ADER and DeC: arbitrarily high order (explicit) methods for PDEs (and ODEs)

Davide Torlo

Inria Bordeaux - Sud Ouest
Team Cardamom

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joint work with Maria Han Veiga and Philipp Öffner

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Outline

1. Motivation
2. DeC
3. ADER
4. Similarities
5. Simulations

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Motivation: high order accurate explicit method

We want to solve a hyperbolic PDE system for $u : \mathbb{R}^+ \times \Omega \to \mathbb{R}^D$

$$\partial_t u + \nabla_{\mathbf{x}} \mathcal{F}(u) = 0. \quad (1)$$

Or ODE system for $\boldsymbol{\alpha} : \mathbb{R}^+ \to \mathbb{R}^S$

$$\partial_t \boldsymbol{\alpha} + F(\boldsymbol{\alpha}) = 0. \quad (2)$$

Applications:

- Fluids/transport
- Chemical/biological processes

How?

- Arbitrarily high order accurate
-

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How?

- Arbitrarily high
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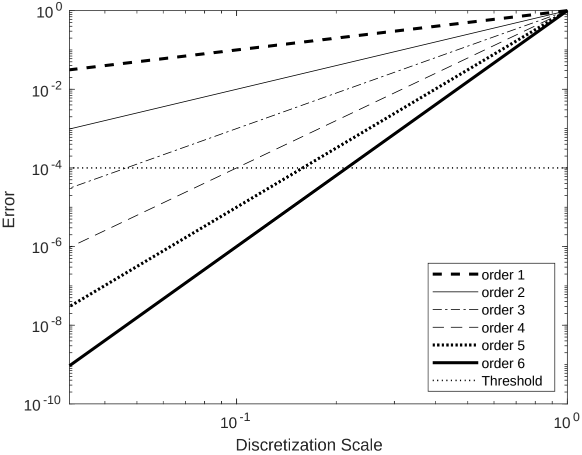

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Applications:

- Fluids/transport
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How?

- Arbitrarily high order accurate
- Explicit (if nonstiff problem)

DeC

Deferred Correction + Residual distribution

- Residual distribution (FV ⇒ FE) ⇒ High order in space
- Prediction/correction/iterations ⇒ High order in time
- Subtimesteps ⇒ High order in time

$$U_\xi^{m,(k+1)} = U_\xi^{m,(k)} - |C_p|^{-1} \sum_{E|\xi\in E} \left(\int_E \Phi_\xi \left(U^{m,(k)} - U^{n,0} \right) \mathrm{d}\mathbf{x} + \Delta t \sum_{r=0}^{M} \theta_r^m \mathcal{R}_\xi^E (U^{r,(k)}) \right),$$

with

$$\sum_{\xi \in E} \mathcal{R}_\xi^E(u) = \int_E \nabla_{\mathbf{x}} F(u) \mathrm{d}\mathbf{x}.$$

ADER

- Cauchy–Kovalevskaya theorem
- Modern automatic version
- Space/time DG
- Prediction/Correction
- Fixed-point iteration process

Prediction: iterative procedure

$$\int_{T^n \times V_i} \theta_{rs}(x,t)\partial_t \theta_{pq}(x,t) z^{pq} \mathrm{d}x\mathrm{d}t + \int_{T^n \times V_i} \theta_{rs}(x,t) \nabla_{\mathbf{x}} \cdot F(\theta_{pq}(x,t) z^{pq}) \mathrm{d}x\mathrm{d}t = 0.$$

Correction step: communication between cells

$$\int_{V_i} \Phi_r \left(u(t^{n+1}) - u(t^n) \right) \mathrm{d}x + \int_{T^n \times \partial V_i} \Phi_r(x) \mathcal{G}(z^-, z^+) \cdot \mathbf{n} \, \mathrm{d}S \, \mathrm{d}t - \int_{T^n \times V_i} \nabla_{\mathbf{x}} \Phi_r \cdot F(z) \, \mathrm{d}x \, \mathrm{d}t = 0,$$

ADER[1] and DeC[2]: immediate similarities

- High order time-space discretization
- Start from a well known space discretization (FE/DG/FV)
- FE reconstruction in time
- System in time, with M equations
- Iterative method / K corrections

- Both high order explicit time integration methods (neglecting spatial discretization)

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DeC high order time discretization: $\mathcal{L}^2$

