Absorbing Boundary Conditions for Wave Problems

A Review of Current Practices and Future Perspectives

Part I: Theoretical Aspects in Current Practices

Bruno Welfert

School of Mathematical & Statistical Sciences
Arizona State University

Computational & Applied Mathematics Proseminar
02-18-2011

In this talk...

- The ABC of ABCs
  1. a review of past and current techniques
  2. Conceptualized ideas in terms of operators... very "mathematical"

In this talk...

- The ABC of ABCs
  1. a review of past and current techniques
  2. Conceptualized ideas in terms of operators... very "mathematical"
- Goals
  1. understand basic approaches in use and their connections
  2. set up a framework for future improvements

Model problem

$$\boxed{-u'' + au = f(t) \text{ for } t > 0, \quad \text{with } \begin{cases} u(0) = 0 \\ \text{BC at } t = \infty \end{cases}}$$

- $t =$ "time" but can represent spatial coordinate
- $a =$ differential operator
  - $a = \Delta < 0$: hyperbolic problem (wave propagation/scattering)
  - $a = -\Delta > 0$: elliptic problem
- f has support in $(0, 1)$
- BC at $t = \infty$

$$|u(\infty)| < \infty \quad \text{or} \quad (u' + \sqrt{a}\, u)(\infty) = 0$$

  (Sommerfeld)
- $\sqrt{a} =$ principal square root of a ($\sqrt{a} := i\sqrt{-a}$ if $a < 0$)

Laplace transform of solution

(shifted) Laplace transform

$$U(s) = \int_1^{+\infty} u(t) e^{-s(t-1)}\, dt = \int_0^{+\infty} f(t+1) e^{-st}\, dt$$

for

$$s \in \mathcal{D} = \begin{cases} \{s \in \mathcal{C}, \Re(s) > 0\} & \text{if } a > 0, \\ \{s \in \mathcal{C}, \Re(s) \geq 0\} & \text{if } a < 0. \end{cases}$$

- $U(s)$ satisfies

$$(s^2 - a)U(s) = su(1) + u'(1)$$

$$\Leftrightarrow \quad U(s) = \frac{1}{2}\left(u(1) + \frac{u'(1)}{\sqrt{a}}\right)\frac{1}{s-\sqrt{a}} + \frac{1}{2}\left(u(1) - \frac{u'(1)}{\sqrt{a}}\right)\frac{1}{s+\sqrt{a}}$$

- For $t \geq 1$

$$u(t) = \frac{1}{2}\left(u(1) + \frac{u'(1)}{\sqrt{a}}\right) e^{\sqrt{a}(t-1)} + \frac{1}{2}\left(u(1) - \frac{u'(1)}{\sqrt{a}}\right) e^{-\sqrt{a}(t-1)}$$

- BC at $t = \infty$ reduces to transparent BC

$$\boxed{u'(1) + \sqrt{a}\, u(1) = 0}$$

Truncated problem

$$\boxed{\begin{cases} -u'' + au = f(t), \quad 0 < t < 1 \\ u(0) = 0, \\ u'(1) + \sqrt{a}\, u(1) = 0. \end{cases}}$$

$-\sqrt{a} =$ Dirichlet-to-Neumann operator DtN.

BUT In general $\sqrt{a}$ global (pseudo-differential) if a local (differential)

$$a = 1 + \partial_{xx} \Rightarrow \sqrt{a} = \sum_{n \geq 0} \binom{1/2}{n} (\partial_{xx})^n = \sum_{n \geq 0} \binom{1/2}{n} \partial_{x^{2n}}$$

However typically $a = a_1 + a_2$ $\begin{cases} a_1 = 1 \\ a_2 = \partial_{xx} \end{cases} \Rightarrow \begin{cases} \sqrt{a_1} = 1 \\ \sqrt{a_2} = \partial_x \end{cases}$

$\Rightarrow$ $\boxed{\text{approximate } \sqrt{a} \text{ in terms of } \sqrt{a_1} \text{ and } \sqrt{a_2}}$

Local ABCs

$$\boxed{u'(1) + \alpha u(1) = 0}$$

- $\alpha \approx \sqrt{a}$
- Solution of problem with ABC for $t > 1$ is

$$\begin{aligned} u(t) &= \frac{1}{2}\left(1 - \frac{\alpha}{\sqrt{a}}\right) u(1) e^{\sqrt{a}(t-1)} + \frac{1}{2}\left(1 + \frac{\alpha}{\sqrt{a}}\right) u(1) e^{-\sqrt{a}(t-1)} \\ &:= u_R(t) + u_T(t) \end{aligned}$$

  the sum of reflected and transmitted components.
- Reflection coefficient

$$r := \frac{u_R(1)}{u_T(1)} = \frac{\sqrt{a} - \alpha}{\sqrt{a} + \alpha} \qquad \begin{array}{lcll} r = -1 & \leftrightarrow & \alpha = \infty & u(1) = 0, \text{ reflection} \\ r = 0 & \leftrightarrow & \alpha = \sqrt{a} & \text{transparent} \\ r = 1 & \leftrightarrow & \alpha = 0 & u'(1) = 0, \text{ transmission} \end{array}$$

