Hybrid Frequency-Time Analysis and Numerical Methods for Time-Dependent Wave Propagation

DOE Howes Scholar Presentation

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July 21, 2021

Thanks to...

- The Department of Energy & The Krell Institute
- The fellows and alumni: those I know and those I haven't yet met
- My thesis advisor Oscar Bruno
  - ...and so many others: Agustin F.-Lado, Emmanuel Garza, Edwin Jimenez, Carlos P.-Arancibia...
- My UMich mentor Shravan Veerapaneni
- Other mentors: Tzanio Kolev @ LLNL; Daniel Toundykov @ UNL; and Peter Petropoulos, Catalin Turc, and David Horntrop @ NJIT.

Time-domain linear PDEs

My universe: wave propagation and scattering in $\mathbb{R}^d$, $d = 2, 3$.
Example, scalar wave equation:

$$\frac{\partial^2 u}{\partial t^2}(\mathbf{r}, t) - c^2 \Delta u(\mathbf{r}, t) = 0, \quad \mathbf{r} \in \Omega \subset \mathbb{R}^d, \tag{1a}$$

$$u(\mathbf{r}, 0) = \frac{\partial u}{\partial t}(\mathbf{r}, 0) = 0 \tag{1b}$$

$$u(\mathbf{r}, t) = h(\mathbf{r}, t) \quad \text{for} \quad (\mathbf{r}, t) \in \Gamma \times [0, T], \tag{1c}$$

Boundary data: $h(\mathbf{r}, t) = -u^{inc}(\mathbf{r}, t)$ (sound-soft **scattering**)

Important classical problem:

- Motivations: nanophotonics, RADAR, communications, imaging systems, elastodynamics, electromagnetism
- Propagation in dispersive materials: $c = c(\omega)$

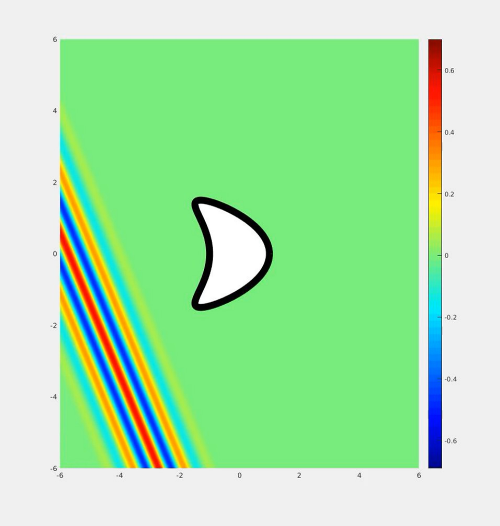
Challenging problem! Previous work

Existing Numerical Methods:

- Finite-difference / Finite-element time domain (FDTD / FETD)
- Time-domain integral equations
- Convolution Quadrature

Our work:

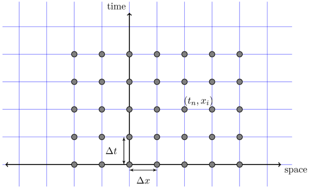
1. TGA, O. P. Bruno, Mark Lyon. High-order, Dispersionless "Fast-Hybrid" Wave Equation Solver. Part I. [SISC 2020]
2. TGA, O. P. Bruno, Mark Lyon. High-order, Dispersionless "Fast-Hybrid" Wave Equation Solver. Part II. [in prep]
3. TGA, O. P. Bruno. "Domain-of-dependence" Bounds and Time Decay of Solutions of the Wave Equation. [arXiv:2010.09002]



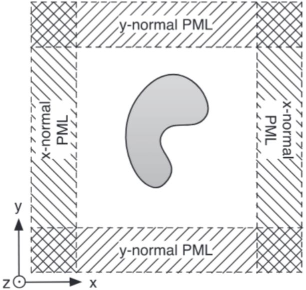
Previous work: Volumetric (FDTD/FETD) methods

- Must discretize entire volumetric grid
- Absorbing boundary conditions / layers
- Time-stepping, implies increasing:
  - **cost** for large time
  - **error** for large time
- Generally low-order methods

Schematic:



Absorbing Layers ([Berenger JCP '94]):



Ref: [Shin et al JCP '12]

Previous work: Time Domain Integral Equations (TDIEs)

Focuses on the representation formula:

$$u(\mathbf{r}, t) = \int_{-\infty}^{t} \int_{\Gamma} G(\mathbf{r} - \mathbf{r}', t - t')\varphi(\mathbf{r}', t')d\sigma(\mathbf{r}')dt' \qquad (2)$$

Density must satisfy the TDIE:

$$\iint\limits_{[-\infty, t]\times\Gamma} G(\mathbf{r} - \mathbf{r}', t - t')\varphi(\mathbf{r}', t')d\sigma(\mathbf{r}')dt' = b(\mathbf{r}, t), \quad (\mathbf{r}, t) \in \Gamma \times [0, T]$$

Overview ([Barnett '20, Ha-Duong '03]):

- Difficult to guarantee stability
- Complex schemes
- Typically low-order convergence

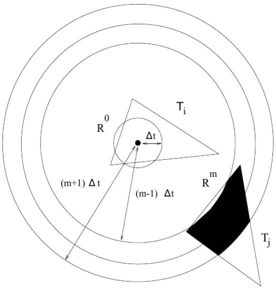


Fig. 2. The domain of spatial integration

$$\iint_{t_l \le |x-y| \le t_{l+1}} (\cdots)\, d\sigma_x\, d\sigma_y,$$

Ref: [Ha-Duong '03]

