Accuracy Estimate, Multilevel Method and Robust Extrapolation Formula for the numerical solution of PDEs

M. Garbey† *and W. Shyy*††

† Department of Computer Science,
University of Houston, USA

†† Department of Mechanical and Aerospace Engineering, University of Florida, USA

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Thanks DOE

Few examples of a posteriori estimates and code verification theories

- AIAA Guide for the Verification and Validation of Computational Fluid Dynamics Simulations.
- the 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.
- Stochastic method in the Baysian framework - ref Glimm et Al..

Challenge

In complex simulation, one cannot afford anything else but coarse grid approximations, and one want to know if the answer is away by 50 percent or one order of magnitude!

Solution procedure should be:

- simple to implement and works with a code independent from the main code procedure.
- with arithmetic cost negligible compare to a direct computation of the 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.

What about Richardson Extrapolation ?

It is a popular method in Computational Fluid Dynamics (**CFD**) because of its straightforward implementation that is code (and " PDE ") independent. However its use raise the following questions:

- are the (3D) meshes fine enough to satisfies accurately 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 aposteriori estimates?

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

- **Problem 1**

  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*

- **Problem 2**

  Using two or three different grid solutions (not necessarily with uniformly increasing mesh resolution), *obtain a solution with improved accuracy*

- **Problem 3**

  Derive reliable aposteriori error bounds from coarse grid approximation of complex PDE problems.

plan of the talk

- Basic properties of Richardson extrapolation method and evaluate its application to CFD.
- Least square extrapolation for PDEs.
- Numerical results for steady incompressible Navier Stokes flows and Heat Transfer.
- Conclusion and future work.

1. Basic Properties of Richardson Extrapolation and Computational Implications

Asymptotic expansion for continuous function in a normed vector space

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,

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

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

For known p, Richardson extrapolation formula,

$$v_r^i = \frac{2^p \ u^{i+1} - u^i}{2^p - 1}, \ i = 1, 2$$

provides improved convergence:

$$||v - v_r^i|| = o(h^p)$$

.

Application of Convergence Order Approximation and Richardson Extrapolation to CFD

- we have several solutions $U^i \in E_i$, with increasing accuracy on non matching embedded grids.
- $$I_i : (E_i, \, || \, ||) \rightarrow (E^0, \, || \, ||)$$
  is an operator that interpolates from M_i to a common very fine mesh M^0:
  $$\tilde{U}^i = I_i[U^i]$$

Requirement: this interpolation does not add significant error to the original PDE'approximation code.

Remark: *centered cells finite volume (**FV**) approximation or finite differences (**FD**) with staggered grids require interpolation.*

Procedure

- Application of RE to the family of flow solutions $\tilde{U^i}$.
- Get convergence order from

$$\frac{h_1^p - h_2^p}{h_2^p - h_3^p} = \frac{||U^1 - U^2||}{||U^2 - U^3||}. \quad (1)$$

- Eventually applies RE with convergence order obtained from (1).
- computation of a numerical approximation of p depending on the norm

  ◇ on a coarse mesh after projection

  ◇ or on the fine mesh after high order interpolation.

data

- two different codes for the steady state, 2-D laminar incompressible lid-driven square cavity flow with the Reynolds number, **Re**, in the range of 20 to 1000 and squared regular meshes.
- first code $C_{\omega-\psi}$: FD approximation of the two dimensional vorticity - stream function formulation with either central finite differences for the convective term or first order upwinding.
- second code, C_{v-p}: FV code with centered cells and velocity-pressure formulation.

  The convective terms are approximated by first order upwind or second order central differences depending on the local cell Reynolds number.

Conclusion

- For most of the cases with low Reynolds number, it can be shown that second order RE reduces the error in discrete L_1, L_2 and L_∞ norm.
- For higher Reynolds number such as $Re = 1000$, RE fails to improve the error in the L_2 norm when the coarse grid is not fine enough.
- Overall, RE can improve the order of accuracy but not consistently.
- RE with computed order of convergence using three grids is numerically unstable.
- for $C_{\omega-\psi}$, poor performance of the code in the neighborhood of the corner of the sliding side for large Reynolds number.
- worst results for the back step test case with a turbulence model.

