Time integration methods based on operator splitting and application to models from nonlinear acoustics

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Theme

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 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.

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. (2014) doi:10.1093/imanum/dru029

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

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

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

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

Subproblem (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

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

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

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 $0 = t_0 < \cdots < t_N \le T$ 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

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

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

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

Second-order Strang splitting method

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

Stability and error analysis of Lie–Trotter splitting method

Approach

Mein Verzicht auf das Restglied war leichtsinnig. (W. ROMBERG, 1979)

Situation. Apply first-order Lie–Trotter splitting method ($p = 1$) to nonlinear evolution equation (Westervelt equation)

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

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) = \mathrm{e}^{\tau_{n-1} D_A}\, \mathrm{e}^{\tau_{n-1} D_B}\, u_{n-1}$$

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

Consider situations where sufficiently regular solution exists (non-degenerate case, regular data, additional compatibility conditions satisfied)

$$\sup_{t \in [0,T]} \|u(t)\|_D \le C.$$

Local error representation. Deduce local error representation suitable for differential equations involving unbounded operators

$$\mathscr{L}_F(\tau, v) = \mathscr{S}_F(\tau, v) - \mathscr{E}_F(\tau, v) = \mathscr{O}\big(\tau^{p+1}, \|v\|_D\big).$$

Convergence analysis. Deduce convergence result by means of stability bounds and local error estimates

$$\|u_N - u(t_N)\|_X \le C\Big(\|u_0 - u(0)\|_X + \tau^p\Big).$$

Approach based on differential equations

Aim. Derivation compact local error expansion for Lie–Trotter splitting method applied to nonlinear evolution equation.

Basic idea. Derivation of differential equation for splitting operator in analogy to differential equation for evolution operator

$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,, \quad t \in (0,T)\,, \quad \mathscr{S}_F(0,\cdot) = I\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t,\cdot) = D_F\,\mathscr{E}_F(t,\cdot) = (D_A + D_B)\,\mathscr{E}_F(t,\cdot)\,, \quad t \in (0,T)\,, \quad \mathscr{E}_F(0,\cdot) = I\,.$$

Main tools. Nonlinear variation-of-constants formula (Alekseev–Gröbner), Lie-commutator.

Theorem (Descombes & Th. 2012)

Local error of Lie–Trotter splitting method admits (formal) integral representation

$$\mathscr{L}_F(t,\cdot) = \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\,\mathrm{e}^{\tau_2 D_B}\,[D_A, D_B]\,\mathrm{e}^{(\tau_1-\tau_2)D_B}\,\mathrm{e}^{(t-\tau_1)D_F}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1$$

$$= \int_0^t \int_0^{\tau_1} \partial_2\mathscr{E}_F\big(t-\tau_1, \mathscr{S}_F(\tau_1,\cdot)\big)\,\partial_2\mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\,[B,A]\big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\big)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,.$$

Compact local error expansion (Linear case, Lie)

Situation. Study Lie–Trotter splitting method applied to linear evolution equation

$$\mathscr{S}_F(t) = \mathrm{e}^{tB}\,\mathrm{e}^{tA} \approx \mathscr{E}_F(t) = \mathrm{e}^{t(A+B)}\,, \quad t \in (0,T)\,.$$

First step. Recall initial value problem for evolution operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t) = (A+B)\,\mathscr{E}_F(t)\,, \quad t \in (0,T)\,, \quad \mathscr{E}_F(0) = I\,.$$

In analogy, rewrite time derivative of splitting operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}_F(t) = B\,\mathscr{S}_F(t) + \mathrm{e}^{tB}\,A\,\mathrm{e}^{tA} = (A+B)\,\mathscr{S}_F(t) + \mathscr{R}(t)\,, \quad \mathscr{R}(t) = \left[\mathrm{e}^{tB}, A\right]\mathrm{e}^{tA}\,, \quad t \in (0,T)\,,$$

and obtain initial value problem for splitting operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}_F(t) = (A+B)\,\mathscr{S}_F(t) + \mathscr{R}(t)\,, \quad t \in (0,T)\,, \quad \mathscr{S}_F(0) = I\,.$$

Apply variation-of-constants formula to arrive at compact integral representation

$$\mathscr{L}_F(t) = \mathscr{S}_F(t) - \mathscr{E}_F(t) = \int_0^t \mathscr{E}_F(t-\tau)\,\mathscr{R}(\tau)\,\mathrm{d}\tau\,, \quad \mathscr{R}(t) = \left[\mathrm{e}^{tB}, A\right]\mathrm{e}^{tA}\,, \quad t \in (0,T)\,.$$

