the PDE. For each specific PDE problem, the right Finite Element (FE) approximation may provide the correct a posteriori error estimate. Unfortunately this approach may require a complete rewriting of an existing CFD code based on Finite Volume (FV) for example and lack generality. While a posteriori estimates in FE can be rigorous and has provided a number of interesting numerical analysis theory, its practical value is often questioned by practitioners. Usually such a posteriori estimators fails if the PDE solution is stiff or if the grid resolution is not adequate. Since grid refinement itself is based on a posteriori estimator, this pose an obvious problem. Large Reynolds number flow are common in many applications, not to mention turbulence problems. For those applications solution verification may not be achievable by the current state of the art of numerical analysis. If the PDE problem gets complicated, for example in the presence of fluid-structure interaction, or other complex multi-physic coupling, one faces the same problem. The general practice in scientific computing is to simulate PDEs for which applied mathematics neither numerical analysis guaranty the result. There is no completed analytical work on the 3D Navier Stokes equation that is a century old! But this model is used every day in fluid flow simulation to design air plane, cars, etc... Because of this time lag between the development of rigorous mathematical tools and the common scientific computing practice, our goal is to improve existing SV tools such as the convergence index of Roache et Al, and the Richardson Extrapolation (RE) technique, that are used daily by practitioner, by something more elaborate and reliable that can take both advantage of existing a posteriori estimators when they are available, and new distributed computing tools since SV is computer intensive.

Our method relies on four main ideas that are (1) the embedding of the problem of error estimation

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into an optimum design framework that can extract the best information from a set of two or three existing numerical results, (2) solving the problem as much as possible as a (non)linear set of discrete equations to produce a general tool, and renounce on using the specific approximation theory used to compute the PDE solution. (3) provide a framework that can reuse any a posteriori estimator if they are available (4) take advantage of distributed computing (or grid computing) to get a cost effective SV.

While it is impossible to review the work done in the theory of a posteriori estimators in few pages, we will give a brief description of this work in the next section.

II.   Background and Context

From the applied mathematics point of view, a posteriori estimates have been studied for many years.[5, 11, 12, 58, 61] There is a vast literature on on this subject. Most of this work has been done in the framework of finite element analysis, but there are some works on finite volume as well as finite differences available.[13, 49] Most of the theory is provided in a rigorous framework for linear operators, mostly linear elliptic operators, and more recently, unsteady problems with diffusion convection. A posteriori estimates are mainly used to drive adaptive mesh refinement and there is, however, still a lack of a reliable error indicators for Euler and Navier Stokes calculations that gives estimates on given meshes. This is especially apparent when the grid resolution is inadequate. Grid refinement in these studies are, in fact, supposed to increase the reliability of the a posteriori estimate computation. As a matter of fact, we recall that straightforward local refinement of grids based on the dominant flow features such as shock waves, slip lines or stagnation points, by using indicators based on large gradients, may even lead to incorrect results.[62]

A standard and well known procedure to establish a posteriori estimates is to solve local residual problems. The so-called "equilibrated residual method" is one of the most reliable and accurate techniques.[2–6, 42] However, theory for this method has been essentially limited to linear PDEs. Examples of the application in the literature include the Poisson problem, linear singular perturbation problem with simple boundary layers, the Stokes and Oseen equation and linear elasticity theory. This family of techniques, that has the advantage of being mathematically rigorous in the finite element framework, can be generalized, up to a certain point and on a case per case basis, to non-linear elliptic problems or hyperbolic equations.[8–10, 17, 18, 20, 21, 23, 44, 55] But it may not apply a priori to finite volumes computation, when there is no equivalence theorem with finite element formulations. We also notice that the estimates given by the theory does not provide quantitative free bound on the error. In practice, the unknown constants in the error estimates obtained by this theory have naturally a bad asymptotic behavior for boundary layer problems as the disparity of scales increases unless one refines the grid. Although, the method has to be significantly modified depending on the existence of additional length scales, such as boundary layers or not,[3] or to take into account the influence of the error in discretization of non-homogeneous boundary conditions.[6]

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 Patera et al[53 54 56 57].[45] Furthermore, this new theory focuses on the fact that one is not necessarily interested in the solution u, but rather in a linear (local) functional output $Q(u)$ or a stress $\sigma(u)$. A posteriori Finite-Element free constant output bounds can be constructed for the Incompressible Navier Stokes equation. The procedure to construct the a posteriori estimate on a given triangular mesh of step 'H', uses as a reference solution a fine grid solution 'h'. The efficiency of this method is demonstrated in the construction of upper and lower bounds of linear-functional outputs of the PDE solution. Examples considered in[45, 46, 53, 57] are the Helmholtz problem and the viscous Burgers equation in one space dimension, 1st order linear convection in two dimensional spaces, and Navier Stokes equation written in Boussinesq approximations in a highly convective flow regime.

