Numerical simulations of first order systems

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joint work with L. Ludwig (TU Dresden), R. Picard (TU Dresden), S. Trostorff (Uni Kiel), M. Waurick (TU Freiberg)

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General class of problems

Let

- H be a real Hilbert space, $\rho > 0$,
- inner product: $\langle f, g \rangle_\rho := \int_{\mathbb{R}} \langle f(t), g(t) \rangle_H \mathrm{e}^{-2\rho t} \, \mathrm{d}t$,
- norm: $\|f\|_\rho := \langle f, f \rangle_\rho^{1/2}$,
- $H_\rho(\mathbb{R}; H) := \{ f : \mathbb{R} \to H \ : \ f \text{ meas.}, \|f\|_\rho < \infty \}$.

Picard: An Elementary Hilbert Space Approach to Evolutionary Partial Differential Equations, *Rend. Istit. Mat. Univ. Trieste*, 2010
Picard, McGhee: Partial Differential Equations: A unified Hilbert Space Approach, *volume 55 of De Gruyter Expositions in Mathematics*, 2011

General class of problems

The problem class

$$\overline{(\partial_t \mathcal{M}_0 + \mathcal{M}_1 + \mathcal{A})} U = F,$$

where

- ∂_t is the time derivative,
- $\mathcal{M}_0$, $\mathcal{M}_1$ are bounded, linear, self-adjoint operators on H,
- $\mathcal{A}$ is an unbounded, skew-selfadjoint operator on H,
- $\exists \rho_0, \gamma > 0 \, \forall \rho \geq \rho_0, x \in H: \qquad \langle (\rho \mathcal{M}_0 + \mathcal{M}_1)x, x \rangle_H \geq \gamma \langle x, x \rangle_H$,

has for each $\rho \geq \rho_0$ and $F \in H_\rho(\mathbb{R}; H)$ a unique solution $U \in H_\rho(\mathbb{R}; H)$ and it holds

$$\|U\|_\rho \leq \frac{1}{\gamma} \|F\|_\rho.$$

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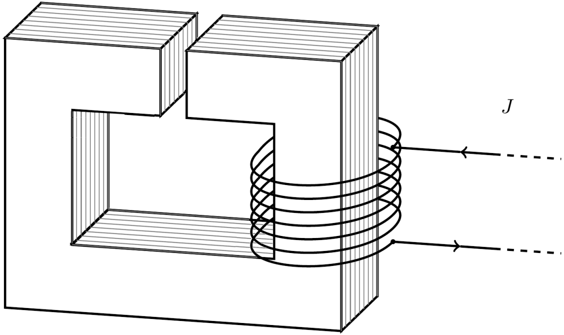
Transformer



Pauly, Picard: A Note on the Justification of the Eddy Current Model in Electrodynamics, *MMAS*, 40(18), 2017

Examples

Maxwell's-equations where $J(t,\boldsymbol{x}) = K(t,\boldsymbol{x}) = 0$ for $t < 0$.

$$\left[\partial_t \begin{pmatrix} \varepsilon & 0 \\ 0 & \mu \end{pmatrix} + \begin{pmatrix} \sigma & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\operatorname{curl} \\ \mathring{\operatorname{curl}} & 0 \end{pmatrix}\right] \begin{pmatrix} E \\ H \end{pmatrix} = \begin{pmatrix} -J \\ K \end{pmatrix}$$

$\mu > 0$, ε, $\sigma \geq 0$, and $\varepsilon + \sigma > 0$
solution space:

$$V = \left\{ (E,H) : \begin{array}{l} E, H \in H^1_\rho\left(\mathbb{R}_+;\ (L^2(\Omega))^d\right) \cap H_\rho\left(\mathbb{R}_+; H(\operatorname{curl},\Omega)\right), \\ \boldsymbol{n} \times E|_{\partial\Omega} = 0 \end{array} \right\}$$

no transmission conditions

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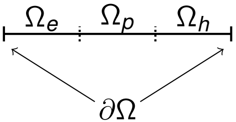
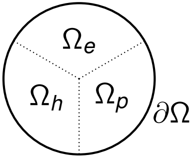
Examples

changing type systems





$$\left[\partial_t \begin{pmatrix} \mathbb{1}_{\Omega_h\cup\Omega_p} & 0 \\ 0 & \mathbb{1}_{\Omega_h} \end{pmatrix} + \begin{pmatrix} \mathbb{1}_{\Omega_e} & 0 \\ 0 & \mathbb{1}_{\Omega_p\cup\Omega_e} \end{pmatrix} + \begin{pmatrix} 0 & \operatorname{div} \\ \mathring{\operatorname{grad}} & 0 \end{pmatrix}\right]\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

