On the development of locally implicit schemes for linear wave problems

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Code Montjoie

- 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, HDG
  - Time schemes: explicit and implicit one step, explicit multi-step.
- Uses several libraries like: Blas, Mumps, Lapack, SuperLU, GSL, ...

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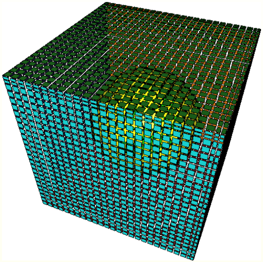
We have developed:

✓ Unconditionally stable implicit schemes (see [Barucq et al., 2017])

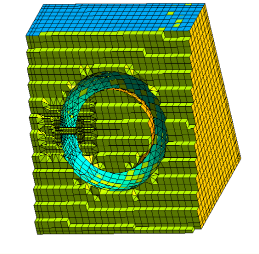
✓ Optimized CFL number explicit schemes (see the thesis [N'diaye, 2017]).

✓ Locally implicit schemes (see the thesis [N'diaye, 2017]).

Implicit and/or explicit high order time schemes?



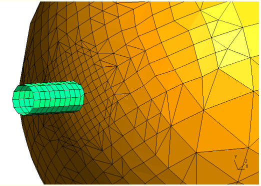
(a) Spherical resonant cavity



(b) Cross-section

24 885 elements

- 3 423 tetrahedra
- 16 571 hexahedra
- 4 246 pyramids
- 645 wedges



(c) Entry of the cavity

Implicit and/or explicit high order time schemes?

We consider the following ODE (Ordinary Differential equation):

$$M_h \frac{dy}{dt} + K_h y = f(t)$$

where M_h is the mass matrix and K_h is the stiffness matrix, obtained after space discretization on Ω.
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.
- ✓ But, implicit methods are highly memory consuming.

Implicit and/or explicit high order time schemes?

Table: Computational resources needed for explicit and implicit schemes for the scattering of the spherical resonant to obtained a relative L^2 error is below $1e-03$ (3D case HDG Acoustic). The direct solver MUMPS is used for implicit schemes. The computational times correspond to the maximal time when using 6 nodes Miriel and 144 cores on the PlaFRIM platform.

$\mathbb{Q}_4$	24 885 elements		1 633 475 degrees of freedom	
Schemes	Memory (GiB)	Factorization (GiB)	Number of time-steps	Computational times
L-ERK$4-2$	1.1	-	24 000	1h08mn25s
L-ERK$8-2$	1.40	-	15 000	1h16mn16s
L-SDIRK$3-1$	35.04	29.38	3 000	1h19mn30s
L-SDIRK$7-2$	35.41	29.38	900	44mn03s
Pade4	68.86	58.67	3 000	40mn31s
Pade8	136.40	117.34	750	20mn08s

Implicit and/or explicit high order time schemes?

How about mixing explicit and implicit schemes ?

Outline

Outline

1. Methodology for the construction of a locally implicit method
   - General idea to construct a locally implicit method
   - Treatment of the coarse region
   - Treatment of the fine region
   - Splitting of the Mesh into fine and coarse region

General idea to construct a locally implicit method

We consider

$$\frac{dy(t)}{dt} = Ay(t) + F(t), \tag{1}$$

with $A = -M_h^{-1}K_h$ and $F(t) = M_h^{-1}f(t)$.

We consider the following splitting

$$y(t) = y^{(c)}(t) + y^{(f)}(t)$$

where

$$y^{(c)} = (I - P)y(t),$$
$$y^{(f)} = Py(t).$$

P is a diagonal matrix with

$$\begin{cases} P_{i,i} = 1, & \text{if } i \text{ is a degree of freedom in the refined mesh} \\ P_{i,i} = 0, & \text{if } i \text{ is a degree of freedom in the coarse mesh} \end{cases}$$

