Extrapolation method and optimum design of solutions

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Solution Verification

Problem

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

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

Assume that the PDE problem is well posed and has a unique solution. We consider an approximation on a family of meshes $M(h)$ parameterized 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 ($||.||$ is a given discrete norm):

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

Comment

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

Manufactured solution

$$f(x) = L[u(x)]$$

- Polynomial solution to verify the code.
  - Test each term of the equation.
  - Useful for parallel codes
- Use of symbolic manipulation languages
- Constraint by conservation of physical quantities
- Principle of nearby exact solution (C.J.Roy and M.M.Hopkins).
- Possible use of image analysis on experimental data.

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 α is a weight function.
• In classical Richardson Extrapolation (RE) α is a constant.
• In our optimized extrapolation method α is a function solution of the following optimization problem:

P_α: *Find* $\alpha \in \Lambda(\Omega) \subset L_\infty$ *such that* $G(\alpha\, U_1 + (1-\alpha)\, U_2)$ *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:
  - ☐ Equilibrated residual method for FE .- see Ainsworth & Oden and ref.
  - ☐ A posteriori Finite-Element free constant output bounds - see Patera and ref.

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_∞.
- $M(h_\infty)$ 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 Physicist and Asymptotic Analysis.
- Reuse Stability Theory from Linear Algebra.

Practical Consequences

- Both coarse grid solutions U_1 and U_2 must be projected onto $M(h_\infty)$. Notation: $\tilde{U}_1$ and $\tilde{U}_2$.

- The objective function is a discrete norm of the residual:

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

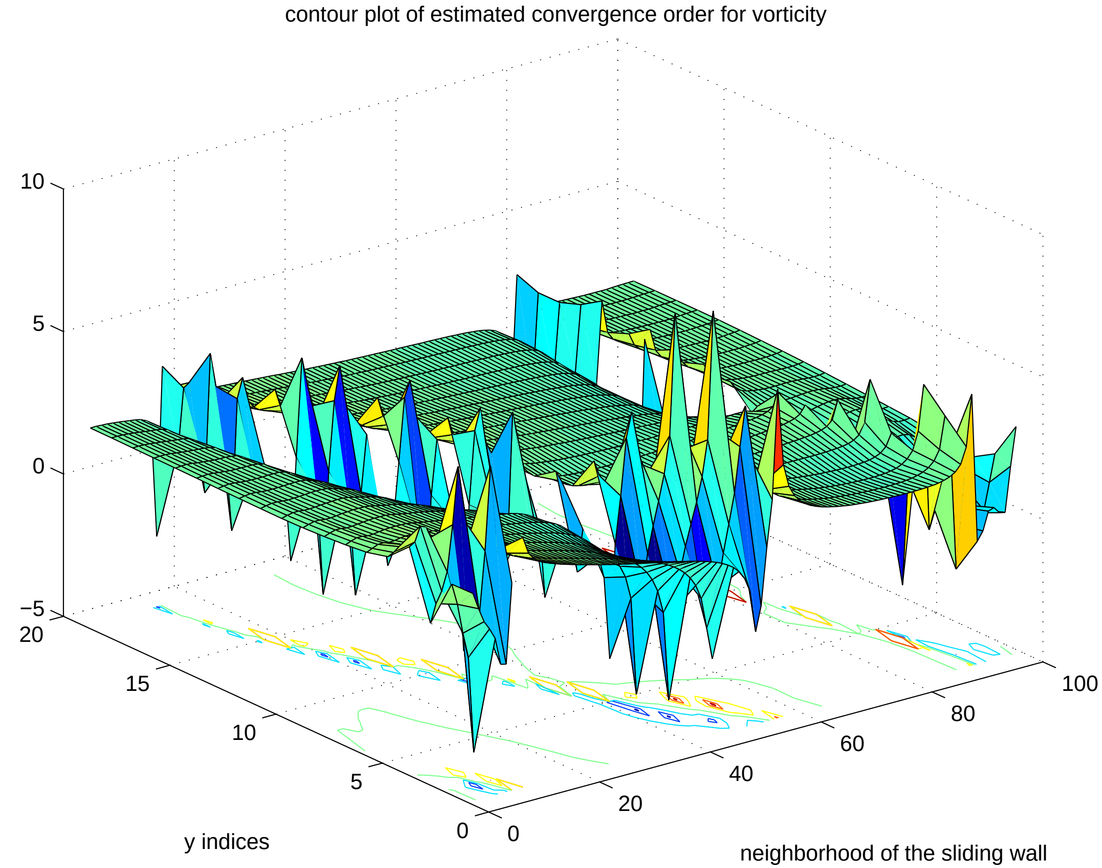
The Optimized Extrapolated Solution (OES) if it exists, is denoted $V_e = \alpha_e U_1 + (1-\alpha_e) U_2$.

