Bendroji metodika, skirta daugiamačių hiperbolinių lygčių nehomogeninėse terpėse skaitinių sprendimo algoritmų analizei

R. Čiegis

Vilniaus Gedimino technikos universitetas
e-mail: rc@vgtu.lt

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Daugelyje Maksvelo elektromagnetinių laukų taikymų tenka spręsti daugiamačius uždavinius nehomogeninėse terpėse.

Nenuostabu, kad jau sukurta daug įvairių skaitinių algoritmų (schemų) jų sprendimui, reguliariai atsiranda nauji algoritmai.

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Kadangi šioje veikloje svarbiais (svarbiausiais) tikslais dažniausiai tampa virtualaus modeliavimo eksperimento atlikimas, technologijų ir prietaisų optimizavimas, tai skaitinių algoritmų teorinis pagrindimas dažniausiai vėluoja.

Šiame seminare supažindinsime su naujausių tyrimų rezultatais. Jų tikslas yra teorinių tyrimų užduotį perkelti į gerokai aukštesnį lygį – sukurti pakankamai bendrą ir universalią metodiką.

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Tada konkrečių schemų analizė tampa šios technikos taikymu. Tenka pripažinti, kad bendrų sąlygų patikrinimas visgi dažniausiai nėra trivialus.

On Construction and Properties of Compact 4th Order Finite-Difference Schemes for the Variable Coefficient Wave Equation

Alexander Zlotnik, Raimondas Čiegis

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We consider the following initial-boundary value problem (IBVP) with the Dirichlet boundary condition for the wave equation in a generalized form

$$\rho(x)\partial_t^2 u(x,t) - (a_1^2\partial_1^2 + \ldots + a_n^2\partial_n^2)u(x,t) = f(x,t) \quad (1)$$
$$\text{in} \quad Q_T = \Omega \times (0,T);$$

$$u|_{\Gamma_T} = g(x,t); \quad u|_{t=0} = u_0(x), \quad \partial_t u|_{t=0} = u_1(x), \quad x \in \Omega. \quad (2)$$

Here $0 < \rho \leq \rho(x)$ in $\bar{\Omega}$, $a_1 > 0, \ldots, a_n > 0$ are constants and $x = (x_1, \ldots, x_n)$, $n \geq 1$.

Also Ω is a bounded domain in $\mathbb{R}^n$, $\partial\Omega$ its boundary and $\Gamma_T = \partial\Omega \times (0,T)$ is the lateral surface of Q_T.

Note that $c(x) = \frac{1}{\sqrt{\rho(x)}}$ is the variable sound speed in the case $a_1 = \ldots = a_n = 1$.

Let H_h be an Euclidean space of functions given on a spatial mesh endowed with an inner product $(\cdot, \cdot)_h$ and the corresponding norm $\| \cdot \|_h$, where h is the parameter related to this mesh.

Let B_h and A_h be linear operators in H_h having the properties $B_h = B_h^* > 0$ and $A_h = A_h^* > 0$.

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As applied to the wave equation (1), B_h is an averaging operator and A_h is an approximation to its elliptic part $-(a_1^2\partial_1^2 + \ldots + a_n^2\partial_n^2)$.

For any operator $C_h = C_h^* > 0$ in H_h, one can define the norm $\|w\|_{C_h} = (C_h w, w)_h^{1/2}$ in H_h generated by it.

We introduce the uniform mesh $\overline{\omega}_{h_t} = \{t_m = mh_t\}_{m=0}^{M}$ on a segment $[0, T]$, with the step $h_t = T/M > 0$ and $M \geq 2$. Let $\omega_{h_t} = \{t_m\}_{m=1}^{M-1}$ be the internal part of $\overline{\omega}_{h_t}$.

