A fast and well-conditioned spectral method for singular integral equations

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Outline

- Singular integral equations:

$$\fint_\Gamma K(x,y)u(y)\,\mathrm{d}y = f(x), \qquad \mathcal{B}u = \mathbf{c},$$

  Classical collocation method [Elliott 1982], hybrid quadrature rules [Alpert 1999], etc,. . . .
- Classical applications
  - Boundary integral equations for Laplace & Helmholtz equations
  - Fracture mechanics
- Contemporary applications
  - Korteweg-de Vries (KdV) and nonlinear Schrödinger (NLS) equation via inverse scattering transform
  - Random matrix theory and orthogonal polynomials by reformulating as a matrix-valued Riemann–Hilbert problem.
- New combination of three key ingredients:
  - use a basis in which singularities are integrated exactly
  - The basis allows for banded linear algebra
  - and low rank bivariate approximants for integral kernels

2D Elliptic PDEs

In this work, we will consider:

- the Laplace equation:

$$-\Delta u(\mathbf{x}) = 0, \qquad \Phi(\mathbf{x},\mathbf{y}) = \frac{1}{2\pi}\log|\mathbf{x}-\mathbf{y}|,$$

- the Helmholtz equation:

$$-(\Delta + k^2)u(\mathbf{x}) = 0, \qquad \Phi(\mathbf{x},\mathbf{y}) = \frac{\mathrm{i}}{4}H_0^{(1)}\left(k|\mathbf{x}-\mathbf{y}|\right),$$

- the gravity Helmholtz equation:

$$-\left(\Delta + E + x_2\right)u(\mathbf{x}) = 0,$$
$$\Phi(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi}\int_0^\infty \exp \mathrm{i}\left[\frac{|\mathbf{x}-\mathbf{y}|^2}{4t} + \left(E + \frac{x_2+y_2}{2}\right)t - \frac{1}{12}t^3\right]\frac{\mathrm{d}t}{t},$$

  where the fundamental solution is derived in [Bracher et al 1998]. Numerical evaluation via the trapezoidal rule [Trefethen and Weideman 2014] on path of steepest descent. Timings of $10^5/\mathrm{s}$ are reported in [Barnett et al. 2014].

Exterior Scattering Problems

Theorem [Vekua 1967] where for analytic coefficients of an elliptic PDO (accomplished with Riemann function):

$$\Phi(\mathbf{x},\mathbf{y}) = A(\mathbf{x},\mathbf{y}) \log|\mathbf{x}-\mathbf{y}| + B(\mathbf{x},\mathbf{y}), \quad \text{where} \quad A(\mathbf{x},\mathbf{x}) = -(2\pi)^{-1}.$$

For any continuous density [Kress 2010] u, let $\mathcal{S}_\Gamma$ and $\mathcal{D}_\Gamma$ define the single- and double-layer potentials:

$$\mathcal{S}_\Gamma u(\mathbf{x}) = \int_\Gamma \Phi(\mathbf{x},\mathbf{y}) u(\mathbf{y})\, \mathrm{d}\Gamma(\mathbf{y}), \quad \text{for} \quad \mathbf{x} \in D,$$

$$\mathcal{D}_\Gamma u(\mathbf{x}) = \int_\Gamma \frac{\partial \Phi(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{y})} u(\mathbf{y})\, \mathrm{d}\Gamma(\mathbf{y}), \quad \text{for} \quad \mathbf{x} \in D.$$

For homogeneous equations $\mathbf{L}[u] = 0$, Green's representation theorem allows for the determination of the exterior solutions given data on the boundary Γ:

$$u(\mathbf{x}) = -\mathcal{S}_\Gamma\left[\partial u/\partial n\right](\mathbf{x}) + \mathcal{D}_\Gamma\left[u\right](\mathbf{x}), \quad \text{for} \quad \mathbf{x} \in D.$$

Dirichlet Problem

Definition (Dirichlet Problem, Kress 2010)

Given $u^i(\mathbf{x}) \in C^2(\mathbb{R}^2)$ satisfying $\mathbf{L}[u^i] = 0$, find $u^s(\mathbf{x}) \in C^2(D) \cap C^{0,\alpha}(\Gamma)$ satisfying $\mathbf{L}[u^s] = 0$ and the radiation condition at infinity, and:

$$u^i(\mathbf{x}) + u^s(\mathbf{x}) = 0, \quad \text{for} \quad \mathbf{x} \in \Gamma.$$