Compact local error expansion (Linear case, Lie)

Second step. Recall definition of remainder and note that relation $r(0) = 0$ suggests further expansion

$$\mathscr{R}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}_F(t) - (A+B)\,\mathscr{S}_F(t) = r(t)\,\mathrm{e}^{tA}\,, \quad r(t) = \left[\mathrm{e}^{tB}, A\right] = \mathrm{e}^{tB}A - A\,\mathrm{e}^{tB}\,, \quad t \in (0,T)\,.$$

Rewrite time derivative of commutator in suitable way to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\,r(t) = B\,\mathrm{e}^{tB}A - AB\,\mathrm{e}^{tB} = B\,r(t) + \left[B, A\right]\mathrm{e}^{tB}\,, \quad t \in (0,T)\,, \quad r(0) = 0\,.$$

Apply variation-of-constants formula to arrive at compact integral representation

$$r(t) = \left[\mathrm{e}^{tB}, A\right] = \int_0^t \mathrm{e}^{\tau B}\left[B, A\right]\mathrm{e}^{(t-\tau)B}\,\mathrm{d}\tau\,, \quad t \in (0,T)\,.$$

Local error expansion. Considerations imply compact local error expansion

$$\mathscr{L}_F(t) = \int_0^t \int_0^{\sigma_1} \mathscr{E}_F(t-\sigma_1)\,\mathrm{e}^{\sigma_2 B}\left[B, A\right]\mathrm{e}^{-\sigma_2 B}\,\mathscr{S}_F(\sigma_1)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,.$$

Provided that integrand bounded for suitable choice of norms, local error estimate follows

$$\|\mathscr{E}_F(\tau_{n-1}-\sigma_1)\,\mathrm{e}^{\sigma_2 B}[B, A]\,\mathrm{e}^{-\sigma_2 B}\,\mathscr{S}_F(\sigma_1)\,u(t_{n-1})\|_X \le C\,\|u(t_{n-1})\|_D$$

$$\Longrightarrow \quad \|\mathscr{L}_F(\tau_{n-1})\,u(t_{n-1})\|_X \le C\,\tau_{n-1}^2\,\|u(t_{n-1})\|_D\,.$$

Compact local error expansion (Nonlinear case, Lie)

Linear case. Recall compact local error expansion obtained for linear case

$$\mathscr{L}_F(t) = \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)(A+B)}\, \mathrm{e}^{(\tau_1-\tau_2)B} \big[B, A\big]\, \mathrm{e}^{\tau_2 B}\, \mathrm{e}^{\tau_1 A}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \,.$$

Extension to nonlinear case. Extend compact local error expansion for Lie–Trotter splitting method to nonlinear evolution equation

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

$$\mathscr{L}_F(t,v) = \mathscr{S}_F(t,v) - \mathscr{E}_F(t,v) = \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, v - \mathrm{e}^{tD_F}\, v\,.$$

Theorem (Descombes & Th. 2012)

Local error of Lie–Trotter splitting method admits (formal) integral representation

$$\begin{aligned}\mathscr{L}_F(t,\cdot) &= \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\, \mathrm{e}^{\tau_2 D_B} \big[D_A, D_B\big]\, \mathrm{e}^{(\tau_1-\tau_2)D_B}\, \mathrm{e}^{(t-\tau_1)D_F}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \\ &= \int_0^t \int_0^{\tau_1} \partial_2 \mathscr{E}_F\big(t-\tau_1, \mathscr{S}_F(\tau_1,\cdot)\big)\, \partial_2 \mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big) \\ &\qquad \times \big[B, A\big]\big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\big)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,.\end{aligned}$$

Application to Westervelt equation

Challenge. Study local error expansion for Westervelt equation

$$\mathscr{L}_F(t,\cdot) = \int_0^t \int_0^{\tau_1} \partial_2 \mathscr{E}_F\big(t-\tau_1, \mathscr{S}_F(\tau_1,\cdot)\big)\, \partial_2 \mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\big[B,A\big]\big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\big)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 .$$

