Fundamental nonlinear wave equations arising in nonlinear acoustics: Analytical and numerical aspects

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Focus in this talk

Splitting methods. Efficient time integration of nonlinear evolution equations by operator splitting methods

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big)\,, & t \in (0,T)\,, \\ u(0) \text{ given}\,, & \end{cases}$$

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau_{n-1} D_A}\, \mathrm{e}^{b_{s+1-j}\tau_{n-1} D_B}\, u_{n-1}$$

$$\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1})\,, \quad n \in \{1,\dots,N\}\,.$$

Applications.

- Nonlinear parabolic equations
- Nonlinear Schrödinger equations (GPS, MCTDHF)
- Nonlinear wave equations with damping (Westervelt equation)

References

Main reference.

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.

Main inspiration.

- Operator splitting methods for nonlinear Schrödinger equations, see various contributions by W. BAO and CH. LUBICH.
- Approach studied in cooperation with S. DESCOMBES.

STÉPHANE DESCOMBES, M. TH.
The Lie–Trotter splitting for nonlinear evolutionary problems with critical parameters. A compact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime.
IMA J. Numer. Anal. 33/2 (2013) 722–745.

Current work.

BARBARA KALTENBACHER, VANJA NIKOLIĆ, M. TH.
Fundamental models in nonlinear acoustics. Part I. Analytical comparison.
Submitted to M3AS.

Westervelt equation

Simulation of models from nonlinear acoustics

Nonlinear acoustics. Investigation of mathematical models for propagation of high intensity ultrasound waves. Applications include

- medical treatment like lithotripsy or thermotherapy and
- industrial applications like ultrasound cleaning or welding and sonochemistry.

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

Challenges.

- Mathematical models arising in nonlinear acoustics involve time-dependent nonlinear partial differential equations.
- Use of transient simulations within mathematical optimisation of high intensity ultrasound devices still beyond scope of existing approaches.

Approach.

- Operator splitting methods known to be efficient time integration methods for other classes of nonlinear partial differential equations.
- Motivates introduction and investigation of splitting methods for classical model from nonlinear acoustics (Westervelt equation).

Westervelt equation

Westervelt equation. Consider nonlinear wave equation with damping for $\psi : \overline{\Omega} \times [0,T] \subset \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \to \mathbb{R} : (x,t) \mapsto \psi(x,t)$

$$\begin{cases} \partial_{tt}\psi(x,t) - \alpha\,\Delta\,\partial_t\psi(x,t) - \beta\,\Delta\,\psi(x,t) \\ \quad = \gamma\,\partial_t\big(\partial_t\psi(x,t)\big)^2 = \delta\,\partial_t\psi(x,t)\,\partial_{tt}\psi(x,t)\,, \quad (x,t) \in \Omega \times (0,T)\,, \end{cases}$$

involving constants $\alpha, \beta > 0$ and $\delta = 2\gamma \neq 0$.

Remarks.

- In view of time integration by first- and second-order splitting methods, assume that solution is sufficiently regular. In particular, suppose that spatial domain and prescribed initial data are sufficiently regular.
- Focus on relevant case of homogeneous Dirichlet boundary conditions.

First step. In regard to introduction and error analysis of operator splitting methods, rewrite Westervelt equation as nonlinear evolution equation and define associated subproblems.

Reformulation as first-order system

Westervelt equation. Recall Westervelt equation for $\psi : \overline{\Omega} \times [0,T] \to \mathbb{R}$

$$\partial_{tt}\psi(x,t) - \alpha\,\Delta\,\partial_t\psi(x,t) - \beta\,\Delta\,\psi(x,t) = \delta\,\partial_t\psi(x,t)\,\partial_{tt}\psi(x,t)\,.$$

Non-degeneracy. Regularity result ensures non-degeneracy of Westervelt equation for initial state of sufficiently small norm

$$0 < 1 - \delta\,\partial_t\psi(x,t) < \infty\,.$$

Obtain equivalent formulation of non-degenerate Westervelt equation

$$\partial_{tt}\psi(x,t) = \alpha\left(1 - \delta\,\partial_t\psi(x,t)\right)^{-1}\Delta\,\partial_t\psi(x,t) + \beta\left(1 - \delta\,\partial_t\psi(x,t)\right)^{-1}\Delta\,\psi(x,t)\,.$$