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We introduce the mesh averages and difference operators

$$\bar{s}_t y = \frac{\check{y} + y}{2}, \ \ s_t y = \frac{y + \hat{y}}{2}, \ \ \bar{\delta}_t y = \frac{y - \check{y}}{h_t}, \ \ \delta_t y = \frac{\hat{y} - y}{h_t},$$
$$\mathring{\delta}_t y = \frac{\hat{y} - \check{y}}{2h_t}, \ \Lambda_t y = \delta_t \bar{\delta}_t y = \frac{\hat{y} - 2y + \check{y}}{h_t^2}$$

with $y^m = y(t_m)$, $\check{y}^m = y^{m-1}$ and $\hat{y}^m = y^{m+1}$.

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The operator of summation with the variable upper limit

$$I_{h_t}^m y = h_t \sum_{l=1}^{m} y^l \ \text{ for } \ 1 \leq m \leq M, \quad I_{h_t}^0 y = 0.$$

We consider the following symmetric three-level in t method with a weight (parameter) σ for the IBVP (1)-(2) with $g = 0$:

$$B_h(\rho \Lambda_t v) + \sigma h_t^2 A_h \Lambda_t v + A_h v = f \quad \text{in} \quad H_h \quad \text{on} \quad \omega_{h_t}, \tag{3}$$

$$B_h(\rho \delta_t v^0) + \sigma h_t^2 A_h \delta_t v^0 + \frac{1}{2} h_t A_h v^0 = u_1 + \frac{1}{2} h_t f^0 \quad \text{in} \quad H_h, \tag{4}$$

where v: $\overline{\omega}_{h_t} \to H_h$ is the sought function and the functions $v^0, u_1 \in H_h$ and f: $\{t_m\}_{m=0}^{M-1} \to H_h$ are given.

For $\sigma < \frac{1}{4}$, we also assume that A_h and B_h are related by the following inequality

$$\|w\|_{A_h} \le \alpha_h \|w\|_{B_h} \quad \forall w \in H_h \quad \Leftrightarrow \quad A_h \le \alpha_h^2 B_h. \tag{5}$$

Clearly the minimal value of α_h^2 is the maximal eigenvalue of the generalized eigenvalue problem

$$A_h e = \lambda B_h e, \quad e \in H_h, \quad e \neq 0. \tag{6}$$

Prieš pateikiant mūsų gautus rezultatus, priminsiu populiarų tokių schemų šabloną, jį sudarė ir pagrindė A. Samarskis.

Gautuosius bendrus stabilumo rezultatus dažnai labai patogu pritaikyti konkrečių schemų pagrindimui.

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Šablonas yra skirtas parabolinių lygčių aproksimacijai, kai naudojame trijų sluoksnių skirtuminius operatorius.

A. Samarskio schemų šablonas

$$B_h \mathring{\delta}_t y + h_t^2 R_h \Lambda_t y + A_h y = \varphi(t^m), \qquad (7)$$
$$y(0) = u^0, \quad y^1 = v^0.$$

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$$B_h(\rho \Lambda_t v) + \sigma h_t^2 A_h \Lambda_t v + A_h v = f \quad \text{in} \quad H_h \quad \text{on} \quad \omega_{h_t},$$

Theorem

Let the operators A_h and B_h commute, i.e. $A_h B_h = B_h A_h$. Let either $\sigma \geq \frac{1}{4}$ and $\varepsilon_0 = 1$, or

$$\sigma < \tfrac{1}{4}, \quad (\tfrac{1}{4} - \sigma) h_t^2 \alpha_h^2 \leq (1 - \varepsilon_0^2) \underline{\rho} \ \text{ for some } \ 0 < \varepsilon_0 < 1. \tag{8}$$

For the solution to method (3)-(4), the following bounds hold: (1) in the strong energy norm

$$\max_{1 \leq m \leq M} \Big[\| \sqrt{\rho} \bar{\delta}_t v^m \|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \| \bar{\delta}_t v^m \|_{B_h^{-1} A_h}^2 + \| \bar{s}_t v^m \|_{B_h^{-1} A_h}^2 \Big]^{1/2}$$

$$\leq \Big(\| v^0 \|_{B_h^{-1} A_h}^2 + \varepsilon_0^{-2} \| \tfrac{1}{\sqrt{\rho}} B_h^{-1} u_1 \|_h^2 \Big)^{1/2} + 2 \varepsilon_0^{-1} \| \tfrac{1}{\sqrt{\rho}} B_h^{-1} f \|_{L^1_{h_t}(H_h)}, \tag{9}$$

