

Aposteriori error analysis of timestepping schemes for the wave equation

using elliptic reconstruction techniques

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a talk based on joint work with

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Adaptive algorithms for computational partial differential equations



University of Birmingham
England UK

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 - The wave equation, backward Euler and energy
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The model linear wave equation

a second order hyperbolic problem

Initial–boundary value problem

$$\partial_{tt}u = \Delta u + f \quad , \quad u|_{\text{spatial boundary}} = 0 \quad \text{and} \quad u(0) = u_0, \quad \partial_t u(0) = v_0.$$

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Simplest timestepping scheme: Backward–Euler for the system (Bernardi and Süli, 2005):

$$\begin{bmatrix} 1 & -k_n \\ +k_n\Delta & 1 \end{bmatrix} \begin{bmatrix} u^n \\ v^n \end{bmatrix} = \begin{bmatrix} u^{n-1} \\ v^{n-1} \end{bmatrix} + \begin{bmatrix} 0 \\ f(t_n) \end{bmatrix}.$$

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Resulting equation form is a 2-step (timestep = k_n) method

$$\frac{u^n - u^{n-1}}{k_n} - \frac{u^{n-1} - u^{n-2}}{k_{n-1}} - k_n \Delta u^n = k_n f(t_n).$$

Goal-oriented duality approach:

W. Bangerth and R. Rannacher (1999) and

Wolfgang Bangerth and Rolf Rannacher (2001)

Direct Galerkin orthogonality with energy approach: Bernardi and Süli (2005)

Semidiscrete analysis:

Picasso (2010)

Heuristic-based adaptive methods:

Wiberg & Li (1998), Schemann & Bornemann (1998),

Romero & Lacoma (2006).

Spatially semidiscrete schemes

Suppose the exact elliptic operator $\mathcal{A} : \text{Dom } \mathcal{A} \rightarrow \text{Ran } \mathcal{A}$, e.g., $-\Delta : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$ is discretized as

$$(8.1) \quad \begin{aligned} A : \mathbb{V} &\rightarrow \mathbb{V} \\ V &\mapsto AV : \langle AV, \Phi \rangle = \langle \mathcal{A}V | \Phi \rangle \quad \forall \Phi \in \mathbb{V} \end{aligned}$$

then a spatially semidiscrete method for the wave equation takes the system form

$$d_t \begin{bmatrix} U(t) \\ V(t) \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ A & 0 \end{bmatrix} \begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} 0 \\ \Pi^{\mathbb{V}} f(t) \end{bmatrix}$$

where $\Pi^{\mathbb{V}}$ is the $L_2(\Omega)$ -orthogonal projection.

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Equation form looks very nice (it is) to analyze

$$d_{tt} U(t) + AU(t) = \Pi^{\mathbb{V}} f(t).$$

Energy methods for the wave equation

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Fully discrete scheme

We consider the fully discrete scheme for the initial value wave problem

$$\text{for each } n = 1, \dots, N, \text{ find } U^n \in V_h^n \text{ such that}$$
$$\langle \partial^2 U^n, V \rangle + a(U^n, V) = \langle f^n, V \rangle \quad \forall V \in V_h^n,$$

where $f^n := f(t^n, \cdot)$, the backward second and first finite differences

$$\partial^2 U^n := \frac{\partial U^n - \partial U^{n-1}}{k_n},$$

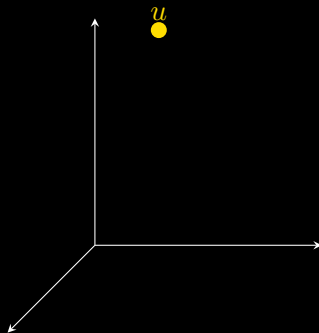
with

$$\partial U^n := \begin{cases} \frac{U^n - U^{n-1}}{k_n}, & \text{for } n = 1, 2, \dots, N, \\ V^0 := \pi^0 u_1 & \text{for } n = 0, \end{cases}$$