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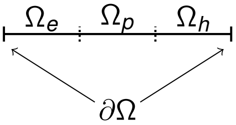

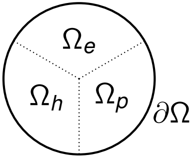

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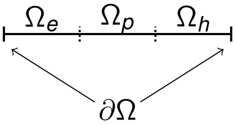

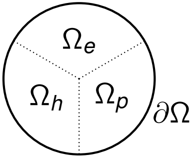

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no transmission conditions

Further problems that fit

- heat-, wave-, Poisson-equations
- Maxwell's equations
- acoustic wave equations,
- (regularised) Stokes equation,
- dynamic linear elasticity,
- piezo-electric models,
- fractional integrals,
- ...

and any combination of above equations.

SF, Waurick: Resolvent estimates and numerical implementation for the homogenisation of one-dimensional periodic mixed type problems, *ZAMM*, 98(7), 2018
SF, Waurick: Homogenisation of parabolic/hyperbolic media,, *BAIL2018 Proceedings*, 2020

Time – Discontinuous Galerkin

continuous form:
Find $U \in V$, such that for all $\Phi \in V$ and $m = 1, \dots, M$

$$\langle (\partial_t \mathcal{M}_0 + \mathcal{M}_1 + \mathcal{A})U, \Phi \rangle_{\rho,m} = \langle F, \Phi \rangle_{\rho,m} ,$$

where $\langle \cdot, \cdot \rangle_{\rho,m}$ is the weighted inner product localised to $I_m := (t_{m-1}, t_m]$.

semidiscrete form:
Find $U^\tau \in \mathcal{V}^\tau := \mathcal{P}_q^{disc}([0,T], H)$, such that for all $\Phi \in \mathcal{V}^\tau$ and m

$$\langle (\partial_t \mathcal{M}_0 + \mathcal{M}_1 + \mathcal{A})U^\tau, \Phi \rangle_{\rho,m} + \langle \mathcal{M}_0 [\![U^\tau]\!]_{m-1}, \Phi_{m-1}^+ \rangle_H = \langle F, \Phi \rangle_{\rho,m} ,$$

where $[\![\cdot]\!]_{m-1}$ is the jump at the time t_{m-1}.
There is exactly one solution for each $F \in H_\rho(\mathbb{R}; H)$.

SF, Trostorff, Waurick: Numerical methods for changing type systems *IMA J. Numer. Anal.*, 39 (2), 2019

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Finite Element Method

discrete form:

Find $U_h \in \mathcal{V}_h^\tau$, such that for all $\Phi \in \mathcal{V}_h^\tau$, $m = 1, \ldots, M$

$$Q\left[(\partial_t \mathcal{M}_0 + \mathcal{M}_1 + \mathcal{A})U_h, \Phi\right]_{\rho,m} + \left\langle \mathcal{M}_0 [\![U_h]\!]_{m-1}, \Phi_{m-1}^+ \right\rangle_H = Q\left[F, \Phi\right]_{\rho,m},$$

where $[\![\cdot]\!]_{m-1}$ is the jump at the time t_{m-1} and $Q\left[\cdot,\cdot\right]_{\rho,m}$ is a weighted right-sided Gauß-Radau quadrature rule exactly for $p \in \mathcal{P}_{2q}(I_m; H)$.

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Choice of discrete space

In *time*, the functions are piecewise polynomials in t of degree q, globally discontinuous.

Depending on $\mathcal{A}$ we choose conforming, piecewise polynomial spaces for the spatial discretisation.

