Uniform accuracy of implicit-explicit methods for stiff hyperbolic relaxation systems and kinetic equations

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Overview

- Stiff PDEs, IMEX methods, uniform accuracy vs. order reduction
- Basic methodology of energy estimates
- Uniform accuracy of IMEX-BDF (J. Hu-RS 21')
- Uniform accuracy of IMEX-RK (J. Hu-RS 25')

Model problems

Stiff kinetic equations

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{Q}(f)$$

- f = f(t, x, v) particle density function, ε Knudsen number
- Q(f): collision operator (Boltzmann, BGK, Landau, ...)
- Hyperbolic relaxation systems (S. Jin-Z. Xin 95')

$$\begin{cases} \partial_t u + \partial_x v = 0, & |F'(u)| < 1 \\ \partial_t v + \partial_x u = \frac{1}{\varepsilon} (F(u) - v), & \text{sub-characteristic condition} \end{cases}$$

Asymptotic limits

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{Q}(f)$$

$$\varepsilon \to 0$$

$$f(v) = M_{\rho, u, T}(v)$$

Taking moments and using the local equilibrium,

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + pI) = 0, \\ \partial_t E + \nabla_x \cdot ((E + p)u) = 0, \end{cases}$$

$$E = \frac{1}{2} \rho u^2 + \frac{d_v}{2} \rho T \qquad p = \rho T$$

next order expansion gives compressible Navier-Stokes

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + \partial_x u = \frac{1}{\varepsilon} (F(u) - v), \end{cases}$$

$$\varepsilon \to 0$$
 $v = F(u)$

Using the local equilibrium in the first equation,

$$\partial_t u + \partial_x F(u) = 0$$

next order expansion gives convection-diffusion

IMEX methods

• Implicit-explicit Runge-Kutta methods (IMEX-RK): U. Ascher-S. Ruuth-R. Spiteri 97', L. Pareschi-G. Russo 05', G. Dimarco-L. Pareschi 13',...

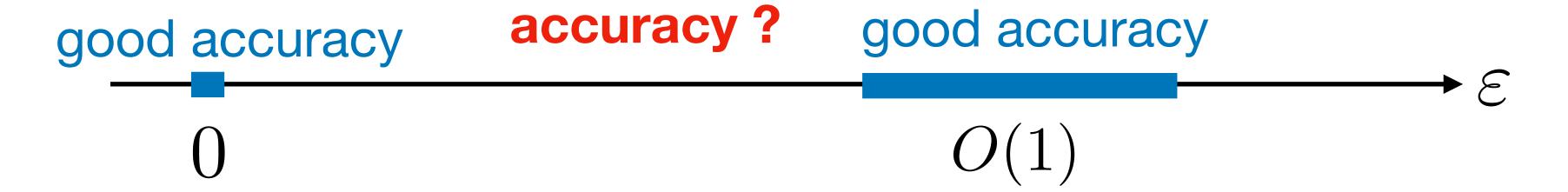
$$f^{(i)} = f^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} v \cdot \nabla_x f^{(j)} + \frac{\Delta t}{\varepsilon} \sum_{j=1}^{i} a_{ij} \mathcal{Q}(f^{(j)}), \quad i = 1, \dots, s$$
$$f^{n+1} = f^n - \Delta t \sum_{j=1}^{s} \tilde{b}_j v \cdot \nabla_x f^{(j)} + \frac{\Delta t}{\varepsilon} \sum_{j=1}^{s} b_j \mathcal{Q}(f^{(j)})$$

Implicit-explicit multistep methods: U. Ascher-S. Ruuth-B. Wetton 95',
 G. Dimarco-L. Pareschi 17', ... One example is IMEX-BDF:

$$\sum_{i=0}^{q} \alpha_i f^{n+i} + \Delta t \sum_{i=0}^{q-1} \gamma_i v \cdot \nabla_x f^{n+i} = \frac{\beta \Delta t}{\varepsilon} \mathcal{Q}(f^{n+q})$$