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- $u(\cdot, t) \in H_0^1(\Omega)$ exact solution at fixed time t

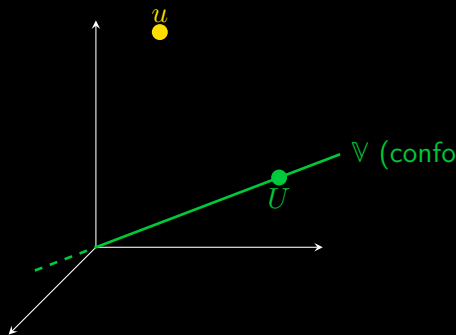
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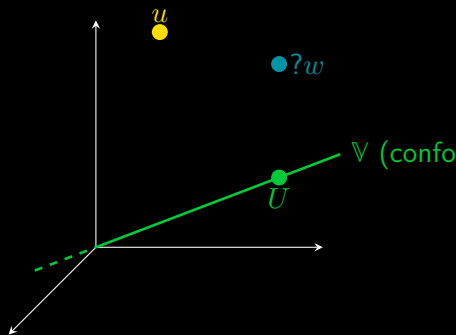
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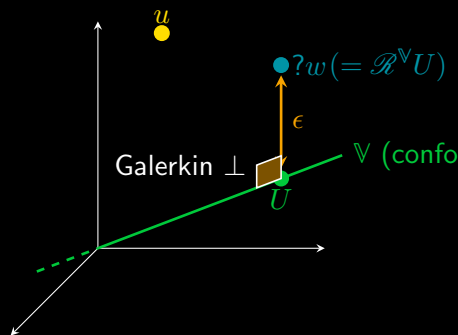
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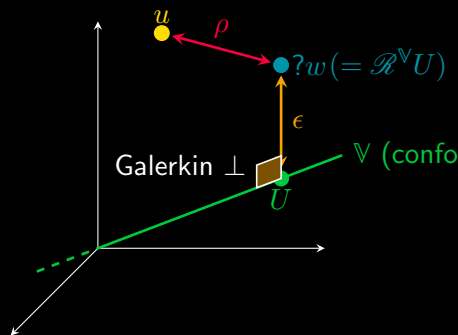
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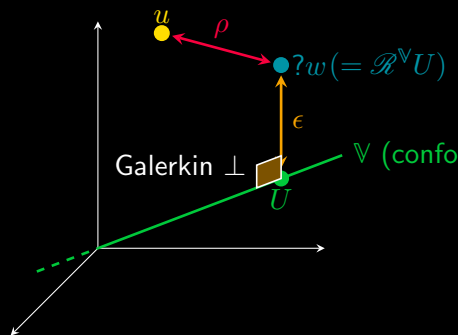
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- but **time dependent error**
 $\rho := w - u$ satisfies original PDE with **computable data**.

$H_0^1(\Omega)$



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$$(25.4) \quad \partial_{tt}[w - u] + \mathcal{A}[w - u] = \partial_{tt}[w - U] + [\Pi^{\vee} - \text{id}]f$$

Elliptic reconstruction: a user's guide (**controlling** ρ)

$$\partial_{tt}\rho + \mathcal{A}\rho = \partial_{tt}\epsilon + \mathcal{A}(w - w^n) + \text{controlled terms}$$

control of the spatial error $\partial_{tt}\epsilon$:

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Example: use relation

$$\partial_{tt}U + \mathcal{A}w^n = \Pi^n f^n$$

leads to explicit a posteriori representation

$$\mathcal{A}w^n := \Pi^n f^n - \partial_{tt}U.$$

A Baker's recipe

introduced by Baker (1976) for $L_\infty(0, T; L_2(\Omega))$ wave equation apriori error estimates

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Theorem (abstract semidiscrete error bound by Georgoulis, Lakkis and Makridakis, 2013)

Let $u(t)$ exact solution, $U(t)$ space-discrete, $\mathcal{R}u(t)$ elliptic reconstruction, and $\epsilon = u - U$. Then