The procedure uses the concept of duality, in which an equivalent dual adjoint formulation of the primal is exploited. The error in the functional can then be related to the local residual errors of the primal solution through the adjoint variable. This method is promising and technically impressive. Its implementation seems, at first sight, complex, and is restricted to the finite element framework with appropriate so-called "broken space" to relate the coarse mesh space with the fine mesh approximation. The results on the bounds hold for $H \to h$ but for all $H < H^*$ where H^* is generally an unknown threshold discretization parameter.[45] A traditional drawback is the fact that the coarse mesh solution H may not be good enough to provide useful information, and that is why the method does use refinement to build confidence in the output results. Therefore, a large Reynolds number is an issue in such a computation. Furthermore, a reliable error estimate on the fine grid solution of step 'h' does not necessarily lead on a reliable error estimate for the

true solution, unless one has external knowledge to guess what will be a good, fine grid solution. Let us noticed that[59] and[60] present a practical solution to the error estimate of functional outputs that is used to drive grid refinement on complex CFD problems. It is also an adjoint-based error correction procedure that is very close to the engineering point of view.

It seems that there is a lot of new activity on a posteriori estimates based on residual methods for the problem and/or its adjoint in the variational theory framework, but recovery methods that rely on building a better solution to derive an a posteriori estimate are still very much in use in the engineering world. Among these methods are the Richardson extrapolation technique[56] and the so-called ZZ[64][65] Super Convergence Patch Recovery Method. These methods are applicable to linear as well as nonlinear problems[14][15].[16] As explained in[5] Sect 4.7 p82, this technique may require that the grid resolves the smallest scale.

A third stream of work strongly related to a posteriori estimates,[36–40, 43] concern real complex phenomena that are nonlinear, stochastic and multiscale with no clear cut between the different scaling. Problems with turbulent flows, flow in porous media, or weather prediction are classical examples. The stochastic method of Glimm et al. for the prediction of complex phenomena divides them into two components. One is the forward problem, starting from the governing equation and initial data; the other is the inverse problem to minimize the uncertainties in the model from given observations of the system. The main thrust of the method is to predict functional output of the solution with coarse grid solution only based on a probability error model that includes numerical errors in the computation, error in the observation or experiments used to calibrate the model, and error in the data used in the model. Randomness occurs at several levels such as the specification of the model or the solution process itself. The solution process and the model must support a probabilistic framework; that is why stochastic PDEs is a natural application field.[43] gives a detailed description of the method applied to scale up flow in porous media. To focus on the role of this method for a posteriori estimate of the numerical error in direct computation of PDEs, the assumption is that the numerical error can be divided into two components: first, a highly variable component with sensitive dependence on data, and second, a systematic component with smooth but also unknown dependence on the data. Both components are present in the random process which models the error. Sensitive dependence of the error on the data must be subsumed within the randomness of the error process. Further, the output functional that is the objective to be predicted must not be sensitive to the global error. The error estimate depends on the specific choice of the error statistic model. It seems that this approach is very useful when uncertainties in the model are dominant versus the numerical error, and when a fine grid solution is never accessible. It is also interesting to notice that in complex numerical methods as PDF/Monte Carlo Methods for turbulent flows,[63] the construction of the model for numerical accuracy is a difficult task. It is also remarkable, that once it is done, one may minimize the main component of the error that is random via time-averaging. Then Richardson extrapolation can provide a significant improvement on the accuracy of the solution.[63] Nevertheless, the theory developed by J.Glimm and co-workers is a giant step toward the understanding of the effect of combined observation errors, model error, and numerical simulation error in effective prediction.

All the works described above are extremely important contributions to the understanding of a posteriori estimates for PDEs. There are advantages and disadvantages for each of the theories described above. Method of choice depends very much on the complexity of the application and the amount of CPU time that is available. The main challenge is still **to estimate numerical accuracy on under-resolved grids**.[52] As a matter of fact, in complex modeling, as described in the ASCI project, best grid solutions provided by our best computing resources are fairly under-resolved at least locally[41].[19] A posteriori estimates should now be redesigned to provide solution verification assessment in this context[1].[7]

Furthermore there are still some basic physical mechanisms on propagation of the error that must be reintroduced in the analysis of the error such as, following[54] (1) diffusion terms cause slow isotropic error decay, but global error pollution may occur from local irregularities, (2) advection terms propagate local errors in the transport direction, but errors decay exponentially in the cross wind direction, and (3) reaction terms cause isotropic exponential error decay, but stiff behavior may occur in the coupling error components. These ideas have been used extensively to build efficient, parallel iterative domain decomposition solvers that optimize fast decay of numerical error introduced at artificial interfaces- for example see[24, 26, 28, 29] and its references. Therefore, it might be useful to keep track of specific error propagation even if for models in which (1) to (3) are present, it is impossible to account for all error interactions by analytical means. Finally, there are still possibilities of catastrophic failures of a posteriori estimates in case of meta-stabilities or bifurcations[22, 25, 27] . A good method for complex modeling should therefore provide numerical indicators

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of ill-conditioning problems and potential catastrophic errors.

We present in this paper an entirely different framework to construct reliable a posteriori estimates for *general* PDEs or system of PDEs.

