A parallel-in-time IMEX multiderivative method

Jochen Schütz and David Seal

PinT 2020

## Outline

- Introduction: Why MD-IMEX?


## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach


## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time


## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time
- Conclusion and outlook


## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time
- Conclusion and outlook


## Low Mach

- Isentropic Euler equations

$$
\rho_{t}+\nabla \cdot(\rho \boldsymbol{u})=0, \quad(\rho \boldsymbol{u})_{t}+\nabla \cdot(\rho \boldsymbol{u} \otimes \boldsymbol{u})+\frac{1}{\varepsilon^{2}} \nabla p(\rho)=0
$$

## Low Mach

- Isentropic Euler equations

$$
\rho_{t}+\nabla \cdot(\rho \boldsymbol{u})=0, \quad(\rho \boldsymbol{u})_{t}+\nabla \cdot(\rho \boldsymbol{u} \otimes \boldsymbol{u})+\frac{1}{\varepsilon^{2}} \nabla p(\rho)=0
$$

- Singular perturbed system of conservation laws

$$
w_{t}+\nabla \cdot f_{\varepsilon}(w)=0, \quad \varepsilon \rightarrow 0
$$

## Low Mach

- Isentropic Euler equations

$$
\rho_{t}+\nabla \cdot(\rho \boldsymbol{u})=0, \quad(\rho \boldsymbol{u})_{t}+\nabla \cdot(\rho \boldsymbol{u} \otimes \boldsymbol{u})+\frac{1}{\varepsilon^{2}} \nabla p(\rho)=0
$$

- Singular perturbed system of conservation laws

$$
w_{t}+\nabla \cdot f_{\varepsilon}(w)=0, \quad \varepsilon \rightarrow 0
$$

- Eigenvalues of $f_{\varepsilon}^{\prime}(w) \cdot \boldsymbol{n}$

$$
\lambda_{0}=\boldsymbol{u} \cdot \boldsymbol{n}, \quad \lambda_{ \pm}=\boldsymbol{u} \cdot \boldsymbol{n} \pm \frac{\sqrt{p^{\prime}(\rho)}}{\varepsilon}
$$

## Low Mach

- Isentropic Euler equations

$$
\rho_{t}+\nabla \cdot(\rho \boldsymbol{u})=0, \quad(\rho \boldsymbol{u})_{t}+\nabla \cdot(\rho \boldsymbol{u} \otimes \boldsymbol{u})+\frac{1}{\varepsilon^{2}} \nabla p(\rho)=0
$$

- Singular perturbed system of conservation laws

$$
w_{t}+\nabla \cdot f_{\varepsilon}(w)=0, \quad \varepsilon \rightarrow 0
$$

- Eigenvalues of $f_{\varepsilon}^{\prime}(w) \cdot \boldsymbol{n}$

$$
\lambda_{0}=\boldsymbol{u} \cdot \boldsymbol{n}, \quad \lambda_{ \pm}=\boldsymbol{u} \cdot \boldsymbol{n} \pm \frac{\sqrt{p^{\prime}(\rho)}}{\varepsilon}
$$

- One slow wave ('convection'), two fast waves ('acoustics').


## IMEX schemes

$$
w_{t}+\nabla \cdot f_{\varepsilon}(w)=0
$$

${ }^{*}$ [Klein 1994], [Degond, Tang 2008], [Haack, Jin, Liu 2012], [Noelle et al. 2014], [Kaiser et al. 2017] ...

## IMEX schemes

$$
w_{t}+\nabla \cdot\left(\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)\right)=0
$$

- $f_{\varepsilon}(w)=\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)$.
- Ideal: $\widehat{f}_{\varepsilon}=$ convection, $\widetilde{f}_{\varepsilon}(w)=$ acoustics ${ }^{*}$.
${ }^{*}$ [Klein 1994], [Degond, Tang 2008], [Haack, Jin, Liu 2012], [Noelle et al. 2014], [Kaiser et al. 2017] ..


