

# A family of Linear Singly Diagonal Runge-Kutta methods and high order Pade's schemes for ODE

Mamadou N'DIAYE  
PhD student Department of Applied Mathematics

University of Pau & INRIA-Bordeaux Sud-Ouest, Team Magique-3D  
Advisors : H el ene BARUCQ & Marc DURUFL E

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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, ...

Here we are concerned with ...

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

# 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.

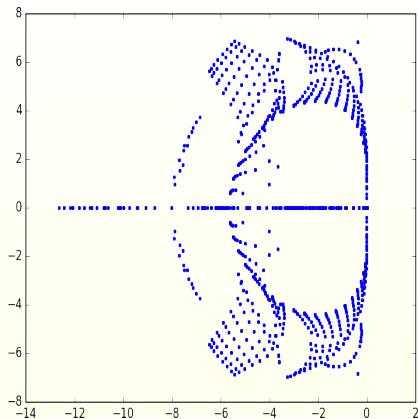
The ODE is stiff because

- 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.

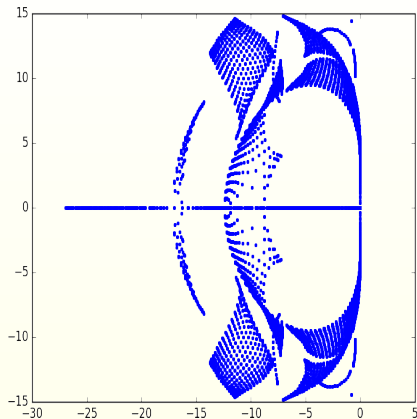
## Consequence

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

# Implicit and/or explicit high order time schemes ?



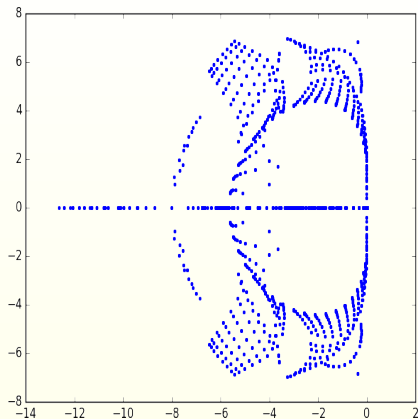
(a) 10 points along x



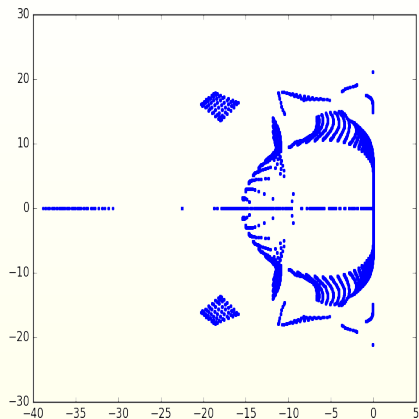
(b) 20 points along x

***Spectrum of  $M_h^{-1}K_h$  for the second order (Q2) FEM method on the regular grid  $[-4, 4]^2$ . Acoustic wave equation with Neumann boundary condition.***

# Implicit and/or explicit high order time schemes ?



(c) Order 2 (Q2)

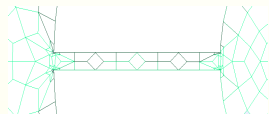


(d) Order 4 (Q4)

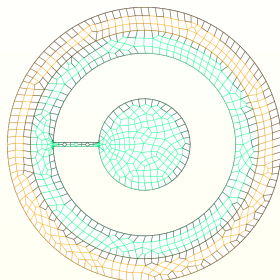
***Spectrum of  $M_h^{-1}K_h$  for FEM method on the regular grid  $[-4, 4]^2$  with 10 points along the  $x$  axis. Acoustic wave equation with Neumann boundary condition.***

