Fast and oblivious algorithms for dissipative and 2D wave equations

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Boundary integral formulation of wave equations

Let $\Omega \subset \mathbb{R}^D$, $D = 2, 3$, be a bounded Lipschitz domain with boundary $\partial\Omega$ and (unbounded) complement $\Omega^c = \mathbb{R}^D \backslash \overline{\Omega}$.
In the particular case $\alpha \geq 0$, let u be the solution to the dissipative wave equation

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\begin{aligned}
\partial_t^2 u(t,x) + \alpha \partial_t u(t,x) - \Delta u(t,x) &= 0, && t \in [0,T], x \in \mathbb{R}^D \setminus \partial\Omega \\
u(t,x) &= g(t,x), && t \in [0,T], x \in \partial\Omega \\
u(0,x) = \partial_t u(0,x) &= 0, && x \in \mathbb{R}^D \setminus \partial\Omega.
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Then u can be represented as a retarded single-layer potential

$$u(x,t) = \int_0^t \int_{\partial\Omega} k\left(t-s, |x-y|\right) \phi(y,s)\, dyds, \quad x \in \mathbb{R}^D \setminus \partial\Omega,\ 0 < t < T.$$

where ϕ is the solution of

$$\int_0^t \int_{\partial\Omega} k(t-s, |x-y|) \phi(y,s)\, dyds = g(x,t), \quad x \in \partial\Omega,\ 0 < t < T.$$

The transfer function

Explicit formulas for $k(t, d)$ are complicated or even unavailable but the Laplace transform of $k(\cdot, d)$ is easily written down explicitly

$$K(\lambda, d) = \begin{cases} \dfrac{1}{2\pi} K_0\left(\sqrt{\lambda^2 + \alpha\lambda}\, d\right), & D = 2 \\ \dfrac{e^{-\sqrt{\lambda^2+\alpha\lambda}d}}{4\pi d}, & D = 3, \end{cases}$$

where K_0 is a modified Bessel function.

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For $\alpha=0$ it is

$$k(t,d)=\begin{cases}\dfrac{\delta(t-d)}{4\pi d}, & D=3,\\[2ex] \dfrac{H(t-d)}{2\pi\sqrt{t^2-d^2}}, & D=2.\end{cases}$$

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Abstract setting for applying Convolution Quadrature

Evaluate c (or solve for ϕ) such that

$$c(t) = \int_0^t k(t-s)\phi(s)\,ds,$$

where for B and D normed vector spaces,

$$k(t) : B \to D, \quad t \in [0, T],$$

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$$c = K(\partial_t)\phi : [0, T] \to D,$$

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The *transfer operator* , $K(\lambda) : B \to D, \quad \operatorname{Re} z \geq \sigma_0,$ is analytic and satisfies

$$\|K(\lambda)\| \leq C|\lambda|^{\mu}, \qquad \operatorname{Re}\lambda \geq \sigma_0,$$

for some $C > 0$ and $\mu \in \mathbb{R}$.

Runge–Kutta Convolution Quadrature (CQ)

Choose an L-stable Runge–Kutta method of s stages and Butcher tableau $\mathbf{A} = (a_{ij})_{i,j=1}^{s} \in \mathbb{R}^{s\times s}$, $\mathbf{b} = (b_i)_{i=1}^{s} \in \mathbb{R}^{s}$ and $\mathbf{c} = (c_j)_{j=1}^{s} \in [0,1]^{s}$.

The CQ based on this Runge–Kutta method approximates

$$\int_0^{t_n} k(t_n-\tau)\phi(\tau)\,d\tau \approx \sum_{j=0}^{n} \boldsymbol{\omega}_{n-j}\cdot\boldsymbol{\phi}_j$$

where $\boldsymbol{\phi}_j = (\phi(t_j + c_i h))_{i=1}^{s}$ and vector-valued weights $\boldsymbol{\omega}_{n-j}$, computed in terms of K, $\mathbf{b}$ and $\mathbf{A}$.

Lubich & Ostermann 1993, Banjai & Lubich 2011

Contour integral representation of the CQ weights

The CQ weights can be written as

$$\omega_n = \frac{h}{2\pi \mathrm{i}} \int_\Gamma K(\lambda) \mathbf{e}_n(h\lambda)\, d\lambda,$$

with

$$\mathbf{e}_n(z) = r(z)^n \mathbf{b}^T (I - z\mathbf{A})^{-1}, \quad n \geq 0,$$

and $r(z)$ the stability function of the Runge–Kutta method

$$r(z) = 1 + z\mathbf{b}^T (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{1}$$

The integration contour Γ is in principle closed, counter-clockwise oriented, and surrounds the poles of $\mathbf{e}_n(h\lambda)$.

