A method of boundary equations for unsteady hyperbolic problems in 3D

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Advances in PDEs: Theory, Computation and Application to CFD

Workshop to honor the memory of Professor Saul Abarbanel

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Collaborators and support

- Collaborators:
  - Sergey Petropavlovsky (National Research University Higher School of Economics (Moscow, Russia) and NCSU)
  - Fouche Smith (NCSU)
  - Eli Turkel (Tel Aviv University)
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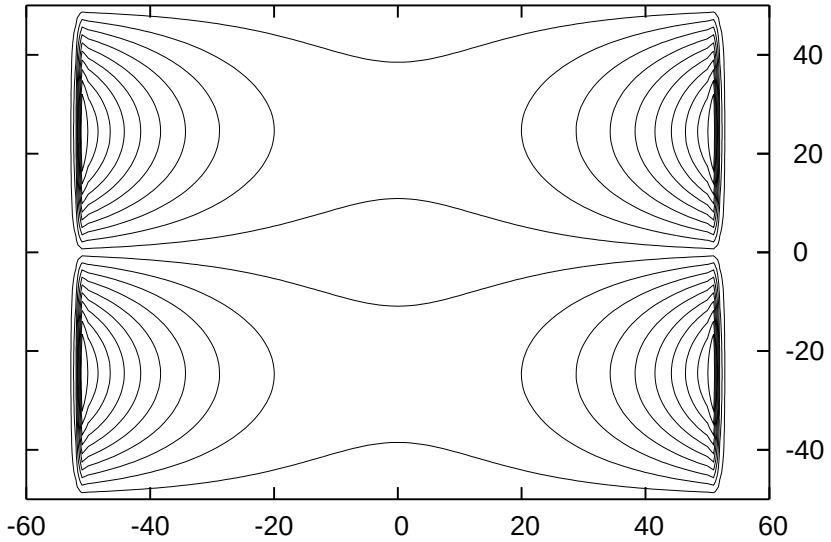
In memory of Saul Abarbanel

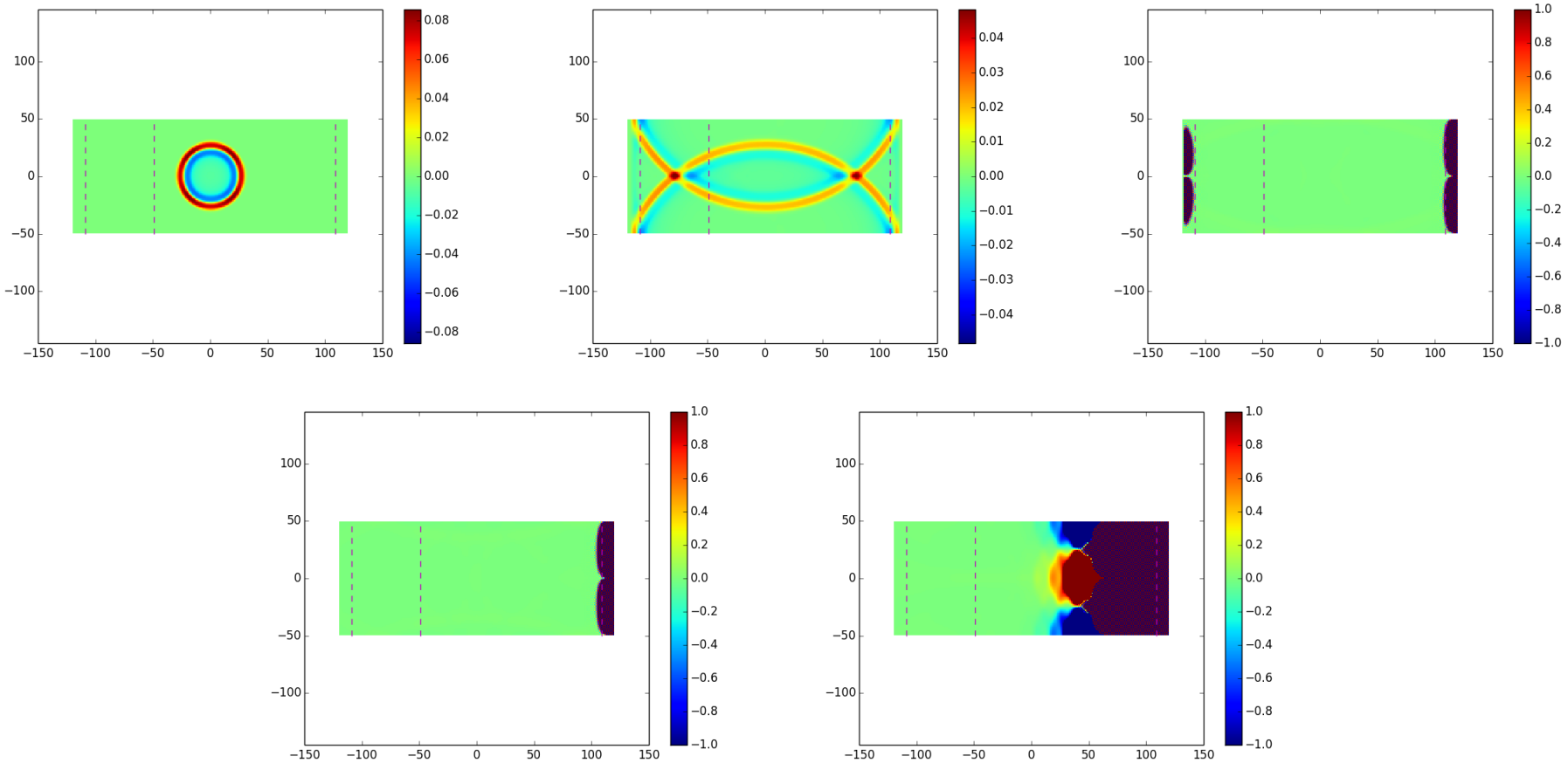
Retrospect

- Weak well-posedness of split-field PMLs for Maxwell's equations [S. Abarbanel and D. Gottlieb, 1997]
- Unsplit PMLs [S. Abarbanel and D. Gottlieb, 1998]
- May still be susceptible to gradually developing instabilities [S. Abarbanel, D. Gottlieb, and J. Hesthaven, 2002]
- Computational study of long-time instabilities of unsplit PMLs [S. Abarbanel, H. Qasimov, and S. Tsynkov, 2009]



Lacunae-based stabilization

- Long-time instabilities may sometimes be attributed to multiple eigenvalues, but this is not always the case.
- Lacunae-based time marching offers a fix regardless of the cause.



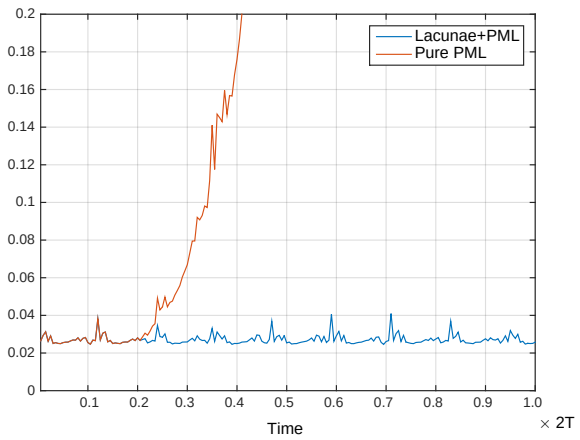
[numerical simulations by Uri Shumlak, U. of Washington]

Lacunae-based stabilization (continued)

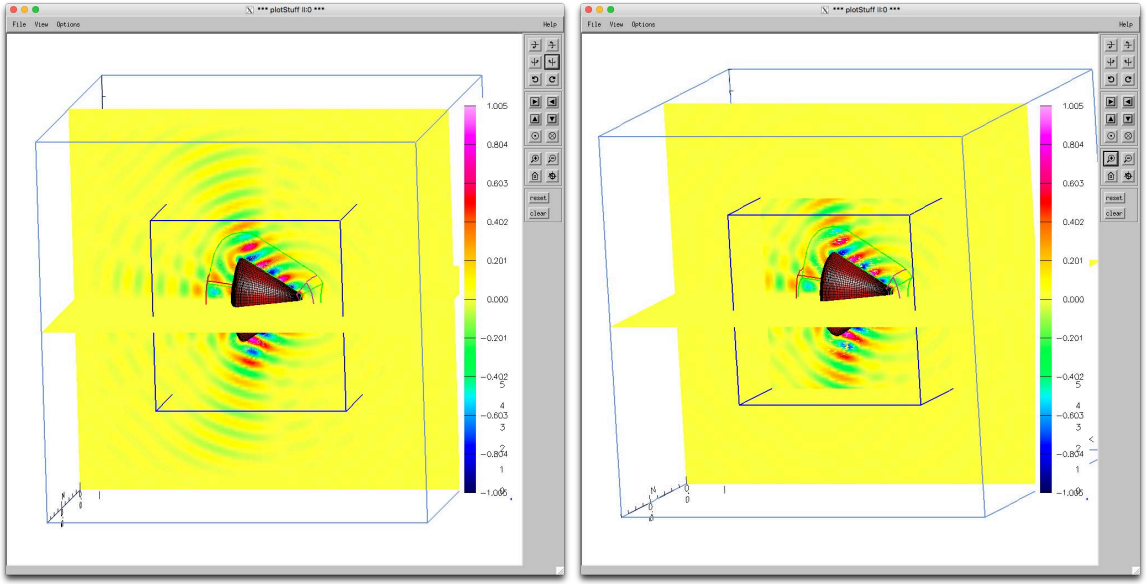
- Lacunae are a manifestation of the Huygens' principle — propagating waves have aft (i.e., trailing) fronts.
  - It was Saul who suggested to use the words "aft fronts."
- The key idea is to partition the problem in time and integrate each component only until the waves have left the domain.
- Thus, the instability is removed before it can develop.
- Works for any PML or ABC as long as the original instability does not develop too rapidly.
- Works independently as well.