Reformulation as first-order system. Employ reformulation as first-order system for $\Psi = (\Psi_1, \Psi_2) = (\psi, \partial_t\psi) : \overline{\Omega} \times [0,T] \to \mathbb{R}^2$

$$\begin{cases} \partial_t\Psi_1(x,t) = \Psi_2(x,t)\,, \\ \partial_t\Psi_2(x,t) = \alpha\left(1 - \delta\,\Psi_2(x,t)\right)^{-1}\Delta\,\Psi_2(x,t) + \beta\left(1 - \delta\,\Psi_2(x,t)\right)^{-1}\Delta\Psi_1(x,t)\,. \end{cases}$$

Reformulation as abstract evolution equation

Reformulation as first-order system. Employ reformulation of non-degenerate Westervelt equation as first-order system for $\Psi = (\Psi_1, \Psi_2) = (\psi, \partial_t \psi) : \overline{\Omega} \times [0, T] \to \mathbb{R}^2$

$$\begin{cases} \partial_t \Psi_1(x,t) = \Psi_2(x,t)\,, \\ \partial_t \Psi_2(x,t) = \alpha \big(1 - \delta\, \Psi_2(x,t)\big)^{-1} \Delta \Psi_2(x,t) + \beta \big(1 - \delta\, \Psi_2(x,t)\big)^{-1} \Delta \Psi_1(x,t)\,. \end{cases}$$

Reformulation as evolution equation. In regard to introduction and error analysis of operator splitting methods rewrite non-degenerate Westervelt equation as nonlinear evolution equation on Banach space for $u : [0, T] \to X : t \mapsto u(t) = \Psi(\cdot, t)$

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = F\big(u(t)\big)\,, \quad t \in (0, T)\,,$$

$$F(v) = \begin{pmatrix} v_2 \\ \alpha \big(1 - \delta\, v_2\big)^{-1} \Delta v_2 + \beta \big(1 - \delta\, v_2\big)^{-1} \Delta v_1 \end{pmatrix}, \quad v = (v_1, v_2) \in D(F)\,.$$

Remark. Domain of nonlinear operator $F : D(F) \subset X \to X$ reflects regularity requirements on solution and imposed boundary conditions.

Associated subproblems (Decomposition I)

Abstract formulation. Employ compact formulation of Westervelt equation as nonlinear evolution equation and define nonlinear operators A, B

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad t \in (0,T),$$

$$A(v) = \begin{pmatrix} v_2 \\ \alpha\,(1-\delta\, v_2)^{-1}\,\Delta v_2 \end{pmatrix}, \quad B(v) = \begin{pmatrix} 0 \\ \beta\,(1-\delta\, v_2)^{-1}\,\Delta v_1 \end{pmatrix}.$$

Subproblem (Nonlinear diffusion equation). Resolution of subproblem associated with A

$$\begin{cases} \partial_t \Psi_1(x,t) = \Psi_2(x,t), \\ \partial_t \Psi_2(x,t) = \alpha\,\big(1-\delta\,\Psi_2(x,t)\big)^{-1}\,\Delta\Psi_2(x,t), \end{cases}$$

amounts to solution of nonlinear diffusion equation for second component $\Psi_2 = \partial_t \psi$

$$\partial_t \Psi_2(x,t) = \alpha\,\big(1-\delta\,\Psi_2(x,t)\big)^{-1}\,\Delta\Psi_2(x,t).$$

First component $\Psi_1 = \psi$ then retained by (pointwise) integration

$$\Psi_1(x,t) = \Psi_1(x,0) + \int_0^t \Psi_2(x,\tau)\,\mathrm{d}\tau.$$

Associated subproblems (Decomposition I)

Abstract formulation. Employ compact formulation of Westervelt equation as nonlinear evolution equation and define nonlinear operators A, B

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big)\,, \quad t \in (0,T)\,,$$

$$A(v) = \begin{pmatrix} v_2 \\ \alpha\,\big(1-\delta\,v_2\big)^{-1}\,\Delta v_2 \end{pmatrix}, \quad B(v) = \begin{pmatrix} 0 \\ \beta\,\big(1-\delta\,v_2\big)^{-1}\,\Delta v_1 \end{pmatrix}.$$

