

# LINEAR MULTISTEP METHODS (LMMs)

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We already gave one example of a (linear) multistep method for solving the (system of) ODE(s):

$$u'(t) = f(u(t), t)$$

namely the Adams-Basforth (AB2) second-order method:

$$u^{n+2} = u^n + \frac{2}{2} (3f^{n+1} - f^n)$$

time step size

This is an explicit two step scheme.

More commonly written as

$$u^{n+1} = u^n + \frac{2}{2} (3f^n - f^{n-1})$$

↑ future      ↑ present      ↓ past

It requires storing  $f^{n-1}$  (but not  $u^{n-1}$ ).

A general  $r$ -step Linear Multistep Method (LMM) takes the form:

$$\sum_{j=0}^r \alpha_j u^{(n+j)} = \bar{z} \sum_{j=0}^r \beta_j f^{(n+j)}$$

For LMMs we will assume  $\bar{z}$  is fixed and not adaptive, as adapting is hard with multistep methods.

Three classes of LMMs:

A) Adams methods

$$\alpha_r = 1, \alpha_{r-1} = -1, \alpha_{j \leq r-2} = 0$$

① Adams - Bashforth

$$\beta_r = 0 \rightarrow \text{explicit}$$

② Adams - Bashforth - Moulton

$$\beta_r \neq 0 \rightarrow \text{implicit}$$

B) Backwards Differentiation Formulas

$$\beta_j = 0, j = 0 \dots r-1 \rightarrow \text{implicit}$$

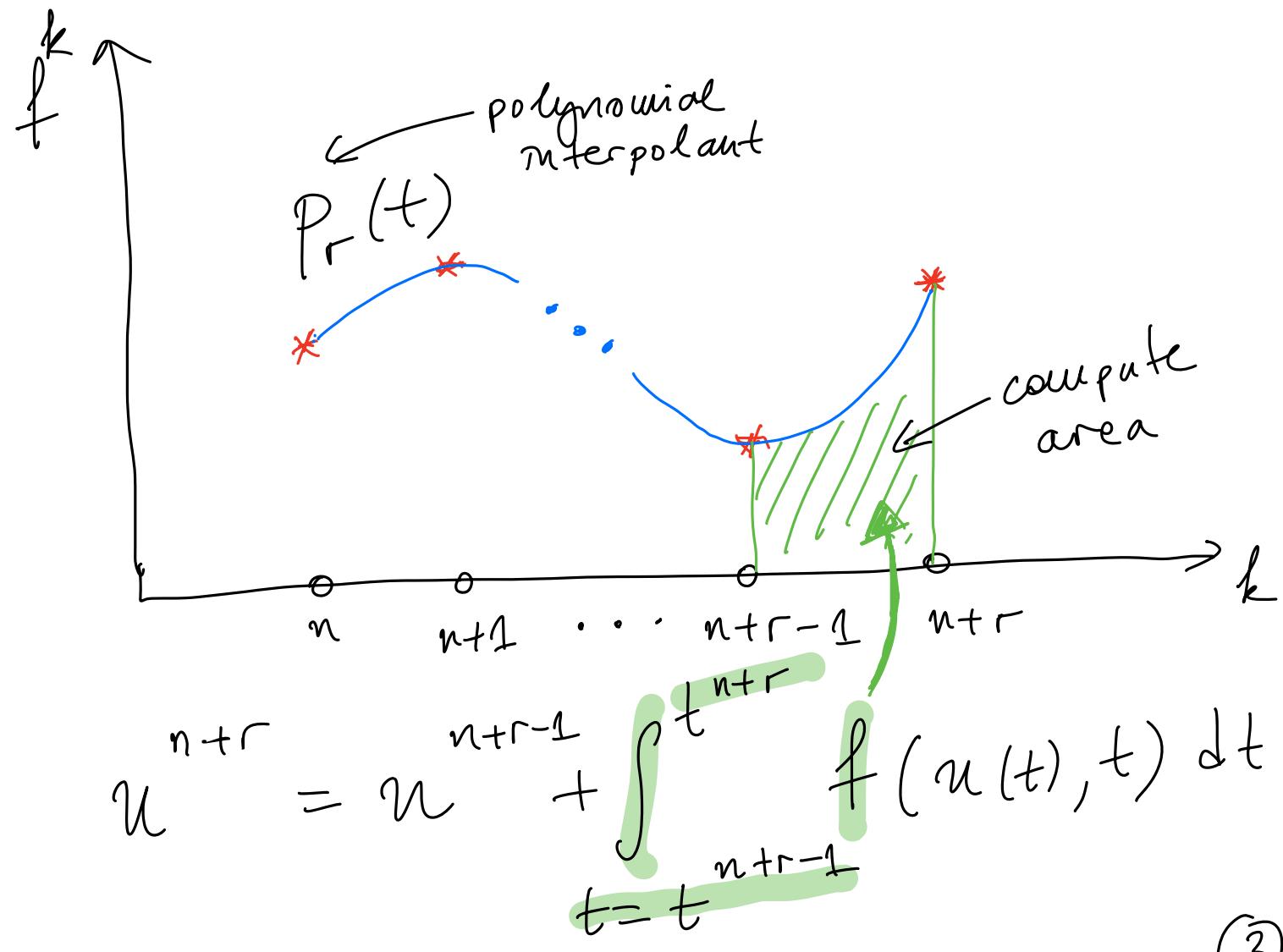
Stores past values of  $u$  not  $f$

②

## Adams Methods

$$u^{n+r} = u^{n+r-1} + \epsilon \sum_{j=0}^r \beta_j f^{n+j}$$

Basic idea: Fit a polynomial of degree  $r-1$  through past values of  $f^k$ : interpolate (+extrapolate) the r.h.s of ODE



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$$u^{n+r} \approx u^n + \int_{t=t^{n+r-1}}^{t=t^{n+r}} p_r(t) dt$$

Simple algebra to compute interpolant. If method is explicit the last time step is extrapolated

**AB3 scheme** (third order)

$$u^{n+3} = u^{n+2} + \frac{2}{12} \left[ 5f^n - 16f^{n+1} + 23f^{n+2} \right]$$

