Numerical Solutions to PDEs

Lecture Notes #8

— Stability for Multistep Schemes —

Schur and von Neumann Polynomials

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Spring 2018

Outline

1. Recap
   - In a previous episode of Math 693b...
2. Stability
   - "Proof" by Picture...
   - Beyond "Proof by Picture" — Building a Theoretical Toolbox
3. Schur and von Neumann Polynomials
   - Definitions and Theorems
   - Examples: Revisited with Theoretical Toolbox in Hand...
   - Algorithm for von Neumann / Schur Polynomials

Previously...

We looked at stability for multistep schemes. — First, we did a complete analysis of the stability picture for the leapfrog scheme,

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} + a\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0$$

in which we found bounds for the roots of

$$g(\theta)^2 + \Big[2ia\lambda\sin(\theta)\Big]g(\theta) - 1 = 0$$

so that $|g_\pm(\theta)| \le 1$ for simple roots and $|g_\pm(\theta)| < 1$ for multiple roots.

The analysis for general multi-step scheme has the same "flavor," but we postponed the development of a unified framework for that analysis until today.

Example: Unnamed Scheme From Last Time

Last time, we boldly stated that the scheme

$$\frac{3v_m^{n+1} - 4v_m^n + v_m^{n-1}}{2k} + a\frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{2h} = f_m^{n+1}$$

with amplification polynomial

$$\Phi(g,\theta) = \left[\frac{3 + 2ia\lambda\sin(\theta)}{2}\right] g^2 - 2g + \frac{1}{2}$$

is unconditionally stable, and order-(2,2) accurate.

Whereas pictures are not proof, the plots of the roots for various values of $a\lambda$ and $\theta \in [-\pi, \pi]$ shown on slide 7 seem to indicate that the stability is indeed unconditional.

Example: Unnamed Scheme From Last Time

Sure, we can take the amplification polynomial

$$\Phi(g,\theta) = \underbrace{\left[\frac{3+2ia\lambda\sin(\theta)}{2}\right]}_{a} g^2 \underbrace{-2}_{b} g + \underbrace{\frac{1}{2}}_{c} = 0$$

and formally apply the quadratic formula

$$g_\pm(\theta) = \frac{-b \pm \sqrt{b^2-4ac}}{2a} = \frac{4 \pm \sqrt{2 - 4\left[\frac{3+2ia\lambda\sin(\theta)}{2}\right]\frac{1}{2}}}{2\left[\frac{3+2ia\lambda\sin(\theta)}{2}\right]}$$

$$\rightsquigarrow g_\pm(\theta) = \frac{2 \pm \sqrt{1-2ia\lambda\sin(\theta)}}{3+2ia\lambda\sin(\theta)}$$

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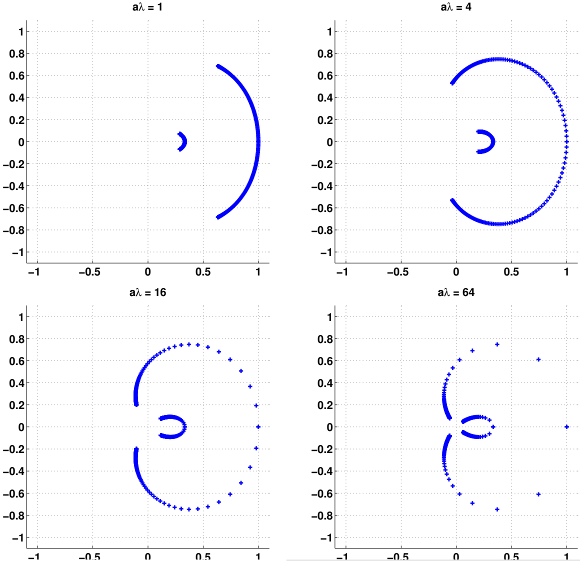
Example: Unnamed Scheme From Last Time

$$g_{\pm}(\theta) = \frac{2 \pm \sqrt{1 - 2ia\lambda \sin(\theta)}}{3 + 2ia\lambda \sin(\theta)}$$

$$\rightsquigarrow g_{\pm}(\theta) = \frac{\left(2 \pm \sqrt{1 - 2ia\lambda \sin(\theta)}\right)(3 - 2ia\lambda \sin(\theta))}{9 + 4(a\lambda)^2 \sin^2(\theta)}$$

Next, define an appropriate branch for the square-root in the complex plane; chase down the various cases... and there it is?!