Subproblem (Explicit representation). For subproblem associated with B

$$\begin{cases} \partial_t \Psi_1(x,t) = 0\,, \\ \partial_t \Psi_2(x,t) = \beta\,\big(1-\delta\,\Psi_2(x,t)\big)^{-1}\,\Delta\Psi_1(x,t)\,, \end{cases}$$

first component remains constant on considered time interval

$$\Psi_1(x,t) = \Psi_1(x,0)\,.$$

Consequently, second component is (pointwise) solution to ODE with explicit representation

$$\partial_t \Psi_2(x,t) = \beta\,\big(1-\delta\,\Psi_2(x,t)\big)^{-1}\,\Delta\Psi_1(x,0)\,,$$

$$\Psi_2(x,t) = \tfrac{1}{\delta}\,\Big(1-\sqrt{\big(1-\delta\,\Psi_2(x,0)\big)^2 - 2\,\beta\,\delta\,t\,\Delta\Psi_1(x,0)}\,\Big).$$

Suitable choice of time increment $t>0$ ensures $(1-\delta\,\Psi_2(x,0))^2 - 2\,\beta\,\delta\,t\,\Delta\Psi_1(x,0) > 0$ and hence $\Psi_2(x,t) \in \mathbb{R}$.

Operator splitting methods for Westervelt equation

Exponential operator splitting methods

Time-stepping approach. Time integration of nonlinear evolution equation on Banach space $(X, \|\cdot\|_X)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big)\,, \quad t \in (0,T)\,, \quad u(0) \text{ given}\,.$$

Approximations at time grid points $0 = t_0 < \cdots < t_N \leq T$ with increments $\tau_{n-1} = t_n - t_{n-1}$ are given by recurrence

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \approx u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1})\,, \quad n \in \{1, \dots, N\}\,.$$

Splitting methods. Operator splitting methods rely on suitable decomposition of right-hand side and presumption that associated subproblems solvable in accurate and efficient manner

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = A\big(v(t)\big)\,, \quad v(t) = \mathrm{e}^{t D_A}\, v(0)\,, \quad t \in (0,T)\,,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\, w(t) = B\big(w(t)\big)\,, \quad w(t) = \mathrm{e}^{t D_B}\, w(0)\,, \quad t \in (0,T)\,.$$

Splitting methods for Westervelt equation

Splitting methods for Westervelt equation. Recall abstract formulation for Westervelt equation (Decomposition I)

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad t \in (0,T),$$

$$A(v) = \begin{pmatrix} v_2 \\ \alpha\,(1-\delta\, v_2)^{-1}\,\Delta v_2 \end{pmatrix}, \quad B(v) = \begin{pmatrix} 0 \\ \beta\,(1-\delta\, v_2)^{-1}\,\Delta v_1 \end{pmatrix}.$$

Solution of subproblem associated with A requires resolution of nonlinear diffusion equation and (pointwise) integration. Explicit (pointwise) representation available for solution to subproblem associated with B.

Lower-order splitting methods. First-order Lie–Trotter splitting method

$$\mathcal{S}_F(t,\cdot) = \mathrm{e}^{tD_B}\,\mathrm{e}^{tD_A}\,.$$

Second-order Strang splitting method

$$\mathcal{S}_F(t,\cdot) = \mathrm{e}^{\frac{1}{2}tD_A}\,\mathrm{e}^{tD_B}\,\mathrm{e}^{\frac{1}{2}tD_A}\,.$$

Stability and error analysis of Lie–Trotter splitting method

Main result (Lie–Trotter splitting)

Convergence result. Employ basic regularity assumption on initial state and additional compatibility conditions

$$u(0) = \big(\psi(\cdot,0), \partial_t \psi(\cdot,0)\big) \in H^6(\Omega) \times H^5(\Omega)\,,$$
$$\|u(0)\|_{H^6 \times H^5} = \|\psi(\cdot,0)\|_{H^6} + \|\partial_t \psi(\cdot,0)\|_{H^5} \leq C_0\,.$$

Apply auxiliary result that ensures regularity and boundedness of solution

$$u(t) \in H^6(\Omega) \times H^5(\Omega)\,, \quad \|u(t)\|_{H^6 \times H^5} \leq C\,, \quad t \in [0,T]\,.$$

Obtain global error estimate for Lie–Trotter splitting method applied to Westervelt equation.