III.   Method

Let us first describe the general concept of our method.[30–33]

A.   General Concept

We consider a boundary value problem (Ω is a polygonal domain and $n = 2$ or 3) :

$$N[u(x)] = f(x),\ x \in \Omega \subset \mathrm{I\!R}^n,\ u = g \text{ on } \partial\Omega. \tag{1}$$

We assume that the PDE problem is well posed and has a unique smooth solution. We consider a finite volume approximation of (1) on a family of meshes $M(h)$ parametrized by $h > 0$ a small parameter. The smaller h the finer should be the discretization. We denote symbolically the corresponding family of linear systems

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

Let p_h denotes the projection of the continuous solution u onto the mesh $M(h)$. We assume a priori that ($||.||$ is a given discrete norm):

$$||U_h - p_h(u)||\ \rightarrow\ 0,\ \text{as } h\ \rightarrow\ 0, \tag{3}$$

Let $M(h_1)$ and $M(h_2)$ be two different meshes used to build two approximations U_1 and U_2 of the PDE problem (1). 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 an unknown space dependent function solution of the following optimization problem, where G is an objective function to be defined:

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

The Optimized Extrapolated Solution (OES) if it exists, is denoted $V_e = \alpha U_1 + (1-\alpha)U_2$. 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 might be derived from any existing a posteriori error estimators if possible. For a number of fluid dynamic methods used in bioengineering such as the immersed boundary technique, or the chimera technique there is no solid theoretical framework that can provides such rigorous a posteriori estimators. For complex bioengineering problems, the fact that there exist a functional space framework to derive a posteriori estimate is more the exception than the generality. Our ambition is to provide a numerical estimate on $||U_j - U_\infty||$, $j = 1, 2$, without computing U_∞ indeed. The solution U_j can be verified then assuming (3). The fine mesh $M(h_\infty)$ should be set such that it captures all the scales of the continuous solution with the level of accuracy required by the application. We have a priori $h_\infty\ <<\ h_1,\ h_2$. Both coarse grid solutions U_1 and U_2 must be projected onto $M(h_\infty)$. We will denote $\tilde{U}_1$ and $\tilde{U}_2$ the corresponding functions. We choose then to minimize the consistency error for the numerical approximation of (1) on a fine mesh $M(h_\infty)$. The objective function is then

$$G(U^\alpha) = ||N_{h_\infty}\,U^\alpha - F_{h_\infty}||,\ \text{where } U^\alpha = \alpha\,\tilde{U}_1\ +\ (1 - \alpha)\,\tilde{U}_2. \tag{4}$$

The choice of the discrete norm should depend on the property of the solution. In the Least Square Extrapolation (LSE) method[30, 31] we chose the discrete L_2 norm. The choice of the L_1 or the L_∞ norm have been tested for stiff elliptic problems.[32]

One of the difficulties encountered with a two-level extrapolation method is that there exists subsets of $M(h_\infty)$ where $\tilde{U}_1$ and $\tilde{U}_2$ 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

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

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 an optimum solution 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.

Let us denote U_j to be one of the coarse grid approximations at our disposal. A global a posteriori estimate of the error $||U_j - p_h(u)||$ may come in two different ways. For the sake of simplicity we will assume that G is the L_2 norm of the residual (4) and N is a linear operator; let us denot A_h its matrix.

• 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 $M(\infty)$ 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,

$$||V_e - p_h(u)||_2 << ||\tilde{U}_j - p_h(u)||_2. \tag{5}$$

Then $||\tilde{U}_j - V_e||_2 \sim ||\tilde{U}_j - p_h(u)||_2$ and $||V_e - \tilde{U}_2||$ is a good error indicator to assess the accuracy on U_2. We have seen in our numerical experiments with steady incompressible Navier Stokes (NS) solutions that this method may give a good *lower* bound error estimate. But we do not know in general if the hypothesis (5) is correct. There is no guarantee that a smaller residual for V_e than for U_2 on the fine grid $M(h_\infty)$ leads to a smaller error.

• Second is a global *upper* bound that follows from a stability estimate with the discrete operator. We have

$$||V_e - U^0|| < \mu\, G(V_e), \text{ where } \mu \geq ||(A_{h_\infty})^{-1}||$$

We conclude then

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

The procedure to derive an estimate for μ uses a combination of standard eigenvalue computation procedures applied to A_{h_j}, $j = 1..3$ and some extrapolation technique designed for scalar functions. (6) is a good global a posteriori error estimator provided that

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

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 $M(h_\infty)$. This is a feasible test because the fine grid solution is never computed in OES. Our verification procedure checks that $||U^0 - U_2||_2$ increases toward an asymptotic limit as $M(h_\infty)$ gets finer.

The algorithm procedure to construct V_e solution of P_α or $P_{\alpha,\beta}$ is straightforward when the operator is linear and the objective function is the discrete L_2 norm of the residual. Let e_i, $i = 1..m$ be a set of basis function of $\Lambda(\Omega)$. The solution process can be decomposed into three steps.

• First, interpolation of the coarse grid solution from $M(h_j)$, $j = 1..p$ to $M(h_\infty)$, with $p = 2$ for the two level method, respectively 3 for the three level method.

• Second, evaluate the residual $R[e_i\ (\tilde{U}_j - \tilde{U}_{j+1})]$, $i = 1..m$, $j = 1..p - 1$, and $R[\tilde{U}_p]$ on the fine grid $M(h_\infty)$.