- grad : $\Rightarrow H^1$-conform,
  piecewise polynomials in $\boldsymbol{x}$ of degree k, globally continuous
- div : $\Rightarrow H(div)$-conform
  Raviart-Thomas or Brezzi-Douglas-Marini elements in $\boldsymbol{x}$ of degree $k-1$
- curl : $\Rightarrow H(curl)$-conform
  Nédélec-elements in $\boldsymbol{x}$ of degree k

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Abstract convergence results

Assuming enough regularity in time and space (roughly $U \in H^1_\rho(\mathbb{R}; H^k(\Omega)) \cap H^{q+2}_\rho(\mathbb{R}; L^2(\Omega))$) we obtain

$$\mathrm{e}^{-2\rho T} \sup_{t\in[0,T]} \|\mathcal{M}_0^{1/2}(U - U_h)(t)\|_H^2 + \|U - U_h\|^2_{Q,\rho} \leq C(\tau^{2(q+1)} + Tg(h)^2)$$

where $g(h)$ represents the approximation quality of the chosen discrete space, depending on k (again roughly $g(h) = h^k$).

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Drawback of this approach

- Even for continuous data there is no continuity in time, although jumps converge towards zero (order $q + 1/2$).
- Dissipative method in the sense (r.h.s $= 0$)

$$e^{-2\rho t}\|\mathcal{M}_0^{1/2}U(t)\|_H^2 + 2\|(\rho\mathcal{M}_0 + \mathcal{M}_1)^{1/2}U\|_{\rho,(0,t)}^2 = \|\mathcal{M}_0^{1/2}U(0)\|_H^2$$

vs.

$$e^{-2\rho t_i}\|\mathcal{M}_0^{1/2}U_{i-}^{\tau}\|_H^2 + 2\|(\rho\mathcal{M}_0 + \mathcal{M}_1)^{1/2}U^{\tau}\|_{\rho,(0,t_i)}^2$$

$$+ 2\sum_{m=1}^{i} e^{-2\rho t_{m-1}}\|\mathcal{M}_0^{1/2}[\![U^{\tau}]\!]_{m-1}^{x_0}\|_H^2 = \|\mathcal{M}_0^{1/2}U_{0-}^{\tau}\|_H^2$$

Alternative: Continuous Galerkin-Petrov instead of dG-methods in time.

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A singularly perturbed problem

Let a singularly perturbed reaction-diffusion problem on $\Omega = (0,1)^2$ be given by

$$-\varepsilon^2 \Delta u + cu = f,\ 0 < \varepsilon \ll 1,\ 0 < c_0 \le c \le c_\infty$$

and $u = 0$ on $\partial\Omega$. Using $\boldsymbol{u} = -\varepsilon \operatorname{grad}^\circ u$ we have the first order system

$$\left[\begin{pmatrix} c & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon \operatorname{div} \\ \varepsilon \operatorname{grad}^\circ & 0 \end{pmatrix}\right] \begin{pmatrix} u \\ \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

We obtain the weak formulation

$$B(U,V) := \langle cu, v\rangle + \varepsilon \langle \operatorname{div} \boldsymbol{u}, v\rangle + \langle \boldsymbol{u}, \boldsymbol{v}\rangle - \varepsilon \langle u, \operatorname{div} \boldsymbol{v}\rangle = \langle f, v\rangle$$

for $U = (u, \boldsymbol{u})$ and $V = (v, \boldsymbol{v}) \in L^2(\Omega) \times H_{\mathrm{div}}(\Omega)$.

SF: Singularly perturbed reaction-diffusion problems as first order systems, *J. Sci. Comput.* 89(38), 2021

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Stronger norm

We have immediately

$$B(U,U) \geq \min\{1, c_0\}\|U\|^2_{L^2(\Omega)} = \min\{1, c_0\}(\|u\|^2_{L^2(\Omega)} + \|\boldsymbol{u}\|^2_{L^2(\Omega)})$$

that is equivalent to coercivity in the energy norm of the initial problem. But we can actually use the stronger norm

$$|||U||| := \left(\|U\|^2_{L^2(\Omega)} + \delta\|\varepsilon \operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)}\right)^{1/2}, \ \delta \leq \frac{c_0}{c_\infty^2}.$$