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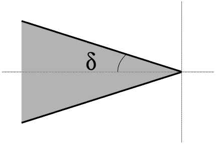
If K is sectorial Γ can be chosen as the left branch of a hyperbola, beginning and ending in the left half plane. Related with the numerical inversion of the Laplace transform and heavily used to design fast and oblivious algorithms. (Lubich, Schädle, Palencia, MLF, 2005-2008)

Sectorial Laplace transforms

We say that a mapping $G(\lambda)$ is sectorial if

G is analytic in a sector $|\arg(\lambda - \sigma)| < \pi - \delta$, for $0 < \delta < \frac{\pi}{2}$,

and in this sector $|G(\lambda)| \leq M|\lambda - \sigma|^{\mu}$, for some $M,\ \mu \in \mathbb{R}$.



Fast and oblivious convolution quadrature

Based on a very efficient quadrature approximation of the CQ weights, a smart splitting of the sums in

$$\sum_{j=0}^{n} \omega_{n-j} \cdot \phi_j,$$

for $n = 1, \ldots, N$, and a sophisticated organization of the computations and bookkeeping. Lubich & Schädle 2002

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Features

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Features

- It reduces the complexity of a direct implementation of CQ from $O(N^2)$ to $O\left(|\log(\varepsilon)| N \log(N)\right)$
  (like modern implementations of CQ for wave problems based on FFT Banjai, Sauter 2008)
- The number of evaluations of the transfer operator K is reduced from $O(N)$ to $O\left(|\log(\varepsilon)| \log(N)\right)$
- The memory requirements are also reduced from $O(N)$ to $O\left(|\log(\varepsilon)| \log(N)\right)$

Key estimates for 2D and damped wave problems

In Banjai & Grüne 2012 it was noticed that

$$\left|e^{\lambda d} K(\lambda, d)\right| \leq \begin{cases} C(d), & D = 3,\ \alpha \geq 0,\ |\arg(\lambda)| < \pi \\ C(d,\delta)|\lambda|^{-1/2}, & D = 2,\ \alpha = 0,\ |\arg(\lambda)| < \pi - \delta, \end{cases}$$

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Thus $e^{\lambda d} K(\lambda, d)$ as a function of λ is sectorial

How to exploit this property?

Our contour

- Our K is not sectorial. The integral along the (infinite) left branch of a hyperbola is divergent.
- $e^{\lambda d} K(\lambda, d)$ is sectorial for every d. (Notice that $\omega_n = \omega_n(d)$).

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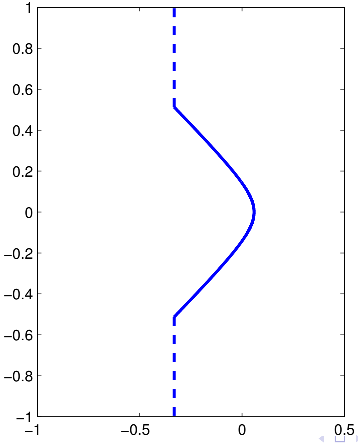

Parameterization and estimates of stability function

We parameterize the finite section of the hyperbola in the picture as

$$\Gamma_0 = \nu\varphi([-a, a]), \qquad \varphi(x) = 1 - \sin(\alpha - \mathrm{i}x), \quad \nu > 0.$$

Γ_0 begins and ends in the left-half complex plane provided that

$$\operatorname{Re}\varphi(a) = (1 - \sin\alpha\cosh a) < 0 \qquad \Longleftrightarrow \qquad \cosh a > 1/\sin\alpha.$$

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Technical Lemma

Let

$$\gamma(\xi) = \inf_{-\xi\le \operatorname{Re} z\le 0} \frac{\log|r(z)|}{\operatorname{Re} z}.$$

Then $\gamma(\xi)\in(0,1]$ for $\xi>0$, it monotonically increases as $\xi\to 0$ and

$$|r(z)| \le |e^{\gamma(\xi)z}|,$$

for all z in the strip $-\xi \le \Re z \le 0$.
Further, there exists $\rho > 0$ such that $|r(z)| \le |e^{2z}|$ for all z in the strip $0 \le \operatorname{Re} z \le \rho$.

Truncation error

Proposition

Let $d, \delta > 0$ and μ be given from the sectorial estimate of $e^{\lambda d} K(\lambda, d)$.

