The “Fast Hybrid Method” for Wave Scattering: New Advances in Time-Domain Integral Equations

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July 17, 2018

Time-domain linear PDEs in homogeneous medium

- Diffusion Equation
- Elastodynamics
- Wave Equation, Maxwell's Equations (including dispersive materials)

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

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

Sound-soft scattering conditions: $h(\mathbf{r}, t) = -u^i(\mathbf{r}, t)$

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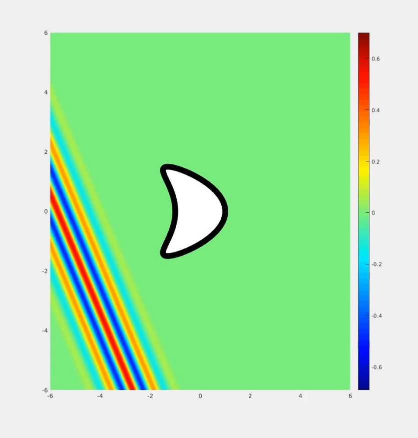
Important classical problem:

- Applications: photovoltaic efficiency, nanophotonics
- Characterization of propagation in dispersive materials
- Defense: RADAR, imaging systems

Challenging problem! Previous work

Existing Numerical Methods:

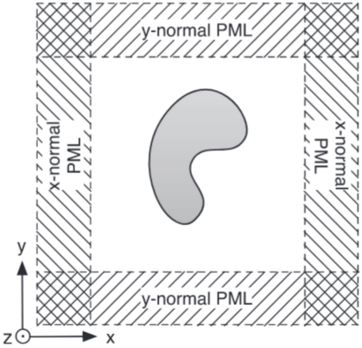
- Finite-difference / Finite-element time domain (FDTD / FETD)
- Direct solution of time-domain integral equations
- Convolution Quadrature



Volumetric (FDTD/FETD) methods

- Must discretize entire volumetric grid
- For exterior problems, absorbing boundary conditions (Perfectly Matched Layers)
- Time-stepping $\implies$ growing cost for large time
- Generally low-order accurate methods $\implies$ computationally expensive
- Numerical dispersion $\implies$ multiple scattering is problematic

PML (Berenger '94):



Ref: Shin et al., JCP (2012)

Convolution Quadrature: A true *Hybrid* method

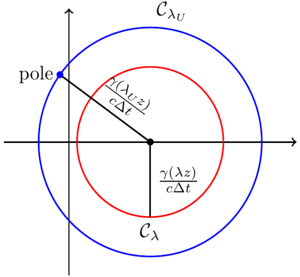
Still a time-stepping method — with connections to discrete Laplace transform. Use Z-transform relations for $\{u_d(t_i, \mathbf{r}) : 1 \leq i \leq N_d\}$:

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

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

$$\Delta U_d - s^2 U_d = 0, \quad U_d|_\Gamma = H_s$$

- Relies on a choice of A-stable integrator: BDF2, RK
- Two sources of temporal approximation error
  - Time-stepping error, smaller Δt
  - Contour integral error, more U_d solutions



Ref: Betcke, SIAM J. Sci. Comput. (2017)

Convolution Quadrature: Discussion

Advantages:

- Hybrid algorithm decouples solution — Parallel in time
- Boundary integral equations: Dimensional reduction!
- Exploits fast frequency-domain solvers

Disadvantages:

- Limited order of accuracy, dispersion due to finite differences
- Fast solvers only demonstrated at low spatial order (linear Galerkin)
- Increasing cost for large time
- Need *many* frequency-domain solutions for full accuracy

Time Domain Integral Equations

Focuses on representation formula:

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

where

$$G(\mathbf{r}, t) = \begin{cases} \frac{H(ct-|\mathbf{r}|)}{2\pi\sqrt{(ct)^2-|\mathbf{r}|^2}} & \text{for} \quad d = 2 \quad \text{and} \\ \frac{\delta(ct-|\mathbf{r}|)}{4\pi|\mathbf{r}|} & \text{for} \quad d = 3. \end{cases} \tag{3}$$

