Fundamental models in nonlinear acoustics

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Nonlinear acoustics

Nonlinear acoustics. Field of nonlinear acoustics concerned with propagation of sound waves in thermoviscous fluids. Applications in high-intensity ultrasonics include

- medical treatment (lithotripsy, thermotherapy) and
- industrial applications (ultrasound cleaning, welding).

Simulations. Numerical simulations provide valuable tools for design and improvement of high-intensity ultrasound devices.

Kidney stones, Lithotripsy. Quotation from https://www.healthline.com/

> *Kidney stones, or renal calculi, are solid masses made of crystals.*
>
> *Kidney stones are known to cause severe pain.*
>
> *Extracorporeal shock wave lithotripsy uses sound waves to break up large stones so they can more easily pass down the ureters into your bladder. This procedure can be uncomfortable and may require light anesthesia. It can cause bruising on the abdomen and back and bleeding around the kidney and nearby organs.*

Our approach

Our approach. Contributions regarding analytical aspects as well as numerical challenges.

- Derivation and analysis of underlying models (PDEs).
- Design of efficient time integration methods.

Mathematical models

Mathematical models. Propagation of high-intensity ultrasound waves in thermoviscous fluids described by nonlinear damped wave equations. Blackstock–Crighton–Brunnhuber–Jordan–Kuznetsov equation has form

$$\begin{cases} \Big(\partial_{ttt} - \beta_1^{(a)}\,\Delta\partial_{tt} + \beta_2^{(a)}(\sigma_0)\,\Delta^2\partial_t - \beta_3\,\Delta\partial_t + \beta_4^{(a)}(\sigma_0)\,\Delta^2\Big)\,\psi^{(a)}(t) \\ \quad + \partial_{tt}\Big(\frac{1}{2}\,\beta_5(\sigma)\,\big(\partial_t\psi^{(a)}(t)\big)^2 + \beta_6(\sigma)\,\big|\nabla\psi^{(a)}(t)\big|^2\Big) = 0\,, \quad t \in (0,T)\,, \\ \psi^{(a)}(0) = \psi_0\,, \quad \partial_t\psi^{(a)}(0) = \psi_1\,, \quad \partial_{tt}\psi^{(a)}(0) = \psi_2\,. \end{cases}$$

Reduced models. Commonly used Kuznetsov and Westervelt equations result when neglecting thermal and local nonlinear effects

$$\begin{cases} \Big(\partial_{tt} - \beta_1^{(0)}\,\Delta\partial_t - \beta_3\,\Delta\Big)\,\psi(t) + \partial_t\Big(\frac{1}{2}\,\beta_5(\sigma)\,\big(\partial_t\psi(t)\big)^2 + \beta_6(\sigma)\,|\nabla\psi(t)|^2\Big) = 0\,, \quad t \in (0,T)\,, \\ \psi(0) = \psi_0\,, \quad \partial_t\psi(0) = \psi_1\,. \end{cases}$$

Numerical challenges. Use of transient numerical simulations within mathematical optimisation of high-intensity ultrasound devices still beyond scope of existing approaches.

Novel approach

Novel approach. Operator splitting methods known to be efficient time integration methods for nonlinear partial differential equations

$$\begin{cases} u'(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), & t \in (0,T)\,, \\ u(0) \text{ given}\,, \end{cases}$$

$$\begin{aligned} u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) &= \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau_{n-1} D_A}\, \mathrm{e}^{b_{s+1-j}\tau_{n-1} D_B}\, u_{n-1} \\ \approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) &= \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1})\,, \quad n \in \{1,\dots,N\}\,. \end{aligned}$$

Motivates introduction and investigation of operator splitting methods for nonlinear damped wave equations arising in nonlinear acoustics.

Remark. Approach reveals underlying parabolic equations.

Our contributions and plans

Former contributions.

BARBARA KALTENBACHER, VANJA NIKOLIĆ, M. TH.
Efficient time integration methods based on operator splitting and application to the Westervelt equation.
IMA J. Numer. Anal. 35/3 (2015) 1092–1124.

