

# Efficient high order time schemes for Maxwell's equations

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- Research code maintained by Marc Duruflé at INRIA (open-source).
- Frequency-domain and time domain modeling for wave propagation.

## Main goals

- Several wave-field propagators
  - Acoustic, electromagnetic, aeroacoustic and elastodynamic.
- Different discretization methods
  - Spatial : FEM, DG
  - Time schemes : explicit and implicit one step, explicit multi-step.
- Uses several libraries like : Blas, Mumps, Lapack, SuperLU, GSL, ...

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- ✓ Implicit time schemes for Maxwell's equations (1D, 2D and 3D).

# Equations of interest

Here we are dealing with the Maxwell's equations

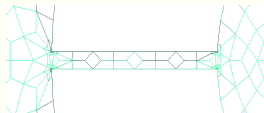
$$\begin{cases} \frac{\varepsilon \partial E}{\partial t} - \nabla \times H + \sigma E = F_E \\ \frac{\mu \partial H}{\partial t} + \nabla \times E = F_H \end{cases} \quad (1)$$

where

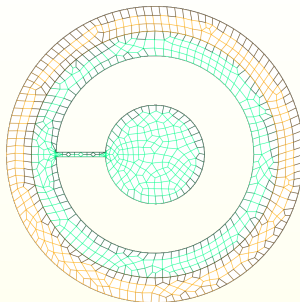
- $E$  is the electric field,
- $H$  is the magnetic field,
- $\sigma$  is the conductivity,
- $\varepsilon$  is the permittivity of the medium,
- $\mu$  is the permeability of the medium,
- $F_E$  and  $F_H$  are respectively the source term for the electric and magnetic fields.

# Implicit and/or explicit high order time schemes ?

- 927 elements
- 1989 edges



(a) Local refinement



(b) Irregular disk resonant mesh.

8<sup>th</sup>-order Padé vs 4<sup>th</sup>-order explicit Runge-Kutta with 6-th order FEM

| Schemes | Time steps                    | Relative errors       | Times   |
|---------|-------------------------------|-----------------------|---------|
| Padé8   | 0.05                          | $4.99 \times 10^{-4}$ | 3mn51s  |
| Padé8   | $\approx 6.67 \times 10^{-3}$ | $1.69 \times 10^{-9}$ | 18mn20s |
| ERK44   | $\approx 6.67 \times 10^{-5}$ | $1.69 \times 10^{-9}$ | 33mn21s |

# Implicit and/or explicit high order time schemes ?

We consider the following ODE (Ordinary Differential equation) :

$$M_h \frac{dU}{dt} + K_h U = F(t)$$

where  $M_h$  is the mass matrix and  $K_h$  is the stiffness matrix, obtained after space discretization.

The ODE is stiff because

- the eigenvalues of  $M_h^{-1} K_h$  can be large,
- due to the presence of small elements in the computational mesh,
- or high-order space discretization.

## Consequence

- ✓ Explicit methods become too expensive.
- ✓ Implicit methods are needed.

# Main goals to achieve

## Objectives

- Develop **locally** implicit time schemes.
- Release stability constraint in given regions and for high order space discretization.
- Improve the accuracy.

## Advantages

- ✓ Reduce the computational costs.
- ✓ Solve realistic problems more accurately.

# Plan

- 1 Numerical stability, amplitude and phase errors
- 2 Selected implicit RK (IRK) schemes
- 3 Padé schemes
- 4 Correct approximation of the source term
- 5 Application to 1D and 2D Maxwell's equations



- 1 Numerical stability, amplitude and phase errors

# Stability function and stability region

We consider the following linear test equation

$$y' = i\lambda y, \quad y(t_0) = y_0, \quad (2)$$

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

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

## Definition

$\forall z \in \mathbb{C}$ ,  $R(z)$  is called the stability function of the numerical scheme. The set

$$S = \{z \in \mathbb{C}; |R(z)| \leq 1\} \quad (3)$$

is called the stability region of the method.

I didn't like all these “strong”, “perfect”, “absolute”, “generalized”, “super”, “hyper”, “complete” and so on in mathematical definitions, I wanted something neutral ; and having been impressed by David Young's “property A”, I chose the term “A-stable”.