- Collaborators/coauthors: A. Fedoseyev, W. Henshaw, E. Kansa, M. Osintcev, S. Petropavlovsky, H. Qasimov, U. Shumlak, E. Turkel
- Industrial partner: Computational Sciences, LLC (Madison, AL).
- Funding: NSF, BSF, AFOSR, ARO (including STTR).

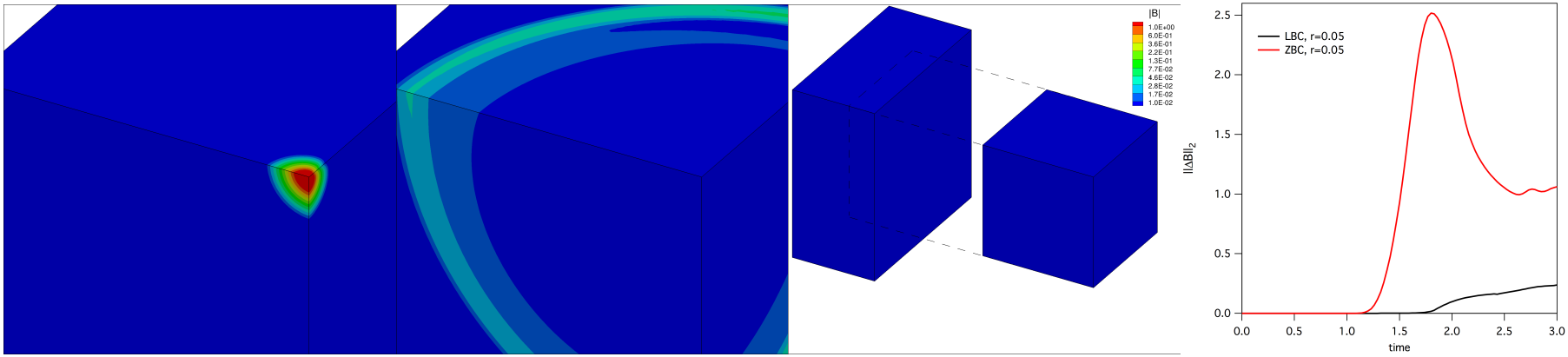
Examples of simulations



in-house code



OVERTURE



WARPX

Next step: Go beyond artificial outer boundaries

Observation:

- The Huygens' principle has proven an efficient computational tool for the treatment of artificial outer boundaries.

Objectives:

- Extend the lacunae-based numerical methodology to solving general unsteady hyperbolic IBVPs.
- Allow for a variety of boundary shapes and boundary conditions.
- Include both interior and exterior formulations.
- Allow for high order accuracy.
- Allow for arbitrarily long time intervals.

In the end of the day:

- Develop a time-dependent counterpart to BIEs/BEM.

Motivation and overview

- BIEs reduce the dimension of the problem:
  - Typically used for elliptic (or predominantly elliptic) problems;
  - Offer substantial flexibility from the standpoint of geometry;
  - Notwithstanding the perpetual debate of reduced dimension vs. dense linear algebra, we will discuss benefits for unsteady problems.
- RPBIEs [Tuong, 2003], [Michielssen, et. al., 2005, 2006], [Abboud, 2011], [Sayas, 2016] generalize BIEs to hyperbolic case:
  - Discretization may be unstable [Epstein, Greengard, Hagstrom, 2016]
  - Become increasingly costly at longer integration times [Lubich, 1994].
- The Huygens' principle removes the main limitation of RPBIEs coupled with convolution quadratures:
  - Enables the derivation of an equivalent boundary operator equation with only finite and non-increasing backward dependence on time.
- Solved by Ryaben'kii's method of difference potentials:
  - Renders parallelization in time on multi-processor systems.
  - Other discretization/solution techniques can be explored.

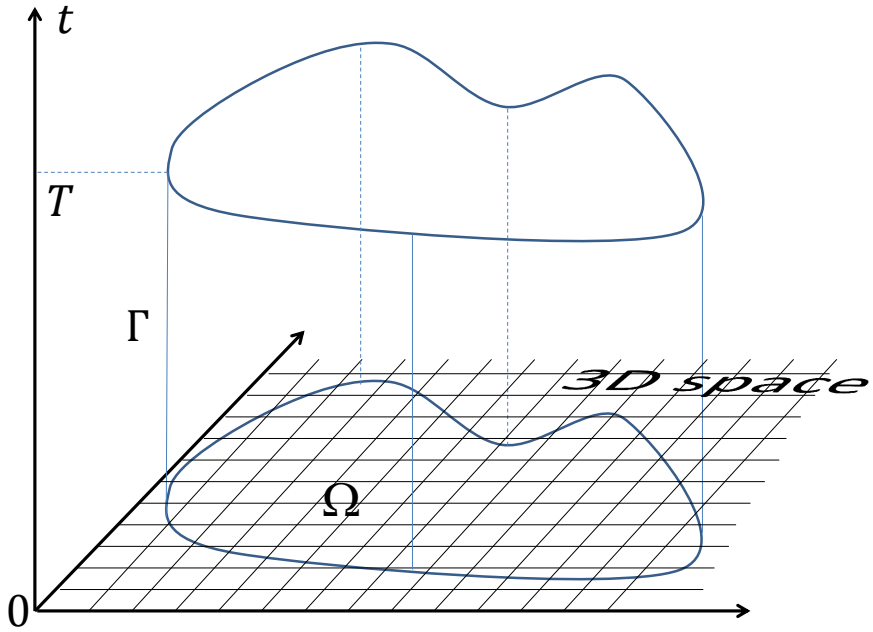
Exterior problem for the d'Alembert equation

An exterior IBVP for the 3D wave equation on $\tilde{\Omega} \stackrel{\text{def}}{=} \mathbb{R}^3 \backslash \bar{\Omega}$:

$$\Box_c u(\boldsymbol{x}, t) \equiv \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \Delta u = 0, \quad (\boldsymbol{x}, t) \in \tilde{\Omega} \times (0, T],$$

$$u\big|_{t=0} = 0, \quad \frac{\partial u}{\partial t}\Big|_{t=0} = 0, \quad \boldsymbol{x} \in \tilde{\Omega},$$

$$\boldsymbol{l}_\Gamma u = \phi, \quad (\boldsymbol{x}, t) \in \Gamma \equiv \partial\tilde{\Omega} \times (0, T].$$



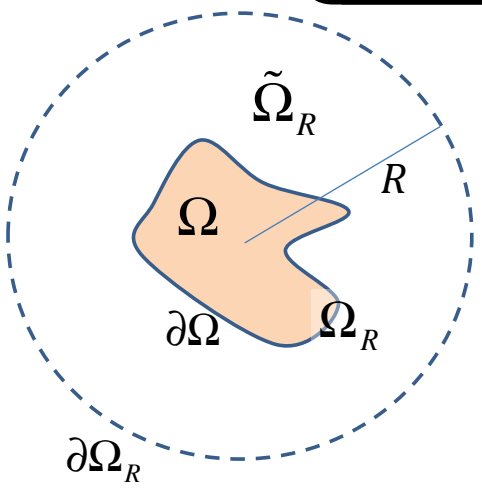
- Homogeneous formulation makes sense on the substance.
- Interior/inhomogeneous allowed.
- Boundary conditions may be of any type and may depend on time.
- Computational time T may be arbitrarily long.
- Equations beyond d'Alembert can be considered (e.g., Maxwell's).

Green's formula

$$u(\boldsymbol{x},t) = \underbrace{\frac{1}{c^2}\int\limits_{\tilde{\Omega}_R}\left\{\frac{\partial u}{\partial t}(\boldsymbol{y},0)G(\boldsymbol{x}-\boldsymbol{y},t) - u(\boldsymbol{y},0)\frac{\partial G}{\partial t}(\boldsymbol{x}-\boldsymbol{y},t)\right\}d\boldsymbol{y}}_{=0}$$

$$+\int\limits_{\Gamma_t}\left\{\frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t') - u(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_y$$

$$\underbrace{+\int\limits_{\Gamma_t^R}\left\{\frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t') - u(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_y}_{=0}.$$



- $\Omega_R \supset \Omega$; $\tilde{\Omega}_R = \Omega_R \backslash \bar{\Omega}$; $\Gamma_t = \partial\Omega \times (0,t]$; $\Gamma_t^R = \partial\Omega_R \times (0,t]$.
- Fundamental solution:
  $G(\boldsymbol{x},t) = \frac{c}{2\pi}\theta(t)\delta(c^2t^2 - |\boldsymbol{x}|^2)$.
- Third integral $= 0 \Leftrightarrow$ no incoming waves at Γ_t^R.
- R arbitrary; hence, the formula holds for entire $\tilde{\Omega}$.