Computing the LTE to confirm the order of accuracy is just as for RK schemes:

Plug exact solution into the scheme and do Taylor series

$$u^{n+1} = u^n + \frac{\bar{\tau}}{2} (3f^n - f^{n-1}) \quad AB2$$

$$u((n+1)\bar{\tau}) = u(n\bar{\tau}) + \frac{\bar{\tau}}{2} \left[ 3f(u(n\bar{\tau}), n\bar{\tau}) - f(u((n-1)\bar{\tau}, (n-1)\bar{\tau})) \right]$$

↑  
expand around  $(u^n, t^n)$

**+ LTE \*  $\bar{\tau}$**

④

$$\begin{cases} u'(t) = f(u(t), t) \\ u''(t) = \frac{\partial f}{\partial u}(u(t), t) u'(t) + \frac{\partial f}{\partial t}(u(t), t) \end{cases} \dots (*)$$

$$u(n\bar{\tau}) + u'(n\bar{\tau})\bar{\tau} + \frac{1}{2}u''(n\bar{\tau})\bar{\tau}^2 + O(\bar{\tau}^3)$$

$$= u(n\bar{\tau}) + \frac{\bar{\tau}}{2} \left\{ 3f(u(n\bar{\tau}), n\bar{\tau}) - \right.$$

$$\left[ f(u(n\bar{\tau}), n\bar{\tau}) + \frac{\partial f}{\partial u}(u(n\bar{\tau}), n\bar{\tau}) \underbrace{(u((n+1)\bar{\tau}) - u(n\bar{\tau}))}_{u'(n\bar{\tau})\bar{\tau}} \right.$$

$$\left. + \frac{\partial f}{\partial t}(u(n\bar{\tau}), n\bar{\tau})\bar{\tau} + O(\bar{\tau}^2) \right] + \text{LTE}$$

Use (\*)

$$f(u(n\bar{\tau}), n\bar{\tau})\bar{\tau} + \frac{\bar{\tau}^2}{2} \left[ \frac{\partial f}{\partial u}(u(t), t) u'(t) + \frac{\partial f}{\partial t}(u(t), t) \right]$$

$$= f(u(n\bar{\tau}), n\bar{\tau})\bar{\tau} + \frac{\bar{\tau}^2}{2} \frac{\partial f}{\partial u}(\dots) + \frac{\bar{\tau}^2}{2} \frac{\partial f}{\partial t}(\dots) +$$

$$+ O(\bar{\tau}^3) + \text{LTE}$$

$$\Rightarrow \text{LTE} = O(\bar{\tau}^3) \Rightarrow \text{third order}$$

These sort of calculations are best done using symbolic algebra (Maple, Mathematica) or, better, use error estimates for polynomial interpolation!

