Oblivious quadrature for long-time computation of waves

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Heriot-Watt University, Edinburgh

LMS-EPSRC Durham symposium, 12th July 2014

Based on work with: Volker Gruhne, María López Fernández (Zurich), Christian Lubich (Tübingen), Francisco-Javier Sayas (Delaware), Achim Schädle (Düsseldorf)

Oblivious quadrature for long-time computation of waves and the coupling of implicit/explicit time-stepping

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Outline

1. A model problem
2. Coupling of different time-discretizations
3. Oblivious quadrature for long time computation
4. Conclusions

A model problem: Damped wave equation

Consider, for some bounded domain Ω with boundary Γ,

$$\begin{aligned} \frac{1}{c(x)^2}\partial_t^2 u + \alpha\partial_t u - \Delta u = f, &\quad \text{in } \Omega \times \mathbb{R}_{>0}, \\ u(\cdot,0) = u_0, \quad \partial_t u(\cdot,0) = v_0, &\quad \text{in } \Omega, \\ \partial_\nu u = -\sqrt{\partial_t^2 + \alpha\partial_t}\, u, &\quad \text{on } \Gamma \times \mathbb{R}_{>0}, \end{aligned}$$

with f, u_0, v_0, $c(x) - 1$, compactly supported in Ω and $\alpha > 0$.

- We can think of this as the damped wave equation with corresponding zero-order absorbing boundary condition.
- Note that $u = 0$ near Γ at time $t = 0$.

Motivation behind the problem

Some properties of the $\sqrt{\partial_t^2 + \alpha\partial_t}$:

- A non-local operator with infinite memory.
- Taking the Laplace transform

$$\left(\mathscr{L}\sqrt{\partial_t^2 + \alpha\partial_t}\right)(s) = \sqrt{s^2 + \alpha s}$$

  we obtain an operator analytic and polynomially bounded in $\mathbb{C} \setminus (-\infty, 0]$ – an operator of parabolic type.

Motivation for considering:

- Similarities with 2D and damped wave equation fundamental solutions:

$$\frac{H(t-r)}{4\sqrt{t^2 - r^2}} \text{ – 2D} \qquad \frac{e^{-\sqrt{s^2+\alpha s}\, r}}{4\pi r} \text{ – 3D damped in Laplace domain.}$$

- Gives a simple example of a coupled linear hyperbolic/parabolic system, where the coupling of different time-discretizations is of interest.

Meaning of $\sqrt{\partial_t^2 + \alpha\partial_t}$.

- For sufficiently smooth causal f and $F(s) = (\mathscr{L}f)(s)$

$$(\mathscr{L}(\partial_t f))\,(s) = sF(s).$$

  Note that $\partial_t f$ can be understood as the convolution

$$\delta' * f.$$

- Similarly

$$\sqrt{\partial_t^2 + \alpha\partial_t}\, f(t) = \int_{\sigma+\mathrm{i}\mathbb{R}} e^{st}\sqrt{s^2+\alpha s}\, F(s)\,\mathrm{d}s$$

  and can also be understood as a convolution, which is continuous and causal if

$$|\mathscr{L}f(s)| \leq C|s|^{-\mu}$$

  for $\mu > 2$ and $\operatorname{Re} s \geq \sigma > 0$.

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Variational formulation and spatial discretization

Let $S_h \subset H^1(\Omega)$ be a piecewise linear finite element space. Find $u_h(\cdot, t) \in S_h$ such that

$$(\partial_t^2 u_h + \alpha \partial_t u_h, v)_{L^2(\Omega)} + (\nabla u_h, \nabla v)_{L^2(\Omega)} + \left\langle \sqrt{\partial_t^2 + \alpha \partial_t}\, u_h, v \right\rangle_{L^2(\Gamma)} = (f, v)_{L^2(\Omega)}$$

and $u_h(0) = u_{0,h}$, $\partial_t u_h(0) = v_{0,h}$.