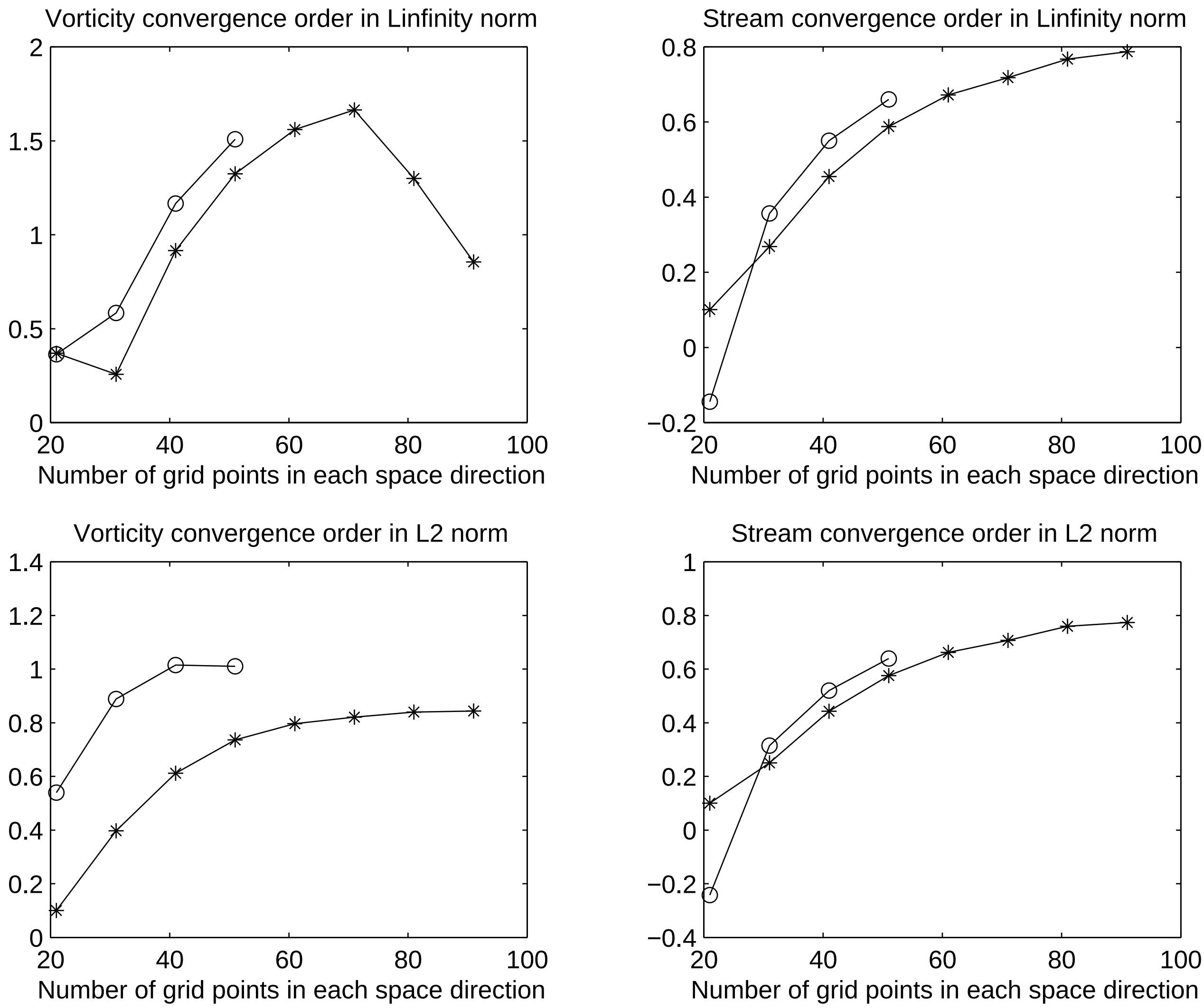

Fig 1 Convergence order approximation for $C_{\omega-\psi}$ code with $Re = 400$. $\circ$ curve for coarse grid projection solution, $*$ curve for fine grid interpolation solution

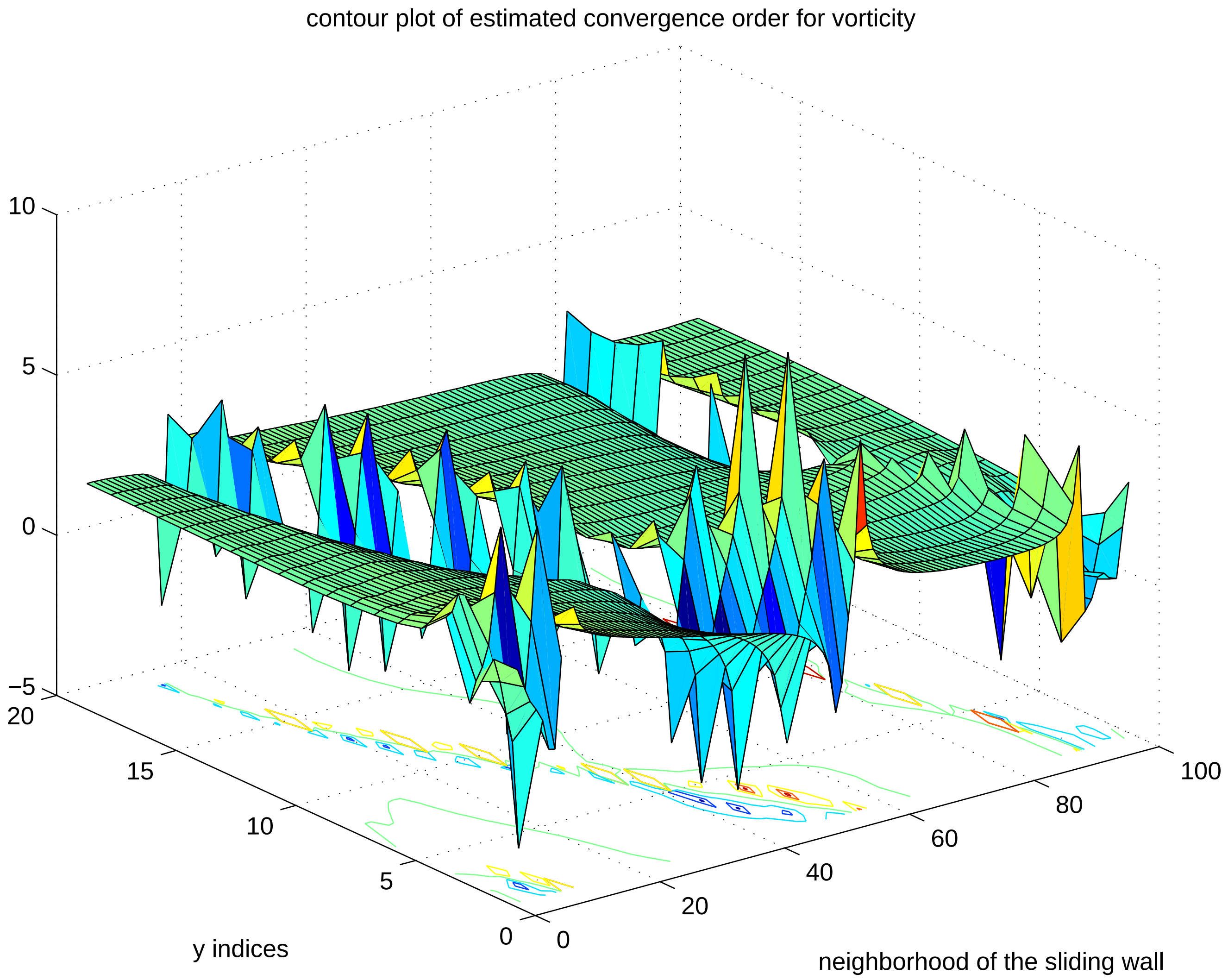

Fig 2 Surface plot of space dependent convergence order approximation for $C_{\omega-\psi}$ code with $Re = 100$.

2. Least Square Extrapolation for PDEs

Idea: use the PDE in the RE process to find an improved solution on the fine grid

Computational Algorithm

Let us denote formally the linear PDE

$L[u] = f, \ with\ u \in (E_a, || \ ||_a)\ and\ f \in (E_b, || \ ||_b),$

and its numerical approximation,

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

parameterized by a mesh step h.

We suppose that we have the stability estimate

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

with s real non necessarily positive.