## AM2 (Adams-Moulton two step):

$$u^{n+2} = u^{n+1} + \frac{1}{12} [-f^n + 8f^{n+1} + 5f^{n+2}]$$

implicit

One can get another explicit 2<sup>nd</sup> order scheme by combining AB2 with AM2 in a predictor-corrector fashion:

### AB2-AM2

two-stage two-step scheme:  
linear multi-stage multi-step

$$\left\{ \begin{array}{l} u^{n+2,*} = u^{n+1} + \frac{1}{2} (3f^{n+1} - f^n) \\ u^{n+2} = u^{n+1} + \frac{1}{12} (-f^n + 8f^{n+1} + 5f(u^{n+2,*}, t^{n+2})) \end{array} \right.$$

AB2 predictor  
AM2 corrector

One could iterate this multiple times but there is rarely a benefit of that - use AM2 with Newton's method solver instead.

LMMs are not self-starting

To do  $r$  initial steps, use a one-step method of order  $p-1$ , if order of LMM is  $p$ .

Order  $p-1$  is OK since we do a finite (small) number of initial steps so error does not accumulate.

- For AB2/AM2 use one step of Euler
- For AB3/AM2 use RK2 (midpoint or trapezoidal)

To avoid any large errors in the initial steps, usually an RK of order  $\underline{E}$  is used in practice.

## Backwards Differentiation Formulas (BDF)

$$\frac{1}{\tau} \sum_{j=0}^r \alpha_j u^{n+j} = f^{n+r} \approx u'((n+r)\tau)$$

finite-difference approximation of derivative  $u'((n+r)\tau)$  using past values of  $u$ .

Interpolate  $r+1$  values of  $u$  with a polynomial of degree  $r$  to get a scheme of order  $r$ :

$$f^{n+r} = p_r'((n+r)\tau)$$

BDF schemes are good for stiff systems of equations.

BDF 1  $\equiv$  Backwards Euler

$$\frac{u^{n+1} - u^n}{\tau} = f(u^{n+1}, (n+1)\tau)$$

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BDF2 scheme ( $2^{\text{nd}}$  order implicit)

$$\frac{3u^{n+2} - 4u^{n+1} + u^n}{2\bar{\tau}} = f^{n+2}$$

$$\Rightarrow u^{n+2} = \frac{1}{3}(4u^{n+1} - u^n + 2\bar{\tau}f^{n+2})$$

Trapezoidal BDF2 : TR-BDF2

$$\left\{ \begin{array}{l} u^{n+1/2,*} = u^n + \frac{\bar{\tau}}{4} (f^n + f^{n+1/2,*}) \\ \text{Trapezoidal to midpoint} \\ \text{(predictor)} \\ u^{n+1} = \frac{1}{3} (4u^{n+1/2,*} - u^n + \bar{\tau}f^{n+1}) \\ \text{BDF2 from } u^n, u^{n+1/2,*} \text{ with} \\ \text{time-step size } \bar{\tau}/2 \text{ (corrector)} \end{array} \right.$$

(One of the simplest) L-stable schemes  
of  $2^{\text{nd}}$  order.

If it is used when solving PDEs

## Zero Stability of LMMs

When do LMMs converge?

Let's apply the scheme to a linear equation

$$\begin{cases} u'(t) = 0 \\ u(0) = 0 \end{cases}$$

A one-step method would give

$$u^k = 0 + k, \text{ so stable.}$$

BUT, in an LMM, not necessarily

Previous  $\tau$  values will have some roundoff errors / perturbations.

We don't want those to grow.

Also, previous values have some error since method is not exact

We should only require initial values to be  $= u^0 \approx u(0)$  as

$$\tau \rightarrow 0.$$

Take an ODE  $u' = f(u, t)$  where  $f$  is Lipschitz continuous in  $u$  and ODE has a unique solution up to time  $T$ .

{ An r-step LMM converges if   
 $\forall u^{\bar{v}}$  s.t.  $\lim_{\bar{\tau} \rightarrow 0} u^{\bar{v}} = u(0), \bar{v}=0, \dots, r-1$    
 $\lim_{\bar{\tau} \rightarrow 0} u^{T/\bar{\tau}} = u(T)$

Here is a non-convergent LMM:

$$u^{n+2} - 3u^{n+1} + 2u^n = -\bar{\tau} f^n$$

Apply to  $f=0$ :

$$u^{n+2} - 3u^{n+1} + 2u^n = 0 \leftarrow \begin{array}{l} \text{recurrence} \\ \text{relation} \end{array}$$

$$\Rightarrow u^n = 2u^0 - u^1 + 2^n (\underbrace{u^1 - u^0}_{\text{non-zero}})$$

which will blow up for  $n \gg 1$ !

