



High order Padé schemes for ODEs

Mamadou N'Diaye

► To cite this version:

Mamadou N'Diaye. High order Padé schemes for ODEs. Journée de l'école doctorale ED211, Jun 2016, Pau, France. hal-01535802

HAL Id: hal-01535802

<https://inria.hal.science/hal-01535802>

Submitted on 9 Jun 2017

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Mamadou N'DIAYE

Advisors : Hélène BARUCQ and Marc DURUFLÉ
Team: Magique-3D INRIA-Bordeaux Sud-Ouest and LMA

Introduction

We consider the following linear test equation

$$y'(t) = i\lambda y(t), \quad y(t_0) = y_0, \quad t \in [t_0, T], \quad (1)$$

which has the exact solution after one step ($h = t_{n+1} - t_n$)

$$y_n = e^{ih\lambda} y_{n-1}.$$

Numerical solution is obtained by approximating

$$e^{ih\lambda} \approx R(ih\lambda).$$

- The scheme is **stable** if $|R(ih\lambda)| \leq 1$,
 - non dissipative** if $|R(ih\lambda)| = 1$,
 - non dispersive** if $\phi(ih\lambda) = ih\lambda - \arg(R(ih\lambda)) = 0$.
- $\forall z \in \mathbb{C}$, $R(z)$ is called the stability function of the numerical scheme.

Main goals

Find $R(z)$ such that the scheme is **unconditionally stable**, **less dissipative** and **less dispersive**.

Diagonal Padé schemes

The $(r+s)^{th}$ -order Padé approximation of e^z [2] is $R_{r,s}(z) = \frac{P_{r,s}(z)}{Q_{r,s}(z)}$, with

$$P_{r,s}(z) = \sum_{k=0}^s \frac{s!(r+s-k)!}{(r+s)!k!(s-k)!} (z)^k \quad \text{and} \quad Q_{r,s}(z) = P_{s,r}(-z).$$

✓ **Diagonal Padé schemes** correspond to the case where $r = s = m$:

Good news

- Diagonal Padé schemes are always stable.
- When applied to the test equation (1) they are not dissipative.