Variational formulation and spatial discretization

Let $S_h \subset H^1(\Omega)$ be a piecewise linear finite element space. Find $u_h(\cdot, t) \in S_h$ such that

$$(\ddot{u}_h + \alpha \dot{u}_h, v)_{L^2(\Omega)} + (\nabla u_h, \nabla v)_{L^2(\Omega)} + \left\langle \sqrt{1 + \alpha \partial_t^{-1}}\, \dot{u}_h, v \right\rangle_{L^2(\Gamma)} = (f, v)_{L^2(\Omega)}$$

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and $u_h(0) = u_{0,h}$, $\dot{u}_h(0) = v_{0,h}$.

- We plan to discretize $\dot{u}$ and ∂_t^{-1} with different discretization schemes.
- Testing with $v = \dot{u}_h$ we obtain the energy identity (for $f = 0$)

$$E(t) = E(0) - \int_0^t \alpha \|\dot{u}_h\|^2_{L^2(\Omega)} d\tau - \int_0^t \left\langle \sqrt{1+\alpha\partial_t^{-1}}\, \dot{u}_h, \dot{u}_h \right\rangle_{L^2(\Gamma)} d\tau.$$

where

$$E(t) = \tfrac{1}{2}\|\dot{u}_h\|^2_{L^2(\Omega)} + \tfrac{1}{2}\|\nabla u_h\|^2_{L^2(\Omega)}.$$

Positivity of the boundary term [LB, Lubich, Sayas 2014]

Lemma

For a sufficiently smooth causal $\varphi(\cdot, t) \in H^{1/2}(\Gamma)$

$$\int_0^t \left\langle \sqrt{1 + \alpha \partial_t^{-1}}\, \varphi, \varphi \right\rangle_{L^2(\Gamma)} d\tau \geq \int_0^t \|\varphi\|^2 d\tau.$$

Proof: For $\sigma > 0$ consider

$$\int_{\mathbb{R}} e^{-2\sigma\tau} \left\langle \sqrt{1 + \alpha \partial_t^{-1}}\, \varphi, \varphi \right\rangle_{L^2(\Gamma)} d\tau = \int_{\mathbb{R}} \sqrt{1 + \alpha s^{-1}} \|\Phi(s)\|^2 d\omega,$$

where, $s = \sigma + i\omega$, $\Phi(s) = \mathscr{L}\varphi(s)$. The proof is finished by noticing that

$$\operatorname{Re} \sqrt{1 + \alpha s^{-1}} \geq 1 \implies$$

$$\int_{\mathbb{R}} e^{-2\sigma\tau} \left\langle \sqrt{1 + \alpha \partial_t^{-1}}\, \varphi, \varphi \right\rangle_{L^2(\Gamma)} d\tau \geq \int_{\mathbb{R}} e^{-2\sigma\tau} \|\varphi\|^2 d\tau.$$

Discretizing $\sqrt{\partial_t^2 + \alpha\partial_t}$ – Convolution quadrature [Lubich '88]

- $\partial_t u(t) \approx \partial_{\Delta t} u(t) = \dfrac{u(t) - u(t-\Delta t)}{\Delta t}$. Then

$$(\mathscr{L}\partial_{\Delta t} u)(s) = \left(\frac{1 - e^{-s\Delta t}}{\Delta t}\right) U(s) = s_{\Delta t} U(s).$$

  Note $s_{\Delta t} = s(1 + O(s\Delta t))$.

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  Note $s_{\Delta t} = s(1 + O(s\Delta t))$.

- Similarly $\sqrt{1 + \alpha\partial_t^{-1}}\, u(t) \approx \sqrt{1 + \alpha\partial_{\Delta t}^{-1}}\, u(t)$ where

$$\left(\mathscr{L}\sqrt{1 + \alpha\partial_{\Delta t}^{-1}}\, u\right)(s) = \sqrt{1 + \alpha s_{\Delta t}^{-1}}\, U(s).$$

  Expanding

$$\sqrt{1 + \alpha s_{\Delta t}^{-1}} = \sum_{j=0}^{\infty} \omega_j e^{-sj\Delta t}$$

  we get that

$$\sqrt{1 + \alpha\partial_{\Delta t}^{-1}}\, u(t) = \sum_{j=0}^{\infty} \omega_j u(t - t_j).$$

Computing the weights ω_j and extensions

- The weights are Taylor coefficients of the analytic function

$$\sqrt{1 + \alpha \frac{\Delta t}{1-z}} = \sum_{j=0}^{\infty} \omega_j z^j$$

  and can hence be efficiently computed using contour integrals and FFTs.
- Similarly higher order $A(\theta)$-stable linear multistep or Runge-Kutta methods can be used as the basis for discretization.