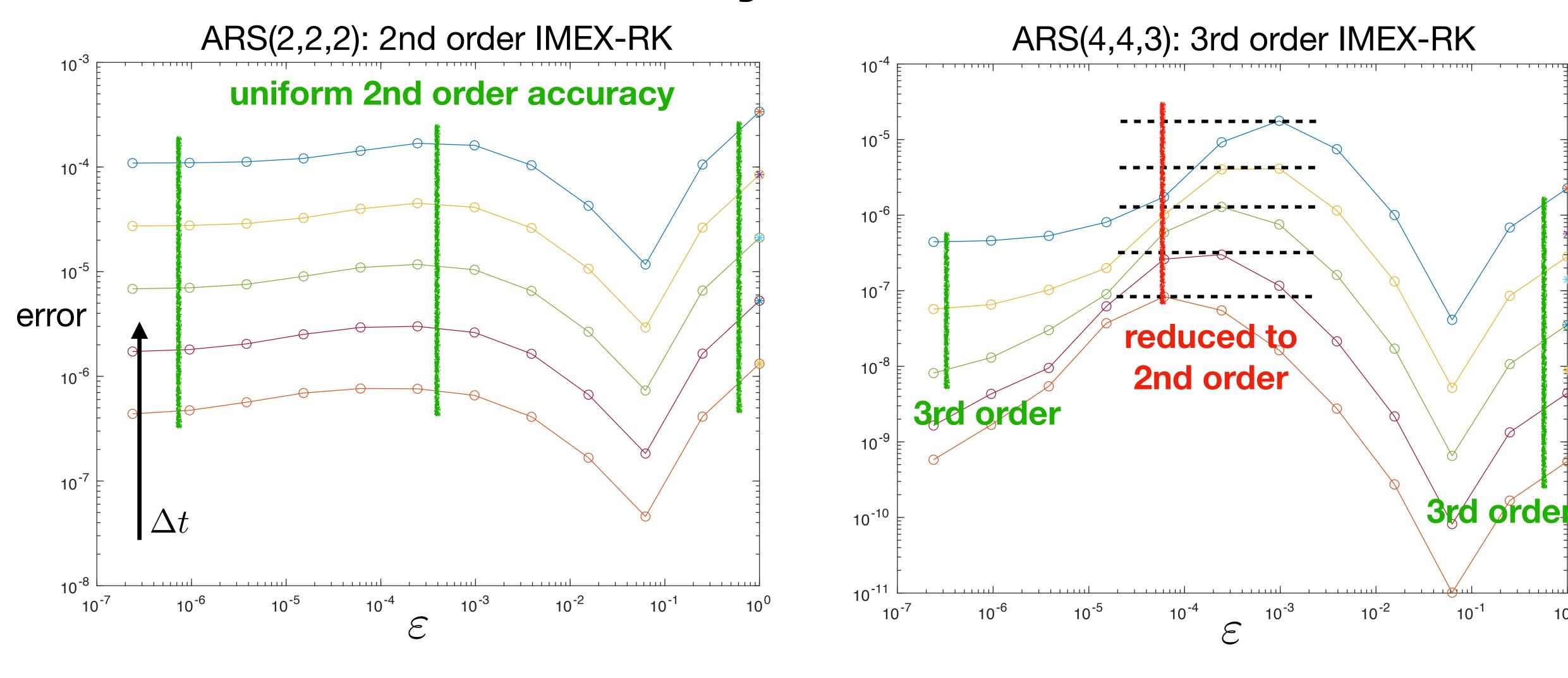
Asymptotic properties

- Asymptotic-preserving (AP) schemes (S. Jin 99'): allow the time step Δt to be chosen independent of ε . Automatically captures the asymptotic limit as $\varepsilon \to 0$
- Accuracy is guaranteed for kinetic regime $\varepsilon = O(1)$ and fluid regime $\varepsilon \to 0$ What happens for intermediate regime?