# Implicit and/or explicit high order time schemes ?

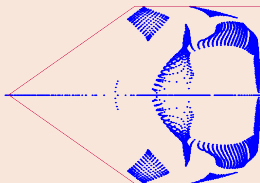
- 927 elements
- 1989 edges



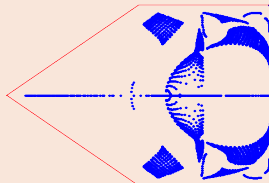
(e) Local refinement



(f) Disk resonant mesh



(g) Spectrum (Absorbing BC)



(h) Spectrum (Neumann BC)

# In this framework...

Consider

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

The exact solution after one step ( $h = t_{n+1} - t_n$ ) is

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

Numerical solution is obtained by approximating

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

- The scheme is **A-stable** if  $|R(z)| \leq 1, \forall z \in \mathbb{C}^-$ ,
- **non dissipative** if  $|R(z)| = 1, \forall z \in \mathbb{C}^-$ ,
- **non dispersive** if  $\phi(z) = z - \arg(R(z)) = 0, \forall z \in \mathbb{C}^-$ .

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

## Main goals

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

- 1 Some classical Runge-Kutta schemes
- 2 Padé schemes
- 3 Application to 1D and 2D Maxwell's equations
- 4 On going... : “Linear” Singly Diagonal Runge-Kutta schemes (Linear-SDIRK)



- 1 Some classical Runge-Kutta schemes

# Some Runge-Kutta schemes

The  $s$ -stage RK scheme applied to  $y'(t) = i\lambda y(t)$  is given by

$$y_{n+1} = y_n + h \sum_{j=1}^s b_j K_j, \quad K_j = i\lambda \left( y_n + h \sum_{l=1}^s a_{j,l} K_l \right). \quad (2)$$

Which is equivalent to

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

where  $R$  is the stability function defined by

$$R(z) = \mathbf{1} + zb^T(I - zA)^{-1}\mathbf{1}, \quad z \in \mathbb{C}. \quad (3)$$

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

# Some Runge-Kutta schemes

Here are some ERK schemes (in Butcher table) :

ERK22

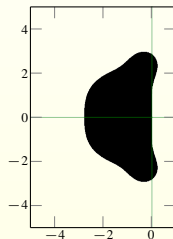
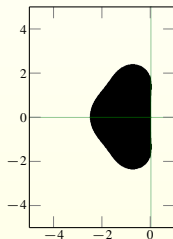
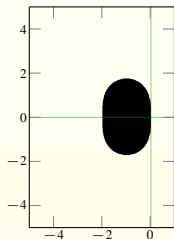
0		
0.5		0.5
-----		
		0    1

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	
-----					
		$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

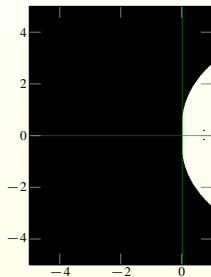


**Stability region, black when  $|R(z)| \leq 1$ .**

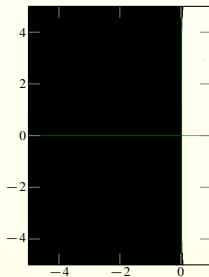
# Some Runge-Kutta schemes

We considered the following IRK methods :

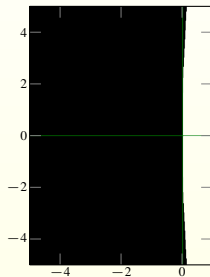
- SDIRK34 of Crouzeix [Hairer and Wanner, 2010].
- S54b of Skvortsov [Skvortsov, 2006].
- SDIRK55 of Cooper & Sayfy [Hairer and Wanner, 2010].



