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

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SISSA Mathlab

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Outline

- Motivation
- 2 DeC
- 3 ADER
- Similarities
- 5 ADER stability and accuracy
- Simulations

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Motivation: high order accurate explicit method

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

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

Or ODE system for $oldsymbol{u}: \mathbb{R}^+
ightarrow \mathbb{R}^S$

$$\partial_t \boldsymbol{u} = F(\boldsymbol{u}). \tag{2}$$

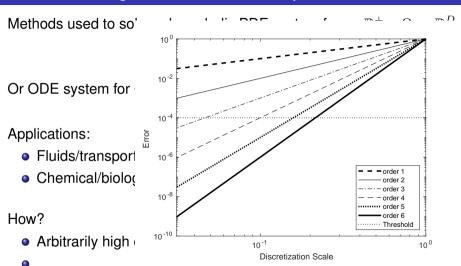
Applications:

- Fluids/transport
- Chemical/biological processes

How?

- Arbitrarily high order accurate
- •

Motivation: high order accurate explicit method



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(1)

(2)

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Applications:

- Fluids/transport
- Chemical/biological processes

How?

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

Classical time integration: Runge-Kutta

$$\boldsymbol{u}^{(1)} := \boldsymbol{u}^n, \tag{3}$$

$$\boldsymbol{u}^{(k)} := \boldsymbol{u}^n + \sum_{s=1}^K a_{ks} F\left(t^n + c_s \Delta t, \boldsymbol{u}^{(s)}\right), \quad \text{for } k = 2, \dots, K,$$
(4)

$$\boldsymbol{u}^{n+1} := \boldsymbol{u}^n + \sum_{s=1}^K b_s F\left(t^n + c_s \Delta t, \boldsymbol{u}^{(s)}\right). \tag{5}$$

ADER vs DeC 5/72

Classical time integration: Explicit Runge-Kutta

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

- 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

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

- 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

ADER and DeC

Two iterative explicit arbitrarily high order accurate methods.

- ADER¹ for hyperbolic PDE, after a first analytic more complicated approach.
- Deferred Correction (DeC): introduced for explicit ODE², extended to implicit ODE³ and to hyperbolic PDE⁴.

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¹M. 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.

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

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

⁴R. 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.

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

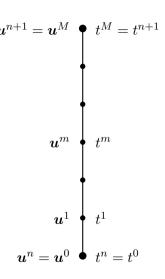
High order in time: we discretize our variable on $[t^n, t^{n+1}]$ in M substeps (u^m) .

$$\partial_t \boldsymbol{u} = F(\boldsymbol{u}(t)).$$

Thanks to Picard-Lindelöf theorem, we can rewrite

$$oldsymbol{u}^m = oldsymbol{u}^0 + \int_{t^0}^{t^m} F(oldsymbol{u}(t)) dt.$$

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

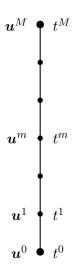


DeC high order time discretization: \mathcal{L}^2

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

$$\mathcal{L}^{2}(\boldsymbol{u}^{0},\ldots,\boldsymbol{u}^{M}) = \begin{pmatrix} \boldsymbol{u}^{M} - \boldsymbol{u}^{0} + \sum_{r=0}^{M} \int_{t^{0}}^{t^{M}} F(\boldsymbol{u}^{r}) \varphi_{r}(s) ds \\ \vdots \\ \boldsymbol{u}^{1} - \boldsymbol{u}^{0} + \sum_{r=0}^{M} \int_{t^{0}}^{t^{1}} F(\boldsymbol{u}^{r}) \varphi_{r}(s) ds \end{pmatrix}$$

- $\mathcal{L}^2 = 0$ is a system of $M \times S$ coupled (non)linear equations
- ullet L² is an implicit method (collocation method: Gauss, LobattoIIIA)
- Not easy to solve directly $\mathcal{L}^2(\underline{\boldsymbol{u}}^*)=0$
- High order ($\geq M+1$), depending on points distribution

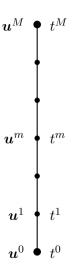


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$$\mathcal{L}^2(oldsymbol{u}^0,\dots,oldsymbol{u}^M) = egin{pmatrix} oldsymbol{u}^M - oldsymbol{u}^0 + \Delta t \sum_{r=0}^M heta_r^M F(oldsymbol{u}^r) \ dots \ oldsymbol{u}^1 - oldsymbol{u}^0 + \Delta t \sum_{r=0}^M heta_r^1 F(oldsymbol{u}^r) \end{pmatrix}$$

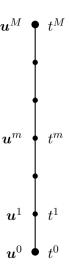
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Instead of solving the implicit system directly (difficult), we introduce a first order scheme $\mathcal{L}^1(\boldsymbol{u}^{n,0},\ldots,\boldsymbol{u}^{n,M})$:

$$\mathcal{L}^1(oldsymbol{u}^0,\dots,oldsymbol{u}^M) = egin{pmatrix} oldsymbol{u}^M - oldsymbol{u}^0 + \Delta t eta^M F(oldsymbol{u}^0) \ dots \ oldsymbol{u}^1 - oldsymbol{u}^0 + \Delta t eta^1 F(oldsymbol{u}^0) \end{pmatrix}$$