Theorem (Dirichlet Solution, Kress 2010)

The scattered solution to the Dirichlet problem is represented everywhere by the single-layer potential. The density $[\partial u / \partial n]$ satisfies:

$$\int_\Gamma \Phi(\mathbf{x}, \mathbf{y}) \left[\frac{\partial u}{\partial n}\right] \mathrm{d}\Gamma(\mathbf{y}) = u^i(\mathbf{x}), \qquad \mathbf{x} \in \Gamma.$$

Practical approximation theory: Chebyshev polynomials

- Chebyshev polynomials:

$$T_n(x) = \cos(n\cos^{-1}(x)), \quad \text{for} \quad n \in \mathbb{N}_0, \quad \text{and} \quad x \in [-1,1].$$

- Interpolants: $p_N(x) = \sum_{n=0}^{N} c_n T_n(x), \quad x \in [-1,1],$
- Interpolation condition:

$$p_N(x_n) = f(x_n) \quad \text{where} \quad x_n = \cos\left(\frac{2n+1}{2N+2}\pi\right), \quad \text{for} \quad n = 0,\ldots,N.$$

- Clenshaw's algorithm for $\mathcal{O}(n)$ evaluation of interpolants,
- DCT for $\mathcal{O}(n\log n)$ transformation of the interpolation condition into approximate projections,
- Convergence depends on regularity.

Ultraspherical spectral method

The ultraspherical spectral method of [Olver and Townsend 2013] represents solutions of linear ordinary differential equations of the form:

$$\mathcal{L}u = f, \qquad \mathcal{B}u = c,$$

where $\mathcal{L}$ is a linear operator of the form:

$$\mathcal{L} = a_N(x)\frac{\mathrm{d}^N}{\mathrm{d}x^N} + \cdots + a_1(x)\frac{\mathrm{d}}{\mathrm{d}x} + a_0(x),$$

and $\mathcal{B}$ contains N linear functionals satisfied by $u(x)$ in Chebyshev expansions:

$$u(x) = \sum_{n=0}^{\infty} u_n T_n(x),$$

where $T_n(x)$ is the Chebyshev polynomial of the first kind of degree n, and $\mathbf{u} = (u_0, u_1, \ldots)^\top$ is a vector of coefficients. Three ingredients we need are:

Differentiation Conversion Multiplication

Differentiation

- Differentiation is banded if we change bases:

$$\frac{\mathrm{d}^\lambda T_n(x)}{\mathrm{d}x^\lambda} = \begin{cases} 0, & 0 \le n \le \lambda - 1, \\ 2^{\lambda-1}(\lambda-1)!\, n\, C^{(\lambda)}_{n-\lambda}(x), & n \ge \lambda, \end{cases}$$

  where $C^{(\lambda)}_n$ represents the ultraspherical polynomial of integral order λ and of degree n.

- This sparse differentiation has the operator representation:

$$\mathcal{D}_\lambda = 2^{\lambda-1}(\lambda-1)! \begin{pmatrix} \overbrace{0 \;\; \cdots \;\; 0}^{\lambda \text{ times}} & \lambda & & & \\ & & \lambda+1 & & \\ & & & \lambda+2 & \\ & & & & \ddots \end{pmatrix},$$

  mapping T_n to $C^{(\lambda)}_n$.

Conversion & Multiplication

- Conversion from T_n to $C_n^{(1)}$ and from $C_n^{(\lambda)}$ to $C_n^{(\lambda+1)}$ is banded:

$$\mathcal{S}_0 = \begin{pmatrix} 1 & 0 & -\frac{1}{2} & & \\ & \frac{1}{2} & 0 & -\frac{1}{2} & \\ & & \frac{1}{2} & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}, \quad \mathcal{S}_\lambda = \begin{pmatrix} 1 & 0 & -\frac{\lambda}{\lambda+2} & & \\ & \frac{\lambda}{\lambda+1} & 0 & -\frac{\lambda}{\lambda+3} & \\ & & \frac{\lambda}{\lambda+2} & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}.$$