(a) SDIRK34



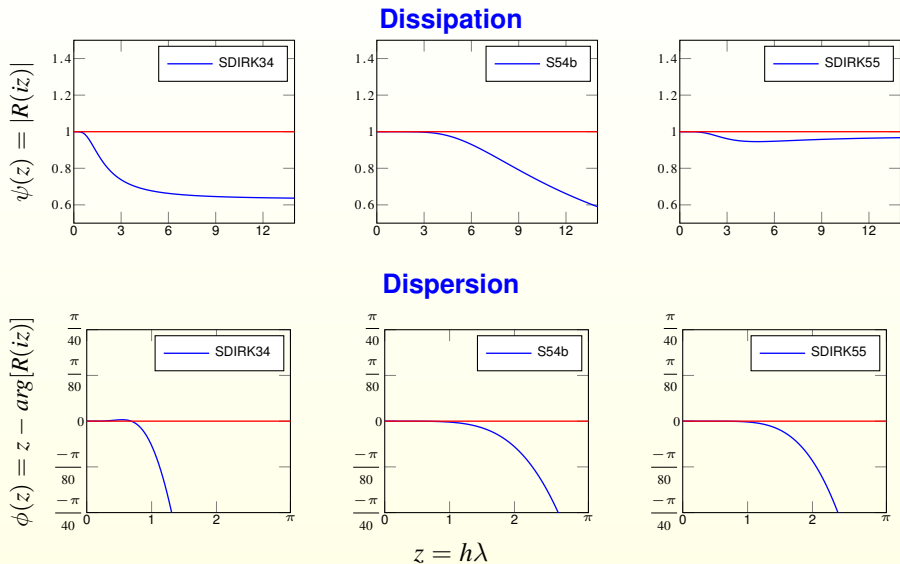
(b) S54b



(c) SDIRK55

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

# Some Runge-Kutta schemes



## 2 Padé schemes

# Stability function of diagonal Padé schemes

The stability function of Padé schemes are defined by

$$R_{r,s}(z) = \frac{P_{r,s}(z)}{Q_{r,s}(z)}, \quad (2)$$

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].

# Stability function 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  $z = ib$ ,  $b \in \mathbb{R}$ ,*

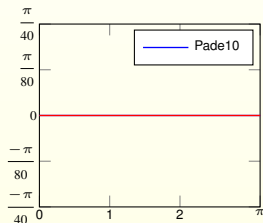
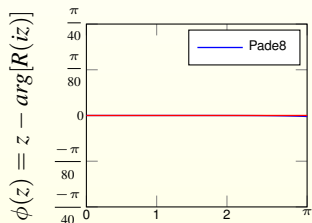
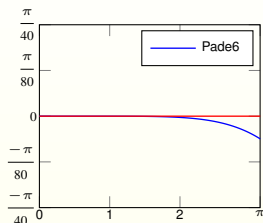
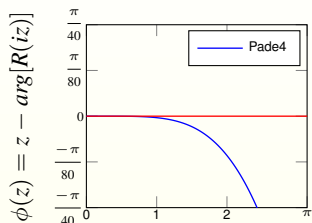
$$|R_{m,m}(z)| = 1, \quad \forall m \in \mathbb{N}.$$

## Consequences

- The Diagonal Padé schemes are “always” stable,
- the Diagonal Padé schemes when applied to the test equation  $y' = i\lambda y$  are not dissipative.



# Stability function of diagonal Padé schemes



$z = h\lambda$

$z = h\lambda$

**Dispersion of diagonal Padé schemes of order 4 to 10.**

- 
- 
- 3 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.

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

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

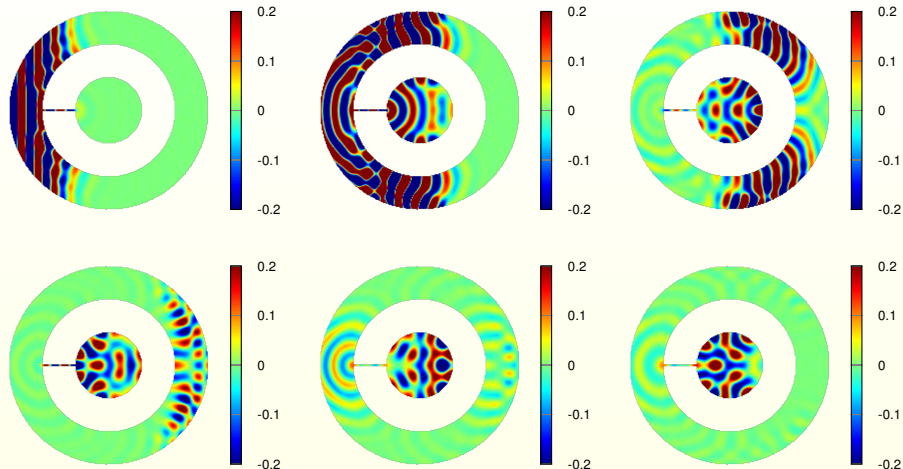
- ✓ 6-th order FEM is used on the irregular mesh resonant disk.
- ✓ Time interval :  $[0, 10]$ .