General idea to construct a locally implicit method

We consider

$$\frac{dy(t)}{dt} = Ay(t) + F(t), \tag{1}$$

After discretization we compute $y(t_n + \xi\Delta t)$ as follows

$$\begin{aligned} y(t_n + \xi\Delta t) = y(t_n) &+ \underbrace{\int_{t_n}^{t_n+\xi\Delta t} A(I-P)y(t)dt + \overbrace{\int_{t_n}^{t_n+\xi\Delta t} (I-P)F(t)dt}^{\text{source term}}}_{\text{Coarse part}} \\ &+ \underbrace{\int_{t_n}^{t_n+\xi\Delta t} APy(t)dt + \overbrace{\int_{t_n}^{t_n+\xi\Delta t} PF(t)dt}^{\text{source term}}}_{\text{Fine part}} \end{aligned} \tag{2}$$

Treatment of the coarse region

For degrees of freedom (dofs) in the coarse region far from the fine region, we obtain the following expression:

$$y_{n+1} = y_n + \Delta t A(I - P) \sum_{j=0}^{m} \alpha_{j+1} \Delta t^j \widetilde{w}_j + \Delta t (I - P) \sum_{i=1}^{s} b_i F_i \tag{3}$$

where α_j are the coefficients of the Optimized CFL number explicit schemes (see the thesis [N'diaye, 2017]), b_i are the weights of a quadrature rule and

$$\widetilde{w}_j \;=\; A^j y(t_n) + \sum_{\ell=1}^{j} A^{j-\ell} Q^{(\ell-1)}(t_n).$$

Q is the polynomial that interpolates F.

Treatment of the fine region

We denote by $\hat{Q}$ the anti-derivative of Q and we approximate the contribution for dofs in the coarse region close to the fine region to obtain:

$$y(t_n + \xi\Delta t) \approx y_n + A(I-P)\sum_{j=0}^{m} \alpha_{j+1}(\xi\Delta t)^{j+1}\widetilde{w}_j + (I-P)\left(\hat{Q}(t_n+\xi\Delta t) - \hat{Q}(t_n)\right) + \int_{t_n}^{t_n+\xi\Delta t} APy(t) + PF(t)dt \tag{4}$$

We introduce $\tau = \xi\Delta$, $\widetilde{y}(\tau) = y(t_n+\tau)$ and differentiate (4), like in [Mehlin et al., 2015], to get:

$$\frac{d\widetilde{y}(\tau)}{d\tau} = \overbrace{A(I-P)\sum_{j=0}^{m}(j+1)\alpha_{j+1}\,\tau^j\widetilde{w}_j + (I-P)Q(t_n+\tau) + PF(t_n+\tau)}^{\text{updated source term}} + AP\widetilde{y}(\tau) \tag{5}$$

We use unconditionally stable implicit method developed in [Barucq et al., 2017] to solve the ODE (5).

Splitting of the Mesh into fine and coarse region

We assume that the domain Ω is meshed with elements K_i such that

$$\Omega = \bigcup K_i.$$

- We define Ω_i containing K_i and adjacent elements,
- then we define the size of K_i by:

$$h_i = \min_{\text{e edge of } \Omega_i} \text{length}(\text{e}).$$

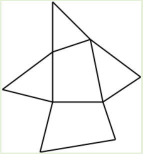


Figure: Example of 2D small meshes Ω_i.

Given a reference size h_{ref}, we split the domain using the following rule:

$$\begin{cases} \text{if } h_i \leq h_{ref},\ K_i \in \Omega^{fine} = \text{ fine region} \\ \text{if } h_i > h_{ref},\ K_i \in \Omega^{coarse} = \text{ coarse region} \end{cases}$$

Outline

Acoustic wave equation

We consider the first order formulation of the acoustic wave equation

$$\begin{cases} \rho\, \partial_t u - \operatorname{div} \mathbf{v} = f, \quad \forall (x,t) \in \Omega \times I \\ \mu^{-1} \partial_t \mathbf{v} - \nabla u = 0, \quad \forall (x,t) \in \Omega \times I \\ u(x,0) = \partial_t u(x,0) = 0, \quad \forall x \in \Omega \quad \text{(null initial conditions)} \\ \mu \partial_n u = 0, \quad x \in \Gamma_N \quad \text{(Neumann condition)} \end{cases} \tag{6}$$

- Ω is the computational domain
- I is the time interval
- u is the pressure field
- $\mathbf{v}$ is the displacement wave field
- $\rho = \frac{1}{\rho_f c^2}$ and $\mu = \frac{1}{\rho_f}$
- ρ_f is the fluid density
- c is the wave speed

Convergence curves

✓ 8^{th} order HDG is used on a regular mesh covering $[-5,5]^2$, and $\rho = \mu = 1$.