BARBARA KALTENBACHER, M. TH.
Fundamental models in nonlinear acoustics. Part I. Analytical comparison.
M3AS 28/12 (2018).

Current work.

BARBARA KALTENBACHER, M. TH.
Part II. Numerical comparison.

Focus in this talk. Analytical aspects.

Analytical aspects

Derivation of general model
Existence and regularity result
Justification of limiting systems

Derivation of general model

Approach

Approach. Derivation of general model relies on physical and mathematical principles.

- Decompose basic state variables of acoustics into constant mean values and space-time-dependent fluctuations

$$\text{mass density} \quad \varrho = \varrho_0 + \varrho_\sim \,, \quad \text{acoustic particle velocity} \quad v = v_\sim \,,$$
$$\text{acoustic pressure} \quad p = p_0 + p_\sim \,, \quad \text{temperature} \quad T = T_0 + T_\sim \,.$$

- Use Helmholtz decomposition of acoustic particle velocity and assign irrotational part to gradient of acoustic velocity potential

$$v_\sim = \nabla \psi + \nabla \times S \,.$$

Approach

- Employ conservation laws for mass, momentum, energy

$$\partial_t \varrho + \nabla \cdot (\varrho\, v) = 0\,,$$
$$\partial_t (\varrho\, v) + v\, \nabla \cdot (\varrho\, v) + \varrho\, (v \cdot \nabla)\, v + \nabla p = \mu\, \Delta v + \big(\mu_B + \tfrac{1}{3}\, \mu\big)\, \nabla (\nabla \cdot v)\,,$$
$$\varrho\, \big(c_V\, \partial_t T + c_V\, v \cdot \nabla T + \tfrac{c_p - c_V}{\alpha_V}\, \nabla \cdot v\big)$$
$$= a\, \Delta T + \big(\mu_B - \tfrac{2}{3}\, \mu\big)\, (\nabla \cdot v)^2 + \tfrac{1}{2}\, \mu\, \big\| \nabla v + (\nabla v)^T \big\|_F^2\,,$$

as well as equation of state for acoustic pressure

$$p_\sim \approx A\, \frac{\varrho_\sim}{\varrho_0} + \frac{B}{2}\, \Big(\frac{\varrho_\sim}{\varrho_0}\Big)^2 + \hat{A}\, \frac{T_\sim}{T_0}\,.$$

Relations in particular involve thermal conductivity $a > 0$ and parameter of nonlinearity $\frac{B}{A} > 0$.

- Accordingly to Blackstock (1963) and Lighthill (1956), take first- and second-order contributions with respect to fluctuating quantities into account.

General model

General model. Above approach leads to general model

$$\begin{aligned}&\partial_{ttt}\psi^{(a)}(t) - \beta_1^{(a)}\,\Delta\partial_{tt}\psi^{(a)}(t) + \beta_2^{(a)}(\sigma_0)\,\Delta^2\partial_t\psi^{(a)}(t)\\ &\quad - \beta_3\,\Delta\partial_t\psi^{(a)}(t) + \beta_4^{(a)}(\sigma_0)\,\Delta^2\psi^{(a)}(t)\\ &\quad + \partial_{tt}\Big(\tfrac{1}{2}\,\beta_5(\sigma)\,\big(\partial_t\psi^{(a)}(t)\big)^2 + \beta_6(\sigma)\,\big|\nabla\psi^{(a)}(t)\big|^2\Big) = 0\,, \qquad t\in(0,T)\,,\end{aligned}$$

where coefficients in particular depend on thermal conductivity $a > 0$ and parameter of nonlinearity $\frac{B}{A} > 0$

$$\beta_1^{(a)} = a\big(1+\tfrac{B}{A}\big) + \nu\Lambda\,, \quad \beta_2^{(a)}(\sigma_0) = a\big(\nu\Lambda + a\,\tfrac{B}{A} + \sigma_0\,\tfrac{B}{A}\,(\nu\Lambda - a)\big)\,,$$
$$\beta_3 = c_0^2\,, \quad \beta_4^{(a)}(\sigma_0) = a\big(1+\sigma_0\,\tfrac{B}{A}\big)\,c_0^2\,,$$
$$\beta_5(\sigma) = \tfrac{1}{c_0^2}\big(2\,(1-\sigma) + \tfrac{B}{A}\big)\,, \quad \beta_6(\sigma) = \sigma\,, \quad \sigma,\sigma_0\in\{0,1\}\,.$$

