A posteriori error estimator framework for PDEs

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Background

1. Master Applied Mathematics, Université de Bordeaux 1, June 2003
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Introduction
- Solution Verification
- A Posteriori error estimates
- Richardson Extrapolation
- Goals

OES for elliptic problems (Garbey, Shyy)
- Definitions
- Results

OES for parabolic equations (Picard, Garbey)
- Formulation
- Thermal Wave 1D
- Reactive Shock Layer

OES for general code (Garbey, Picard)
- General OES
- Algorithm/Result with No detail code knowledge
- Heat Transfer problem

Distributed computation (Picard, Garbey)

Conclusion
Impact of numerical simulation

Figure: 1999 : Storm system Lothar over Europe
Simulation is a bridge between theory and experiments
DOE report from D. Keyes.

How to make them reliable?

How reliable decision can be based on the outcome of a software expressing a mathematical model?

These issues raise the concept of Solution Validation and Verification.
A posteriori error estimator framework for PDEs

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Introduction

Solution Verification

Concept of solution verification

Definition

Quantitative evaluation of the numerical error of a given solution to the PDEs (ref. Oberkampf, Trucano)

- Estimate the accuracy of a given solution is the primary goal of solution verification
- It is often impossible to perform a complete and rigorous analysis for complex PDEs.
- The problem can be addressed by
  1. Explicit discretization robustness and convergence studies
  2. Formal error estimation procedures
  3. Inference from test problem suites and from previous experience
- Numerical error estimation is strongly dependent on the quality and completeness of code verification.
Concept of A posteriori error estimates

Definition

From word-net: **A posteriori**: involving reasoning from facts or particulars to general principals or from effects to causes.

Consequently, A Posteriori error estimates make use of

- A priori information
- Computational results from a previous numerical solution using the same numerical algorithm on the same PDE and initial and boundary data.
- Information extracted can be estimates or convergence characteristics.
Examples of A Posteriori estimates

- AIAA Guide for the Verification and Validation of Computational Fluid Dynamics Simulations.
- Finite Elements
  - ZZ recovery method - see Zienkiewicz et Al, and ref.
  - Equilibrated residual method for FE - see Ainsworth & Oden and ref.
  - A posteriori Finite-Element free constant output bounds - see Patera and ref.
- Extrapolation Based methods
  - Richardson Extrapolation (h-extrapolation)
  - Order Extrapolation (p-extrapolation)
- Stochastic method in the Bayesian framework - ref Glimm et Al.
It is a popular method in Computational Fluid Dynamics (CFD) because of its straightforward implementation that is code (and " PDE ") independent.

It uses a sequence of meshes with distinct refinement to estimate the spatial discretization error.

Can be extend to temporal discretization.

Can be apply to large variety of discretization method.
Overview of RE

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

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

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

- For known $p$, Richardson extrapolation formula,

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

- Provides improved convergence:

$$||v - v^i_r|| = o(h^p)$$
Potential pitfalls

- Are the (3D) meshes fine enough to satisfy the a priori convergence estimates that are only asymptotic relations in nature?
- What can be done, if the order of convergence of a PDE code is space dependent and eventually physical parameter’s dependent?
- Can we afford three grid levels with a coarse grid solution that has a satisfactory level of accuracy, to be used in RE?
- Can we use RE to provide a posteriori error estimates?
- Richardson’s method produces different estimates of error and uses different norms
**Problem**

A code that provides a set of discrete approximations of a (set of) PDE(s) for example Navier Stokes equations or Heat transfer equations.