Calderon's operators

- Calderon's potential for $\boldsymbol{x} \in \tilde{\Omega}$:

$$\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x},t) = \int_{\Gamma_t} \left\{ \xi_1(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t') - \xi_0(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t') \right\} dt'dS_{\boldsymbol{y}}.$$

- The density $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$ is defined on the space-time boundary Γ_t.
- Vector trace of the potential is Calderon's projection:

$$\boldsymbol{P}_{\Gamma_t} \overset{\text{def}}{=} \boldsymbol{Tr}_{\Gamma_t}\boldsymbol{P}_{\tilde{\Omega}}, \quad \text{where} \quad \boldsymbol{Tr}_{\Gamma_t} w \overset{\text{def}}{=} \left(w, \frac{\partial w}{\partial \boldsymbol{n}} \right)\Big|_{\Gamma_t}.$$

- Calderon's boundary equation with projection (BEP):

$$\boldsymbol{P}_{\Gamma_t}\boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{\xi}_{\Gamma_t}$$

holds if and only if $\boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{Tr}_{\Gamma_t} u$, where $\Box_c u = 0$ on $\tilde{\Omega}$.

- Advantages: physical sources and independence of the BCs.
- The BC $l_{\Gamma_t} u = \phi$ is added to the BEP to form a combined system.

Partition in time

- As the time elapses, the boundary Γ_t extends (unlike elliptic!).
- Let $0 \leqslant t \leqslant K \cdot T_0 \equiv T$. Partition the boundary Γ_T into K equal parts:

$$\Gamma_T = \Gamma_1 \cup \Gamma_2 \cup \ldots \cup \Gamma_K, \quad \text{where} \quad \Gamma_k = \partial\Omega \times \big((k-1)T_0, kT_0\big].$$

- Represent the density as a sum:

$$\boldsymbol{\xi}_{\Gamma_T} = \boldsymbol{\xi}_{\Gamma_1} + \boldsymbol{\xi}_{\Gamma_2} + \ldots + \boldsymbol{\xi}_{\Gamma_K}, \quad \text{where} \quad \boldsymbol{\xi}_{\Gamma_k}(\boldsymbol{x}, t) = \begin{cases} \boldsymbol{\xi}_{\Gamma_T}(\boldsymbol{x}, t), & (\boldsymbol{x}, t) \in \Gamma_k, \\ \boldsymbol{0}, & (\boldsymbol{x}, t) \in \Gamma_T \backslash \Gamma_k. \end{cases}$$

- The system of boundary equations to be solved:

$$\boldsymbol{P}_{\Gamma_T} \boldsymbol{\xi}_{\Gamma_T} = \boldsymbol{\xi}_{\Gamma_T} \quad \& \quad \boldsymbol{l}_{\Gamma_T} \boldsymbol{\xi}_{\Gamma_T} = \phi.$$

  It is equivalent to the original IBVP.
- Can we recast this system to determine $\boldsymbol{\xi}_{\Gamma_k}$ consecutively?

Partition in time (continued)

- Separate the last component Γ_K from the rest of Γ_T:

$$\boldsymbol{Tr}_{\Gamma_{T-T_0}} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_T} = \boldsymbol{\xi}_{\Gamma_{T-T_0}} \quad \text{and} \quad \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_T} = \boldsymbol{\xi}_{\Gamma_K}.$$

- Due to causality, the first equation can be replaced with

$$\boldsymbol{Tr}_{\Gamma_{T-T_0}} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_{T-T_0}} = \boldsymbol{\xi}_{\Gamma_{T-T_0}}$$

  and supplemented with the "truncated" boundary condition:

$$\boldsymbol{l}_{\Gamma_{T-T_0}} \boldsymbol{\xi}_{\Gamma_{T-T_0}} = \phi.$$

- The same system as before except for a shorter interval $T - T_0$.
- Assuming that $\boldsymbol{\xi}_{\Gamma_{T-T_0}}$ is known, we would like to determine $\boldsymbol{\xi}_{\Gamma_K}$.
- Equivalently, all $\boldsymbol{\xi}_{\Gamma_k}$, $k = 1, 2, \ldots, K-1$, are assumed known.

Partition in time (continued)

- Using the linearity (the terms $k = 1, 2, \ldots, K-1$ are known):

$$\boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_K} + \sum_{k=1}^{K-1} \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_k} = \boldsymbol{\xi}_{\Gamma_K}.$$

- All constructs withstand translation in time:

$$\boldsymbol{\xi}_{\Gamma_K}(\boldsymbol{x}, t) = \boldsymbol{\xi}_{\Gamma_{T_0}}(\boldsymbol{x}, t-(K-1)T_0); \quad G = G(\cdot, t-t'); \quad \int_{T-T_0}^{T} \ldots \mapsto \int_{0}^{T_0} \ldots$$

- Then, $\boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \sum_{k=1}^{K-1} \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_k} = \boldsymbol{\xi}_{\Gamma_K}$, where $\underbrace{\boldsymbol{P}_{\Gamma_{T_0}} = \boldsymbol{P}_{\Gamma_t}\big|_{t=T_0}}_{\text{does not depend on } K}$.

- The BC is time-dependent: $\boldsymbol{l}_{\Gamma_K} \boldsymbol{\xi}_{\Gamma_K} = \phi$.
- A system of equations to determine $\boldsymbol{\xi}_{\Gamma_K}$. Completes the solution for the entire time interval of length $T = KT_0$.
- T and K arbitrary. Can continue consecutive updates $K \mapsto K+1$.
- Still full backward dependence on time: $\boldsymbol{\xi}_{\Gamma_K} = \boldsymbol{\xi}_{\Gamma_K}(\boldsymbol{\xi}_{\Gamma_{K-1}}, \ldots, \boldsymbol{\xi}_{\Gamma_1})$.

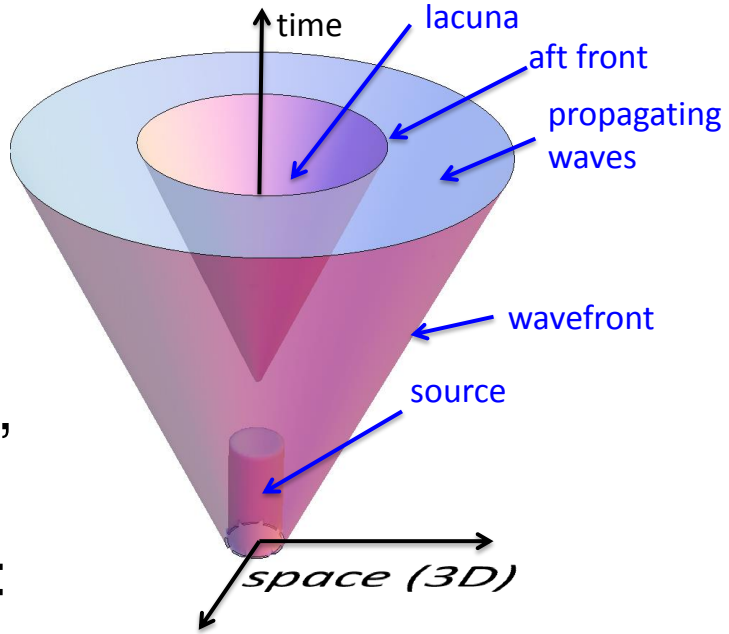
The Huygens' principle and lacunae

- The fundamental solution $G(\boldsymbol{x},t)=\frac{c}{2\pi}\theta(t)\delta(c^2t^2-|\boldsymbol{x}|^2)$ is an expanding spherical layer with "empty" interior — lacuna.
- 3D wave equation with a compactly supported RHS, $\Box_c u=f$, $\operatorname{supp} f\subseteq Q$, has a secondary lacuna of the solution:

$$u(\boldsymbol{x},t)\equiv 0\quad \forall(\boldsymbol{x},t)\in\bigcap_{(\boldsymbol{\xi},\tau)\in Q}\left\{(\boldsymbol{x},t)\middle||\boldsymbol{x}-\boldsymbol{\xi}|<c(t-\tau),\ t>\tau\right\}\stackrel{\text{def}}{=}\Lambda.$$

- Implication of the Kirchhoff integral:

$$u(\boldsymbol{x},t)=\frac{1}{4\pi}\iiint\limits_{|\boldsymbol{x}-\boldsymbol{\xi}|\leqslant ct}\frac{f(\boldsymbol{\xi},t-|\boldsymbol{x}-\boldsymbol{\xi}|/c)}{|\boldsymbol{x}-\boldsymbol{\xi}|}d\boldsymbol{\xi}.$$



- Overall, a rare phenomenon. Its opposite, the diffusion of waves, is more common.
- Yet important applications are Huygens': electromagnetic and acoustic waves.
- Have been used for the treatment of artificial outer boundaries.