(35.1)

$$\begin{aligned} \|e\|_{L^\infty(0, T; L^2(\Omega))} &\leq \|\epsilon\|_{L^\infty(0, T; L^2(\Omega))} + \sqrt{2} \left(\|u_0 - U(0)\| + \|\epsilon(0)\| \right) \\ &\quad + 2 \int_0^T \|\epsilon_t\| + C_{a, T} \|u_1 - U_t(0)\|, \end{aligned}$$

where $C_{a, T} := \min\{2T, \sqrt{2C_\Omega/\alpha_{\min}}\}$, where C_Ω is the constant of the Poincaré–Friedrichs inequality $\|v\|^2 \leq C_\Omega \|\nabla v\|^2$, for $v \in H_0^1(\Omega)$.

Proof: test with $v(\cdot, t) = \int_\tau^t \rho(\cdot, s) \, ds$ for each τ and then take \max_τ .

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- ② To analyze the fully discrete scheme we also need:
 - Discrete Baker's test function.
 - a special cubic time-reconstruction satisfying a crucial vanishing moment property

Theorem (abstract fully-discrete error bound by Georgoulis, Lakkis and Makridakis, 2013)

Let w^n be the elliptic reconstruction of U^n , $n = 0, \dots, N$, and consider the $C^{1,1}$ -piecewise quadratic extension w, U , of both functions respectively,

$$(42.1) \quad U(t) := \frac{t - t^{n-1}}{k_n} U^n + \frac{t^n - t}{k_n} U^{n-1} - \frac{(t - t^{n-1})(t^n - t)^2}{k_n} \partial^2 U^n \quad \text{and} \quad \partial^2 U^n := \frac{\partial U^n - \partial U^{n-1}}{k_n}$$

$$\epsilon := w - u \quad \text{and} \quad e := u - U$$

where w is the elliptic reconstruction of u and $\eta_1(\tau), \dots, \eta_4(\tau)$ be appropriate (time τ -dependent) error indicators then

$$(42.2) \quad \|e\|_{L^\infty(0, t^N; L^2(\Omega))} \leq \| \epsilon \|_{L^\infty(0, t^N; L^2(\Omega))} + \sqrt{2} \left(\|u_0 - U(0)\| + \| \epsilon(0) \| \right)$$

$$+ 2 \left(\int_0^{t^N} \| \epsilon_t \| + \sum_{i=1}^4 \eta_i(t^N) \right) + C_{a,N} \|u_1 - V^0\|,$$

where $C_{a,N} := \min\{2t^N, \sqrt{2C_\Omega/\alpha_{\min}}\}$, C_Ω is Poincaré–Friedrichs inequality constant.

Error indicators I

For any $\tau \in (t^{m-1}, t^m]$

mesh change indicator

$\eta_1(\tau) := \eta_{1,1}(\tau) + \eta_{1,2}(\tau)$, with

$$\eta_{1,1}(\tau) := \sum_{j=1}^{m-1} \int_{t^{j-1}}^{t^j} \|(I - \Pi^j)U_t\| + \int_{t^{m-1}}^{\tau} \|(I - \Pi^m)U_t\|,$$

$$\eta_{1,2}(\tau) := \sum_{j=1}^{m-1} (\tau - t^j) \|(\Pi^{j+1} - \Pi^j)\partial U^j\| + \tau \|(I - \Pi^0)V^0(0)\|,$$

Error indicators II

evolution error indicator

$$\eta_2(\tau) := \int_0^\tau \|\mathcal{G}\|,$$

where $\mathcal{G} : (0, T] \rightarrow \mathbb{R}$ with $\mathcal{G}|_{(t^{j-1}, t^j]} := \mathcal{G}^j$, $j = 1, \dots, N$ and

$$\mathcal{G}^j(t) := \frac{(t^j - t)^2}{2} \partial g^j - \left(\frac{(t^j - t)^4}{4k_j} - \frac{(t^j - t)^3}{3} \right) \partial^2 g^j - \gamma_j,$$

with

$$g^n := A^n U^n - \Pi^n f^n + \bar{f}^n,$$

$$\gamma_j := \begin{cases} 0 & \text{for } j = 0 \\ \gamma_{j-1} + \frac{k_j^2}{2} \partial g^j + \frac{k_j^3}{12} \partial^2 g^j & \text{if } j = 1, \dots, N. \end{cases}$$