This norm is equivalent to the weighted H^2-norm $\|u\|_{L^2} + \varepsilon\|\operatorname{grad}^\circ u\|_{L^2} + \varepsilon^2\|\Delta u\|_{L^2}$, and even a balanced version of this norm

$$|||U|||_{bal} := \left(\|u\|^2_{L^2(\Omega)} + \varepsilon^{-1}\|\boldsymbol{u}\|^2_{L^2(\Omega)} + \delta\varepsilon^{-1}\|\varepsilon \operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)}\right)^{1/2}$$

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Stronger convergence

No coercivity with stronger norm, but for each $\delta \leq \frac{c_0}{c_\infty^2}$ there exists a constant $\beta > 0$, such that for all $V \in \mathcal{U}_N$ it holds

$$\sup_{\chi \in \mathcal{U}_N} \frac{B(V,\chi)}{\|\chi\|_{L^2(\Omega)}} \geq \beta \,|||V|||\,.$$

Using interpolation error estimates for each term on a properly chosen layer adapted rectangular mesh, we obtain for $RT_k(K) = \mathcal{Q}_{k+1,k}(K) \times \mathcal{Q}_{k,k+1}(K)$

$$|||U - U_N|||_{bal} \lesssim (h + N^{-1} \max|\psi'|)^{k+1} (\ln N)^{1/2}.$$

and $BDM_k(K) := (\mathcal{P}_k(K))^2 \oplus \text{span}\{\text{curl}(x^{k+1}y), \text{curl}(xy^{k+1})\}$

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Stronger convergence

No coercivity with stronger norm, but for each $\delta \leq \frac{c_0}{c_\infty^2}$ there exists a constant $\beta > 0$, such that for all $V \in \mathcal{U}_N$ it holds

$$\sup_{\chi \in \mathcal{U}_N} \frac{B(V, \chi)}{\|\chi\|_{L^2(\Omega)}} \geq \beta \, |||V||| \, .$$

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Example

$$-\varepsilon^2 \Delta u + \left(1 + x^2 y^2 e^{xy/2}\right) u = f,$$

where

$$u = \left(\cos\left(\frac{\pi x}{2}\right) - \frac{e^{-x/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}}\right) \cdot \left(1 - y - \frac{e^{-y/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}}\right)$$

Errors $|||U - U_h|||_{bal}$ for fixed $\varepsilon = 10^{-4}$ in the Raviart-Thomas case.

N	$k=1$		$k=2$		$k=3$	
8	9.250e-03		1.059e-03		1.640e-04	
16	2.304e-03	2.01	1.518e-04	2.80	1.238e-05	3.73
32	5.679e-04	2.02	2.023e-05	2.91	8.433e-07	3.88
64	1.402e-04	2.02	2.603e-06	2.96	5.480e-08	3.94
128	3.479e-05	2.01	3.298e-07	2.98	3.488e-09	3.97
256	8.657e-06	2.01	4.148e-08	2.99	2.198e-10	3.99
512	2.158e-06	2.00				

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Errors $|||U - U_h|||_{bal}$ for fixed $\varepsilon = 10^{-4}$ in the Brezzi-Douglas-Marini case.

N	$k = 1$		$k = 2$		$k = 3$	
8	8.406e-01		1.520e-02		2.700e-03	
16	6.451e-01	0.38	3.420e-03	2.15	3.624e-04	2.90
32	3.519e-01	0.87	8.492e-04	2.01	4.606e-05	2.98
64	1.796e-01	0.97	2.144e-04	1.99	5.553e-06	3.05
128	7.124e-02	1.33	5.403e-05	1.99	6.631e-07	3.07
256	2.186e-02	1.70	1.356e-05	1.99	8.129e-08	3.03
512	5.906e-03	1.89	3.390e-06	2.00	1.027e-08	2.98
1024	1.566e-03	1.92				