Direct solution:

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

- Difficult to ensure stability
- Complex schemes
- Low-order convergence

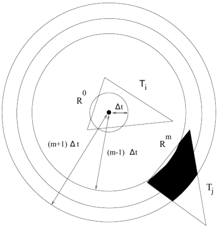


Fig. 2. The domain of spatial integration

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

Ref: Ha-Duong, Topics in Comput. Wave Propag. (2003)

Frequency-domain solvers: Boundary integral equations

Solution Method for Frequency-domain (Fourier-Time Transform) Analysis

$$\Delta U + \omega^2 U = 0 \quad \text{in} \quad \Omega \tag{4a}$$

$$U = U^i \quad \text{on} \quad \Gamma = \partial\Omega \tag{4b}$$

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Notation:

$$G_\omega(\mathbf{r}) = \begin{cases} \frac{i}{4} H_0^1(\omega|\mathbf{r} - \mathbf{r}'|) & \text{for} \quad d = 2 \quad \text{and} \\ \frac{e^{i\omega|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} & \text{for} \quad d = 3. \end{cases} \tag{5}$$

Layer Potentials: $U(\mathbf{r}) = \int_\Gamma G_\omega(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}')d\sigma$ — a solution to (4) for all ψ!

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Layer Potentials: $U(\mathbf{r}) = \int_\Gamma G_\omega(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}')d\sigma$ — a solution to (4) for all ψ!To satisfy boundary conditions, must satisfy for $\mathbf{r} \in \Gamma$:

1st-kind integral equation: $$(S_\omega \psi)(\mathbf{r}) = \int_\Gamma G_\omega(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}')d\sigma = U^i(\mathbf{r})$$

2nd-kind integral equation: $$\left[-\frac{1}{2} I + K_\omega^* + i\eta S_\omega\right](\psi)(\mathbf{r}) = \partial_\nu U^i(\mathbf{r}) + i\eta U^i(\mathbf{r})$$

A Hybrid Approach

Use Fourier transformation:

$$u(\mathbf{r}, t) = \int_{-\infty}^{\infty} U(\mathbf{r}, \omega) e^{-i\omega t} d\omega, \tag{6}$$

Can use any frequency-domain solution, but for integral equations,

$$U(\mathbf{r}, \omega) = \int_{\Gamma} \psi(\mathbf{r}', \omega) G_{\omega}(\mathbf{r}, \mathbf{r}') d\sigma(\mathbf{r}'). \tag{7}$$

Frequency-domain solutions are obtained via transforming incident fields and solving, e.g. with layer potentials,

$$(S_{\omega}\psi)(\mathbf{r}, \omega) = -U^{i}(\mathbf{r}, \omega) \tag{8}$$

Questions to address:

- How do we best exploit a Hybrid approach for HPC?
- What quadrature rule is used?
- How many frequency-domain problems need be solved? Relationship to t?

Evaluating (Oscillatory) Fourier integrals

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

$$u(t) = \int_{-\infty}^{\infty} U(\omega) e^{-i\omega t} d\omega$$

Classical quadrature algorithms: *Trapezoidal rule*

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

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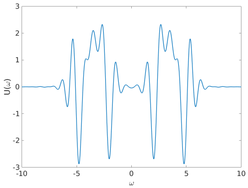
- Implies periodicity in $u(t)$, fails to handle structure of Fourier kernel.
- To manage spurious periodicity: refine ω discretization $\implies$ $\mathcal{O}(N)$ large-time cost and expensive frequency-domain solves.
- Requires global regularity and periodicity for high-order convergence.