Auxiliary results. Derive auxiliary regularity results for Westervelt equation, associated subproblems and variational equations, as well as estimate for Lie-commutator

$$\|\mathscr{E}_F(t,v)\|_{H^{k+6}\times H^{k+5}} \le \mathrm{e}^{Ct}\, \|v\|_{H^{k+6}\times H^{k+5}}, \quad k \in \mathbb{N}_{\ge 0},$$

$$\|\mathscr{E}_A(t,v)\|_{H^{k+4}\times H^{k+2}} \le \mathrm{e}^{Ct}\, \|v\|_{H^{k+4}\times H^{k+2}}, \quad k \in \mathbb{N}_{\ge 0},$$

$$\|\mathscr{E}_B(t,v)\|_{H^{k+2}\times H^{k}} \le \mathrm{e}^{Ct}\, \|v\|_{H^{k+2}\times H^{k}}, \quad k \in \mathbb{N}_{\ge 0},$$

$$\|\partial_2 \mathscr{E}_F(t,v)\, w\|_{H^{\ell+1}\times H^{\ell}} \le \mathrm{e}^{C(\|v\|_{H^4\times H^4})t}\, \|w\|_{H^{\ell+1}\times H^{\ell}}, \quad \ell = 0,1,2,3,$$

$$\|\partial_2 \mathscr{E}_A(t,v)\, w\|_{H^{k+2}\times H^{k}} \le \begin{cases} \mathrm{e}^{C(\|v\|_{H^5\times H^3})t}\, \|w\|_{H^{k+2}\times H^{k}}, & k = 0,1,2, \\ \mathrm{e}^{C(\|v\|_{H^7\times H^5})t}\, \|w\|_{H^{k+2}\times H^{k}}, & k \in \mathbb{N}_{\ge 3}, \end{cases}$$

$$\|\partial_2 \mathscr{E}_B(t,v)\, w\|_{H^{k+2}\times H^{k}} \le \mathrm{e}^{C(\|v\|_{H^{k+4}\times H^{k+2}})t}\, \|w\|_{H^{k+2}\times H^{k}}, \quad k \in \mathbb{N}_{\ge 0},$$

$$\|[A,B](v)\|_{H^{k+2}\times H^{k}} \le C\big(\|v\|_{H^{k+4}\times H^{k+2}}\big), \quad k \in \mathbb{N}_{\ge 0}.$$

Remark. Obtained regularity results imply stability estimate for splitting methods. Global error estimate follows by standard approach.

Main result

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

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

Apply auxiliary result that ensures regularity and boundedness of solution

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

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

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

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.

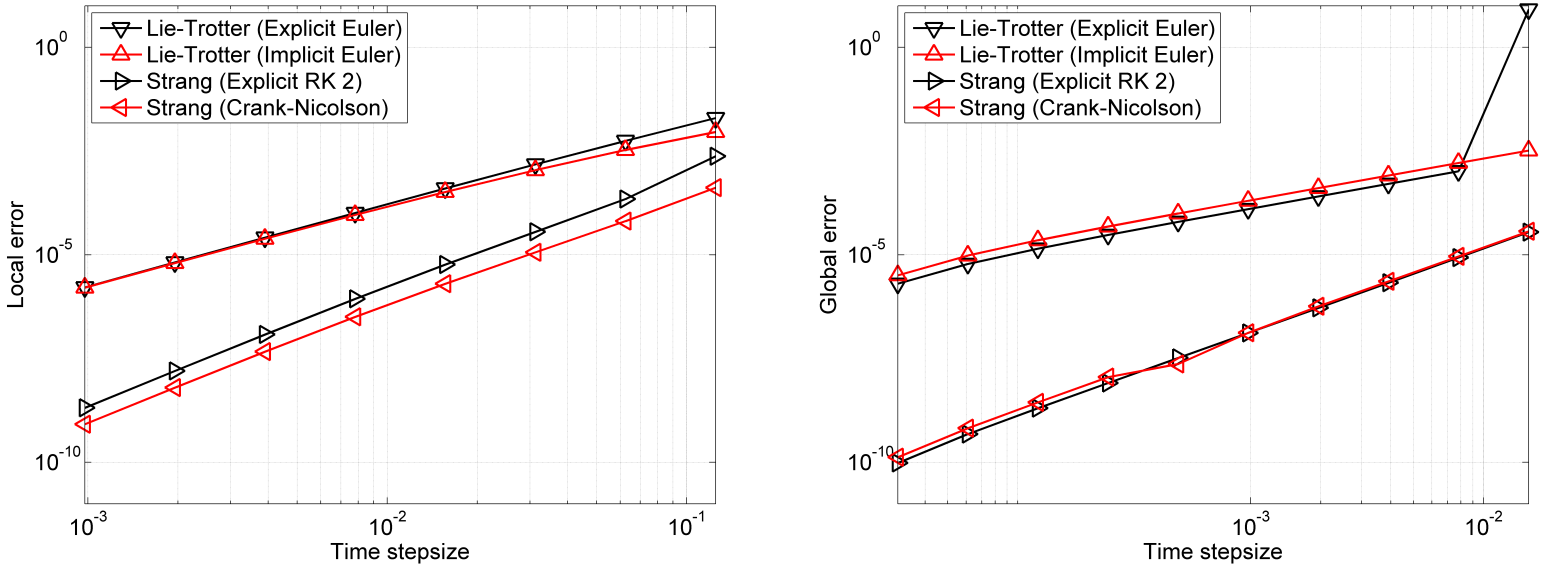
- Chose spatial grid width sufficiently fine such that global error dominated by time discretisation error ($M = 100$).