Previous work: Convolution Quadrature—a true *Hybrid* method

Still a time-stepping method — with connections to discrete (Z-) Laplace transform.

$$U_d(z;\mathbf{r}) = \sum_{n=0}^{\infty} u_d(t_n,\mathbf{r}) z^n \quad \xLeftrightarrow{\text{Z-transform}} \quad u_d(t_n,\mathbf{r}) = \int_{\mathcal{C}_\lambda} \frac{U_d(z;\mathbf{r})}{z^{n+1}} dz.$$

Hybrid frequency/time method — decoupled modified Helmholtz problems for U_d:

$$\Delta U_d - s_n^2 U_d = 0, \quad U_d|_\Gamma = B_{s_n}, \quad n = 1,\ldots,N_f$$

Ref: [Betcke '17, Banjai '10, Lubich '94]

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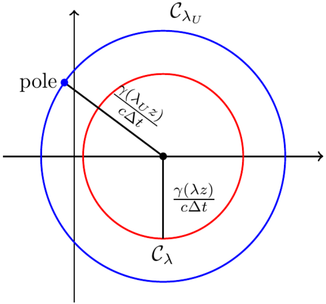
Ref: [Betcke '17, Banjai '10, Lubich '94]

- Relies on a choice of A-stable integrator: BDF2, RK
- Two sources of temporal approximation error
  - Time-stepping error: $\Delta t \to 0$
  - Contour integral error: $N_f \to \infty$.
    - Error ↑ as integration contour C_λ approaches analyticity boundary C_{λ_U} of unknown location



Ref: [Betcke et al SISC '17]

Fourier Frequency/Time Hybrid Approach

Use Fourier transformation on incident wave:

$$U^i(\mathbf{r},\omega) = \int_{-\infty}^{\infty} u^{inc}(\mathbf{r},t)\,\boxed{e^{i\omega t}}\,dt$$

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$$u(\mathbf{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(\mathbf{r},\omega)\boxed{e^{-i\omega t}}\,d\omega$$

Questions to address:

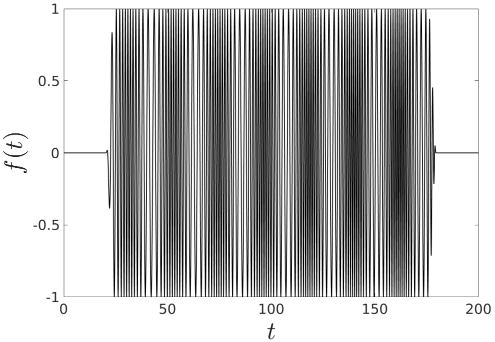
1. Forward transform: How many frequency-domain problems need be solved? Relationship to T^{inc}, the duration of u^{inc}?
2. Inverse transform: Need to evaluate for large times, multiple scattering. Relationship between t and # of frequency-domain problems?

- Of course, this has been done;
  - . . . see [Rokhlin ’83, Douglas ’93, Zirilli et al ’00, Klaseboer et al ’17]
  - [Jensen et al ’11, §8.2] discusses, but does not address, difficulties
- Note: When solving wave equation in $\mathbb{R}^2$, nonsmooth behavior as $\omega \to 0^\pm$.

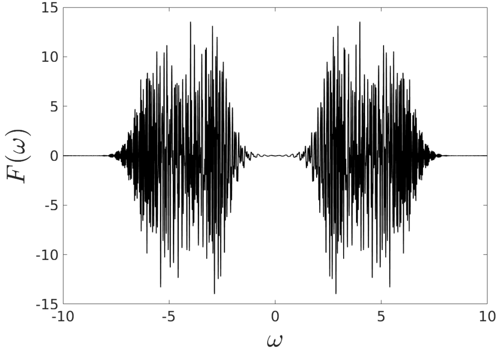
Long-duration incident waves

- Dominant cost of Hybrid method: Frequency-domain solutions
  - Number of solutions dependent on Freq-complexity of incident field

Challenge when time-dependent field has long duration:



Smooth linear chirp signal, large t



Fourier transform of linear chirp

Need to resolve this in Frequency Domain(!) :-(

Temporal Partition of Unity

Recall problem:

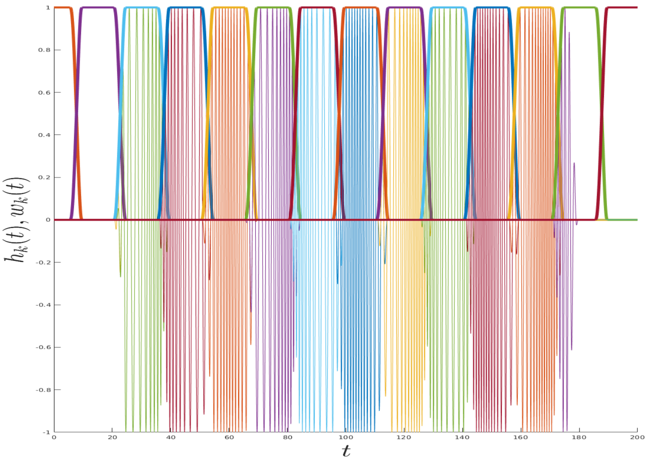
$$\frac{\partial^2 u}{\partial t^2}(\mathbf{r}, t) - c^2 \Delta u(\mathbf{r}, t) = 0, \quad \mathbf{r} \in \Omega,$$
$$u(\mathbf{r}, t) = b(\mathbf{r}, t) \quad \text{for} \quad (\mathbf{r}, t) \in \Gamma \times [0, T].$$

Define a partition of unity of *time*.
Let $s_k \in [0, T]$ and windowing functions $w_k \in C_c^\infty$:

1. $w_k(t) = 1$ in neighborhood of $t = s_k$,
2. $w_k(t) = 0$ for $|t - s_k| > H$,
3. $\sum_{k=1}^{K} w_k(t) = 1$ for all $t \in [0, T]$.