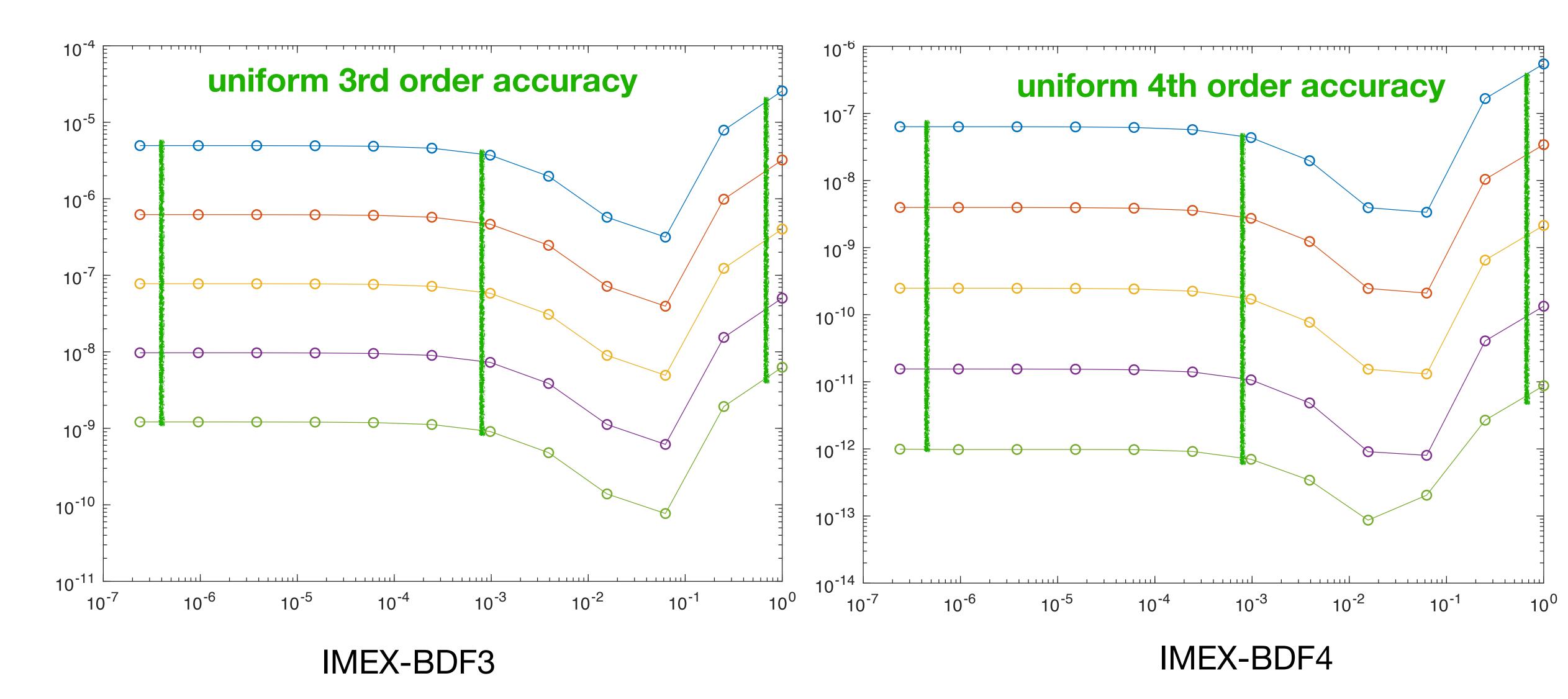
• Uniform accuracy of order q: $error = O(\Delta t^q)$ uniformly in ε

Uniform accuracy vs. order reduction



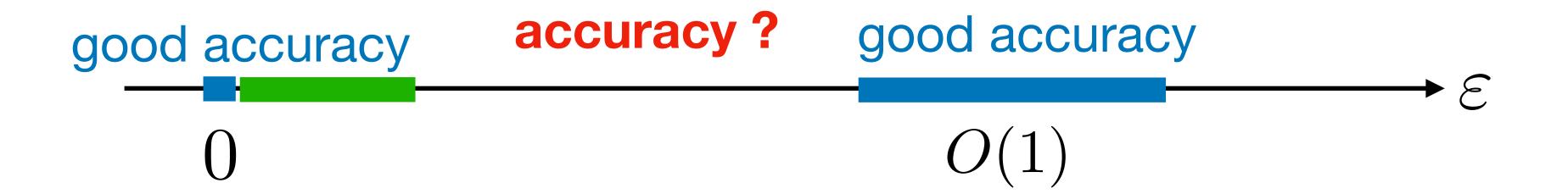
schemes from U. Ascher-S. Ruuth-R. Spiteri 97'

Uniform accuracy of IMEX-BDF



Uniform accuracy vs. order reduction

- One way to understand order reduction for IMEX-RK is to design schemes which captures the next order expansion (S. Boscarino 07', S. Boscarino-G. Russo 09', S. Boscarino-L. Pareschi 17', J. Hu-X. Zhang 17')
- However, this may not be sufficient to give uniform accuracy



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The model problem

Linear hyperbolic relaxation equations

$$\begin{cases} \partial_t u + \partial_x v = 0, & |b| < 1 \\ \partial_t v + \partial_x u = \frac{1}{\varepsilon} (bu - v), \end{cases}$$

• Change of variable w = v - bu

$$\begin{cases} \partial_t u + \partial_x (bu + w) = 0, \\ \partial_t w + \partial_x ((1 - b^2)u - bw) = -\frac{1}{\varepsilon} w. \end{cases}$$

Asymptotic limit

$$\partial_t u + \partial_x (bu) = 0$$

Lemma (J. Hu-RS 21'): Assume initial data is smooth. Then, after an initial layer, we have the regularity estimate

$$\|\partial_t^{r_1} \partial_x^{r_2} u(t, \cdot)\|^2 \le C$$
$$\|\partial_t^{r_1} \partial_x^{r_2} w(t, \cdot)\|^2 \le C\epsilon$$

 $\|\cdot\|$ denotes L^2 norm in x

Fully discretized scheme

• The spatial domain is discretized by Fourier-Galerkin method:

$$\mathbb{P}_{N} = \operatorname{span}\{e^{ikx}| - N \le k \le N\},$$

$$\mathcal{P}_{N}f(x) = \sum_{k=-N}^{N} \hat{f}_{k}e^{ikx} \in \mathbb{P}_{N}, \quad \hat{f}_{k} = \langle f, e^{ikx} \rangle.$$