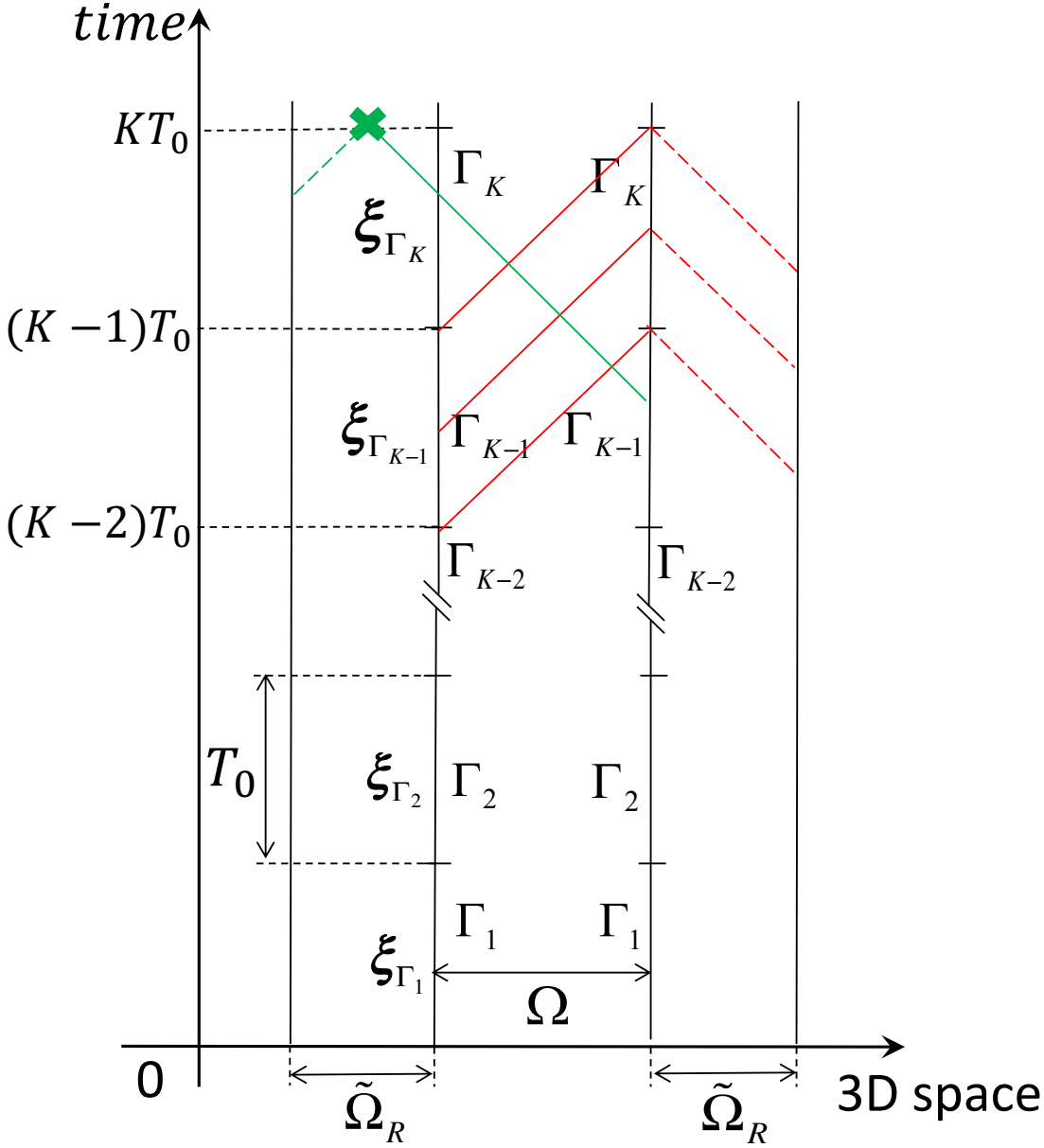
Application of lacunae to IBVPs

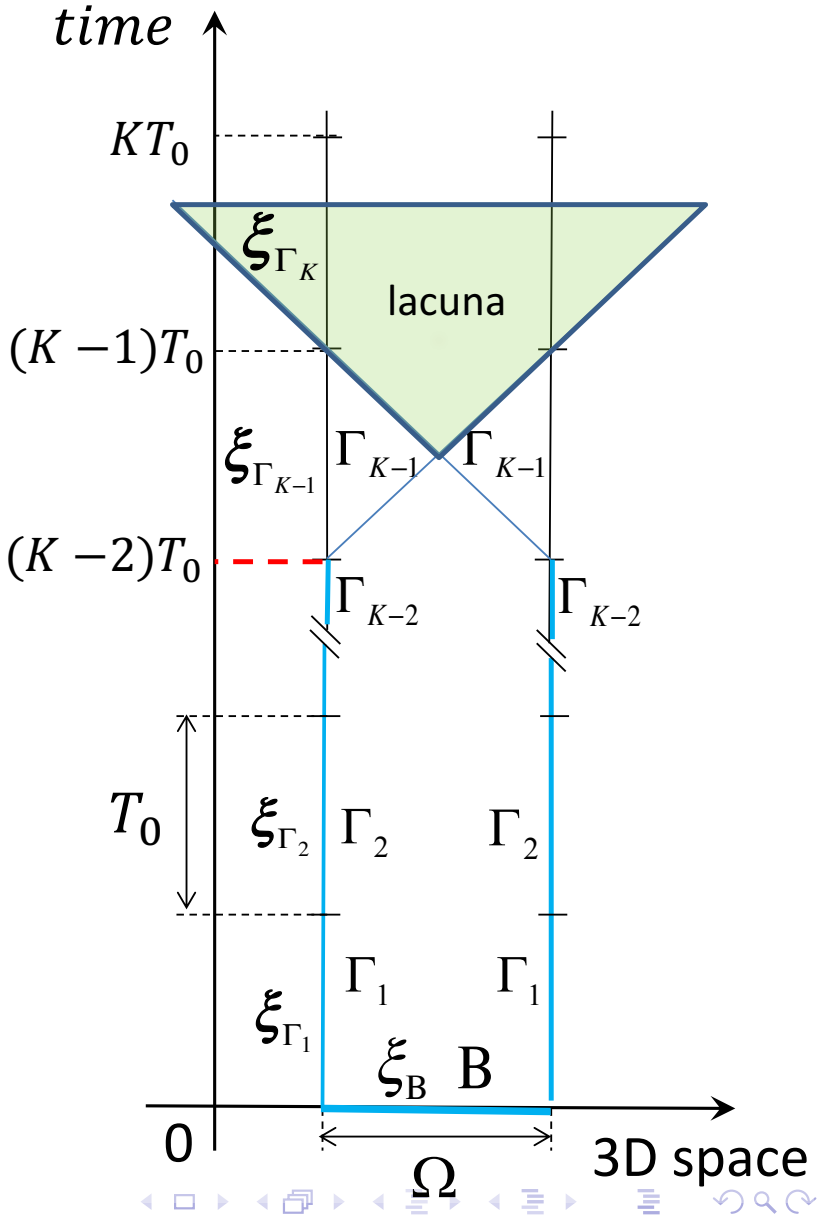
- Choose $T_0 \geqslant \frac{1}{c}\operatorname{diam}\Omega$. As $\boldsymbol{P}_{\tilde{\Omega}}$ is convolution with G, there will be no contribution from any of $\boldsymbol{\xi}_{\Gamma_k}$, $k = K-2, \ldots, 1$. Therefore,

$$\boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \underbrace{\boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}}}_{\boldsymbol{R}_{\Gamma_{T_0}}} \boldsymbol{\xi}_{\Gamma_{K-1}} = \boldsymbol{\xi}_{\Gamma_K}.$$

  Thus, $\boldsymbol{\xi}_{\Gamma_K}$ depends only on the immediately preceding $\boldsymbol{\xi}_{\Gamma_{K-1}}$.
- To actually determine $\boldsymbol{\xi}_{\Gamma_K}$, one also needs the BC: $\boldsymbol{l}_{\Gamma_K} \boldsymbol{\xi}_{\Gamma_K} = \phi$.
- Effective time marching with respect to K, $\boldsymbol{\xi}_{\Gamma_{K-1}} \mapsto \boldsymbol{\xi}_{\Gamma_K}$:
  - Performed along a $(2+1)$-dimensional lateral boundary.
- The limited backward dependence on time is a direct implication of the Huygens' principle:
  - Calderon's operators take advantage of the lacuna of G;
  - This enables the two-step time-matching algorithm: $K-1 \mapsto K$.

Application of lacunae to IBVPs (schematic)





Semi-discretization

- Basis on Γ_{K-1} and Γ_K, $\{\boldsymbol{\psi}_{0,s} = (\psi_s, 0)$ and $\boldsymbol{\psi}_{1,s} = (0, \psi_s)\}$:

$$\boldsymbol{\xi}_{\Gamma_{K-1}} = \sum_s c^{(\mathrm{I})}_{0,s}\boldsymbol{\psi}_{0,s} + c^{(\mathrm{I})}_{1,s}\boldsymbol{\psi}_{1,s}, \qquad \boldsymbol{\xi}_{\Gamma_K} = \sum_s c^{(\mathrm{II})}_{0,s}\boldsymbol{\psi}_{0,s} + c^{(\mathrm{II})}_{1,s}\boldsymbol{\psi}_{1,s}.$$

- $\boldsymbol{\xi}_{\Gamma_{K-1}}$ is known; hence, $c^{(\mathrm{I})}_{0,s}$ and $c^{(\mathrm{I})}_{1,s}$ are available. Then,

$$\sum_s c^{(\mathrm{II})}_{0,s} \underbrace{\left\{\boldsymbol{P}_{\Gamma_{T_0}} - \boldsymbol{I}\right\}}_{\boldsymbol{Q}_{\Gamma_{T_0}}} \boldsymbol{\psi}_{0,s} + c^{(\mathrm{II})}_{1,s} \underbrace{\left\{\boldsymbol{P}_{\Gamma_{T_0}} - \boldsymbol{I}\right\}}_{\boldsymbol{Q}_{\Gamma_{T_0}}} \boldsymbol{\psi}_{1,s}$$
$$= -\sum_s c^{(\mathrm{I})}_{0,s}\boldsymbol{R}_{\Gamma_{T_0}}\boldsymbol{\psi}_{0,s} + c^{(\mathrm{I})}_{1,s}\boldsymbol{R}_{\Gamma_{T_0}}\boldsymbol{\psi}_{1,s}.$$