- 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)

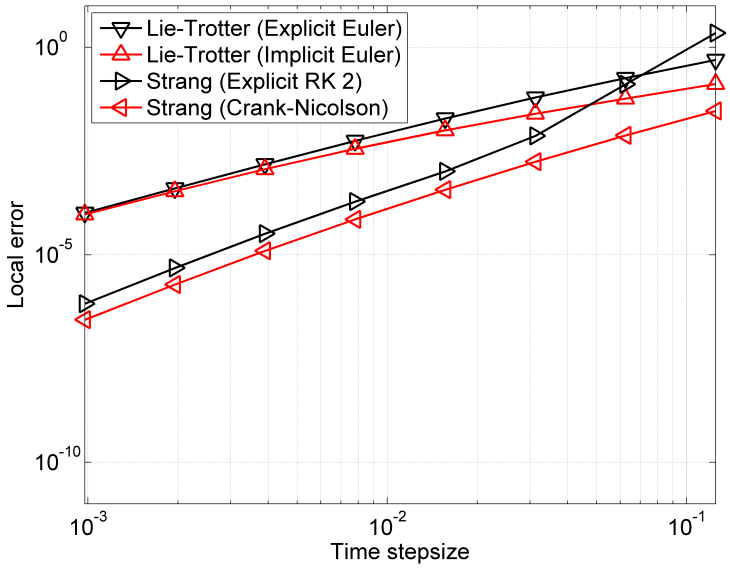
Numerical results ($L^2 \times L^2$-norm). Time integration of Westervelt equation by Lie–Trotter and Strang splitting methods (Decomposition I). Comparison of different methods for numerical solution of subproblems. Computation of local (left) and global (right) errors with respect to $L^2 \times L^2$-norm. Nonstiff orders of convergence retained.

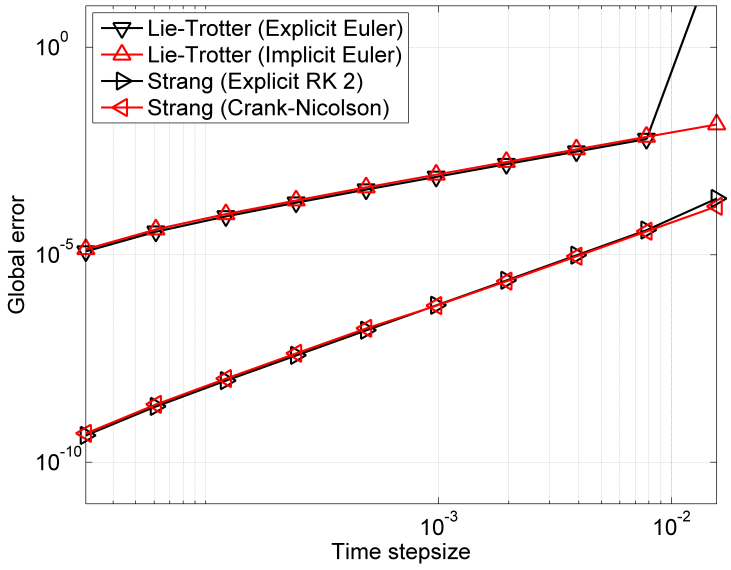


Remark. Consider different ranges of time stepsizes for local error (include larger time stepsizes to study stability behaviour) and global error (include smaller time stepsizes to study attainable accuracy).

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).

Illustration (Solution behaviour)

Situation.