Furthermore, dispersion error decreases with high order

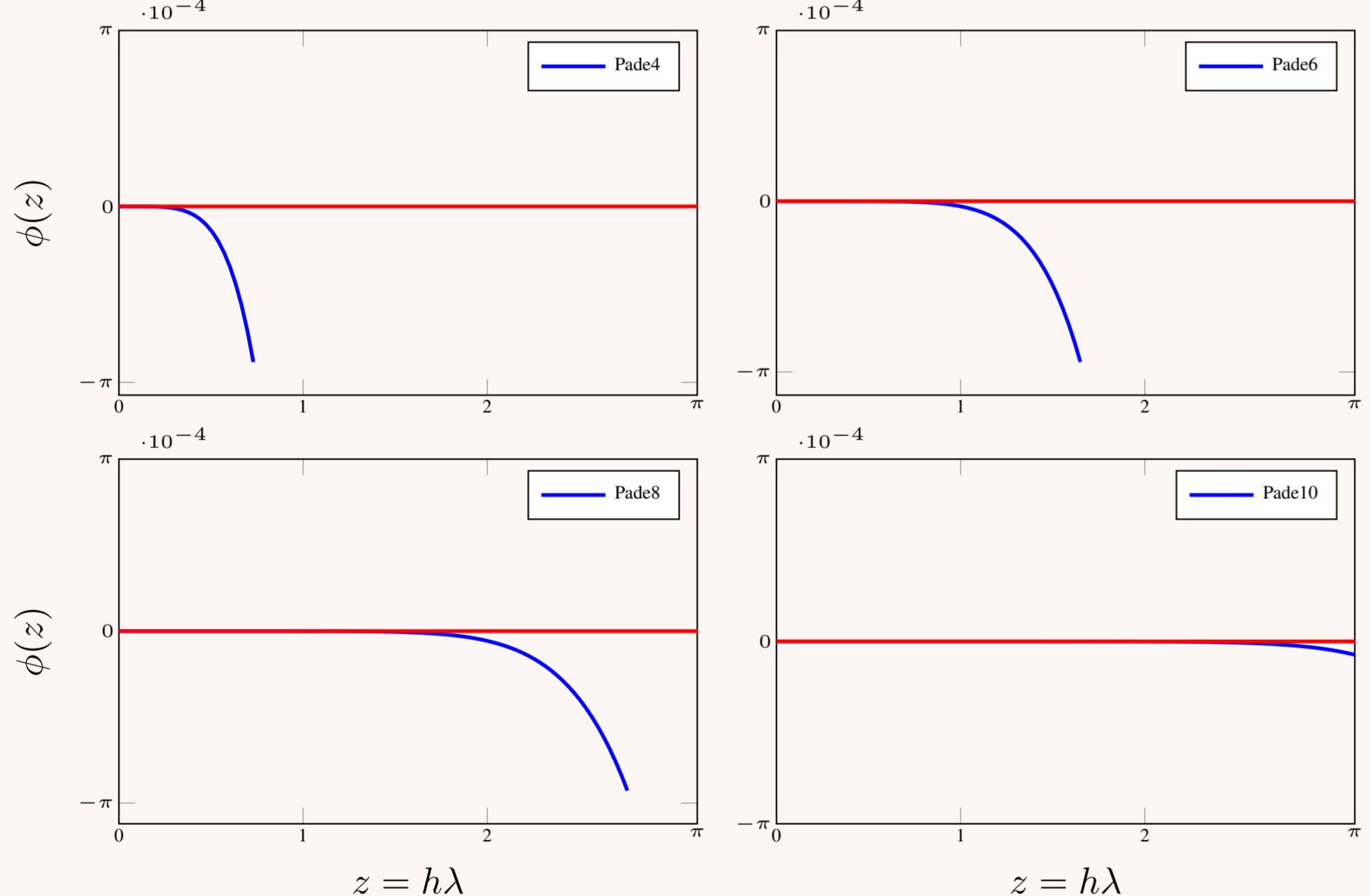


Fig. 1: Dispersion error of diagonal Padé schemes

Further research and perspectives

- Development of high order implicit time schemes for ODEs, application to Maxwell's equations (conference ICOSAHOM2016 Rio June, 27th–July, 1st),
- CFL optimization for explicit time schemes (Runge-Kutta and Runge-Kutta-Nyström),
- development of locally implicit time schemes,
- modeling of seismolectric waves,
- teaching: 64 hours (helping class and TD).

References

- [1] Ernst Hairer and Gerhard Wanner, "Solving ordinary differential equations II Stiff and differential-algebraic problems", Springer, 2010.
- [2] John C. Butcher, "Numerical methods for ordinary differential equations second edition", John Wiley & Sons Ltd, 2008.
- [3] Marc Duruflé, "Intégration numérique et éléments finis d'ordre élevé appliqués aux équations de Maxwell en régime harmonique", PhD Thesis of University Paris Dauphine, 2006.

Undesirable effects of time schemes

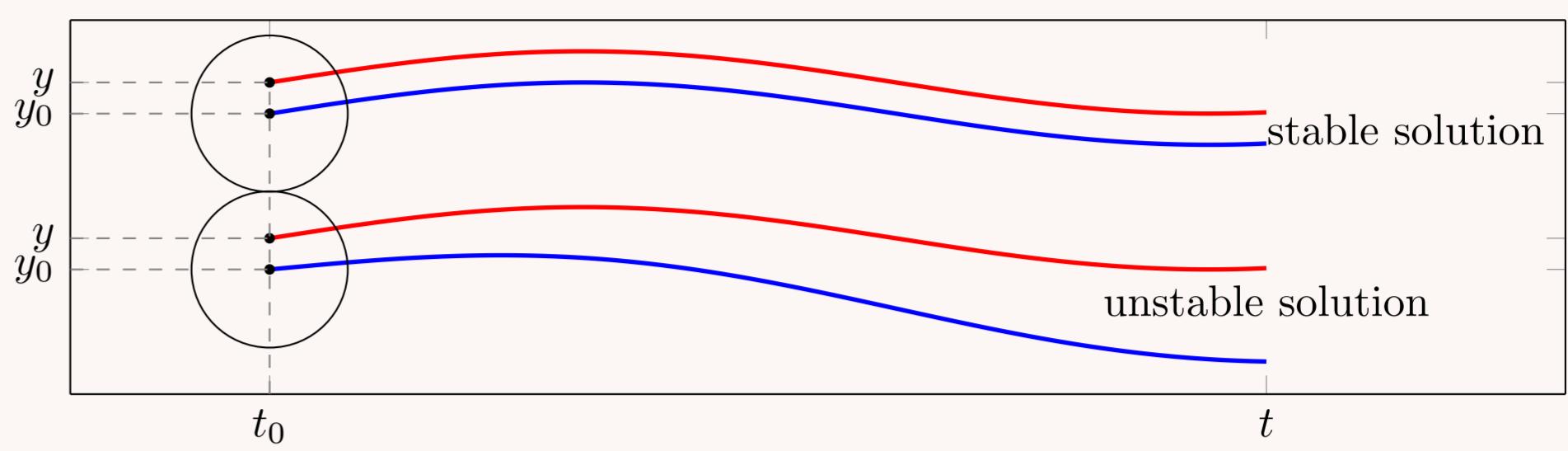


Fig. 2: Stability and instability effects

- Unstable scheme: the numerical solution grows more rapidly than the physical solution.