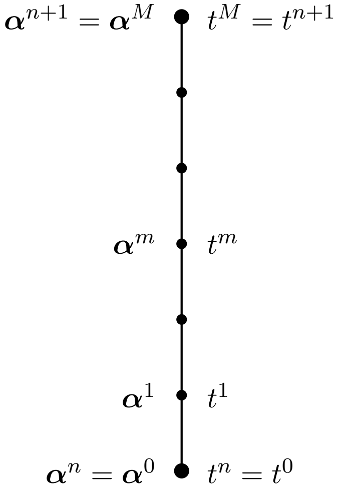
High order in time: we discretize our variable on $[t^n, t^{n+1}]$ in M substeps ($\boldsymbol{\alpha}^m$).

$$\partial_t \boldsymbol{\alpha} + F(\boldsymbol{\alpha}(t)) = 0.$$

Thanks to Picard–Lindelöf theorem, we can rewrite

$$\boldsymbol{\alpha}^m = \boldsymbol{\alpha}^0 - \int_{t^0}^{t^m} F(\boldsymbol{\alpha}(t))dt.$$

and if we want to reach order $r+1$ we need $M = r$.

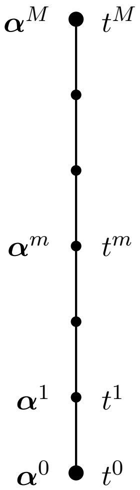


DeC high order time discretization: $\mathcal{L}^2$

More precisely, for each σ we want to solve $\mathcal{L}^2(\boldsymbol{\alpha}^{n,0},\dots,\boldsymbol{\alpha}^{n,M})=0$, where

$$\mathcal{L}^2(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M)=\begin{pmatrix}\boldsymbol{\alpha}^M-\boldsymbol{\alpha}^0-\sum_{r=0}^M\int_{t^0}^{t^M}F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s\\ \vdots\\ \boldsymbol{\alpha}^1-\boldsymbol{\alpha}^0-\sum_{r=0}^M\int_{t^0}^{t^1}F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s\end{pmatrix}$$

- $\mathcal{L}^2=0$ is a system of $M\times S$ coupled (non)linear equations
- $\mathcal{L}^2$ is an implicit method
- Not easy to solve directly $\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*)=0$
- High order ($\geq M+1$), depending on points distribution



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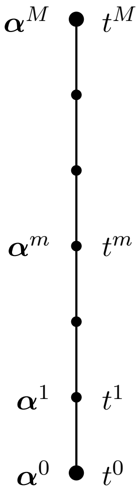
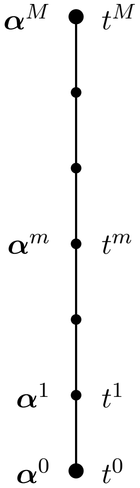


DeC low order time discretization: $\mathcal{L}^1$

Instead of solving the implicit system directly (difficult), we introduce a first order scheme $\mathcal{L}^1(\boldsymbol{\alpha}^{n,0},\dots,\boldsymbol{\alpha}^{n,M})$:

$$\mathcal{L}^1(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M)=\begin{pmatrix}\boldsymbol{\alpha}^M-\boldsymbol{\alpha}^0-\Delta t\beta^M F(\boldsymbol{\alpha}^0)\\ \vdots \\ \boldsymbol{\alpha}^1-\boldsymbol{\alpha}^0-\Delta t\beta^1 F(\boldsymbol{\alpha}^0)\end{pmatrix}$$

- First order approximation
- Explicit Euler
- Easy to solve $\mathcal{L}^1(\underline{\boldsymbol{\alpha}})=0$



How to combine two methods keeping the accuracy of the second and the stability and simplicity of the first one?

- $\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) = 0$, first order accuracy, easily invertible.
- $\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) = 0$, high order $M+1$.

$$\boldsymbol{\alpha}^{0,(k)} := \boldsymbol{\alpha}(t^n), \quad k = 0, \dots, K,$$

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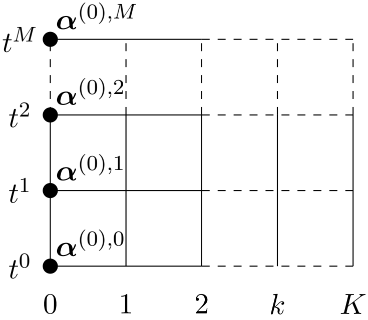
$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)})$ with $k = 1, \dots, K$.