Two-point BVP in $(0,1)$.

ooooooooooooooo

P_α**: Find** $\alpha \in \Lambda(0,1) \ \subset \ L_\infty$ **such that**

$$L_h[\alpha\tilde{U}^1 + (1-\alpha)\tilde{U}^2] - f_h$$

is minimum in $L_2(M^0)$.

ooooooooooooooo

and

ooooooooooooooo

$P_{\alpha,\beta}$**: Find** $\alpha, \beta \in \Lambda(0,1)$ **such that**

$$L_h[\alpha\tilde{U}^1 + \beta\tilde{U}^2 + (1-\alpha-\beta)\tilde{U}^3] - f_h$$

is minimum in $L_2(M^0)$.

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- Space of approximation for unknown weight function is either trigonometric polynomial or smooth piecewise polynomial.
- A priori no BC on weight functions!

Extension to multidimensional problem

- straightforward on tensorial product of grids.
- for complex geometry (under development): We extend artificially the functions $\tilde{U}^i(x)$ and U for $x \in \Omega \cap M^0$ to grid functions defined on M^0. There are generally no Boundary conditions on weight functions α, β.
- One can use domain decomposition, to do refinement in sub-domains with regular grids.
- However extension to irregular meshes is to be worked out.

Few remarks of importance

- *it is essential that the interpolation operator gives a smooth interpolant.*
- *For conservation laws, one may require that the interpolation operator satisfies the same conservation properties.*
- *For chemical problems, one may require that the interpolant preserve the positivity of species.*
- *For elliptic problems, it is convenient to postprocess the interpolated functions* $\tilde{U}^i$*, by few steps of the relaxation scheme*

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

  with appropriate artificial time step δt*.*

Generalization to non-linear PDE problem, via a Newton-like loop

Let the non linear problem be

$$N[u] = f,$$

linearized into,

$$J(u)[v] = g.$$

Algorithm for the two-level extrapolation case:

oooooooooooo

P_{α^k}: *Find* $\alpha^k \in \Lambda \subset L_\infty$ *such that*

$$J_h(\alpha^k \tilde{U}^1 + (1-\alpha^k)\tilde{U}^2)[\alpha^{k+1}\tilde{U}^1 + (1-\alpha^{k+1})\tilde{U}^2] - g_h$$

is minimum in $L_2(M^0)$,

starting from initial condition $\alpha^0 \equiv 0$, until $||\alpha^{k+1} - \alpha^k||$ is less than some tolerance number.

ooooooooooooo

The algorithm is coded in a stand alone procedure as:

- **step 1**: one compute the spline interpolation of each grid solution onto a common fine grid solution M^0.
- **step 2**: one compute once and for all with the basis functions e_i of Λ:

$$L[e_i\,(\tilde{U}^1 - \tilde{U}^2)],$$

  for the two-level case, and additionally

$$L[e_i\,(\tilde{U}^2 - \tilde{U}^3)],$$

  for the three-level case.
- **step 3**: one solve the least square problem P_α or $P_{\alpha,\beta}$.

• If the problem is nonlinear, then we repeat steps 1 to 3 as many Newton iterations are computed.

• *If we keep M, the overall cost of computation is modest.*

3. Numerical Evaluation

abbreviations:

- G1 for direct numerical solution, without any extrapolation, on grid $N_1 \times N_1$,
- G2 for direct numerical solution on grid $N_2 \times N_2$,... etc,
- R1 for Richardson extrapolation assuming first order convergence using G2 and G3 data,
- R2 for Richardson extrapolation assuming second order convergence using G2 and G3 data,
- LS1 for two-level least square extrapolation using G2 and G3 data,
- LS2 for three-levels least square extrapolation using G1, G2, G3 data.

(i) 2D Turning Point Problem

$$\epsilon\,\Delta u + a(x,y)\frac{\partial u}{\partial x} = 0,\ x \in (0,\pi)^2,$$

Dirichlet BC of opposit signs at $x = 0$ respt $x = \pi$, and homogeneous Neumann at $y = 0/\pi$.

$$a(x,y) = x - (\frac{\pi}{2} + 0.3(y - \frac{\pi}{2})).$$

- Transition layer of ϵ order thickness centered on the curve $a(x,y) = 0$, is not parallel to the x or y axis.
- 2^{sd} central FD diffusion term and 1^{st} upwinding for convection term.
- either direct sparse LU linear or GMRES solver.

Conclusion LS2 is an efficient numerical extrapolation that can gain more than one order of convergence with as little as 2 grid points in TL on G3.

(ii) The Square Cavity Flow Problem

The steady problem writes in $\Omega = (0,1)^2$,

$$N_1[u,v,p] \;=\; -\frac{1}{Re}\Delta u + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = 0,$$

$$N_2[u,v,p] \;=\; -\frac{1}{Re}\Delta v + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = 0,$$

submitted to the divergence free constraint.

The flow speed is zero on all walls except on the sliding wall $u(x,1) = g(x),\ x\ \in (0,1)$.

Neither the projected flow field or the extrapolated flow field, satisfy a priori the divergence free condition.

We define then the following mapping:

$$(u,v) \;\rightarrow\; \Psi \;\rightarrow\; (U,V), \text{where}$$

$$U = \frac{\partial \Psi}{\partial y},\ V = -\frac{\partial \Psi}{\partial x},$$

$$\Delta\Psi = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x},\ \Psi = 0 \text{ on } \partial\Omega.$$

LSE for Navier Stokes

The least square extrapolation problem with two levels writes then

Find α_1 *and* $\alpha_2 \in \Lambda(\Omega) \subset L_\infty(\Omega)$ such that

$$N^0[\alpha_1 \tilde{\Psi}_1 + (1-\alpha_1)\tilde{\Psi}_2, \alpha_2 \tilde{p}_1 + (1-\alpha_2)\tilde{p}_2]$$

is minimum in $L_2(M^0)$,

with

$$N^0[\Psi, p] = (N_1^0[U, V, p], N_2^0[U, V, p]).$$

Since this problem is non linear, we use a Newton loop to construct a sequence of weight functions (α_1^n, α_2^n) that may converge to the solution.

The iterative procedure starts from the finest coarse grid solution at our disposal.