• Fully discretized Backward-forward Euler method (1st order)

$$\begin{cases} U_N^{n+1} - U_N^n + \Delta t \partial_x (bU_N^n + W_N^n) = 0, \\ W_N^{n+1} - W_N^n + \Delta t \partial_x ((1-b^2)U_N^n - bW_N^n) = -\frac{\Delta t}{\varepsilon} W_N^{n+1}. \end{cases}$$

Subscript N will be omitted later

How to do energy estimate?

$$\Delta t \left| \int U^{n+1} \partial_x U^n dx \right| = \Delta t \left| \int (U^{n+1} - U^n) \partial_x U^n dx \right| \le c \|U^{n+1} - U^n\|^2 + C \Delta t^2 \|\partial_x U^n\|^2$$

$$\leq c\|U^{n+1}-U^n\|^2+C\Delta t\|U^n\|^2$$
 under a CFL condition $\Delta t \leq c_{CFL}/N^2$

$$||U^{n+1}||^2 - ||U^n||^2 + ||U^{n+1} - U^n||^2 + 2\Delta t \int U^{n+1} \partial_x (bU^n + W^n) dx = 0$$

$$||W^{n+1}||^2 - ||W^n||^2 + ||W^{n+1} - W^n||^2 + 2\Delta t \int W^{n+1} \partial_x ((1-b^2)U^n - bW^n) dx = -2\frac{\Delta t}{\varepsilon} ||W^{n+1}||^2$$

Combine to get

$$(1 - b^2) \|U^{n+1}\|^2 + \|W^{n+1}\|^2 \le (1 + C\Delta t)((1 - b^2)\|U^n\|^2 + \|W^n\|^2)$$

Use Gronwall to get uniform stability

$$(1 - b^2) ||U^n||^2 + ||W^n||^2 \le C(T)((1 - b^2) ||u_{in}||^2 + ||w_{in}||^2)$$

 Uniform accuracy follows from the same procedure applied on the evolution of error, with the local truncation error taken into consideration

$$(1-b^2)\|U_e^n\|^2+\|W_e^n\|^2\leq C(T)\Delta t^2$$
 here, first order uniform accuracy

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Uniform accuracy of IMEX-BDF

$$\begin{cases} \sum_{i=0}^{q} \alpha_{i} U_{N}^{n+i} + \Delta t \sum_{i=0}^{q-1} \gamma_{i} \partial_{x} (b U_{N}^{n+i} + W_{N}^{n+i}) = 0, \\ \sum_{i=0}^{q} \alpha_{i} W_{N}^{n+i} + \Delta t \sum_{i=0}^{q-1} \gamma_{i} \partial_{x} ((1-b^{2}) U_{N}^{n+i} - b W_{N}^{n+i}) = -\frac{\beta \Delta t}{\varepsilon} W_{N}^{n+q}. \end{cases}$$

• Theorem (J. Hu-RS 21'): for q=1,2,3,4, assume the initial data is "consistent", then under CFL condition $\Delta t \leq c_{CFL}/N^2$, IMEX-BDF-q for linear hyperbolic relaxation system has uniform q-th order accuracy:

$$\|u(t_n)-U_N^n\|^2+\|w(t_n)-W_N^n\|^2\leq C(T)\left(\Delta t^{2q}+\frac{1}{N^{4q}}\right)$$
 follows from stability due to stage order temporal error spatial error

- Accuracy follows from stability due to stage order
- Generalized to linear hyperbolic systems by Z. Ma-J. Huang-W. Yong 25'

$$2W^{n+1} \times W^{n+1} - W^n + \Delta t \partial_x ((1-b^2)U^n - bW^n) = -\frac{\Delta t}{\varepsilon} W^{n+1}$$

$$\|W^{n+1}\|^2 - \|W^n\|^2 + \|\underline{W^{n+1} - W^n}\|^2 + 2\Delta t \int W^{n+1} \partial_x ((1-b^2)U^n - bW^n) dx = -2\frac{\Delta t}{\varepsilon} \|W^{n+1}\|^2$$
 good terms

$$\left(W^{n+q} - \sum_{i=1}^{q-1} \eta_i W^{n+i}\right) \times \sum_{i=0}^{q} \alpha_i W^{n+i} + \Delta t \sum_{i=0}^{q-1} \gamma_i \partial_x ((1-b^2)U^{n+i} - bW^{n+i}) = -\frac{\beta \Delta t}{\varepsilon} W^{n+q}$$

$$G(W^{n+1}, \dots, W^{n+q}) - G(W^n, \dots, W^{n+q-1}) + \|\cdot\|^2 + \text{transport terms}$$