- 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 subdomain.

Three level methods (1)



Cancelation phenomenon: surface plot of space dependent convergence order approximation for $\omega - \psi$ code with Re=100.

Three level methods (2)

- There are subset of Ω where $\tilde{U}_1 - \tilde{U}_2 << h^k$, with k expected order of convergence.

- Optimized two-level extrapolation problem is ill posed.

Three levels OES *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.*

- 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.

- Robustness of the 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.

A Posteriori Error

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:

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

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

- Heuristic: 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 μ 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.

Stability estimate (1)

- Let $(E, ||.||_E)$ and $(F, ||.||_F)$ be two normed linear space, $N \in L(E, F)$ be the operator corresponding to the CFD problem.

- 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 ρ 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 $\varepsilon \in$ such that $\varepsilon = o(1)$.

- Let $(V_i^{\mp})_{i=1..N}$, be the family of solutions of the following problems $N(U_h \mp \varepsilon V_i) = S + \rho \mp \varepsilon b_i$.

Stability estimate (2)

- We get from finite differences the approximation

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

- Fundamental tool: compact representation of the solution via a projection: trigonometric polynomial or wavelet or spectral elements for example.
- One get the error estimate in this smaller space only.
- The size of the space is fixed adaptively according to the quality of the approximation of trigonometric polynomial/wavelets of the FE solution!.
- Both stability estimate and OES construction relies on several hundred of residual/smoothing computation that are extremely fast and have embarassing parallelism $\rightarrow$ distributed computing !!!

Algorithm/Result with detail code knowledge

Windows Grid

General Principle(1)

- Assume that 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.

- Step 1: interpolation of the coarse grid solution from $M(h_j), \ j = 1..p$, to $M(h_\infty)$ and postprocessing to smooth out the "spurious modes".

- Step 2: 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 $M(h_\infty)$.

- Step 3: solution of the least square linear algebra problem that has m unknowns for each weight coefficient α and β.

General Principle(2)

- Compact representation of unknown weight functions: m is much lower than the number of grid points on any coarse grid used.

