Frequency-independent solvers for linear ODEs

James Bremer

University of Toronto

June 25, 2024

Linear scalar differential equations in the high-frequency regime

$$y^{(n)}(t) + q_{n-1}(t)y^{(n-1)}(t) + \cdots + q_1(t)y'(t) + q_0(t)y(t) = 0$$

$$\begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ -q_0(t) & -q_1(t) & \cdots & -q_{n-1}(t) \end{pmatrix}$$

The complexity of typical solutions grow linearly with "frequency:"

$$\Omega = \max_{j=1,\ldots,n} \int |\Lambda_j(t)| \; dt$$

Eigenvalues : $\Lambda_1(t), \ldots, \Lambda_n(t)$

Frequency-independent exponential representations

Riccati equation:

$$y''(t) + \lambda^2 q(t) y(t) = 0, \quad y(t) = \exp\left(\int \psi(t)\, dt\right)$$

$$\psi'(t) + (\psi(t))^2 + \lambda^2 q(t) = 0.$$

WKB approximation:

$$\psi(t) = \sum_{j=0}^{n} \lambda^{1-j} \psi_j(t) + \mathcal{O}\left(\frac{1}{\lambda^n}\right) \quad \text{where the } \psi_j \text{ depend on } q \text{ but not } \lambda$$

Implication:

If q is nonoscillatory, then at high enough frequencies, we can treat the Riccati equation as if it has a slowly-varying solution.

Frequency-independent exponential representations

Zhu Heitman, B— and Vladimir Rokhlin. "On the existence of nonoscillatory phase functions for second order differential equations in the high-frequency regime," *Journal of Computational Physics* 290 (2015), 1-27.

The gist:

If q is slowly-varying, $\psi'(t) + (\psi(t))^2 + \lambda^2 [\ q(t) + \mathcal{O}(\exp(-C\lambda))\ ] = 0$ admits a slowly-varying solution.

Implication:

For numerical purposes,

$$\psi'(t) + (\psi(t))^2 + \lambda^2 q(t) = 0$$

always admits a slowly-varying solution.

Frequency-independent exponential representations

Zhu Heitman, B— and Vladimir Rokhlin. "On the existence of nonoscillatory phase functions for second order differential equations in the high-frequency regime," *Journal of Computational Physics* 290 (2015), 1-27.

The gist:

If q is slowly-varying, $\psi'(t) + (\psi(t))^2 + \lambda^2 [\ q(t) + \mathcal{O}(\exp(-C\lambda))\ ] = 0$ admits a slowly-varying solution.

Implication:

For numerical purposes,

$$\psi'(t) + (\psi(t))^2 + \lambda^2 q(t) = 0$$

always admits a slowly-varying solution.

When λ is small, all solutions are slowly-varying.

Frequency-independent exponential representations

Zhu Heitman, B— and Vladimir Rokhlin. "On the existence of nonoscillatory phase functions for second order differential equations in the high-frequency regime," *Journal of Computational Physics* 290 (2015), 1-27.

Effectively 0 when λ is even of modest size.

The gist:

If q is slowly-varying, $\psi'(t) + (\psi(t))^2 + \lambda^2 [\ q(t) + \mathcal{O}(\exp(-C\lambda))\ ] = 0$ admits a slowly-varying solution.

Implication:

For numerical purposes,

$$\psi'(t) + (\psi(t))^2 + \lambda^2 q(t) = 0$$

always admits a slowly-varying solution.

When λ is small, all solutions are slowly-varying.