- Provided that one can obtain the definition of the residual of the PDE approximation, the existence of a stability estimate on the approximation of the PDE’s problem and two grid solutions, **find automatically the order of convergence**
- Using two or three different grid solutions (not necessarily with uniformly increasing mesh resolution), **obtain a solution with improved accuracy**
- Derive reliable a posteriori error bounds from coarse grid approximation of complex PDE problems.
Solution Procedure

- Simple to implement and works with a code independent from the main code procedure.
- With arithmetic cost negligible compare to a direct computation of a very fine grid solution.
- A general tool that can be applied to variational, FV or FD formulations, with irregular meshes, non linearities etc...
- Able to enhance the numerical accuracy and efficiency of simulation with complex physical model and trust in the context of code verification.
- Able to increase the overall numerical efficiency of the solution procedure when combined to multilevel procedure.
Problem

- This concept was introduced by Garbey and Shyy in 2002.
- Boundary value problem ($\Omega$ is a polygonal domain and $n = 2$ or 3):

\[
L[u(x)] = f(x), \quad x \in \Omega \subset \mathbb{R}^n, \quad u = g \quad \text{on} \quad \partial \Omega.
\]

- Assume that the PDE problem is well posed and has a unique solution.
- We consider an approximation on a family of meshes $M(h)$ parametrized by $h > 0$ a small parameter.
- We denote symbolically the corresponding family of linear systems

\[
A_h U_h = F_h.
\]

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

\[
\|U_h - p_h(u)\| \to 0, \quad \text{as} \quad h \to 0,
\]
Optimized Extrapolation Technique

- Let $M(h_1)$ and $M(h_2)$ be two $\neq$ meshes used to build two approximations $U_1$ and $U_2$ of the PDE problem.
- A consistent linear extrapolation writes

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

where $\alpha$ is a weight function.
- In classical Richardson Extrapolation (RE) $\alpha$ is a constant.
- In our optimized extrapolation method $\alpha$ is a function solution of the following optimization problem:

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

- For computational efficiency, $\Lambda(\Omega)$ should be a finite vector space of very small dimension compared to the dimension of $A_h$. 
General Idea

- One can choose to work with a posteriori FE error estimates:
- **From now on, and to make our technique general, we will work with discrete value functions and discrete norms:** Why is it possible?
- Our ambition: a numerical estimate on $||U_j - U_\infty||, j = 1, 2$, without computing $U_\infty$.
- $M(h_\infty)$ should capture a priori all the scales needed.
- In practice $h_\infty << h_1, h_2$.
- The solution $U_j$ can be verified, assuming convergence of the approximation method, i.e $U_\infty \rightarrow u$, as $h_\infty \rightarrow 0$.
- Reuse extensive knowledge of Physics and Asymptotic Analysis.
- Reuse Stability Theory from Linear Algebra.
Practical Consequences

- Both coarse grid solutions $U_1$ and $U_2$ must be projected onto $M(h_\infty)$.
- The objective function is a discrete norm of the residual:
  \[ G(U^\alpha) = \| A_{h_\infty} U^\alpha - F_{h_\infty} \|, \text{ where } U^\alpha = \alpha \tilde{U}_1 + (1 - \alpha) \tilde{U}_2 \]

The Optimized Extrapolated Solution (OES) if it exists, is denoted $V_e = \alpha_e U_1 + (1 - \alpha_e) U_2$.

- The choice of the discrete norm depends on the property of the solution.
- One can choose to work in a subspace:
  - Estimate on a functional of the solution.
  - Estimate in sub-domain.
\[
div(\rho \nabla u) = f
\]

Figure: Stiff poisson problem on a fine grid (Garbey and Shyy)

- \( \rho \approx 100 \) in the disc, \textbf{one} elsewhere.
- Domain has a L-shape.
- Coarse grid solutions: \( h_1 = 1/14, h_2 = 1/20, h_3 = 1/26 \).
- Fine grid: \( h^0 = 1/128 \).
Error Estimate in $L_2$ norm

Figure: Error estimation in $L_2$ norm (Garbey and Shyy)
Problem setup I

- Assumption: well posed parabolic problem with a unique solution.