• Third, the solution of the least square linear algebra problem that has m unknowns for each weight coefficient α and β used in the extrapolation procedure. In practice, m is much lower than the number of grid points on any coarse grid used.

We have generalized the LSE method to non-linear elliptic problems via a Newton like loop.[30,31] We have also obtained preliminary results for unsteady parabolic problems.[33] Most of this work has been done on solutions produced by our own code on a fairly large variety of linear and nonlinear PDE problems on structured grids. To apply these techniques on solution produced by commercial code that have thousands of lines, and work with unstructured grids requires a more general and abstract approach, that we present in the next section.

B.   Solution Verification of off the shelf CFD code

We propose to generalize our method to time independent, i.e steady, CFD solutions produced by existing code. The challenge is that in most commercial codes, one cannot rely on the exact knowledge of the discretization method, neither have access to information on the internal structure of the code. What we propose is fundamentally different than existing methods. We describe in the following the main ideas without seeking an exact formal mathematical description of a given specific PDE problem.

Let $(E, ||.||_E)$ and $(F, ||.||_F)$ be two normed linear space, $\mathcal{C} : E \to F$ be the operator corresponding to the CFD problem. Further let us denote $S \in F$ the input data of the CFD code and $U \in E$ the solution we are looking for.

In practice we look for an approximation of the accuracy of the solution U_h on the mesh $M(h)$ produced by the code $\mathcal{C}$ that operates on the data S_h: $\mathcal{C} : S_h \to U_h$. The objective is still to get an error estimate versus a very fine grid solution U_∞ that is never computed, because the cost is prohibitive. We will skip the index h when it is not essential. The space E, F have (very large) finite dimensions indeed since they are for the discrete solutions on $M(h_\infty)$, and discrete data S_{h_∞}.

We assume that the code $\mathcal{C}$ has a procedure that provides the residual, i.e $V \to \rho = N(U_h) - N(V)$, where $V \in E$, $\rho \in F$. We note that this hypothesis is realistic, since most of the commercial code offer this feature or either provides a (first order explicit) time stepping procedure:

$$\frac{U_h^{n+1} - U_h^n}{dt} = N(U_h^n) - S, \tag{8}$$

The residual is then $\rho = \frac{U_h^1 - U_h}{dt}$. We assume that the following problem

$$N(u) = s, \ \forall s \in B(S, d).$$

is well posed for $s \in B(S, d)$, where B is a ball of center S and diameter d in $(F, ||.||_F)$. There should exist a unique solution for all data in $B(S, d)$ and the dependency of the solution on these data is supposed to be smooth enough to use a second order Taylor expansion.

Let us suppose that $N(U_h) \in B(S, d)$, that is

$$||\rho||_F = ||N(U_h) - S||_F < d. \tag{9}$$

We would like to get an error estimate on $e = U_h - U_\infty = \mathcal{C}(U_h) - \mathcal{C}(U_\infty)$. A Taylor expansion writes

$$\mathcal{C}(S) = \mathcal{C}(S + \rho) - (\rho \cdot \nabla_s)\mathcal{C}(S + \rho) + \frac{1}{2}\rho \cdot [\rho \cdot R(S)] \tag{10}$$

$$\text{where } ||R(S)||_E \leq K = \sup_{s \in B(S,d)} ||\nabla_s^2 \mathcal{C}(s)||_E. \tag{11}$$

Therefore

$$||e||_E \leq ||\rho||_F \ (||\nabla_s \mathcal{C}(S + \rho)||_E + \frac{K}{2}||\rho||_F). \tag{12}$$

This completely general error estimate point out to two different tasks:
• Task 1: get an accurate upper bound on $||\nabla_S \mathcal{C}(S + \rho)||$
• Task 2: obtain a solution $U_\infty + e$ that gives a residual $||\rho||$ small enough to make the estimate useful, i.e compatible with (9).
Task 2 is the purpose of the OES method, while Task 1 can be achieve by a perturbation method that can reuse the code.

C.   Task 1: Stability Estimate

Let $\{b_i^E, \ i = 1 \dots n\}$, (resp. $\{b_i^F, \ i = 1 \dots n\}$) be a basis of E_h, (resp. F_h) and $\varepsilon \in I\!R$ such that $\varepsilon = o(1)$. Let $(V_i^\mp)_{i=1..n}$, be the family of solutions of the following problems: $N(U_h \mp \varepsilon V_i) = S + \rho \mp \varepsilon b_i$. We get from finite differences the approximation

$$C_{h_\infty} = ||\nabla_S \mathcal{C}(S + \rho)|| \approx ||(\frac{1}{2}(V_j^+ - V_j^-))_{j=1\dots n}|| + O(\varepsilon^2).$$

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We can get in a similar manner an approximation of the norm of the Hessian $\nabla_s^2 \mathcal{C}(S + \rho)$. For ρ small enough, we can verify that the upper bound is given essentially by:

$$||e||_E \ \preceq \ C_{h_\infty}||\rho||_F. \tag{13}$$

The column vectors $V_j^\mp$ can be computed with embarrassing parallelism. It is however unrealistic to compute these solutions that lies on the fine grid $M(h_\infty)$.