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Homogenisation with PDEs – Maxwell's equations in 2d

$$(\partial_t M_{0,n} + M_{1,n} + A)U_n = F,$$

Where the coefficients are stratified, i.e. they oscillate only in one direction. Let

$$\mathbb{1}_n(x) := \begin{cases} 1, & \exists i \in \mathbb{Z} : x \in \left[\frac{2i}{n}, \frac{2i+1}{n}\right) \\ 0, & otherwise \end{cases}$$

be the oscillating indicator and $\Omega = (-2,2)^2$, $D = (-1,1)^2$, $\mathbb{I} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$. Then

$$M_{0,n} := \chi_D \cdot \begin{pmatrix} 1 + \mathbb{1}_n & 0 \\ 0 & (1 - \mathbb{1}_n)\mathbb{I} \end{pmatrix} + (1 - \chi_D) \cdot \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & \mu_0 \mathbb{I} \end{pmatrix},$$

$$M_{1,n} := \chi_D \cdot \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1}_n \mathbb{I} \end{pmatrix}, \quad A := \begin{pmatrix} 0 & \operatorname{div} \\ \operatorname{grad}^\circ & 0 \end{pmatrix}, \quad F := \begin{pmatrix} \sin(2\pi t) \\ 0 \end{pmatrix}$$

Ongoing joint work with M. Waurick

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Maxwell's equations in 2d – homogenised equation

$$(\partial_t M_0^{hom} + M_1^{hom} + A)U_{hom} = F,$$

where

$$M_0^{\text{hom}} := \chi_D \cdot \begin{pmatrix} \frac{3}{2} & 0 \\ 0 & \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix} + (1-\chi_D) \cdot \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & \mu_0 \mathbb{I} \end{pmatrix},$$

$$M_1^{\text{hom}} := \chi_D \cdot \begin{pmatrix} 0 & 0 \\ 0 & \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 2-2(1+\partial_t)^{-1} \end{pmatrix} \end{pmatrix}.$$

Thus, by the limit process we obtain an operator with a memory term.

Maxwell's equations in 2d – memory term

Let us define an intrinsic variable w with $w(t,x) = 0$ for $t \leq 0$ by

$$(1+\partial_t)^{-1} v_2 = w \quad \Leftrightarrow \quad v_2 = (1+\partial_t) w \quad \Leftrightarrow \quad \partial_t w + w - v_2 = 0.$$

$$(\partial_t \widehat{M}_0^{\text{hom}} + \widehat{M}_1^{\text{hom}} + \widehat{A}) \widehat{U}^{\text{hom}} = \widehat{F},$$

where $\widehat{U}^{\text{hom}} = (u^{\text{hom}}, v^{\text{hom}}, w^{\text{hom}})^\top$, $\widehat{F} = (f, g, 0)^\top$ and

$$\widehat{M}_0^{\text{hom}} := \chi_D \cdot \begin{pmatrix} M_0^{hom} & 0 \\ 0 & 2 \end{pmatrix} + (1-\chi_D) \cdot \begin{pmatrix} M_0^{hom} & 0 \\ 0 & 0 \end{pmatrix}, \quad \widehat{A} := \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix},$$

$$\widehat{M}_1^{\text{hom}} := \chi_D \cdot \begin{pmatrix} 0 & 0 & 0 \\ 0 & \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{pmatrix} & \begin{pmatrix} 0 \\ -2 \end{pmatrix} \\ 0 & \begin{pmatrix} 0 & -2 \end{pmatrix} & 2 \end{pmatrix} + (1-\chi_D) \cdot \begin{pmatrix} M_1^{hom} & 0 \\ 0 & 1 \end{pmatrix}$$

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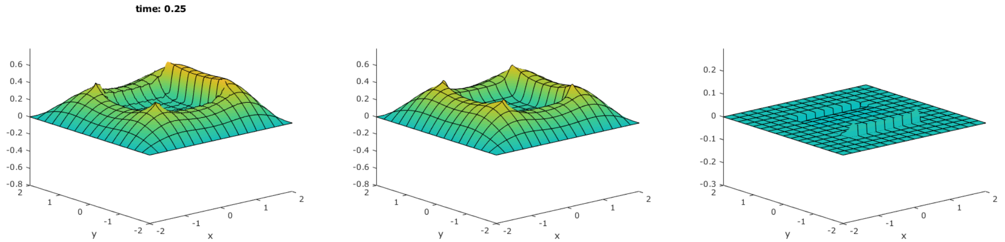
Maxwell's equations in 2d – snapshots of u_8, u^{hom}, w^{hom}