Theorem (Convergence DeC)

- $\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*) = 0$
- *If $\mathcal{L}^1$ coercive with constant C_1*
- *If $\mathcal{L}^1 - \mathcal{L}^2$ Lipschitz with constant $C_2 \Delta t$*

Then $\|\underline{\boldsymbol{\alpha}}^{(K)} - \underline{\boldsymbol{\alpha}}^*\| \leq C(\Delta t)^K$

[3] A. Dutt, L. Greengard, and V. Rokhlin. BIT Numerical Mathematics, 40(2):241–266, 2000.

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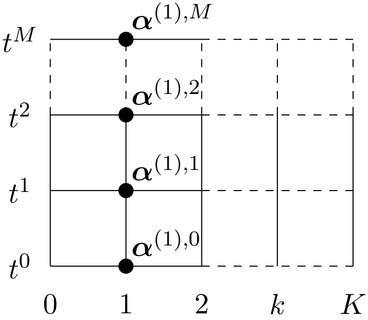

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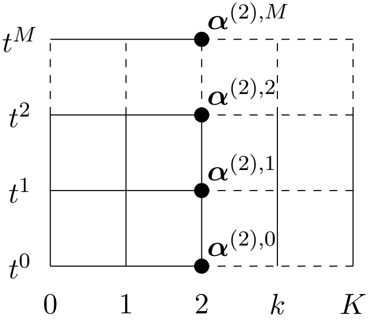

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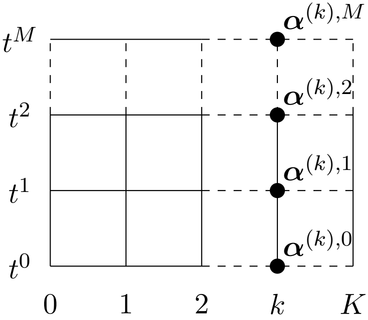

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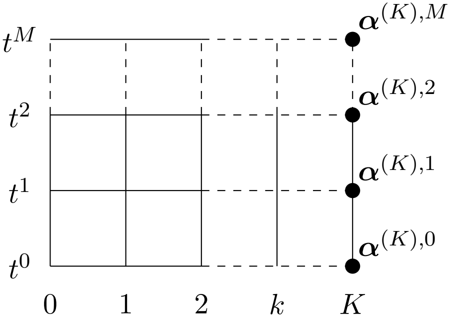

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DeC and Residual Distribution

In practice

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For $m = 1, \dots, M$

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- Operators can be extended for space time discretization.
- The $\mathcal{L}^2$ operator contains also the complications of the spatial discretization (e.g. mass matrix)
- $\mathcal{L}^1$ operator further simplified up to a first order approximation (e.g. **mass lumping**)

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ADER: space-time discretization

Originally exploitation of Cauchy–Kovalevskaya theorem (many computations)

Modern approach is DG in space time for hyperbolic problem

$$\partial_t u(x,t) + \nabla \cdot F(u(x,t)) = 0, \qquad x \in \Omega \subset \mathbb{R}^d,\ t > 0. \tag{3}$$

Defining $\theta_{rs}(x,t) = \Phi_r(x)\phi_s(t)$ basis functions in space and time

$$\int_{T^n \times V_i} \theta_{rs}(x,t)\partial_t \theta_{pq}(x,t) u^{pq} \mathrm{d}x\mathrm{d}t + \int_{T^n \times V_i} \theta_{rs}(x,t)\nabla \cdot F(\theta_{pq}(x,t)u^{pq})\mathrm{d}x\mathrm{d}t = 0. \tag{4}$$

This leads to

$$\underline{\underline{\mathrm{M}}}_{rspq} u^{pq} = \underline{r}(\underline{\mathbf{u}})_{rs}, \tag{5}$$

solved with fixed point iteration method.
+ Correction step where cells communication is allowed (derived from (4)).

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ADER: time integration method

Simplify!

$$\int_{T^n} \psi(t)\partial_t \boldsymbol{\alpha}(t)dt + \int_{T^n} \psi(t)F(\boldsymbol{\alpha}(t))dt = 0, \quad \forall \psi : T^n = [t^n, t^{n+1}] \to \mathbb{R}.$$

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \int_{T^n} \underline{\phi}(t)\partial_t \underline{\phi}(t)^T \underline{\boldsymbol{\alpha}} dt + \int_{T^n} \underline{\phi}(t) F(\underline{\phi}(t)^T \underline{\boldsymbol{\alpha}})dt = 0$$

$$\underline{\phi}(t) = (\phi_0(t), \dots, \phi_M(t))^T$$

Quadrature. . .