To make this task manageable, we have to reduce the dimension of the problem. We use the following two observations. While the solution of the CFD problem can be very much grid dependent, the conditioning number of the problem is in general much less sensitive to the grid. The idea is then to compute an approximation of C_{h_∞} by extrapolation from an estimate of two or three coarse grid computation of C_{h_j}. Further, let us assume that the fine grid $M(h_\infty)$ is a regular Cartesian grid. The number of terms to represent accurately the projected solution $\tilde{U}_j$, $j = 1 \ldots 3$ with a spectral expansion or a wavelet approximation at a given accuracy is much less than the dimension of the coarse grid used in a Finite Element/Finite Volume computation. We propose to use preferably a grid M_{h_∞} that has enough regularity to allow a representation of the solution U_∞ with some form of reduced representation, using either trigonometric expansion or wavelets.

The grid M_{h_∞} may have many more grid points than necessary, and therefore might not be computationally efficient for a true fine grid computation. But we do not have to do this computation anyway.

Further, regular grids are far more easy to construct. If for some reasons M_{h_∞} has to be unstructured, we can also use spectral elements.

Let us denote $\hat{E}$ and $\hat{F}$ the spaces corresponding to one of these reduced representation of the solution and residual. Let $(\hat{b}_j^{E/F}, j = 1 \ldots \hat{n})$, be the corresponding base with $\hat{n} << n$. Let $q_{E/F}$ be a mapping $E/F \rightarrow \hat{E}/\hat{F}$, respectively $q_{\hat{E}/\hat{F}}$ be a mapping $\hat{E}/\hat{F} \rightarrow E/F$ and let $\hat{C} : \hat{S}_h \rightarrow \hat{U}_h$ be the code that uses this postprocessing of the residual and solution. To summarize the procedure for Task 1, The estimate on C_{h_∞} will be applied to verify the code $\hat{C}$ based on the computation of $(\hat{V}_j^\mp, j = 1 \ldots \hat{n})$ vectors on the coarse grids $M(h_j)$, $j = 1 \ldots 3$ done by the code $\hat{C}$. We notice that the computation of the vector $\hat{V}_j^\mp$ can be done with embarrassing parallelism. Further because ε is small the code $\hat{C}$ can use as an initial guess in its iterative process the solution U_h that is hopefully very close to the unknown $\hat{U}_h \pm \hat{V}_j^\mp$.

There are several issues that needs to be carefully investigated in the future development of this method. Let us mention two of them. First our method relies on the fact that the spectral properties of the operator follows some fairly regular asymptotic properties for the coarse meshes under consideration as $h \rightarrow 0$. This hypothesis should be verified. Second ε should be chosen adaptively and carefully as a function of the mesh size, in order to avoid a dramatic inaccuracy on the stability estimate of C_{h_∞}. Since we are only looking for an order of magnitude of C_{h_∞} and not its true value, we feel confident in our approach.

Let us discuss our second task that is to compute a solution on the fine grid that is good enough to recover an error estimate.

D. Task 2: Optimized Extrapolation

We use here an optimized extrapolation method. To reduce the dimension of this problem we search for the unknown weight functions in a small space that can be described either by trigonometric expansion, or wavelet expansion, or possibly spectral elements. If Ω is the physical domain for the CFD solution, the unknown weight function can be search in a square domain $(0, 1)^2$ modulo a change of variables. As a matter of fact no boundary conditions are required on the unknown weight functions. Let $\{\theta_j, \ j = 1..m\}$ be the set of basis function of $\Lambda(\Omega)$.

We look for the solution of the optimization problem in the two level case

$$\text{Find } (\alpha_j) \in I\!\!R^m, \text{such that } ||G([\sum_{j=1..m} \alpha_j \Theta_j]\tilde{U}_1 + [1 - \sum_{j=1..m} \alpha_j \Theta_j]\tilde{U}_2)||_F \text{ is minimum.} \tag{14}$$

We have a similar formulation for the three level OES. Following the same argument than before we will rather look for this minimum in $\hat{F}$. As shown in,[30, 31] we need a filtering process of the solution to have this minimization process numerically efficient. The postprocessing q_F is then useful. We can obtain easily the result when the weight function is a scalar function. To make this computation robust we use a surface response methodology[50] that is rather trivial in the scalar case. This procedure consist to compute a lower order polynomial best fit of the function $||G(\alpha\tilde{U}_1 + (1 - \alpha)\tilde{U}_2)||$ by sampling α according to the

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expected convergence order range of the code. The minimization on α is then done with this polynomial approximation by a standard method. The sampling process is a cumbersome embarrassing parallel process that can take advantage of a computational grid.[47]

It is however impractical when the dimension of the problem for the α search is more than few units. We are planning to use a combination of genetic algorithm and local optimization search to solve the nonlinear optimization problem (14). There is an extensive knowledge and set of available optimization softwares[48] that we can reuse indeed. The main difficulty in this process is to solve the nonlinear minimization problem (14) using the proper method : if the solution provided by the CFD code is very coarse, the use of space dependent weight functions might not be required. Similarly, if the solution is very accurate and the code has uniform convergence, we do not need either space dependent weight function. But, in the case of stiff problem we would like to get some adaptivity on the construction of the weight function. This is a fairly open problem.