(*G. Dahlquist, in 1979* [Hairer and Wanner, 2010])

## Definition

(Dahlquist 1963). A method, whose stability region satisfies

$$S \supset \mathbb{C}^- = \{z \in \mathbb{C}, \text{Re}(z) \leq 0\} \quad (4)$$

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is called A-stable.

But ...

A-stability is not the whole answer to wave propagation problems.

# Amplitude and phase errors formulae

Let  $z = h\lambda$  in (2). Then the following ratio in trigonometric form reads

$$\frac{R(iz)}{e^{iz}} = |R(iz)|e^{-\phi(z)} \quad \text{with } \phi(z) = -\arg[R(iz)e^{-iz}].$$

## Amplitude (or dissipation) error

The dissipation error of a time scheme applied to the test equation (2) is defined by

$$\psi(z) = |R(iz)| \quad (\text{must be } =1). \quad (5)$$

## Phase (or dispersion) error

The dispersion error of a time scheme applied to the test equation (2) is defined by

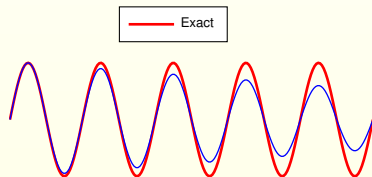
$$\phi(z) := \arg \left[ \frac{e^{iz}}{R(iz)} \right] = z - \arg[R(iz)] \quad (\text{must be } =0). \quad (6)$$

# Amplitude and phase errors formulae

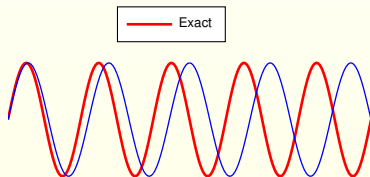
Let  $z = h\lambda$  in (2). Then the following ratio in trigonometric form reads

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Let us recall the dissipation and dispersion error effects on the numerical solution :



(a) Dissipation



(b) Dispersion

## 2 Selected implicit RK (IRK) schemes

# Some Runge-Kutta schemes

The  $s$ -stage RK scheme applied to (2) is given by

$$y_{n+1} = y_n + h \sum_{j=1}^s b_j K_j, \quad K_j = i\lambda \left( y_n + h \sum_{l=1}^s a_{j,l} K_l \right). \quad (5)$$

Which is equivalent to

$$y_{n+1} = R(ih\lambda)y_n$$

where  $R$  is the stability function defined by

$$R(z) = \mathbf{1} + zb^T(I - zA)^{-1}\mathbf{1}, \quad z \in \mathbb{C}. \quad (6)$$

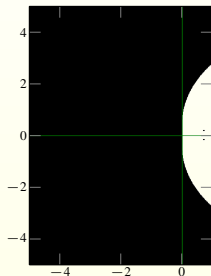
$A$  is the matrix  $(a_{j,l})$  and  $b$  is the vector  $(b_j)$ .



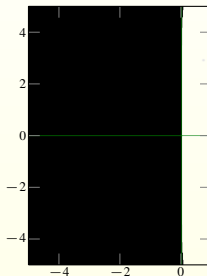
# Some Runge-Kutta schemes

We consider the following IRK methods :

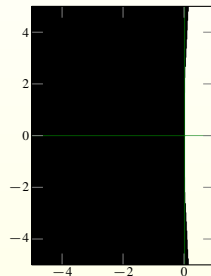
- SDIRK34 of Crouzeix [Hairer and Wanner, 2010].
- S54b of Skvortsov [Skvortsov, 2006].
- SDIRK55 of Cooper & Sayfy [Hairer and Wanner, 2010].



(a) SDIRK34



(b) S54b

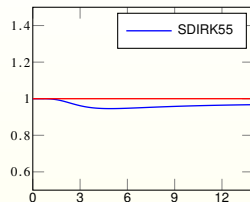
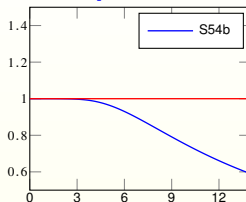
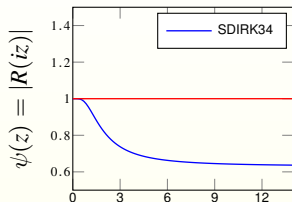


