ADER and DeC: arbitrarily high order explicit time integration methods

Davide Torlo

Universität Zürich
Institut für Mathematik

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joint work with Maria Han Veiga and Philipp Öffner

Outline

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Motivation: high order accurate explicit method

We want to solve an ODE system for $\boldsymbol{\alpha} : \mathbb{R}^+ \to \mathbb{R}^S$

$$\partial_t \boldsymbol{\alpha} + F(\boldsymbol{\alpha}) = 0. \tag{1}$$

Applications:

- Semidiscretized PDEs
- Chemical/biological processes

How?

- Arbitrarily high order accurate
-

Motivation: high order accurate explicit method

We want to

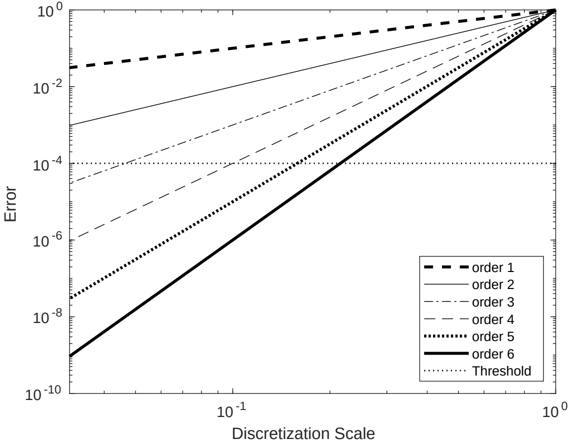
(1)

Application

- Semid
- Chemi

How?

- Arbitra
-



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Applications:

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How?

- Arbitrarily high order accurate
- Explicit

Classical time integration: Runge–Kutta

$$\boldsymbol{\alpha}^{(1)} := \boldsymbol{\alpha}^n, \tag{2}$$

$$\boldsymbol{\alpha}^{(k)} := \boldsymbol{\alpha}^n + \sum_{s=1}^{K} A_{ks} F\left(t^n + b_s \Delta t, \boldsymbol{\alpha}^{(s)}\right), \quad \text{for } k = 2, \dots, K, \tag{3}$$

$$\boldsymbol{\alpha}^{n+1} := \sum_{k=1}^{K} \gamma_k \boldsymbol{\alpha}^{(k)}. \tag{4}$$

Classical time integration: Explicit Runge–Kutta

$$\boldsymbol{\alpha}^{(k)} := \boldsymbol{\alpha}^n + \sum_{s=1}^{k-1} A_{ks} F\left(t^n + b_s \Delta t, \boldsymbol{\alpha}^{(s)}\right), \quad \text{for } k = 2, \dots, K.$$

- Easy to solve
- High orders involved:
  - Order conditions: system of many equations
  - Stages $K \geq d$ order of accuracy (e.g. RK44, RK65)

Classical time integration: Implicit Runge–Kutta

$$\boldsymbol{\alpha}^{(k)} := \boldsymbol{\alpha}^n + \sum_{s=1}^{K} A_{ks} F\left(t^n + b_s \Delta t, \boldsymbol{\alpha}^{(s)}\right), \quad \text{for } k = 2, \dots, K.$$

- More complicated to solve for nonlinear systems
- High orders easily done:
  - Take a high order quadrature rule on $[t^n, t^{n+1}]$
  - Compute the coefficients accordingly, see Gauss–Legendre or Gauss–Lobatto polynomials
  - Order up to $d = 2K - 1$

ADER and DeC

Two iterative explicit arbitrarily high order accurate methods.

- ADER[1] for hyperbolic PDE, after a first analytic more complicated approach.
- Deferred Correction (DeC): introduced for explicit ODE[2], extended to implicit ODE[3] and to hyperbolic PDE[4].

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[1] M. Dumbser, D. S. Balsara, E. F. Toro, and C.-D. Munz. A unified framework for the construction of one-step finite volume and discontinuous galerkin schemes on unstructured meshes. Journal of Computational Physics, 227(18):8209–8253, 2008.

[2] A. Dutt, L. Greengard, and V. Rokhlin. Spectral Deferred Correction Methods for Ordinary Differential Equations. BIT Numerical Mathematics, 40(2):241–266, 2000.

[3] M. L. Minion. Semi-implicit spectral deferred correction methods for ordinary differential equations. Commun. Math. Sci., 1(3):471–500, 09 2003.