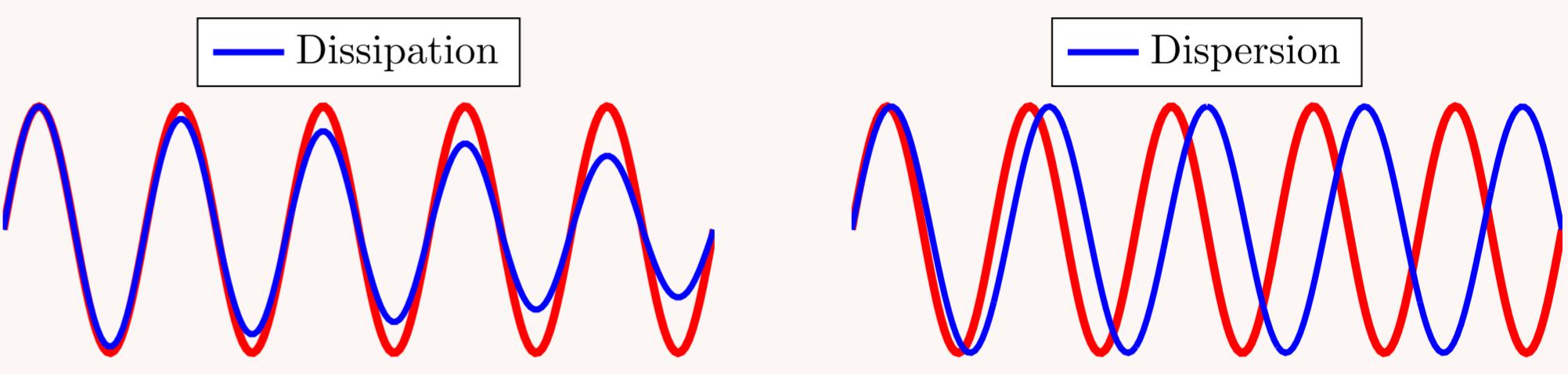


Fig. 3: Dissipation and dispersion effects

- Dissipative scheme: numerical solution has amplitude error.
- Dispersive scheme: numerical solution has phase error.

Application to Maxwell's equations

We consider

$$\begin{cases} \frac{\varepsilon \partial E}{\partial t} - \nabla \times H + \sigma E = F_E, \\ \mu \partial H / \partial t + \nabla \times E = F_H, \end{cases} \quad (2)$$

- E (F_E) and H (F_H) are respectively the electric and magnetic fields (source term),
- ε is the permittivity of the medium, μ is the permeability of the medium and σ is the conductivity.

Efficiency in term of computational time

We performed numerical tests with the C++ code Montjoie [3].

- 10-th order FEM on regular mesh $[-4, 4]^2$.
- Time interval: $[0, 10]$.

Schemes	Time steps	Relative errors	Times in s
Padé2	0.003	0.001241	1713.04
Padé4	0.054	0.000988	181.09
Padé6	0.153	0.000871	183.84
Padé8	0.285	0.001051	149.50
SDIRK34 [1]	0.0166	0.001030	985.66
SDIRK55 [1]	0.066	0.001244	455.39

We have compared computational times of different schemes after imposing 0.1% of errors.

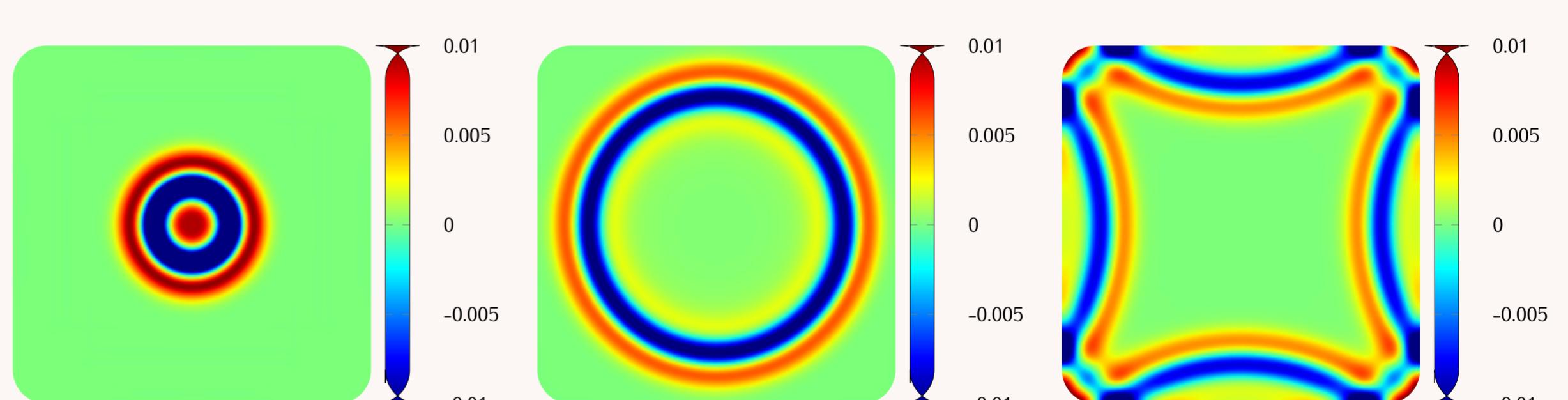


Fig. 4: Simulation results of Maxwell's equations in 2D on regular square mesh at $t = 1, 2, 3$.