New Quadrature Algorithm: Fourier Expansion

Idea: expand integrand in new basis

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



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

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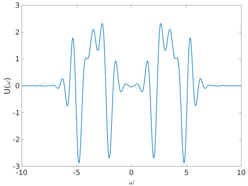

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Then, evaluating term-by-term *exactly*,

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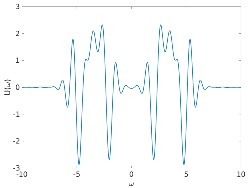

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Integrating exactly and evaluating on $t_\ell = \ell \Delta t$,

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

Fourier Quadrature: Generalizing

On $[a, b]$, more generally,

$$I_a^b[F](t_\ell) = \int_a^b F(\omega) e^{-i\omega t_\ell} d\omega$$

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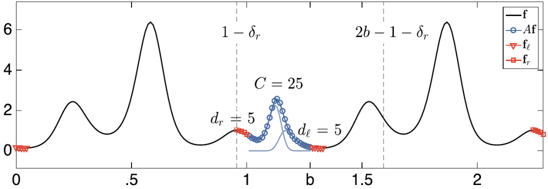
- If $F \notin C_{per}([a, b])$, use Fourier Continuation to produce Fourier coefficients.
  - High-order (10^{th}-order and higher) interpolation.



Ref: Amlani & Bruno, JCP (2016)

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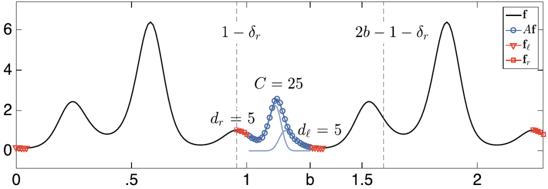

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Fourier series interpolant in $[a, b]$:

$$F^c(\gamma + \delta\omega) = \sum_{m=-N/2}^{N/2-1} c_m e^{i\frac{2\pi}{P} m\omega}$$

- Use $F^c \approx F$ for quadrature rule.

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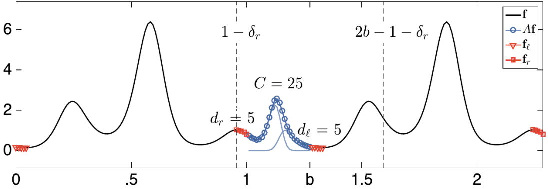

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Generalized Fourier Quadrature Rule: Analysis

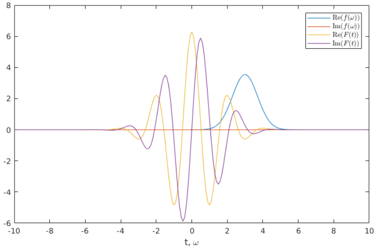
We have the quadrature rule:

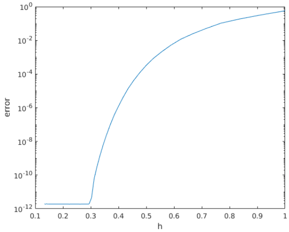
$$I_a^b[F](t_\ell) = \delta e^{-it_\ell \gamma} \sum_{m=-N/2}^{N/2-1} c_m \int_{-W}^{W} e^{-i\frac{2\pi}{P}(\beta\ell - m)}\, d\omega, \quad \beta = \frac{\delta P}{2\pi}\Delta t$$

$$= \delta e^{-it_\ell \gamma} \sum_{m=-N/2}^{N/2-1} c_m b_{\beta m - \ell}, \quad \text{where} \quad b_q := 2W\,\mathrm{sinc}(\frac{2W}{P}q)$$

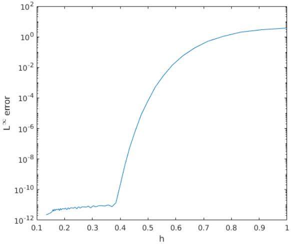
- For $L_1 \leq \ell \leq L_2$, defines a *scaled convolution*. Fast algorithms exist to evaluate in $O(M \log M)$ time, $M = max(N, L_2 - L_1)$.
  - Uses *Fractional Fourier Transforms* and FFTs. Ref: Nascov & Logafotu (2009).
- Quadrature rule requires $\mathcal{O}(1)$ coefficients for **uniform error** as $t \to \infty$.
  - **Dispersionless**
- For $F \in C_{per}$, $\mathcal{O}(e^{-\alpha N})$ convergence.
- For $F \notin C_{per}$, cf. Trapezoidal rule: $\mathcal{O}(1/N)$ convergence.
  - We observe high order convergence, e.g. $\mathcal{O}(1/N^{10})$.
  - Still a spectral (dispersionless) method

Numerical results: Fourier quadrature rule (periodic)





Maximum error as a function of time discretization h_t (Forward).