[4] R. Abgrall. High order schemes for hyperbolic problems using globally continuous approximation and avoiding mass matrices. Journal of Scientific Computing, 73(2):461–494, Dec 2017.

Outline

DeC

Discretization of each time step $[t^n, t^{n+1}]$.

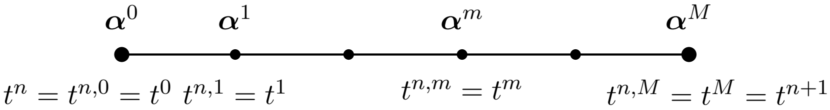

Figure: Subtime intervals

High order approximation of the equation in the Picard–Lindelöf form

$$\boldsymbol{\alpha}^m = \boldsymbol{\alpha}^0 - \int_{t^0}^{t^m} F(\boldsymbol{\alpha}(t))dt. \tag{5}$$

DeC: $\mathcal{L}^2$ operator

$$\mathcal{L}^2(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M) = \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \int_{t^0}^{t^M} \mathcal{I}_M(F(\boldsymbol{\alpha}^0),\dots,F(\boldsymbol{\alpha}^M))ds \\ \dots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \int_{t^0}^{t^1} \mathcal{I}_M(F(\boldsymbol{\alpha}^0),\dots,F(\boldsymbol{\alpha}^M))ds \end{cases}$$

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

$$= \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \Delta t \sum_{r=0}^M \theta_r^M F(\boldsymbol{\alpha}^r) \\ \dots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \Delta t \sum_{r=0}^M \theta_r^1 F(\boldsymbol{\alpha}^r) \end{cases}$$

DeC: $\mathcal{L}^2$ operator

Goal: find $\underline{\boldsymbol{\alpha}}^* = (\boldsymbol{\alpha}^0, \dots, \boldsymbol{\alpha}^m, \dots, \boldsymbol{\alpha}^M)^*$: $\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*) = 0$.

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

DeC: $\mathcal{L}^1$ operator

$$\mathcal{L}^1(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M) := \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \beta^M \Delta t F(\boldsymbol{\alpha}^0) \\ \vdots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \beta^1 \Delta t F(\boldsymbol{\alpha}^0) \end{cases} \qquad \beta^m := \frac{t^m - t^0}{t^M - t^0}. \tag{6}$$

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

DeC: Iterative process

K iterations where the iteration index is the superscript (k), with $k = 0, \dots, K$

1. Define $\boldsymbol{\alpha}^{(0),m} = \boldsymbol{\alpha}^n = \boldsymbol{\alpha}(t^n)$ for $m = 0, \dots, M$
2. Define $\boldsymbol{\alpha}^{(k),0} = \boldsymbol{\alpha}(t^n)$ for $k = 0, \dots, K$
3. Find $\underline{\boldsymbol{\alpha}}^{(k)}$ as $\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)}) = \mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k-1)})$
4. $\boldsymbol{\alpha}^{n+1} = \boldsymbol{\alpha}^{(K),M}$.

Theorem (Convergence DeC)

- *If $\mathcal{L}^1$ coercive with constant C_1*
- *If $\mathcal{L}^1 - \mathcal{L}^2$ Lipschitz with constant $C_2 \Delta t$*

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

Hence, choosing $K = M + 1$, then $\|\boldsymbol{\alpha}^{(K),M} - \boldsymbol{\alpha}^{ex}(t^{n+1})\| \leq C \Delta t^K$

DeC – Proof

Proof.

Let $\underline{\boldsymbol{\alpha}}^*$ be the solution of $\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*)=0$. We know that $\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^*)=\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^*)-\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*)$ and $\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k+1)})=\left(\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)})-\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k)})\right)$, so that

$$\begin{aligned}
C_1||\underline{\boldsymbol{\alpha}}^{(k+1)}-\underline{\boldsymbol{\alpha}}^*|| \leq & ||\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k+1)})-\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^*)|| = \\
= & ||\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^{(k)})-\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^{(k)})-(\mathcal{L}^1(\underline{\boldsymbol{\alpha}}^*)-\mathcal{L}^2(\underline{\boldsymbol{\alpha}}^*))|| \leq \\
\leq & C_2\Delta t||\underline{\boldsymbol{\alpha}}^{(k)}-\underline{\boldsymbol{\alpha}}^*||.
\end{aligned}$$

$$||\underline{\boldsymbol{\alpha}}^{(k+1)}-\underline{\boldsymbol{\alpha}}^*|| \leq \left(\frac{C_2}{C_1}\Delta t\right)||\underline{\boldsymbol{\alpha}}^{(k)}-\underline{\boldsymbol{\alpha}}^*|| \leq \left(\frac{C_2}{C_1}\Delta t\right)^{k+1}||\underline{\boldsymbol{\alpha}}^{(0)}-\underline{\boldsymbol{\alpha}}^*||.$$