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



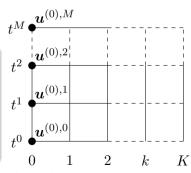
How to combine two methods keeping the accuracy of the second and the stability and simplicity of the first one?

$$\begin{split} \boldsymbol{u}^{0,(k)} &:= \boldsymbol{u}(t^n), \quad k = 0, \dots, K, \\ \boldsymbol{u}^{m,(0)} &:= \boldsymbol{u}(t^n), \quad m = 1, \dots, M \\ \mathcal{L}^1(\underline{\boldsymbol{u}}^{(k)}) &= \mathcal{L}^1(\underline{\boldsymbol{u}}^{(k-1)}) - \mathcal{L}^2(\underline{\boldsymbol{u}}^{(k-1)}) \text{ with } k = 1, \dots, K. \end{split}$$

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

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

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



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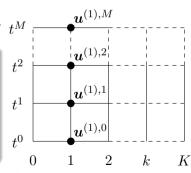
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Theorem (Convergence DeC)

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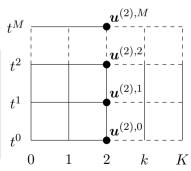
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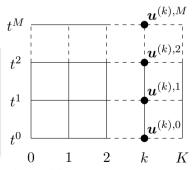
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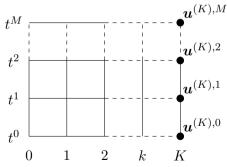
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DeC - Proof

Proof.

Let f^* be the solution of $\mathcal{L}^2(\underline{\boldsymbol{u}}^*)=0$. We know that $\mathcal{L}^1(\underline{\boldsymbol{u}}^*)=\mathcal{L}^1(\underline{\boldsymbol{u}}^*)-\mathcal{L}^2(\underline{\boldsymbol{u}}^*)$, so that



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$$\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{(k+1)}) - \mathcal{L}^{1}(\underline{\boldsymbol{u}}^{*}) = \left(\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{(k)}) - \mathcal{L}^{2}(\underline{\boldsymbol{u}}^{(k)})\right) - \left(\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{*}) - \mathcal{L}^{2}(\underline{\boldsymbol{u}}^{*})\right)$$

$$\frac{\boldsymbol{C_{1}}||\underline{\boldsymbol{u}}^{(k+1)} - \underline{\boldsymbol{u}}^{*}|| \leq ||\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{(k+1)}) - \mathcal{L}^{1}(\underline{\boldsymbol{u}}^{*})|| =$$

$$= ||\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{(k)}) - \mathcal{L}^{2}(\underline{\boldsymbol{u}}^{(k)}) - (\mathcal{L}^{1}(\underline{\boldsymbol{u}}^{*}) - \mathcal{L}^{2}(\underline{\boldsymbol{u}}^{*}))|| \leq$$

$$\leq \underline{\boldsymbol{C_{2}}} \Delta ||\underline{\boldsymbol{u}}^{(k)} - \underline{\boldsymbol{u}}^{*}||.$$

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

After K iteration we have an error at most of $\left(\frac{C_2}{C_1}\Delta\right)^K ||\underline{\boldsymbol{u}}^{(0)}-\underline{\boldsymbol{u}}^*||$.

In practice

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

$$\mathbf{u}^{(k),\underline{m}} \cdot \mathbf{u}^{0} - \beta^{m} \Delta t F(\mathbf{u}^{0}) - \mathbf{u}^{(k-1),m} + \mathbf{u}^{0} + \beta^{m} \Delta t F(\mathbf{u}^{0})$$
$$+ \mathbf{u}^{(k-1),\underline{m}} \cdot \mathbf{u}^{0} - \Delta t \sum_{r=0}^{M} \theta_{r}^{m} F(\mathbf{u}^{(k-1),r}) = 0$$

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DeC and residual distribution

Deferred Correction + Residual distribution

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

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

with

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

- The \mathcal{L}^2 operator contains also the complications of the spatial discretization (e.g. mass matrix)
- ullet \mathcal{L}^1 operator further simplified up to a first order approximation (e.g. **mass lumping**)

\mathcal{L}^1 with mass lumping

Define \mathcal{L}^1 as

$$\mathcal{L}^1(oldsymbol{u}^0,\dots,oldsymbol{u}^M) = egin{pmatrix} oldsymbol{u}^M - oldsymbol{u}^0 - \Delta t eta^M F(oldsymbol{u}^0) \ dots \ oldsymbol{u}^1 - oldsymbol{u}^0 - \Delta t eta^1 F(oldsymbol{u}^0) \end{pmatrix}$$