- Dual ABC

$$\boxed{\text{primal ABC}} \quad u'(1) + \alpha u(1) = 0 \quad \text{vs} \quad \boxed{\text{dual ABC}} \quad \alpha u'(1) + a u(1) = 0$$

PML analogy

- The solution $u(t)$ vanishes for

$$\Delta t := t - 1 = \begin{cases} -\ln(-r)/(2\sqrt{a}) & \text{if } 0 < a < \alpha^2, \\ \arctan(\sqrt{-a}/\alpha)/\sqrt{-a} & \text{if } a < 0 \text{ and } \alpha \text{ real.} \end{cases}$$

- The model problem can then be solved in $[0, 1 + \Delta t]$ with Dirichlet BC

$$u(1 + \Delta t) = 0$$

$[1, 1 + \Delta t]$ = PML, Bérenger 1994

Rational approximation of $\sqrt{a}$

Rewrite

$$\sqrt{a} = \sqrt{a_1} \Big/ \sqrt{1 - \frac{a_2}{a}}$$

Approximation

$$\sqrt{1-z} \approx \frac{p(z)}{q(z)} \quad \Rightarrow \quad \alpha = \sqrt{a_1}\,\frac{q(a_2/a)}{p(a_2/a)}$$

- Enquist & Majda (1977): Taylor at $z = 0$
- Trefethen & Halpern (1986): Padé at $z = 0$
- Halpern & Trefethen (1988): other z's (Chebyshev, Neumann points), least-squares (L^2), Chebyshev (L^∞), and Chebyshev-Padé
- Example

$$\begin{cases} p(z) = p_0 + p_1 z \\ q(z) = 1 \end{cases} \quad \Rightarrow \quad \begin{cases} (p_0 a + p_1 a_2)u'(1) + a\sqrt{a_1}\,u(1) = 0 & \text{(primal)} \\ \sqrt{a_1}\,u'(1) + (p_0 a + p_2 a_2)u(1) = 0 & \text{(dual)} \end{cases}$$

ABCs based on characteristics

$$\begin{cases} v := u' + \sqrt{a_1}u \\ w := \sqrt{a_2}u \end{cases} \quad \Rightarrow \quad \begin{bmatrix} v' \\ w' \end{bmatrix} = \begin{bmatrix} \sqrt{a_1} & \sqrt{a_2} \\ \sqrt{a_2} & -\sqrt{a_1} \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} := A \begin{bmatrix} v \\ w \end{bmatrix},$$

- Giles (1990)
  characteristic direction associated to outgoing information is given by left eigenvector
  $$\begin{bmatrix} \sqrt{a_2}/s \\ -1 + \sqrt{1 - a_2/s^2} \end{bmatrix}$$
  of A^{-1} associated to eigenvalue $-1/s = -1/\sqrt{a}$
- Expand in Taylor series in terms of powers of $\sqrt{a_2}/s \Rightarrow p(z) + q(z) = 2$.

$$p(z) = \begin{cases} 1 - z/4 & \text{first-order} \\ 1 - z/4 - z^2/8 & \text{second-order} \end{cases}$$

Additive, partial fractions form

- Lindman (1975)

$$\frac{1}{\sqrt{1-z}} \approx \frac{q(z)}{p(z)} := 1 + z \sum_{n=1}^{N} \frac{\alpha_n}{1-\beta_n z}.$$

- Coefficients α_n and β_n by minimizing $L^2_{(1-z)^{1/4}}$-norm of reflection coefficient r
- Yields ABC

$$u'(1) + \sqrt{a_1}u(1) = -\sum_{n=0}^{N} \alpha_n u_n(1),$$

with

$$(a - \beta_n a_2)u_n(1) = a_2\sqrt{a_1}u(1), \quad n = 0, \dots, N.$$

  - differential system posed on boundary $t = 1$
  - $au_n(1) \to u_n''(1)$ requires solution in an interval $[1-\delta, 1]$ large enough to numerically approximate u_n'', which is not as efficient.
  - Renaut (1992): detailed analysis of Lindman's approach and dual ABC starting from an approximation of $\sqrt{1-z}$ instead.