Space of approximation for weight functions

The space of unknown weight function is the set of trigonometric polynomial functions

$$\alpha = \Sigma_{i=1..m,j=1..m} \alpha_{i,j} e^i \, e^j,$$

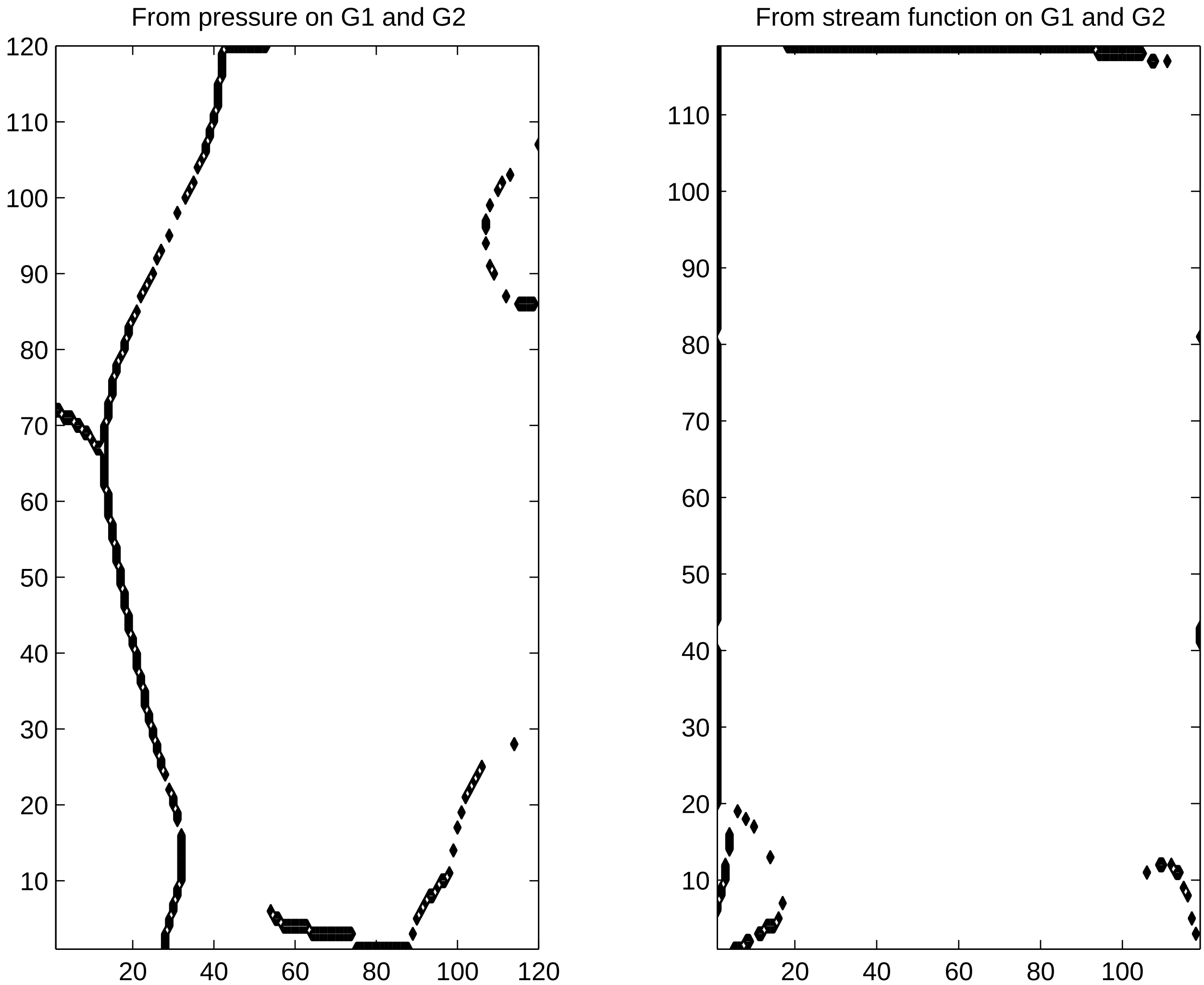
with

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

This set of trigonometric functions allows us to approximate at second order in L^2 norm any smooth non periodic functions of $C^1[(0,1)^2]$, - ref Gottlieb et Al.

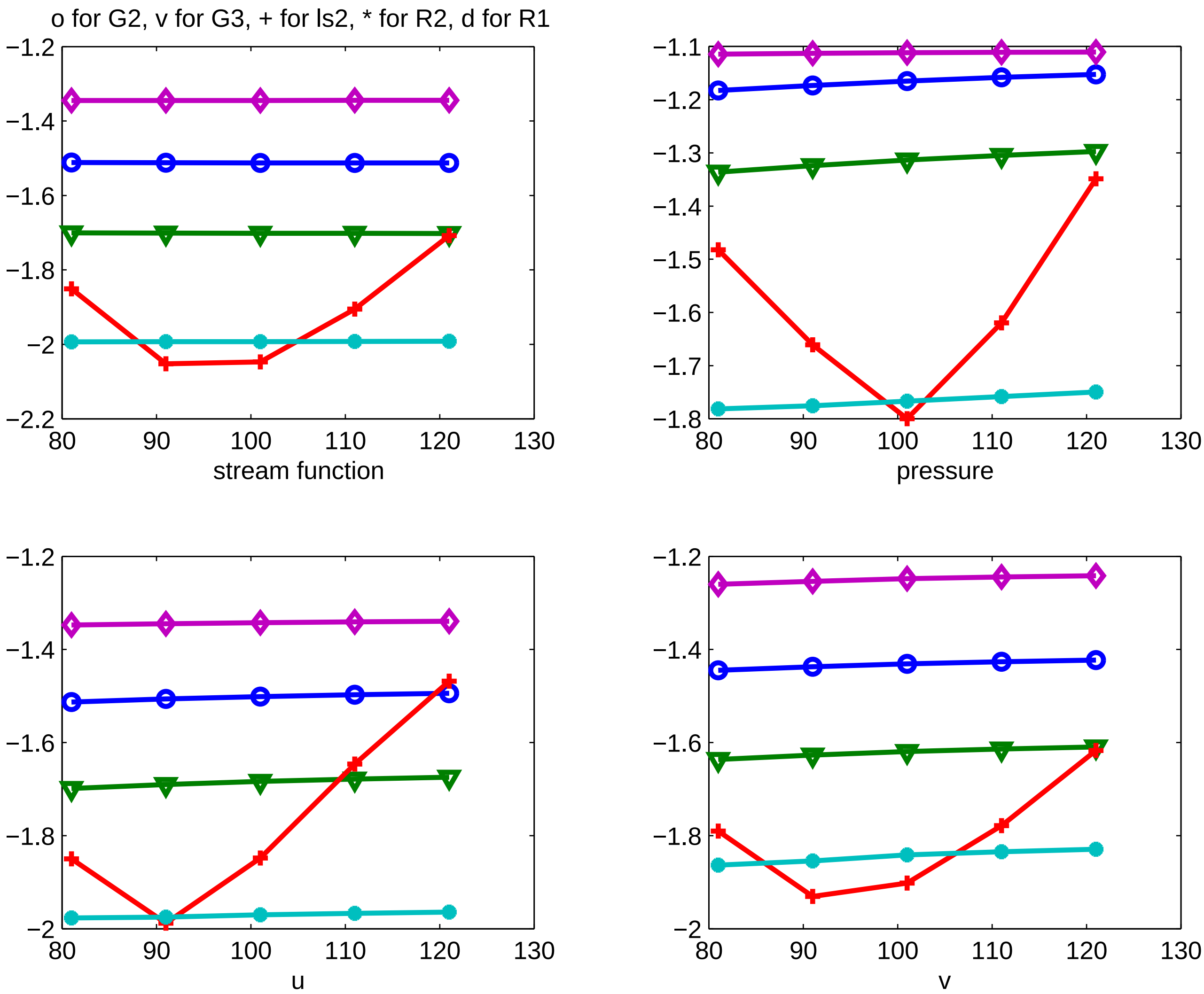
The main advantage of this choice of approximation space for the weight function, is that it allows us easily to interpret our numerical result in term of frequencies.