Maximum error as a function of frequency discretization h_ω (Inverse).

Overall hybrid algorithm

Given (incoming) boundary conditions: $u^{inc}(\mathbf{r}, t)$, $\mathbf{r} \in \Gamma$

1. Fourier transform to obtain $U^{inc}(\mathbf{r}, \omega)$.
2. Solve frequency-domain problems for relevant ω

$$\left[-\frac{1}{2}I + K_\omega^* + i\eta S_\omega\right](\psi)(\mathbf{r}, \omega) = -\left(\partial_\nu U^{inc}(\mathbf{r}, \omega) + i\eta U^{inc}(\mathbf{r}, \omega)\right)$$

3. For each desired point $\mathbf{r} \in \Omega$, compute

$$U(\mathbf{r}, \omega) = \int_\Gamma \psi(\mathbf{r}', \omega) G_\omega(\mathbf{r}, \mathbf{r}')\, d\sigma(\mathbf{r}').$$

4. Inverse transform:

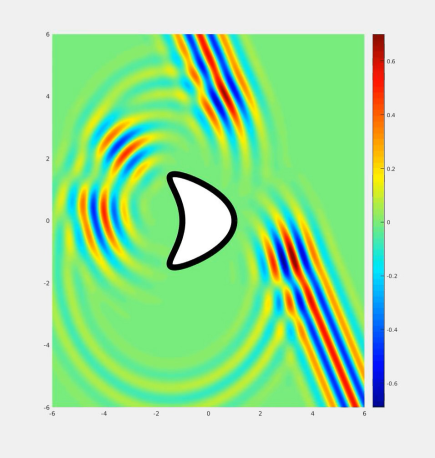
$$u(\mathbf{r}, t) = \int_{-\infty}^{\infty} U(\mathbf{r}, \omega) e^{-i\omega t}\, d\omega, \quad (9)$$

- When solving wave equation in $\mathbb{R}^2$, nonsmooth behavior as $\omega \to 0^{\pm}$. Use Filon-Clenshaw-Curtis and nonperiodic Fourier rule.

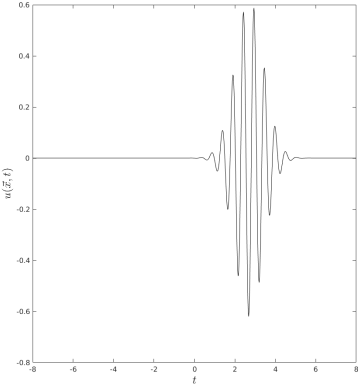
Plane wave incident on kite scatterer in $\mathbb{R}^2$

Hybrid method solution with Gaussian-modulated plane wave incidence:

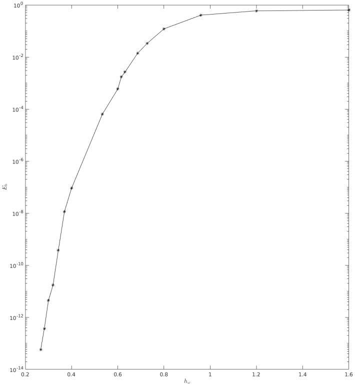
$$U^{inc}(\mathbf{r},\omega) = e^{-\frac{(\omega-\omega_0)^2}{\sigma^2}} e^{i\omega \frac{\mathbf{k}}{||\mathbf{k}||}\cdot \mathbf{r}}, \quad \text{where} \quad \omega_0 = 12, \sigma = 2, \mathbf{k} = \mathbf{e}_x + \frac{1}{2}\mathbf{e}_y.$$



Convergence



Solution trace at observation point (2,2).