(2) in the weak energy norm

$$\max_{0\le m\le M} \max\Big\{ \Big[\|\sqrt{\rho} v^m\|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \|v^m\|^2_{B_h^{-1}A_h} \Big]^{1/2}, \ \|I^m_{h_t} \bar{s}_t v\|_{B_h^{-1}A_h} \Big\}$$

$$\le \Big[\|\sqrt{\rho} v^0\|_h^2 + (\sigma - \tfrac{1}{4}) h_t^2 \|v^0\|^2_{B_h^{-1}A_h} \Big]^{1/2}$$

$$+ 2\|(A_h B_h)^{-1/2} u_1\|_h + 2\|(A_h B_h)^{-1/2} f\|_{L^1_{h_t}(H_h)}. \qquad (10)$$

We notice that *the discrete energy conservation law* is valid

$$
\begin{aligned}
&\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + (\sigma - \tfrac{1}{4})h_t^2\|\bar{\delta}_t v^m\|^2_{B_h^{-1}A_h} + \|\bar{s}_t v^m\|^2_{B_h^{-1}A_h} \\
&\quad = \big(B_h^{-1}A_h v^0, s_t v^0\big)_h + \big(B_h^{-1}u_1, \delta_t v^0\big)_h + \tfrac{1}{2}h_t\big(B_h^{-1}f^0, \delta_t v^0\big)_h \\
&\qquad + 2I_{h_t}^{m-1}(B_h^{-1}f, \mathring{\delta}_t v)_h, \quad 1 \le m \le M. \qquad (11)
\end{aligned}
$$

It itself has the independent interest. This natural form is obtained, in particular, due to equation (4) for v^1.

Construction and properties of compact finite-difference schemes of the 4th order of approximation

We define the Numerov-type averaging operators and approximation of f

$$s_N := I + \frac{1}{12}(h_1^2\Lambda_1 + \ldots + h_n^2\Lambda_n), \quad s_{N\widehat{j}} := I + \frac{1}{12}\sum_{1\le i\le n,\, i\ne j} h_i^2\Lambda_i,$$

$$A_N := -(a_1^2 s_{N\widehat{1}}\Lambda_1 + \ldots + a_n^2 s_{N\widehat{n}}\Lambda_n), \quad f_N := s_N f + \frac{1}{12}h_t^2\Lambda_t f,$$

where I is the identity operator; note that $s_{N\widehat{1}} = I$ for $n = 1$.

Lemma

Let the coefficient ρ and solution u to the IBVP (1)-(2) be sufficiently smooth respectively in $\bar{\Omega}$ and $\bar{Q}_T$. Then the following formulas hold

$$s_N(\rho\Lambda_t u) - \frac{1}{12}h_t^2(a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n)\Lambda_t u + A_N u - f_N = \mathcal{O}(|h|^4),$$

$$s_N(\rho\delta_t u)^0 - \frac{h_t^2}{12}(a_1^2\Lambda_1 + \ldots + a_n^2\Lambda_n)(\delta_t u)^0 + \frac{h_t}{2}A_N u_0 - u_{1N} - \frac{h_t}{2}f_N^0 = \mathcal{O}(|h|^4)$$

Preliminarily we consider the scheme of the form

$$s_N(\rho \Lambda_t v) - \frac{1}{12} h_t^2 (a_1^2 \Lambda_1 + \ldots + a_n^2 \Lambda_n) \Lambda_t v + A_N v = f_N \quad \text{on} \quad \omega_h,$$

$$s_N(\rho \delta_t v^0) - \frac{1}{12} h_t^2 (a_1^2 \Lambda_1 + \ldots + a_n^2 \Lambda_n) v^0 + \frac{1}{2} h_t A_N v^0 = u_{1N} + \frac{1}{2} h_t f_N^0.$$

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It belongs to the template

$$B_h(\rho \Lambda_t v) + \sigma h_t^2 A_h \Lambda_t v + A_h v = f \quad \text{in} \quad H_h \quad \text{on} \quad \omega_{h_t},$$

only for $n = 1$.