Example for $\alpha = 1/2$, $\Delta t = 1/100$:

j	0	1	2	3
ω_j	1.0024969	0.0024938	0.0024907	0.0024876

Fully discrete system

Writing $t_j = j\Delta t$ and u_j an approximation of $u_h(t_j)$ the fully discrete system reads

$$\frac{1}{\Delta t^2}(u_{n+1} - 2u_n + u_{n-1}, v) + (\alpha \dot{u}_n, v) + (\nabla u_n, \nabla v) + \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_n), v \right\rangle = (f_n, v),$$

where $\dot{u}_n = \frac{1}{2\Delta t}(u_{n+1} - u_{n-1})$.

- To obtain an energy identity test again with $v = \dot{u}_n$ (for $f = 0$) and sum over n to obtain

$$E_{N+1/2} = E_{1/2} - \Delta t \sum_{n=0}^{N} \alpha \|\dot{u}_n\|^2 - \Delta t \sum_{n=0}^{N} \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_n), \dot{u}_n \right\rangle,$$

  where the discrete energy

$$E_{n+1/2} = \frac{1}{2} \left\| \frac{u_{n+1} - u_n}{\Delta t} \right\|^2 + \frac{1}{2}(\nabla u_n, \nabla u_{n+1})$$

  is positive under the usual CFL condition.

Positivity of the discretized boundary term [LB, Lubich, Sayas 2014]

Lemma

We have

$$\sum_{n=0}^{N} \left\langle \sqrt{1+\alpha \partial_{\Delta t}^{-1}}\, v(t_n), v_n \right\rangle \geq 0.$$

Proof is similar and requires that

$$\mathrm{Re}\, \sqrt{1+\alpha/s^{\Delta t}} > 0.$$

- This is true as long as $s^{\Delta t}$ avoids the negative real axis.
- For $s = \mathrm{i}\omega$, $s^{\Delta t}$ traverses the boundary of the stability region, hence the above holds for $A(\theta)$-stable methods.

Different time-steps: version 1

The time-step may be severely restricted by the CFL condition. So use

$$\kappa = \Delta t / k, \qquad k \in \mathbb{N},$$

in the interior. Denote $t_{n,\ell} = n\Delta t + \ell\kappa = n\Delta t + (\ell/k)\Delta t$ and $u_{n,\ell}$ the corresponding approximation.

$$\frac{1}{\kappa^2}(u_{n,\ell+1} - 2u_{n,\ell} + u_{n,\ell-1}, v) + (\alpha \dot{u}_{n,\ell}, v) + (\nabla u_{n,\ell}, \nabla v) \\ + \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_{n,\ell}), v \right\rangle = (f_{n,\ell}, v),$$

where $\dot{u}_{n,\ell} = \frac{1}{2\kappa}(u_{n,\ell+1} - u_{n,\ell-1})$.

- To obtain an energy identity test again with $v = \dot{u}_{n,\ell}$ and sum over n *and* ℓ to obtain

$$E_{N,1/2} = E_{0,1/2} - \kappa \sum_{\ell=0}^{k-1} \sum_{n=0}^{N} \alpha \|\dot{u}_n\|^2 - \kappa \sum_{\ell=0}^{k-1} \sum_{n=0}^{N} \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_{n,\ell}), \dot{u}_{n,\ell} \right\rangle$$

Comments on version 1

- Note

$$\sqrt{1+\alpha\partial_{\Delta t}^{-1}}\,\dot{u}(t_{n,\ell}) = \sum_{j=0}^{\infty} \omega_j \dot{u}_{n-j,\ell}.$$

- The boundary term is again positive since it is positive for each ℓ:

$$\sum_{n=0}^{N} \left\langle \sqrt{1+\alpha\partial_{\Delta t}^{-1}}\,\dot{u}(t_{n,\ell}), \dot{u}_{n,\ell} \right\rangle \geq 0.$$

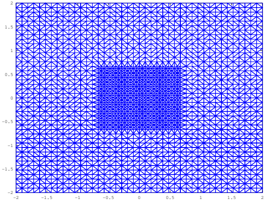
- Only need to compute N weights and each convolution requires N multiplications, rather than kN.
- But we still need to compute the whole convolution for each $t_{n,\ell}$. Can this be improved?