## 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  $t = 2, \dots, 7$ .**

- 4 On going... : “Linear” Singly Diagonal Runge-Kutta schemes (Linear-SDIRK)

# Stability function of “Linear”-SDIRK schemes

The stability function of the  $(\mathbf{s}+1)^{th}$ -order “Linear”-SDIRK schemes is given by

$$R_s^m(z) = 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^s}{s!} + \frac{z^{s+1}}{(s+1)!} + \frac{\alpha_1 z^{s+2} + \cdots + \alpha_s z^{2s+1}}{(1-\gamma z)^{s+m}}.$$

where  $s$  is a fixed number of stage and  $m$  represent the number of additional stages.

$R_s^m(z)$  is found by minimizing the coefficient  $\eta_0$  such that

$$e^z - R_s^m(z) = \eta_0 z^{s+1} + \cdots + \eta_m z^{s+m+1},$$

subject to  $|R_s^m(z)| \leq 1$  (A-stability condition).



# Stability function of “Linear”-SDIRK schemes

$$R_s^m(z) = 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^s}{s!} + \frac{z^{s+1}}{(s+1)!} + \frac{\alpha_1 z^{s+2} + \cdots + \alpha_s z^{2s+1}}{(1 - \gamma z)^{s+m}}.$$

For  $m = 0$  :

- No free parameter (no optimization),
- reduce to the common denominator and find the roots of the polynomial in  $\gamma$  that satisfies order conditions,
- choose  $\gamma$  such that  $|R_s^m(z)| \leq 1$ .

Minimal stage linear SDIRK of order $s+1$		
s	Value for $\gamma$	comment
1	0.5	-
2	0.788675134594813	-
3	1.068579021301629	-
4	x	No A-stable schemes
5	0.473268391258295	-
6	x	No A-stable schemes
$r \geq 7$	x	No A-stable schemes

# Stability function of “Linear”-SDIRK schemes

$$R_s^m(z) = 1 + z + \frac{z^2}{2!} + \dots + \frac{z^s}{s!} + \frac{z^{s+1}}{(s+1)!} + \frac{\alpha_1 z^{s+2} + \dots + \alpha_s z^{2s+1}}{(1-\gamma z)^{s+m}}.$$

For  $m = 1$  :

- One free parameter  $\gamma$ ,
- choose  $\gamma$  such that  $|R_s^m(z)| \leq 1$ .

Linear SDIRK of order $s+1$ with one additional stage		
s	interval for $\gamma$	$\gamma_{opt}$
1	$[\frac{1}{4}, \infty[$	leads to third order
2	$[\frac{1}{3}, 1.06866]$	leads to fourth order
3	$[0.39434, 1.28057]$	<b>0.394337567297406</b>
4	$[\cdot24651, \cdot3618] \cup [\cdot42079, \cdot47326]$	leads to sixth order
5	$[0.28407, 0.5409]$	<b>0.284064638011798</b>
6	x	No A-stable schemes
<b>7</b>	$[0.21705, 0.26471]$	<b>0.217049743094303</b>
$r \geq 8$	x	No A-stable schemes

# Stability function of “Linear”-SDIRK schemes

$$R_s^m(z) = 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^s}{s!} + \frac{z^{s+1}}{(s+1)!} + \frac{\alpha_1 z^{s+2} + \cdots + \alpha_s z^{2s+1}}{(1 - \gamma z)^{s+m}}.$$

For  $m = 2$  :

- Two free parameters  $\gamma$  and  $\alpha_1$ .