Thus for $n = 3$ we replace s_N with $\bar{s}_N$

$$\bar{s}_N := \prod_{k=1}^{n} s_{kN}, \quad s_{kN} := I + \frac{1}{12} h_k^2 \Lambda_k,$$

and pass to the scheme

$$\bar{s}_N(\rho \Lambda_t v) + \frac{1}{12} h_t^2 A_N \Lambda_t v + A_N v = f_N \quad \text{on} \quad \omega_h,$$

$$\bar{s}_N(\rho \delta_t v^0) + \frac{1}{12} h_t^2 A_N \delta_t v^0 + \frac{1}{2} h_t A_N v^0 = u_{1N} + \frac{1}{2} h_t f_N^0.$$

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$$\bar{s}_N(\rho \delta_t v^0) + \tfrac{1}{12} h_t^2 A_N \delta_t v^0 + \tfrac{1}{2} h_t A_N v^0 = u_{1N} + \tfrac{1}{2} h_t f_N^0.$$

Still no way to use a spliting technique and 1D factorization in the implementation of this scheme.

How to solve the PDE problem for any $n \geq 1$ (if possible)?

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We replace A_N with $\bar{A}_N$

$$\bar{A}_N := -(a_1^2 \bar{s}_{N\hat{1}} \Lambda_1 + \ldots + a_n^2 \bar{s}_{N\hat{n}} \Lambda_n),$$
$$\bar{s}_{N\hat{l}} := \prod_{1 \leq k \leq n,\, k \neq l} s_{kN},$$

and get the following unified scheme

$$\bar{s}_N(\rho \Lambda_t v) + \frac{1}{12} h_t^2 \bar{A}_N \Lambda_t v + \bar{A}_N v = f_N \quad \text{on} \quad \omega_h, \qquad (12)$$
$$\bar{s}_N(\rho \delta_t v^0) + \frac{1}{12} h_t^2 \bar{A}_N \delta_t v^0 + \frac{1}{2} h_t \bar{A}_N v^0 = u_{1N} + \frac{1}{2} h_t f_N^0. \qquad (13)$$

Implementation

We solve systems of linear equations

$$\bar{s}_N(\rho w^m) + \frac{1}{12} h_t^2 \bar{A}_N w^m = b \ \text{ on } \ \omega_h,$$

for different right-hand sides b.

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for different right-hand sides b.

We consider effective iterative methods to solve such systems.

Theorem

Let the parameters β, γ and θ be chosen such that $B_h > 0$ and $A_h > 0$ in H_h, and $A_h \le \alpha_h^2 B_h$ with some α_h for the scheme in 3D. Let also $0 < \varepsilon_0 < 1$, and the condition

$$\frac{1}{6} h_t^2 \alpha_h^2 \le (1 - \varepsilon_0^2)\underline{\rho}, \tag{14}$$

is valid for the scheme in 3D, or the explicit condition

$$h_t^2 \Big(\frac{a_1^2}{h_1^2} + \ldots + \frac{a_n^2}{h_n^2} \Big) \le (1 - \varepsilon_0^2)\underline{\rho} \tag{15}$$

for the general scheme $n \ge 1$. Then, for any free terms f_N and $u_{1N} \in H_h$ the solutions to both schemes satisfy the following two stability bounds:

$$
\begin{aligned}
\max_{1\le m\le M} & \left(\varepsilon_0^2 \|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + \|\bar{s}_t v^m\|^2_{B_h^{-1}A_h}\right)^{1/2} \\
& \le \left(\|v^0\|^2_{B_h^{-1}A_h} + \varepsilon_0^{-2} \|\tfrac{1}{\sqrt{\rho}} B_h^{-1} u_{1N}\|_h^2\right)^{1/2} \\
& \quad + 2\varepsilon_0^{-1} \|\tfrac{1}{\sqrt{\rho}} B_h^{-1} f_N\|_{L^1_{h_t}(H_h)},
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
\max_{0\le m\le M} \max \left\{\varepsilon_0 \|\sqrt{\rho} v^m\|_h,\ \|I^m_{h_t} \bar{s}_t v\|_{B_h^{-1}A_h}\right\} & \le \|\sqrt{\rho} v^0\|_h \\
+ 2\|B_h^{-1/2} A_h^{-1/2} u_{1N}\|_h + 2\|B_h^{-1/2} A_h^{-1/2} f_N\|_{L^1_{h_t}(H_h)}.
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
&\max_{1\le m\le M}\Big(\varepsilon_0^2\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2+\|\bar{s}_t v^m\|^2_{B_h^{-1}A_h}\Big)^{1/2}\\
&\quad\le\Big(\|v^0\|^2_{B_h^{-1}A_h}+\varepsilon_0^{-2}\|\tfrac{1}{\sqrt{\rho}}B_h^{-1}u_{1N}\|_h^2\Big)^{1/2}\\
&\qquad+2\varepsilon_0^{-1}\|\tfrac{1}{\sqrt{\rho}}B_h^{-1}f_N\|_{L^1_{h_t}(H_h)},
\end{aligned}
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$$

$$
\begin{aligned}
&\max_{0\le m\le M}\max\big\{\varepsilon_0\|\sqrt{\rho}v^m\|_h,\ \|I^m_{h_t}\bar{s}_t v\|_{B_h^{-1}A_h}\big\}\le\|\sqrt{\rho}v^0\|_h\\
&\qquad+2\|B_h^{-1/2}A_h^{-1/2}u_{1N}\|_h+2\|B_h^{-1/2}A_h^{-1/2}f_N\|_{L^1_{h_t}(H_h)}.
\end{aligned}
\tag{17}
$$

The proof follows directly from the general stability Theorem 1, for B_h and A_h listed in the statement.

Unconditionally stable HO schemes

We generalize a well-known two-level scheme, which was proposed for $n = 2$ case:

$$\bar{\delta}_t v = c^2 \left[I - \frac{1}{12} h_t^2 L_h(c^2 I) \right] \bar{s}_t w + d \quad \text{in} \quad H_h, \tag{18}$$

$$\bar{\delta}_t w = \left[L_h - \frac{1}{12} h_t^2 L_h(c^2 L_h) \right] \bar{s}_t v + \tilde{f} \quad \text{in} \quad H_h, \tag{19}$$

where $c^2 = 1/\rho(x)$ and

$$L_h := s_{1N}^{-1} \Lambda_1 + s_{2N}^{-1} \Lambda_2 = -\bar{s}_N^{-1} A_N \quad \text{for} \quad n = 2.$$

We exclude w from this system

$$\rho \Lambda_t v + A_h v^{(1/4)} = f_h \quad \text{on} \quad \omega_{h_t}, \tag{20}$$

where we have set

$$v^{(1/4)} \equiv \frac{1}{4}(\hat{v} + 2v + \check{v}),$$

$$A_h := \Big[I - \frac{1}{12} h_t^2 L_h(c^2 I)\Big](-L_h)\Big(I - \frac{1}{12} h_t^2 c^2 L_h\Big),$$

$$f_h := \Big[I - \frac{1}{12} h_t^2 L_h(c^2 I)\Big] s_t \tilde{f} + \rho \delta_t d.$$