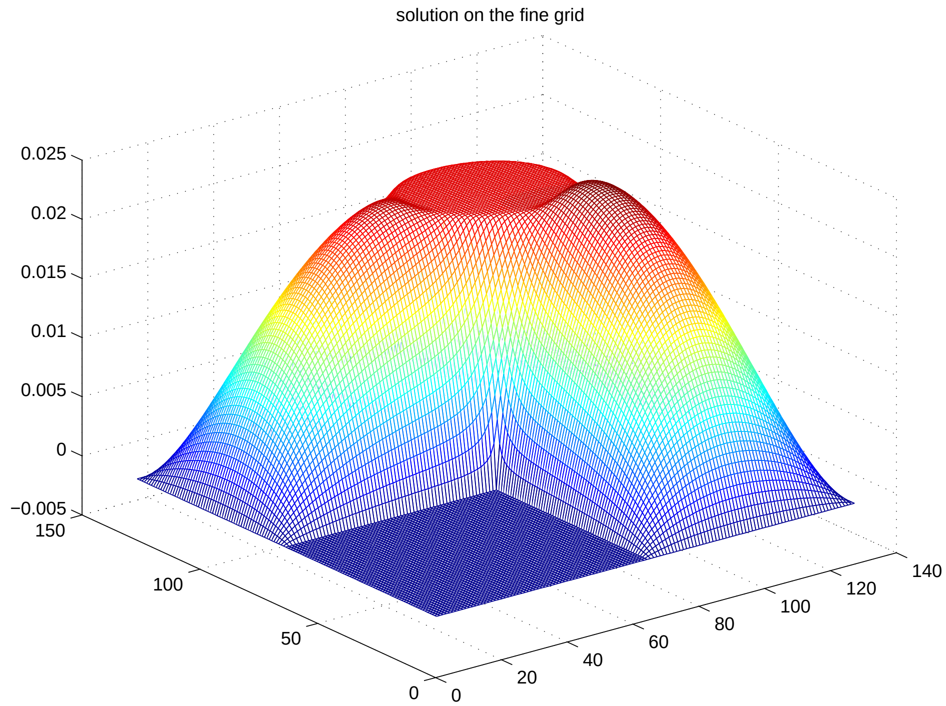
- Estimate on the number of iterates to regularized $\tilde{U}_j, \; j = 1..p$

- 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.

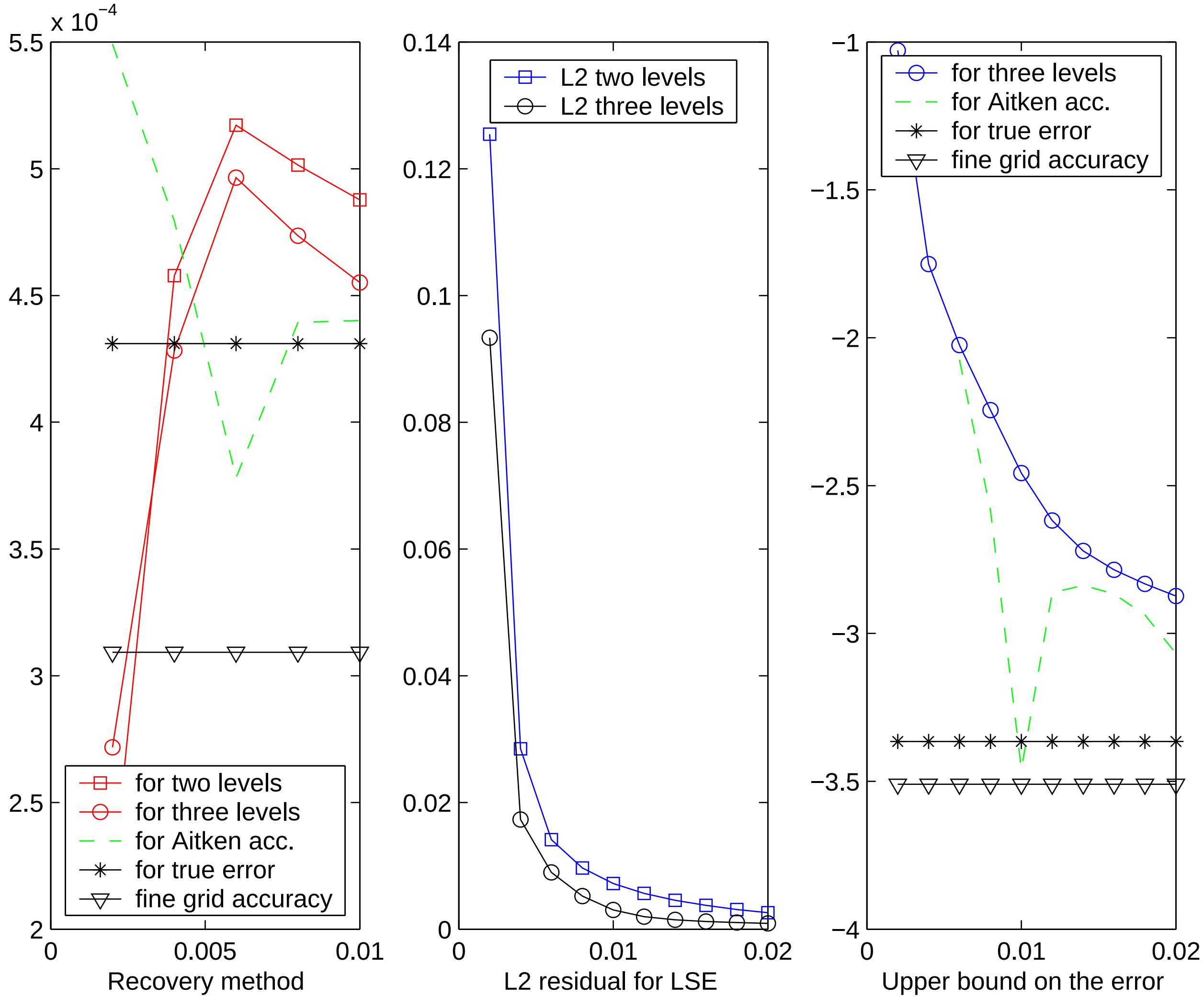
- Generalization to L_1 and L_∞ with appropriate minimization procedure.