A bad version

Let us throw caution to the wind and try

$$\frac{1}{\kappa^2}(u_{n,\ell+1} - 2u_{n,\ell} + u_{n,\ell-1}, v) + (\alpha \dot{u}_{n,\ell}, v) + (\nabla u_{n,\ell}, \nabla v) + \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_n), v \right\rangle = (f_{n,\ell}, v),$$

First compute with the stable version:



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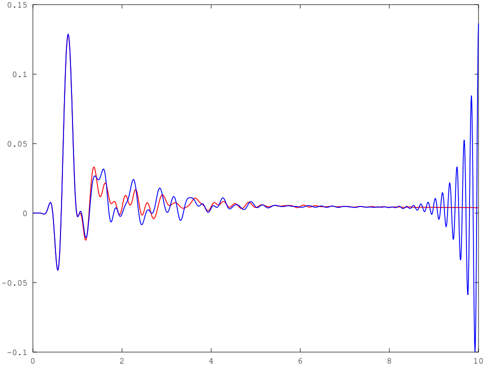
$$\frac{1}{\kappa^2}(u_{n,\ell+1} - 2u_{n,\ell} + u_{n,\ell-1}, v) + (\alpha \dot{u}_{n,\ell}, v) + (\nabla u_{n,\ell}, \nabla v) + \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \dot{u}(t_n), v \right\rangle = (f_{n,\ell}, v),$$

Instability occurs eventually with the ad-hoc version:



Version 2: cheaper and stable

Idea: Apply the boundary operator to a different approximation of $\dot{u}$:

$$\frac{1}{\kappa^2}(u_{n,\ell+1} - 2u_{n,\ell} + u_{n,\ell-1}, v) + (\alpha \dot{u}_{n,\ell}, v) + (\nabla u_{n,\ell}, \nabla v) + \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \widetilde{\dot{u}}(t_n), v \right\rangle = (f_{n,\ell}, v).$$

- Testing with $v = \dot{u}_{n,\ell}$ we obtain

$$E_{N,1/2} = E_{0,1/2} - \kappa \sum_{\ell=1}^{k} \sum_{n=0}^{N} \alpha \|\dot{u}_n\|^2 - \kappa \sum_{\ell=1}^{k} \sum_{n=0}^{N} \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \widetilde{\dot{u}}(t_n), \dot{u}_{n,\ell} \right\rangle$$

$$= E_{0,1/2} - \Delta t \sum_{n=0}^{N} \alpha \|\dot{u}_n\|^2 - \Delta t \sum_{n=0}^{N} \left\langle \sqrt{1 + \alpha \partial_{\Delta t}^{-1}}\, \widetilde{\dot{u}}(t_n), \frac{1}{k} \sum_{\ell=1}^{k} \dot{u}_{n,\ell} \right\rangle.$$

- Energy balance is obtained by choosing

$$\widetilde{\dot{u}}_n = \frac{1}{k} \sum_{\ell=1}^{k} \dot{u}_{n,\ell}.$$

Comments on version 2

- Now the convolution is only evaluated N times.
- The convergence order has been reduced.
- The boundary and domain values of u are strongly coupled.
- In [Abboud et al. ,2011] the authors consider a predictor-corrector strategy to solve a similar system.
- With all the versions the memory connected to the boundary is infinite.