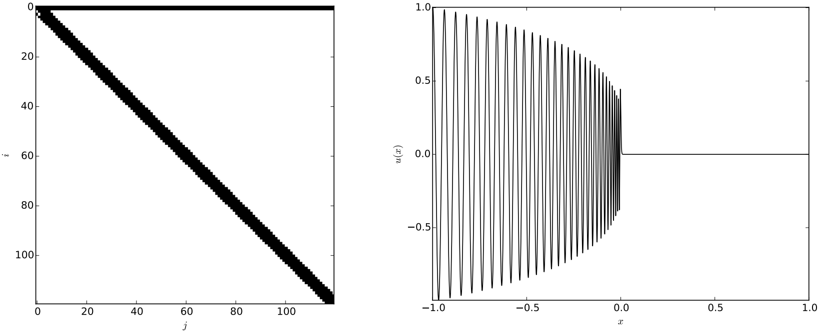
- Multiplication is banded:

$$\mathcal{M}_0[a] = \frac{1}{2}\left[\begin{pmatrix} 2a_0 & a_1 & a_2 & \cdots \\ a_1 & 2a_0 & a_1 & \ddots \\ a_2 & a_1 & 2a_0 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & \cdots \\ a_1 & a_2 & a_3 & \cdots \\ a_2 & a_3 & a_4 & \iddots \\ \vdots & \iddots & \iddots & \iddots \end{pmatrix}\right].$$

Using the recurrence relation for the ultraspherical polynomials, multiplication operators are built in higher order bases as needed.

Ultraspherical spectral method: Example

We solve $\epsilon(\epsilon + x^2)u''(x) = x\,u(x)$, $u(-1) = 1$, $u(1) = 0$ in as little as $\sim 0.0057\,\mathrm{s}$ in `Chebfun` or `ApproxFun.jl`.



Left: the structure of the system. Right: a plot of the solution for $\epsilon = 10^{-4}$. In this case, a Chebyshev expansion of degree 3,276 is required to approximate the solution to double precision.

Singular integral equations

Consider the SIE:

$$\frac{1}{\pi}⨎_{-1}^{1}\left(\frac{K_1(x,y)}{(y-x)^2}+\frac{K_2(x,y)}{y-x}\right.$$
$$\left.+\log|y-x|K_3(x,y)+K_4(x,y)\right)u(y)\,\mathrm{d}y=f(x),$$

- where K_1, K_2, K_3 and K_4 are continuous bivariate kernels,
- f is a known continuous function,
- and integration is interpreted by the Cauchy principal value or Hadamard finite-part.

For the ultraspherical spectral method, we require **singular integral operators** and **bivariate kernels**.

Hilbert transform

- We have the finite Hilbert transform [King 2009]:

$$\mathcal{H}_{(-1,1)}\left[\frac{T_n(x)}{\sqrt{1-x^2}}\right] = \begin{cases} 0, & n=0, \\ C^{(1)}_{n-1}(x), & n\geq 1, \end{cases}$$

- Integrating with respect to x, we obtain the log transform:

$$\mathcal{L}_{(-1,1)}\left[\frac{T_n(x)}{\sqrt{1-x^2}}\right] = \begin{cases} -\log 2, & n=0, \\ -\dfrac{T_n(x)}{n}, & n\geq 1, \end{cases}$$

- Differentiating:

$$\mathcal{H}'_{(-1,1)}\left[\frac{T_n(x)}{\sqrt{1-x^2}}\right] = \begin{cases} 0, & n=0,1, \\ C^{(2)}_{n-2}(x), & n\geq 2, \end{cases}$$

- Integration (divided by π):

$$\Sigma_{(-1,1)}\left[\frac{T_n(x)}{\sqrt{1-x^2}}\right] = \begin{cases} 1, & n=0, \\ 0, & n\geq 1. \end{cases}$$