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

\[
u|_{\partial \Omega} = g(t), \quad t \in (0, T),
\]

\[
u(x, 0) = v(x), \quad x \in \Omega.
\]

- The coarse grid solution used in the numerical solution corresponding to the discretization \((h, dt), (h/2, dt), (h, dt/2), (h/2, dt/2)\) are \(v^j_{dx, dt}, j = 1 \ldots 3\)

- The fine grid \(M(h_\infty)\) used in OES corresponds to \((h/4, dt/4)\).

- The coarse grid solutions \(v^j_{dx, dt}\) are projected on the fine grid with second (or third order) accuracy. We denote them by \(\tilde{U}^j_{dx, dt}\).
OES Formulation

- Find the three weight functions $\alpha_j, j = 1..3$ such that the residual
  \[ \sum_{j=1..4} \alpha_j \tilde{U}^{n+1}_{dx,dt} - H\left( \sum_{j=1..4} \alpha_j \tilde{U}^n_{dx,dt} \right), \]
  is minimum in the discrete norm on the space time grid
  \[ \{idx\}_{i=1...N} \times \{t^n, t^n + dt, t^n + 2dt, t^n + 3dt, t^{n+1} \} \]
  where $H$ is some objective function

- The asymptotic expansion writes
  \[ U_{dx,dt} - u = C_1 dx^{p_x} + C_2 dt^{p_t} + O(dx^{q_x}, dt^{q_t}), \quad (4) \]
Theorem on continuous functions

**Theorem**

If \( \alpha_j \in C^0(\Omega_x \times \Omega_t), j = 1 \ldots 3 \), and \( v_j^{dx,dt} - v_4^{dx,dt} = O(dx^{p_x}, dt^{p_t}) \) then there exists \( M \) such that

\[
\begin{align*}
\sum_{j=1}^{4} \alpha_j^M v_j^{dx,dt} + O(dx^{p_x}, dt^{p_t}) \times O(M^{-1})
\end{align*}
\]

In practice only an approximation to order \( \varepsilon = M^{-1} \) is needed to compute \( \alpha_i \).
Richardson Extrapolation in space and time

Theorem

There exists a unique linear combination of the coarse grid solutions $U_{i,n}$ with constant weights $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ such that

$$\alpha_1 U_{1,1} + \alpha_2 U_{2,1} + \alpha_3 U_{1,2} + \alpha_4 U_{2,2} - u = O(dx^{p_x}) + O(dt^{p_t}), \quad (6)$$

The $(\alpha_i)_{i=1...3}$ are:

$$\alpha_1 = \frac{1}{(2p_x - 1)(2p_t - 1)}, \quad \alpha_2 = -\frac{2^{p_t}}{(2p_x - 1)(2p_t - 1)},$$
$$\alpha_3 = -\frac{2^{p_x}}{(2p_x - 1)(2p_t - 1)}$$

Further, the consistency of the extrapolation formula implies

$$\alpha_4 = 1 - \alpha_1 - \alpha_2 - \alpha_3.$$
On the precision of OES

Theorem

If the following two assumptions are true

- the asymptotic expansion is valid in the discrete $L^2$ norm for the coarse grid solution used in OES,
- the consistency error for the one-step scheme is asymptotically equivalent to the error on the solution

then the OES solution for the $\alpha_j$ coefficients is asymptotically equivalent to the RE solution within order 2.
Problem Definition

- **Thermal wave problem similar to Ropp et Al in JCP 2004,**
  \[
  \frac{\partial T}{\partial t} = \Delta T - 2T(T - 1)(2T - 1).
  \]

- Benchmark problem exhibits a traveling wave
  \[
  T(x, y, t) = 1 - \tanh(x + y - 2t)
  \]
  with wave speed is of order one.