Example: Unnamed Scheme From Last Time



Example #2: Another Second-Order Accurate Scheme

The second order accurate scheme

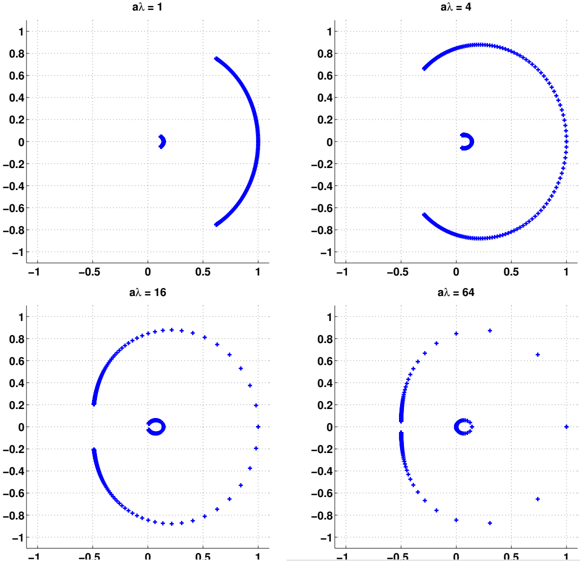
$$\frac{7v_m^{n+1} - 8v_m^n + v_m^{n-1}}{6k} + a\delta_0 \left[\frac{2v_m^{n+1} + v_m^n}{3}\right] = f_m^{n+2/3}$$

has the amplification polynomial

$$\Phi(g) = \left[7 + 4i\beta\right] g^2 - \left[8 - 2i\beta\right] g + 1$$

where $\beta = a\lambda \sin(\theta)$. Also seems to have pretty decent stability properties (see next slide).

Example #2: Root Plots



Example #3: An Order-(3,4) Accurate Scheme

The (3,4)-order accurate scheme

$$\frac{23v_m^{n+1} - 21v_m^n - 3v_m^{n-1} + v_m^{n-2}}{24k} + \left[1 + \frac{h^2}{6}\delta^2\right]^{-1} \cdot$$
$$\left[a\delta_0\left(\frac{v_m^{n+1} + v_m^n}{2}\right) + \frac{k^2a^2}{8}\delta^2\left(\frac{v_m^{n+1} - v_m^n}{k}\right)\right] = f_m^{n+1/2},$$

has the amplification polynomial

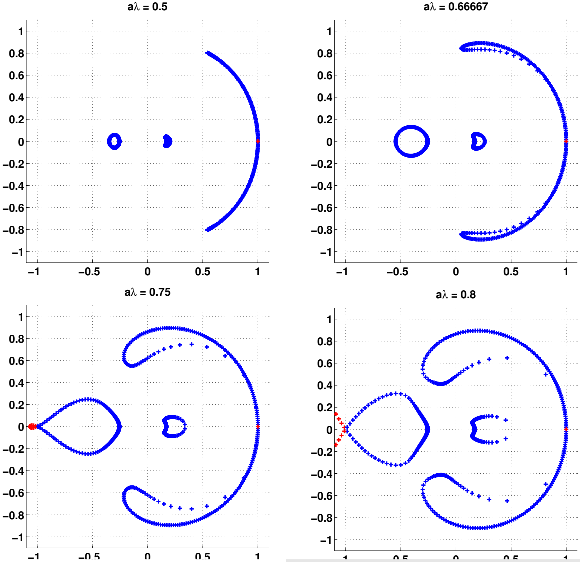
$$\Phi(g) = \Big[23 - 12\alpha + 12i\beta\Big]g^3 - \Big[21 - 12\alpha - 12i\beta\Big]g^2 - 3g + 1,$$

where

$$\alpha = \frac{a^2\lambda^2\sin^2\left(\frac{\theta}{2}\right)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)}, \quad \beta = \frac{a\lambda\sin(\theta)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)}.$$

Does not seem to be unconditionally stable...