2D: Tensor and SVD

- In 2D, we scale with $\mathcal{O}(mn)$ function samples and $\mathcal{O}(\min(mn\log n, nm\log m))$ arithmetic via fast 2D transforms.
- Consider the function $f \in C([-1,1]^2)$, then the two dimensional interpolant takes the form:

$$p_{m,n}(x,y) = \sum_{i=0}^{m-1}\sum_{j=0}^{n-1} A_{i,j}T_i(x)T_j(y).$$

- Using the SVD: $\mathbf{A} = \mathbf{U\Sigma V}^*$, we reveal the rank of $\mathbf{A}$:

$$p_{\mathrm{SVD}}(x,y) = \sum_{i=1}^{k} \sigma_i u_i(x) v_i^*(y),$$

  where σ_i are the singular values, and $u_i(x)$ and $v_i^*(y)$ are univariate approximations and $\mathbf{A}$ the optimal rank-k approximant in $L^2([-1,1]^2)$.
- Can we get a low rank form without computing the 2D matrix of coefficients or the SVD?

2D: Continuous GE [Townsend and Trefethen 2013]

- Given $f(x,y) \in C([-1,1]^2)$ and a **tol**, we find f_k such that $\|f - f_k\| < \textbf{tol}$.
- Set $e_0(x,y) = f(x,y)$, $f_0(x,y) = 0$, $k = 0$.

  while $|e_k(x_k, y_k)| = \max(|e_k(x,y)|) > \textbf{tol}$

  $$e_{k+1}(x,y) = e_k(x,y) - \frac{e_k(x_k,y)e_k(x,y_k)}{e_k(x_k,y_k)}$$

  $$f_{k+1}(x,y) = f_k(x,y) + \frac{e_k(x_k,y)e_k(x,y_k)}{e_k(x_k,y_k)}$$

  $$k = k+1$$

  end

  Result: $p_{\mathrm{GE}}(x,y) = \sum_{i=1}^{k} A_i(x)B_i(y)$,
- Scales with a search over $\mathcal{O}(mn)$ function samples and $\mathcal{O}(k\,(m\log m + n\log n))$ arithmetic via fast one-dimensional transforms.

SingularIntegralEquations.jl

Low rank approximations are separable models:

$$K_\lambda(x,y) = \sum_{i=1}^{k_\lambda} A_{\lambda,i}(x) B_{\lambda,i}(y), \quad \text{for} \quad \lambda = 1,2,3,4,$$

then:

$$\mathcal{H}'_{(-1,1)}[K_1] = \sum_{i=1}^{k_1} \mathcal{M}_2[A_{1,i}(x)]\mathcal{H}'_{(-1,1)}\mathcal{M}_0[B_{1,i}(y)], \qquad \mathcal{H}_{(-1,1)}[K_2] = \sum_{i=1}^{k_2} \mathcal{M}_1[A_{2,i}(x)]\mathcal{H}_{(-1,1)}\mathcal{M}_0[B_{2,i}(y)]$$

$$\mathcal{L}_{(-1,1)}[K_3] = \sum_{i=1}^{k_3} \mathcal{M}_0[A_{3,i}(x)]\mathcal{L}_{(-1,1)}\mathcal{M}_0[B_{3,i}(y)], \qquad \Sigma_{(-1,1)}[K_4] = \sum_{i=1}^{k_4} \mathcal{M}_0[A_{4,i}(x)]\Sigma_{(-1,1)}\mathcal{M}_0[B_{4,i}(y)],$$

and ultimately:

$$\left(\mathcal{H}'_{(-1,1)}[K_1] + \mathcal{S}_1\mathcal{H}_{(-1,1)}[K_2] + \mathcal{S}_1\mathcal{S}_0(\mathcal{L}_{(-1,1)}[K_3] + \Sigma_{(-1,1)}[K_4])\right)\mathbf{u} = \mathcal{S}_1\mathcal{S}_0\mathbf{f}.$$

- Affine maps from $(-1,1)$ to (a,b) allow general intervals in $\mathbb{C}$.
- Union of disjoint intervals by interlacing operators & coefficients.