Let us describe now the design of the software that we are developing as a solution verification system independent of the CFD code.

IV. Software and Numerical Examples

Let us present first the algorithm.

A. Algorithm

The algorithm of our method writes in its simplest version

1. *Call coarse Mesh* : generate the (coarse) meshes $M(h_1)$ and $M(h_2)$. If h_i is the average space step for the grid $M(h_i)$ we should have $h_2 < h_1$ but this is not necessary.

2. *Call fine Mesh* : generate a fine mesh $M(h_\infty)$ that is supposed to solve all the scales of the problem. $M(h_\infty)$ is preferably a structured mesh. We must have $h_\infty << h_1, h_2$.

3. *Call Solver* : solve the problem on $M(h_1)$ and $M(h_2)$, possibly in parallel.

4. *Call Projection* : project the coarse solutions U_1 and U_2 onto G_∞ and post-process them to avoid spurious oscillations due to the interpolant.

5. *Solve minimization problem* (14) : we can create for example sample solutions $U_\alpha = [\alpha \tilde{U}_1 + (1-\alpha)\tilde{U}_2]$ or use an off the shelf optimization package.

6. *Get Stability Constant*: compute in parallel an increasing set of perturbed solutions $U_h \pm \varepsilon V_i^{\pm}$ until convergence of the stability estimate.

We will use the standard discrete vector norm $|| \; ||_2$, to measure the numerical error on the trace of the numerical solution at those points. To be more specific

$$||(f_j)_{j=1..M}||_2 \; = \; \sqrt{\sum_j (f_j)^2}$$

This norm is unrelated to the FE space used in ADINA calculation. Our verification procedure follows the spirit of an experimental measurement where one can get information at pointwise values.

B. Application

To illustrate the pertinence of our methodology, let us present two examples that are (1) a Navier Stokes back step flow, (2) a heat transfer problem for a thermal battery. While our goal is to solve three dimensional problems, we present here preliminary results in two space dimensions. The computation is done with ADINA. The ADINA system is a comprehensive finite element software that enable analysis of structures, fluids simulations , and fluid flows simulations with structural interactions. It allows to solve a wide variety of problem including simulation of blood flow that are one of our main interest.[34, 35]
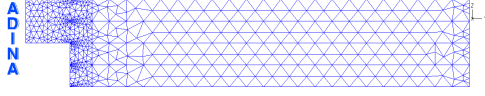
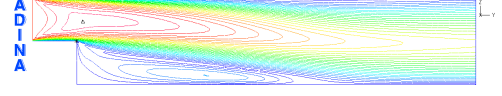**Figure 1.** Coarse unstructured mesh with Adina R&D.

Figure 2. Contour line of the amplitude of the velocity field.

Figure 1 shows an example of an unstructured mesh calculation of the back flow step problem at Reynolds number 500. In this simulation, the number of elements are respectively 10347 on the fine grid G^{∞}, 1260 on the coarse grid $M(h_1)$, and 2630 on the coarse grid $M(h_2)$.

The steady solutions are obtained using a transient scheme for the incompressible Navier-Stokes equation.
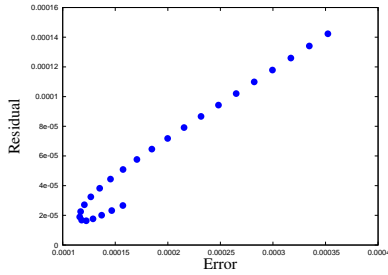
Figure 3. LSE: error and residual for Adina in L_2 norm.
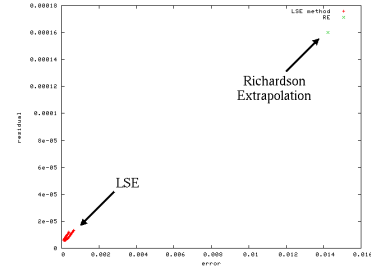
Figure 4. Performance of LSE and Richardson Extrapolation.

For this test case OES outperforms the accuracy of the RE method by one order of magnitude.

In figure 5, we look at the stability constant as the function of the size of the approximation space. In this example, the basis functions of the reduced space used to perturb the source term of the PDE are the sine functions. The x-axis of the figure give the total number of functions used to evaluate the stability coefficient. It is also the number of times the perturbed problem is solved. We observed that the stability constant reach a threshold when the size of the approximation space increase. It is therefore unnecessary to take a larger number of basis functions to evaluate the stability constant.