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$$\mathcal{L}^{1}(\boldsymbol{u}^{0},\ldots,\boldsymbol{u}^{M}) = \begin{pmatrix} \boldsymbol{u}^{M} - \boldsymbol{u}^{0} - \Delta t \beta^{M} \left(F(\boldsymbol{u}^{0}) + \partial_{\boldsymbol{u}} F(\boldsymbol{u}^{0}) (\boldsymbol{u}^{M} - \boldsymbol{u}^{0}) \right) \\ \vdots \\ \boldsymbol{u}^{1} - \boldsymbol{u}^{0} - \Delta t \beta^{1} \left(F(\boldsymbol{u}^{0}) + \partial_{\boldsymbol{u}} F(\boldsymbol{u}^{0}) (\boldsymbol{u}^{1} - \boldsymbol{u}^{0}) \right) \end{pmatrix}$$
$$= \begin{pmatrix} \boldsymbol{u}^{M} - \boldsymbol{u}^{0} - \Delta t \beta^{M} \partial_{\boldsymbol{u}} F(\boldsymbol{u}^{0}) \boldsymbol{u}^{M} \\ \vdots \\ \boldsymbol{u}^{1} - \boldsymbol{u}^{0} - \Delta t \beta^{1} \partial_{\boldsymbol{u}} F(\boldsymbol{u}^{0}) \boldsymbol{u}^{1} \end{pmatrix}$$

$$\mathcal{L}^{1,m}(\boldsymbol{u}^0,\ldots,\boldsymbol{u}^M) = \boldsymbol{u}^m - \boldsymbol{u}^0 - \Delta t \beta^m \partial_{\boldsymbol{u}} F(\boldsymbol{u}^0) \boldsymbol{u}^m$$
$$\mathcal{L}^{2,m}(\boldsymbol{u}^0,\ldots,\boldsymbol{u}^M) = \boldsymbol{u}^m - \boldsymbol{u}^0 - \Delta t \sum_{r} \theta_r^m F(\boldsymbol{u}^r)$$

DeC as RK

$$u^{(k),m} - u^0 - \Delta t \sum_{r=0}^{M} \theta_r^m F(u^{(k-1),r}) = 0$$

DeC as RK

DeC as RK

We can write DeC as RK defining $\underline{\theta}_0 = \{\theta_0^m\}_{m=1}^M$, $\underline{\theta}^M = \theta_r^M$ with $r \in 1, \ldots, M$, denoting the vector $\underline{\theta}_r^{M,T} = (\theta_1^M, \ldots, \theta_M^M)$. The Butcher tableau for an arbitrarily high order DeC approach is given by:

Idea: study the RK version!

$$u' = \lambda u \qquad \Re(\lambda) < 0. \tag{7}$$

$$u_{n+1} = R(\lambda \Delta t)u_n, \qquad R(z) = 1 + zb^T (I - zA)^{-1} \mathbf{1}, \qquad z = \lambda \Delta t$$
 (8)

Goal: find $z \in \mathbb{C}$ such that |R(z)| < 1.

Recall: stability function for explicit RK methods is a polynomial, indeed the inverse of (I-zA) can be written in Taylor expansion as

$$(I - zA)^{-1} = \sum_{r=0}^{\infty} z^r A^s = I + zA + z^2 A^2 + \dots,$$
 (9)

and, since A is strictly lower triangular, it is nilpotent. Hence, R(z) is a polynomial in z with degree at most equal to S.

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Theorem

If the RK method is of order P, then

$$R(z) = 1 + z + \frac{z^2}{2!} + \dots + \frac{z^P}{P!} + O(z^{P+1}).$$
 (10)

The first P+1 terms of the stability functions $R(\cdot)$ for explicit DeCs of order P are known.

Theorem

The stability function of any explicit DeC of order P (with P iterations) is

$$R(z) = \sum_{r=0}^{P} \frac{z^r}{r!} = 1 + z + \frac{z^2}{2!} + \dots + \frac{z^P}{P!}$$
 (11)

and does not depend on the distribution of the subtimenodes.

Proof (1/3)

$$A = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ \star & 0 & 0 & \dots & 0 & 0 \\ \star & \star & 0 & \dots & 0 & 0 \\ \star & 0 & \star & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \star & 0 & 0 & \dots & \star & 0 \end{pmatrix},$$

Block structure of the matrix A

* are some non-zero block matrices and the 0 are some zero block matrices.

The number of blocks in each line and row of these matrices is P, the order of the scheme.

Proof (2/3)

By induction, A^k has zeros in the upper triangular part, in the main block diagonal, and in all the k-1 block diagonals below the main diagonal, i.e.,

$$(A^k)_{i,j} = 0 \quad , \text{if } i < j + k,$$

where the indexes here refer to the blocks. Indeed, it is true that $A_{i,j} = 0$ if i < j + 1. Now, let us consider the entry $(A^{k+1})_{i,j}$ with i < j + k + 1, i.e., i - k < j + 1. It is defined as

$$(A^{k+1})_{i,j} = \sum_{w} (A^k)_{i,w} A_{w,j}.$$
(12)

Now, we can prove that all the terms of the sum are 0. Let w < j + 1, then $A_{w,j} = 0$ because of the structure of A; while, if $w \ge j + 1 > i - k$, we have that i < w + k, so $(A^k)_{i,w} = 0$ by induction.