Applications: the Faraday cage

- Consider n infinitesimally thin plates located at the n roots of unity [Chapman, Hewett and Trefethen 2015]. We seek to find the solution to the Laplace equation such that:

$$
\begin{aligned}
u(\mathbf{x}) &= u_0 && \text{for} \quad \mathbf{x} \in D, \\
u(\mathbf{x}) &= \log|\mathbf{x} - \mathbf{x}_0| + \mathcal{O}(1), && \text{as} \quad |\mathbf{x} - \mathbf{x}_0| \to 0, \\
u(\mathbf{x}) &= \log|\mathbf{x}| + o(1), && \text{as} \quad |\mathbf{x}| \to \infty.
\end{aligned}
$$

- We can split the solution $u = u^i + u^s$ as in a scattering problem, where:

$$u^i(\mathbf{x}) = \log|\mathbf{x} - (2,0)|,$$

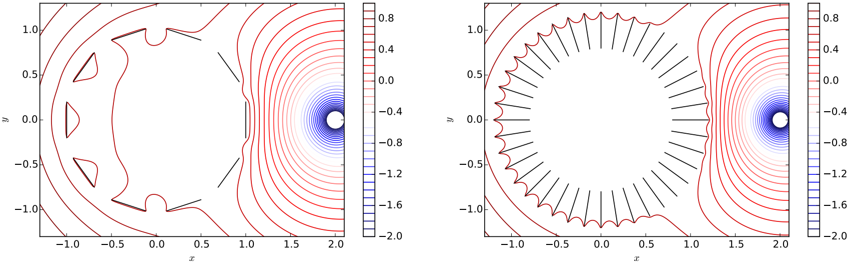
is the source term with strength 2π located at $(2,0)$.

- Dirichlet boundary conditions on Γ. We augment our system with the zero sum condition on the total charge:

$$\int_\Gamma \left[\frac{\partial u(\mathbf{y})}{\partial n}\right] \mathrm{d}\Gamma(\mathbf{y}) = 0,$$

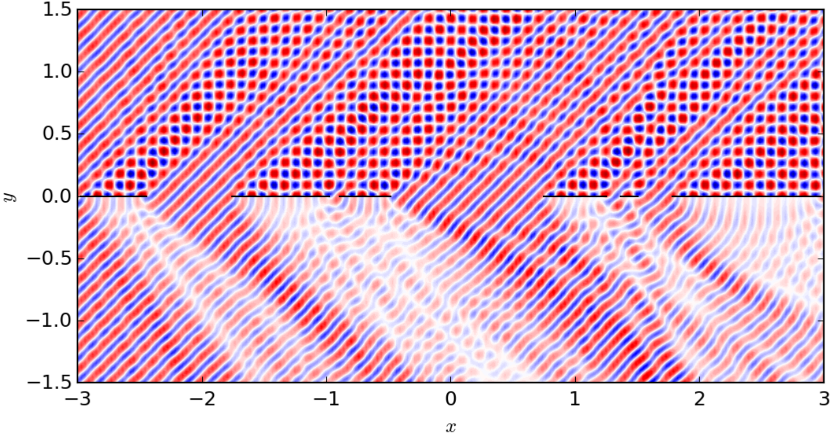
and the unknown constant u_0 to accommodate this condition.

Applications: the Faraday cage



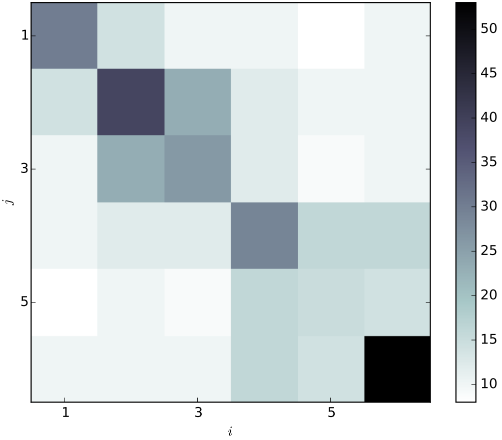
Left: a plot of the solution $u(\mathbf{x})$ with 10 normal plates with radial parameter $r = 10^{-1}$. Right: a plot of the solution $u(\mathbf{x})$ with 40 tangential plates with the same radial parameter.

Applications: acoustic scattering



Acoustic scattering with Neumann boundary conditions from an incident wave with $k = 50$ and $\mathbf{d} = (1/\sqrt{2}, -1/\sqrt{2})$.