Error indicators III

data error indicator

$$\eta_3(\tau) := \frac{1}{2\pi} \sum_{j=1}^{m-1} \left(\int_{t^{j-1}}^{t^j} k_j^3 \|\bar{f}^j - f\|^2 \right)^{1/2} + \left(\int_{t^{m-1}}^{\tau} k_m^3 \|\bar{f}^m - f\|^2 \right)^{1/2};$$

time reconstruction error indicator

$$\eta_4(\tau) := \frac{1}{2\pi} \sum_{j=1}^{m-1} \left(\int_{t^{j-1}}^{t^j} k_j^3 \|\mu^j \partial^2 U^j\|^2 \right)^{1/2} + \left(\int_{t^{m-1}}^{\tau} k_m^3 \|\mu^m \partial^2 U^m\|^2 \right)^{1/2}.$$

What is μ^n ? I

Proposition (fully-discrete error relation)

Denote $\rho := u - w$ ($w := \mathcal{R}u$) and $t \in (t^{n-1}, t^n]$, $n = 1, \dots, N$, we have

$$(46.1) \quad \langle e_{tt}, v \rangle + a(\rho, v) = \langle (I - \Pi^n)U_{tt}, v \rangle + \mu^n \langle \partial^2 U^n, \Pi^n v \rangle \\ + a(w - w^n, v) + \langle \bar{f}^n - f, v \rangle$$

for all $v \in H_0^1(\Omega)$, with $\Pi^n : L^2(\Omega) \rightarrow V_h^n$ denoting the orthogonal L^2 -projection operator onto V_h^n , I is the identity mapping in $L^2(\Omega)$, and

$$\mu^n(t) := -6k_n^{-1}(t - t^{n-\frac{1}{2}}),$$

where $t^{n-\frac{1}{2}} := \frac{1}{2}(t^n + t^{n-1})$.

What is μ^n ? II

Remark (vanishing moments)

Crucially the functions μ^n satisfy:

$$\int_{t^{n-1}}^{t^n} \mu^n(t) dt = 0.$$

so when integrating in time

$$(46.2) \quad \langle e_{tt}, v \rangle + a(\rho, v) = \langle (I - \Pi^n)U_{tt}, v \rangle + \mu^n \langle \partial^2 U^n, \Pi^n v \rangle \\ + a(w - w^n, v) + \langle \bar{f}^n - f, v \rangle$$

*the μ^n terms disappear leading to **optimal order** error indicators.*

Verlet, leapfrog and cosine methods

analysis is useful for useful methods Georgoulis, Lakkis, Makridakis and Virtanen, 2014

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- Further generalizable to **family of cosine methods**, in similar spirit to exponential methods for first order DE's.

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- Størmer (1907) in electromagnetics.
- Also known as the **Newmark schemes**.
- Rediscovered and popularized amongst modern physicists (for molecular dynamics) with modern computers in 1960's by **Loup Verlet** as a two-step method:

(61.1)

$$\ddot{u} = A(u), u(0) = u_0, \dot{u}(0) = v_0 \Leftrightarrow \begin{cases} \dot{u} = v & u(0) = u_0 \\ \dot{v} = A(u) & v(0) = v_0 \end{cases}$$

$$u^1 := u_0 + v_0 k + \frac{1}{2} A(u_0) (k)^2$$

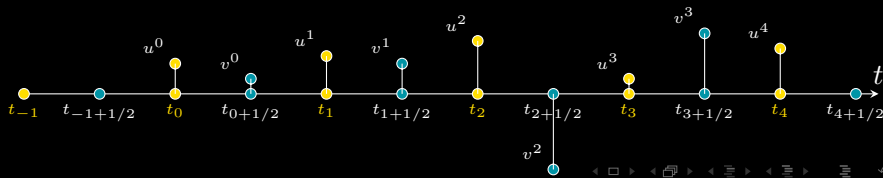
$$u^{n+1} k = 2u^n - u^{n-1} + A(u^n) (k)^2$$