$div(\rho \nabla u) = f$



- $\rho \approx 100$ in the disc, **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



Algorithm/Result with No detail code knowledge

General Principle(1)

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_∞ that is supposed to solve all the scales of the problem. G_∞ 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.

General Principle(2)

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

- Step 5 *Create sample* : We create sample solutions $u_\alpha^\infty = [\alpha \tilde{u}_1^\infty + (1-\alpha)\tilde{u}_2^\infty]$. 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_α^∞. The choice of the Optimum Design Space in which α is taken is one the main item of our research.

- Step 6 We compute the best α that minimizes the L_2 norm of the residual. We may use a surface response technique.

Benchmark Problems

- Laminar flow over a backward facing step

The flow problem has the following characteristics:

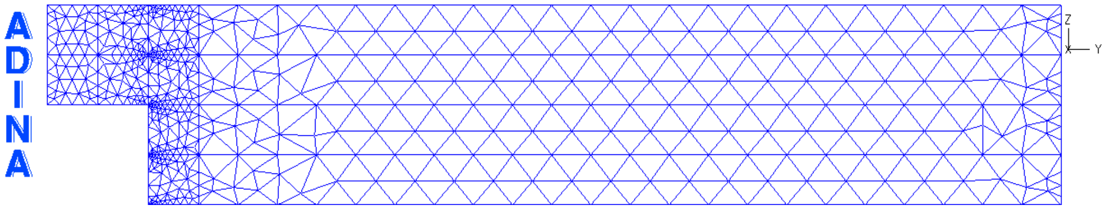
Density	1	Length of the pipe	10
Viscosity	0.01	Inflow diameter	1
Maximum Inflow Velocity	U=1	Outflow diameter	2
Reynold Number	500		

- Heat Transfer in a composite material (Sandia Nat. Lab.)

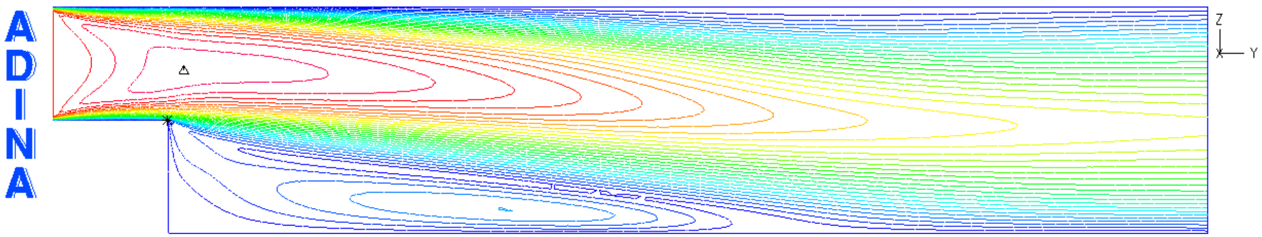
$$\frac{\partial}{\partial x_i}(k_{ij}(T))\frac{\partial T}{\partial x_i} + Q(T) = 0 \text{ in } \Omega \times (0, T)$$

The boundary conditions are of robin type to describe radiations effects. Remark : The problem is very stiff and the solution is near discontinuous between material.