$$= -A(W^{n+2}, \dots, W^{n+q}) + A(W^{n+1}, \dots, W^{n+q-1}) - \|\cdot\|^2$$

G, A positive definite quadratic forms

$$\left(W^{n+q} - \sum_{i=1}^{q-1} \eta_i W^{n+i}\right) \times \sum_{i=0}^{q} \alpha_i W^{n+i} + \Delta t \sum_{i=0}^{q-1} \gamma_i \partial_x ((1-b^2)U^{n+i} - bW^{n+i}) = -\frac{\beta \Delta t}{\varepsilon} W^{n+q}$$

$$G(W^{n+1},\dots,W^{n+q})-G(W^n,\dots,W^{n+q-1}) \underbrace{+\parallel\cdot\parallel^2}_{\mbox{good term 1}} + \mbox{transport terms} \\ = -A(W^{n+2},\dots,W^{n+q}) + A(W^{n+1},\dots,W^{n+q-1}) \underbrace{-\parallel\cdot\parallel^2}_{\mbox{good term 2}} + \mbox{good term 2}$$

- Requirements on the multiplier:
 - Gives G with good term 1 (Nevanlinna-Odeh 81' up to q=5)
 - Gives A with good term 2
 - Good term 1 controls the transport terms

For q = 1, the coefficients are given by

$$g_{11} = \frac{1}{2}, \quad d_1 = \frac{1}{2}, \quad c_1 = 1.$$
 (3.32)

For q=2, the coefficients are given by

$$\eta_1 = 0, \quad g_{11} = \frac{1}{6}, \quad g_{22} = \frac{5}{6}, \quad g_{12} = -\frac{1}{3}, \quad d_1 = \frac{1}{6}, \quad d_2 = \frac{3}{2}, \quad a_{11} = 0, \quad c_2 = 1, \quad c_1 = 0.$$
(3.33)

For q=3, the coefficients g_{ij} , η_i , d_i are given by

New multiplier!

$$g_{11} = \frac{\sqrt{30}}{187} + \frac{8}{187}, \quad g_{22} = \frac{\sqrt{30}}{34} + \frac{95}{187}, \quad g_{33} = \frac{\sqrt{30}}{22} + \frac{7}{11},$$

$$g_{12} = -\frac{3\sqrt{30}}{187} - \frac{24}{187}, \quad g_{13} = \frac{3\sqrt{30}}{187} + \frac{24}{187}, \quad g_{23} = -\frac{6\sqrt{30}}{187} - \frac{9}{17},$$

$$\eta_2 = -\frac{2\sqrt{30}}{17} + \frac{18}{17}, \quad \eta_1 = \frac{\sqrt{30}}{17} - \frac{9}{17}, \quad d_1 = -\frac{\sqrt{30}}{22} + \frac{4}{11}, \quad d_2 = \frac{11\sqrt{30}}{102} + \frac{44}{51}.$$

$$(3.34)$$

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IMEX-RK

$$\begin{split} U^{(i)} &= U^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} (b \partial_x U^{(j)} + \partial_x W^{(j)}) \\ W^{(i)} &= W^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} ((1-b^2) \partial_x U^{(j)} - b \partial_x W^{(j)}) - \frac{\Delta t}{\varepsilon} \sum_{j=1}^{i} a_{ij} W^{(j)} \\ U^{n+1} &= U^n - \Delta t \sum_{j=1}^{s} \tilde{b}_j (b \partial_x U^{(j)} + \partial_x W^{(j)}) \\ W^{n+1} &= W^n - \Delta t \sum_{j=1}^{s} \tilde{b}_j ((1-b^2) \partial_x U^{(j)} - b \partial_x W^{(j)}) - \frac{\Delta t}{\varepsilon} \sum_{j=1}^{s} a_{sj} W^{(j)} \end{split}$$

Butcher tables

implicit explicit $c_1 = 0$ $a_{22} 0 0$ c_2 $ilde{a}_{32}$ $ilde{a}_{31}$ a_{32} a_{31} c_3 $ilde{a}_{42}$ \tilde{a}_{43} \tilde{a}_{41} a_{41} a_{42} c_4 $ilde{b}_4$ $ilde{b}_2$ \tilde{b}_3 b_2 b_1 b_1

$$\gamma = 1 - \frac{\sqrt{2}}{2}, \delta = 1 - \frac{1}{2\gamma}$$

$$c_i = \sum_j a_{ij} = \sum_j \tilde{a}_{ij}$$

Implicitly Stiffly Accurate (ISA):

