Fundamental models in nonlinear acoustics: analytical and numerical aspects

Mechthild Thalhammer Leopold–Franzens Universität Innsbruck, Austria

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Overview on current research activities

Within the core of numerics.

- S. BLANES (Valencia), F. CASAS (Castellón), C. GONZÁLEZ (Valladolid) Involvement in Spanish research project
- J. A. CARRILLO (Oxford) BritInn–Fellowship
- Hamiltonian systems, Schrödinger equations, Parabolic equations, Kinetic equations (Vlasov–Maxwell–Poisson systems) Project proposal submitted (FWF)



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Overview on current research activities

Beyond numerics - towards dynamical systems and stochastics.

- E. HAUSENBLAS (Leoben) Stochastic partial differential equations (Reaction-diffusion systems, pattern formation)
- CH. KÜHN (Munich) Network dynamics (models for epidemics) Stochastic partial differential equations (Rough paths) Special issue contribution Involvement in submitted project proposal (DFG) Project proposal in preparation (FWF, 2021)

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Overview on current research activities

Beyond numerics - towards modelling and analysis.

 B. KALTENBACHER (Klagenfurt) Nonlinear damped wave equations Special issue contribution Project proposal in preparation (DA)

... theme of this talk ...

Why this theme?

- My current research focus because of
 - contribution to special issue (with BARBARA KALTENBACHER),
 - planning of DA research proposal (initiated by TOM LAHNER).
- Comprehensive and demanding theme that includes various aspects of applied mathematics (modelling, analysis, numerics).
 - fascinating phenomena,
 - beautiful mathematics,
 - numerical challenges.
- Open questions remain, e.g.
 - derivation and theoretical analysis of fundamental models,

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• design and convergence analysis of numerical methods.

Our contributions and work in process

B. KALTENBACHER, M. TH. Fundamental models in nonlinear acoustics. Part I. Analytical comparison. M3AS 28/12 (2018) 2403–2455.

- Derivation of fundamental models
- Existence and regularity of solutions
- Rigorous justification of limiting models

... some details on our derivation of the most general model ...

Our contributions and work in process

- B. KALTENBACHER, V. 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.
- B. KALTENBACHER, M. TH. Fundamental models in nonlinear acoustics. Part II. Numerical comparison. In preparation.
- B. KALTENBACHER, M. TH.

Convergence of implicit Runge–Kutta time discretisation methods for fundamental models in nonlinear acoustics. In preparation.

... some details on numerical issues and our different approaches to resolve them ...

General model

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Theme ... getting familiar ...

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Nonlinear acoustics

• Field of nonlinear acoustics concerned with propagation of sound waves in thermoviscous fluids.

High-intensity ultrasound applications

- Focus on applications of high-intensity ultrasound such as
 - medical treatment (lithotripsy, thermotherapy),
 - industrial applications (ultrasound cleaning, welding).
- Term ultrasound used for sound waves with frequencies above range of human hearing.

• Realistic models given by nonlinear partial differential equations.

Our most general model ... and how we have deduced it ...

Derivation of fundamental models

Relevant quantities. Consider basic state variables of acoustics

mass density ρ , acoustic particle velocity v, acoustic pressure p, temperature T.

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Derivation of fundamental models

Approach. Derivation of fundamental models relies on physical and mathematical principles.

- Employ decomposition of state variables into constant mean values ρ_0, ν_0, p_0, T_0 and space-time-dependent fluctuations $\rho_{\sim}, \nu_{\sim}, p_{\sim}, T_{\sim}$.
- Use Helmholtz decomposition of acoustic particle velocity and assign irrotational part to gradient of acoustic velocity potential

$$v_{\sim} = \nabla \boldsymbol{\psi} + \nabla \times S.$$

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Derivation of general model

• Employ conservation laws for mass, momentum, energy

$$\begin{split} \partial_t \varrho + \nabla \cdot (\varrho v) &= 0, \\ \partial_t (\varrho v) + v \nabla \cdot (\varrho v) + \varrho (v \cdot \nabla) v + \nabla p &= \mu \Delta v + \left(\mu_B + \frac{1}{3} \mu \right) \nabla (\nabla \cdot v), \\ \varrho (c_V \partial_t T + c_V v \cdot \nabla T + \frac{c_p - c_V}{\alpha_V} \nabla \cdot v) \\ &= a \Delta T + \left(\mu_B - \frac{2}{3} \mu \right) (\nabla \cdot v)^2 + \frac{1}{2} \mu \left\| \nabla v + (\nabla v)^T \right\|_F^2, \end{split}$$