The fundamental idea

We construct a collection of slowly-varying phases which represent a basis in space of solutions of the ordinary differential equation by solving the obvious "Riccati" equation numerically.

$$\left\{ u_j(t) = \exp\left(\int \psi_j(t)\, dt \right) : j = 1, \ldots, n \right\}$$

$$y''(t) + q_1(t)y'(t) + q_0(t)y(t) = 0, \qquad y(t) = \exp\left(\int \psi(t)\, dt \right)$$

$$\psi'(t) + (\psi(t))^2 + q_1(t)\psi(t) + q_0(t) = 0$$

The fundamental idea

We construct a collection of slowly-varying phases which represent a basis in space of solutions of the ordinary differential equation by solving the obvious "Riccati" equation numerically.

$$\left\{ u_j(t) = \exp\left(\int \psi_j(t)\, dt \right) : j = 1, \ldots, n \right\}$$

$$y'''(t) + q_2(t) y''(t) + q_1(t) y'(t) + q_0(t) y(t) = 0, \qquad y(t) = \exp\left(\int \psi(t)\, dt \right)$$

$$\psi''(t) + 3\psi'(t)\psi(t) + q_2(t)\psi'(t) + (\psi(t))^3 + q_2(t)(\psi(t))^2 + q_1(t)\psi(t) + q_0(t) = 0$$

The fundamental idea

We construct a collection of slowly-varying phases which represent a basis in space of solutions of the ordinary differential equation by solving the obvious "Riccati" equation numerically.

$$\left\{ u_j(t) = \exp\left(\int \psi_j(t)\, dt \right) : j = 1, \ldots, n \right\}$$

$$y''''(t) + q_3(t) y'''(t) + q_2(t) y''(t) + q_1(t) y'(t) + q_0(t) y(t) = 0, \quad y(t) = \exp\left(\int r(t)\, dt \right)$$

$$\begin{aligned} &\psi'''(t) + 4\psi''(t)\psi(t) + 3(\psi'(t))^2 + 6\psi'(t)(\psi(t))^2 + q_3(t)\psi''(t) + 6\psi'(t)(\psi(t))^2 \\ &+ q_3(t)\psi''(t) + 3q_3(t)\psi'(t)\psi(t) + q_2(t)\psi'(t) \\ &+ (\psi(t))^4 + q_3(t)(\psi(t))^3 + q_2(t)(\psi(t))^2 + q_1(t)\psi(t) + q_0(t) = 0 \end{aligned}$$

How can we construct slowly-varying solutions of the Riccati equation?

$$\psi'(t) + (\psi(t))^2 + q(t) = 0$$

Newton-Kantorovich iterations:

$$\psi_0(t) = i\sqrt{q(t)}$$

$$\psi_1(t) = \psi_0(t) + \delta(t), \quad \delta'(t) + 2i\sqrt{q(t)}\delta(t) = -\frac{q'(t)}{2\sqrt{q(t)}}$$

$$\vdots$$

$$\psi_{j+1}(t) = \psi_j(t) + \delta(t), \quad \delta'(t) + 2\psi_j(t)\delta(t) = -\left(\psi_j'(t) + (\psi_j(t))^2 + q(t)\right)$$

$$\vdots$$

How can we construct slowly-varying solutions of the Riccati equation?

$$\psi'(t) + (\psi(t))^2 + q(t) = 0$$

These are slowly-varying.

Newton-Kantorovich iterations:

$$\psi_0(t) = i\sqrt{q(t)}$$

$$\psi_1(t) = \psi_0(t) + \delta(t), \quad \delta'(t) + 2i\sqrt{q(t)}\delta(t) = -\frac{q'(t)}{2\sqrt{q(t)}}$$

$$\vdots$$

$$\psi_{j+1}(t) = \psi_j(t) + \delta(t), \quad \delta'(t) + 2\psi_j(t)\delta(t) = -\left(\psi_j'(t) + (\psi_j(t))^2 + q(t)\right)$$

$$\vdots$$

How can we construct slowly-varying solutions of the Riccati equation?

$$\psi'(t) + (\psi(t))^2 + q(t) = 0$$

These are slowly-varying.

Newton-Kantorovich iterations:

$$\psi_0(t) = i\sqrt{q(t)}$$

$$\psi_1(t) = \psi_0(t) + \delta(t), \quad \delta'(t) + 2i\sqrt{q(t)}\delta(t) = -\frac{q'(t)}{2\sqrt{q(t)}}$$

$$\vdots$$

$$\psi_{j+1}(t) = \psi_j(t) + \delta(t), \quad \delta'(t) + 2\psi_j(t)\delta(t) = -\left(\psi_j'(t) + (\psi_j(t))^2 + q(t)\right)$$

$$\vdots$$

As long as the coefficient and the residual are slowly-varying, there is a slowly-varying solution.