The “simplest” Verlet method

$$(62.1) \quad \ddot{u} = A(u), \quad u(0) = u_0, \quad \dot{u}(0) = v_0 \Leftrightarrow \begin{cases} \dot{u} = v & u(0) = u_0 \\ \dot{v} = A(u) & v(0) = v_0 \end{cases}$$
$$u^1 := u_0 + v_0 k + \frac{1}{2} A(u_0) (k)^2$$
$$u^{n+1} k = 2u^n - u^{n-1} + A(u^n) (k)^2$$

Using **staggered time-grid** idea we can write it as a system by introducing sequence of “velocities”:

$$v^0 := v_0 + \frac{1}{2} A(x_0) k \text{ and } v^{n+1/2} := \frac{u^{n+1} - u^n}{k}, \text{ for each } n = 1, \dots, N-1.$$



Leapfrog for wave

$$(63.1) \quad \partial_{tt}u + \mathcal{A}u = f, \quad u(0) = u_0 \text{ and } v(0) = v_0,$$

where \mathcal{A} is elliptic operator (including boundary conditions).

Leapfrog for wave

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where \mathcal{A} is elliptic operator (including boundary conditions). We can now write the method (semidiscrete in time) as a system in the staggered form considered in Hairer, Lubich and Wanner, 2003:

$$(64.2) \quad \begin{aligned} \partial U^n - V^{n-1/2} &= 0, \\ \partial V^{n-1/2} + \mathcal{A}U^{n-1} &= f^{n-1}, \end{aligned}$$

for $n = 1, \dots, N$.

Time-discrete analysis

including the spatial reconstructions

Consider $U : [-k_1, T] \rightarrow \text{Dom } \mathcal{A}$ continuous piecewise affine interpolant of $(U^n)_{n \in n=-1, \dots, N}$ then $U_1 : [0, T] \rightarrow \text{Dom } \mathcal{A}$ the same for the values $U^{n-1/2} := U(t_{n-1/2})$, for $n = 0, \dots, N$. Similarly, but on the staggered mesh build functions V and V_1 .

$$(65.1) \quad \begin{aligned} \partial_t U - I_0 V_1 &= R_V, \\ \partial_t V + \mathcal{A} \tilde{I}_0 U_1 &= \tilde{I}_0 f + R_U, \end{aligned}$$

where we define the interpolators

$$(65.2) \quad \begin{aligned} \tilde{I}_0 &: \text{piecewise constant midpoint interpolator on } \{(t^{n-1/2}, t^{n+1/2})\}_{n=0}^{N-1}, \\ I_0 &: \text{piecewise constant midpoint interpolator on } \{(t^{n-1}, t^n)\}_{n=1}^{N-1}. \end{aligned}$$

Time reconstructions

$$(66.1) \quad \hat{V}(t) := V^{n-1/2} + \int_{t_{n-1/2}}^t (-\mathcal{A}U_1 + \tilde{I}_1 f + \rho_U),$$

and

$$(66.2) \quad \hat{U}(t) := U^{n-1} + \int_{t_{n-1}}^t (V_1 + \rho_V).$$

Setting $\hat{e}_U := u - \hat{U}$ and $\hat{e}_V := u' - \hat{V}$, we deduce

$$(66.3) \quad \begin{aligned} \hat{e}'_V + \mathcal{A}\hat{e}_U &= \mathcal{R}_1 + \mathcal{R}_f \\ \hat{e}'_U - \hat{e}_V &= \mathcal{R}_2, \end{aligned}$$