Cancelation Phenomenon



Local minima of $\tilde{p}_2 - \tilde{p}_1$ on the left and $\tilde{\psi}_2 - \tilde{\psi}_1$ on the right .

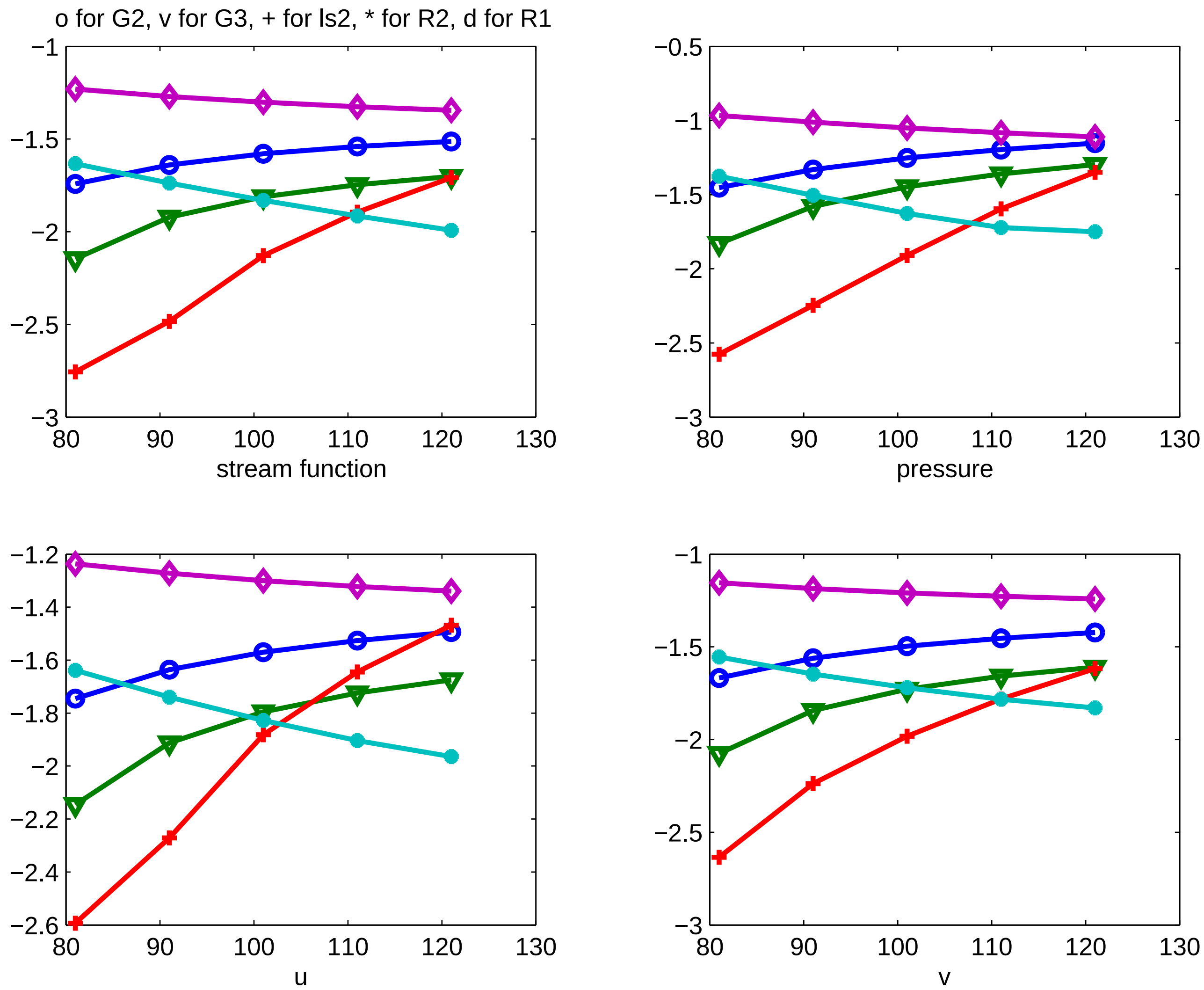
- $N = 50, ..70,\ Re = 400$, and $g(x) = -1$.
- Strong singularities of the flow field at the corner.
- LS2 more robust and more accurate than LS1.



x axis is for the number of grid points N in each space direction for the fine grid M^0.

'o' for G_2 solution, 'v' for G_3 solution, $\star$ for R2, '$\diamond$' for R1, $+$ for LS2.