How do we obtain initial guesses for higher order equations?

The eigenvalues $\Lambda_1(t), \dots, \Lambda_n(t)$ of

$$\begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ -q_0(t) & -q_1(t) & \cdots & -q_{n-1}(t) \end{pmatrix}$$

are asymptotic approximations of solutions of the Riccati equation obtained by inserting

$$y(t) = \exp\left(\int \psi(t)\, dt\right)$$

into

$$y^{(n)}(t) + q_{n-1}(t) y^{(n-1)}(t) + \cdots + q_1(t) y'(t) + q_0(t) y(t) = 0.$$

How do we obtain initial guesses for higher order equations?

$$\begin{pmatrix} 0 & 1 \\ -q_0(t) & -q_1(t) \end{pmatrix} \qquad \psi'(t) + \boxed{(\psi(t))^2 + \psi(t)q_1(t) + q_0(t) = 0}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -q_0(t) & -q_1(t) & -q_2(t) \end{pmatrix} \qquad \begin{array}{l} \psi''(t) + 3\psi'(t)\psi(t) + q_2(t)\psi'(t) + \\ \boxed{(\psi(t))^3 + q_2(t)(\psi(t))^2 + q_1(t)\psi(t) + q_0(t) = 0} \end{array}$$

Robust algorithm for computing the eigenvalues:

J. Aurentz, T. Mach, R. Vanderbril and D. S. Watkins, "Fast and backward stable computation of the roots of polynomials," *SIAM Journal on Matrix Analysis and Applications* 36 (2015), 942-973.

What can go wrong?

Turning points: (i.e., locations where the eigenvalues coalesce)

The Riccati equation need not have solutions which extend across turning points and which are slowly-varying on both sides.

Low-frequency regions:

On intervals where the frequency is small, the linearized equations do not admit unique slowly-varying solutions.

What can go wrong?

Subdivide the solution domain as needed.

Turning points: (i.e., locations where the eigenvalues coalesce)

The Riccati equation need not have solutions which extend across turning points and which are slowly-varying on both sides.

Low-frequency regions:

On intervals where the frequency is small, the linearized equations do not admit unique slowly-varying solutions.

What can go wrong?

Subdivide the solution domain as needed.

Turning points: (i.e., locations where the eigenvalues coalesce)

The Riccati equation need not have solutions which extend across turning points and which are slowly-varying on both sides.

Low-frequency regions:

On intervals where the frequency is small, the linearized equations do not admit unique slowly-varying solutions.

Only apply in high-frequency regions and use ODE solvers to extend the solutions.

A frequency-indendent solver

Assumption:

$\Lambda_1(t), \ldots, \Lambda_n(t)$ are distinct on $[a, b]$ and either of large magnitude on the interval $[a_0, b_0]$, or are of small magnitude throughout $[a, b]$.

(in other words: if one of the Λ_j is large anywhere on $[a, b]$, it is large on $[a_0, b_0]$)

Algorithm:

Compute initial values for $\psi_1, \ldots, \psi_n$ on $[a_0, b_0]$:

- Compute $\Lambda_1(t), \ldots, \Lambda_n(t)$ at the k-point Chebyshev grid on a subinterval $[a_0, b_0]$.
- For each j, use Newton-Kantorovich iterations to construct a solution ψ_j of the Riccati equation over $[a_0, b_0]$. The linearized equations are solved via the obvious Chebyshev spectral method.

Use an ODE solver to construct piecewise Chebyshev expansions of the phase functions $\psi_1, \ldots, \psi_n$ over $[a, b]$.

Key properties of the solver

- Running time bounded independent of frequency.
- Phase functions are computed to near machine precision accuracy regardless of frequency.
- ODE solutions are computed to accuracy consistent with their condition number of evaluation.
- Allows for the rapid evaluation of the solution, in time independent of frequency, anywhere in the solution domain.
- Allows for the solution of boundary value problems as well as initial value problems.
- Highly parallelizable (although no experiments shown here exploit this).