Example #3: Root Plots



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Example #4: An Order-(4,4) Accurate Scheme

The (4,4)-order accurate scheme

$$\frac{v_m^{n+2} - v_m^{n-2}}{4k} + a\left[1 + \frac{h^2}{6}\right]^{-1} \delta_0 \left(\frac{2v_m^{n+1} - v_m^n + 2_m^{n-1}}{3}\right) = \frac{2f_m^{n+1} - f_m^n + 2f_m^{n-1}}{3},$$

has the amplification polynomial

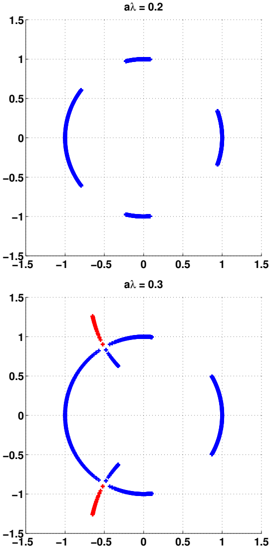
$$\Phi(g) = g^4 + \frac{4}{3} i\beta\left(2g^3 - g^2 + 2g\right) - 1,$$

where

$$\beta = \frac{a\lambda \sin\left(\theta\right)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)}.$$

Does not seem to be unconditionally stable...

Example #4: Root Plots



Moving Beyond "Proof By Picture"

Looking at the expressions and corresponding figures in the previous examples, it is quite clear that the analysis, *i.e.* the determination and bounding of the roots of these polynomials is quite a task.

The good news is that there is a well-developed theory and an algorithm for checking whether the roots of these polynomials satisfy the stability conditions: —

Theorem (Stability of Multistep Schemes)

If the amplification polynomial $\Phi(g, \theta)$ is explicitly independent of h and k, then the necessary and sufficient condition for the finite difference scheme to be stable is that all roots, $g_\nu(\theta)$, satisfy the following conditions:

(a) $|g_\nu(\theta)| \leq 1$, *and*

(b) *if* $|g_\nu(\theta)| = 1$, *then* $g_\nu(\theta)$ *must be a simple root.*

Building the Toolbox — Definitions, 1 of 2

Let $\varphi_d(z) = a_d z^d + \cdots + a_0 = \sum_{\ell=0}^{d} a_\ell z^\ell$ be a polynomial of degree d. If $a_d \neq 0$, then φ is of exact degree d.

Definition (Schur Polynomial)

The polynomial φ is a Schur polynomial if all its roots, r_ν, satisfy $|r_\nu| < 1$.

Definition (von Neumann Polynomial)

The polynomial φ is a von Neumann polynomial if all its roots, r_ν, satisfy $|r_\nu| \leq 1$.

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Building the Toolbox — Definitions, 2 of 2

Let $\varphi_d(z) = a_d z^d + \cdots + a_0 = \sum_{\ell=0}^{d} a_\ell z^\ell$ be a polynomial of degree d. If $a_d \neq 0$, then φ is of exact degree d.

Definition (Simple von Neumann Polynomial)

The polynomial φ is a simple von Neumann polynomial if φ is a von Neumann polynomial, and its roots on the unit circle are simple roots.

Definition (Conservative Polynomial)

The polynomial φ is a conservative polynomial if all its roots lie on the unit circle, *i.e.* $|r_\nu| = 1$.

Building the Toolbox — The Polynomial $\varphi^*(z)$

For a polynomial of exact degree d, we define the polynomial

$$\varphi^*(z) = \sum_{\ell=0}^{d} \overline{a}_{d-\ell} z^{\ell} \equiv \overline{\varphi(1/\overline{z})} z^d,$$

where $\overline{z}$ is the complex conjugate of z.

We recursively define the polynomial φ_{d-1} of exact degree $d-1$ by

$$\varphi_{d-1}(z) = \frac{\varphi_d^*(0)\varphi_d(z) - \varphi_d(0)\varphi_d^*(z)}{z} \equiv \frac{\overline{a}_d \varphi_d(z) - a_0 \varphi_d^*(z)}{z}.$$

We are now ready to state theorems which provide tests for Schur and simple von Neumann polynomials.

Building the Toolbox — Polynomial Tests

Theorem (Schur Polynomial Test)

φ_d is a Schur polynomial of exact degree d if and only if φ_{d-1} is a Schur polynomial of exact degree $d-1$ and $|\varphi_d(0)| < |\varphi_d^*(0)|$.

Theorem (Simple von Neumann Polynomial Test)

φ_d is a simple von Neumann polynomial if and only if either

(a) *$|\varphi_d(0)| < |\varphi_d^*(0)|$ and φ_{d-1} is a simple von Neumann polynomial,* **or**

(b) *φ_{d-1} is identically zero and φ_d' is a Schur polynomial.*

The (somewhat lengthy) proofs, which depend on **Rouché's theorem** (complex analysis) are in Strikwerda pp. 110−114.