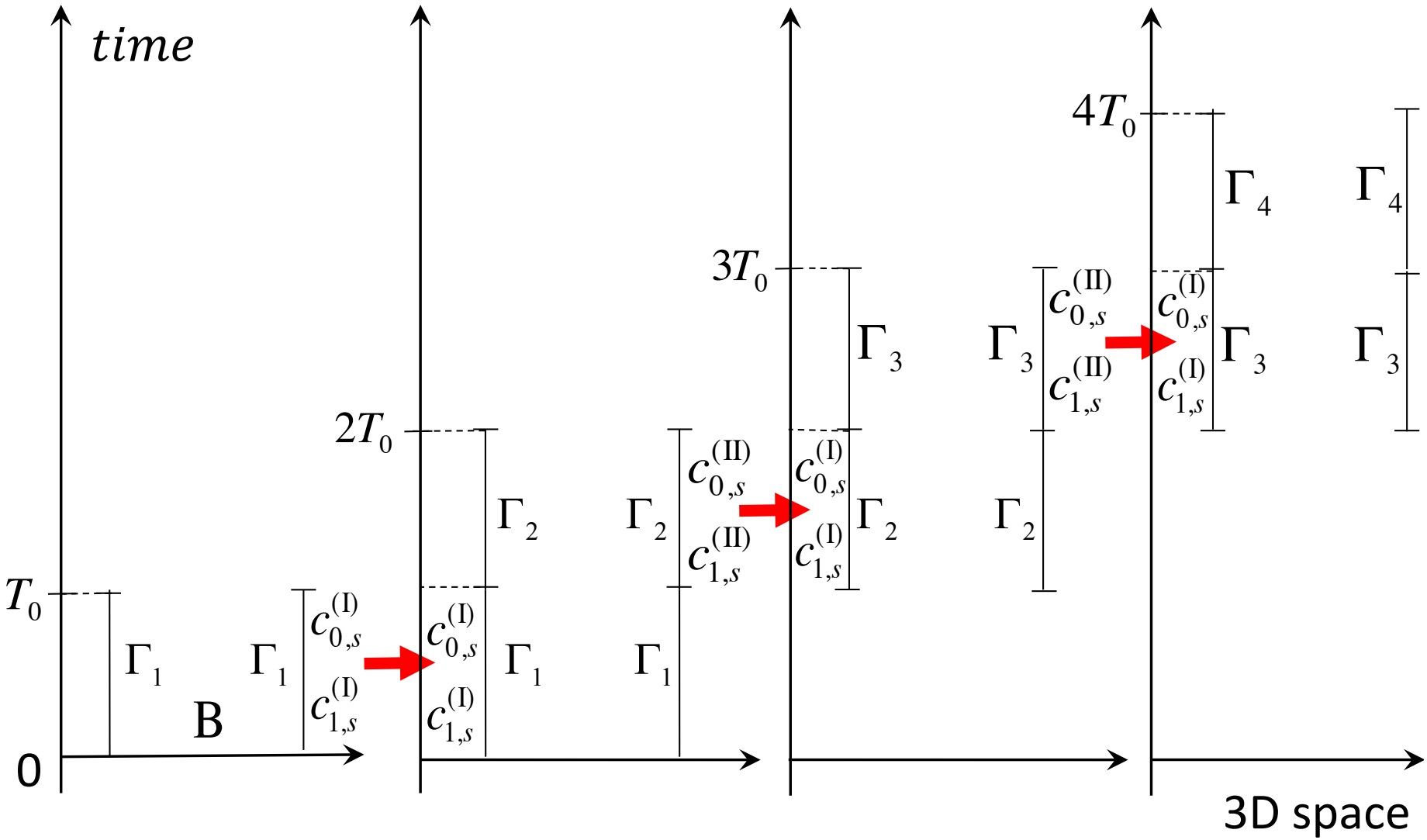
- Boundary condition on Γ_K:

$$\boldsymbol{l}_{\Gamma_K} \sum_s c^{(\mathrm{II})}_{0,s}\boldsymbol{\psi}_{0,s} + c^{(\mathrm{II})}_{1,s}\boldsymbol{\psi}_{1,s} = \phi \equiv \sum_s c^{(\phi)}_s \psi_s.$$

Time marching w.r.t. to K

- The operators $\boldsymbol{Q}_{\Gamma_{T_0}}$ and $\boldsymbol{R}_{\Gamma_{T_0}}$ do not depend on K.
- The basis functions $\psi_{0,s}$ and $\psi_{1,s}$ are also the same for all K.
- Hence, $\boldsymbol{Q}_{\Gamma_{T_0}}\psi_{0,s}$, $\boldsymbol{Q}_{\Gamma_{T_0}}\psi_{1,s}$ and $\boldsymbol{R}_{\Gamma_{T_0}}\psi_{0,s}$, $\boldsymbol{R}_{\Gamma_{T_0}}\psi_{1,s}$ stay unchanged for any two consecutive partition elements $K-1$ and K:
  - Can be precomputed, which yields major gains in performance.
- In time marching, the coefficients $c_{0,s}^{(\mathrm{II})}$ and $c_{1,s}^{(\mathrm{II})}$ are the unknowns, whereas $c_{0,s}^{(\mathrm{I})}$, $c_{1,s}^{(\mathrm{I})}$, and $c_s^{(\phi)}$ represent the available data.
- After the coefficients $c_{0,s}^{(\mathrm{II})}$ and $c_{1,s}^{(\mathrm{II})}$ have been determined, we perform one time step: $c_{0,s}^{(\mathrm{I})} \leftarrow\!\shortmid\, c_{0,s}^{(\mathrm{II})}$, $c_{1,s}^{(\mathrm{I})} \leftarrow\!\shortmid\, c_{1,s}^{(\mathrm{II})}$.
- Then, the procedure repeats itself.
- Important: we always solve only for the coefficients $c_{0,s}^{(\mathrm{II})}$ and $c_{1,s}^{(\mathrm{II})}$ of an expansion at the boundary.

Time marching w.r.t. to K (schematic)



Alternative definition of operators

- Let $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$ be given. Let $w = w(\boldsymbol{x}, t)$ be compactly supported in space (on Ω_R) and satisfy $\boldsymbol{Tr}_{\Gamma_t} w = \boldsymbol{\xi}_{\Gamma_t}$. Then, for $\boldsymbol{x} \in \tilde{\Omega}_R$:

$$w(\boldsymbol{x},t) = \frac{1}{c^2}\int\limits_{\tilde{\Omega}_R}\left\{\frac{\partial w}{\partial t}(\boldsymbol{y},0)G(\boldsymbol{x}-\boldsymbol{y},t) - w(\boldsymbol{y},0)\frac{\partial G}{\partial t}(\boldsymbol{x}-\boldsymbol{y},t)\right\}d\boldsymbol{y}$$
$$+\int\limits_{\Gamma_t}\left\{\underbrace{\frac{\partial w}{\partial \boldsymbol{n}}(\boldsymbol{y},t')}_{\xi_1}G(\boldsymbol{x}-\boldsymbol{y},t-t') - \underbrace{w(\boldsymbol{y},t')}_{\xi_0}\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_{\boldsymbol{y}}$$
$$+\int\limits_0^t\int\limits_{\tilde{\Omega}_R} G(\boldsymbol{x}-\boldsymbol{y},t-t')\Box_c w(\boldsymbol{y},t')d\boldsymbol{y}dt'.$$

- The second integral defines the Calderon potential $\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x},t)$.
- The first and third integrals together yield the solution to a Cauchy problem for the wave equation on $\mathbb{R}^3$.

Alternative definition of operators (continued)

- Thus, we have $\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x},t) = w(\boldsymbol{x},t) - \tilde{v}(\boldsymbol{x},t) \equiv v(\boldsymbol{x},t)$, where $\tilde{v}(\boldsymbol{x},t)$ solves the following Cauchy (initial value) problem on $\mathbb{R}^3$:

$$\frac{1}{c^2}\frac{\partial^2 \tilde{v}}{\partial t^2} - \Delta \tilde{v} = \begin{cases} \square_c w, & \boldsymbol{x} \in \tilde{\Omega}_R, \\ 0, & \boldsymbol{x} \notin \tilde{\Omega}_R, \end{cases}$$

$$\tilde{v}\big|_{t=0} = \begin{cases} w\big|_{t=0}, & \boldsymbol{x} \in \tilde{\Omega}_R, \\ 0, & \boldsymbol{x} \notin \tilde{\Omega}_R, \end{cases} \qquad \left.\frac{\partial \tilde{v}}{\partial t}\right|_{t=0} = \begin{cases} \frac{\partial w}{\partial t}\big|_{t=0}, & \boldsymbol{x} \in \tilde{\Omega}_R, \\ 0, & \boldsymbol{x} \notin \tilde{\Omega}_R. \end{cases}$$

- Accordingly, $v(\boldsymbol{x},t)$ solves the complimentary Cauchy problem, which we call the auxiliary problem (AP):

$$\frac{1}{c^2}\frac{\partial^2 v}{\partial t^2} - \Delta v = \begin{cases} \square_c w, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega, \end{cases}$$

$$v\big|_{t=0} = \begin{cases} w\big|_{t=0}, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega, \end{cases} \qquad \left.\frac{\partial v}{\partial t}\right|_{t=0} = \begin{cases} \frac{\partial w}{\partial t}\big|_{t=0}, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega. \end{cases}$$