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Weights and inverse Laplace transform

- Another representation of ω_js is useful for $n > 1$

$$\omega_n = \frac{\Delta t}{2\pi \mathrm{i}} \int_{\sigma + \mathrm{i}\mathbb{R}} \sqrt{1 + \alpha/s}\, e_n(s\Delta t) \mathrm{d}s$$

where for Backward Euler

$$e_n(z) = \frac{1}{(1-z)^{n+1}}, \qquad \text{Note: } \frac{1}{1-z} = e^z + O(z^2).$$

- Similar to inverse Laplace computations use

$$\omega_n = \frac{\Delta t}{2\pi \mathrm{i}} \int_{\Gamma} \sqrt{1 + \alpha/s}\, e_n(s\Delta t) \mathrm{d}s,$$

with Γ a hyperbola or Talbot contour and discretize by a truncated trapezoid rule.

- To obtain uniform quadrature errors us different contours Γ_i for

$$t_n \in [B^{n-1}\Delta t, 2B^n \Delta t).$$

Oblivious quadrature [Schädle, López Fernández, Lubich 2005]

Split the discrete convolution as

$$v_{n+1} = \sum_{j=0}^{n} \omega_{n-j} u_j = v_{n+1}^{(0)} + \cdots + v_{n+1}^{L},$$

with

$$v_{n+1}^{(0)} = \omega_0 u_n \text{ and } v_{n+1}^{(i)} = \sum_{j=b_i}^{b_{i-1}-1} \omega_{n-j} u_j,$$

where $b_0 = N$, $b_L = 0$, and
for $i \in [b_i, b_{i-1} - 1]$ we have $n - j \in [B^{i-1}, 2B^i - 2]$.

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where $b_0 = N$, $b_L = 0$, and
for $i \in [b_i, b_{i-1} - 1]$ we have $n - j \in [B^{i-1}, 2B^i - 2]$.

$$v_{n+1}^{(i)} = \sum_{j=b_i}^{b_{i-1}-1} \omega_{n-j} u_j = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_i} e_{n-(b_{i-1}-1)}(sh) \sqrt{1 + \alpha/s}\, y^{(i)}(hs) ds$$

with

$$y^{(i)}(hs) = h \sum_{j=b_i}^{b_{i-1}-1} e_{(b_{i-1}-1)-j}(hs) u_j.$$

Oblivious quadrature [Schädle, López Fernández, Lubich 2005]

Some comments regarding the algorithm:

- $y^{(i)}(hs)$ is the Backward-Euler approximation at $t = b_{i-1}h$ to

$$u' = sy + g(t), \qquad y(b_i h) = 0.$$

- This ODE needs to be solved for L contours Γ_i and the corresponding $2K+1$ quadrature points $s_k^{(i)} = \varphi_i(x_k)$.
- There are only $(2K+1)L = O(\log N \log \frac{1}{\epsilon})$ evaluations of $\sqrt{1+\alpha/s}$ ($(K+1)L$ when using symmetry).
- To compute N steps *after* $t_n > r$, required number of multiplications is $O(N \log N)$ with $O(\log N)$ memory stored.

Relation to time-domain boundary integral equations

Laplace domain fundamental solutions $K(r,s) = (\mathscr{L}k)(r,s)$

$$\text{2D: } K(r,s) = \frac{1}{2\pi} K_0(rs), \qquad \text{damped 3D: } K(r,s) = \frac{e^{-\sqrt{s^2+\alpha s}\,r}}{4\pi r}.$$

- Note $K(s,r)e^{sr}$ bounded for $\operatorname{Re} s > 0$ – causality. But more is true.

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Late-time behaviour of fundamental solution [LB,Gruhne 2011]

Dissipative and 2D wave equations have infinite memory but the kernel has a parabolic behaviour for $t > r$:

$$|K(r,s)e^{rs}| \leq C|s|^{\mu}, \qquad s \in \mathbb{C} \setminus (-\infty, 0]$$

$\mu = -1/2$ for $K_0(\cdot)$ and $\mu = 0$ for 3D dissipative wave equation.

For how to combine this observation with oblivious quadrature ideas see work in progress with López-Fernández and Schädle.

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Conclusions

- Coupling of explicit/implicit schemes based on energy balance.
- Relevant also to the coupling of FEM/BEM in the time domain as the time-domain boundary integral equations are discretizaed by implicit mehods.
- Oblivious quadrature reduces memory requirements and is also applicable to wave propagation problems and time-domain boundary integral equations.