Applications: acoustic scattering



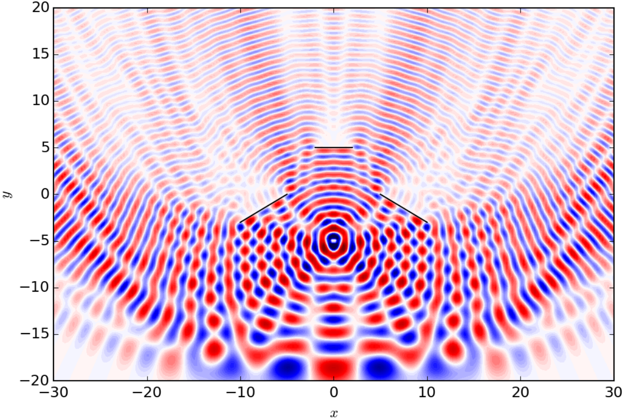
Acoustic scattering with Neumann boundary conditions from an incident wave with $k = 50$ and $\mathbf{d} = (1/\sqrt{2}, -1/\sqrt{2})$.

Applications: gravity Helmholtz

Scattering in a linearly stratified medium $-(\Delta + E + x_2)u(\mathbf{x}) = 0$.

- Fourier transform from time-energy $\Rightarrow$ an interpretation as the Schrödinger equation with linear potential
- Models quantum particles of fixed energy in a uniform gravitational field [Barnett et al. 2014]
- Classical Hamiltonian $\Rightarrow$ rays are *parabolic* instead of linear
- Every point in the "classically allowed" region is illuminated twice

Applications: gravity Helmholtz



In the figure $E = 20$ and source located at $(0, -5)$.

Diagonal preconditioner for compactness

The space $\ell^2_\lambda \subset \mathbb{C}^\infty$ is defined as the Banach space with norm:

$$\|\mathbf{u}\|_{\ell^2_\lambda} = \sqrt{\sum_{k=0}^{\infty} |u_k|^2 (k+1)^{2\lambda}} < \infty.$$

Lemma

If $\Phi = A(\mathbf{x},\mathbf{y}) \log|\mathbf{x}-\mathbf{y}| + B(\mathbf{x},\mathbf{y})$ *and if:*

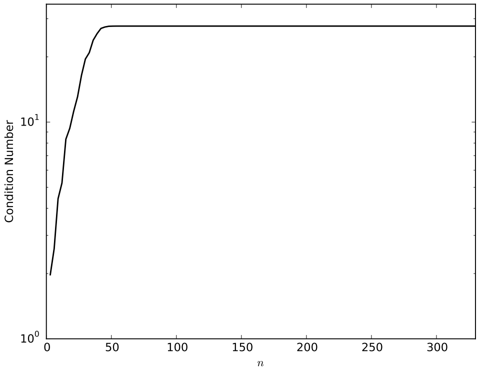
$$\mathcal{R} = \begin{pmatrix} \frac{1}{2\log 2} & & & \\ & 2 & & \\ & & 4 & \\ & & & \ddots \end{pmatrix} : \ell^2_\lambda \to \ell^2_{\lambda-1},$$

then:

$$\left(\mathcal{L}_{(-1,1)}[\pi A] + \Sigma_{(-1,1)}[\pi B]\right)\mathcal{R} = I + \mathcal{K},$$

where $\mathcal{K} : \ell^2_\lambda \to \ell^2_\lambda$ *is compact for* $\lambda = 1, 2, \ldots$.

Diagonal preconditioner for compactness



Fast Chebyshev multiplication + banded operators = fast operator-function products $\Rightarrow$ continuous Krylov methods.

Conclusion & Outlook

- `SingularIntegralEquations.jl` is an open-source framework for solving singular integral equations. It requires open-source `ApproxFun.jl` and is written in free & open-source Julia.
- Fractal screens have a non-trivial solution to the Dirichlet problem, but a zero-solution for the Neumann problem. No Numerical results! Approach: symmetrized Woodbury matrix identity & Schur complement to hierarchically assemble and annihilate off-diagonal low rank compact operators.
- Polynomially mapped domains can be treated via the spectral mapping theorem.
- Fundamental solution is known for Helmholtz equation with a parabolic refractive index. Models Gaussian beams in optical fibres.
- Special thanks to Lloyd Nick Trefethen, Dave Hewett, and the Chebfun team for stimulating discussions

Thank you all very much for your time!

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