with the following **residuals**

$$(66.4) \quad \begin{aligned} \mathcal{R}_1 &:= -\mathcal{A}(\hat{U} - U_1) - \rho_U, \\ \mathcal{R}_2 &:= \hat{V} - V_1 - \rho_V, \\ \mathcal{R}_f &:= f - \tilde{I}_1 f. \end{aligned}$$

$$\begin{aligned} (67.1) \quad \frac{1}{2} \frac{d}{dt} \|\|(\hat{e}_U, \hat{e}_V)\|\|^2 &= (((\hat{e}'_U, \hat{e}'_V), (\hat{e}_U, \hat{e}_V))) \\ &= (\mathcal{A}\hat{e}'_U, \hat{e}_U) + (\hat{e}'_V, \hat{e}_V) \\ &= (\mathcal{A}\hat{e}_V, \hat{e}_U) + (\mathcal{A}\mathcal{R}_2, \hat{e}_U) - (\mathcal{A}\hat{e}_U, \hat{e}_V) \\ &\quad + (\mathcal{R}_1, \hat{e}_V) + (\mathcal{R}_f, \hat{e}_V) \\ &= (\mathcal{A}\mathcal{R}_2, \hat{e}_U) + (\mathcal{R}_1, \hat{e}_V) + (\mathcal{R}_f, \hat{e}_V), \end{aligned}$$

Theorem

Let u be the solution of the wave equation, $\hat{e}_U := u - \hat{U}$ and $\hat{e}_V := u' - \hat{V}$. Then, the following a posteriori error estimate holds (68.1)

$$\sup_{t \in [0, t^N]} \|\|(\hat{e}_U, \hat{e}_V)(t)\|\|^2 \leq 2\|\|(\hat{e}_U, \hat{e}_V)(0)\|\|^2 + 4\left(\int_0^{t^N} \|\|(\mathcal{R}_2, \mathcal{R}_1 + \mathcal{R}_f)\|\| dt\right)^2,$$

where \mathcal{R}_2 , \mathcal{R}_1 , and \mathcal{R}_f are defined in (66.4).

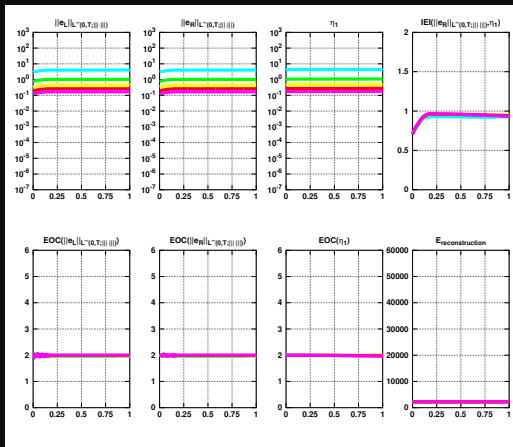
An immediate Corollary is an a posteriori bound for the error $\sup_{[0, t^N]} \|\|(u - U, u' - V)\|\|$.

Numerics with known exact solution

$$u(t, x) := \sum_{j,k=1}^3 \sin(\pi k x) \sin(\pi j y) (\alpha_{k,j} \cos(\pi \xi_{k,j} t) + \beta_{k,j} \sin(\xi_{k,j} \pi t))$$

numerics for $c = 1.0, \alpha_{1,1} = \beta_{1,1} = 15.0, \beta_{k,j} = \alpha_{k,j} = 0$

Errors, estimator and inverse effectivity indexes (IEIs) are plotted on the top row while experimental orders of convergence (EOCs) and energy of the reconstructed solution on the bottom row over time (abscissa). Results are computed on the sequence of uniform meshes with mesh size h , fixed time step $k = 0.4h/(p+1)^2$ and $p = 2$. The IEI behaviour indicates that the error is well estimated by the estimator and the convergence rate of the estimator remains near to $\text{EOC} \approx 2$, i.e., to that of the errors e_L and e_R .