## IMEX schemes

$$
w_{t}+\nabla \cdot\left(\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)\right)=0
$$

- $f_{\varepsilon}(w)=\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)$.
- Ideal: $\widehat{f}_{\varepsilon}=$ convection, $\widetilde{f}_{\varepsilon}(w)=$ acoustics ${ }^{*}$.
- Treat implicitly and explicitly:

$$
\frac{w^{n+1}-w^{n}}{\Delta t}+\nabla \cdot\left(\widetilde{f}_{\varepsilon}\left(w^{n+1}\right)+\widehat{f}_{\varepsilon}\left(w^{n}\right)\right)=0
$$

${ }^{*}$ [Klein 1994], [Degond, Tang 2008], [Haack, Jin, Liu 2012], [Noelle et al. 2014], [Kaiser et al. 2017] ..

## IMEX schemes

$$
w_{t}+\nabla \cdot\left(\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)\right)=0
$$

- $f_{\varepsilon}(w)=\widetilde{f}_{\varepsilon}(w)+\widehat{f}_{\varepsilon}(w)$.
- Ideal: $\widehat{f}_{\varepsilon}=$ convection, $\widetilde{f}_{\varepsilon}(w)=$ acoustics ${ }^{*}$.
- Treat implicitly and explicitly:

$$
\frac{w^{n+1}-w^{n}}{\Delta t}+\nabla \cdot\left(\widetilde{f}_{\varepsilon}\left(w^{n+1}\right)+\widehat{f}_{\varepsilon}\left(w^{n}\right)\right)=0
$$

- This talk: Time integration $w^{\prime}(t)=\Phi(w)$.
${ }^{*}$ [Klein 1994], [Degond, Tang 2008], [Haack, Jin, Liu 2012], [Noelle et al. 2014], [Kaiser et al. 2017] .


## IMEX schemes

$$
\frac{w^{n+1}-w^{n}}{\Delta t}=\Phi_{\mathrm{I}}\left(w^{n+1}\right)+\Phi_{\mathrm{E}}\left(w^{n}\right)
$$

- Higher order versions exist:
- IMEX-RK
- IMEX-BDF


## IMEX schemes

$$
\frac{w^{n+1}-w^{n}}{\Delta t}=\Phi_{\mathrm{I}}\left(w^{n+1}\right)+\Phi_{\mathrm{E}}\left(w^{n}\right)
$$

- Higher order versions exist:
- IMEX-RK
- IMEX-BDF
- Issues:
- Storage requirements?
- Really high order extensions?
- Stability?
- Parallel capabilities?
- Asymptotic consistency/accuracy?



## Multiderivative approach

$$
w^{\prime}(t)=\Phi(w)
$$

- 'Classical' methods: Use $w^{\prime} \equiv \Phi(w)$ only.
- Multiderivatives: Use

$$
\begin{aligned}
w^{\prime \prime} & \equiv \dot{\Phi}(w):=\Phi^{\prime}(w) \Phi(w) \\
w^{\prime \prime \prime} & \equiv \ddot{\Phi}(w):=\ldots
\end{aligned}
$$

- Example: $3^{\text {rd }}$-order Euler:

$$
w^{n+1}=w^{n}+\Delta t \Phi\left(w^{n}\right)+\frac{\Delta t^{2}}{2} \dot{\Phi}\left(w^{n}\right)+\frac{\Delta t^{3}}{6} \ddot{\phi}\left(w^{n}\right) .
$$

## Advertisement

$$
w^{\prime}(t)=\Phi(w)
$$

- Advantages:
- Storage efficient
- Easy construction of high order, stable methods
- Rather natural for PDEs


## Advertisement

$$
w^{\prime}(t)=\Phi(w) \equiv \Phi_{I}(w)+\Phi_{E}(w)
$$

- Advantages:
- Storage efficient
- Easy construction of high order, stable methods
- Rather natural for PDEs

But: How to construct stable MD-IMEX schemes?

## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time
- Conclusion and outlook


## Preliminaries: An integral approximation

$$
w^{\prime}(t)=\Phi(w), \quad w^{\prime \prime}(t)=\dot{\Phi}(w)
$$

- Two-derivative integral approximation:

$$
\int_{t^{n}}^{t^{n+1}} \Phi(t) \mathrm{d} t=\underbrace{\frac{\Delta t}{2}\left(\Phi^{n}+\Phi^{n+1}\right)+\frac{\Delta t^{2}}{12}\left(\dot{\Phi}^{n}-\dot{\Phi}^{n+1}\right)}_{=: I\left[\phi^{n} ; \phi^{n+1}\right]}+\mathcal{O}\left(\Delta t^{5}\right)
$$

- Relatively old ideas*.