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We need to understand when linear recurrence relations blow up.

Consider

$$(\star\star) \dots \sum_{j=0}^r \alpha_j n^{n+j} = 0 \quad (\text{since } f \equiv 0)$$

For every simple root  $\xi_i$  of

$$\left\{ \begin{array}{l} g(\xi) = \sum_{j=0}^r \alpha_j \xi^j - \text{characteristic polynomial of LMR} \\ g(\xi_i) = 0 \end{array} \right.$$

a linearly independent solution of

$$(\star\star) \text{ is } u^n = \xi_i^n$$

For a double (repeated) root,

$$g(\xi_j) = 0 \quad \& \quad g'(\xi_j = 0)$$

two linearly independent solutions of  $(\star\star)$  are

$$u^n = \xi_j^n \quad \& \quad u^n = n \xi_j^n$$

etc. for roots of multiplicity  $> 2$ .  
 General solution of (\*4):

$$u^n = \sum_{j=1}^{n_1} c_j^{(1)} \xi_j^n + \sum_{k=1}^{n_2} c_k^{(2)} n \xi_k^n + \dots + \sum_{l=1}^{n_3} c_l^{(3)} n^2 \xi_l^n + \dots$$

We want the coefficients not to grow with time. This requires that

$$|\xi_j| \leq 1 \text{ for simple roots}$$

$$|\xi_j| < 1 \text{ for repeated roots}$$

To see why take a double root. If  $|\xi_k| = 1$ , then we get a term

$$u^n = \dots + n O(\bar{\tau}) \Rightarrow$$

$$u^{T/\bar{\tau}} = \dots + O(N \bar{\tau}) = \dots + O(T)$$

not convergent

## Adams methods:

$$S(\xi) = \xi^r - \xi^{r-1} = (\xi - 1) \xi^{r-1}$$

$\Rightarrow \begin{cases} \xi_1 = 1 & \text{is a simple root} \\ \xi_2 = 0 & \text{is a root of multiplicity } r-1 \end{cases}$

$\Rightarrow$  All Adams methods are zero-stable

Note that  $\xi_1 = 1$  is always a root for any consistent LMM.

$$\sum_{j=0}^r \alpha_j u^{(n+j)} = \bar{\epsilon} \sum_{j=0}^r \beta_j f^{(n+j)}$$

$$\sum_j \alpha_j (n^n + j\bar{\epsilon} + O(\bar{\epsilon}^2)) = \bar{\epsilon} \sum_j \beta_j (f^n + O(\bar{\epsilon})) \Rightarrow$$

$$\begin{cases} O(\bar{\epsilon}^0) : \sum_j \alpha_j = 0 \\ O(\bar{\epsilon}^1) : \sum_j j \alpha_j = \sum_j \beta_j \end{cases}$$

$$\delta(\xi) = \sum_j \beta_j \xi^j$$

$$\begin{cases} O(\bar{\tau}^0) : \quad g(1) = 0 \Rightarrow 1 \text{ is a root} \\ O(\bar{\tau}^+) : \quad g'(1) = \delta(1) \end{cases}$$

Dahlquist equivalence theorem

consistency + zero stability  $\Leftrightarrow$  convergence

Note: A one step method has only one root  $\xi_1 = 1$  so it is convergent, as we proved earlier.

## Absolute stability of LMMs

Zero stability is about the limit  $\tau \rightarrow 0$ , and we want a finite  $\tau$ . So we need to look at absolute stability:

$$u' = \lambda u$$

$$\sum_{j=0}^r d_j u^{n+j} = \bar{\tau} \sum_{j=0}^r \beta_j \lambda u^{n+j}$$

recurrence relation  $\Rightarrow \sum_{j=0}^r (d_j - \bar{\tau} \beta_j) u^{n+j} = 0$

where recall  $\bar{\tau} = \lambda \tau$

Define polynomial

$$\pi(\xi; \tau) = s(\xi) - \tau b(\xi)$$

LMM is absolutely stable if roots of  $\pi$  satisfy root conditions  $(| \text{simple roots} | \leq 1, | \text{multiple roots} | < 1)$