Key properties of the solver

High-accuracy computation of zeros, Gaussian quadrature weights, barycentric interpolation weights, etc.

- Running time bounded independent of frequency.
- Phase functions are computed to near machine precision accuracy regardless of frequency.
- ODE solutions are computed to accuracy consistent with their condition number of evaluation.
- Allows for the rapid evaluation of the solution, in time independent of frequency, anywhere in the solution domain.
- Allows for the solution of boundary value problems as well as initial value problems.
- Highly parallelizable (although no experiments shown here exploit this).

Key properties of the solver

High-accuracy computation of zeros, Gaussian quadrature weights, barycentric interpolation weights, etc.

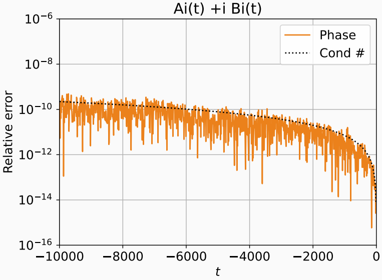
- Running time bounded independent of frequency.
- Phase functions are computed to near machine precision accuracy regardless of frequency.
- ODE solutions are computed to accuracy consistent with their condition number of evaluation.
- Allows for the rapid evaluation of the solution, in time independent of frequency, anywhere in the solution domain.
- Allows for the solution of boundary value problems as well as initial value problems.
- Highly parallelizable (although no experiments shown here exploit this).

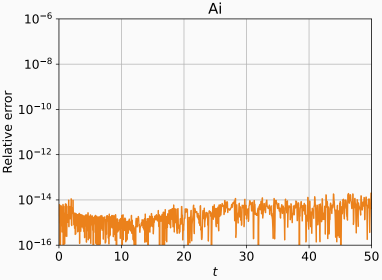
Compare with step methods that sample below the Nyquist rate.

Airy's Equation

$$y''(t) - ty(t) = 0, \qquad -10,000 \leqslant t \leqslant 50$$

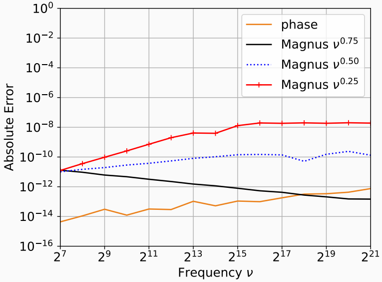
400 coefficients   0.22 milliseconds

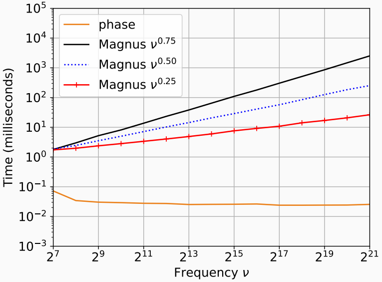




Legendre's differential equation

$$y''(t) + \left(\frac{1}{(1-t^2)^2} + \frac{\nu(\nu+1)}{1-t^2} \right) y(t) = 0, \quad 0 \leqslant t \leqslant 0.9$$

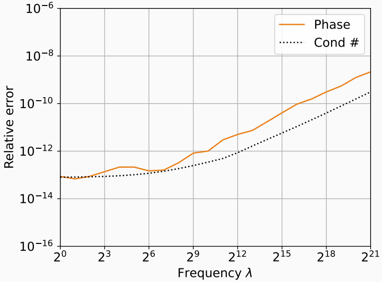


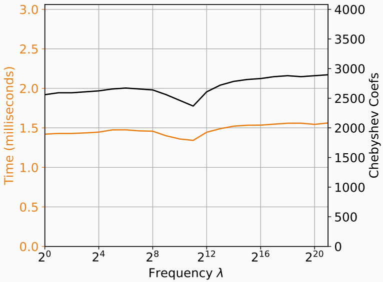


Associated Legendre functions

$$y''(t) + \left(-\mu^2 + \nu(\nu+1)\cosh^2(t)\right) y(t) = 0, \quad \mu = 10,000, \quad -\alpha < t < \alpha$$

$$\widetilde{P}^{\mu}_{\mu+\lambda}(\tanh(t)) + \frac{2i}{\pi}\widetilde{Q}^{\mu}_{\mu+\lambda}(\tanh(t))$$