- **Experiment with constant extrapolation coefficient.**
- **Post-processing of fine grid solution by few SSOR.**
- **We use the unconstrained minimization subroutine of matlab,**
  to compare results with different choices of the norm, i.e
  either discrete \( L_2 \) norm or maximum norm.
- **We have three unknown coefficients and start the search**
  from the set of RE coefficients.
Figure: Evolution of the residual of in time with a Crank Nicholson scheme

Figure: Optimization path from Richardson Extrapolation in red to the LSE optimum solution in blue for a Crank-Nicholson scheme
Problem Definition

- The model we are using is the one proposed by Majda

\[
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} [F(u) - q_0 Z] = \varepsilon \frac{\partial^2 u}{\partial x^2}
\]

(7)

\[
Z_x = \varepsilon^{-1} \phi(u) Z
\]

(8)

- Experiment with constant extrapolation coefficient.
- Post-processing of fine grid solution by few SSOR.
- We use the unconstrained minimization subroutine of matlab, to compare results with different choices of the norm, i.e either discrete $L_2$ norm or maximum norm.
- We have three unknown coefficients and start the search from the set of RE coefficients.
A posteriori error estimator framework for PDEs

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OES for elliptic problems (Garbey, Shyy)
OES for parabolic equations (Picard, Garbey)
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Reactive Shock Layer
OES for general code (Garbey, Picard)
Distributed computation (Picard, Garbey)
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Figure: Solution for Reactive Shock Layer equation using finite differences

PDE solution using FDM
Figure: Optimization path for Reactive Shock Layer equation using finite differences
Solution using PPM

Figure: Solution for Reactive Shock Layer equation using PPM
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Figure: Optimization path for Reactive Shock Layer equation using PPM
Conclusions

- RE does not work on the fine grid $G^*$, but may work well on the coarse grid $G_{1,1}$ at time steps $kdT$, where $dT$ is the coarse time step.

- One requires few SSOR smoothing of $\tilde{U}_{i,j}$ on $G^*$ solutions to have OES performing better than the fine grid solution $\tilde{U}_{2,2}$.

- One can have OES better than RE for $G^*$ and in the same time OES worst than RE as an approximation of the exact solution.

- the higher the order of the scheme, and/or the finer the discretization, the more iterates of SSOR we need.

- OES gives best results for under resolved solutions with low order scheme.

- smaller residual on $G^*$ does not lead to smaller errors. The post-processing step with SSOR is then essential to recover this monotonic relationship between residual and errors.

- filtering the residual and/or the solution in space, might be beneficial for large time step.
### General Principle (1)

- Let us assume that $V_e$ exists and has been computed.
- Let $U_j$ be one of the coarse grid approximations; We look for a global a posteriori estimate of the error

$$\| \tilde{U}_j - p_h(u) \|$$

- Recovery method:

$$\text{IF} \| V_e - p_h(u) \|_2 \ll \| \tilde{U}_j - p_h(u) \|_2,$$

$$\text{THEN} \| \tilde{U}_j - V_e \|_2 \sim \| \tilde{U}_j - p_h(u) \|_2$$

provides a good lower bound on the error in our numerical experiments with steady incompressible Navier Stokes (NS).

- But 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.
General Principle (2)

- From a stability estimate with the discrete operator:
  \[ \| V_e - U_\infty \| < \mu_\infty G(V_e), \text{ where } \mu \geq \| (A_{h_\infty})^{-1} \|. \]

- We conclude
  \[ \| \tilde{U}_2 - U_\infty \|_2 < \mu G(V_e) + \| V_e - \tilde{U}_2 \|_2. \]

- Uses extrapolation on \( \mu_1, \mu_2, \mu_3 \) to get \( \approx \mu_\infty \).

- \( L_2 \) norm: the estimate on \( \mu \) uses a standard eigenvalue iterative procedure to get the smallest eigenvalue.

- \( L_1 \) norm: see N J. Higham papers.

- Additional Test: Verify that the upper bound on \( \| U_\infty - U_2 \| \) increases toward an asymptotic limit as \( M(h_\infty) \) gets finer.