Partition incident wave (...then Fourier transform)

$$b(\mathbf{r}, t) = \sum_{k=1}^{K} b_k(\mathbf{r}, t) \implies u(\mathbf{r}, t) = \sum_{k=1}^{K} u_k(\mathbf{r}, t)$$


1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
20
40
60
80
100
120
140
160
180
200
$h_k(t), w_k(t)$
t

Temporal Partitions of Unity & Fourier Transforms

The key relationship:

$$B_k(\mathbf{r},\omega) = \int_{-\infty}^{\infty} w_k(t) b(\mathbf{r},t) e^{i\omega t}\,dt = \int_{-H}^{H} b_k(\mathbf{r}, t+s_k) e^{i\omega(t+s_k)}\,dt$$

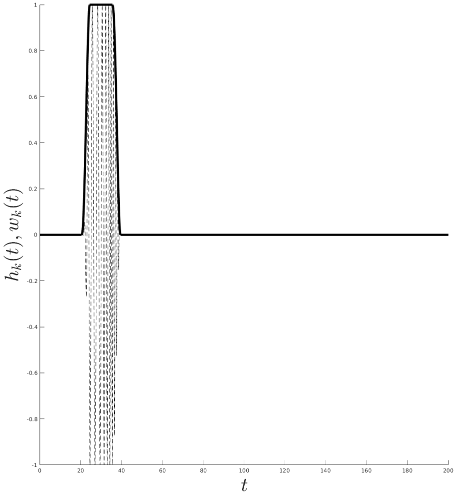
Factoring out $e^{i\omega s_k}$ we obtain a "slow"-varying quantity:

$$B_k^{slow}(\mathbf{r},\omega) = e^{-i\omega s_k} B_k(\mathbf{r},\omega).$$

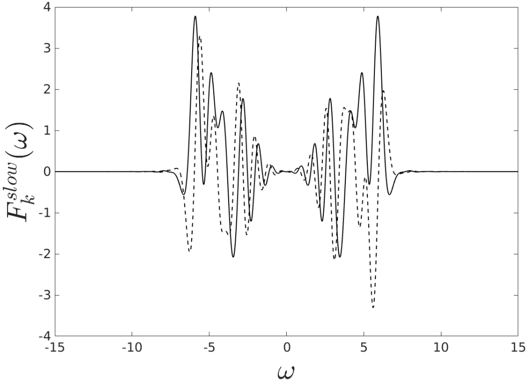
The same then holds for the frequency-domain solution:

$$U_k^{slow}(\mathbf{r},\omega) = e^{-i\omega s_k} U_k(\mathbf{r},\omega), \quad (k = 1,\ldots,K)$$

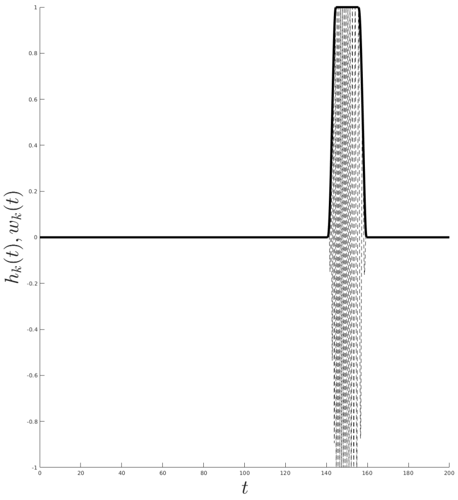
- . . . But: how do we generate all the K (time-partition) solutions U_k^{slow}?
  - Do we need $K = \mathcal{O}(T)$ frequency-domain (integral equation) solutions?



Windowed real signal.



Windowed Fourier Transform, partition $s_k = 35$.



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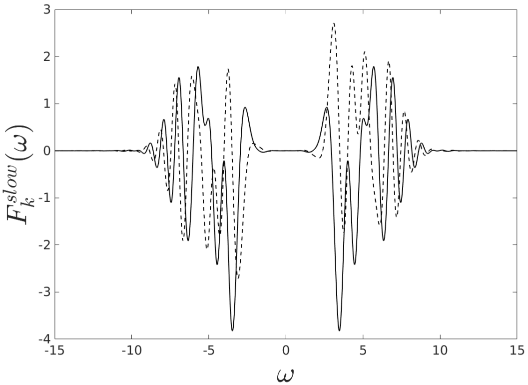

Windowed Fourier Transform,
partition $s_k = 155$.