Adina Software

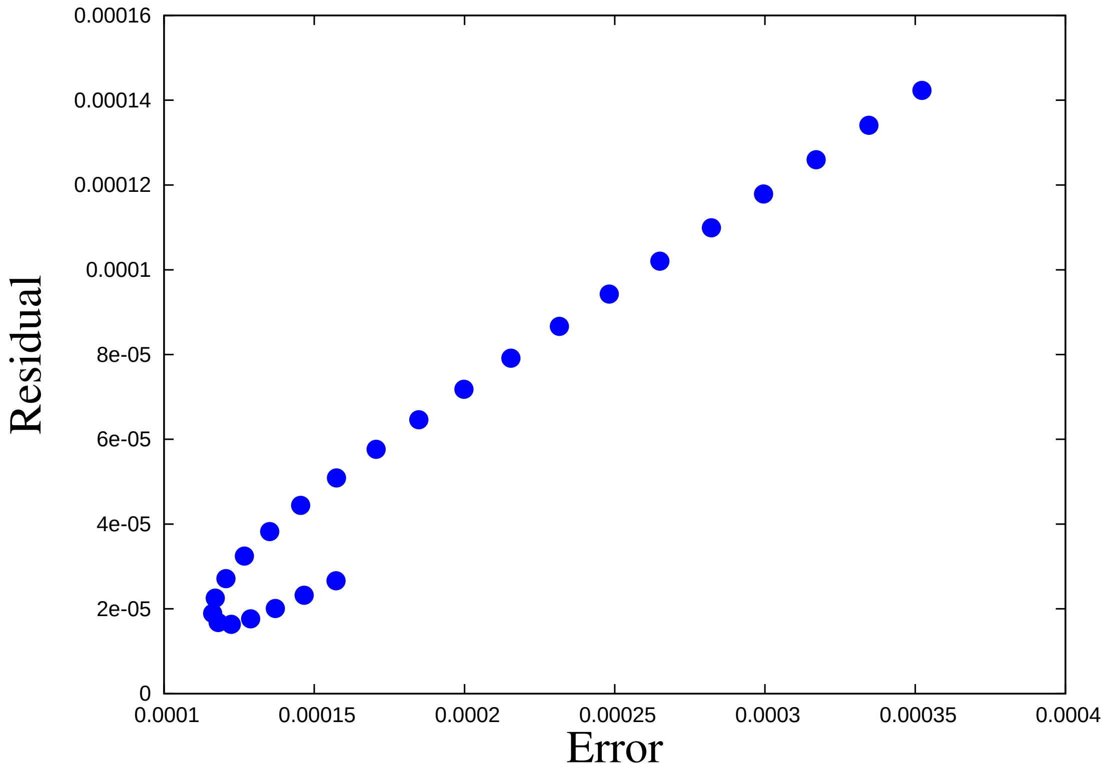


In this simulation, the number of elements are respectively 10347 on the fine grid G^{∞}, 1260 on the coarse grid G_1, and 2630 on the coarse grid G_2.