Stability region  $S$  for an LMM

$$S = \left\{ z \in \mathbb{C} \mid \begin{array}{l} |\text{simple roots}| \leq 1 \\ \text{or } |\pi(\xi; z)| < 1 \\ |\text{multiple roots}| < 1 \end{array} \right\}$$

We can plot the boundary of  $S$  by rendering the parametric curve:

$$\pi(e^{i\theta}; z) = 0, \quad 0 < \theta \leq 2\pi$$

$$\Rightarrow z(\theta) = \frac{s(e^{i\theta})}{\sigma(e^{i\theta})}, \quad 0 < \theta \leq 2\pi$$

is the boundary of  $S$ .

Take BDF methods, for example:

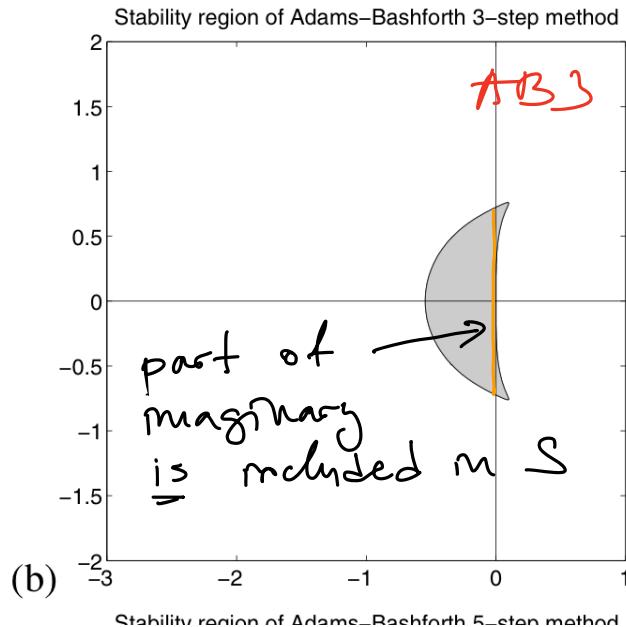
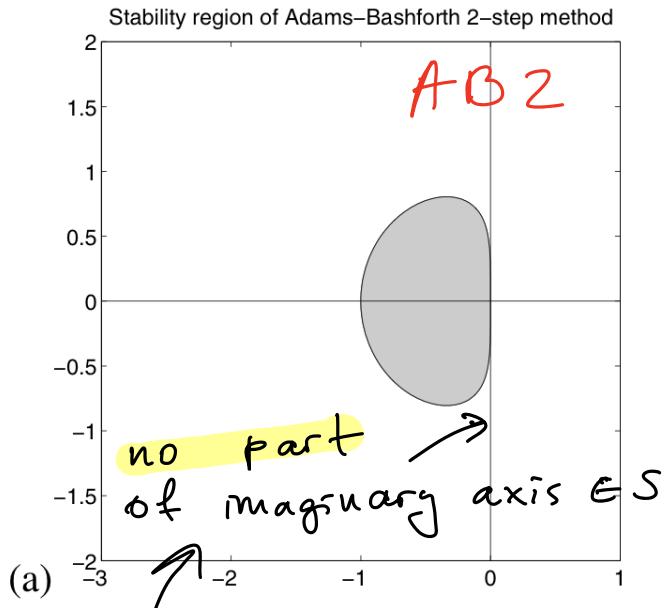
$$\sigma(\xi) = \prod \xi^r$$

$$\text{As } |z| \rightarrow \infty \Rightarrow \pi(\xi; z) \rightarrow -z \sigma(\xi)$$

so roots of  $\pi$  match roots of  $\sigma$  as  $|z| \rightarrow \infty$ . But the only root of  $\sigma(\xi)$  is  $\xi_r = 0 \Rightarrow$