Going back to time: evaluating (oscillatory) Fourier integrals

Task: Accurately approximate highly oscillatory integrands at $\mathcal{O}(1)$ cost:

$$u(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(\omega)e^{-i\omega t}\,d\omega$$

Classical quadrature algorithms: *Trapezoidal rule*

$$u(t_k) = \frac{1}{2\pi}\int_{-W/2}^{W/2} U(\omega)e^{-i\omega t_k}\,d\omega \approx \frac{T}{2\pi m}\sum_{j=0}^{m-1} U(\omega_j)e^{-i\omega_j t_k}$$

- Can be accelerated with FFTs (and fast fractional DFTs)

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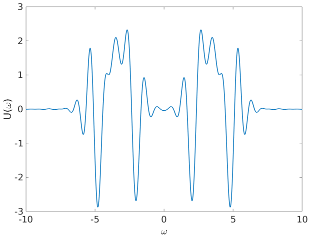
- Implies periodicity in $u(t)$, fails to handle structure of Fourier kernel.
- To manage spurious periodicity: refine ω discretization $\implies$ $\mathcal{O}(N)$ large-time cost and expensive frequency-domain solves.
- Requires global regularity and periodicity for high-order convergence.

New Quadrature Rule: Fourier Expansion

Fourier basis for **frequency-domain**

$$U(\omega) \approx \sum_{m=-N/2}^{N/2-1} c_m e^{i\frac{\pi}{W}m\omega}$$



A signal $U(\omega)$ with finite bandlimit.

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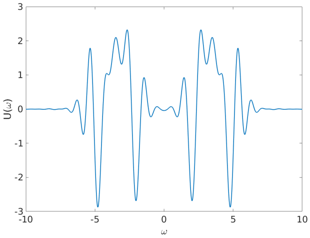

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Then, evaluating term-by-term *exactly*,

$$u(t) = \int_{-W}^{W} U(\omega)e^{-i\omega t}\,d\omega \approx \sum_{m=-N/2}^{N/2-1} c_m \int_{-W}^{W} e^{i\frac{\pi}{W}(m-\frac{W}{\pi}t)\omega}\,d\omega$$

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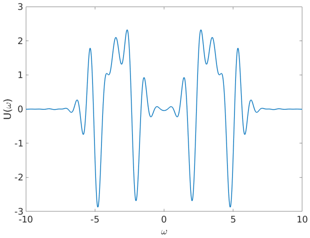

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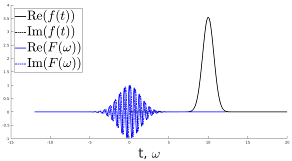
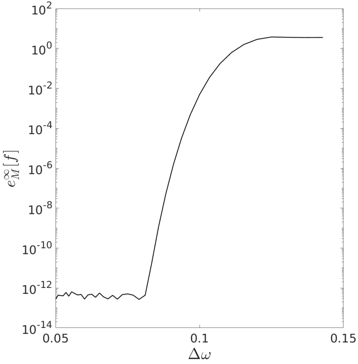
Can evaluate on $t_\ell = \ell \Delta t$; **arbitrary grid** *(Δt has no CFL limitations)*,

$$u(t_\ell) = \sum_{m=-N/2}^{N/2-1} c_m b_{\beta\ell - m}, \quad \text{where} \quad \beta = \frac{W}{\pi}\Delta t \quad \text{and} \quad b_q = 2W \operatorname{sinc}(q)$$

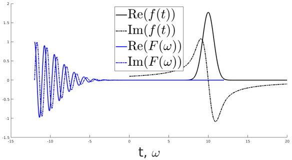
Numerical results: (inverse) Fourier quadrature rule

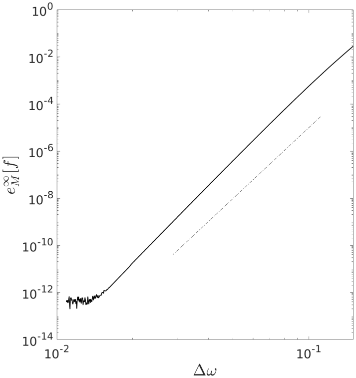
Fourier (periodic) quadrature.





FC (non-periodic) quadrature.





Overall Convergence Analysis

Overall solution description:

$$u(\mathbf{r}, t) = \sum_k u_k(\mathbf{r}, t) \approx \sum_{k=1}^{K} u_k^{W,J}(\mathbf{r}, t)$$

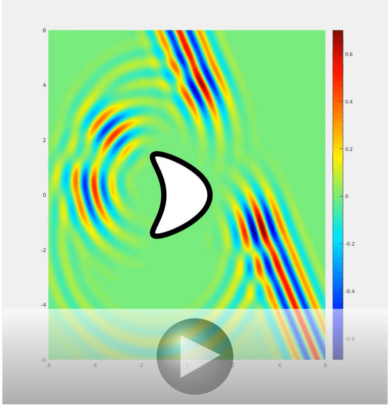
Two errors contributing (assuming smooth incident data):

- Frequency truncation parameter W: Error decreases *superalgebraically* as numerical bandwidth $W \to \infty$.
- # J of Frequency Domain problems solved, $J = \mathcal{O}(1)$ as $t \to \infty$:
  - 2D: Fixed, high-order convergence, e.g. 10th order as $J \to \infty$.
    - ★ Relies on general-purpose numerical algs introduced in [Amlani & Bruno '16, Dominguez '13].
  - 3D: Superalgebraic as $J \to \infty$.