Full discretization: Difference potentials

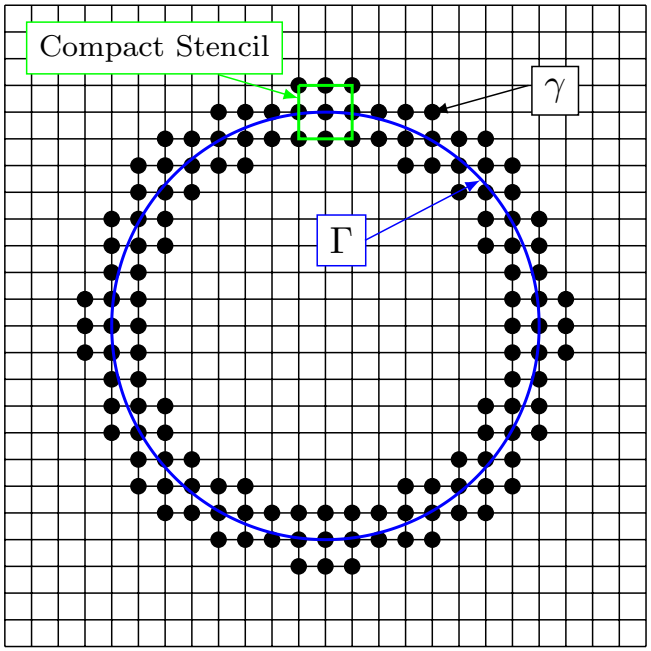
- Surface integrals have been replaced with a plain Cauchy problem.
- This problem (the AP) is solved by finite differences:
  - One can use any scheme deemed convenient and appropriate;
  - We have used 2nd order central differences and 4th order compact;
  - The scheme can be built on a regular structured grid (Cartesian);
  - The shape of the boundary can be non-conforming.
- Solution of the difference AP yields discrete counterparts of Calderon's operators:
  - Discrete Calderon's operators do not depend on the BCs;
  - Specific boundary conditions are later added to the overall system;
  - No approximation of the boundary conditions on the grid is required.
- The boundary is coupled to the grid via extension operators:
  - Constructed by means of equation-based Taylor formulae;
  - Sufficient order of extension enables approximation of continuous potentials by difference potentials.

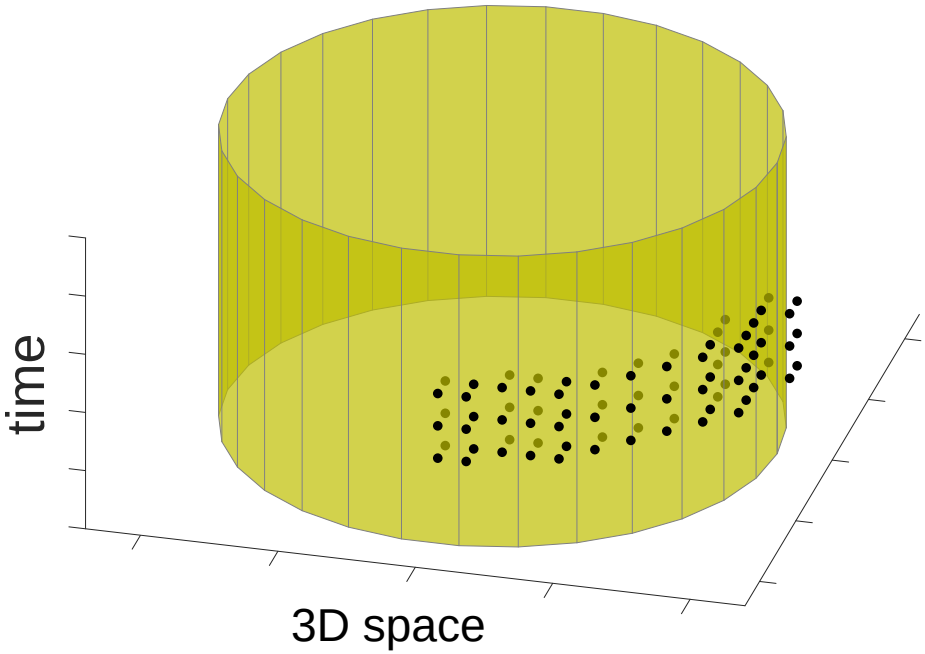
Discrete AP

- An initial value (Cauchy) problem on the entire $\mathbb{R}^3$.
- All the data (both initial data and the source term) are compactly supported on Ω in space.
- Sufficient to solve for $0 \leqslant t \leqslant 2T_0$ to compute discrete counterparts to both $\boldsymbol{Q}_{\Gamma_{T_0}}$ and $\boldsymbol{R}_{\Gamma_{T_0}}$:
  - A direct implication of the Huygens' principle.
- Hence, no treatment of the artificial outer boundary is required:
  - A larger computational domain that would guarantee no reflection before the computation is terminated at $t = 2T_0$.

Discrete Calderon's operators

- The grid boundary γ_t straddles the continuous boundary Γ_t. γ_t depends on the scheme stencil.





- Difference boundary projection $\boldsymbol{P}_{\gamma_t}$ is an operator in the space of grid functions defined on γ_t — obtained by solving the discrete AP.
- The discrete BEP $\boldsymbol{P}_{\gamma_t}\xi_{\gamma_t} = \xi_{\gamma_t}$ holds iff there is a solution $u^{(h)}$ of the discrete wave equation such that $u^{(h)}\big|_{\gamma_t} = \xi_{\gamma_t}$.

Equation-based extension

- Extension relates the continuous and discrete densities, $\boldsymbol{\xi}_{\Gamma_t}$ & ξ_{γ_t}.
- Let $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)\big|_{\Gamma_t}$ be given. In the vicinity of Γ_t define:

$$v(\boldsymbol{x}, t) = \sum_{p=0}^{P} \frac{1}{l!} \frac{\partial^p v}{\partial \boldsymbol{n}^p}(\boldsymbol{x}_0, t)\rho^p,$$

  where $v(\boldsymbol{x}_0, t) = \xi_0(\boldsymbol{x}_0, t)$, $\frac{\partial v}{\partial \boldsymbol{n}}(\boldsymbol{x}_0, t) = \xi_1(\boldsymbol{x}_0, t)$, and higher order derivatives are obtained via the d'Alembert equation.
- Specifically, $\frac{\partial^2 v}{\partial \boldsymbol{n}^2}(\boldsymbol{x}_0, t) = \frac{1}{c^2}\frac{\partial^2 v}{\partial t^2}(\boldsymbol{x}_0, t) - \tilde{\Delta} v(\boldsymbol{x}_0, t)$, where $\tilde{\Delta}$ contains no derivatives w.r.t. $\boldsymbol{n}$ higher than first order:
  - Derivatives beyond $\frac{\partial^2 v}{\partial \boldsymbol{n}^2}$ are obtained by further differentiation.
- If $\exists u = u(\boldsymbol{x}, t)$: $\Box_c u = 0$ and $\boldsymbol{Tr}_{\Gamma_t} u = \boldsymbol{\xi}_{\Gamma_t}$, then $\|v - u\| = \mathcal{O}(|\rho|^{P+1})$:
  - Otherwise, the extension can be applied to any pair $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$.
- Evaluating the extension at the nodes of γ_t, we define the operator

$$\xi_{\gamma_t} = \boldsymbol{Ex}\boldsymbol{\xi}_{\Gamma_t}.$$

Numerical algorithm

- For the continuous basis functions $\psi_{0,s}$ and $\psi_{1,s}$, compute:

$$\boldsymbol{P}_{\gamma_{T_0}}\boldsymbol{Ex}\boldsymbol{\psi}_{0,s},\quad \boldsymbol{P}_{\gamma_{T_0}}\boldsymbol{Ex}\boldsymbol{\psi}_{1,s},\quad \boldsymbol{R}_{\gamma_{T_0}}\boldsymbol{Ex}\boldsymbol{\psi}_{0,s},\ \text{and}\ \ \boldsymbol{R}_{\gamma_{T_0}}\boldsymbol{Ex}\boldsymbol{\psi}_{1,s}.$$

  This requires repeated solution of the difference AP.
- Use the resulting column vectors to form the discrete operators:

$$\boldsymbol{Q}^{(0)}_{\gamma_{T_0}} \equiv \boldsymbol{P}^{(0)}_{\gamma_{T_0}} - \boldsymbol{I},\quad \boldsymbol{Q}^{(1)}_{\gamma_{T_0}} \equiv \boldsymbol{P}^{(1)}_{\gamma_{T_0}} - \boldsymbol{I},\quad \boldsymbol{R}^{(0)}_{\gamma_{T_0}},\ \text{and}\ \ \boldsymbol{R}^{(1)}_{\gamma_{T_0}}.$$