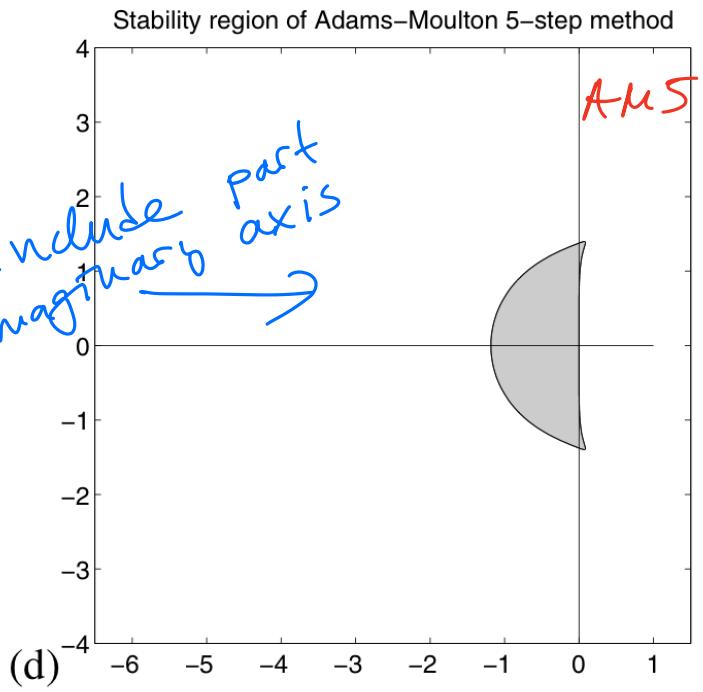
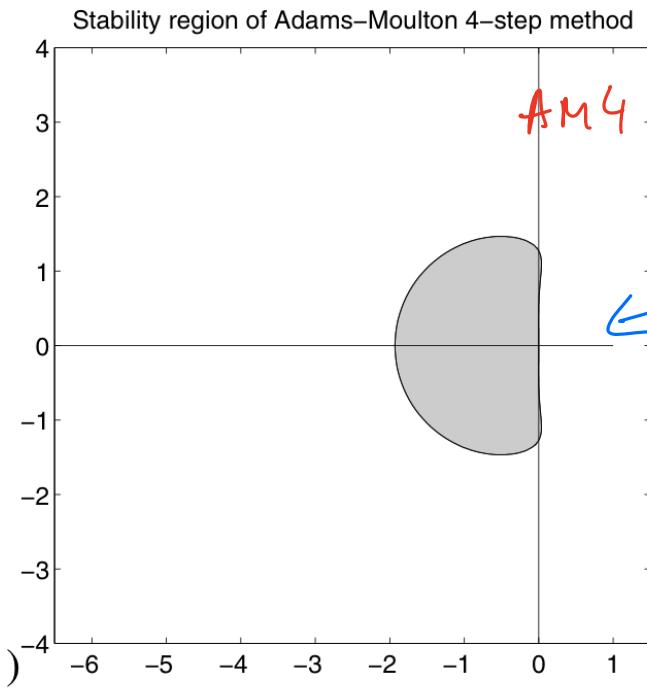
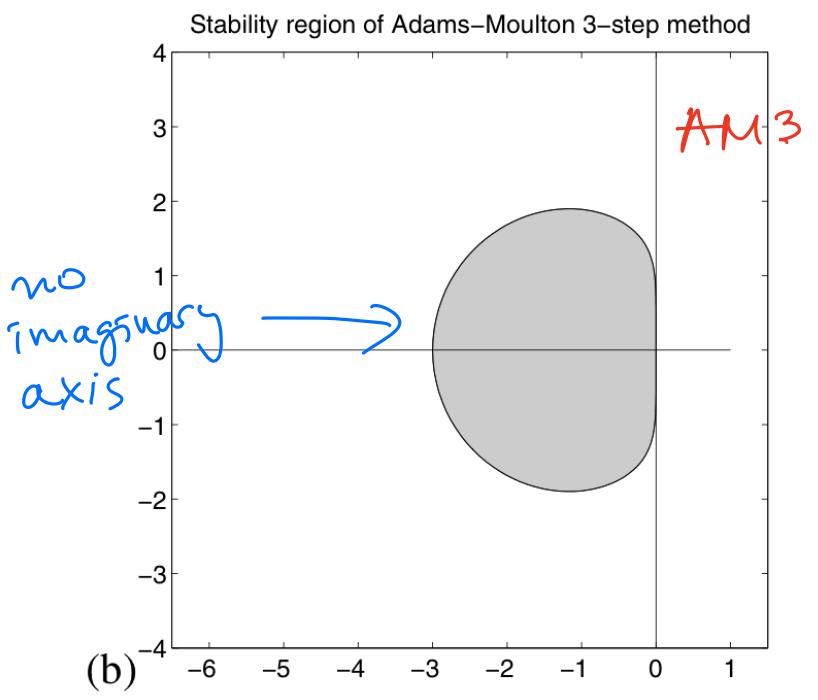
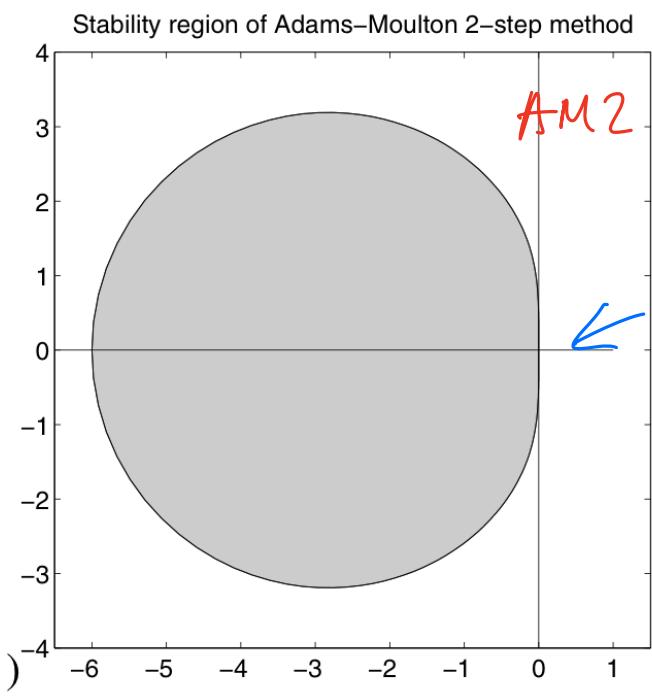
All BDF methods are stable as  $|z| \rightarrow \infty$