Proof (3/3)

In particular, this means that $A^P = \underline{0}$, because i is always smaller than j + P as P is the number of the block matrices that we have. Hence,

$$(I - zA)^{-1} = \sum_{r=0}^{\infty} z^r A^s = \sum_{r=0}^{P-1} z^r A^s = I + zA + z^2 A^2 + \dots + z^{P-1} A^{P-1}.$$
 (13)

Plugging this result into $R(z)=1+zb^T(I-zA)^{-1}\mathbf{1}$, the stability function R(z) is a polynomial of degree P, the order of the scheme. All terms of order lower or equal to P must agree with the expansion of the exponential function, so it must be

$$R(z) = \sum_{r=0}^{P} \frac{z^r}{r!} = 1 + z + \frac{z^2}{2!} + \dots + \frac{z^P}{P!}.$$
 (14)

Note: no assumption on the distribution of the subtimenodes.

D. Torlo (SISSA) ADER vs DeC 32/72

CODE

- Choice of iterations (P) and order
- Choice of point distributions t^0, \dots, t^M
- Computation of θ
- Loop for timesteps
- Loop for correction
- Loop for subtimesteps

Outline

- Motivation
- 2 DeC
- 3 ADER
- Similarities
- ADER stability and accuracy
- Simulations

ADER

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

Modern approach is DG in space time for hyperbolic problem

$$\partial_t u(x,t) + \nabla \cdot F(u(x,t)) = 0, \ x \in \Omega \subset \mathbb{R}^d, \ t > 0.$$
 (15)

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

Correction step: communication between cells

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

ADER: space-time discretization

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

$$\int_{T^n \times V_i} \theta_{rs}(x,t) \partial_t \theta_{pq}(x,t) u^{pq} dx dt + \int_{T^n \times V_i} \theta_{rs}(x,t) \nabla \cdot F(\theta_{pq}(x,t) u^{pq}) dx dt = 0.$$
 (16)

This leads to

$$\underline{\underline{\underline{\underline{M}}}}_{rspq} u^{pq} = \underline{\underline{\underline{r}}}(\underline{\underline{\underline{u}}})_{rs}, \tag{17}$$

solved with fixed point iteration method

+ Correction step where cells communication is allowed (derived from (16)).

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$$\int_{T^n \times V_i} \theta_{rs}(x,t) \partial_t \theta_{pq}(x,t) u^{pq} dx dt + \int_{T^n \times V_i} \theta_{rs}(x,t) \nabla \cdot F(\theta_{pq}(x,t) u^{pq}) dx dt = 0.$$
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solved with fixed point iteration method.

+ Correction step where cells communication is allowed (derived from (16)).

ADER: time integration method

Simplify! Take
$$m{u}(t) = \sum_{m=0}^M \phi_m(t) m{u}^m = \underline{\phi}(t)^T \underline{m{u}}$$

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

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

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

Quadrature...

$$\mathcal{L}^{2}(\underline{\boldsymbol{u}}) := \underline{\underline{\mathbf{M}}}\underline{\boldsymbol{u}} - \underline{r}(\underline{\boldsymbol{u}}) = 0 \Longleftrightarrow \underline{\underline{\mathbf{M}}}\underline{\boldsymbol{u}} = \underline{r}(\underline{\boldsymbol{u}}). \tag{18}$$

Nonlinear system of $M \times S$ equations

ADER: Mass matrix

What goes into the mass matrix? Use of the integration by parts

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

$$\underline{\phi}(t^{n+1}) \underline{\phi}(t^{n+1})^{T} \underline{\boldsymbol{u}} - \underline{\phi}(t^{n}) \boldsymbol{u}^{n} - \int_{T^{n}} \partial_{t} \underline{\phi}(t) \underline{\phi}(t)^{T} \underline{\boldsymbol{u}} - \int_{T^{n}} \underline{\phi}(t) F(\underline{\phi}(t)^{T} \underline{\boldsymbol{u}}) dt$$

$$\underline{\underline{M}} = \underline{\phi}(t^{n+1}) \underline{\phi}(t^{n+1})^{T} - \int_{T^{n}} \partial_{t} \underline{\phi}(t) \underline{\phi}(t)^{T}$$

$$\underline{r}(\underline{\boldsymbol{u}}) = \underline{\phi}(t^{n}) \boldsymbol{u}^{n} + \int_{T^{n}} \underline{\phi}(t) F(\underline{\phi}(t)^{T} \underline{\boldsymbol{u}}) dt$$

$$\underline{\underline{M}} \underline{\boldsymbol{u}} = \underline{r}(\underline{\boldsymbol{u}})$$

ADER: Fixed point iteration

Iterative procedure to solve the problem for each time step

$$\underline{\underline{\boldsymbol{u}}}^{(k)} = \underline{\underline{\underline{M}}}^{-1}\underline{\underline{r}}(\underline{\underline{\boldsymbol{u}}}^{(k-1)}), \quad k = 1, \dots, \text{convergence}$$
 (19)

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

Reconstruction step

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

- Convergence?
- How many steps K?
- Accuracy L²?