✓ The source term in space is $f(x,y) = exp(-\alpha_0(x^2+y^2))$, $\alpha_0 \approx -\dfrac{\log(10^{-6})}{4}$.

✓ $I = [0,200]$, the temporal source is a Ricker, with frequency $f_0 = 0.48$.

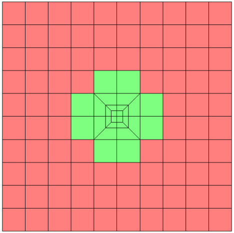
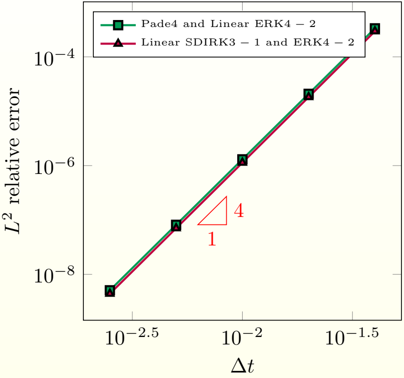


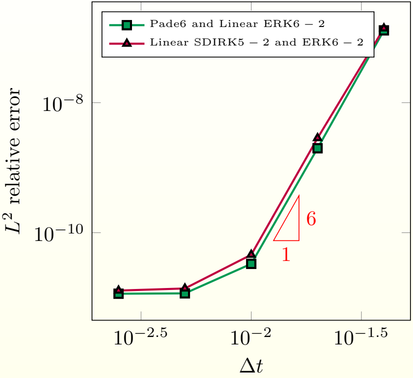
Figure: Mesh used for the convergence curves of the locally implicit method. Fine region in green.

- 116 elements
- 2 268 degrees of freedom
- $\Delta t_{max} \approx 0.005$ for classical ERK4
- $\Delta t_{max} \approx 0.0133$ for optimized ERK4 with 2 additional stages.
- $\Delta t_{max} \approx 0.04$ for the locally implicit method of order 4.

Convergence curves



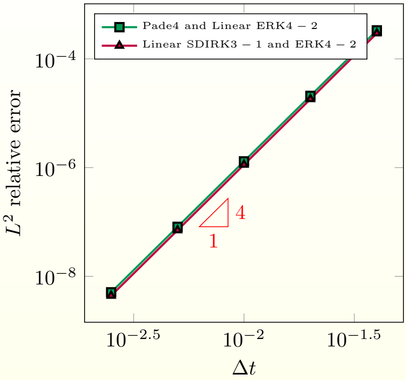
(a) Order 4



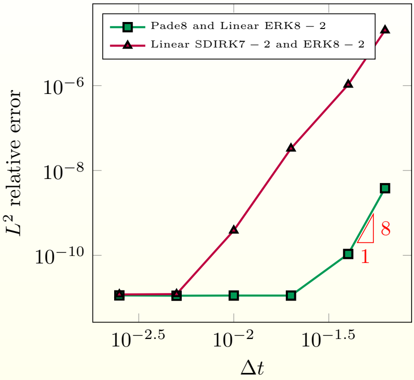
(b) order 6

Figure: Relative L^2 error between numerical solution and the reference solution for $t = 200$ with respect to the time step. Comparison of locally implicit methods of order 4 and 6 (Padé and Linear-SDIRK schemes combined with Linear-ERK schemes). The space discretization error is about 10^{-11}.

Convergence curves



(a) Order 4



(b) Order 8

Figure: Relative L^2 error between numerical solution and the reference solution for $t = 200$ with respect to the time step. Comparison of locally implicit methods of order 4 and 8 (Padé and Linear-SDIRK schemes combined with Linear-ERK schemes). The space discretization error is about 10^{-11}.

On going works and perspectives

On going works

- Parallelization of the locally implicit method.
- Comparison of explicit, implicit and locally implicit methods for 3D problems.

Perspectives

- Comparison of locally implicit and the local time stepping technique.
- Combine locally implicit methods with the local time stepping technique.

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- Combine locally implicit methods with the local time stepping technique.

Thank you for your attention.

Questions?

Outline

References

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