Fundamental question. Use of reduced model for $a \to 0_+$ justified?

Hierarchy

Hierarchy. Overview of considered hierachy of nonlinear damped wave equations.

$$\begin{array}{ccc}
\text{Brunnhuber–Jordan–Kuznetsov (BJK)} & \xrightarrow{\sigma=0} & \text{Brunnhuber–Jordan–Westervelt (BJW)} \\
\downarrow \sigma_0=0 & & \downarrow \sigma_0=0 \\
\text{Blackstock–Crighton–Kuznetsov (BCK)} & \xrightarrow{\sigma=0} & \text{Blackstock–Crighton–Westervelt (BCW)} \\
\downarrow a\to 0_+ & & \downarrow a\to 0_+ \\
\text{Kuznetsov (K)} & \xrightarrow{\sigma=0} & \text{Westervelt (W)}
\end{array}$$

Remarks.

- BJK cast into general formulation with $\sigma = \sigma_0 = 1$.
- BCK describes monatomic gases (quantity $(\nu\Lambda - a)\,\frac{B}{A}$ negligible).
- Kuznetsov equation results as limiting system.
- Westervelt-type equations additionally do not take into account local nonlinear effects (term $c_0^2\,|\nabla\psi|^2 - (\partial_t\psi)^2$ negligible).

Illustration (General model)

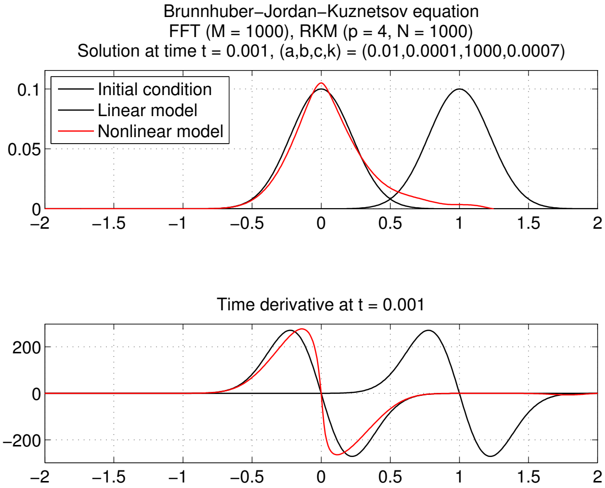
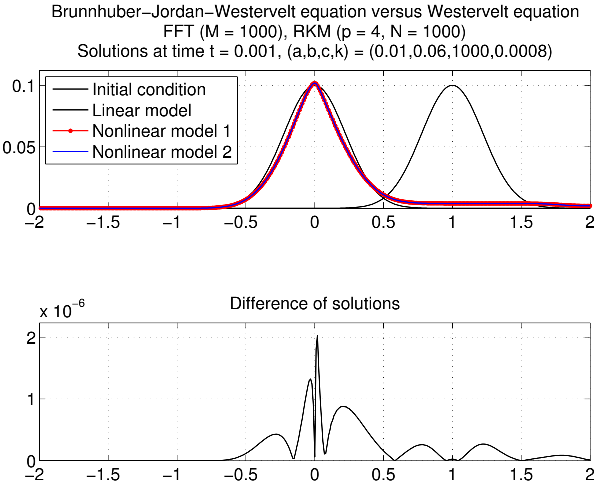


Illustration (General versus reduced model)



Existence and regularity result

Existence and regularity result

Initial-boundary value problem.