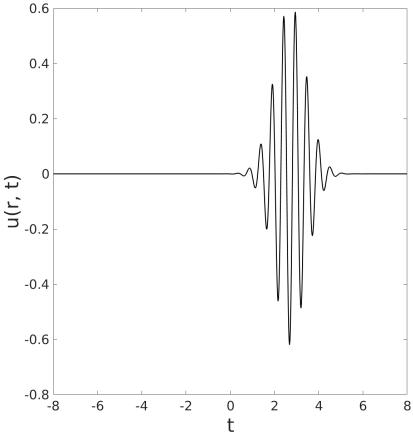
Plane wave incident on kite scatterer in $\mathbb{R}^2$

Hybrid method solution with Gaussian-modulated plane wave incidence:

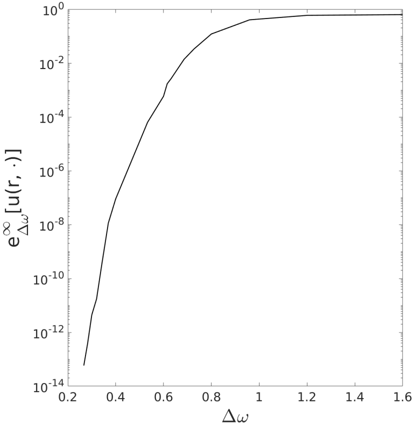
$$U^{inc}(\mathbf{r},\omega) = e^{-\frac{(\omega-\omega_0)^2}{\sigma^2}} e^{i\omega \frac{\mathbf{k}}{||\mathbf{k}||}\cdot\mathbf{r}}, \quad \text{where} \quad \omega_0 = 12, \sigma = 2, \mathbf{k} = \mathbf{e}_x + \frac{1}{2}\mathbf{e}_y.$$



Convergence

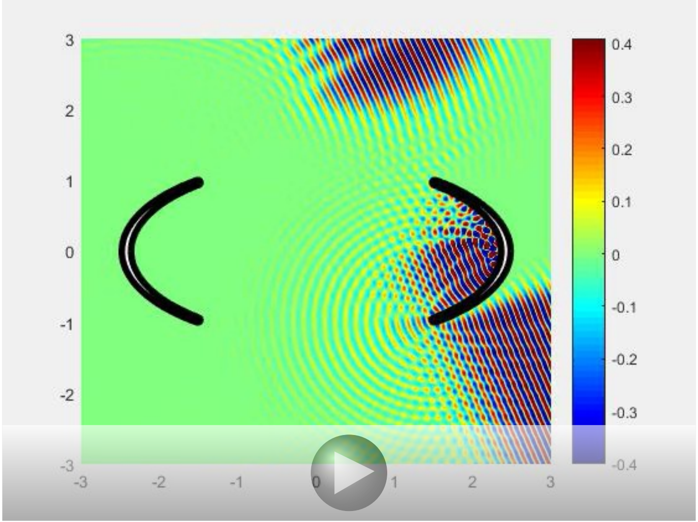


Solution trace at observation point (2,2).



All-time L^{∞} error as function of freq. discretization refinement $\Delta\omega$.

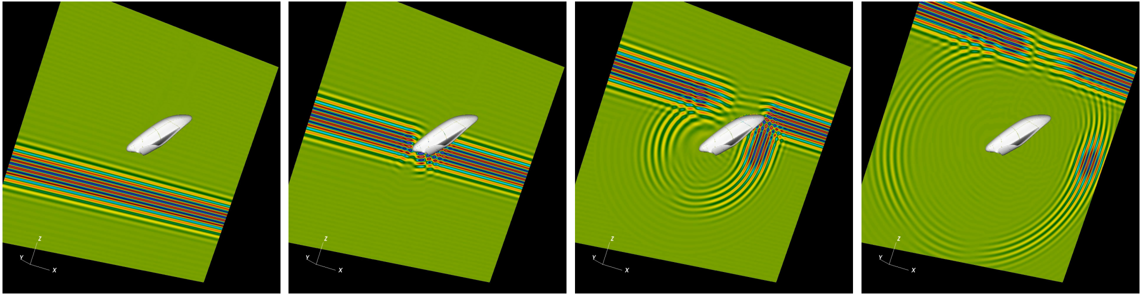
Long-time simulations: Whispering Gallery



Three-dimensional scattering: II

Pulse incident field:

$$U^{inc}(\mathbf{r},\omega) = e^{-\frac{(\omega-\omega_0)^2}{\sigma^2}} e^{i\omega \frac{\mathbf{k}}{||\mathbf{k}||}\cdot\mathbf{r}}, \quad \text{where} \quad \omega_0 = 15, \sigma = 2, \mathbf{k} = \mathbf{e}_z.$$



Cost comparisons: TDIEs / Convolution Quadrature

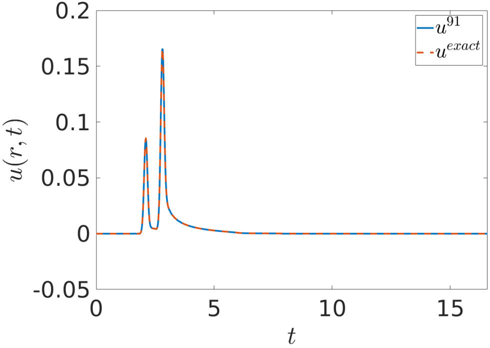
Sphere of radius $a = 1.0$, incident field:

$$u^{inc}(\mathbf{r}, t) = -0.33 \sum_{i=1}^{3} \exp\left[\frac{(t - \mathbf{e}_i \cdot \mathbf{r} - 0.60 - 1)^2}{.01}\right].$$