All-time L^∞ error as function of freq. discretization refinement h_ω.

Long-duration incident waves

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

Challenge when time-dependent field has long duration:

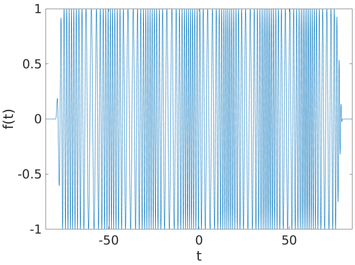


Figure: Smooth linear chirp signal, large t

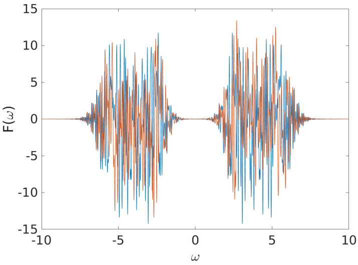


Figure: Fourier transform of linear chirp

Temporal Partition of Unity

Recall problem:

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

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

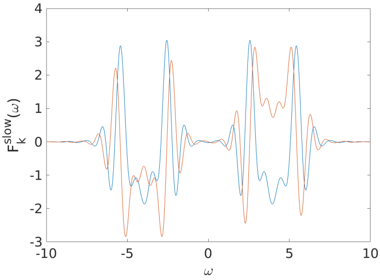
1. $w_k(t) = 1$ in neighborhood of $t = s_k$,
2. $w_k(t) = 0$ for $|t - s_k| > H$,
3. $\sum_{k=1}^{K} w_k(t) = 1$ for all $t \in [0, T]$.

Partition incident wave

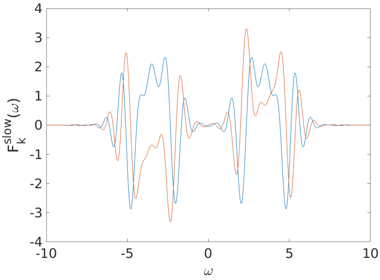
$$H_k(\mathbf{r}, \omega) = \int_{-\infty}^{\infty} w_k(t) h(\mathbf{r}, t) e^{i\omega t}\, dt, \quad H_k^{slow}(\mathbf{r}, \omega) = e^{-i\omega s_k} H_k(\mathbf{r}, \omega).$$

Apply hybrid method: solve frequency-domain problems for U_k with H_k boundary conditions.

What does the partition of unity yield?



Windowed Fourier Transform, partition $s_k = 0$.



Windowed Fourier Transform, partition $s_k = -55$.

Temporal Partition of Unity II

Build time-partitioned solutions using Fourier shifting:

$$u_k(\mathbf{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U_k(\mathbf{r},\omega)e^{-i\omega t}\,d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} U_k^{slow}(\mathbf{r},\omega)e^{-i\omega(t+s_k)}\,d\omega.$$

In practice,

$$u_k^W(\mathbf{r},t) = \int_{-W}^{W} U_k^{slow}(\mathbf{r},\omega)e^{-i\omega(t+s_k)}\,d\omega$$

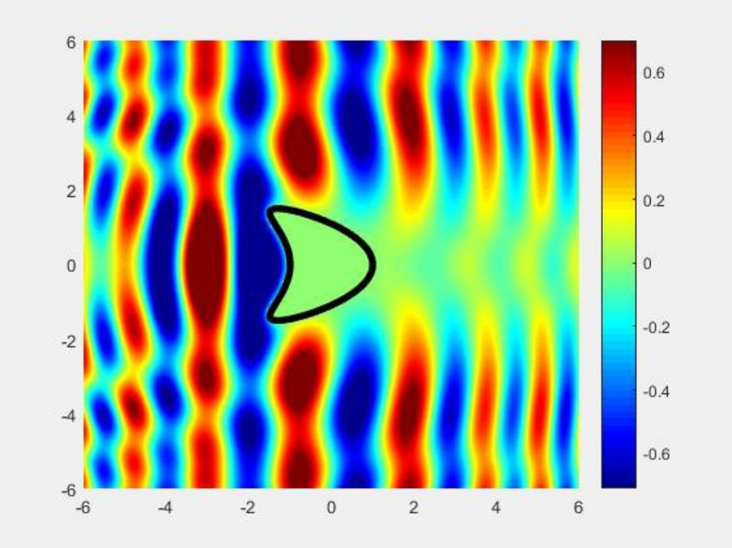
and the overall solution is reconstituted as:

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

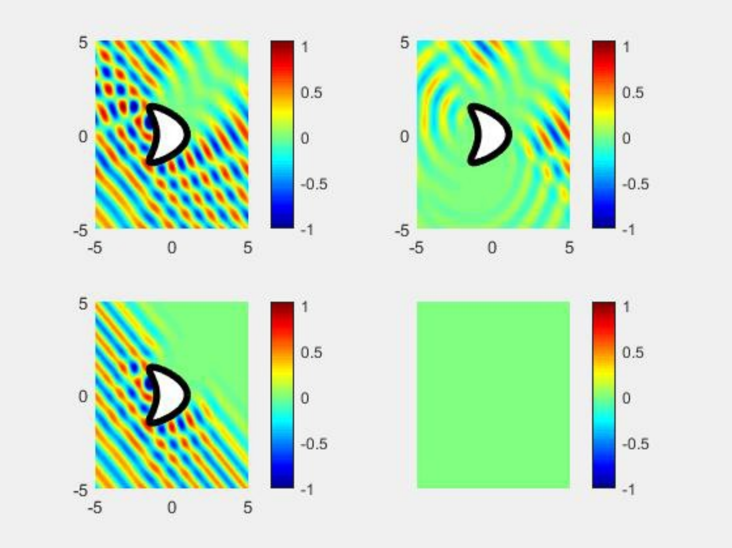
Overall this allows efficient long-time computation.

- Note: $H_k^{slow}(\mathbf{r},\omega) = e^{-i\omega s_k}H_k(\mathbf{r},\omega)$
  - Implies we can **re-use frequency-domain solutions!** Use linearity..
- Need not compute $u_k^W(\mathbf{r},t)$ for every $\mathbf{r}$, t. Track when windows are *active*.
  - Reliant on geometrical considerations and BIE densities.

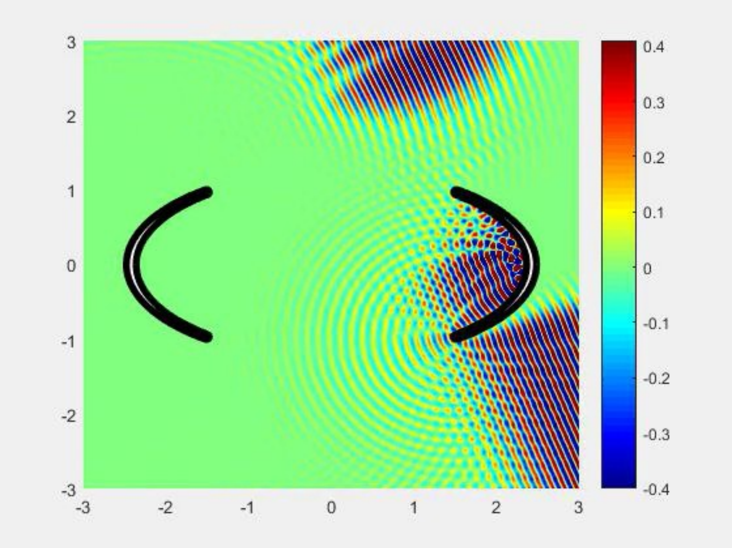
Time-partitioning for long incident duration



Time-tracking of active windows



Example: Whispering Gallery



Acknowledgements

I would like to especially thank and acknowledge:

- Department of Energy and the CSGF program
- Krell Institute staff
- My advisor Oscar Bruno and collaborator Mark Lyon
- Practicum advisor Tzanio Kolev and Lawrence Livermore National Laboratory
- The many fellows and alums of the program

Thank you!

Questions?