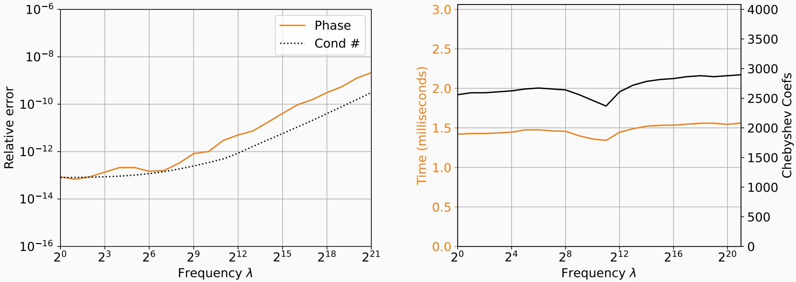




$$y''(t) + \left(-\mu^2 + \nu(\nu+1)\cosh^2(t)\right) y(t) = 0, \quad \mu = 10{,}000, \quad -\alpha < t < \alpha$$

$$\widetilde{P}^{\mu}_{\mu+\lambda}(\tanh(t)) + \frac{2i}{\pi}\widetilde{Q}^{\mu}_{\mu+\lambda}(\tanh(t))$$

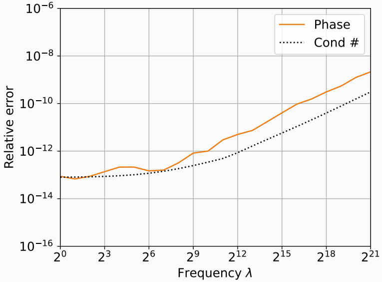
chosen such that $P(\pm\alpha) \approx 10^{-150}$

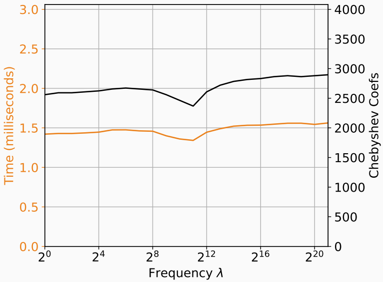


$$y''(t) + \left(-\mu^2 + \nu(\nu+1)\cosh^2(t)\right) y(t) = 0, \quad \mu = 10{,}000, \quad -\alpha < t < \alpha$$

$$\widetilde{P}^{\mu}_{\mu+\lambda}(\tanh(t)) + \frac{2i}{\pi}\widetilde{Q}^{\mu}_{\mu+\lambda}(\tanh(t))$$

chosen such that $P(\pm\alpha) \approx 10^{-150}$



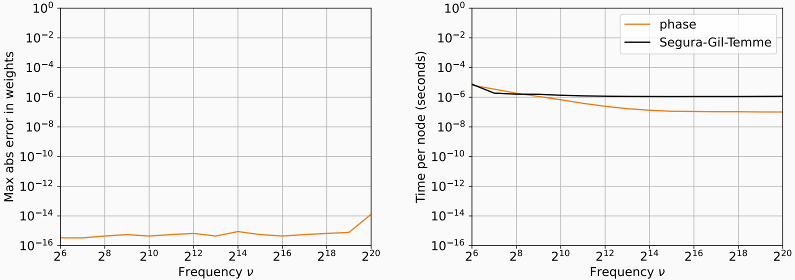


High relative accuracy for both P and Q in the oscillatory and nonoscillatory regimes

Computation of Gauss-Jacobi quadrature rules

$$y''(t) + q(t)y(t) = 0$$

$$q(t) = \frac{1}{4}\left(\operatorname{sech}^2(w)(a+b+2\nu)(a+b+2\nu+2) - 2\left(a^2 + (a-b)(a+b)\tanh(w) + b^2\right)\right)$$