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Building the Toolbox — 3 More Theorems

Theorem (von Neumann Polynomial Test)

φ_d *is a von Neumann polynomial of degree* d, *if and only if either*

(a) $|\varphi_d(0)| < |\varphi_d^*(0)|$ *and* φ_{d-1} *is a von Neumann polynomial of degree* $d-1$, **or**

(b) φ_{d-1} *is identically zero and* φ_d' *is a von Neumann polynomial.*

Theorem (Conservative Polynomial Test)

φ_d *is a conservative polynomial if and only if* φ_{d-1} *is identically zero and* φ_d' *is a von Neumann polynomial.*

Theorem (Simple Conservative Polynomial Test)

φ_d *is a simple conservative polynomial if and only if* φ_{d-1} *is identically zero and* φ_d' *is a Schur polynomial.*

Example #1: Revisited

The scheme had the amplification polynomial

$$\varphi_2(z) = \left[\frac{3 + 2ia\lambda\sin(\theta)}{2}\right] z^2 - 2z + \frac{1}{2}.$$

It is stable exactly when $\varphi_2(z)$ is a simple von Neumann polynomial. We make repeated use of the simple-von-Neumann-polynomial-test in order to check stability of the scheme.

We first test $|\boldsymbol{\varphi_2(0)}|^2 = \frac{\mathbf{1}}{\mathbf{4}} < \frac{\mathbf{1}}{\mathbf{4}}\left(\mathbf{3^2} + \mathbf{4a^2}\lambda^2\sin^2(\theta)\right) = |\boldsymbol{\varphi_2^*(0)}|^2$, then define, with $(c + di)$ being the coefficient in front of z^2 in $\varphi_2(z)$:

$$\begin{aligned}\varphi_1(z) &= \frac{1}{z}\left[(c - di)\left((c + di)z^2 - 2z + \frac{1}{2}\right) - \frac{1}{2}\left((c - di) - 2z + \frac{1}{2}z^2\right)\right] \\ &= \left(d^2 + c^2 - \frac{1}{4}\right) z + (1 - 2\,c + 2\,id)\end{aligned}$$

Example #1: Revisited

Now, $\varphi_1(z)$ is a simple von Neumann polynomial as long as

$$\left(d^2 + c^2 - \frac{1}{4}\right)^2 \geq (1-2c)^2 + 4d^2 = 1 + 4c^2 + 4d^2 - 4c$$

where $c = \frac{3}{2}$, and $d = a\lambda \sin(\theta)$.

Plugging in we must have

$$a^4\lambda^4 \sin^4(\theta) + 4\,a^2\lambda^2 \sin^2(\theta) + 4 \geq 4\,a^2\lambda^2 \sin^2(\theta) + 4$$

Which holds strictly for $\sin(\theta) \neq 0$, and with equality when $\sin(\theta) = 0$.

Conclusion: The scheme is unconditionally stable.

Example #2: Revisited

The scheme had the amplification polynomial

$$\varphi_2(z) = \left[7 + 4i\beta\right] z^2 - \left[8 - 2i\beta\right] z + 1$$

it is stable exactly when $\varphi_2(z)$ is a simple von Neumann polynomial. We make repeated use of the simple-von-Neumann-polynomial-test in order to check stability of the scheme.

With $\beta = a\lambda\sin(\theta)$, we first test $|\varphi_2^*(\mathbf{0})| = |\mathbf{7} - \mathbf{4i}\beta| > \mathbf{1} = |\varphi_\mathbf{2}(\mathbf{0})|$, then define

$$\begin{aligned}\varphi_1(z) = \frac{1}{z}\Big[&(7-4i\beta)\left(\left[7+4i\beta\right]z^2 - \left[8-2i\beta\right]z + 1\right) \\ &- 1\left(\left[7-4i\beta\right] - \left[8+2i\beta\right]z + z^2\right)\Big] \\ &= 4\left(\left(12+4\beta^2\right)z + \left(\left(2\beta^2-12\right) + 12\,i\beta\right)\right).\end{aligned}$$

Example #2: Revisited

$$\varphi_1(z) = 4\left((12+4\beta^2)\,z + ((2\,\beta^2 - 12) + 12\,i\beta)\right)$$

is a simple von Neumann polynomial if and only if

$$|\varphi_1(0)|^2 = |(2\,\beta^2 - 12) + 12\,i\beta|^2 = (12 - 2\beta^2)^2 + 12^2\beta^2$$
$$= \mathbf{144} + \mathbf{96}\beta^{\mathbf{2}} + \mathbf{4}\beta^{\mathbf{4}} \leq |\varphi_1^*(0)|^2 = (12{+}4\beta^2)^2 = \mathbf{144} + \mathbf{96}\,\beta^{\mathbf{2}} + \mathbf{16}\,\beta^{\mathbf{4}}$$

The inequality holds strictly as long as $\beta \neq 0$, in which case we get equality.