(c) SDIRK55

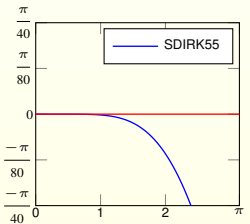
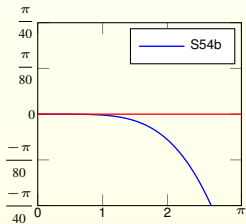
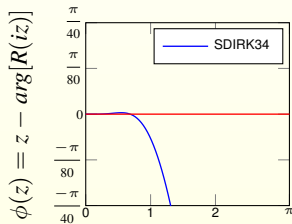
**Stability region, black when  $|R(z)| \leq 1$ .**

# Some Runge-Kutta schemes

## Dissipation



## Dispersion



$$z = h\lambda$$

## 3 Padé schemes

# Stability function of Padé schemes

The stability function is defined by

$$R_{r,s}(z) = \frac{P_{r,s}(z)}{Q_{r,s}(z)}, \quad (5)$$

where

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

It represents a  $(r+s)$ -th order approximation of  $e^z$  [Butcher, 2008].

# Particular case of Diagonal Padé schemes

Diagonal Padé schemes correspond to the case where  $r = s = m$ .

## Fourth-order Padé approximation

For  $m = 2$  the fourth-order approximation reads

$$R_{2,2}(z) = \frac{P_{2,2}(z)}{Q_{2,2}(z)} = \frac{1 + \frac{1}{2}z + \frac{1}{12}z^2}{1 - \frac{1}{2}z + \frac{1}{12}z^2}. \quad (6)$$

## Sixth-order Padé approximation

For  $m = 3$  the sixth-order approximation reads

$$R_{3,3}(z) = \frac{P_{3,3}(z)}{Q_{3,3}(z)} = \frac{1 + \frac{1}{2}z + \frac{1}{12}z^2 + \frac{1}{120}z^3}{1 - \frac{1}{2}z + \frac{1}{10}z^2 - \frac{1}{120}z^3}. \quad (7)$$

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For  $m = 2$  the fourth-order approximation reads

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Let's  $z = a + ib$ , with  $a \leq 0$  then

$$|R_{2,2}(z)| = \frac{\left| 1 + \frac{a}{2} + \frac{a^2 - b^2}{12} + i \left( \frac{b}{2} + \frac{2ab}{12} \right) \right|}{\left| 1 - \frac{a}{2} + \frac{a^2 - b^2}{12} + i \left( -\frac{b}{2} + \frac{2ab}{12} \right) \right|} \leq 1.$$

# Particular case of Diagonal Padé schemes

Diagonal Padé schemes correspond to the case where  $r = s = m$ .

## Proposition

*The stability function of numerical schemes obtained using the diagonal Padé approximation verify :  $\forall z \in \mathbb{C}^-$*

$$|R_{m,m}(z)| \leq 1, \quad \forall m \in \mathbb{N}.$$

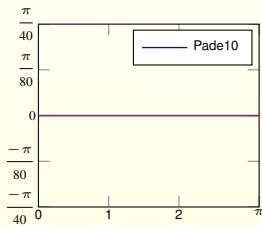
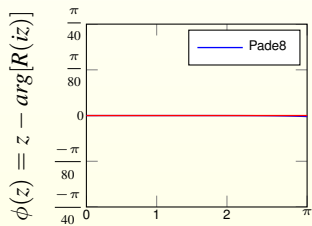
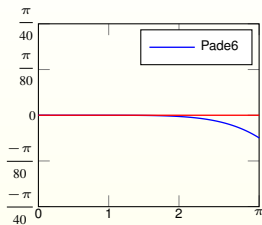
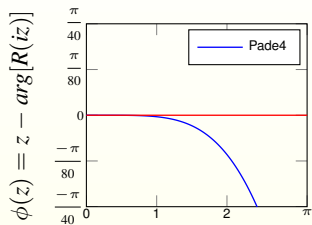
*Furthermore, if  $z = ib$ ,  $b \in \mathbb{R}$ ,*

$$|R_{m,m}(z)| = 1, \quad \forall m \in \mathbb{N}.$$

## Consequences

- The Diagonal Padé schemes are always  $A$ -stable,
- the Diagonal Padé schemes when applied to the test equation (2) are not dissipative.