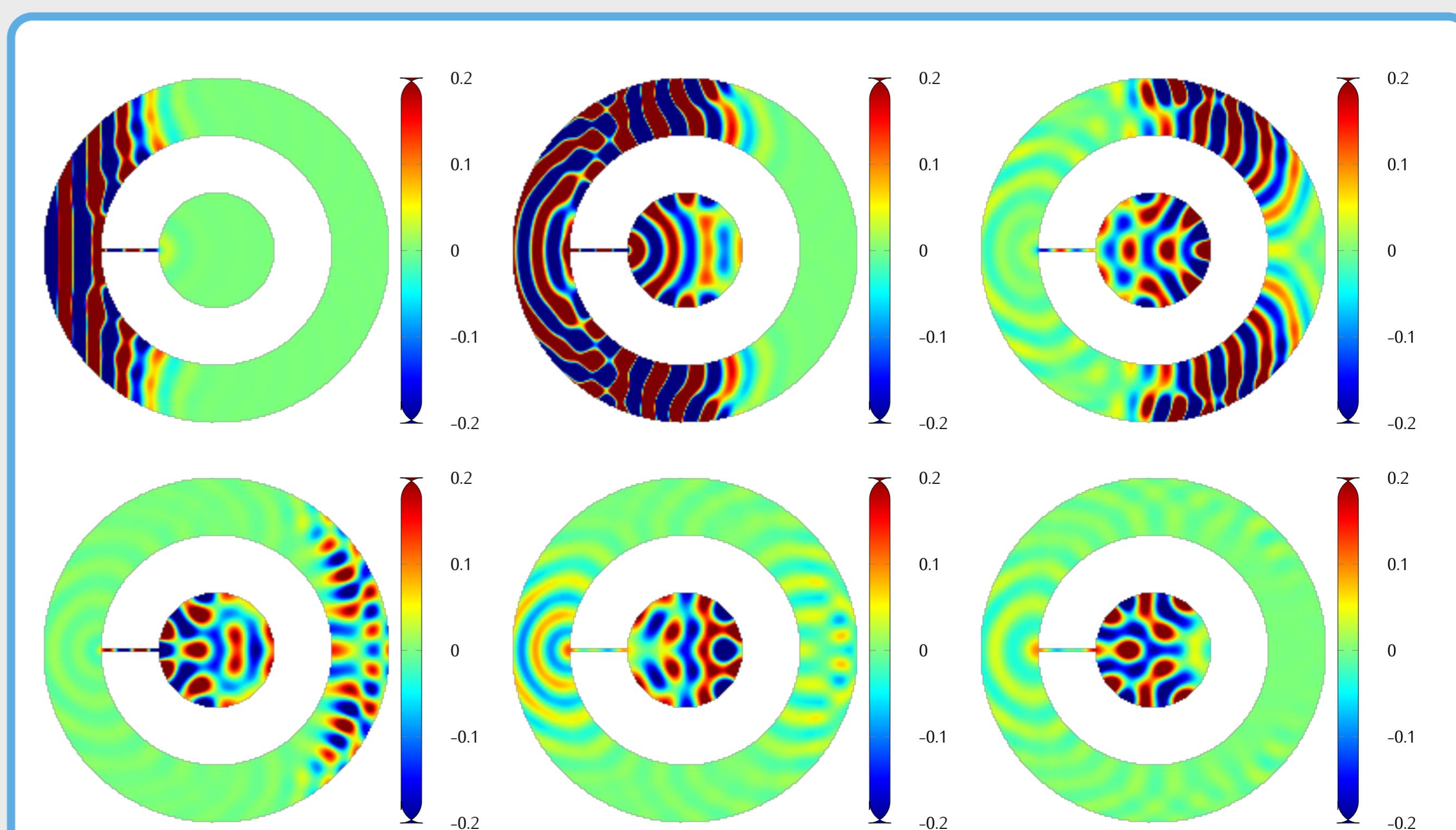


Fig. 5: Simulation results of Maxwell's equations in 2D on irregular mesh resonant disk at $t = 2, \dots, 7$.