Theorem

For the solution to method (20), $n \geq 1$, the following stability bounds hold:

$$\max_{1 \le m \le M} \left(\|\sqrt{\rho}\bar{\delta}_t v^m\|_h^2 + \|\bar{s}_t v^m\|_{A_h}^2 \right)^{1/2}$$

$$\le \left(\|v^0\|_{A_h}^2 + \varepsilon_0^{-2} \Big\| \frac{1}{\sqrt{\rho}} u_{1h} \Big\|_h^2 \right)^{1/2} + 2 \Big\| \frac{1}{\sqrt{\rho}} f_h \Big\|_{L^1_{h_t}(H_h)},$$

$$\max_{0 \le m \le M} \max \left\{ \|\sqrt{\rho} v^m\|_h, \; \|I_{h_t}^m \bar{s}_t v\|_{A_h} \right\} \le \|\sqrt{\rho} v^0\|_h$$

$$+ 2\|(-L_h)^{-1/2} w^0\|_h + \frac{h_t}{2} \|(-L_h)^{-1/2} \tilde{f}^1\|_h$$

$$+ 2 I_{h_t}^{M-1} \|(-L_h)^{-1/2} s_t \tilde{f}\|_h + 2 I_{h_t}^{M} \|\sqrt{\rho} d\|_h.$$

Iterative methods

We solve a system of equations:

$$B_h(\rho w) + \frac{1}{12} h_t^2 A_h w = b \quad \text{in} \quad H_h, \tag{21}$$

with any commuting operators $B_h^* = B_h > 0$ and $A_h^* = A_h > 0$.

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with any commuting operators $B_h^* = B_h > 0$ and $A_h^* = A_h > 0$.
We first consider the one-step iterative method with a constant parameter $\theta > 0$:

$$B_h\Big(\rho \frac{w^{(l+1)} - w^{(l)}}{\theta}\Big) + B_h(\rho w^{(l)}) + \frac{1}{12} h_t^2 A_h w^{(l)} = b, \quad l \geq 0, \tag{22}$$

where B_h serves as a preconditioner.

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where B_h serves as a preconditioner.
Its equivalent practical form is

$$w^{(l+1)} = (1-\theta) w^{(l)} - \frac{\theta}{\rho} B_h^{-1}\big(\frac{1}{12} h_t^2 A_h w^{(l)} - b\big), \; l \geq 0.$$

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In the case of the general HO scheme the preconditioner operator $B_h = \bar{s}_N$ is defined in the splitting (factorized) form, and then implementation of B_h^{-1} is reduced to a sequential solving 1D algebraic systems with tridiagonal matrices.

Example 1. The 3D wave propagation is studied in the three-layer medium with the sound speeds $s_1 = 1500, s_2 = 1000$ and $s_3 = 3000$ m/s, respectively in its left, middle and right layers in x of the same thickness. Here we take $X = 3\,km$.

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The source is defined as the 3D Ricker-type wavelet

$$\varphi(x, y, z, t) = \delta(x - x_0, y - y_0, z - z_0)\sin(50t)e^{-200t^2},$$

where $\delta(x - x_0, y - y_0, z - z_0)$ is the Dirac distribution located at the center of domain $(x_0, y_0, z_0) = (1.5\,km, 1.5\,km, 1.5\,km)$. Also we take $u_0 = u_1 = 0$.

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It follows from our computational experiments, that the dynamics of the wave is complicated even in 2D case. Now we solve numerically a 3D modification of this test problem.

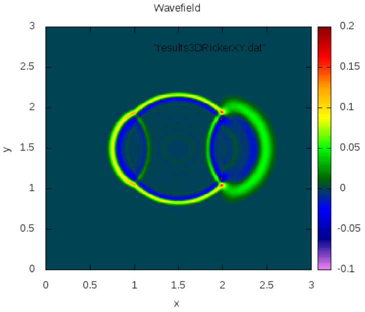

FIGURE: Snapshots of z-section of wavefields computed by the scheme $\bar{S}$ at (a) $t = 0.7\ s$, (b) $t = 0.8\ s$