Corollary: An A-stable LMM is L-stable  
 This is why BDF is great for  
very stiff equations.



Not good for hyperbolic PDEs

↑  
 good for hyperbolic PDEs



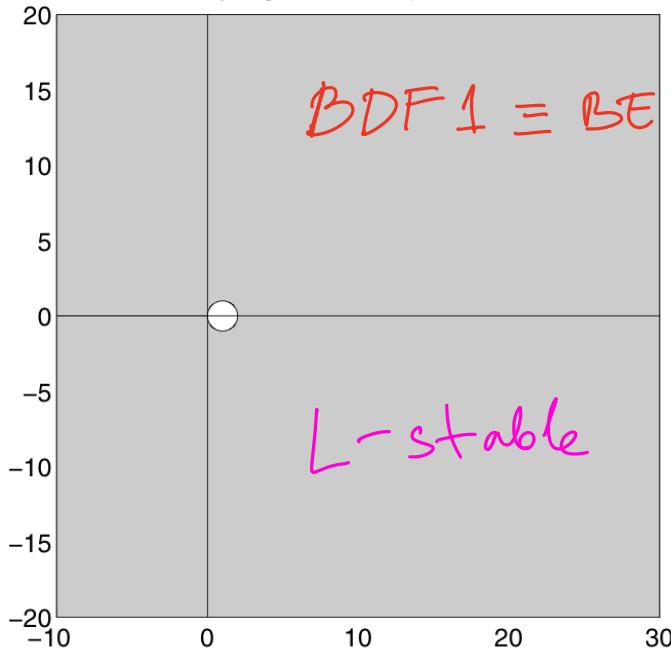
**Figure 7.3.** Stability regions for some Adams–Moulton methods.

General rule : For non-A-stable classes of methods (e.g., explicit), the stability region shrinks as the order of accuracy increases.