Multiplicative, factored form

- Higdon (1986, 1987)

$$\left[\left(\prod_{n=0}^{N}(\sqrt{a_1} + c_n\partial_t)\right) u\right](1) = 0$$

- $c_n = \cos\theta_n$ and $0 \leq \theta_0 < \cdots < \theta_N \leq \pi/2$
- Equivalent to interpolation conditions

$$\sqrt{1 - z_n} = \frac{p(z_n)}{q(z_n)}, \quad z_n := \sin^2\theta_n$$

- Reflection coefficient associated to angle θ

$$r(c) = \prod_{n=0}^{N} \frac{c - c_n}{c + c_n}, \quad c := \cos\theta$$

- Transparent for waves with angles of incidence θ_n
- Reduces to $(N+1, N)$-Padé approximation of $\sqrt{1-z}$ at $z = 0$ for $\theta_n = 0$
- Equivalence to Lindman's approach: each choice of p, q of total degree $N+1$ corresponds to a choice of (possibly complex) angles θ_n

Refinements on Higdon's approach

- Reformulate as system

$$\phi_0 = u, \quad \left(\sqrt{a_1} + c_n \partial_t\right) \phi_n = \phi_{n+1}, \quad \phi_{N+1}(1) = 0,$$

  - Collino (1997), Grote & Keller (1996), Hagstrom & Hariharan (1998), Givoli & Neta (2003)
  - avoids high-order differential operators

Refinements on Higdon's approach

- Reformulate as system

$$\phi_0 = u, \quad \left(\sqrt{a_1} + c_n \partial_t\right) \phi_n = \phi_{n+1}, \quad \phi_{N+1}(1) = 0,$$

  - Collino (1997), Grote & Keller (1996), Hagstrom & Hariharan (1998), Givoli & Neta (2003)
  - avoids high-order differential operators
- Balanced formulation

$$\phi_0 = u, \quad \left(\sqrt{a_1} + c_n \partial_t\right) \phi_n = \left(\sqrt{a_1} - c_n \partial_t\right) \phi_{n+1}, \quad \phi_{N+1}(1) = 0$$

  - Hagstrom & Warburton (2004) , Bécache & Givoli & Hagstrom (2010)
  - better accuracy in repeated differentiation
  - $\phi_n \to \phi_{n+1}$ is now associated to a contribution $r = \frac{c-c_n}{c+c_n} / \left(\frac{c-(-c_n)}{c+(-c_n)}\right) = \left(\frac{c-c_n}{c+c_n}\right)^2$
  - Recurrence relation on boundary $t = 1$

$$a_1 \left(\frac{\phi_{n+1} - \phi_n}{c_n} + \frac{\phi_n - \phi_{n-1}}{c_{n-1}} \right) = a \Big(c_n(\phi_{n+1} + \phi_n) - c_{n-1}(\phi_n + \phi_{n-1}) \Big)$$

  - $\phi_n \to 0 \Rightarrow$ error estimate for choice of N
  - Hagstrom et al. (2008): c_n = Gauss-Radau points (non-dispersive pbs), complex (Klein-Gordon)

Multiplicative, continued fraction form

- ABS of the form $u'(1) + \alpha u(1) = 0$ with

$$\alpha = \alpha_N := \beta_N a / \sqrt{a_1}$$

and

$$\beta_0 = c_0, \quad \beta_n = c_n - \frac{c_n^2 - (1 - a_2/a)}{c_n + \beta_{n-1}}, \quad n = 1, \ldots, N.$$

  - Engquist and Majda (1979) ($c_n = 1$), Guddati and Tassoulas (2000)
  - Savadatti and Guddati (2010): PML version
  - Welfert (2010): interpret as successive projections onto primal/dual forms

$$(\sqrt{a_1} + c_n \partial_t)(u' + \alpha_{n-1} u) = (c_n + \beta_{n-1})(\alpha_n u' + au)$$

  - Some equivalence to factored form

Pole condition

Recall

$$U(s) = \frac{su(1) + u'(1)}{s^2 - a}$$
$$= \frac{1}{2}\left(u(1) + \frac{u'(1)}{\sqrt{a}}\right)\frac{1}{s - \sqrt{a}} + \frac{1}{2}\left(u(1) - \frac{u'(1)}{\sqrt{a}}\right)\frac{1}{s + \sqrt{a}}$$

Then

$$\text{TBC } u'(1) + \sqrt{a}\, u(1) = 0 \quad \Leftrightarrow \quad s = -\sqrt{a} \text{ not a pole of } U(s)$$