- Let $a \in (0, \overline{a}]$.
- Consider nonlinear damped wave equation

$$\begin{cases} \partial_{ttt}\psi^{(a)}(t) - \beta_1^{(a)}\,\Delta\partial_{tt}\psi^{(a)}(t) + \beta_2^{(a)}(\sigma_0)\,\Delta^2\partial_t\psi^{(a)}(t) \\ \quad - \beta_3\,\Delta\partial_t\psi^{(a)}(t) + \beta_4^{(a)}(\sigma_0)\,\Delta^2\psi^{(a)}(t) \\ \quad + \partial_{tt}\Big(\tfrac{1}{2}\,\beta_5(\sigma)\,\big(\partial_t\psi^{(a)}(t)\big)^2 + \beta_6(\sigma)\,\big|\nabla\psi^{(a)}(t)\big|^2\Big) = 0\,, \quad t \in (0,T)\,, \\ \psi^{(a)}(0) = \psi_0, \quad \partial_t\psi^{(a)}(0) = \psi_1\,, \quad \partial_{tt}\psi^{(a)}(0) = \psi_2\,. \end{cases}$$

- Impose homogeneous Dirichlet boundary conditions

$$\partial_{tt}\psi(t)\big|_{\partial\Omega} = 0\,, \quad \Delta\partial_t\psi(t)\big|_{\partial\Omega} = 0\,, \quad \Delta\psi(t)\big|_{\partial\Omega} = 0\,,$$
$$\partial_{ttt}\psi(t)\big|_{\partial\Omega} = 0\,, \quad \Delta\partial_{tt}\psi(t)\big|_{\partial\Omega} = 0\,.$$

Existence and regularity result

Assumptions.

- Suppose that prescribed initial data satisfy regularity and compatibility conditions

$$\psi_0, \psi_1 \in H^3(\Omega) \cap H_0^1(\Omega), \quad \Delta\psi_0, \Delta\psi_1, \psi_2 \in H_0^1(\Omega).$$

- Assume that for $\|\Delta\psi_0\|_{L_2}$, $\|\nabla\Delta\psi_0\|_{L_2}$, and upper bounds $\overline{e}_0, \overline{e}_1 > 0$ on initial energies

$$\|\psi_2\|_{L_2}^2 + \beta_2^{(a)}(\sigma_0)\,\|\Delta\psi_1\|_{L_2}^2 + \|\nabla\psi_1\|_{L_2}^2 \leq \overline{e}_0\,,$$
$$\|\nabla\psi_2\|_{L_2}^2 + \beta_2^{(a)}(\sigma_0)\,\|\nabla\Delta\psi_1\|_{L_2}^2 + \|\Delta\psi_1\|_{L_2}^2 \leq \overline{e}_1\,,$$

following quantity is sufficiently small

$$M(\overline{e}_0, \overline{e}_1) = \frac{C_{\mathrm{PF}}^2\, C_{L_4 \hookleftarrow H^1}^2\, \beta_5(\sigma)}{\underline{\beta}_1} \sqrt{\overline{e}_0} + C_0\, \overline{e}_1 + \frac{C_2}{\underline{\beta}_1}\left(\|\Delta\psi_0\|_{L_2}^2 + C_3\, T^2\, \overline{e}_1\right) + C_4\left(\tfrac{1}{2}\,\|\nabla\Delta\psi_0\|_{L_2} + \sqrt{\overline{e}_1}\right).$$

Existence and regularity result

Theorem (Kaltenbacher, Th., 2018)