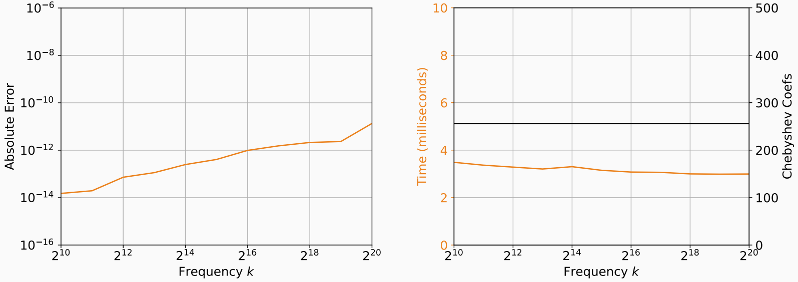


$$a = b = \pi - 0.5$$

A third order scalar equation

$$y'''(t) - \frac{1+t^2}{1+t^4}\sin(t)y''(t) + k^2\frac{\exp(2t)}{(1+t^2)^2}y'(t) - k^2\frac{\exp(2t)\sin(t)}{1+t^2+t^4+t^6}y(t) = 0$$

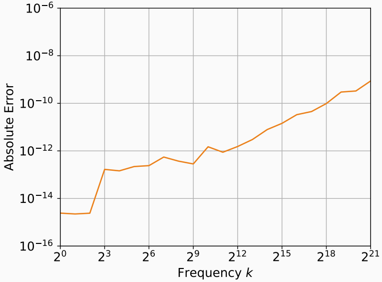
$$\Lambda_1(t) = \sin(t)\frac{1+t^2}{1+t^4}, \quad \Lambda_2(t) = ik\frac{\exp(t)}{1+t^2} \quad \text{and} \quad \Lambda_3(t) = -ik\frac{\exp(t)}{1+t^2}.$$

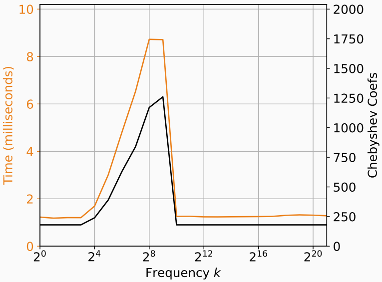


A system of linear ordinary differential equations

$$\mathbf{y}'(t) = \begin{pmatrix} \frac{1+t^2}{1+t^4} & \frac{1}{1+t^4} \\ -k\left(\frac{1}{1+t^2}\right) & -ik\left(\frac{2+t}{5+t}\right) \end{pmatrix} \mathbf{y}(t), \quad -1 < t < 1, \quad \mathbf{y}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\Lambda_1(0) \sim -\frac{2k}{5}i - \frac{5}{2}i + \mathcal{O}\left(\frac{1}{k}\right), \quad \Lambda_2(0) \sim 1 + \frac{5}{2}i + \mathcal{O}\left(\frac{1}{k}\right)$$

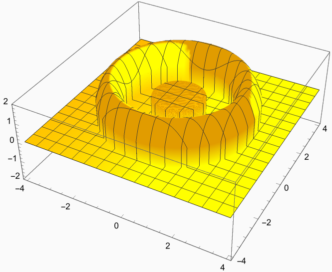


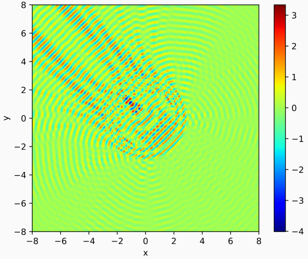


Scattering from a radially symmetric potential

$$\Delta u(x) + k^2 \left(1 + q(r)\right) u(x) = 0$$

$$u(x) = u_i(x) + u_s(x) \qquad \begin{cases} u_i(r\exp(it)) = \exp\left(ikr\cos\left(t - \frac{\pi}{4}\right)\right) \\ \lim_{r\to\infty} \sqrt{r}\left|\frac{\partial u_s}{\partial r}(r,t) - iku_s(r,t)\right| = 0 \end{cases}$$