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - \underline{r}(\underline{\boldsymbol{\alpha}}) = 0 \iff \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} = \underline{r}(\underline{\boldsymbol{\alpha}}). \tag{6}$$

Nonlinear system of $M \times S$ equations

ADER: Fixed point iteration

Iterative procedure to solve the problem for each time step

$$\underline{\boldsymbol{\alpha}}^{(k)} = \underline{\underline{\mathrm{M}}}^{-1}\underline{r}(\underline{\boldsymbol{\alpha}}^{(k-1)}), \quad k = 1, \dots, \text{convergence} \tag{7}$$

with $\underline{\boldsymbol{\alpha}}^{(0)} = \boldsymbol{\alpha}(t^n)$.
Reconstruction step

$$\boldsymbol{\alpha}(t^{n+1}) = \boldsymbol{\alpha}(t^n) - \int_{T^n} F(\boldsymbol{\alpha}^{(K)}(t))dt.$$

- Convergence?
- How many steps K?

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ADER as DeC

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\underline{\boldsymbol{\alpha}}),$$
$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\boldsymbol{\alpha}(t^n)).$$

$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)}), \qquad k = 1, \dots, K,$$

$$\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k)} - r(\boldsymbol{\alpha}^{(k),0}) - \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)} + r(\boldsymbol{\alpha}^{(k-1),0}) + \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)} - r(\underline{\boldsymbol{\alpha}}^{(k-1)}) = 0$$

ADER as DeC

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\underline{\boldsymbol{\alpha}}),$$
$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\boldsymbol{\alpha}(t^n)).$$

$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)}), \qquad k = 1, \dots, K,$$

$$\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k)} - \cancel{r(\boldsymbol{\alpha}^{(k),0})} - \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)} + \cancel{r(\boldsymbol{\alpha}^{(k-1),0})} + \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)} - r(\underline{\boldsymbol{\alpha}}^{(k-1)}) = 0$$

ADER as DeC

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}\boldsymbol{\alpha}} - r(\underline{\boldsymbol{\alpha}}),$$
$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}\boldsymbol{\alpha}} - r(\boldsymbol{\alpha}(t^n)).$$

$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)}), \qquad k = 1, \dots, K,$$

$$\underline{\underline{\mathrm{M}}\boldsymbol{\alpha}}^{(k)} - \cancel{r(\boldsymbol{\alpha}^{(k),0})} - \cancel{\underline{\underline{\mathrm{M}}\boldsymbol{\alpha}}^{(k-1)}} + \cancel{r(\boldsymbol{\alpha}^{(k-1),0})} + \cancel{\underline{\underline{\mathrm{M}}\boldsymbol{\alpha}}^{(k-1)}} - r(\underline{\boldsymbol{\alpha}}^{(k-1)}) = 0$$

ADER as DeC

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\underline{\boldsymbol{\alpha}}),$$
$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\boldsymbol{\alpha}(t^n)).$$

$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)}), \qquad k = 1, \dots, K,$$

$$\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k)} - \cancel{r(\boldsymbol{\alpha}^{(k),0})} - \cancel{\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)}} + \cancel{r(\boldsymbol{\alpha}^{(k-1),0})} + \cancel{\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k-1)}} - r(\underline{\boldsymbol{\alpha}}^{(k-1)}) = 0$$
$$\underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}}^{(k)} - r(\underline{\boldsymbol{\alpha}}^{(k-1)}) = 0.$$

ADER as DeC

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\underline{\boldsymbol{\alpha}}),$$
$$\mathcal{L}^1(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - r(\boldsymbol{\alpha}(t^n)).$$

Apply the DeC Convergence theorem!