as well as equation of state for acoustic pressure

$$p_{\sim} \approx A \frac{\rho_{\sim}}{\rho_0} + \frac{B}{2} \left(\frac{\rho_{\sim}}{\rho_0}\right)^2 + \hat{A} \frac{T_{\sim}}{T_0}.$$

- Accordingly to BLACKSTOCK (1963) and LIGHTHILL (1956), take firstand second-order contributions with respect to fluctuating quantities into account.
- Express resulting equations in terms of acoustic velocity potential.

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Fundamental models

 General model. Above approach leads to general model (compact formulation, Blackstock–Crighton–Brunnhuber–Jordan–Kuznetsov equation with additional term and particular structure of linear part)

$$\begin{split} & \left(\partial_{ttt} - \beta_1^{(a)} \,\Delta \partial_{tt} + \beta_2^{(a)}(\sigma_0) \,\Delta^2 \partial_t - \beta_3 \,\Delta \partial_t + \beta_4^{(a)}(\sigma_0) \,\Delta^2\right) \psi^{(a)}(t) \\ & + \,\partial_{tt} \left(\frac{1}{2} \,\beta_5(\sigma) \left(\partial_t \psi^{(a)}(t)\right)^2 + \beta_6(\sigma) \left|\nabla \psi^{(a)}(t)\right|^2\right) = 0, \quad t \in (0,T) \,. \end{split}$$

• **Reduced models.** Commonly used Kuznetsov and Westervelt equations result when neglecting thermal effects $(a \rightarrow 0_+)$

$$\begin{aligned} \left(\partial_{tt} - \beta_1^{(0)} \Delta \partial_t - \beta_3 \Delta\right) \psi(t) \\ + \partial_t \left(\frac{1}{2} \beta_5(\sigma) \left(\partial_t \psi(t)\right)^2 + \beta_6(\sigma) \left|\nabla \psi(t)\right|^2\right) &= 0, \quad t \in (0, T). \end{aligned}$$

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• **Contribution.** Rigorous justification as limiting models based on existence and regularity result (KALTENBACHER, TH., 2018).

Our most general model ... to get some intuition ...

General model

Numerical illustration (1D). Study effect of nonlinearity for (rather) realistic parameter values. Observe expected solution profile (sharper peak, sawtooth-like derivative).



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Our most general model ... relevant applications ...

Propagation of ultrasound waves inside human body

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.

https://www.healthline.com https://www.slideshare.net/aaaa-2012/ renal-stones-55054355





Need for optimal design of high-intensity ultrasound devices!

Numerical issues

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Numerical challenges

Practical realisation - a demanding task ...

- Mathematical optimisation of high-intensity ultrasound devices based on transient numerical simulations still beyond scope of existing approaches.
- Numerical challenges are
 - complexity of underlying nonlinear damped wave equations,
 - treatment of most relevant case of three space dimensions,
 - different magnitudes of physical parameters.

Numerical approach

Standard numerical approach.

• Use finite differences and explicit methods.

Our (first) straightforward numerical approach.

• Combine fast Fourier techniques (high resolution, computation of space derivatives) and explicit Runge–Kutta methods.

... our code works in 3D ... in principle ...

Linear damped wave equation

Simple special case.

• Consider linear damped wave equation (Westervelt, $\alpha_3 \rightarrow 0$)

 $\partial_{tt}\psi(t)-\alpha_2\,\Delta\partial_t\,\psi(t)-\alpha_1\,\Delta\psi(t)+\alpha_3\,\partial_t\psi(t)\,\partial_{tt}\psi(t)=0\,,\quad t\in(0,T)\,.$

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• Use solution representation by elementary functions (teaching talk).

Linear damped wave equation

Linear damped wave equation.