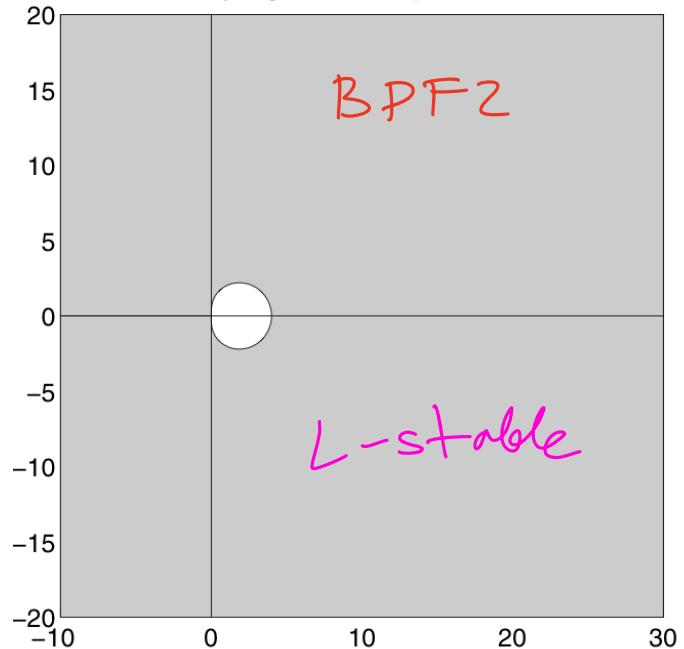
Explicit methods are never A-stable

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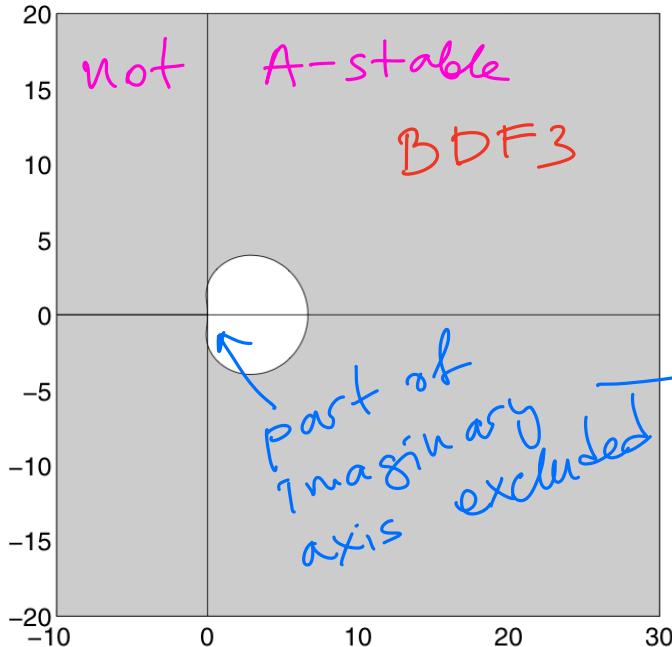
Stability region of 1-step BDF method



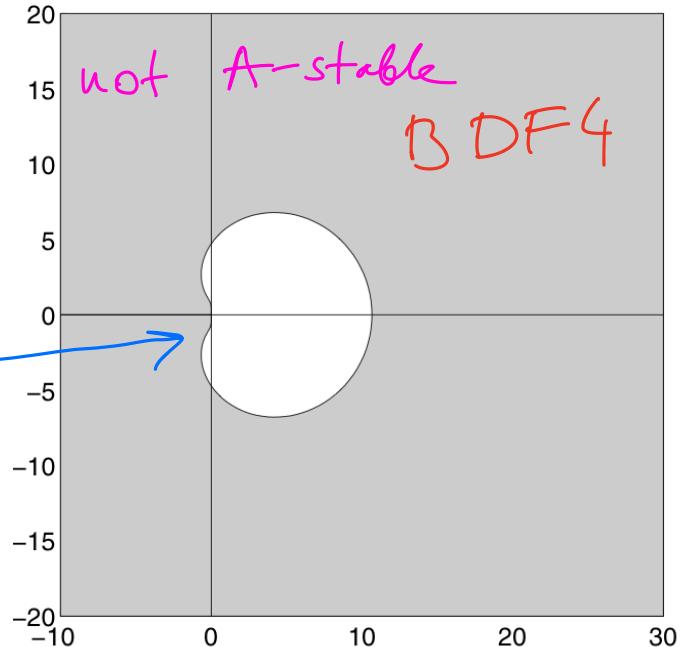
Stability region of 2-step BDF method



Stability region of 3-step BDF method



Stability region of 4-step BDF method



Lesson : Going higher order brings issues with absolute stability.  
To be good for ODES with purely imaginary eigenvalues, explicit schemes must be at least 3<sup>rd</sup> order

These can be turned into theorems called the **Dahlquist order barriers**

① A zero-stable  $r$ -step LMM can at most have order of accuracy:

If **implicit**  $\left\{ \begin{array}{l} r+1 \text{ if } r \text{ is odd} \\ r+2 \text{ if } r \text{ is even} \end{array} \right.$

For **explicit** :  $r$

② An explicit LMM cannot be A-stable (same as for RK)

③ An implicit A-stable LMM cannot be more than 2<sup>nd</sup> order accurate (so best is BDF2 !)