Let a and $\alpha \in (0, \pi/2 - \delta)$ be given such that $\cosh a > 1/\sin\alpha$.

Then for h, $\nu_0 > 0$, $m > \mu$, $0 < \nu \leq \nu_0$ and $t_{n-m} > d/\gamma(\xi)$ with $\xi = h\nu_0 |\operatorname{Re}\varphi(a)|$,

$$\left| \boldsymbol{\omega}_n(d) - \frac{h}{2\pi \mathrm{i}} \int_{\Gamma_0} K(\lambda, d) \mathbf{e}_n(\lambda h)\, d\lambda \right| \leq C |\nu\varphi(a)|^{\mu - m} h^{-m} e^{\nu \operatorname{Re}\varphi(a)(\gamma(\xi) t_{n-m} - d)},$$

where $C = \text{const} \cdot C(d)$, with $C(d)$ in the estimate of $e^{\lambda d} K(\lambda, d)$.

Trapezoidal Quadrature on $[-a, a]$

Lemma

Let f be analytic and bounded as $|f(z)| \leq M$ for

$$z \in R_{\tau_0} = \{w \in \mathbb{C} : -a - \tau_0 \leq \operatorname{Re} w \leq a + \tau_0, \ -b < \operatorname{Im} w < b\}$$

and some $\tau_0 > 0$. Further, let

$$I = \int_{-a}^{a} f(x)dx, \qquad I_L = \frac{a}{L} \sum_{k=-L}^{L} f(x_k),$$

where $x_k = k\tau$, $\tau = a/L$ and $0 < \tau \leq \tau_0$. Then

$$|I - I_L| \leq \frac{2M}{e^{2\pi b/\tau} - 1} + \frac{\log 2}{\pi} \tau \sup_{y \in [-b,b]} |g_{\tau/2}(y)|,$$

where $g_{\tau/2}(y) = f(a + \tau/2 + \mathrm{i}y) - f(-a - \tau/2 + \mathrm{i}y)$.

The proof is a modification of the one in Javed & Trefethen 2014

Total error estimate in the approximation of the weights

We approximate the CQ weight $\omega_n(d)$ by applying trapezoidal quadrature to

$$\frac{h}{2\pi \mathrm{i}} \int_{\Gamma_0} K(\lambda, d) \mathbf{e}_n(h\lambda)\, d\lambda = \frac{\nu h}{2\pi \mathrm{i}} \int_{-a}^{a} K(\nu\varphi(x), d) \mathbf{e}_n(h\nu h\varphi(x))\varphi'(x)\, dx$$

with L quadrature points and nodes $x_k = k\tau$. Denote the error by Err_L.

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Theorem

Under technical assumptions and with ξ the left most point of

$$h\nu\varphi([-a, a] + \mathrm{i}[-b, b]), \qquad \text{with } 0 < b < \min(\alpha, \pi/2 - (\delta + \alpha))$$

we can bound

$$|Err_L| \leq C \left(h \frac{\mathrm{e}^{2t_n\nu}}{\mathrm{e}^{2\pi b/\tau} - 1} + (1 + \tau) \left(h\nu \cosh a\right)^{-m} \mathrm{e}^{\nu(1-\sin(\alpha-b)\cosh a)(\gamma(\xi)t_{n-m}-d)} \right),$$

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We borrow many estimates from MLF & Palencia 2005, MLF, Palencia & Schädle 2006

Uniform error estimate and parameter choice

Given $\Lambda \geq 1$ and $n_0 \geq 1$, the same contour can be used to compute all CQ weights $\omega_n(d)$, for $n_0 \leq n \leq \Lambda n_0$. The estimate is also uniform in $0 \leq d \leq \gamma(\xi) t_0$.

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Corollary

For every $\theta \in (0,1)$, the following choice of parameters

$$\tau = \frac{a(\theta)}{L} \qquad \nu = \frac{\pi b L \theta}{\Lambda t_0 a(\theta)}.$$

with

$$a(\theta) = \operatorname{acosh}\left(\frac{\gamma(\xi)(1-D)\theta + 2\Lambda(1-\theta)}{\gamma(\xi)(1-D)\theta \sin(\alpha - b)}\right)$$

yields the uniform error estimate

$$|Err_L| \leq C \exp\left(-\frac{2\pi b L(1-\theta)}{a(\theta)}\right),$$

where C includes all non exponentially growing terms in the bound.