Linear SDIRK of order $s+1$ with two additional stages			
s	$\gamma_{opt}$	$\alpha_{1,opt}$	comment
$1 \leq s \leq 4$	-	-	No unicity
5	0.20394	0.000198393849206349	-
6	-	-	leads to eighth order
7	0.16688	$2.92592592592593e^{-06}$	-
8	x	x	No A-stable schemes
9	0.1419402	$2.29828167588584e^{-08}$	-
$r \geq 10$	x	x	No A-stable schemes

# Stability function of “Linear”-SDIRK schemes

$$R_s^m(z) = 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^s}{s!} + \frac{z^{s+1}}{(s+1)!} + \frac{\alpha_1 z^{s+2} + \cdots + \alpha_s z^{2s+1}}{(1 - \gamma z)^{s+m}}.$$

For  $m = 3$  :

- Three free parameters  $\gamma$ ,  $\alpha_1$  and  $\alpha_2$ .

Linear SDIRK of order $s+1$ with three additional stages			
$s$	$\gamma_{opt}$	$\alpha_{1opt}$	$\alpha_{2opt}$
$1 \leq s \leq 6$	-	-	-
7	0.13588	$2.76727843915344e^{-06}$	$-3.45238095238095e^{-06}$
8	-	-	-
9	0.15176	$2.4583633958634e^{-08}$	$-4.31522566939234e^{-08}$
10	x	x	x
11	0.134	$1.65054852554853e^{-10}$	$-2.93702705657071e^{-10}$
$r \geq 12$	x	x	x

## On going works

- Optimization of CFL for explicit methods to be combined with the implicit one.
- Comparison of Padé schemes and Linear-SDIRK schemes.

## Perspectives

- Develop **locally** implicit method.
- Perform validation tests with realistic wave problems.

## On going works

- Optimization of CFL for explicit methods to be combined with the implicit one.
- Comparison of Padé schemes and Linear-SDIRK schemes.

## Perspectives

- Develop **locally** implicit method.
- Perform validation tests with realistic wave problems.

**Thank you for your attention.**

**Questions ?**

## 5 References



Butcher, J. C. (2008).

*Numerical Methods for Ordinary Differential Equations SECOND EDITION.*

John Willey & Sons Ltd.



Hairer, E. and Wanner, G. (2010).

*Solving ordinary differential equations II Stiff and differential-algebraic problem.*

Springer.



Skvortsov, L. M. (2006).

Diagonally implicit runge-kutta methods for stiff problems.

*Computational Mathematics and Computational Physics*, 46 :2110–2123.



- 6 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.

# 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

$$\psi(z) = |R(iz)| \quad (\text{must be } =1). \quad (4)$$

## Phase (or dispersion) error

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

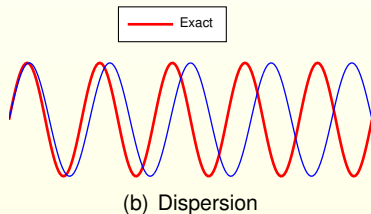
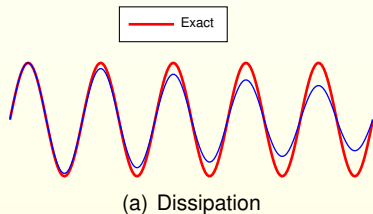
$$\phi(z) := \arg \left[ \frac{e^{iz}}{R(iz)} \right] = z - \arg[R(iz)] \quad (\text{must be } =0). \quad (5)$$

# Amplitude and phase errors formulae

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

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

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



# Stability region of some classical ERK schemes

Here are some ERK schemes (in Butcher table) :