# Dispersion of some Padé schemes



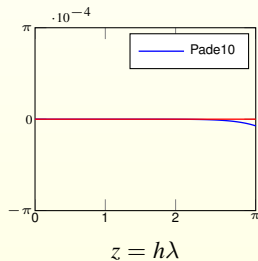
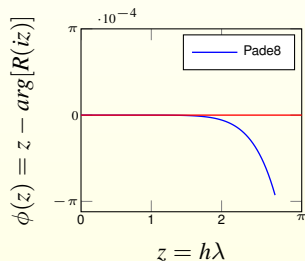
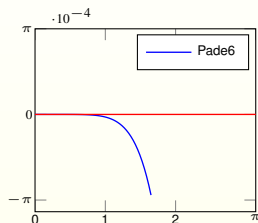
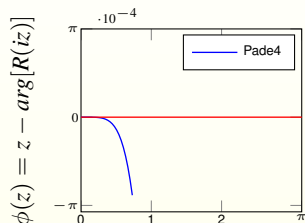
$z = h\lambda$

$z = h\lambda$



# Dispersion of some Padé schemes

## Zoom



## 4 Correct approximation of the source term

We recall

$$M_h \frac{dX}{dt} + K_h X = F(t), \quad t \in (0, T]$$

where  $M_h$  is the mass matrix and  $K_h$  is the stiffness matrix, obtained after space discretization.

The exact solution is given by :

$$X(t) = e^{tA} \left( X_0 + \int_0^t e^{-sA} M_h^{-1} F(u) du \right) \quad (6)$$

where  $A = -M_h^{-1} K_h$ . The  $(r + s)$ -th order Padé schemes is given by

$$e^{tA} \approx R_{r,s}(tA) = [Q_{r,s}(tA)]^{-1} P_{r,s}(tA).$$

# Padé schemes for homogeneous ODE

When  $F(t) = 0$ , we have

$$X(t) = X_0 e^{tA}, \quad t \in (0, T]. \quad (7)$$

If  $t_n = n\Delta t = \frac{nT}{N}$ , where  $N$  is a given positive integer, (7) implies that

$$X(t_{n+1}) = e^{\Delta t A} X(t_n). \quad (8)$$

Let  $C = \Delta t A$ . The  $r + s$  order Padé scheme reads

$$Q_{r,s}(C)X_{n+1} = P_{r,s}(C)X_n \quad (9)$$

where  $X_n \approx X(t_n)$  and  $X_0 \approx X(t_0)$ .

# Padé for inhomogeneous ODE

When  $F(t) \neq 0$ , we are supposed to compute :

$$\int_0^t e^{-sA} M_h^{-1} F(u) \, du.$$

We consider  $t_n = n\Delta t$ , and  $C = \Delta t A$ ,  $X_n \approx X(t_n)$  and the Padé scheme is

$$X_{n+1} = [Q_{r,s}(C)]^{-1} P_{r,s}(C) \left( X_n + \int_{t_n}^{t_{n+1}} e^{-sA} M_h^{-1} F(u) \, du \right). \quad (10)$$

Let's define

$$\mathcal{F} = Q_{r,s}(C)X_{n+1} - P_{r,s}(C)X_n. \quad (11)$$

$\mathcal{F}$  is the quantity of interest.

# Source approximation

The Taylor expansion of  $X(t_n + \Delta t)$  and  $X(t_n)$  around  $t_n + \frac{\Delta t}{2}$  at order  $2m$  allows us to write :

$$\mathcal{F} = \sum_{i=0}^m \sum_{k=0}^{2m} C_{i,k}^m \Delta t^k X^{(k)} z^i + O(\Delta t^{2m+1}).$$

## Proposition

*The expression of  $\mathcal{F}$  is equivalent to*

$$\mathcal{F} = \sum_{r=0}^{m-1} A^r \Delta t^{r+1} \sum_{l=0}^{2m-r-1} \alpha_l^r \Delta t^l F^{(l)} + O(\Delta t^{2m+1}), \quad (12)$$

$\alpha_l^r$  can be computed explicitly, but how about  $F^{(l)}$  ?