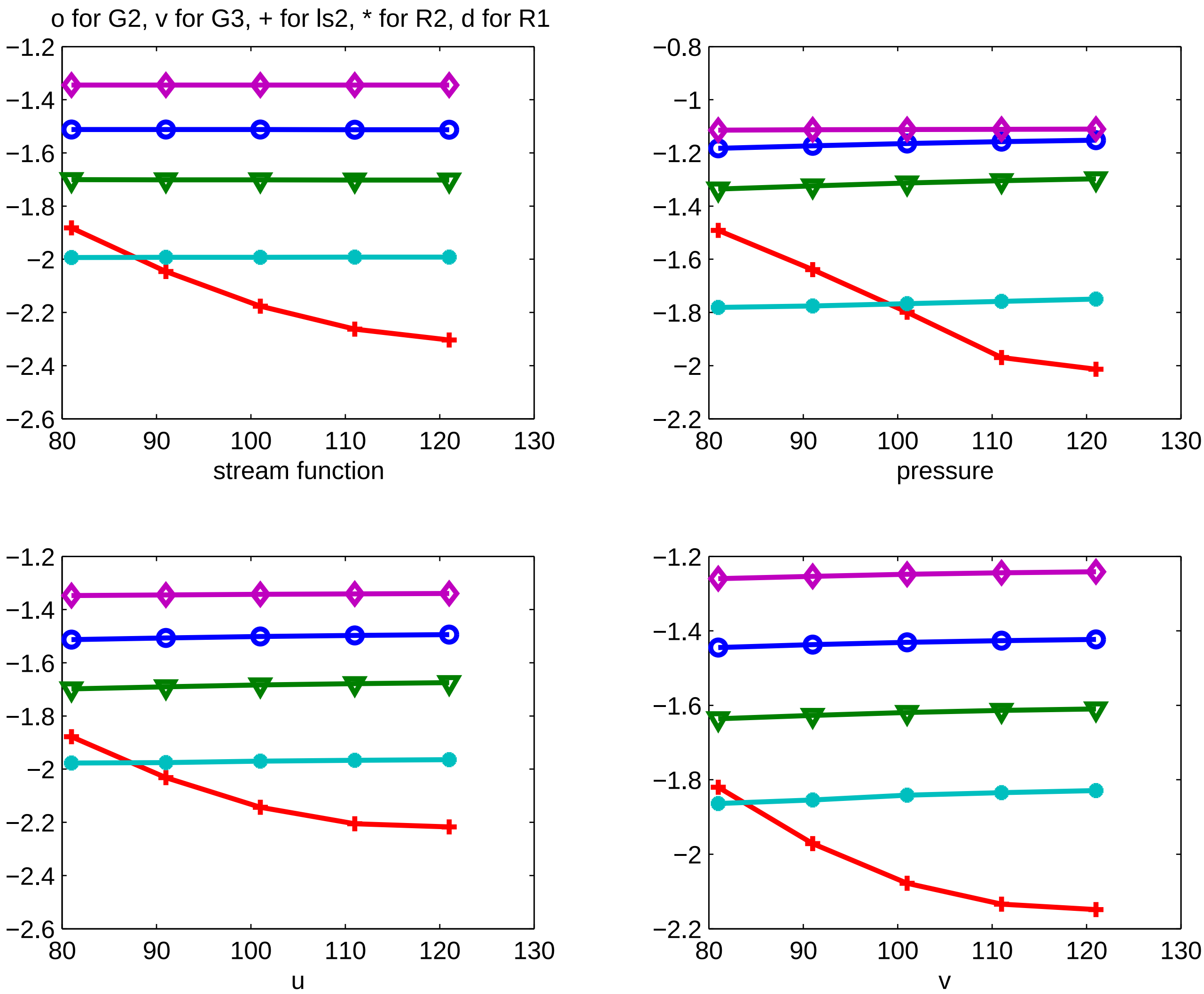
- Numerical locking of the LSE method to predict solution when the grid M^0 gets significantly finer than G_3: Smaller residual does not imply smaller error!



• LSE gives good prediction of the solution on a near by finer grid, but as M^0 gets finer:

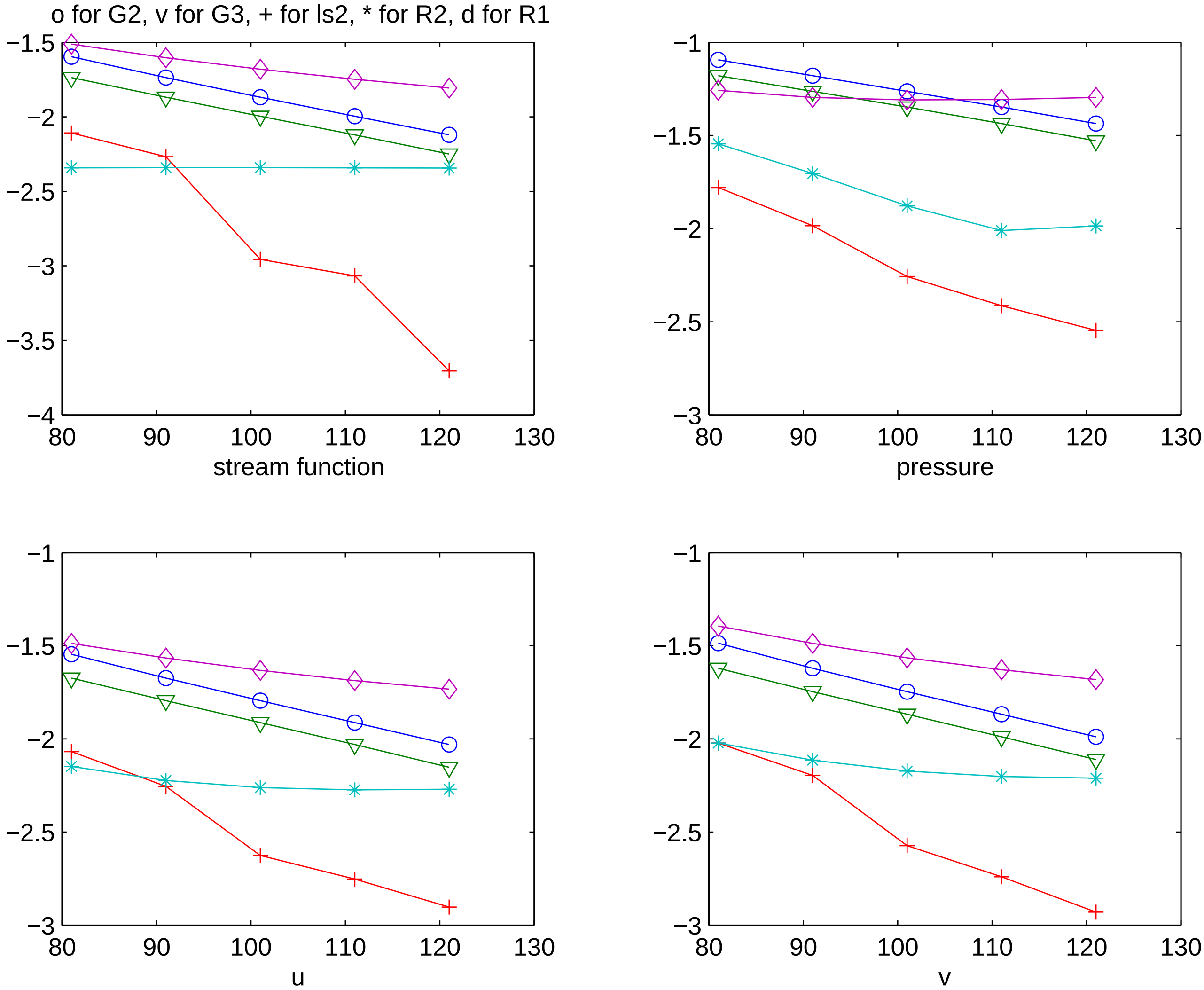
• the Interpolation on the fine grid M^0 adds high spurious wave number terms.