Figure 6 gives the error computed in the reduced space to the fine grid solution in L_2 norm. The error curve (red curve) use as reference is the error in L_2 norm given by the OES obtained previously. The error evaluated is directly correlated to the stability conditions shows on figure 5, as anticipated by (13). The fundamental result in this figure is that we are able to evaluate an upper bound on the numerical error of simulation within 10% of the 'true' error.
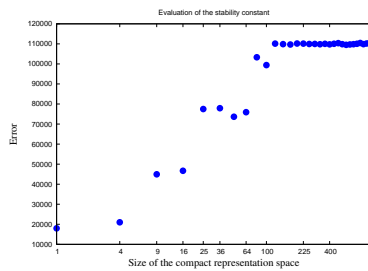

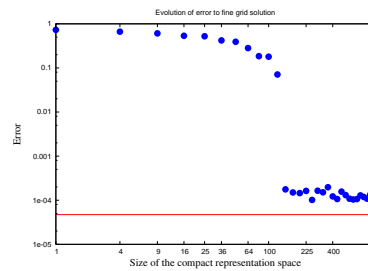**Figure 5.** Evaluation of the stabiltiy constant.

Figure 6. Evolution of the error.

The model, for our second example is governed by the energy equation:

$$\frac{\partial}{\partial x_i}\left(k_{ij}(T)\frac{\partial T}{\partial x_j}\right) + Q(T) = \rho c_p(T)\frac{\partial T}{\partial t} \text{ on } \Omega \times (0, t)$$

in a Cartesian reference frame with i, j running from 1 to 2 for this model. T is the temperature, t is time, ρ is the material density, c_p is the specific heat as a function of T, Q is the volumetric heat source as a function of t, and k_{ij} is the thermal conductivity tensor as a function of T.

The boundary conditions are *Neumann* conditions:

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- $-\left(k_{ij}\frac{\partial T}{\partial x_j}\right)\cdot n = h_1(T)(T - T_\infty) + \sigma\varepsilon_1\left(T^4 - T_\infty^4\right)$, on Γ_{N_1} (radiation, convection);

- $-\left(k_{ij}\frac{\partial T}{\partial x_j}\right)\cdot n = h_2(T)(T - T_\infty) + \sigma\varepsilon_2\left(T^4 - T_\infty^4\right)$, on Γ_{N_2} (radiation, convection);

- $-\left(k_{ij}\frac{\partial T}{\partial x_j}\right)\cdot n = h_3(T)(T - T_\infty)$, on Γ_{N_3} (convection),

where $T_\infty = 313.0K$, $\varepsilon_1 = \varepsilon_2 = 0.25$, $\sigma = 5.670\times 10^{-8}$ is the Stefan-Boltzmann constant ($W\cdot m^{-2}\cdot K^{-1}$), and $h_3 = 1.0$ ($W \cdot m^{-2} \cdot K^{-1}$). The functions $h_1(T)$, $h_2(T)$, and c_p are given by tables.

The temperature is initialized to $T_0 = 313.0K$ in the structure. The difficulty of this study is due to the fact that the structure is compounded of different materials, for which coefficients might depend on space and temperature, and finally, two regions will undergo a phase change. The problem is therefore very stiff and the solution is almost discontinuous near the wall.

To simulate the heat transfer in this structure, we have used quad elements in each subdomain. The number of elements in the grids $M(h_j)$, $j = 1..2$, are respectively 8767 and 21072. To validate our result we compute a fine grid solution and use 57258 elements for $M(h_\infty)$. All meshes here are unstructured and present large aspect ratio. The fine grid computation is 10 times more expensive than the two coarse grid solution process. This fine grid computation becomes intractable in 3D unless one use a large parallel system. In this case also we have shown that OES out performs LSE. We have been able to get a robust upper bound on the error following the strategy described in Section C that is reliable even with relatively coarse grids $M(h_i)$, $i = 1, 2$.

Figures 7 and 8 gives respectively the stability constant as the function of the size of the approximation space and the error computed in the reduced space to the fine grid solution in L_2 norm. Once again this result shows that the evaluation an upper bound on the numerical error of simulation can be done within 10% of the 'true' error. Using this method, we are able to estimate a solution with a absolute error of 0.2 Kelvin, using coarse grid solutions with absolute errors of 10 Kelvin.

The interesting point in those two results is that the same framework is used for two different set of PDEs and lead to similar results.

Moreover, this evaluation can be done efficiently since the estimations are done on an approximate space of dimension 400, to compare to the size of the fine grid (57258 elements). Each computation involving an element of the basis of the approximation space was done in an average time of 2 minutes, leading to a cost of 20 hours for the error estimate. The fine grid computation is also taking on its own 20 hours. Each element of the approximate space can be computed independently of the others, so the estimation algorithm can be fully parallelized. But we can speed up dramatically the error estimate with distributed computing.[47] We will recall the design of this parallel implementation in the next section.
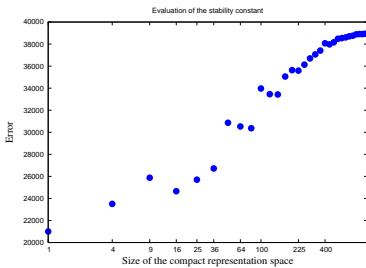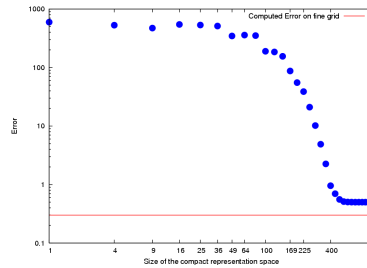

Figure 7.   Evaluation of the stabiltiy constant.