## Proposition

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The source function for the fourth-order Padé scheme ( $m = 2$ ) is given by

$$\mathcal{F} = \Delta t \left( F + \frac{\Delta t^2}{24} F^{(2)} \right) - A \frac{\Delta t^3}{12} F^{(1)} + O(\Delta t^5).$$

## Proposition

The expression of  $\mathcal{F}$  is equivalent to

$$\mathcal{F} = \sum_{r=0}^{m-1} A^r \Delta t^{r+1} \sum_{l=0}^{2m-r-1} \alpha_l^r \Delta t^l F^{(l)} + O(\Delta t^{2m+1}), \quad (12)$$

The source function for the sixth-order Padé scheme ( $m = 3$ ) is given by

$$\begin{aligned} \mathcal{F} = & \Delta t \left( F + \frac{\Delta t^2}{24} F^{(2)} + \frac{\Delta t^5}{1920} F^{(4)} \right) - A \Delta t^2 \left( \frac{\Delta t}{12} F^{(1)} + \frac{\Delta t^3}{480} F^{(3)} \right) \\ & + A^2 \Delta t^3 \left( \frac{1}{60} F + \frac{\Delta t^2}{480} F^{(2)} \right) + O(\Delta t^7). \end{aligned}$$



# Numerical approximation of the source

We consider the following approximation :

$$\sum_{i=0}^{2m} \alpha_i^r \Delta t^i F^{(i)} \left( t_n + \frac{\Delta t}{2} \right) \approx \sum_{i=0}^{2m} \omega_i^r F \left( t_n + \Delta t c_i + \frac{\Delta t}{2} \right), \quad (13)$$

where  $c_i$  are quadrature points chosen in  $\left[ -\frac{1}{2}, \frac{1}{2} \right]$  and  $\omega_i^r$  are the weights.

- We choose Gauss-Lobatto points for  $c_i$ ,
- $\omega_i^r$  are solution of linear system of type Vandermonde.

Finally we replace  $c_i$  and  $\omega_i^r$  in (13) to approximate  $\mathcal{F}$  (12).

## 5 Application to 1D and 2D Maxwell's equations

# Simulation results for Maxwell's equations in 1D

## 1D test case

- ✓ 10-th order FEM is used in space.
- ✓ Time interval :  $[0, 40]$ , domain with  $20 \lambda$  and 10,000 dofs.

## Comparison of selected implicit Runge-Kutta schemes

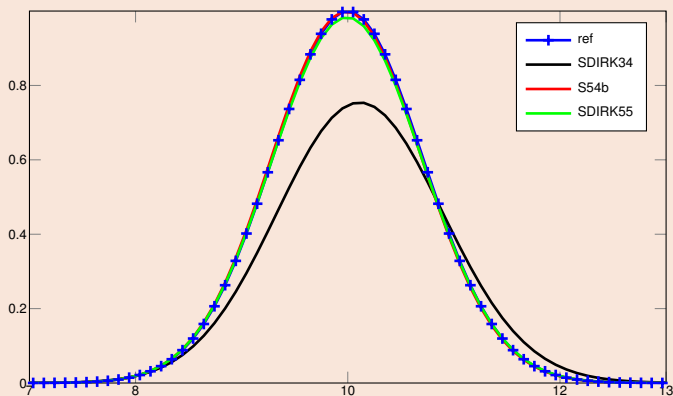
- We take  $\Delta t = 0.08$  for  $s = 5$  as the reference.
- For a  $s$ -stage RK method, we take  $\Delta t_s = \frac{\Delta t}{5} \times s$ .
- RK<sub>sr</sub> refers to  $s$ -stage  $r$ -th order RK scheme.

| Numerical error per scheme |   |                      |                  |
|----------------------------|---|----------------------|------------------|
| Schemes                    | s | Time steps           | Relatives errors |
| SDIRK34                    | 3 | $\Delta t_s = 0.048$ | 0.3376           |
| S54b                       | 5 | $\Delta t_s = 0.08$  | 0.0216           |
| SDIRK55                    | 5 | $\Delta t_s = 0.08$  | 0.0195           |

# Simulation results for Maxwell's equations in 1D

## Comparison of selected implicit Runge-Kutta schemes

Modulus of the numerical solution at  $t = 40$ .



# Simulation results for Maxwell's equations in 1D

## Validation tests of the Padé schemes (1D test case)

- RK $s$  $r$  refers to  $s$ -stage  $r$ -th order RK scheme.
- Padé $N$  refers to  $N$ -th order diagonal Padé scheme.