Note: Since $\varphi_1(z)$ only has **one** root, it is sufficient to bound that root by "≤ 1" in order for $\varphi_1(z)$ to be a simple von Neumann polynomial.

Conclusion: The scheme is unconditionally stable.

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Example #3: Revisited

In this case the amplification polynomial is given by

$$\varphi_3(z) = \Big[23 - 12\alpha + 12i\beta\Big] z^3 - \Big[21 - 12\alpha - 12i\beta\Big] z^2 - 3z + 1$$

where

$$\alpha = \frac{a^2\lambda^2 \sin^2\left(\frac{\theta}{2}\right)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)} \in [\mathbf{0},\ \mathbf{3a^2}\lambda^2], \quad \beta = \frac{a\lambda\sin(\theta)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)} \in [-\mathbf{a}\lambda\sqrt{\mathbf{3}},\ \mathbf{a}\lambda\sqrt{\mathbf{3}}].$$

The first check $|\varphi_3(0)| < |\varphi_3^*(0)|$ can be expressed as $|\varphi_3^*(0)|^2 - |\varphi_3(z)|^2 > 0$, and we get

$$|\varphi_3^*(0)|^2 - |\varphi_3(0)|^2 = 24(2-\alpha)(11-6\alpha) + 12^2\beta^2$$

we see that we must require $\mathbf{0} \leq \alpha \leq \frac{\mathbf{11}}{\mathbf{6}}$ for stability.

Example #3: Revisited

The polynomial $\varphi_2(z)$ is (after division by the common factor 24)

$$\varphi_2(z) = \Big[(11-6\alpha)(2-\alpha)+6\beta^2)\Big] z^2 - 2\Big[(2-\alpha)(5-3\alpha)-3\beta^2-(11-6\alpha)i\beta\Big] z - (2-\alpha-2i\beta),$$

and

$$|\varphi_2^*(0)|^2 - |\varphi_2(0)|^2 = 4(5-3\alpha)\Big[3(2-\alpha)^3+\beta^2(13-6\alpha)\Big] + 36\beta^4.$$

This now requires that $\mathbf{0} \leq \alpha \leq \mathbf{\frac{5}{3}} < \frac{11}{6}$ for stability.

Example #3: Revisited

Finally, the polynomial $\varphi_1(z)$ is

$$\varphi_1(z) = \left[120-252\alpha+198\alpha^2-69\alpha^3+9\alpha^4(18\alpha^2-69\alpha+65)\beta^2+9\beta^4\right] z$$
$$+9\beta^4+6(5-3\alpha)i\beta^3+(3\alpha-5)\beta^2-\left(18\alpha^3+102\alpha^2+192\alpha-120\right)i\beta$$
$$-9\alpha^4+69\alpha^3-198\alpha^2+252\alpha-120$$

The root-condition $|\varphi_1^*(0)|^2 - |\varphi_1(0)|^2 > 0$ translates to

$$12\beta^4(5-3\alpha)\left[6\beta^2+(11-6\alpha)(2-\alpha)\right] > 0$$

This holds in the range $\mathbf{0} \leq \alpha \leq \mathbf{\frac{5}{3}}$; our strictest bound on α.

Example #3: Revisited

We now have that

$$\alpha = |a\lambda|^2 \underbrace{\frac{\sin^2\left(\frac{\theta}{2}\right)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)}}_{\in[0,3]} \leq \frac{5}{3}$$

and it follows that the scheme is stable if and only if

$$|\mathbf{a}\lambda| \leq \frac{\sqrt{\mathbf{5}}}{\mathbf{3}} \approx 0.7454\ldots$$

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Example #4: Revisited

$$\varphi_4(z) = z^4 + \frac{4}{3} i\beta \left(2z^3 - z^2 + 2z\right) - 1, \quad \beta = \frac{a\lambda \sin(\theta)}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)} \in [-a\lambda\sqrt{3}, a\lambda\sqrt{3}].$$

Here, $|\varphi_4(0)| = |\varphi_4^*(0)| = 1$. But $\varphi_3(z) \equiv 0$, hence there is still hope, for $\varphi_4(z)$ being a simple von Neumann polynomial. We must test whether $\psi_3(z) = \frac{3}{4}\varphi_4'(z) = 3z^3 + i\beta(6z^2 - 2z + 2)$ is a **Schur** polynomial.