Theorem (Lie–Trotter splitting method, Decomposition I)

Assume that initial state fulfills above requirements and that intial approximation u_0 remains bounded in $H^5(\Omega) \times H^3(\Omega)$. Then, Lie–Trotter splitting method applied to Westervelt equation satisfies global error estimate

$$\|u_N - u(t_N)\|_{H^3 \times H^1} \leq C\Big(\|u_0 - u(0)\|_{H^3 \times H^1} + \tau\Big)\,, \quad t_N = N\tau \in [0,T]\,,$$

with constant depending on bounds for $\|u\|_{\mathscr{C}([0,t_N],H^6 \times H^5)}$, $\|u_0\|_{H^5 \times H^3}$, and final time t_N.

Remark. Straightforward extension to variable time stepsizes.

Illustration (Global error)

Situation.

- Consider Westervelt equation in single space dimension (facilitates computations)

$$a = 8\,, \quad \alpha = 1\,, \quad \beta = 1\,, \quad \gamma = \tfrac{1}{2}\,, \quad \delta = 2\gamma = 1\,,$$
$$\partial_{tt}\psi(x,t) - \alpha\,\partial_{xxt}\psi(x,t) - \beta\,\partial_{xx}\psi(x,t) = \delta\,\partial_t\psi(x,t)\,\partial_{tt}\psi(x,t)\,,$$
$$\psi(x,0) = \mathrm{e}^{-x^2}\,, \quad \partial_t\psi(x,0) = -\,x\,\mathrm{e}^{-x^2}\,, \quad (x,t) \in [-a,a]\times[0,T]\,,$$

  and impose homogeneous Dirichlet boundary conditions. Note that for chosen data solution to Westervelt equation is regular.

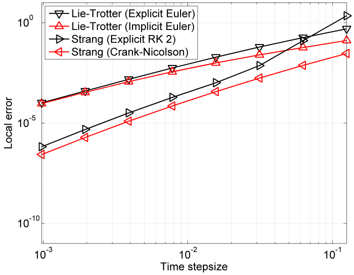
- Chose spatial grid width sufficiently fine such that global error dominated by time discretisation error ($M = 100$).

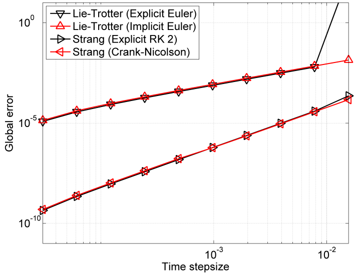
- Compare accuracy of Lie–Trotter and Strang splitting methods. For numerical solution of parabolic subproblem apply explicit and implicit time integrators of same order as underlying splitting method, i.e. combine Lie–Trotter splitting method with explicit and implicit Euler methods and Strang splitting method with second-order explicit Runge–Kutta method and Crank–Nicolson scheme. Note that use of explicit solvers requires sufficiently small time increments to avoid instabilities.

- Display local and global errors at time $T = 1$.

Illustration (Local and global errors)

Numerical results ($H^3 \times H^1$-norm). Time integration of Westervelt equation by Lie–Trotter and Strang splitting methods (Decomposition I). Comparison of different methods for numerical solution of subproblems. Computation of local (left) and global (right) errors with respect to $H^3 \times H^1$-norm. Nonstiff orders retained in accordance with convergence result.





Remark. Consider different ranges of time stepsizes for local error (include larger time stepsizes to study stability behaviour) and global error (include smaller time stepsizes to study attainable accuracy).

Conclusions and future work

Summary.

- Efficient time integration of Westervelt equation by operator splitting methods.
- Rigorous stability and error analysis for Lie–Trotter splitting method.

Relevant questions.

- Study of more involved models arising in nonlinear acoustics.

  Convergence of general model to reduced models such as Kuznetsov and Westervelt equations.
- Application of higher-order splitting methods (complex coefficients).
- Reliable and efficient time integration based on adaptive time stepsize control.

Thank you!