$$b_j = a_{sj}$$

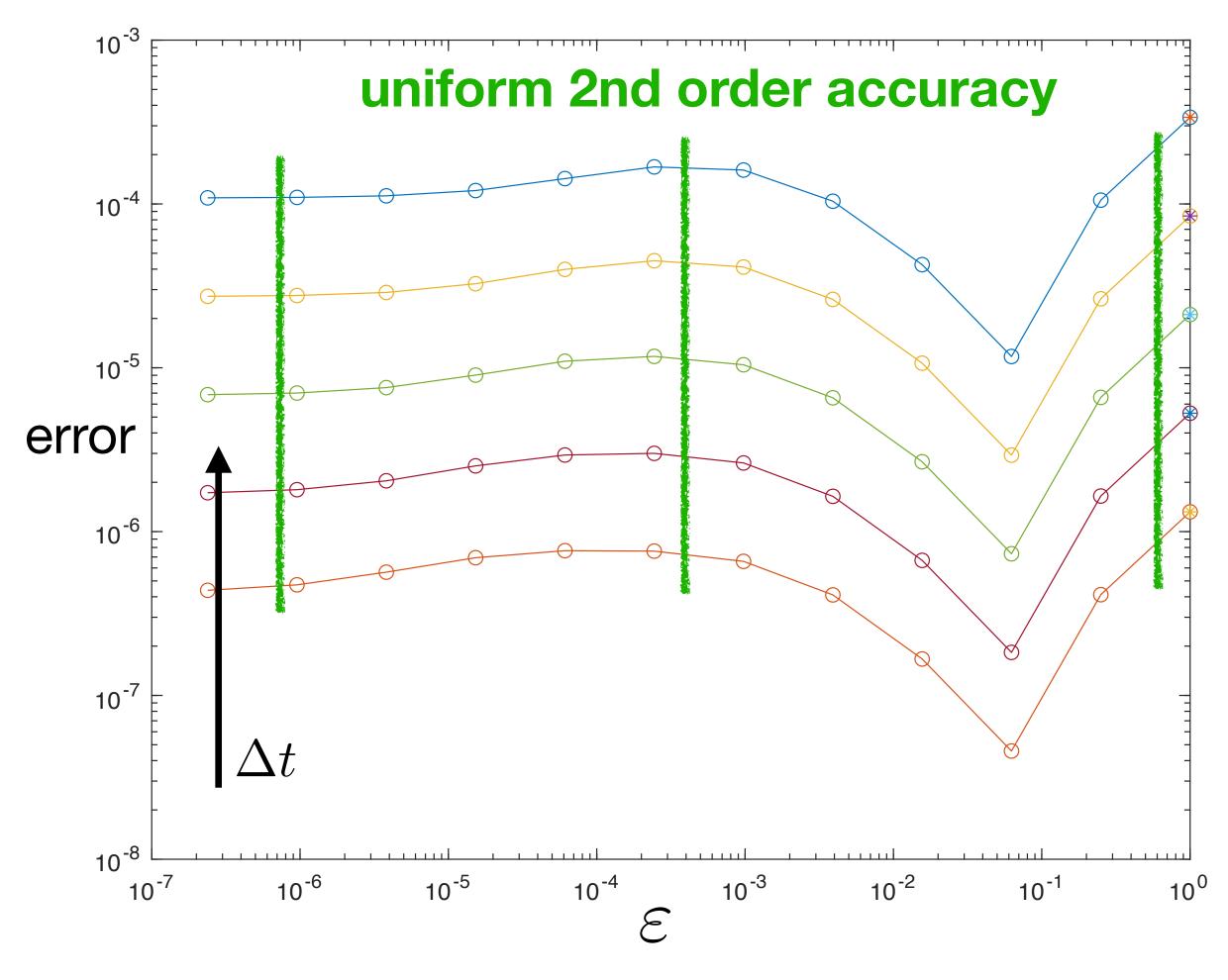
Globally Stiffly Accurate (GSA):

$$b_j = a_{sj}, \, \tilde{b}_j = \tilde{a}_{sj}$$

ARS(4,4,3): 3rd order IMEX-RK

0	0	0	0	0	0	0	0	0	0	0	0
1/2	1/2	0	0	0	0	1/2	0	1/2	0	0	O
2/3	11/18	1/18	0	0	0	2/3	0	1/6	1/2	0	O
						1/2					
1	1/4	7/4	3/4	-7/4	0	1	0	3/2	-3/2	1/2	1/2
	1/4	7/4	3/4	-7/4	0		0	3/2	-3/2	1/2	1/2

Uniform accuracy vs. order reduction



10⁻⁵ 10⁻⁶ 10⁻⁷ reduced to 10⁻⁸ 2nd order 3rd order 3rd order 10⁻⁵

ARS(2,2,2): 2nd order IMEX-RK

ARS(4,4,3): 3rd order IMEX-RK

Second order uniform accuracy

• **Theorem** (J. Hu-RS 25'): assume the initial data is "consistent" and under CFL condition $\Delta t \leq c_{CFL}/N^2$. IMEX-RK (type CK, ISA) for linear hyperbolic relaxation system has second order uniform accuracy:

$$||u(t_n) - U_N^n||^2 + ||w(t_n) - W_N^n||^2 \le C(T) \left(\Delta t^4 + \frac{1}{N^8}\right)$$

if the following are true:

1.
$$c_i = \sum_j a_{ij} = \sum_j \tilde{a}_{ij}$$

- 3. Existence of a multiplier matrix M
- This applies to ARS(2,2,2) and ARS(4,4,3)

- 2. Usual second order conditions
- 4. Last component of \vec{v} is 0 null space of A

(related to the L-stability)

An IMEX-RK with third order uniform accuracy

• S. Boscarino-G. Russo 09': third order IMEX-RK of type CK, ISA

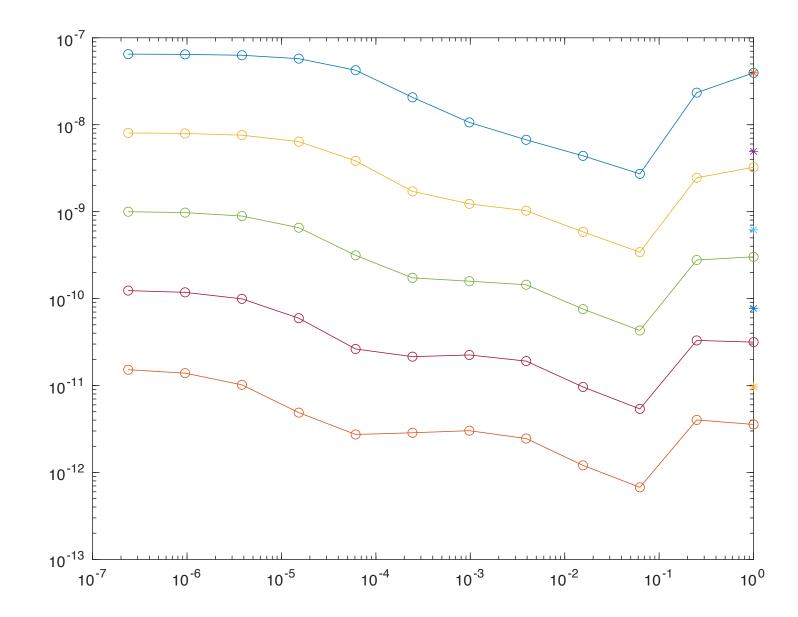
	0	0	0	0	0	0	0	0	0	0	0
0.	.8717	0.8717	0	0	0	0	0.4359	0.4359	0	0	0
0.	.8717	0.4359	0.4359	0	0	0	0.4359	0	0.4359	0	0
1.	.5000	0.2095	0	1.2905	0	0	0.5236	0	0.5405	0.4359	0
1.	.0000	0.3177	-0.3629	1.1960	-0.1508	0	0.3694	0	0.3629	-0.1681	0.4359
		0.3694	0	0.3629	-0.1681	0.4359	0.3694	0	0.3629	-0.1681	0.4359

stage order 1

stage order 2

the 'less accurate' stage is not used directly

Third order uniform accuracy is observed



Third order uniform accuracy

- Theorem (J. Hu-RS 25'): further assume
 - 1. Usual third order conditions

2. Stages (3)-(s) have stage order 2

3.
$$\tilde{b}_2 = 0$$
 $a_{i,2} = 0, i = 3, 4, \dots, s$

Then we have third order uniform accuracy

$$||u(t_n) - U_N^n||^2 + ||w(t_n) - W_N^n||^2 \le C(T) \left(\Delta t^6 + \frac{1}{N^{12}}\right)$$

Proof of stability

$$U^{(i)} = U^{n} - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} (b\partial_{x} U^{(j)} + \partial_{x} W^{(j)})$$

$$W^{(i)} = W^{n} - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} ((1 - b^{2})\partial_{x} U^{(j)} - b\partial_{x} W^{(j)}) - \frac{\Delta t}{\varepsilon} \sum_{j=1}^{i} a_{ij} W^{(j)}$$

Vector form

$$\vec{U} = U^{(1)}\vec{e} - \Delta t \tilde{A}(b\partial_x \vec{U} + \partial_x \vec{W})$$

$$\vec{W} = W^{(1)}\vec{e} - \Delta t \tilde{A}((1 - b^2)\partial_x \vec{U} - b\partial_x \vec{W}) - \frac{\Delta t}{\varepsilon} A \vec{W}$$

• Use a multiplier to do energy estimate?