After K iteration we have an error at most of $\eta^K\cdot||\underline{\boldsymbol{\alpha}}^{(0)}-\underline{\boldsymbol{\alpha}}^*||$. □

DeC: Second order example

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DeC in FEM

Operators can be extended for space time discretization.

Example: PDEs, FEM discretization

The $\mathcal{L}^2$ operator contains also the complications of the spatial discretization (e.g. mass matrix)

The $\mathcal{L}^1$ operator can simplify everything up to a first order approximation (e.g. mass lumping)

Outline

ADER: space-time discretization

Originally exploitation of Cauchy–Kovalevskaya theorem (many computations)

Modern approach is DG in space time for hyperbolic problem

$$\partial_t u(x,t) + \nabla \cdot F(u(x,t)) = 0, \qquad x \in \Omega \subset \mathbb{R}^d,\ t > 0. \tag{7}$$

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

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

This leads to

$$\underline{\underline{\mathrm{M}}}_{rspq} u^{pq} = \underline{r}(\underline{\mathbf{u}})_{rs}, \tag{8}$$

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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...

$$\mathcal{L}^2(\underline{\boldsymbol{\alpha}}) := \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} - \underline{r}(\underline{\boldsymbol{\alpha}}) = 0 \Longleftrightarrow \underline{\underline{\mathrm{M}}}\underline{\boldsymbol{\alpha}} = \underline{r}(\underline{\boldsymbol{\alpha}}). \tag{9}$$

Nonlinear system of $M \times S$ equations

ADER: Fixed point iteration

Iterative procedure to solve the problem for each time step

$$\underline{\boldsymbol{\alpha}}^{(k)} = \underline{\underline{\mathrm{M}}}^{-1} \underline{r}(\underline{\boldsymbol{\alpha}}^{(k-1)}), \quad k = 1, \dots, \text{convergence} \tag{10}$$

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

- Convergence?
- How many steps K?

Outline

ADER as DeC

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

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

defining $\boldsymbol{\alpha}^{(k),0} = \boldsymbol{\alpha}(t^n)$, $\forall k$. Hence, we can explicitly write it as

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

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ADER as DeC

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

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 $\underline{\boldsymbol{\alpha}}^*$

DeC as ADER

$$\mathcal{L}^2(\boldsymbol{\alpha}^0,\dots,\boldsymbol{\alpha}^M) := \begin{cases} \boldsymbol{\alpha}^M - \boldsymbol{\alpha}^0 - \int_{t^0}^{t^M} \mathcal{I}_M(F(\boldsymbol{\alpha}^0),\dots,F(\boldsymbol{\alpha}^M)) \\ \vdots \\ \boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^0 - \int_{t^0}^{t^1} \mathcal{I}_M(F(\boldsymbol{\alpha}^0),\dots,F(\boldsymbol{\alpha}^M)) \end{cases}$$

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and focus on the m-th line, which reads

$$\boldsymbol{\alpha}^m - \boldsymbol{\alpha}^0 - \sum_{r=0}^M F(\boldsymbol{\alpha}^r) \int_{t^0}^{t^m} \varphi_r(t)\mathrm{d}t = 0.$$

DeC as ADER

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

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

$$\chi_{[t^0,t^m]}(t) = \begin{cases} 1, & \text{if} \quad t \in [t^0, t^m], \\ 0, & \text{else.} \end{cases} \tag{11}$$

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

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

DeC as ADER

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

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DeC as ADER

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

DeC – ADER

Both are

- Iterative processes (only iterations $K = d$ order of accuracy)
- Arbitrarily high order accurate
- Explicit

ADER as DeC iterative process

- The operators $\mathcal{L}^1$ and $\mathcal{L}^2$ can be written
- Convergence results hold
- We know in practice how many iteration K