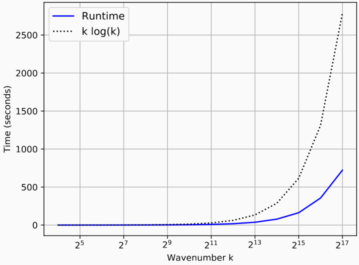




Scattering from a radially symmetric potential

$$\Delta u(x) + k^2 (1 + q(r))\, u(x) = 0$$

k	Maximum absolute error	Time (in seconds)
2^8	2.20×10^{-12}	9.58×10^{-01}
2^9	5.95×10^{-12}	$1.93 \times 10^{+00}$
2^{10}	6.50×10^{-12}	$4.06 \times 10^{+00}$
2^{11}	2.04×10^{-11}	$8.57 \times 10^{+00}$
2^{12}	4.31×10^{-11}	$1.77 \times 10^{+01}$
2^{13}	2.27×10^{-10}	$3.70 \times 10^{+01}$
2^{14}	1.90×10^{-10}	$7.79 \times 10^{+01}$
2^{15}	3.48×10^{-10}	$1.62 \times 10^{+02}$
2^{16}	7.33×10^{-10}	$3.56 \times 10^{+02}$
2^{17}	1.95×10^{-09}	$7.22 \times 10^{+02}$



Many other applications ...

- Fast evaluation of special functions.

  B—. "An algorithm for the numerical evaluation of the associated Legendre functions that runs in time independent of degree and order," *Journal of Computational Physics* 360 (2018), 15-38.

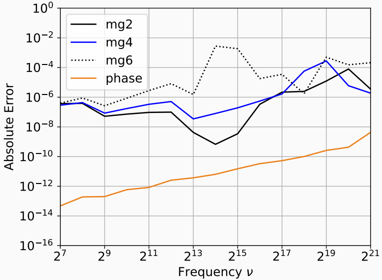
  B—. On the numerical evaluation of the prolate spheroidal wave functions of order zero. Applied and Computational Harmonic Analysis 60 (2022), 53-76.

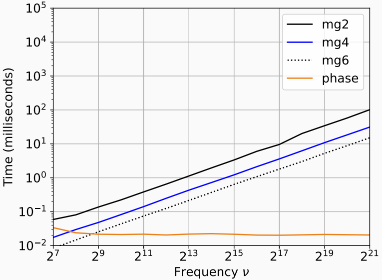
- Fast application of Sturm-Liouville eigentransforms.

  B—, Ze Chen and Haizhao Yang. "Rapid Application of the Spherical Harmonic Transform via Interpolative Decomposition Butterfly Factorization," *SIAM Journal on Scientific Computing* 43 (2021), A3789-A3808.

Comparison with Magnus expansions in a simple case

$$y''(t) + \nu^2 \left(1 + t^2\right) y(t) = 0, \quad 0 \leqslant t \leqslant 1.0$$

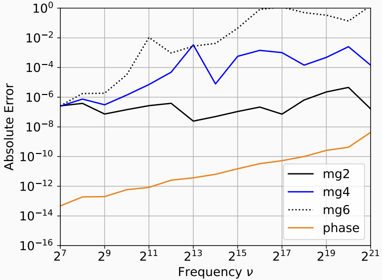


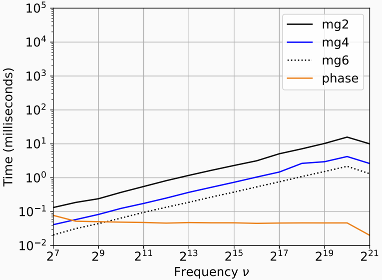


$$h \sim \nu^{-0.75}$$

Comparison with Magnus expansions in a simple case

$$y''(t) + \nu^2 \left(1 + t^2\right) y(t) = 0, \quad 0 \leqslant t \leqslant 1.0$$





$$h \sim \nu^{-0.50}$$