• Study linear damped wave equation

PDE: $\partial_{tt}\psi(t) - \alpha_2 \Delta \partial_t \psi(t) - \alpha_1 \Delta \psi(t) = 0$.

• Apply Fourier spectral method to reveal system of decoupled ordinary differential equations

$$\begin{split} \psi(t) &= \sum_{m \in \mathbb{Z}} \psi_m(t) \,\mathscr{F}_m \,, \\ \Delta \mathscr{F}_m &= \lambda_m \,\mathscr{F}_m \,, \quad \lambda_m \propto -m^2 \,, \quad m \in \mathbb{Z} \,, \\ \sum_{m \in \mathbb{Z}} \left(\psi_m''(t) - \alpha_2 \,\lambda_m \,\psi_m'(t) - \alpha_1 \,\lambda_m \,\psi_m(t) \right) &= 0 \,. \end{split}$$

• Study equation for linear damped oscillation

ODE:
$$\psi_m''(t) - \alpha_2 \lambda_m \psi_m'(t) - \alpha_1 \lambda_m \psi_m(t) = 0$$

Linear damped wave equation

Solution representation.

• Decisive quantities (exponents)

$$c_1 = c_1(\lambda_m, \alpha_1, \alpha_2) = \frac{1}{2} \left(\alpha_2 \lambda_m + \sqrt{\alpha_2^2 \lambda_m^2 + 4 \alpha_1 \lambda_m} \right),$$

$$c_2 = c_2(\lambda_m, \alpha_1, \alpha_2) = \frac{1}{2} \left(\alpha_2 \lambda_m - \sqrt{\alpha_2^2 \lambda_m^2 + 4 \alpha_1 \lambda_m} \right).$$

Solution given by

$$\begin{split} \psi_0(t) &= \psi_0(0) + t \,\psi_0'(0)\,,\\ \psi_m(t) &= \frac{1}{c_2 - c_1} \left(\left(c_2 \,\mathrm{e}^{c_1 t} - c_1 \,\mathrm{e}^{c_2 t} \right) \psi_m(0) + \left(\mathrm{e}^{c_2 t} - \mathrm{e}^{c_1 t} \right) \psi_m'(0)\,, \quad m \in \mathbb{Z} \setminus \{0\}\,. \end{split}$$

Linear damped wave equation

Numerical illustration (1D). Verification of time integration method by solution representation for linear wave equation ($\alpha_2 = \alpha_3 = 0$) and linear damped wave equation ($\alpha_3 = 0$) (and vice versa).



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Numerical issues

Small adaptation of code works for Westervelt equation.

http://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_Westervelt_3.m4v Suitable adaptation of code works for general model.

http://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_GeneralModel_30.m4v

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Numerical issues

Numerical illustration (1D). Numerical study of linear wave equations shows that application of explicit (Runge–Kutta) methods successful, but only under severe restrictions. Sufficiently small time stepsizes needed to ensure stability!

Linear wave equation without damping

Time step	2.50e-02	1.25e-02	6.25e-03	3.12e-03	1.56e-03
Error	1.47e+18	1.04e-08	6.50e-10	4.06e-11	2.54e-12
Order	—	3.99e+00	3.99e+00	4.00e+00	4.00e+00

Linear wave equation with damping As range of eigenvalues larger, smaller time stepsizes needed.

Time step	1.25e-04	6.25e-05
Error	NaN	3.09e-14

Our alternative approaches

... operator splitting, what else stiffly accurate implicit Runge–Kutta methods ...

Operator splitting

Basic idea and theoretical result. Employ *splitting* of Westervelt equation into nonlinear diffusion equation and simple *remainder*

 $\partial_{tt}\psi(t) - \left(1 + \alpha_3 \partial_t \psi(t)\right)^{-1} \alpha_2 \Delta \partial_t \psi(t) - \left(1 + \alpha_3 \partial_t \psi(t)\right)^{-1} \alpha_1 \Delta \psi(t) = 0.$

$$\Psi = \partial_t \psi, \quad \partial_t \Psi(t) - \left(1 + \alpha_3 \Psi(t)\right)^{-1} \alpha_2 \Delta \Psi(t) = 0.$$

Benefits. Requires adaptation of existing code (only) in few places. Weaker stepsize restrictions for explicit solvers (for realistic parameters).