Proof of stability

$$\vec{U}^{\top}M \times \vec{U} = U^{(1)}\vec{e} - \Delta t \tilde{A}(b\partial_x \vec{U} + \partial_x \vec{W})$$

$$\vec{W}^{\top}M \times \vec{W} = W^{(1)}\vec{e} - \Delta t \tilde{A}((1-b^2)\partial_x \vec{U} - b\partial_x \vec{W}) - \frac{\Delta t}{\varepsilon} A \vec{W}$$

$$(W^{(s)})^2 = (W^n)^2 - \underline{\vec{W}^{\top}M_*\vec{W}} - \frac{\Delta t}{\varepsilon} \vec{W}^{\top}MA\vec{W} - \Delta t \vec{W}^{\top}M\tilde{A}((1-b^2)\partial_x \vec{U} - b\partial_x \vec{W})$$

$$= \text{good terms (hopefully)}$$

$$M_* := M \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & -1 \end{pmatrix}$$

• Requirements on the multiplier matrix M:

$$ec{W}^{ op} M_* ec{W}$$
 , $ec{W}^{ op} M A ec{W}$ are semi-positive-definite

For all the previously mentioned schemes, we can construct such M

Proof of accuracy

- Proof of accuracy is NOT obvious because the stage order is lower than the desired uniform accuracy order
- Say, to prove second order uniform accuracy, the evolution of error is

$$\vec{U}_e = U_e^{(1)} \vec{e} - \Delta t \tilde{A} (b \partial_x \vec{U}_e + \partial_x \vec{W}_e) + \vec{E}_U \qquad \text{L.T.E., } O(\Delta t^2) \text{ for some stages}$$

$$\vec{W}_e = W_e^{(1)} \vec{e} - \Delta t \tilde{A} ((1 - b^2) \partial_x \vec{U}_e - b \partial_x \vec{W}_e) - \frac{\Delta t}{\varepsilon} A \vec{W}_e + \vec{E}_W$$

 Directly applying multiplier, local truncation error (L.T.E.) will pollute the estimate and only gives first order uniform accuracy

Proof of accuracy

$$\underline{\vec{U}_e} = U_e^{(1)} \vec{e} - \Delta t \tilde{A} (b \partial_x \vec{U}_e + \partial_x \vec{W}_e) + \underline{\vec{E}_U}$$

$$\underline{\vec{W}_e} = W_e^{(1)} \vec{e} - \Delta t \tilde{A} ((1 - b^2) \partial_x \vec{U}_e - b \partial_x \vec{W}_e) - \frac{\Delta t}{\varepsilon} A \vec{W}_e + \underline{\vec{E}_W}$$

Use a change of variables to absorb the L.T.E.

$$\vec{U}_{e*} := \underline{\vec{U}_e} - \underline{\vec{E}_U}, \quad \left(I + \frac{\Delta t}{\varepsilon} A\right) \vec{W}_{e*} := \left(I + \frac{\Delta t}{\varepsilon} A\right) \vec{W}_e - \underline{\vec{E}_W}$$

$$\vec{U}_{e*} = U_e^{(1)} \vec{e} - \Delta t \tilde{A} (b \partial_x \vec{U}_{e*} + \partial_x \vec{W}_{e*}) - \underline{\Delta t} \tilde{A} \vec{F}_U$$
 some linear combination of L.T.E.
$$\vec{W}_{e*} = W_e^{(1)} \vec{e} - \Delta t \tilde{A} ((1 - b^2) \partial_x \vec{U}_{e*} - b \partial_x \vec{W}_{e*}) - \frac{\Delta t}{\varepsilon} A \vec{W}_{e*} - \underline{\Delta t} \tilde{A} \vec{F}_W$$

• Notice that now the L.T.E. terms has a factor Δt on it!

Proof of accuracy

 Then the multiplier techniques work as before. But finally we need to change back to the original variables...

$$U_e^{n+1} = U_{e*}^{(s)} - \Delta t(\tilde{b}^{\top} - \tilde{A}_s)(b\partial_x \vec{U}_{e*} + \partial_x \vec{W}_{e*}) - \Delta t(\tilde{b}^{\top} - \tilde{A}_s)\vec{F}_U + E_U^{n+1}$$

$$W_e^{n+1} = W_{e*}^{(s)} - \Delta t(\tilde{b}^{\top} - \tilde{A}_s)((1-b^2)\partial_x \vec{U}_{e*} - b\partial_x \vec{W}_{e*}) - \Delta t(\tilde{b}^{\top} - \tilde{A}_s)\vec{F}_W - \frac{\Delta t}{\varepsilon}A_s(I + \frac{\Delta t}{\varepsilon}A)^{-1}\vec{E}_W + E_W^{n+1}$$

all the difficulties are here

• Then one needs a careful study of the matrix

$$\frac{\Delta t}{\varepsilon} A (I + \frac{\Delta t}{\varepsilon} A)^{-1}$$

- This gives second order uniform accuracy by some energy estimate
- For third order, one needs to do the change of variables twice...
- Generalized to linear hyperbolic systems by Z. Ma-J. Huang 25'