- Feasible test because the fine grid solution is never computed in OES.
General Principle (3)

- \( N \) non linear (discrete) operator from \( E \) to \( F \).
- Assuming the problem \( N(u) = s \) is well posed for \( s \in B(S,d) \), and \( N(U_h) \in B(S,d) \), for some discrete solution \( U_h \).
- Defining \( \rho \) the residual and \( e \) the error, an upper bound of the error is given by

\[
\| e \|_E \leq \| \rho \|_F (\| \nabla s N^{-1} (S + \rho) \|_E + \frac{K}{2} \| \rho \|_F).
\]

- Let \( \{ b_i^E, \ i = 1..N \} \), be a basis of \( E \), and \( \varepsilon \in \mathbb{R} \) such that \( \varepsilon = o(1) \).
- Let \( (V_i^\pm)_{i=1..N} \), be the family of solutions of the following problems \( N(U_h \pm \varepsilon V_i) = S + \rho \pm \varepsilon b_i \).
- We get from finite differences the approximation

\[
\| \nabla s N^{-1} (S + \rho) \| \approx \|(\frac{1}{2} (V_j^+ - V_j^-))_{j=1..N}\| + O(\varepsilon^2).
\]
Stability estimates

- \( \hat{q}_E \) is least square approximation of the solution \( u \) in \( \hat{E} \), acting as a filter on the solution
- \( q_E \) is a projection in \( E \).

The construction of \( q_E \) and \( \hat{q}_E \), respectively \( q_F \) and \( \hat{q}_F \) does not consider the nature of the approximation space of the code \( C \) since the implementation details are most of the time unavailable: the mappings involve only the discrete representations of the functions.
Algorithm : Idea

- Compact representation of unknown weight functions: $m$ is much lower than the number of grid points on any coarse grid used.
- Estimate on the number of iterates to regularized $\tilde{U}_j, j = 1..p$
- Generalization to non-linear elliptic problems via a Newton like loop.
- Difficulties: A posteriori Error estimate depends then on the function used to linearized the operator.
- Generalization to $L_1$ and $L_\infty$ with appropriate minimization procedure.
Let us denote $N[u] = 0$ the supposedly well posed PDE problem to be solved, and its unsteady companion problem, $\partial_t u = N[u]$.

The algorithm is as follow:

Step 1 *Call coarse Mesh*: We generate the (coarse) meshes $G_1$ and $G_2$. If $h_i$ is the average space step for the grid $G_i$ we should have $h_2 < h_1$ but this is not necessary.

Step 2 *Call fine Mesh*: We generate a fine mesh $G_\infty$ that is supposed to solve all the scales of the problem. $G_\infty$ might be a structured mesh or not. We must have $h_\infty << h_1, h_2$.

Step 3 *Call Solver*: We solve the problem on $G_1$ and $G_2$, possibly in parallel. The solutions are denoted respectively $u_1$ and $u_2$ on $G_1$ and $G_2$. 

Algorithm(1)
Step 4 *Call Projection*: We project these coarse solutions \( u_1 \) and \( u_2 \) onto \( G_\infty \). We denote these projections \( \tilde{u}_1^\infty \) and \( \tilde{u}_2^\infty \).

Step 5 *Create sample*: We create sample solutions

\[
u_\alpha^\infty = \left[ \alpha \tilde{u}_1^\infty + (1 - \alpha) \tilde{u}_2^\infty \right].
\]

We smooth out the spurious high frequency components of the build solution with few explicit time steps of \( \partial_t u = N(u) \) starting from the initial condition: \( u_\alpha^\infty \). The choice of the Optimum Design Space in which \( \alpha \) is taken is one the main item of our research.