ADER 2nd order

Example with 2 Gauss Legendre points, Lagrange polynomials and 2 iterations Let us consider the timestep interval $[t^n, t^{n+1}]$, rescaled to [0, 1].

Gauss-Legendre points quadrature and interpolation (in the interval [0,1])

$$\underline{t}_q = (t_q^0, t_q^1) = (t^0, t^1) = \left(\frac{\sqrt{3} - 1}{2\sqrt{3}}, \frac{\sqrt{3} + 1}{2\sqrt{3}}\right), \quad \underline{w} = (1/2, 1/2).$$

$$\underline{\phi}(t) = (\phi_0(t), \phi_1(t)) = \left(\frac{t - t^1}{t^0 - t^1}, \frac{t - t^0}{t^1 - t^0}\right).$$

Then, the mass matrix is given by

$$\underline{\underline{\underline{M}}}_{m,l} = \phi_m(1)\phi_l(1) - \phi'_m(t^l)w_l, \quad m, l = 0, 1,$$

$$\underline{\underline{\underline{M}}} = \begin{pmatrix} 1 & \frac{\sqrt{3}-1}{2} \\ -\frac{\sqrt{3}+1}{2} & 1 \end{pmatrix}.$$

ADER 2nd order

The right hand side is given

$$r(\underline{\boldsymbol{u}})_m = \alpha(0)\phi_m(0) + \Delta t F(\alpha(t^m))w_m, \quad m = 0, 1.$$

$$\underline{r}(\underline{\boldsymbol{u}}) = \alpha(0)\underline{\phi}(0) + \Delta t \begin{pmatrix} F(\alpha(t^1))w_1 \\ F(\alpha(t^2))w_2. \end{pmatrix}.$$

Then, the coefficients \underline{u} are given by

$$\underline{\boldsymbol{u}}^{(k+1)} = \underline{\underline{\mathbf{M}}}^{-1}\underline{r}(\underline{\boldsymbol{u}}^{(k)}).$$

Finally, use $\underline{\boldsymbol{u}}^{(k+1)}$ to reconstruct the solution at the time step t^{n+1} :

$$\boldsymbol{u}^{n+1} = \underline{\phi}(1)^T \underline{\boldsymbol{u}}^{(k+1)} = \boldsymbol{u}^n + \int_{T^n} \underline{\phi}(t)^T dt \, F(\underline{\boldsymbol{u}}^{(k)}).$$

- Choice: φ Lagrangian basis functions
- Different subtimesteps: Gauss-Legendre, Gauss-Lobatto, equispaced
- ullet Precompute $\underline{\underline{M}}$
- Precompute the rhs vector part using quadratures after a further approximation

$$\underline{r}(\underline{\boldsymbol{u}}) = \underline{\phi}(t^n) \underline{\boldsymbol{u}}^n + \int_{T^n} \underline{\phi}(t) F(\underline{\phi}(t)^T \underline{\boldsymbol{u}}) dt \approx \underline{\phi}(t^n) \underline{\boldsymbol{u}}^n + \underbrace{\int_{T^n} \underline{\phi}(t) \underline{\phi}(t)^T dt}_{\text{Can be stored}} F(\underline{\boldsymbol{u}})$$

ullet Precompute the reconstruction coefficients $\phi(1)^T$

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- 6 ADER stability and accuracy
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ADER⁶ and DeC⁷: 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)

D. Torlo (SISSA) ADER vs DeC 44/72

⁶M. 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.

⁷R. 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.

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

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

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

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$$\mathcal{L}^{1}(\underline{\boldsymbol{u}}) := \underline{\underline{\mathbf{M}}} \underline{\boldsymbol{u}} - r(\boldsymbol{u}(t^{n})).$$

Apply the DeC Convergence theorem!

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

DeC as ADER

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

DeC as ADER

DeC as ADER

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

$$\chi_{[t^{0},t^{m}]}(t^{m})\boldsymbol{u}^{m} - \chi_{[t^{0},t^{m}]}(t_{0})\boldsymbol{u}^{0} - \int_{t^{0}}^{t^{m}} \chi_{[t^{0},t^{m}]}(t) \sum_{r=0}^{M} F(\boldsymbol{u}^{r})\varphi_{r}(t)dt = 0$$

$$\int_{t^{0}}^{t^{M}} \chi_{[t^{0},t^{m}]}(t)\partial_{t}(\boldsymbol{u}(t))dt - \int_{t^{0}}^{t^{M}} \chi_{[t^{0},t^{m}]}(t) \sum_{r=0}^{M} F(\boldsymbol{u}^{r})\varphi_{r}(t)dt = 0,$$

$$\int_{T^{n}} \psi_{m}(t)\partial_{t}\boldsymbol{u}(t)dt - \int_{T^{n}} \psi_{m}(t)F(\boldsymbol{u}(t))dt = 0.$$

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

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

$$\int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t)\partial_t (\boldsymbol{u}(t)) dt - \int_{t^0}^{t^M} \chi_{[t^0,t^m]}(t) \sum_{r=0}^M F(\boldsymbol{u}^r)\varphi_r(t) dt = 0,$$

$$\int_{T^n} \psi_m(t)\partial_t \boldsymbol{u}(t) dt - \int_{T^n} \psi_m(t)F(\boldsymbol{u}(t)) dt = 0.$$

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

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Stability

Since ADER can be written as a DeC, the stability functions are given by the same formula as for DeC and the stability regions are the following.