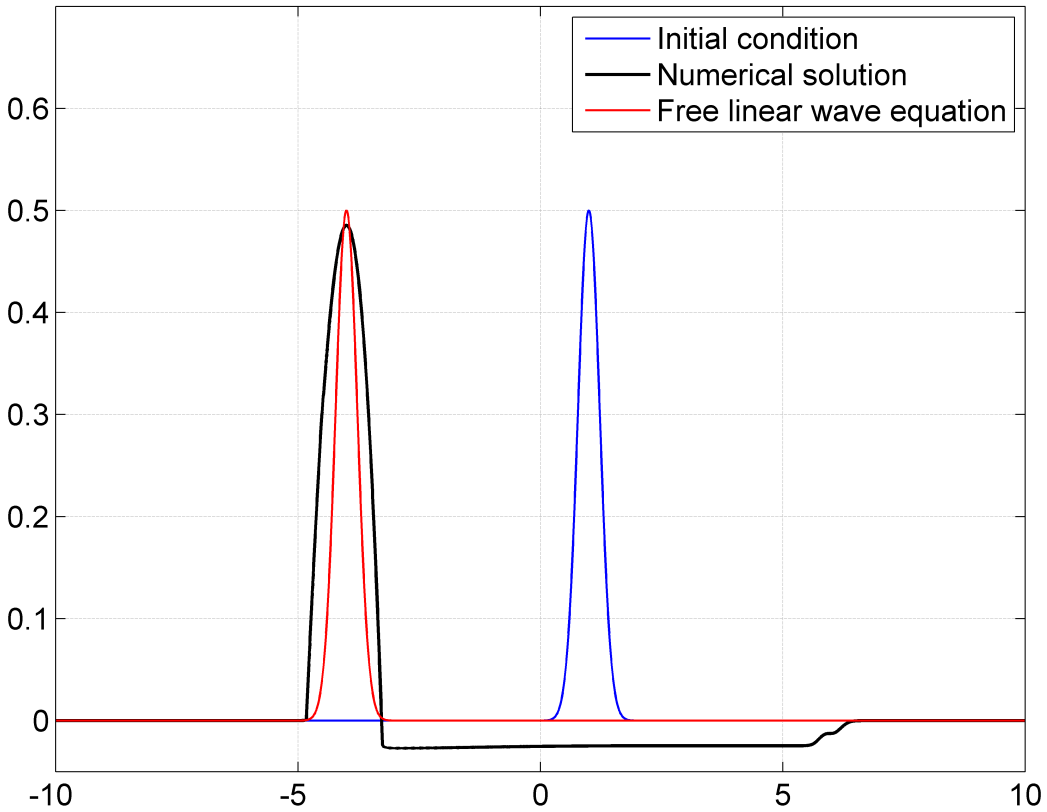
- Illustrate behaviour of solution $\psi : [-a, a] \times [0, T] \to \mathbb{R}$ to one-dimensional Westervelt equation with more realistic parameter, geometry, and excitation values

$$a = 15\,, \quad \alpha = 10^{-2}\,, \quad c = 10^3\,, \quad \beta = c^2 = 10^6\,, \quad \delta = 2 \cdot 10^{-4}\,,$$
$$\partial_{tt}\psi(x,t) - \alpha\,\partial_{xxt}\psi(x,t) - \beta\,\partial_{xx}\psi(x,t) = \delta\,\partial_t\psi(x,t)\,\partial_{tt}\psi(x,t)\,,$$
$$\psi(x,0) = \tfrac{1}{2}\,\mathrm{e}^{-10(x-1)^2}\,, \quad \partial_t\psi(x,0) = c\,\partial_x\psi(x,0) = -10\,c\,(x-1)\,\mathrm{e}^{-10(x-1)^2}\,.$$

- Display solution profile at time $t = 5 \cdot 10^{-3}$, computed by Lie–Trotter splitting method (Decomposition I, $N = 5 \cdot 10^4$, explicit Euler method) combined with Fast Fourier techniques ($M = 6 \cdot 10^3$).
- Observe travelling wave (to left) and slight one-sided steepening of pulse over time. Compare nonlinear model with simplified linear model (free linear wave equation)

$$\alpha = 0 = \delta : \qquad \partial_{tt}\psi(x,t) - c^2\,\partial_{xx}\psi(x,t) = 0\,.$$

Illustration (Solution behaviour)



Profile of acoustic velocity potential ψ at time $t = 5 \cdot 10^{-3}$ and comparison with solution to free linear wave equation.

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.

Open questions.

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

Thank you!