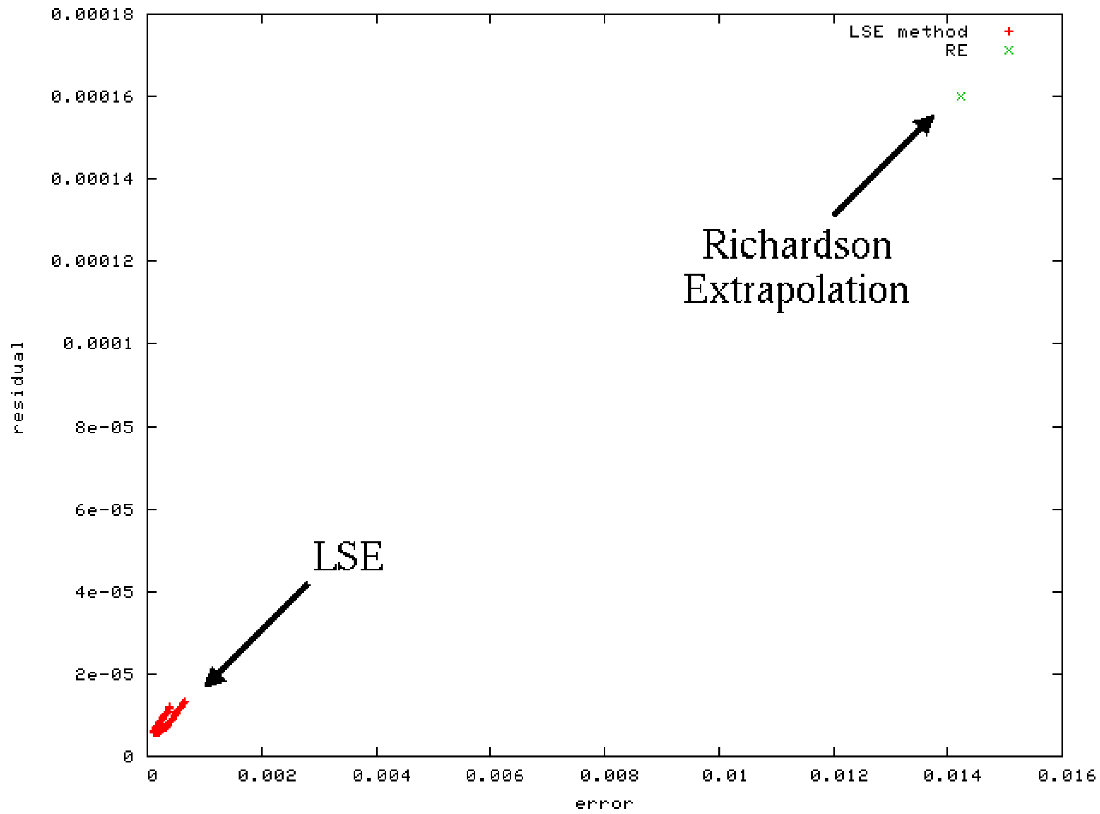
Contour of velocity magnitude on fine grid: Adina R&D
The steady solutions are obtained using a transient scheme for the incompressible Navier-Stokes equation.

Results(1)



LSE: error and residual for Adina R&D in L_2 norm

Results(2)