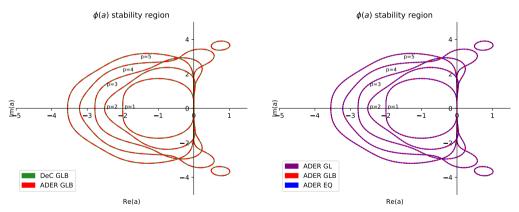


Figure: Stability region

Accuracy of ADER \mathcal{L}^2 operators

The two things that determine the accuracy of the ADER method are the iterations P and the accuracy of \mathcal{L}^2 .

Accuracy of ADER \mathcal{L}^2 for different distributions

- ullet Equispaced: boring, minimum accuracy possible M+1 nodes p=M+1
- ullet Guass-Lobatto: this generates the LobattoIIIC methods, M+1 nodes p=2M
- ullet Gauss-Legendre: this does not generate Gauss methods, M+1 nodes p=2M+1

\mathcal{L}^2 ADER as RK

Here, we see \mathcal{L}^2 as an implicit RK

$$\mathcal{L}^{2,m}(\underline{\boldsymbol{u}}) = \underline{\underline{\mathbf{M}}}_{j}^{m} \boldsymbol{u}^{(j)} - \underline{\phi}^{m}(t^{n}) \boldsymbol{u}^{n} - \underbrace{\int_{T^{n}} \underline{\phi}^{m}(t) \underline{\phi}(t)_{j} dt}_{\Delta t \underline{\underline{\mathbf{R}}}_{j}^{m}} F(\boldsymbol{u}^{(j)}) = 0$$

$$\tilde{\mathcal{L}}^{2,z}(\underline{\boldsymbol{u}}) = \boldsymbol{u}^{(z)} - (\underline{\underline{\mathbf{M}}}^{-1})_{m}^{z} \underline{\phi}^{m}(t^{n}) \boldsymbol{u}^{n} - \Delta t (\underline{\underline{\mathbf{M}}}^{-1})_{m}^{z} \underline{\underline{\mathbf{R}}}_{j}^{m} F(\boldsymbol{u}^{(j)}) = 0$$

$$\boldsymbol{u}^{(z)} = \boldsymbol{u}^{n} + \Delta t a_{z,j} F(\boldsymbol{u}^{(j)})$$

- $\bullet \ a_{mj} = (\underline{\underline{\mathbf{M}}}^{-1})_m^z \underline{\underline{\mathbf{R}}}_j^m$
- \bullet Prove that $(\underline{\underline{\mathbf{M}}}^{-1})_{m}^{z}\underline{\phi}^{m}(t^{n})=1$ for every z
- $c^m = \sum_r a_{mr} = t^m$
- $b_r = \frac{1}{\Delta t} \int_{T^m} \phi_r(t) dt = w_r$ quadrature weights

\mathcal{L}^2 ADER as RK

\mathcal{L}^2 ADER as RK

BCD conditions (Butcher 1964)

Define the conditions

$$B(p):$$

$$\sum_{i=1}^{s} b_i c_i^{z-1} = \frac{1}{z},$$
 $z = 1, \dots, p;$ (20)

$$C(\eta):$$

$$\sum_{j=1}^{s} a_{ij} c_j^{z-1} = \frac{c_i^z}{z}, \qquad i = 1, \dots, s, \ z = 1, \dots, \eta;$$
 (21)

$$D(\zeta): \qquad \sum_{i=1}^{s} b_i c_i^{z-1} a_{ij} = \frac{b_j}{z} (1 - c_j^z), \qquad j = 1, \dots, s, \ z = 1, \dots, \zeta.$$
 (22)

Theorem (Butcher 1964)

If the coefficients b_i, c_i, a_{ij} of a RK scheme satisfy B(p), $C(\eta)$ and $D(\zeta)$ with $p \leq \eta + \zeta + 1$ and $p \leq 2\eta + 2$, then the method is of order p.

D. Torlo (SISSA) ADER vs DeC 60/72

$$C(s-1) D(s-1)$$

Lemma

 \mathcal{L}^2 operator of ADER defined by Gauss–Lobatto or Gauss–Legendre points and quadrature (they coincide) with s=M+1 stages satisfies C(s-1) and D(s-1).

Proof (1/4).

Interpolation with ϕ^j is exact for polynomials of degree s-1.

The quadrature is exact for polynomials of degree 2s - 3.