Comparison with results from Fast 3D CQM work:

—	$\|\|e\|\|_\infty$	Time	Mem.
This work	$2.2 \cdot 10^{-4}$	4.3	1.6
BK '14	$2.1 \cdot 10^{-3}$(†)	40.1	56.8

(Errors are in time-domain compared with Mie theory, Comp. Time in CPU-hours, Memory usage in GB)



Ref: [Banjai & Kachanovska JCP '14] "Fast convolution quadrature for the wave equation in three dimensions"

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Sphere of radius $a = 1.6$, incident field:

$$u^{inc}(\mathbf{r}, t) = T(t - \widehat{k} \cdot \mathbf{r}), \quad T(t) = e^{-(t-6)^2/2}.$$

Comparison with results from recent TDIE work:

—	$\|\|e\|\|_\infty$	Time	Mem.
This work	$1.6 \cdot 10^{-7}$	4.1	1.2
BGH '20	$\approx 10^{-7}$	101.75	290

(Errors are in time-domain compared with Mie theory, Comp. Time in minutes, Memory usage in GB)

Ref: [Banjai & Kachanovska JCP '14] "Fast convolution quadrature for the wave equation in three dimensions"

Ref (†): [M. Kachanovska '19]: private communication to TGA.

Ref: [Barnett, Greengard, & Hagstrom JCP '20] "High-order discretization of a stable time-domain integral equation for 3D acoustic scattering"

Generic boundary data

Before: frequency-domain problems...

$$\Delta U_{\mathbf{p}} + \omega_j^2 U_{\mathbf{p}} = 0 \quad \text{in} \quad \Omega$$

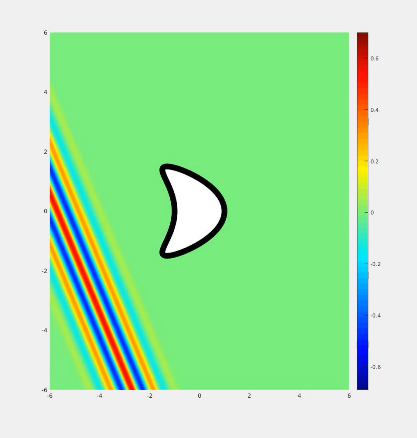
$$U_{\mathbf{p}} = e^{i\kappa(\omega_j)\mathbf{p}\cdot\mathbf{r}} \quad \text{on} \quad \Gamma = \partial\Omega$$

...assuming separability for incident wave:

$$u^{inc}(\mathbf{r}, t) w_k(t) = -b_k(\mathbf{r}, t),$$

$$b_k(\mathbf{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} B_k(\omega) e^{i\frac{\omega}{c}(\mathbf{p}\cdot\mathbf{r} - ct)} d\omega$$

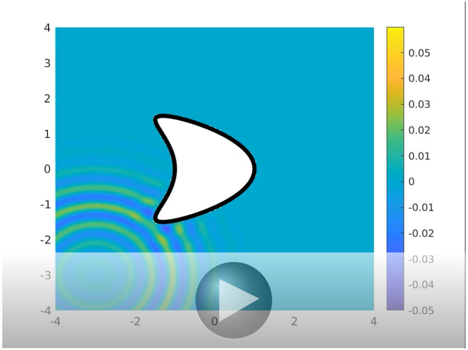
What if it's not as simple as this?



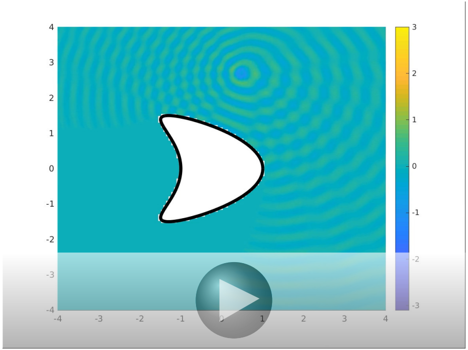
What if direction **p** varies across time?

Generic boundary data

- Generally, need to solve for many directions, at each frequency.
  - With frequency cutoff W and physical size a, $\mathcal{O}((W \cdot a)^{d-1})$-bounded solves.
  - Efficiency relies on fast direct solvers
    - Think: LU factorizations; but really $\mathcal{H}$-matrices, $\mathcal{H}^2$-matrices, etc.



Stationary point-source scattering

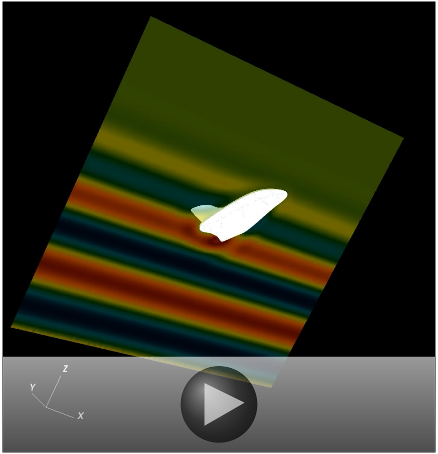


Moving point-source scattering.

- Compared with single-incidence: $N = 80$ solves, 2.5% solve time increase.