Performance of LSE and Richardson Extrapolation

Results : stability and error for backstep flow

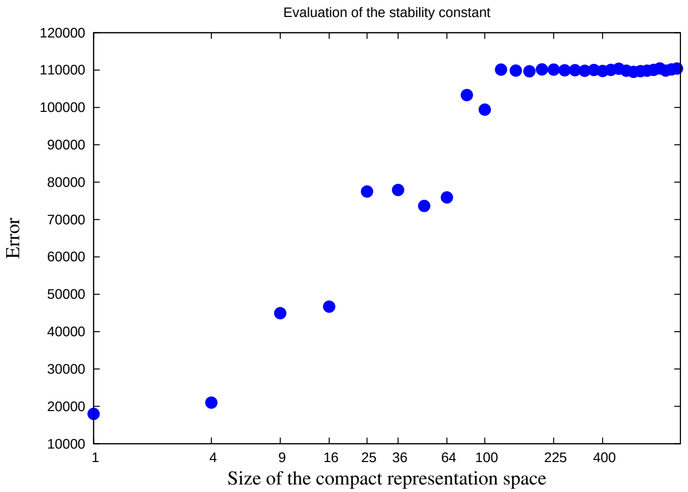


Figure 1: Evaluation of the stability constant

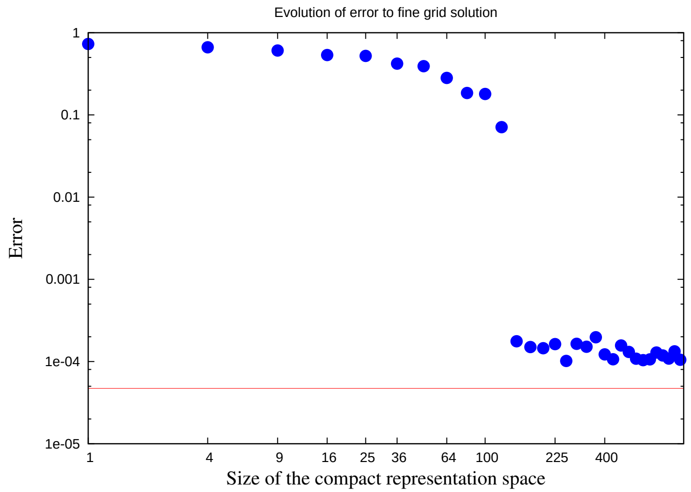


Figure 2: Evaluation of the error upper bound

Results : stability and error for the battery

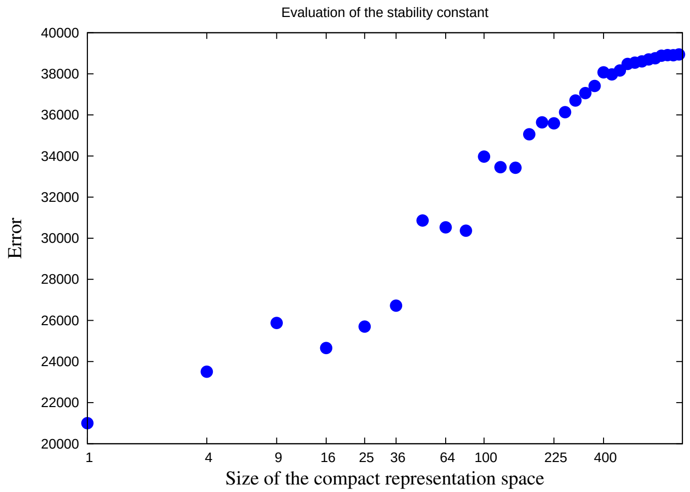


Figure 3: Evaluation of the stability constant