Recall that $\underline{A} = \underline{\mathrm{MR}}$, Condition C(s-1) reads

$$\underline{\underline{A}}\underline{c^{z-1}} = \frac{1}{z}\underline{c^z} \Longleftrightarrow \underline{\underline{R}}\underline{c^{z-1}} = \frac{1}{z}\underline{\underline{M}}\underline{c^z} \Longleftrightarrow \underline{\mathcal{X}} := \underline{\underline{R}}\underline{c^{z-1}} - \frac{1}{z}\underline{\underline{M}}\underline{c^z} = \underline{0}, \qquad z = 1, \dots, s-1.$$

Recall $b_m=t^m$, $c_m=w_m$, $\underline{\underline{\underline{R}}}_{i,j}=\delta_{i,j}w_i$ and the definition of $\underline{\underline{\underline{M}}}$

$$\mathcal{X}_m := w_m(t^m)^{z-1} - \frac{1}{z} \left(\phi^m(1) \phi^j(1) (t^j)^z - \int_0^1 \frac{d}{d\xi} \phi^m(\xi) \phi^j(\xi) (t^j)^z d\xi \right).$$

D. Torlo (SISSA) ADER vs DeC 61/72

Proof (2/4).

Now, the interpolation of t^z with $z \le s-1$ with basis functions ϕ^j is exact. Hence, we can substitute $\phi^j(\xi)(t^j)^z = \xi^z$ for all $z=1,\ldots,s-1$, obtaining

$$\mathcal{X}_m = w_m(t^m)^{z-1} - \frac{1}{z} \left(\phi^m(1) 1^z - \int_0^1 \frac{d}{d\xi} \phi^m(\xi) \xi^z d\xi \right).$$

Using the exactness of the quadrature for polynomials of degree 2s-3, both true for Gauss–Lobatto and Gauss–Legendre, we know that the previous integral is exactly computed as $\frac{d}{d\xi}\phi^m(\xi)$ is of degree at most s-2 and ξ^z is at most s-1. So, we can use integration by parts and obtain

$$\mathcal{X}_m = w_m(t^m)^{z-1} - \frac{1}{z} \left(\phi^m(0)0^z + \int_0^1 \phi^m(\xi) \frac{d}{d\xi} \xi^z d\xi \right) = w_m(t^m)^{z-1} - \int_0^1 \phi^m(\xi) \xi^{z-1} d\xi = 0$$

by the exactness of the quadrature rule and the definition of w_m . Note that the condition is sharp, since the interpolation is not anymore exact for z=s, hence C(s) is not satisfied.

Proof (3/4).

To prove D(s-1), we write explicitly the condition in matricial form, for all $z=1,\ldots,s-1$

$$\underline{bc^{z-1}}\underline{\underline{A}} = \frac{1}{z}\underline{b(1-c^z)} \Longleftrightarrow \underline{bc^{z-1}}\underline{\underline{\mathbf{M}}}^{-1}\underline{\underline{\mathbf{R}}} = \frac{1}{z}\underline{b(1-c^z)} \Longleftrightarrow \underline{bc^{z-1}} = \frac{1}{z}\underline{b(1-c^z)}\underline{\underline{\mathbf{R}}}^{-1}\underline{\underline{\mathbf{M}}}.$$

Note that $b^m=w_m$ and $\underline{\underline{\mathbb{R}}}_r^m=w_m\delta_r^m$, so $\underline{b(1-c^z)}\underline{\underline{\mathbb{R}}}^{-1}=\underline{(1-c^z)}$. It is left to prove that

$$\mathcal{Y} := \underline{bc^{z-1}} - \frac{1}{z} \underline{(1 - c^z)} \underline{\underline{\mathbf{M}}} = \underline{0}.$$

$$\mathcal{Y}_m = w_m(t^m)^{z-1} - \frac{1}{z} \sum_{i=1}^s \left(1 - (t^j)^z \right) \left(\phi^j(1) \phi^m(1) - \int_0^1 \frac{d}{d\xi} \phi^j(\xi) \phi^m(\xi) d\xi \right).$$

Proof (4/4).

Let us observe that, since $z \leq s-1$, the polynomial is exactly represented by the Lagrangian interpolation $t^z = \sum_{j=1}^s \phi(t) (t^m)^z$. Hence, using the exactness of the quadrature for polynomials of degree at most 2s-3, we have

$$\mathcal{Y}_m = w_m(t^m)^{z-1} - \frac{1}{z} \left(1 - (1)^z \right) \phi^m(1) + \frac{1}{z} \int_0^1 \frac{d}{d\xi} \left(1 - (\xi)^z \right) \phi^m(\xi) d\xi$$
$$= w_m(t^m)^{z-1} - \frac{1}{z} \int_0^1 z \, \xi^{z-1} \phi^m(\xi) d\xi = w_m(t^m)^{z-1} - w_m(t^m)^{z-1} = 0.$$

Hence, ADER-Legendre and ADER-Lobatto satisfy D(s-1). Note that the condition is sharp, since the interpolation is not anymore exact for z=s, hence D(s) is not satisfied.