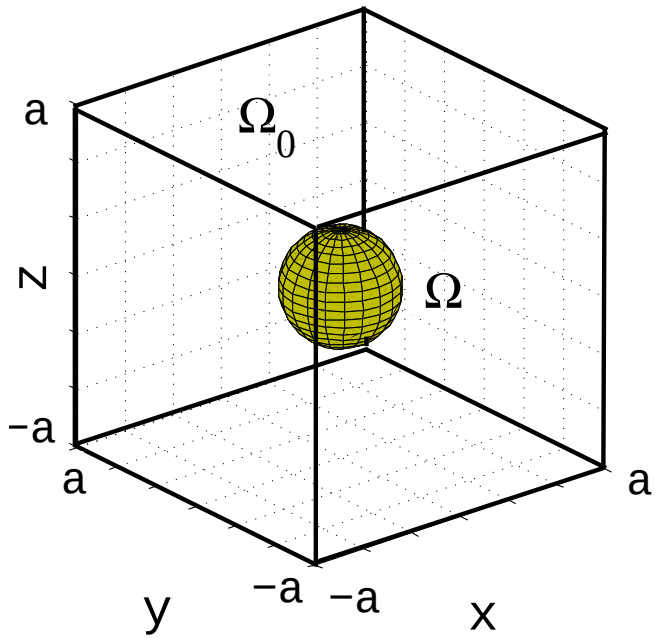
- Solve by least squares for the unknown $\boldsymbol{c}_0^{(\mathrm{II})}=\{c_{0,s}^{(\mathrm{II})}\}$ and $\boldsymbol{c}_1^{(\mathrm{II})}=\{c_{1,s}^{(\mathrm{II})}\}$:

$$\boldsymbol{Q}^{(0)}_{\gamma_{T_0}}\boldsymbol{c}_0^{(\mathrm{II})} + \boldsymbol{Q}^{(1)}_{\gamma_{T_0}}\boldsymbol{c}_1^{(\mathrm{II})} = -\boldsymbol{R}^{(0)}_{\gamma_{T_0}}\boldsymbol{c}_0^{(\mathrm{I})} - \boldsymbol{R}^{(1)}_{\gamma_{T_0}}\boldsymbol{c}_1^{(\mathrm{I})},$$

$$l_{\Gamma_K}\sum_s c_{0,s}^{(\mathrm{II})}\psi_{0,s} + c_{1,s}^{(\mathrm{II})}\psi_{1,s} = \sum_s c_s^{(\phi)}\psi_s.$$

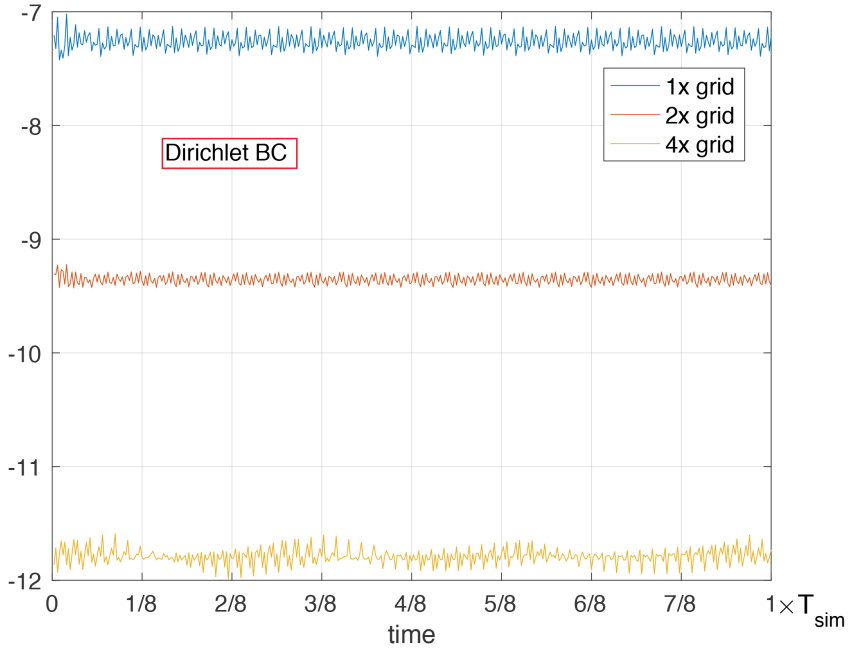
  Note: the boundary condition is never approximated on the grid.
- Reassign the coefficients: $\boldsymbol{c}_0^{(\mathrm{I})} \leftarrow \boldsymbol{c}_0^{(\mathrm{II})}$, $\boldsymbol{c}_1^{(\mathrm{I})} \leftarrow \boldsymbol{c}_1^{(\mathrm{II})}$, and solve again.

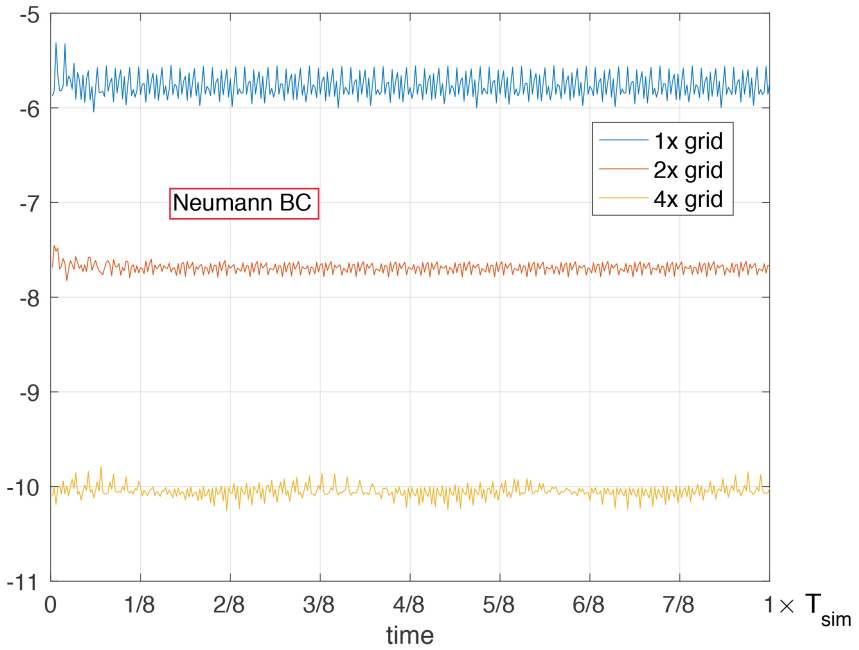
Numerical simulations

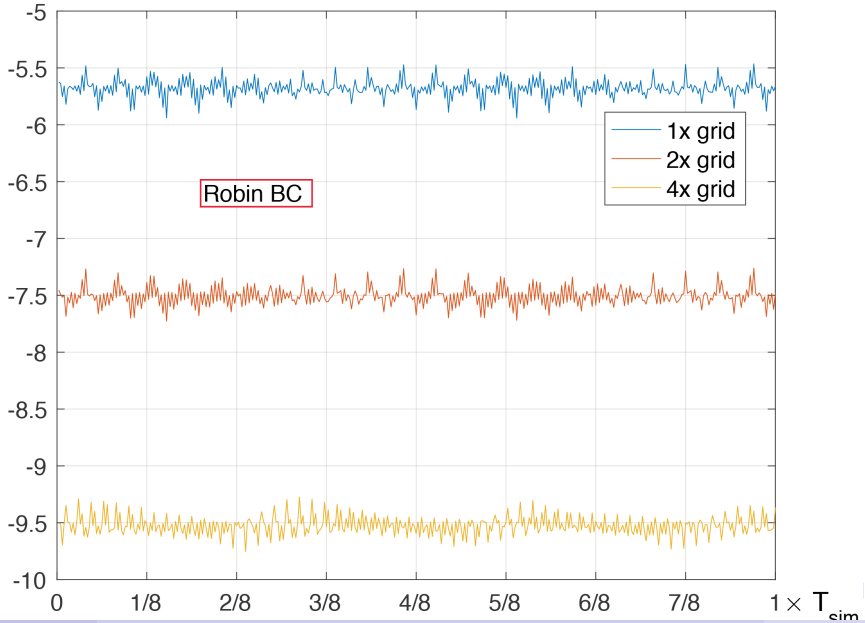


- Ω is a sphere; AP domain Ω_0 is a cube; Cartesian grids are used.
- Boundary conditions: Dirichlet, Neumann, and Robin.
- Incident field: two plane waves with $\omega_1/\omega_2 = \sqrt{2}$.
- Basis functions: $\psi_{nlm} = T_n(t)Y_{lm}(\theta,\varphi)$, $n = 0,\ldots,N$, $l = 0,\ldots,L$.
- Computational time T is 4000 diameters of Ω divided by c.

Second order scheme: Grid convergence







Second order scheme: Error and complexity

Grid	Dirichlet		Neumann		Robin	
	Mean error	Rate	Mean error	Rate	Mean error	Rate
1x	6.55×10^{-3}	-	1.84×10^{-2}	-	2.02×10^{-2}	-
2x	1.52×10^{-3}	4.27	4.84×10^{-3}	3.81	5.74×10^{-3}	3.52
4x	2.91×10^{-4}	5.25	9.69×10^{-4}	4.99	1.41×10^{-3}	4.06

Actual values of the error and convergence rates.