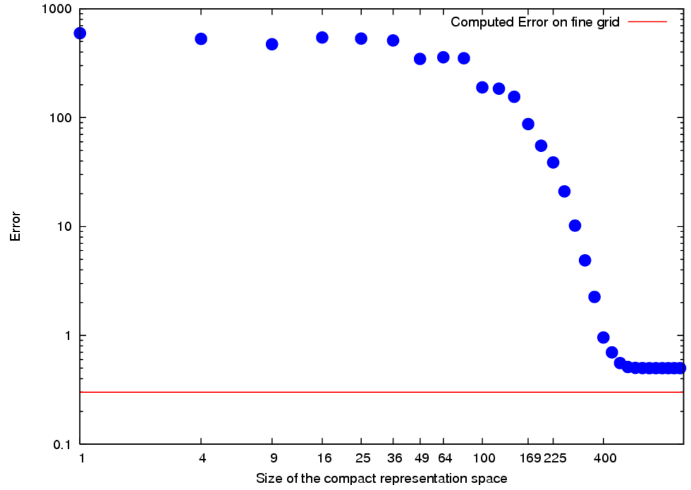
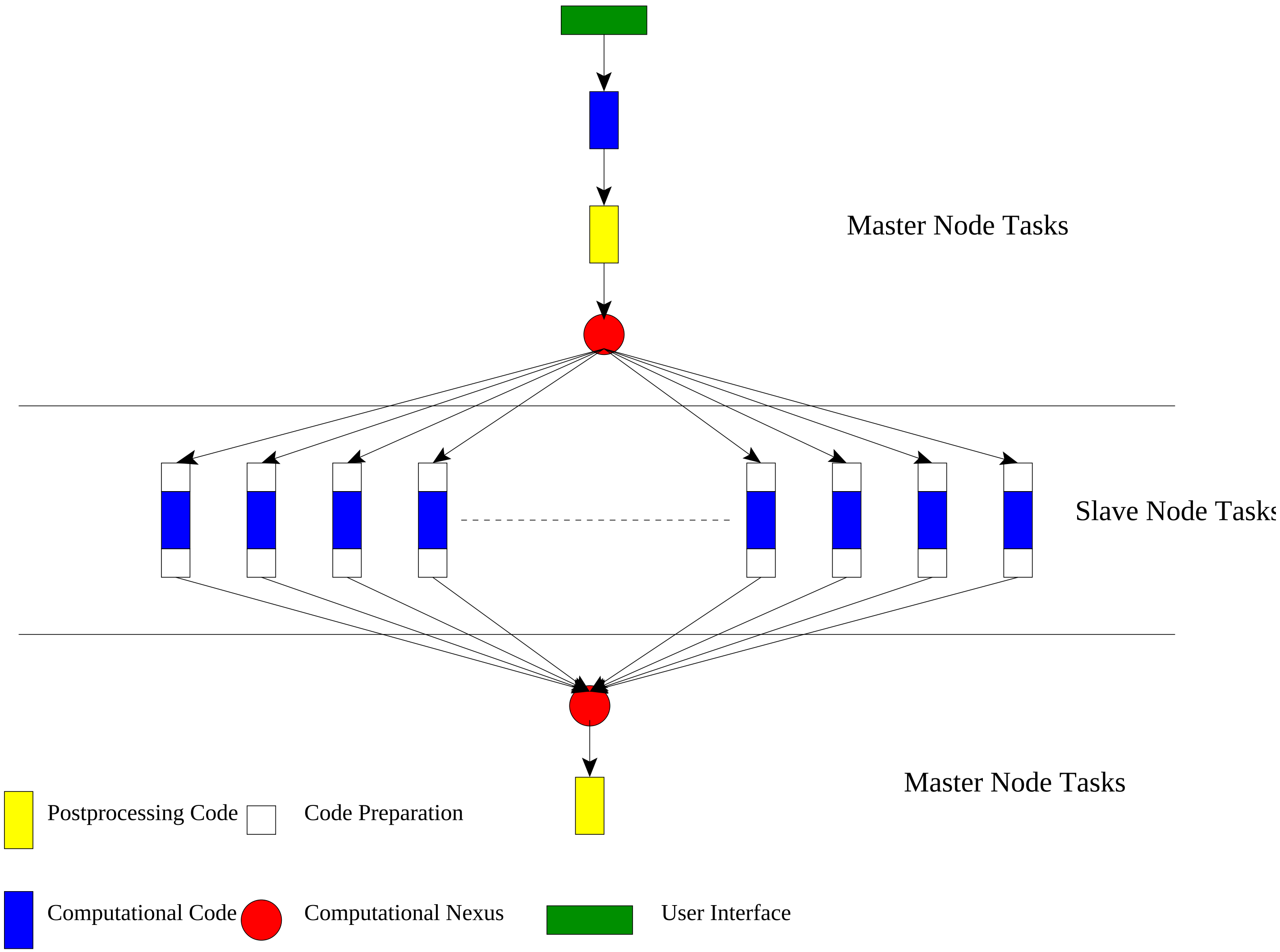


Figure 4: Evaluation of the error upper bound

Software Architecture



Conclusion

Conclusions

- A new extrapolation methods 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.
- Toward a Solution Verification Method with Hands off Coding.
- Toward a system that is user friendly and scalable.
- Time dependent problem currently under investigation.