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The actual error will be bounded from below by

$$|Err_L| \geq C \exp(-\xi^*(\gamma(\xi^*)t_{n_0-m} - d))$$

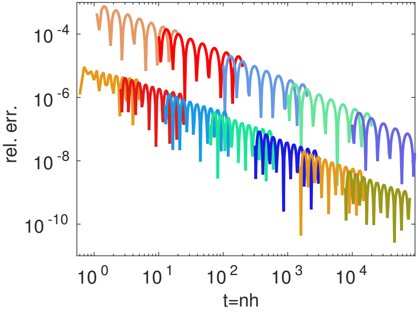
No contradiction with our theory, since with this strategy we are ignoring the (highly nonlinear) relation between $a = a(\theta^*)$ and ξ^*.

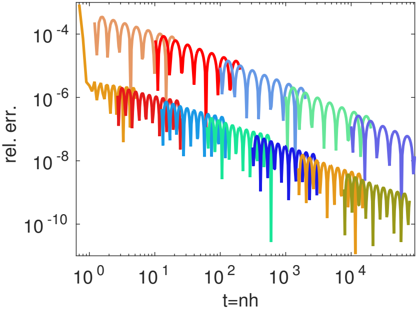
Effective approximation of the weights

We consider

$$K(\lambda, d) = K_0(\lambda d)$$

where $K_0(\cdot)$ is a modified Bessel function. Here $\delta = 0$, $\mu = -1/2$.

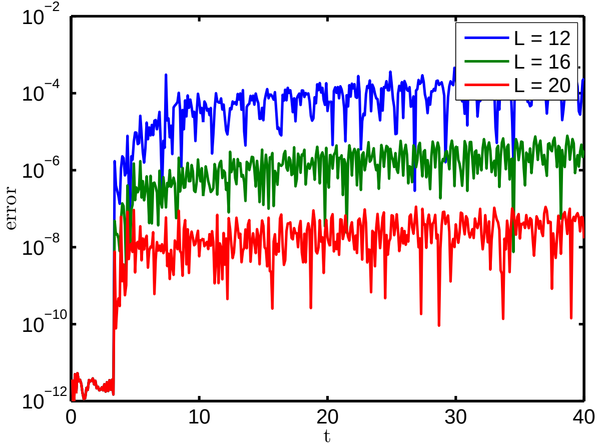




Approximation error along intervals $[hn_0 + hB^\ell, hn_0 + 2hB^{\ell+1}]$ with $B = 10$, $L = 10$ (up), and $B = 5$, $L = 15$ (down).
Left: $d = 0.01$, Right: $d = 0.1$.

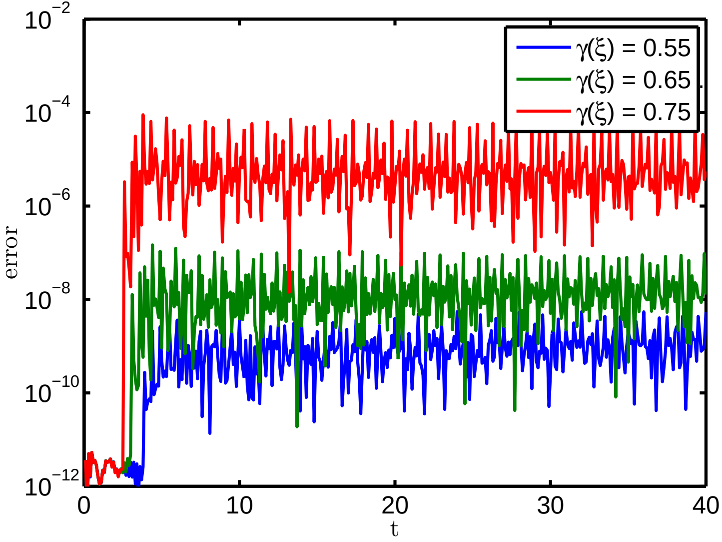
Wave equation in 2D, no damping ($\alpha = 0$)

We take Ω a disk of radius one and $g(x,t) = t^4 e^{-2t}$. $T = 40$, $N = 400$ time steps, $M = 100$ patches for the spatial discretization.
Basis $B = 5$, offset $n_0 = \lceil d/(h\gamma(\xi)) \rceil$, two distance classes: $d \in [0, \sqrt{2}]$ or $d \in [\sqrt{2}, 2]$, Fixed $\gamma(\xi) = 0.6$.



Evolution of the error for different γ

Fixed $L = 26$.



Error behaviour w.r.t. L