ERK22

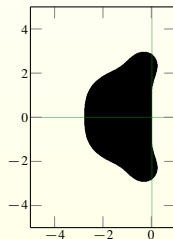
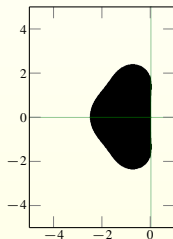
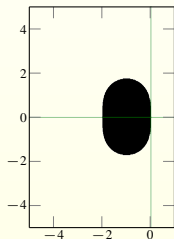
0		
0.5		0.5
-----		0 1

ERK33

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

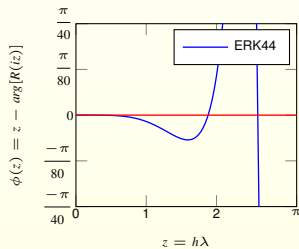
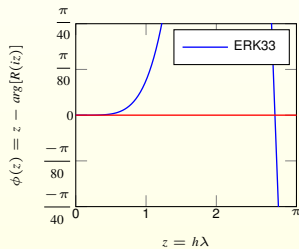
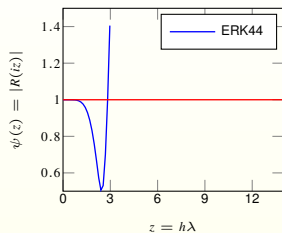
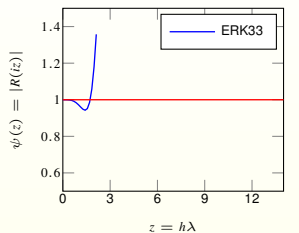
ERK44

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

$$\left\{ \begin{array}{l} \nabla \cdot D = \rho_v \quad \text{Gauss's law} \\ \nabla \cdot B = 0 \quad \text{Gauss Magnetism law} \\ \nabla \times H = \frac{\varepsilon \partial E}{\partial t} + J \quad \text{Amper's law} \\ \nabla \times E = -\frac{\partial B}{\partial t} \quad \text{Faraday's law} \end{array} \right. \quad (4)$$

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

$$\Delta E = \mu \varepsilon \frac{\partial^2 E}{\partial t^2}. \quad (5)$$



# Diagonal Padé schemes applied to the semi-discrete ODE

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

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

# Diagonal Padé schemes applied to the semi-discrete ODE

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

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

If  $t_n = n\Delta t = \frac{nT}{N}$ , where  $N$  is a given positive integer, then

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

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

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

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

# Diagonal Padé schemes applied to the semi-discrete 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

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

Let's define

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

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

# Diagonal Padé schemes applied to the semi-discrete ODE

For  $r = s = m$ , 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 :

## Proposition

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

$$\mathcal{F} = \sum_{r=0}^{m-1} A^r \Delta t^{r+1} \sum_{l=0}^{2m-r-1} \alpha_l^r \Delta t^l F^{(l)} + O(\Delta t^{2m+1}), \quad (6)$$

## Example with the fourth-order Padé

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

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

# 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*

$$\mathcal{F} = \sum_{r=0}^{m-1} A^r \Delta t^{r+1} \sum_{l=0}^{2m-r-1} \alpha_l^r \Delta t^l F^{(l)} + O(\Delta t^{2m+1}), \quad (7)$$

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

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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

$$\mathcal{F} = \sum_{r=0}^{m-1} A^r \Delta t^{r+1} \sum_{l=0}^{2m-r-1} \alpha_l^r \Delta t^l F^{(l)} + O(\Delta t^{2m+1}), \quad (7)$$

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

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

We consider the following approximation :

$$\sum_{i=0}^{2m} \alpha_i^r \Delta t^i F^{(i)} \left( t_n + \frac{\Delta t}{2} \right) \approx \sum_{i=0}^{2m} \omega_i^r F \left( t_n + \Delta t c_i + \frac{\Delta t}{2} \right), \quad (8)$$

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 (8) to approximate  $\mathcal{F}$  (7).