• The LSE method minimizes the L^2 norm of a residual polluted by high frequencies.



x axis is for the number of grid points N in each space direction for the fine grid M^0. Labels of curves are as follows: 'o' for G_2 solution, 'v' for G_3 solution, $\star$ for R2, '$\diamond$' for R1, + for LS2.

- Result obtained by filtering out the high wave components of the residual.

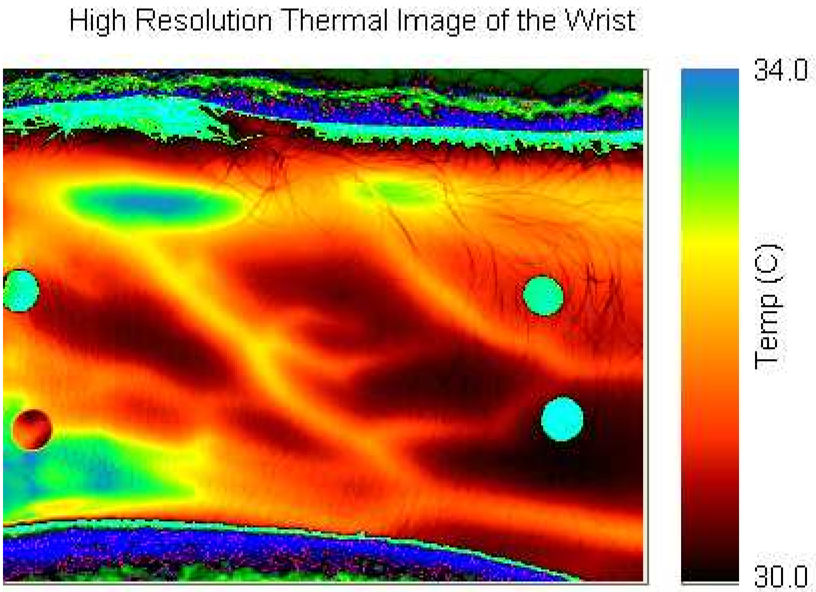


• LSE improves much faster than RE prediction as *coarse grid* gets finer .

• Minimum coarse grid to get reliable error estimate?

• Note: much better results for smoother problems.

(iii) Bioheat transfer Problem: preliminary results



Challenge Recover blood flow rate and heart pulsation from thermal video.

Let us consider the steady problem in $(0,1)^2$,

$$-\frac{\partial}{\partial x}(K(z)\frac{\partial \theta}{\partial x}) - \frac{\partial}{\partial z}(K(z)\frac{\partial \theta}{\partial z}) =$$

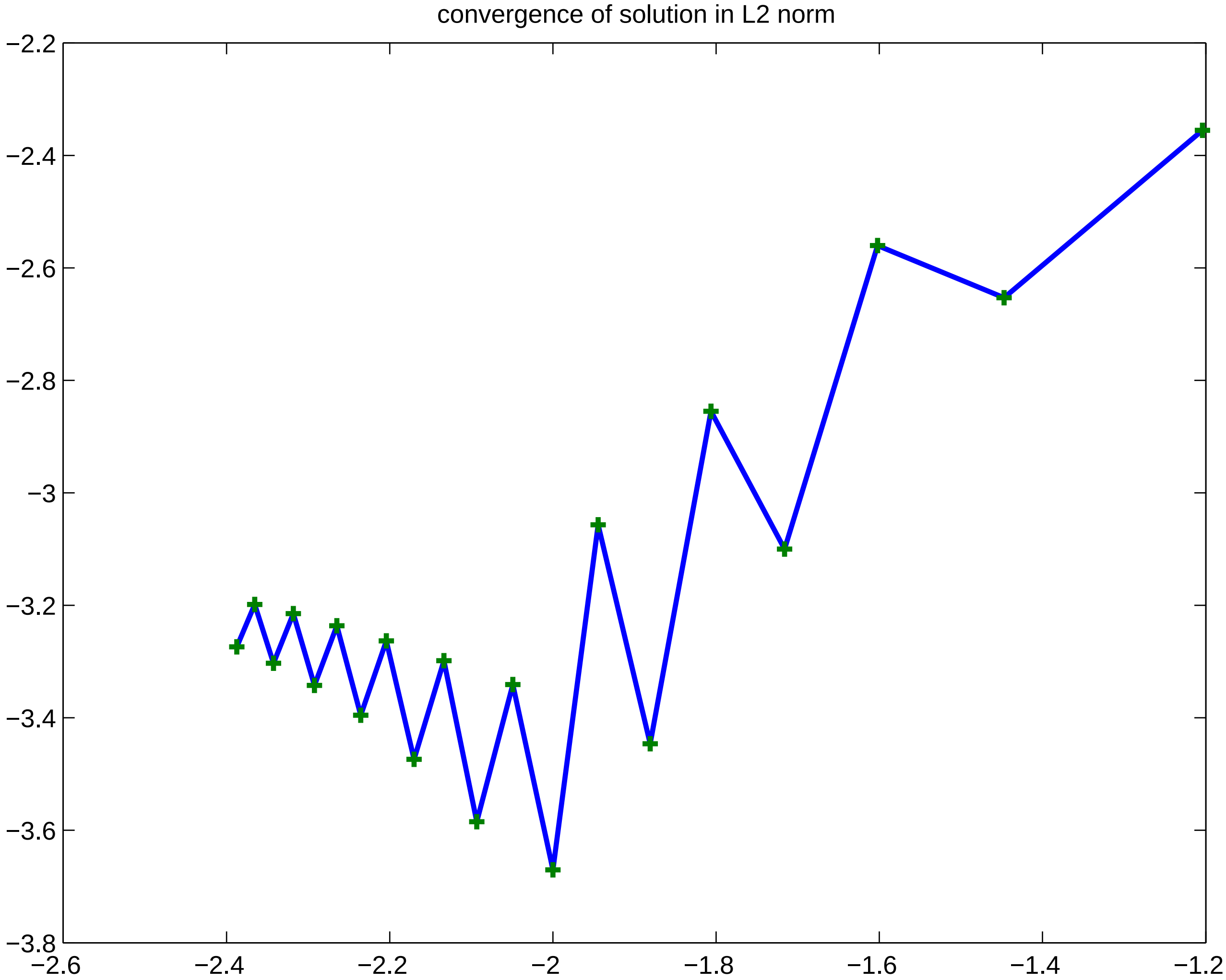
$$\mu\, u(t)\,(1-\theta)\exp(-\frac{(z-S(x))^2}{\eta}) + q^M(x,z),$$