Figure 8.   Evolution of the error.

C.   Scientific Software Design

Step 5 and Step 6 of our algorithm give rise to a large set of cumbersome computations that can be done in parallel with a minimum of synchronization. This is a key feature to make our solution verification cost effective.

We are developing a network oriented interface that allow our solution verification method to be executed remotely on several processing units. We follow the following principle:

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- (i) a three-tier client server model architecture: it allows the system to be transparent, the user should not have to worry about technical details, to be open, each subsystem is open to interaction with the others, and to be scalable, the system should be easy to modify as the number of resources, users, softwares evolved.

- (ii) portability : to be able to run on UNIX/Linux/Windows platform -see Figure 10

- (iii) security in data transfer, because industrial applications as well as computation on clinical data require that the data be protected.

- (iv) friendly user interface.

The slave platform are CFD code dependent. Indeed, in order to build an effective distributed verification tools, we have to ensure that the simulation code we wish to verify can be run on the targeted platforms. Many of the existing simulation softwares were developed only on some specific platform, and therefore limit the possible performances gained of a distributed computation.

The second issue that is encounter is the transfer of data between slaves and master. For large problem, we might have to transfer several megabytes of data using files between hundred of nodes, thus making the application sensitive to firewall and server configurations, temporary network failures, data corruption, or data stealing.
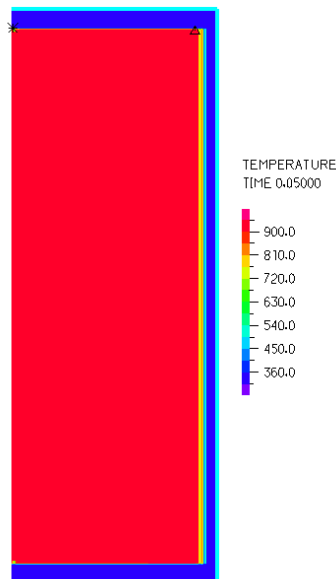
Figure 9.   Final Temperature in the Battery
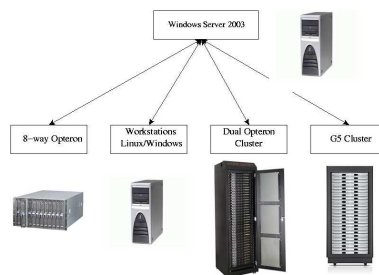
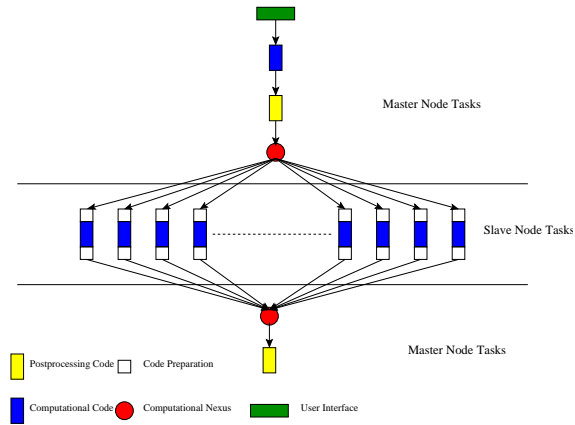**Figure 10.   Distributed Computing System**
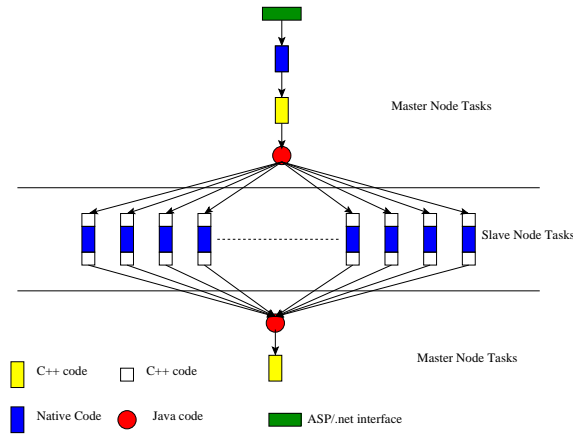
Figure 11.   Softwares

Figure 12.   Languages

Performance analysis of this software design,[47] will be reported in a companion paper. Let us now conclude this study.

V.   Conclusion

In this paper, we explore a new framework for extrapolation method for PDEs. This framework provides a better tool for solution verification than Richardson Extrapolation when the convergence order is space dependent or far from the asymptotic rate of convergence. It also enable an easy way to evaluate numerically the stability condition for complex and different in nature PDEs. The strength of the method is that no specific implementation knowledge or discretization details are necessary to be able to obtain an a posteriori error estimate. This a posteriori error estimate refer however to a very fine grid solution (never computed) but obtained with the same approximation framework. We do have to assume then that the code does converge, and we assume that the code itself has been verified with for example manufactured solutions.

The second key point is that the embarrassing parallelism that is intrinsic to our method can be exploited to improve dramatically the computational efficiency of our solution verification procedure.

The combination of this two aspects leads to a postprocessing method that is fairly versatile, general and friendly to the user.

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Acknowledgment:

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