Theorem (B. KALTENBACHER, V. NIKOLIĆ, M. TH. (2015))

First-order splitting method applied to Westervelt equation with regular and consistent initial data satisfies global error estimate

$$\|\psi_N - \psi(t_N)\|_{H^3 \times H^1} \le C \left(\|\psi_0 - \psi(0)\|_{H^3 \times H^1} + \tau \right), \quad \tau = T/N.$$

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Work in progress. Extension to general model.

Suitable methods for variational equations

Basic idea and theoretical result. Implicit Runge–Kutta and Galerkin methods are ideal for variational approach. Proof of convergence (with rate).

Work in progress to honour J. Gwinner (Univ. Bundeswehr München)

• B. KALTENBACHER, M. TH.

Convergence of implicit Runge–Kutta time discretisation methods for fundamental models in nonlinear acoustics

In preparation for Journal of Applied and Numerical Optimization – Special Issue on Nonsmooth Variational Problems and Optimal control.

Dedicated to Joachim Gwinner on the occasion of his 70th birthday.

Our main inspiration and former work

J. GWINNER, M. TH.

Full discretisations for nonlinear evolutionary inequalities based on stiffly accurate Runge–Kutta and hp-finite element methods.

Found. Comput. Math. 14 (2014) 913-949.

Dedicated to John Butcher on the occasion of his 80th birthday.

Conclusions

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My perspective

My motivation.

• Relevant theme from applied mathematics

My starting point.

• Mathematical model in form of nonlinear partial differential equation (or related evolutionary problem)

My expertise.

- Design reliable and efficient numerical methods
- Provide rigorous stability and error analysis

Nonlinear partial differential equations: A comprehensive and demanding theme with fascinating applications in various fields

Thank you!

Aim. Prove existence and regularity of weak solution to most general model (BJK) under standard assumptions and smallness requirement on initial energies.

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

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

• Impose homogeneous Dirichlet boundary conditions

$$\begin{split} \partial_{tt}\psi(t)|_{\partial\Omega} &= 0, \quad \Delta\partial_t\psi(t)|_{\partial\Omega} = 0, \quad \Delta\psi(t)|_{\partial\Omega} = 0, \\ \partial_{ttt}\psi(t)|_{\partial\Omega} &= 0, \quad \Delta\partial_tt\psi(t)|_{\partial\Omega} = 0. \end{split}$$

• Suppose that prescribed initial data satisfy regularity and compatibility conditions

$$\psi_0,\psi_1\in H^3(\Omega)\cap H^1_0(\Omega)\,,\quad \Delta\psi_0,\Delta\psi_1,\psi_2\in H^1_0(\Omega)\,.$$

Smallness requirement.

• 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

$$\begin{aligned} \left\| \psi_{2} \right\|_{L_{2}}^{2} + \beta_{2}^{(a)}(\sigma_{0}) \left\| \Delta \psi_{1} \right\|_{L_{2}}^{2} + \left\| \nabla \psi_{1} \right\|_{L_{2}}^{2} \leq \overline{e}_{0}, \\ \left\| \nabla \psi_{2} \right\|_{L_{2}}^{2} + \beta_{2}^{(a)}(\sigma_{0}) \left\| \nabla \Delta \psi_{1} \right\|_{L_{2}}^{2} + \left\| \Delta \psi_{1} \right\|_{L_{2}}^{2} \leq \overline{e}_{1}, \end{aligned}$$

following quantity is sufficiently small

$$\begin{split} M\left(\overline{e}_{0},\overline{e}_{1}\right) &= \frac{C_{\mathrm{PF}}^{2}C_{L_{4}}^{2} - \mu^{1}\beta_{5}(\sigma)}{\underline{\beta}_{1}}\sqrt{\overline{e}_{0}} + C_{0}\overline{e}_{1} \\ &+ \frac{C_{2}}{\underline{\beta}_{1}}\left(\left\|\Delta\psi_{0}\right\|_{L_{2}}^{2} + C_{3}T^{2}\overline{e}_{1}\right) + C_{4}\left(\frac{1}{2}\left\|\nabla\Delta\psi_{0}\right\|_{L_{2}} + \sqrt{\overline{e}_{1}}\right). \end{split}$$

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There exists a weak solution

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

to the associated equation

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

obtained by integration with respect to time.