with prescribed temperature at the core, i.e $z=1$, no heat flux at $x=0/1$ and radiative boundary condition at $z=0$.

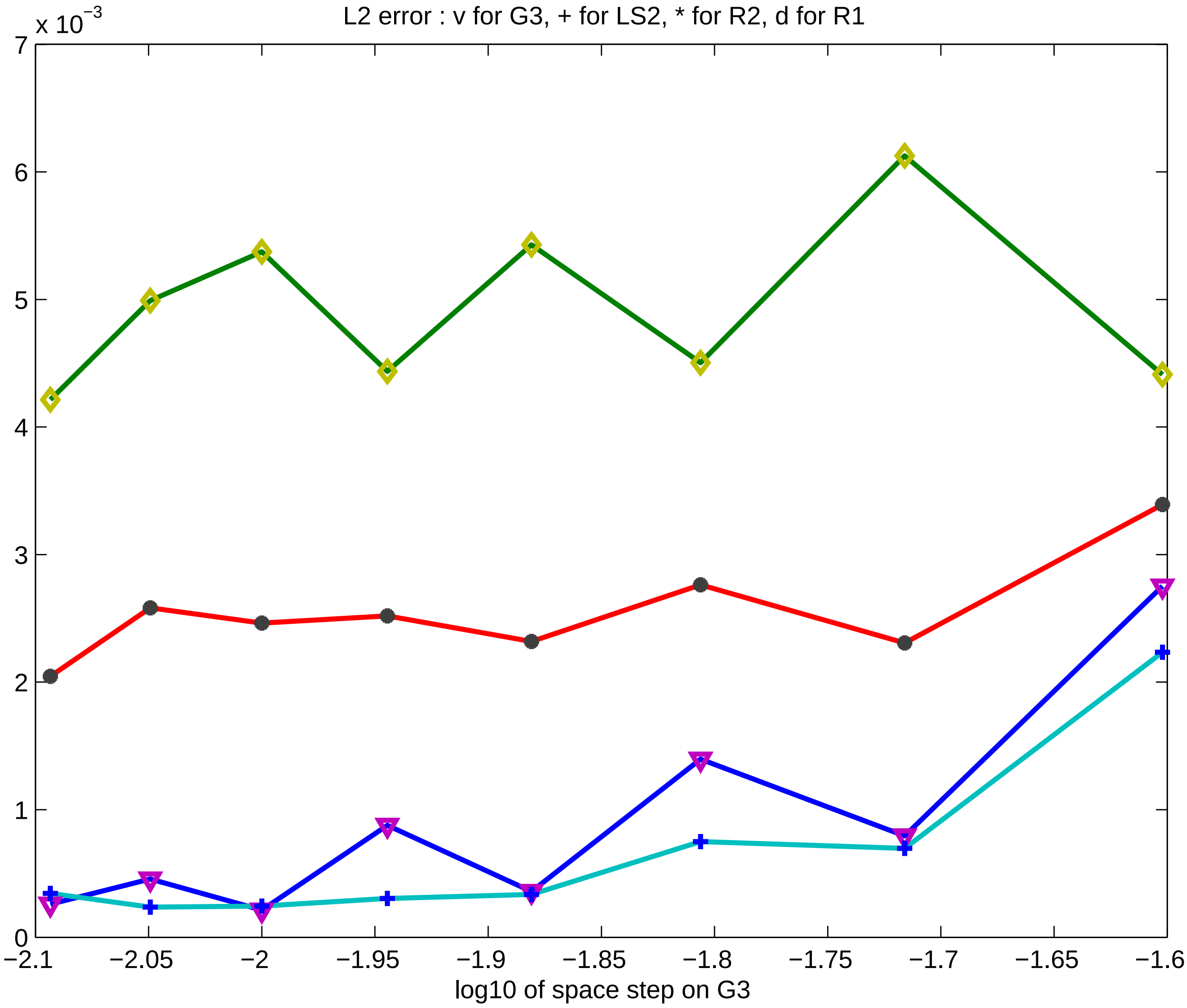
We use a four layer skin method: K is discontinuous at interfaces.

The solution is C^1 but has second order derivative in z direction with finite jump at the line of discontinuities $z = C^t$ of the thermal conductivity K.

We use a Finite Volume (**FV**) approximation with centered cells on a regular space grid.



• Spline interpolation ruins convergence because the solution is NOT C^2



• RE1 and RE2 are worst than coarse grids solutions G1 and/or G2 while LS1 retrieves the best coarse grid solution from G1 and G2.

4. Conclusions and Discussions

- a new extrapolation method for PDEs.
- a better tool for code verification than Richardson extrapolation when the convergence order of a CFD code is space dependent.

ToDo list

- Used generalized least square method, and possibly other objective functions for the extrapolation.
- Adaptive domain decomposition may lead to better choices of representation of the unknown weight function in the extrapolation formula.
- Criteria to relax the constraint on the accuracy of the coarse grid data for efficient least square extrapolation need be further developed.
- Extend the application of our least square extrapolation method to unstructured meshes.