Computational times after imposing 1% of errors

| Schemes | Time steps | Relative errors | Times in s |
|---------|------------|-----------------|------------|
| Padé2   | 0.004      | 0.009692        | 1.535      |
| Padé4   | 0.069      | 0.010023        | 0.379      |
| Padé6   | 0.196      | 0.009752        | 0.242      |
| Padé8   | 0.350      | 0.008919        | 0.195      |
| ERK44   | 0.006      | 0.009978        | 1.665      |
| SDIRK34 | 0.022      | 0.011980        | 0.845      |
| SDIRK55 | 0.08       | 0.009847        | 0.439      |

# Simulation results for Maxwell's equations in 2D

## 2D test case on regular square mesh

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

## Validation tests of the Padé schemes (2D regular square mesh)

Computational times after imposing 0.1% of errors.

| 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 | 0.0166     | 0.001030        | 985.66     |
| SDIRK55 | 0.066      | 0.001244        | 455.39     |

# Simulation results for Maxwell's equations in 2D

## 2D test case on irregular mesh

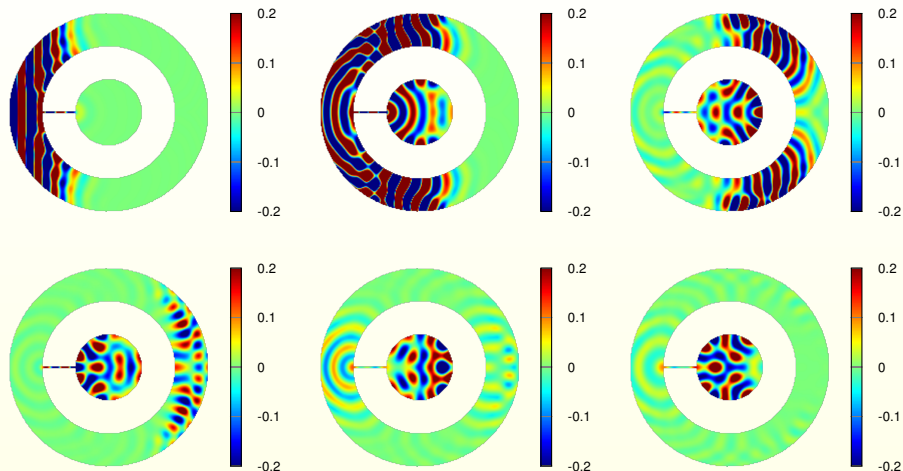
- ✓ 6-th order FEM is used on the irregular mesh resonant disk.
- ✓ Time interval :  $[0, 10]$ .

## Simulation results on the irregular mesh resonant disk

Comparison Padé vs ERK44

| Schemes | Time steps            | Relative errors        | Times in s |
|---------|-----------------------|------------------------|------------|
| Padé4   | 0.0077                | $4.97 \times 10^{-4}$  | 8mn02s     |
| Padé6   | 0.0286                | $4.62 \times 10^{-4}$  | 4mn42s     |
| Padé8   | 0.05                  | $4.99 \times 10^{-4}$  | 3mn51s     |
| Padé4   | $5.00 \times 10^{-4}$ | $1.90 \times 10^{-9}$  | 296mn19s   |
| Padé6   | $1.67 \times 10^{-3}$ | $1.69 \times 10^{-9}$  | 61mn01s    |
| Padé8   | $6.67 \times 10^{-3}$ | $1.69 \times 10^{-9}$  | 18mn20s    |
| ERK44   | $7.20 \times 10^{-5}$ | $39.13 \times 10^{+3}$ | 30mn55s    |
| ERK44   | $6.67 \times 10^{-5}$ | $1.69 \times 10^{-9}$  | 33mn21s    |

# Simulation results for Maxwell's equations in 2D



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



# On going works and perspectives

## On going works

- Optimization of CFL for explicit methods to be combined with the implicit one.
- Development of continuous Padé schemes.

## Perspectives

- Padé schemes for 3D Maxwell's equations.
- Develop **locally** implicit method.
- Perform validation tests with realistic wave problems.