Theorem

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This solution satisfies a priori energy estimates of the form

$$\mathcal{E}_{0}(\psi(t)) = \left\|\partial_{tt}\psi(t)\right\|_{L_{2}}^{2} + \beta_{2}^{(a)}(\sigma_{0})\left\|\Delta\partial_{t}\psi(t)\right\|_{L_{2}}^{2} + \left\|\nabla\partial_{t}\psi(t)\right\|_{L_{2}}^{2},$$

$$\mathcal{E}_{1}(\psi(t)) = \left\|\nabla\partial_{tt}\psi(t)\right\|_{L_{2}}^{2} + \beta_{2}^{(a)}(\sigma_{0})\left\|\nabla\Delta\partial_{t}\psi(t)\right\|_{L_{2}}^{2} + \left\|\Delta\partial_{t}\psi(t)\right\|_{L_{2}}^{2},$$

$$\sup_{\epsilon[0,T]}\mathcal{E}_{0}(\psi(t)) \leq \overline{E}_{0}, \quad \sup_{t\in[0,T]}\mathcal{E}_{1}(\psi(t)) \leq \overline{E}_{1}, \quad \int_{0}^{T}\left\|\Delta\partial_{tt}\psi(t)\right\|_{L_{2}}^{2} dt \leq \overline{E}_{2},$$

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

$$0 < \underline{\alpha} = \frac{1}{2} \le \left\| 1 + \beta_5(\sigma) \,\partial_t \psi \right\|_{L_{\infty}([0,T], L_{\infty}(\Omega))} \le \overline{\alpha} = \frac{3}{2},$$

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

Main tools of proof.

• Derivation of a priori bound for higher-order energy functional

$$\begin{split} \sup_{t \in [0,T]} \left(\left\| \nabla \partial_{tt} \psi^{(a)}(t) \right\|_{L_{2}}^{2} + \beta_{2}^{(a)}(\sigma_{0}) \left\| \nabla \Delta \partial_{t} \psi^{(a)}(t) \right\|_{L_{2}}^{2} + \left\| \Delta \partial_{t} \psi^{(a)}(t) \right\|_{L_{2}}^{2} \right) \\ + \int_{0}^{T} \left\| \Delta \partial_{tt} \psi^{(a)}(t) \right\|_{L_{2}}^{2} \mathrm{d}t \leq C \,. \end{split}$$

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

Basic ideas

Splitting methods.

• Study linear ordinary differential equation with natural decomposition of right-hand side

$$u'(t) = (A+B) u(t), \quad t \in (0,T).$$

Solution given by matrix exponential

$$u(t) = e^{t (A+B)} u(0), \quad t \in [0, T].$$

• Lie-Trotter splitting yields first-order approximation

$$\mathbf{e}^{tB} \mathbf{e}^{tA} \approx \mathbf{e}^{t(A+B)}$$

• Strang splitting yields second-order approximation

$$\mathbf{e}^{\frac{t}{2}A}\mathbf{e}^{tB}\mathbf{e}^{\frac{t}{2}A} \approx \mathbf{e}^{t(A+B)}$$

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Basic ideas

Local error analysis.

• For Lie–Trotter splitting, employ compact local error representation

$$e^{tB} e^{tA} - e^{t(A+B)} = \int_0^t \int_0^{\tau_1} e^{(t-\tau_1)(A+B)} e^{(\tau_1-\tau_2)B} [B, A] e^{\tau_2 B} e^{\tau_1 A} d\tau_2 d\tau_1,$$

deduced and exploited with S. DESCOMBES in context of linear and nonlinear Schrödinger equations in semiclassical regime.

Extension.

• Extend approach to Westervelt equation involving two unbounded nonlinear operators

$$\partial_{tt}\psi(t) - \left(1 + \alpha_3 \partial_t \psi(t)\right)^{-1} \alpha_2 \Delta \partial_t \psi(t) - \left(1 + \alpha_3 \partial_t \psi(t)\right)^{-1} \alpha_1 \Delta \psi(t) = \mathbf{0}.$$

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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).