DeC as ADER

- $\mathcal{L}^2$ is the same up to the choice of basis and test functions in time

Outline

A–Stability

$$y'(t) = \lambda y(t) \tag{12}$$
$$y(0) = 1 \tag{13}$$

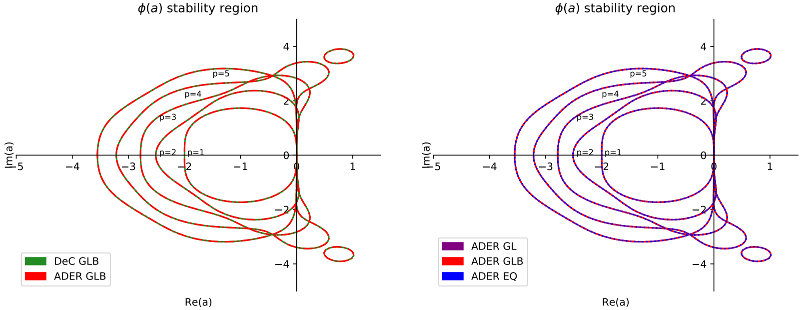
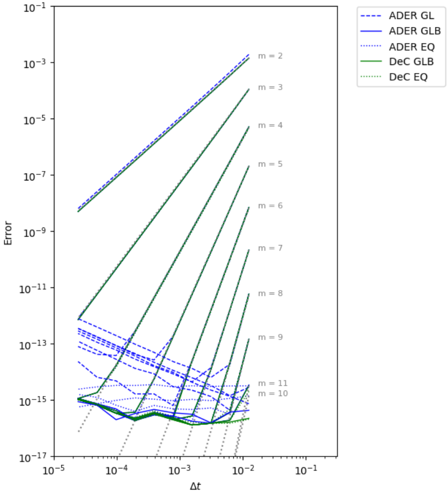


Figure: Stability region

Convergence

$$\begin{aligned} & y'(t) = -|y(t)|y(t), \\ & y(0) = 1, \\ & t \in [0, 0.1]. \end{aligned} \tag{14}$$

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



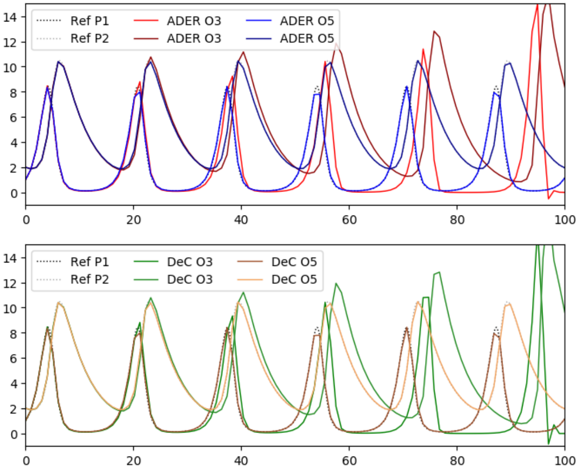


Figure: Numerical solution of the Lotka-Volterra system using ADER (top) and DeC (bottom) with Gauss-Lobatto nodes with timestep $\Delta T = 1$.

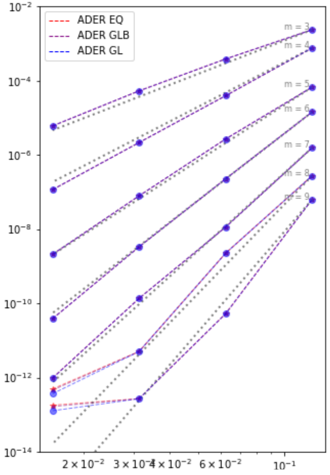


Figure: ADER

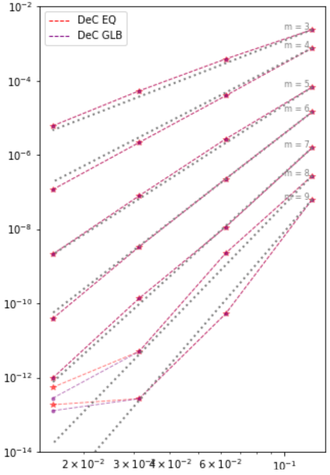


Figure: DeC

Thanks for the attention!
Questions?