$|\psi_3^*(0)| - |\psi_3(0)| = 3 - |2\beta| > 0$, as long as $|\beta| < \mathbf{\frac{3}{2}}$.

We form

$$\psi_2(z) = (9 - 4\beta^2)z^2 + (4\beta^2 + 18i\beta)z - 12\beta^2 - 6i\beta$$

$|\psi_2^*(0)|^2 - |\psi_2(0)|^2 > 0$ if and only if $(9 - 4\beta^2)^2 > (12\beta^2)^2 + (6\beta)^2$, which gives $\beta^{\mathbf{2}} < \mathbf{\frac{9}{64}\left[\sqrt{41} - 3\right]} < \frac{9}{4}$.

Example #4: Revisited

Next, we form

$$\psi_1(z) = \left(81-108\beta^2-128\beta^4\right)z+\left(\left[32\beta^4 + 144\beta^2\right]-i \left[264\beta^3 - 162\beta\right] \right)$$

The one root is inside the unit circle only if

$$\left(81-108\beta^2-128\beta^4\right)^2-\left(\left[32\beta^4 + 144\beta^2\right]^2 + \left[264\beta^3 - 162\beta\right]^2\right) \geq 0.$$

This expression can be factored as

$$3\left(9 - 4\beta^2\right)\left(3 - 16\beta^2\right)\left(\underbrace{\beta^2(80\beta^2 - 72) + 81}_{>0}\right) \geq 0.$$

Hence, $\psi_1(z)$ is a Schur polynomial for

$$\beta^{\mathbf{2}} < \frac{\mathbf{3}}{\mathbf{16}} < \frac{9}{64}\left[\sqrt{41} - 3\right].$$

Example #4: Revisited

Hence, our final stability condition is

$$|\beta| = \frac{|a\lambda \sin(\theta)|}{1 - \frac{2}{3}\sin^2\left(\frac{\theta}{2}\right)} < \frac{\sqrt{3}}{4}.$$

The maximum occurs when $\cos(\theta) = -1/2$, and the scheme is stable when $|\mathbf{a}\lambda| < \mathbf{\frac{1}{4}}$.

Note that even though the scheme is implicit, it is **not** unconditionally stable.

Algorithm for von Neumann / Schur Polynomials

Algorithm

Start with $\varphi_d(z)$ of exact degree d, and set $\mathrm{NeumannOrder} = 0$.

while ($d > 0$**) do**

1. Construct $\varphi_d^*(z)$
2. Define $c_d = |\varphi_d^*(0)|^2 - |\varphi_d(0)|^2$. **(*)**
3. Construct the polynomial $\psi(z) = \frac{1}{z}(\varphi_d^*(0)\varphi_d(z) - \varphi_d(0)\varphi_d^*(z))$.

4.1. If $\psi(z) \equiv 0$, then increase $\mathrm{NeumannOrder}$ by 1, and set $\varphi_{d-1}(z) := \varphi_d'(z)$.

4.2. Otherwise, if the coefficient of degree $d-1$ in $\psi(z)$ is 0, then the polynomial is **not** a von Neumann polynomial of any order, **terminate algorithm**.

4.3. Otherwise, set $\varphi_{d-1}(z) := \psi(z)$.

end-while (decrease d **by 1)**

(*) Enforce appropriate conditions on c_d.

Comments on the Algorithm

At the end of the algorithm, if the polynomial has not been rejected by 4.2 —

- The polynomial is a von Neumann polynomial of the resulting order $(\mathrm{NeumannOrder})$ provided that all the parameters c_d satisfy the appropriate inequalities. — These inequalities provide the stability conditions.
- For first-order PDEs, the amplification polynomial must be a von Neumann polynomial of order 1 for the scheme to be stable.
- For second-order PDEs, the amplification polynomial must be a von Neumann polynomial of order 2 for the scheme to be stable.
- Schur polynomials are von Neumann polynomials of order 0.

This analysis can be automated using a symbolic toolbox. — Again, we have reduced something complicated to a deterministic "recipe."