- $\mathcal{L}^1$ is coercive because $\underline{\underline{\mathrm{M}}}$ is always invertible
- $\mathcal{L}^1 - \mathcal{L}^2$ is Lipschitz with constant $C\Delta t$ because they are consistent approx of the same problem
- Hence, after K iterations we obtain a Kth order accurate approximation of $\underline{\boldsymbol{\alpha}}^*$

$$\mathcal{L}^2(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M) := \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \sum_{r=0}^M \int_{t^0}^{t^M} F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s \\ \dots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \sum_{r=0}^M \int_{t^0}^{t^1} F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s \end{cases}.$$

$$\chi_{[t^0,t^m]}(t^m)\boldsymbol{\alpha}^m - \chi_{[t^0,t^m]}(t_0)\boldsymbol{\alpha}^0 - \int_{t^0}^{t^m} \chi_{[t^0,t^m]}(t)\sum_{r=0}^M F(\boldsymbol{\alpha}^r)\varphi_r(t)\mathrm{d}t = 0$$

$$\int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t)\partial_t\left(\boldsymbol{\alpha}(t)\right)\mathrm{d}t - \int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t)\sum_{r=0}^M F(\boldsymbol{\alpha}^r)\varphi_r(t)\mathrm{d}t = 0,$$

$$\int_{T^n} \psi_m(t)\partial_t\boldsymbol{\alpha}(t)\mathrm{d}t - \int_{T^n}\psi_m(t)F(\boldsymbol{\alpha}(t))\mathrm{d}t = 0.$$

DeC as ADER

$$\mathcal{L}^2(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M) := \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \sum_{r=0}^M \int_{t^0}^{t^M} F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s \\ \dots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \sum_{r=0}^M \int_{t^0}^{t^1} F(\boldsymbol{\alpha}^r)\varphi_r(s)\mathrm{d}s \end{cases}.$$

$$\chi_{[t^0,t^m]}(t^m)\boldsymbol{\alpha}^m - \chi_{[t^0,t^m]}(t_0)\boldsymbol{\alpha}^0 - \int_{t^0}^{t^m} \chi_{[t^0,t^m]}(t) \sum_{r=0}^M F(\boldsymbol{\alpha}^r)\varphi_r(t)\mathrm{d}t = 0$$

$$\int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t)\partial_t\left(\boldsymbol{\alpha}(t)\right)\mathrm{d}t - \int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t) \sum_{r=0}^M F(\boldsymbol{\alpha}^r)\varphi_r(t)\mathrm{d}t = 0,$$

$$\int_{T^n} \psi_m(t)\partial_t\boldsymbol{\alpha}(t)\mathrm{d}t - \int_{T^n} \psi_m(t)F(\boldsymbol{\alpha}(t))\mathrm{d}t = 0.$$

Runge Kutta vs DeC–ADER

Classical Runge Kutta (RK)

- One step method
- Internal stages

Explicit Runge Kutta

+ Simple to code
- Not easily generalizable to arbitrary order
- Stages $>$ order

Implicit Runge Kutta

+ Arbitrarily high order
- Require nonlinear solvers for nonlinear systems
- May not converge

DeC – ADER

- One step method
- Internal subtimesteps
- Can be rewritten as explicit RK (for ODE)

+ Explicit
+ Simple to code
+ Iterations $=$ order
+ Arbitrarily high order
- Large memory storage

Outline

1 Motivation

2 DeC

3 ADER

4 Similarities

5 Simulations

$$y'(t) = \lambda y(t) \qquad y(0) = 1$$

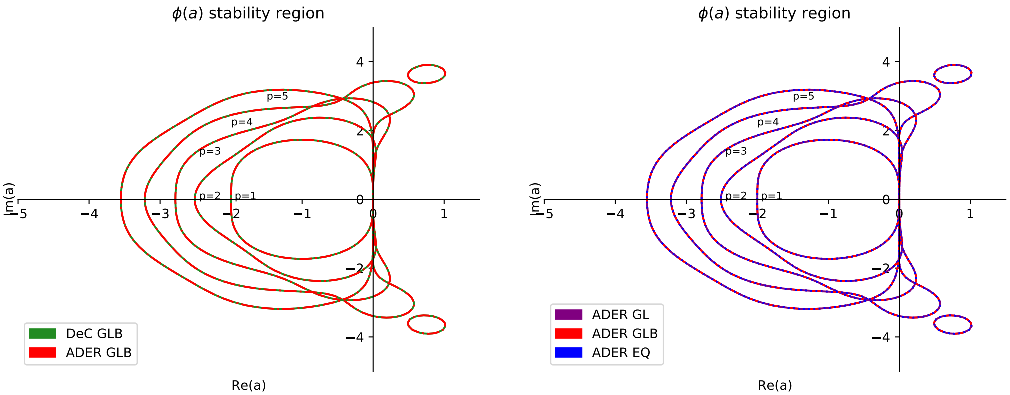
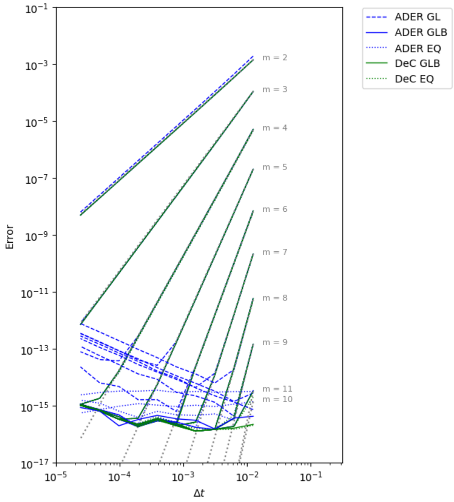