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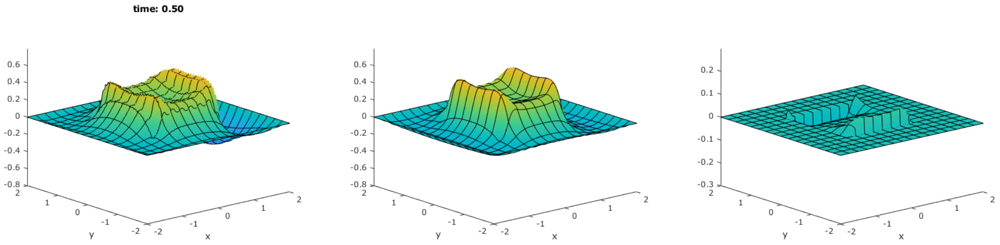

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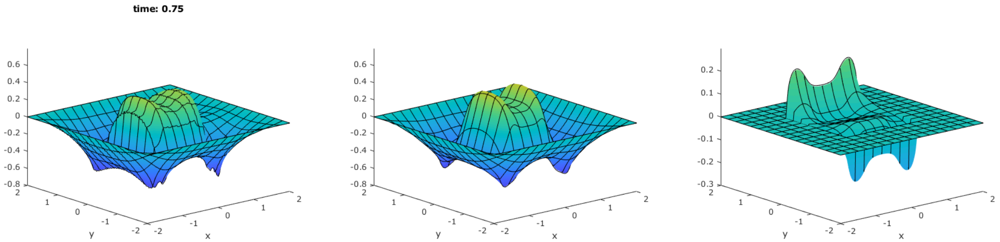

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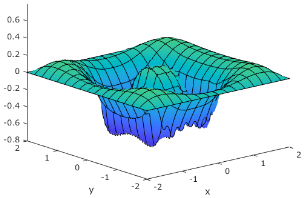
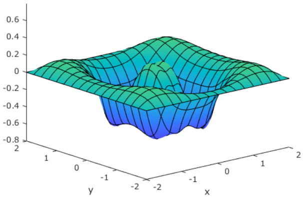
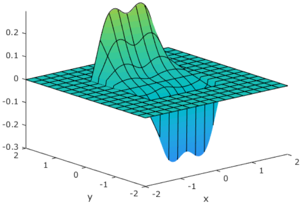
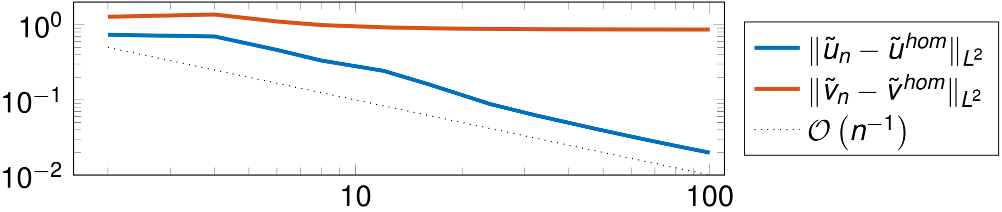
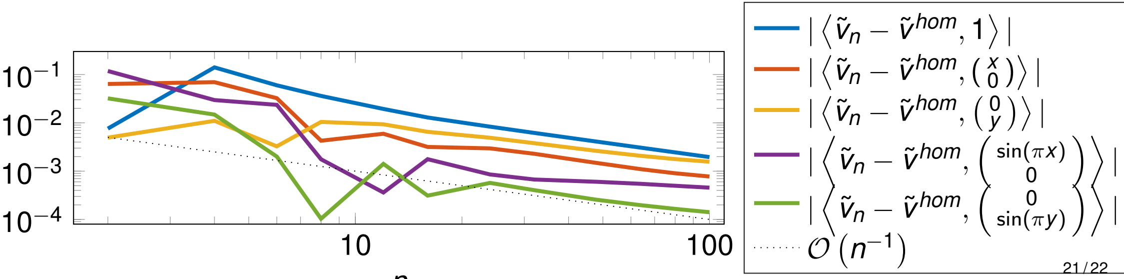






Maxwell's equations in 2d – convergence in n





Conclusion

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- numerical discretisation by discontinuous in time Galerkin methods
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    https://doi.org/10.1093/imanum/dry007 and
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Thank you for your attention!

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