Step 6 We compute the best \( \alpha \) that minimizes the \( L_2 \) norm of the residual. We may use a surface response technique.
In this simulation, the number of elements are respectively 10347 on the fine grid $G^\infty$, 1260 on the coarse grid $G_1$, and 2630 on the coarse grid $G_2$. The steady solutions are obtained using a transient scheme for the incompressible Navier-Stokes equation.
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Figure: LSE: error and residual for Adina R&D in $L_2$ norm

Figure: Performance of LSE and Richardson Extrapolation

Results
Error bound for the back-step flow

**Figure:** Evaluation of the stability constant

**Figure:** Evaluation of the error upper bound
Solution I

The energy equation (9) that governs the model is:

\[
\frac{\partial}{\partial x_i} \left( k_{ij}(T) \frac{\partial T}{\partial x_j} \right) + Q(T) = \rho c_p(T) \frac{\partial T}{\partial t}
\]

on \( \Omega \times (0, t) \)
Solution II

The boundary conditions

• \[- \left( k_{ij} \frac{\partial T}{\partial x_j} \right) \cdot n = h_1(T)(T - T_\infty) + \sigma \varepsilon_1 \left( T^4 - T^4_\infty \right) \text{ on } \Gamma_{N_1} \]

(radiation, convection)

• \[- \left( k_{ij} \frac{\partial T}{\partial x_j} \right) \cdot n = h_2(T)(T - T_\infty) + \sigma \varepsilon_2 \left( T^4 - T^4_\infty \right) \text{ on } \Gamma_{N_2} \]

(radiation, convection)

• \[- \left( k_{ij} \frac{\partial T}{\partial x_j} \right) \cdot n = h_3(T)(T - T_\infty) \text{ on } \Gamma_{N_3} \]

(convection)

• Symmetric boundary condition on \( \Gamma_{N_4} \)
Figure: Steady state solution of the heat transfer problem.
Solution

Figure: Evolution of the error versus the fine grid solution with the $L_2$ norm for the heat transfer problem
Computational cost

- In our procedure, there is a need to compute form a large number of solution in order ot perform the minimization.
- These computations have an embarrassing parallelism.
- On the other hand, given a code that is portable to different platform, there is a large amount of resources that are available.
- The question to be answered is can a distributed version of the verification procedure be designed to take advantage of this two facts?
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Figure: Software Architecture
Figure: Time performances: OES versus computation of fine grid solution with a Pentium 4, 2.4GhZ, running a Linux OS.
Error control and secure data transfer
Conclusions

- A new extrapolation method for PDEs.
- A better tool for solution verification than RE when the convergence order is space dependent or far from the asymptotic rate of convergence.
- Solution Verification Method with Hands off Coding.
Expand OES to other multiphysics case, ie Chimera method and IBM.

Expand OES to compute stability estimates for unsteady problems.

Integrate OES in applications as a plugin/tool.
Publications I

Conference

1. Aitken like acceleration of the Schwarz algorithm for overset methods: application to Incompressible Navier Stokes flow - 7th Symposium on Overset Composite Grid and Solution Technology - Huntington Beach, California, USA , October 5-7, 2004


Publications II


Proceedings


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Publications III


Publications IV

7 Parallel implementation for solution verification of CFD code - C. Picard and M. Garbey - 16th International Conference on Software Engineering and Data Engineering - Las Vegas, Nv - July 9-11, 2007

• Journal

1 M.Garbey and C.Picard, Toward a General Solution Verification Method for Complex PDE problem with Hands of Coding, Computer and Fluids - Submitted

2 C.Picard and M.Garbey, Optimized extrapolation method for parabolic equations. In preparation

3 C.Picard and M.Garbey, Distributed computation of optimized extrapolation. In preparation
Activities

1. Investigation on numerical method for heterogeneous domain decomposition.
2. Investigation on numerical method for fluid-structure interaction
3. From Fall 2006 to Fall 2007: Instructor for COSC 3661 and COSC 3662 (Numerical Analysis)
4. Development of the Intelligent Data and Visualization Desk: Application for a patent 2483-00501
Thank you