## Preliminaries: Euler methods

$$
w^{\prime}(t)=\Phi(w) \equiv \Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)
$$

- explicit Euler (first order):

$$
w^{n+1}=w^{n}+\Delta t \Phi\left(w^{n}\right)
$$

- implicit Euler (first order):

$$
w^{n+1}=w^{n}+\Delta t \Phi\left(w^{n+1}\right)
$$

- IMEX Euler (first order):

$$
w^{n+1}=w^{n}+\Delta t\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{n+1}\right)\right)
$$

## Preliminaries: Euler methods

$$
w^{\prime}(t)=\Phi(w) \equiv \Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)
$$

- explicit Euler (second order):

$$
w^{n+1}=w^{n}+\Delta t \Phi\left(w^{n}\right)+\frac{\Delta t^{2}}{2} \dot{\Phi}\left(w^{n}\right)
$$

- implicit Euler (second order):

$$
w^{n+1}=w^{n}+\Delta t \Phi\left(w^{n+1}\right)-\frac{\Delta t^{2}}{2} \dot{\Phi}\left(w^{n+1}\right)
$$

- IMEX Euler (second order):

$$
w^{n+1}=w^{n}+\Delta t\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{n+1}\right)\right)+\frac{\Delta t^{2}}{2}\left(\dot{\Phi}_{\mathrm{E}}\left(w^{n}\right)-\dot{\Phi}_{\mathrm{I}}\left(w^{n+1}\right)\right)
$$

## Overall method

1. Predict:

$$
w^{[0]}:=w^{n}+\Delta t\left(\phi_{1}\left(w^{[0]}\right)+\phi_{E}\left(w^{n}\right)\right)+\frac{\Delta t^{2}}{2}\left(\dot{\Phi}_{E}\left(w^{n}\right)-\dot{\phi}_{1}\left(w^{[0]}\right)\right) .
$$

## Overall method

1. Predict:

$$
w^{[0]}:=w^{n}+\Delta t\left(\Phi_{\mathrm{I}}\left(w^{[0]}\right)+\Phi_{\mathrm{E}}\left(w^{n}\right)\right)+\frac{\Delta t^{2}}{2}\left(\dot{\Phi}_{\mathrm{E}}\left(w^{n}\right)-\dot{\Phi}_{\mathrm{I}}\left(w^{[0]}\right)\right) .
$$

2. Correct: $\left(0 \leq k \leq k_{\max }-1\right)$

$$
w^{[k+1]}:=w^{n}+\Delta t\left(\phi_{1}^{[k+1]}-\phi_{1}^{[k]}\right)-\frac{\Delta t^{2}}{2}\left(\dot{\Phi}_{1}^{[k+1]}-\dot{\phi}_{1}^{[k]}\right)+\mathcal{I}\left[\phi^{n} ; \phi^{[k]}\right]
$$

## Overall method

1. Predict:

$$
w^{[0]}:=w^{n}+\Delta t\left(\phi_{1}\left(w^{[0]}\right)+\Phi_{E}\left(w^{n}\right)\right)+\frac{\Delta t^{2}}{2}\left(\dot{\Phi}_{E}\left(w^{n}\right)-\dot{\Phi}_{1}\left(w^{[0]}\right)\right) .
$$

2. Correct: $\left(0 \leq k \leq k_{\max }-1\right)$

$$
w^{[k+1]}:=w^{n}+\Delta t\left(\phi_{1}^{[k+1]}-\phi_{1}^{[k]}\right)-\frac{\Delta t^{2}}{2}\left(\dot{\phi}_{1}^{[k+1]}-\dot{\phi}_{1}^{[k]}\right)+\mathcal{I}\left[\phi^{n} ; \phi^{[k]}\right]
$$

3. Update: Set $w^{n+1}:=w^{\left[k_{\max }\right]}$.

## How does it work?



- Different colors $=$ different time intervals


## Consistency analysis

- Classical consistency analysis*:

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Second-order Euler predictor
- Correction
- Accuracy of I.


## Consistency analysis

- Classical consistency analysis*:

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Second-order Euler predictor
- Correction
- Accuracy of I.
- Given $k_{\max } \geq 2$ :

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{4}\right)
$$

## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,


## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,
- I.
- Why take $k_{\max } \geq 2$ ?


## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,
- Why take $k_{\max } \geq 2$ ?



## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,
- I.
- Why take $k_{\max } \geq 2$ ?



## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,
- I.
- Why take $k_{\max } \geq 2$ ?



## Consistency analysis (ctd.)

$$
\frac{\left|w\left(t^{n+1}\right)-\tilde{w}^{n+1}\right|}{\Delta t}=\mathcal{O}\left(\Delta t^{2} \cdot \Delta t^{k}\right)+\mathcal{O}\left(\Delta t^{4}\right)
$$

- Tweaking possibilities:
- Prediction,
- Correction,
- I.
- Why take $k_{\max } \geq 2$ ?


Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time
- Conclusion and outlook


## Method



- Different colors $=$ different time intervals


## A time-parallel alternative

$$
\rightarrow w^{1,[0]}
$$

- Different colors $=$ different processes.
- Not equivalent to original method!


## Performance?

$$
y^{\prime}(t)=z, \quad z^{\prime}(t)=\frac{g(y, z)}{\varepsilon}
$$




$$
\varepsilon=1 \text { (left) and } \varepsilon=10^{-4} \text { (right) }
$$

$$
\begin{aligned}
u_{t} & =\left(\left(1+u^{2}\right) u_{x}\right)_{x}+h(x, t), \\
u(x, 0) & =\sin (\cos (4 x)+\sin (2 x))
\end{aligned}
$$



$$
\begin{aligned}
u_{t} & =\left(\left(1+u^{2}\right) u_{x}\right)_{x}+h(x, t) \\
u(x, 0) & =\sin (\cos (4 x)+\sin (2 x))
\end{aligned}
$$



Spectral method, $N_{k}=60$

$$
\begin{aligned}
u_{t} & =\left(\left(1+u^{2}\right) u_{x}\right)_{x}+h(x, t) \\
u(x, 0) & =\sin (\cos (4 x)+\sin (2 x))
\end{aligned}
$$



Spectral method, $N_{k}=60$

## Outline

- Introduction: Why MD-IMEX?
- Predictor/corrector approach
- Parallelism in time
- Conclusion and outlook


## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{I}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{l}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{1}^{\prime}\left(w^{[0]}\right)\left(\Phi_{E}\left(w^{n}\right)+\Phi_{I}\left(w^{[0]}\right)\right)
$$

## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{l}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{I}^{\prime}\left(w^{[0]}\right)\left(\Phi_{E}\left(w^{n}\right)+\Phi_{I}\left(w^{[0]}\right)\right)
$$

- Stability? Convergence?


## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{I}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{\mathrm{I}}^{\prime}\left(w^{[0]}\right)\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{[0]}\right)\right)
$$

- Stability? Convergence?
- Other higher-order methods?


## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{l}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{\mathrm{I}}^{\prime}\left(w^{[0]}\right)\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{[0]}\right)\right)
$$

- Stability? Convergence?
- Other higher-order methods?
- Error estimation through variable $k_{\max }$ ?


## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{l}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{\mathrm{I}}^{\prime}\left(w^{[0]}\right)\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{[0]}\right)\right)
$$

- Stability? Convergence?
- Other higher-order methods?
- Error estimation through variable $k_{\text {max }}$ ?
- Extension to low-Mach Navier-Stokes?


## Conclusion and outlook

- Typically: $\Phi_{\mathrm{I}}(w)$ is linear.

$$
\dot{\Phi}_{\mathrm{I}}(w)=\Phi_{\mathrm{l}}^{\prime}(w)\left(\Phi_{\mathrm{E}}(w)+\Phi_{\mathrm{I}}(w)\right)
$$

- Substitute

$$
\dot{\Phi}_{I}\left(w^{[0]}\right) \approx \Phi_{\mathrm{I}}^{\prime}\left(w^{[0]}\right)\left(\Phi_{\mathrm{E}}\left(w^{n}\right)+\Phi_{\mathrm{I}}\left(w^{[0]}\right)\right)
$$

- Stability? Convergence?
- Other higher-order methods?
- Error estimation through variable $k_{\text {max }}$ ?
- Extension to low-Mach Navier-Stokes?


## Thank you!

Thank you for your attention!


Financial support by BOF@UHasselt and Office of Naval Research is gratefully acknowledged.