$s = \sqrt{a}$ known as dispersion relation

ABC based on pole condition

- Expand

$$U(s) = \sum_{n\geq 0} a_n (s-\alpha)^n, \quad \alpha \approx \sqrt{a}$$

Assume α and a commute

$$a_n = \frac{1}{2}\left(u(1) + \frac{u'(1)}{\sqrt{a}}\right)\frac{(-1)^n}{(\alpha-\sqrt{a})^{n+1}} + \frac{1}{2}\left(u(1) - \frac{u'(1)}{\sqrt{a}}\right)\frac{(-1)^n}{(\alpha+\sqrt{a})^{n+1}}$$

$$\alpha \approx \sqrt{a} \quad \Rightarrow \quad \text{as } n \to \infty \quad \begin{cases} \text{second term } \to 0 \\ \text{first term dominates unless TBC holds} \end{cases}$$

- Set $\boxed{a_N = 0}$
  - Hohage, Schmidt & Zschiedrich (2003,2008), Ruprecht et al. (2008)
  - Equivalent to

$$u'(1) + \alpha_N u(1) = 0, \quad \alpha_N := \frac{1+(-r)^{N+1}}{1-(-r)^{N+1}}\sqrt{a}$$

  - Reflection coefficient is $-(-r)^{N+1} \to 0$
  - Can be viewed as order acceleration strategy for any classical ABC

ABC based on pole condition: practical implementation

- Sustitute expansion into $(s^2 - a)U(s) = su(1) + u'(1)$ and compare powers

$$\begin{cases} a_{-1} := -u(1), \\ (\alpha^2 - a)a_0 = \alpha u(1) + u'(1), \\ (\alpha^2 - a)a_n + 2\alpha a_{n-1} + a_{n-2} = 0 \quad \text{for } n \geq 1. \end{cases}$$

(classical differential system)

- Hohage et al.(2003): use ansatz

$$U(s) = \frac{2\alpha}{s+\alpha} \sum_{n \geq 0} b_n \left(\frac{s-\alpha}{s+\alpha}\right)^n = (1-\sigma) \sum_{n \geq 0} b_n \sigma^n \quad \text{with } \sigma := \frac{s-\alpha}{s+\alpha}$$

(Möbius transform)

  - correct behavior $U(s) \to 0$ for $s \to \infty$
  - leads to symmetric system

$$\begin{cases} (\alpha^2 - a)b_0 = \alpha u(1) + u'(1), \\ (\alpha^2 - a)b_1 + 2(\alpha^2 + a)b_0 = \alpha u(1) - u'(1), \\ (\alpha^2 - a)b_{n+1} + 2(\alpha^2 + a)b_n + (\alpha^2 - a)b_{n-1} = 0 \quad \text{for } n \geq 1. \end{cases}$$

  - $\boxed{\text{Welfert (2010): } b_n = (a - \alpha^2)^n a_{2n} \Rightarrow b_N = 0 \Leftrightarrow a_{2N} = 0}$

ABC based on pole condition:

- Gander and Schädle (2010):
  - continued fraction form

$$\gamma_n := \frac{1}{2}\left(1 - \frac{\alpha_n}{\alpha}\right) \quad \Rightarrow \quad [\gamma_N] = \left[\frac{\gamma_1}{1-\gamma_{N-1}}\right] := \frac{\gamma_1}{1-}[\gamma_{N-1}] = \left(\frac{\gamma_1}{1-}\right)^N [0]$$

  - b_N is $(N+1, N)$-Padé approximation of

$$\sqrt{1+\lambda} = 1/(1/\sqrt{1-(-\lambda)})$$

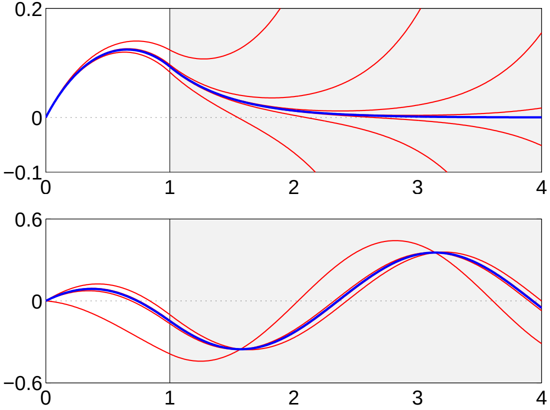
- $\boxed{\text{Welfert (2010): } \alpha_{2N+\delta} \text{ is } (N, N+\delta)\text{-Padé approximant}}$ of

$$\sqrt{a} = \frac{\alpha}{\sqrt{1-(1-\alpha^2)/a}}$$

Pole condition: example

$$-u'' + au = \chi_{[0,1]}, \quad u(0) = 0, \quad u'(1) + \alpha u(1) = 0$$

Solve for increasing N



$a = 4, \alpha = 1$

$a = -4, \alpha = i$