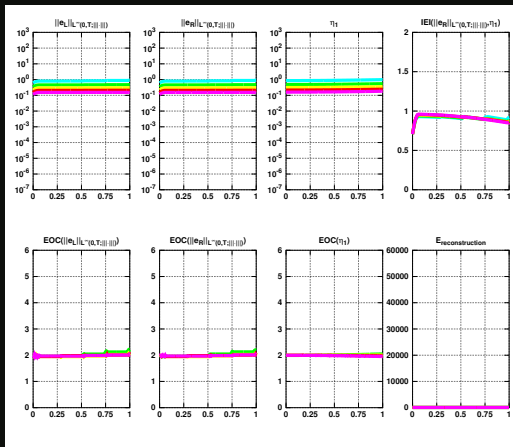


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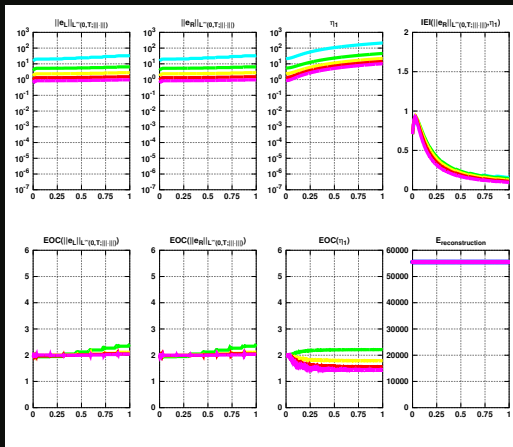


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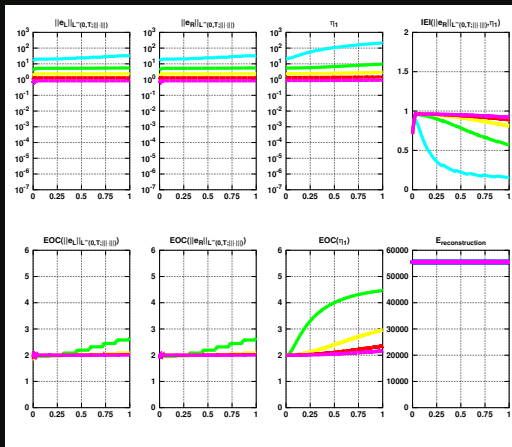


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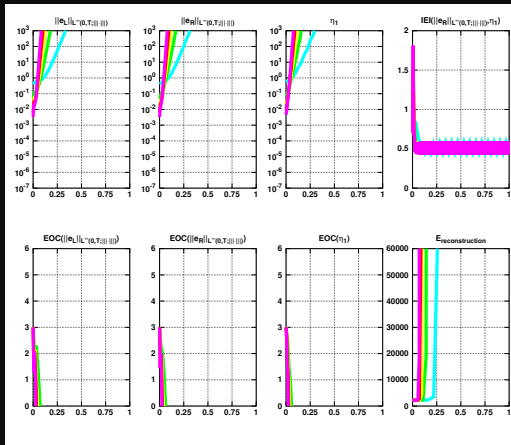


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numerics for $c = 1.0$, $\alpha_{1,1} = \beta_{1,1} = 15.0$, $\beta_{k,j} = \alpha_{k,j} = 0$ violation of the CFL condition

Violation of the CFL condition. Errors, estimator and IEI are depicted on the top row and EOCs and energy of the reconstructed solution on the bottom row against time in abscissa. Results are computed on the sequence of uniform meshes with mesh size h and time step $k = 2.0h/(p + 1)^2$ and $p = 3$. The IEI's behaviour indicates that the error is overestimated by the estimator but follows the error behaviour.



Conclusions

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- ⑤ Practical estimates must be derived for practical schemes. Backward Euler is an academic exercise, but leapfrog/Verlet and more generally cosine/Newmark methods must be analyzed. A first step by Georgoulis, Lakkis, Makridakis and Virtanen (2014) with the staggered timestepping.

Credits

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