Long-time 3D simulations

$$u^{tot} = u^{inc} + \sum_{k=1}^{12} u_k$$



$$u_k^{inc} + u_k, \ k = 1, \ldots, 6.$$

A natural question: *Do we need to evaluate all windows k in the sum?*

Estimating field sizes: boundary densities as a proxy

Given: Space-time patch to evaluate u: $\mathcal{R} \times \mathcal{T}$.
Let $r_{\max} = \max_{\mathbf{r} \in \mathcal{R}, \mathbf{r}' \in \Gamma} |\mathbf{r} - \mathbf{r}'|$.

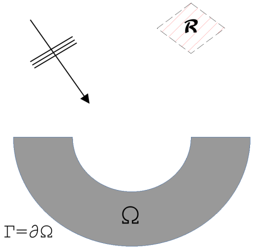
Proposition (Pointwise Kirchhoff-formula bounds)

For each $\mathbf{r} \in \mathcal{R}$, *if*

$$\|\psi_k(\cdot, t)\|_{L^\infty(\Gamma)} < C(\mathbf{r})\varepsilon$$

for $t > T_o$, *then*

$$|u_k(\mathbf{r}, t)| \leq \varepsilon \quad \textit{for all} \quad t > T_o + r_{\max}/c.$$



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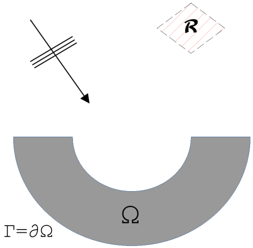

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$$\|\psi_k(\cdot, t)\|_{L^\infty(\Gamma)} < C(\mathbf{r})\varepsilon$$

for $t > T_o$, then

$$|u_k(\mathbf{r}, t)| \leq \varepsilon \quad \text{for all} \quad t > T_o + r_{\max}/c.$$

- Q: Is it possible to estimate the density $\|\psi_k(\cdot, t)\|$ for all $t > T_o$?
  - Better: Using information we can *easily observe and efficiently compute*?
    - A *domain-of-dependence* time interval equal of length $\mathrm{diam}(\Gamma)/c$.
  - Why: Conclude $\|\psi_k(\cdot, t)\| < \varepsilon$ for $t > T_o$ and then don't compute u_k.
    - Can analyze the error committed by solution at large times and show it is bounded.

Domain-of-dependence ψ estimate: "T-Superalg. decay"

Theorem (A. & Bruno '20)

Let n be an arbitrary positive integer and let Γ be the boundary of an obstacle that satisfies a q-growth condition. Let I be a domain-of-dependence interval laying before an "observation time" T_o. For smooth incident data the surface density satisfies the pointwise temporal bound

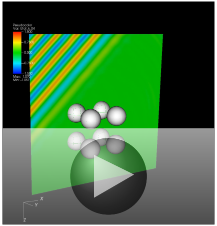
$$\sup_{t > T_o + T} \|\psi_k(\cdot, t)\|_{L^2(\Gamma)} \leq C(\Gamma, n)\, T^{1-n} \, \|\psi_k\|_{H^{n(q+1)+1}(I;\, L^2(\Gamma))} \,.$$

Notes:

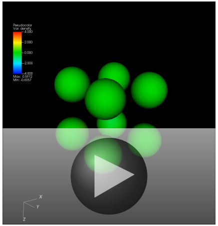
- Superalgebraic decay estimate for any finite q-growth obstacle.
- Uses only q-growth frequency-domain condition on *real*-ω axis.
  - Equivalent to polynomially-bounded resolvent-operator norm as frequency ω grows

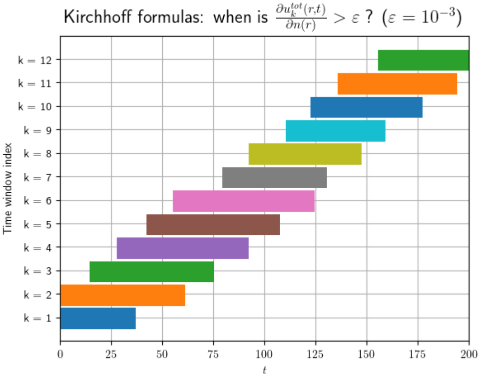
Array of spheres: Tracking the densities

Scattering: u_k^{tot}, $k = 4$ (1 window).



$\frac{\partial u_k^{tot}}{\partial \mathbf{n}(\mathbf{r})}(\mathbf{r}, t)$ on Γ, $k = 4$





- Numerics+Theory agree: u_k can be neglected to ε-tolerance based on $|\psi_k| < \varepsilon$.
  - $\varepsilon = 10^{-3}$, max u_k error: $7.6 \cdot 10^{-4}$.