Under the above assumptions, there exists a weak solution

$$\psi \in X = H^2\big([0,T], H^2_\diamond(\Omega)\big) \cap W^2_\infty\big([0,T], H^1_0(\Omega)\big) \cap W^1_\infty\big([0,T], H^3_\diamond(\Omega)\big),$$
$$H^2_\diamond(\Omega) = \big\{\chi \in H^2(\Omega) : \chi \in H^1_0(\Omega)\big\}, \quad H^3_\diamond(\Omega) = \big\{\chi \in H^3(\Omega) : \chi, \Delta\chi \in H^1_0(\Omega)\big\},$$

to the associated equation

$$\partial_{tt}\psi(t) - \psi_2 - \beta_1^{(a)}\,\Delta\big(\partial_t\psi(t) - \psi_1\big) + \beta_2^{(a)}(\sigma_0)\,\Delta^2\big(\psi(t) - \psi_0\big) - \beta_3\,\Delta\big(\psi(t) - \psi_0\big)$$
$$+ \beta_4^{(a)}(\sigma_0)\int_0^t \Delta^2\psi(\tau)\,\mathrm{d}\tau + \beta_5(\sigma)\big(\partial_{tt}\psi(t)\,\partial_t\psi(t) - \psi_2\,\psi_1\big)$$
$$+ 2\,\beta_6(\sigma)\big(\nabla\partial_t\psi(t)\cdot\nabla\psi(t) - \nabla\psi_1\cdot\nabla\psi_0\big) = 0,$$

obtained by integration with respect to time.

Existence and regularity result

Theorem (Kaltenbacher, Th., 2018)

This solution satisfies a priori energy estimates of the form

$$\mathscr{E}_0\big(\psi(t)\big) = \big\|\partial_{tt}\psi(t)\big\|_{L_2}^2 + \beta_2^{(a)}(\sigma_0)\,\big\|\Delta\partial_t\psi(t)\big\|_{L_2}^2 + \big\|\nabla\partial_t\psi(t)\big\|_{L_2}^2\,,$$
$$\mathscr{E}_1\big(\psi(t)\big) = \big\|\nabla\partial_{tt}\psi(t)\big\|_{L_2}^2 + \beta_2^{(a)}(\sigma_0)\,\big\|\nabla\Delta\partial_t\psi(t)\big\|_{L_2}^2 + \big\|\Delta\partial_t\psi(t)\big\|_{L_2}^2\,,$$
$$\sup_{t\in[0,T]} \mathscr{E}_0\big(\psi(t)\big) \leq \overline{E}_0\,, \quad \sup_{t\in[0,T]} \mathscr{E}_1\big(\psi(t)\big) \leq \overline{E}_1\,, \quad \int_0^T \big\|\Delta\partial_{tt}\psi(t)\big\|_{L_2}^2\,\mathrm{d}t \leq \overline{E}_2\,,$$

which hold uniformly for $a \in (0,\overline{a}]$. *In particular, the quantity* $M(\overline{E}_0,\overline{E}_1)$ *remains sufficiently small to ensure uniform boundedness and hence non-degeneracy of the first time derivative*

$$0 < \underline{\alpha} = \tfrac{1}{2} \leq \big\|1 + \beta_5(\sigma)\,\partial_t\psi\big\|_{L_\infty([0,T],L_\infty(\Omega))} \leq \overline{\alpha} = \tfrac{3}{2}\,,$$
$$0 < \tfrac{1}{\overline{\alpha}} = \tfrac{2}{3} \leq \Big\|\big(1 + \beta_5(\sigma)\,\partial_t\psi\big)^{-1}\Big\|_{L_\infty([0,T],L_\infty(\Omega))} \leq \tfrac{1}{\underline{\alpha}} = 2\,.$$

Existence and regularity result

Main tools. Introduction of higher-order energy functional

$$\mathscr{E}_1\big(\psi^{(a)}(t)\big) = \big\|\nabla\partial_{tt}\psi^{(a)}(t)\big\|_{L_2}^2 + \beta_2^{(a)}(\sigma_0)\,\big\|\nabla\Delta\partial_t\psi^{(a)}(t)\big\|_{L_2}^2 + \big\|\Delta\partial_t\psi^{(a)}(t)\big\|_{L_2}^2 .$$

Derivation of a priori bound of form

$$\sup_{t\in[0,T]} \mathscr{E}_1\big(\psi^{(a)}(t)\big) + \int_0^T \big\|\Delta\partial_{tt}\psi^{(a)}(t)\big\|_{L_2}^2 \,\mathrm{d}t \leq C .$$

Application of fixed point theorem by Schauder (weak formulation).