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**Thank you for your attention.**  
**Questions ?**

## 6 References

# References I



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# Stability region of some classical ERK schemes

Here are some ERK schemes (in Butcher table) :

ERK22

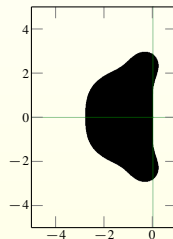
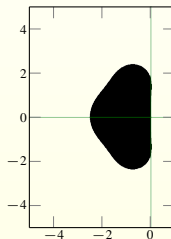
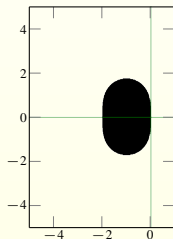
|     |     |   |
|-----|-----|---|
| 0   |     |   |
| 0.5 | 0.5 |   |
|     | 0   | 1 |

ERK33

|     |               |               |               |
|-----|---------------|---------------|---------------|
| 0   |               |               |               |
| 0.5 | 0.5           |               |               |
| 1   | -1            | 2             |               |
|     | $\frac{1}{6}$ | $\frac{2}{3}$ | $\frac{1}{6}$ |

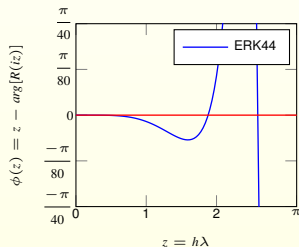
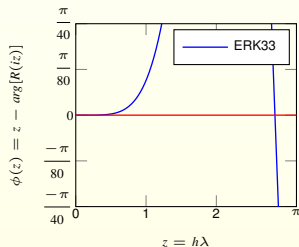
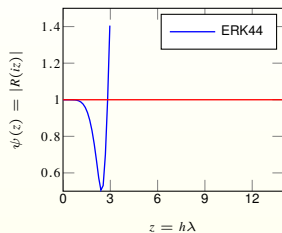
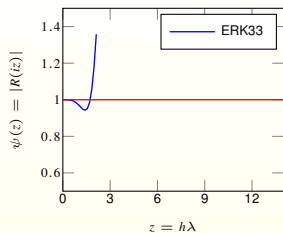
ERK44

|     |               |               |               |               |
|-----|---------------|---------------|---------------|---------------|
| 0   |               |               |               |               |
| 0.5 | 0.5           |               |               |               |
| 0.5 | 0             | 0.5           |               |               |
| 1   | 0             | 0             | 1             |               |
|     | $\frac{1}{6}$ | $\frac{1}{3}$ | $\frac{1}{3}$ | $\frac{1}{6}$ |



**Stability region, black when  $|R(z)| \leq 1$ .**

# Dissipation and dispersion of classical ERK schemes



# Maxwell's equations

$$\left\{ \begin{array}{ll} \nabla \cdot D = \rho_v & \text{Gauss's law} \\ \nabla \cdot B = 0 & \text{Gauss Magnetism law} \\ \nabla \times H = \frac{\varepsilon \partial E}{\partial t} + J & \text{Amper's law} \\ \nabla \times E = -\frac{\partial B}{\partial t} & \text{Faraday's law} \end{array} \right. \quad (14)$$

where

- $E$  is the electric field,
- $H$  is the magnetic field,
- $J = \sigma E$ , from Ohm's law, is the electric current density,
- $D = \varepsilon E$  is the electric flux density with  $\varepsilon$  the permittivity of the medium,
- $B = \mu H$  is the magnetic flux density with  $\mu$  the permeability of the medium,
- $\sigma$  is the electric conductivity of the medium.

# Derivation of the wave equations

We consider the vector identity

$$\nabla \times \nabla \times H = \nabla(\nabla \cdot H) - \Delta H.$$

We suppose we are in a free source region, then

$$\nabla(\nabla \cdot H) = 0.$$

From Faraday's law, we have

$$\nabla \times \nabla \times E = -\mu \frac{\partial}{\partial t}(\nabla \times H).$$

By substituting in Amper's law, we get

$$\begin{aligned}\nabla \times \nabla \times E &= -\Delta E = -\mu \frac{\partial}{\partial t}(\nabla \times H) \\ &= -\mu \varepsilon \frac{\partial}{\partial t} \left( \frac{\partial E}{\partial t} + J \right).\end{aligned}$$

Since  $J = 0$  because of source free region, the vector wave equation reads

$$\Delta E = \mu \varepsilon \frac{\partial^2 E}{\partial t^2}. \quad (15)$$