Implications for numerical analysis of hybrid methods

Theorem (A. & Bruno '20)

Let Γ be the boundary of an obstacle that satisfies a q-growth condition. For smooth incident data, a region of space $\mathcal{R}$ of diameter D_r and a time interval $\mathcal{T}$ of length D_t, there exist for every $\varepsilon_{\mathrm{tol}} > 0$ an integer $M(\varepsilon_{\mathrm{tol}}, D_r, D_t)$ and certain integers M_i and M_f satisfying $M_f - M_i = M$ so that for all incident wavefields

$$\sup_{\substack{t\in\mathcal{T}\\ \mathbf{r}\in\mathcal{R}}} \left| u(\mathbf{r},t) - \sum_{k=M_i}^{M_f-1} u_k(\mathbf{r},t) \right| \leq C(\Gamma, D_r, D_t)\varepsilon_{\mathrm{tol}}.$$

Note:

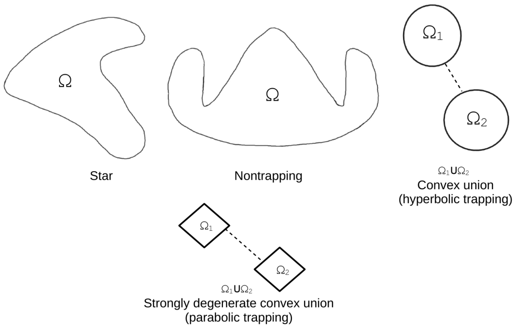
- Number of sum-terms M is independent of $\#$ of windows $K = \mathcal{O}(T)$
  - $\rightsquigarrow \mathcal{O}(1)$ numerical method.
- Inclusion in sum determined by domain-of-dependence norm $\|\psi_k\|_{H^s(I;L^2(\Gamma))}$.

Decay of waves: Geometry & Resonances

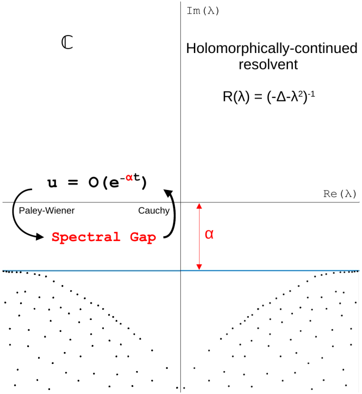
- Q: Is it possible to predict uniform $t \to \infty$ decay rates?

  - '59 Wilcox: sphere
  - '63 Lax-Morawetz-Phillips: star-shaped domain
  - '67 Lax-Phillips: Trapping $\overset{??}{\Longleftrightarrow}$ pole sequence approaching $\mathrm{Im}(\lambda) = -\alpha = 0$
  - '69 Ralston: For trapping geometries, cannot have

$$E(u,t) \leq e^{-\alpha t} E(u,0)$$

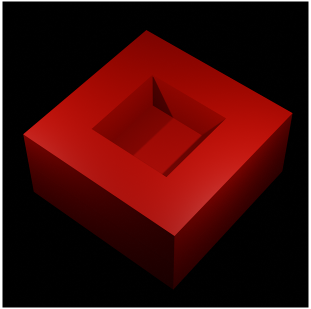


  - '77 Morawetz-Ralston-Strauss: C^∞ "nontrapping" domain
  - '82 Ikawa: Convex-union trapping domains (counterexample to Lax '67)
  - '85 Ikawa: degenerate convex-union domain $\rightsquigarrow \alpha = 0$.

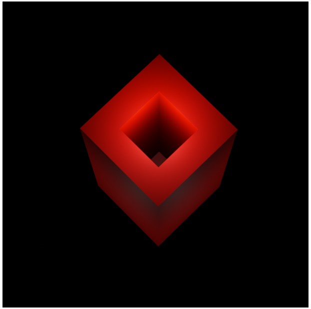


New decay estimates for trapping domains

"Parallel trapping obstacles":



Cube with smaller cube removed.



Deep rectangular cavity.

- Only known decay estimate for a connected trapping obstacle or cavity
- Cases when Lax-Phillips theory yields exponential rate $\alpha = 0$.

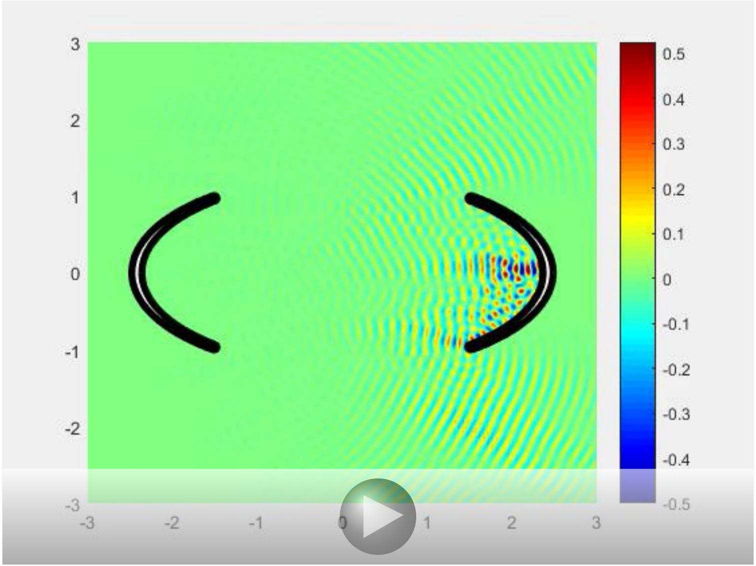
Future Directions (on this theme)

I am currently interested in:

- Large-scale HPC implementations with accelerated freq. domain solvers
- Transient electromagnetics / elastodynamics
- Transient wave propagation in dispersive and/or inhomogeneous media
- Resonant cavities & complex/coupled structures
- Inverse source problems
- Laplace-transform IVPs / low-regularity pulses
- Sharpening decay rates for trapping obstacles
- New trapping-domain q-growth type estimates – Morawetz identities etc.

Also, @ Michigan:

- Volume-potential based solvers, fluid dynamics, optimal mixing of fluids, fractional PDEs



Thank you for your attention!!