Remark. Second term in energy functional associated with Bochner–Sobolev space

$$W_\infty^1\big([0,T], H^3(\Omega)\big) .$$

Due to fact that $\beta_2^{(a)}(\sigma_0) \to 0$ as $a \to 0_+$, only convergence in weaker sense

$$\psi^{(a)} \overset{*}{\rightharpoonup} \psi^{(0)} \text{ in } H^2\big([0,T], H^2(\Omega)\big)$$

can be achieved.

Justification of limiting systems

Justification of limiting systems

Additional assumption. In above situation, assume in addition that prescribed initial data satisfy consistency condition

$$\psi_2 - \beta_1^{(0)}\,\Delta\psi_1 - \beta_3\,\Delta\psi_0 + \beta_5(\sigma)\,\psi_2\,\psi_1 + 2\,\beta_6(\sigma)\,\nabla\psi_1\cdot\nabla\psi_0 = 0\,.$$

For any $a \in (0,\overline{a}]$, let $\psi^{(a)} : [0,T] \to L_2(\Omega)$ denote solution to nonlinear damped wave equation or of reformulation obtained by integration

$$\begin{aligned}
&\partial_{tt}\psi^{(a)}(t) - \beta_1^{(0)}\,\Delta\partial_t\psi^{(a)}(t) - \big(\beta_1^{(a)} - \beta_1^{(0)}\big)\big(\Delta\partial_t\psi^{(a)}(t) - \Delta\psi_1\big)\\
&\quad + \beta_2^{(a)}(\sigma_0)\big(\Delta^2\psi^{(a)}(t) - \Delta^2\psi_0\big) - \beta_3\,\Delta\psi^{(a)}(t) + \beta_4^{(a)}(\sigma_0)\int_0^t \Delta^2\psi^{(a)}(\tau)\,\mathrm{d}\tau\\
&\quad + \beta_5(\sigma)\,\partial_{tt}\psi^{(a)}(t)\,\partial_t\psi^{(a)}(t) + 2\,\beta_6(\sigma)\,\nabla\partial_t\psi^{(a)}(t)\cdot\nabla\psi^{(a)}(t) = 0\,.
\end{aligned}$$

Justification of limiting systems

Theorem

Under the above assumptions, as $a \to 0_+$*, the family* $(\psi^{(a)})_{a \in (0,\overline{a}]}$ *converges to the solution* $\psi^{(0)} : [0,T] \to L_2(\Omega)$ *of the limiting system*

$$\begin{aligned}&\partial_{tt}\psi^{(0)}(t) - \beta_1^{(0)}\,\Delta\partial_t\psi^{(0)}(t) - \beta_3\,\Delta\psi^{(0)}(t)\\&\quad + \beta_5(\sigma)\,\partial_{tt}\psi^{(0)}(t)\,\partial_t\psi^{(0)}(t) + 2\,\beta_6(\sigma)\,\nabla\partial_t\psi^{(0)}(t)\cdot\nabla\psi^{(0)}(t) = 0\,.\end{aligned}$$

More precisely, for the solution to the associated weak formulation, obtained by testing with $v \in L_1([0,T], H_0^1(\Omega))$ *and performing integration-by-parts, convergence is ensured in the following sense*

$$\psi^{(a)} \overset{*}{\rightharpoonup} \psi^{(0)} \text{ in } X_0 \text{ as } a \to 0_+\,.$$

Conclusions and future work

Summary.

- Rigorous justification of Kuznetsov and Westervelt equations as limiting systems.

Relevant open questions.

- Numerical methods for more involved models arising in nonlinear acoustics.
- Application of higher-order splitting methods involving complex coefficients.
- Reliable and efficient time integration based on adaptive time stepsize control.

Thank you!