Figure: Stability region

Convergence

$$\begin{aligned} y'(t) &= -|y(t)|y(t), \\ y(0) &= 1, \\ t &\in [0, 0.1]. \end{aligned} \tag{8}$$

Convergence curves for ADER and DeC, varying the approximation order and collocation of nodes for the subtimesteps for a scalar nonlinear ODE



Lotka–Volterra

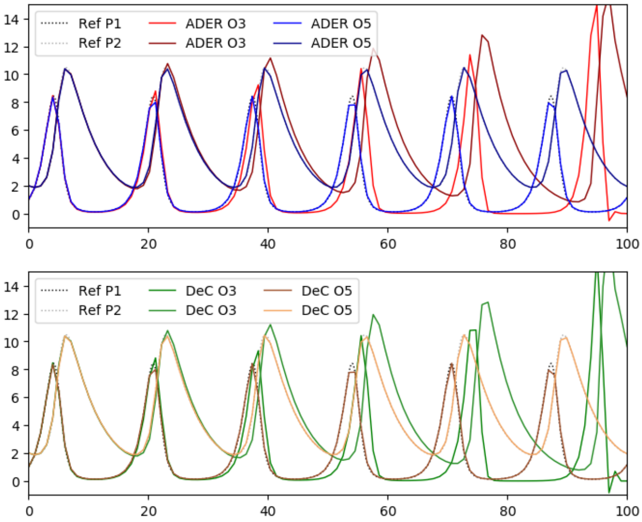


Figure: Numerical solution of the Lotka-Volterra system using ADER (top) and DeC (bottom) with Gauss-Lobatto nodes with timestep $\Delta T = 1$.

PDE: Burgers with spectral difference

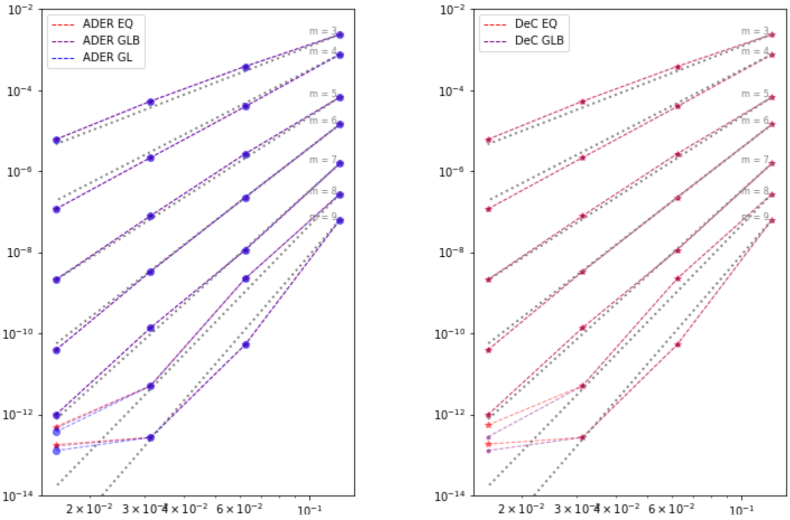


Figure: Convergence error for Burgers equations: Left ADER right DeC. Space discretization with spectral difference

Extensions

Other versions

- Other spatial discretizations (FV/DG ADER, FEM/DG DeC)
- Implicit or implicit–explicit time discretizations (implicit DeC and implicit ADER by making implicit $\mathcal{L}^1$)
- Positivity preserving versions (modified Patankar DeC)
- ...

On going projects

- Stability study of implicit versions
- Entropy stable high order ADER DeC

Thanks for the attention!
Questions?