ADER Gauss–Legendre \mathcal{L}^2

Remark (ADER-Legendre is no collocation method)

From the proof of previous Lemma, we can observe that ADER-Legendre methods do not satisfy C(s), hence, the methods are not collocation methods and they do not coincide with Gauss-Legendre implicit RK methods.

Theorem

 \mathcal{L}^2 of ADER with Gauss–Legendre is of order 2s-1.

Proof.

ADER-Legendre with s=M+1 stages satisfies B(2s) for the quadrature rule and, hence, it satisfies B(2s-1). For previous Lemma it also satisfies C(s-1) and D(s-1). Hence, Butcher's (1964) Theorem ($p \le \eta + \zeta + 1$ and $p \le 2\eta + 2$) guarantees that the method is of order 2s-1, since it is satisfied with p=2s-1 and $\eta=\zeta=s-1$.

ADER Gauss–Lobatto \mathcal{L}^2

Theorem

 \mathcal{L}^2 of ADER with Gauss-Lobatto is of order 2s-2.

Proof.

The condition for B(2s-2) is satisfied as (c,b) is the Gauss–Lobatto quadrature with order 2s-2. Previous Lemma guarantees that ADER-Lobatto satisfies B(2s-2), C(s-1) and D(s-1), so Butcher's (1964) Theorem ($p \le \eta + \zeta + 1$ and $p \le 2\eta + 2$) is satisfied for order p = 2s-2 and $\eta = \zeta = s-1$.



ADER Gauss–Lobatto \mathcal{L}^2

Theorem

 \mathcal{L}^2 of ADER with Gauss-Lobatto is LobattoIIIC.

The Lobatto IIIC method is defined using the condition

$$a_{i1} = b_1$$
 for $i = 1, \dots, s$. (23)

Lemma

 \mathcal{L}^2 of ADER with Gauss-Lobatto satisfies (23).

Theorem (Chipman 1971)

Lobatto IIIC schemes (in particular RK a_{ij}) are uniquely determined by Gauss-Lobatto quadrature rule (c,b), condition (23) and by C(s-1).

ADER Gauss–Lobatto \mathcal{L}^2

Lemma

 \mathcal{L}^2 of ADER with Gauss-Lobatto satisfies (23).

Proof.

$$a_{i1} = \sum_{j} (\underline{\underline{\mathbf{M}}}^{-1})_{ij} \mathbb{R}_{j1} = b_{1} = w_{1} \iff$$

$$\sum_{i,j} \underline{\underline{\mathbf{M}}}_{ki} (\underline{\underline{\mathbf{M}}}^{-1})_{ij} \mathbb{R}_{j1} = \sum_{i} \underline{\underline{\mathbf{M}}}_{ki} w_{1} \iff$$

$$\delta_{k1} w_{1} = \mathbb{R}_{k1} = \sum_{i} \underline{\underline{\mathbf{M}}}_{ki} w_{1}$$

$$\sum_{i} \underline{\underline{\mathbf{M}}}_{ki} w_{1} = \phi^{m}(1) w_{1} - \int_{0}^{1} \frac{d}{dt} \phi^{m}(\xi) w_{1} dt = w_{1} \phi^{m}(0) = w_{1} \delta_{m,1}.$$

Outline

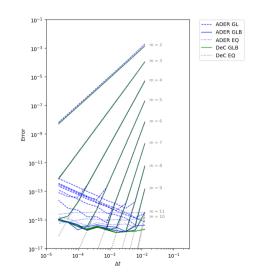
- Motivation
- 2 DeC
- 3 ADER
- Similarities
- 6 ADER stability and accuracy
- 6 Simulations

Convergence

$$y'(t) = -|y(t)|y(t),$$

 $y(0) = 1,$ (24)
 $t \in [0, 0.1].$

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



Lotka-Volterra

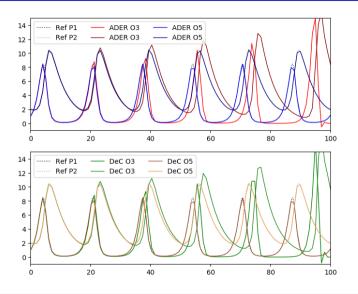
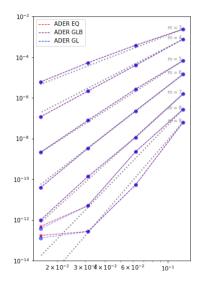


Figure: Numerical solution of the Lotka-Volterra system using ADER (top) and DeC (bottom) with Gauss-Lobatto nodes with timestep $\Delta T=1$.

PDE: Burgers with spectral difference



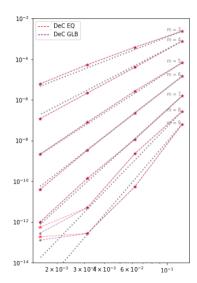


Figure: Convergence error for Burgers equations: Left ADER right DeC. Space discretization with spectral difference