Grid	volumetric method+PML		MDP+lacunae	
	CPU time, sec	scaling rate	CPU time, sec	scaling rate
1x	1.26	-	0.0474	-
2x	19.8	15.7	0.421	8.87
4x	322	16.3	3.56	8.46

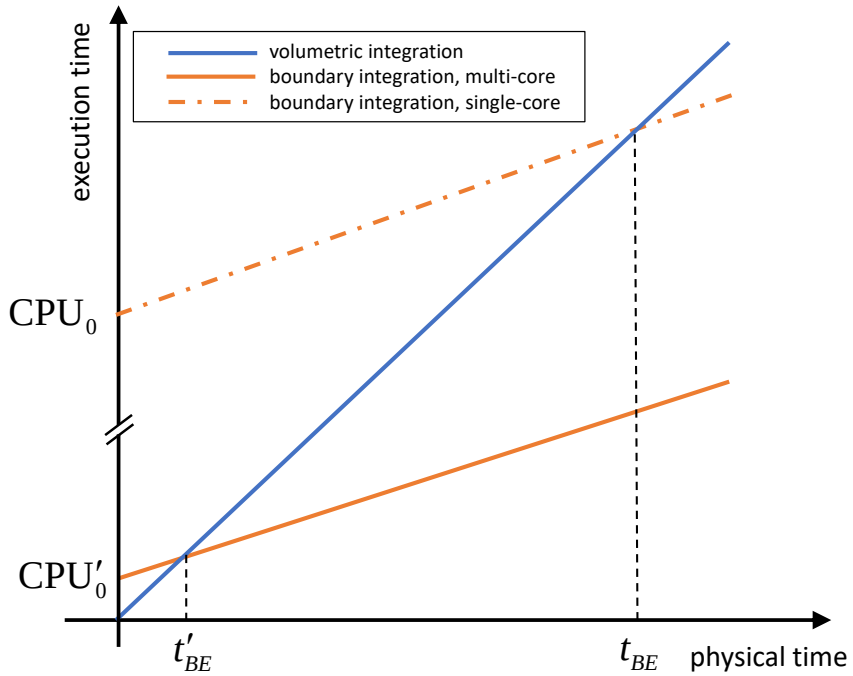
Cost comparison against a volumetric method per unit time T_0.

- MDP+lacunae show sub-linear complexity vs. volumetric scheme.
- MDP+lacunae offer two orders of magnitude performance gains.

Second order scheme: Break even times

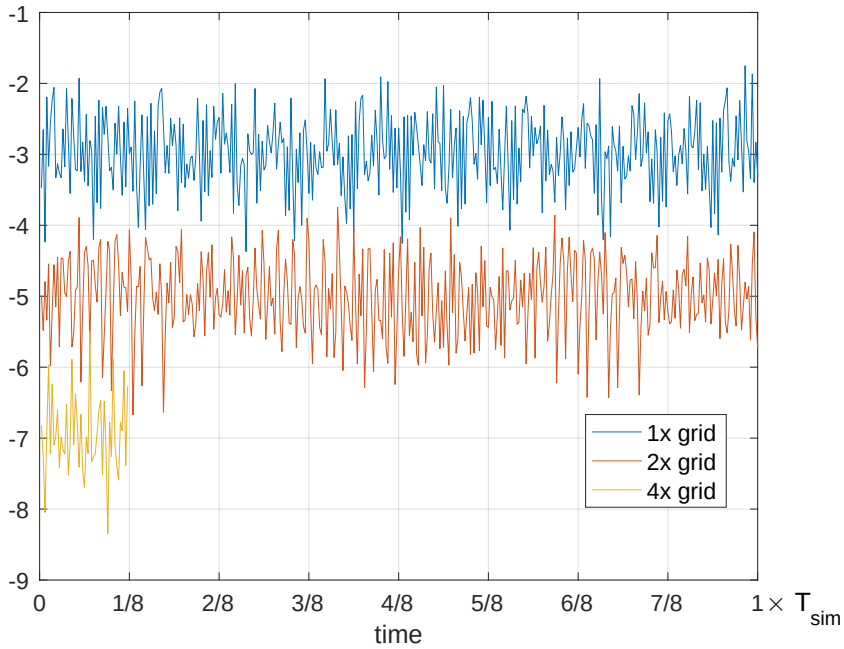
Grid	CPU time for computing Q and R, sec	t'_{BE}, in T_0
1x	1283.62	1018
2x	20152.9	1061
4x	328492	1027

Taking into account the cost of pre-computing the operators.

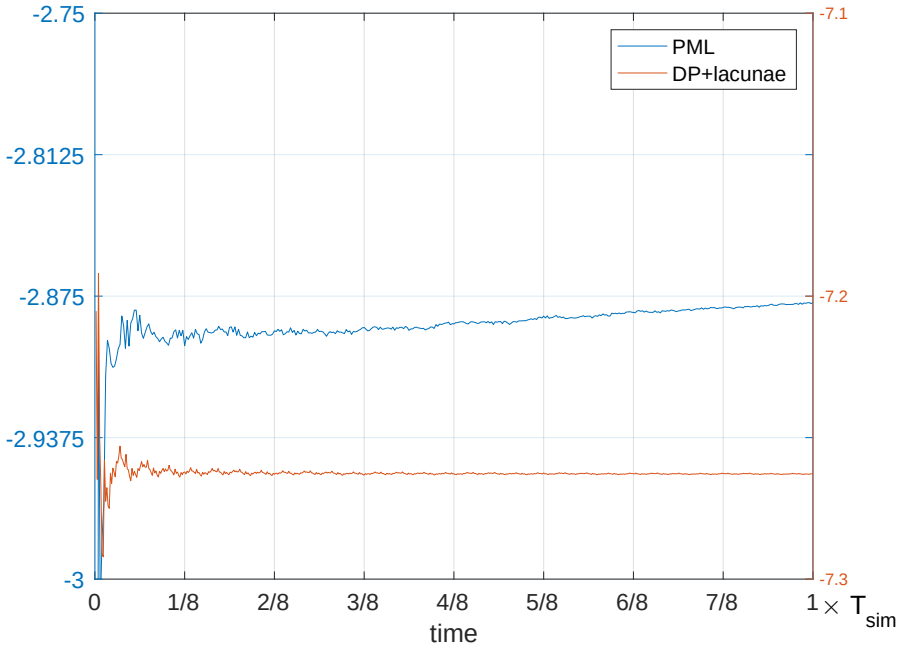


Effective parallelization in time.

Second order scheme: Comparison with PML



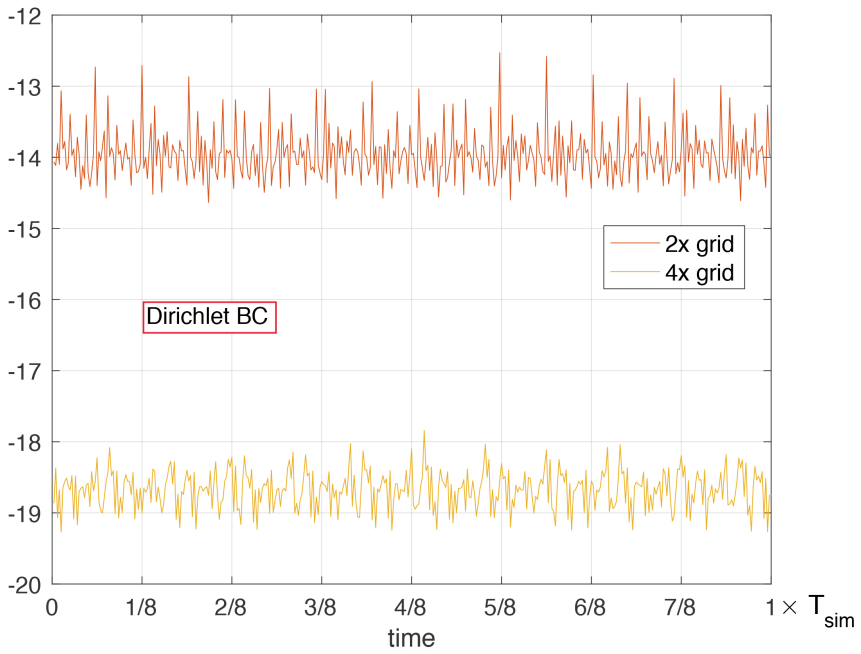
Grid convergence for PML.

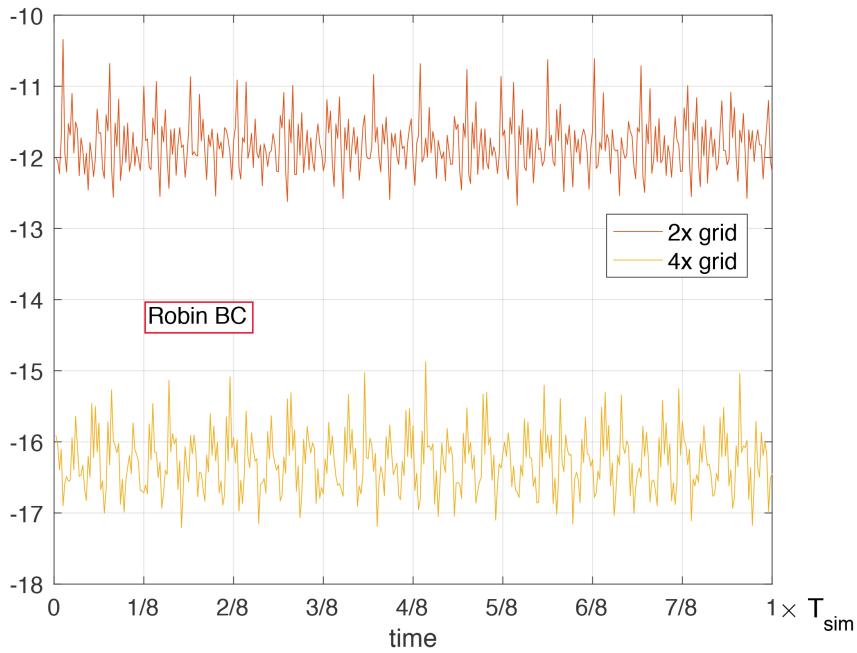


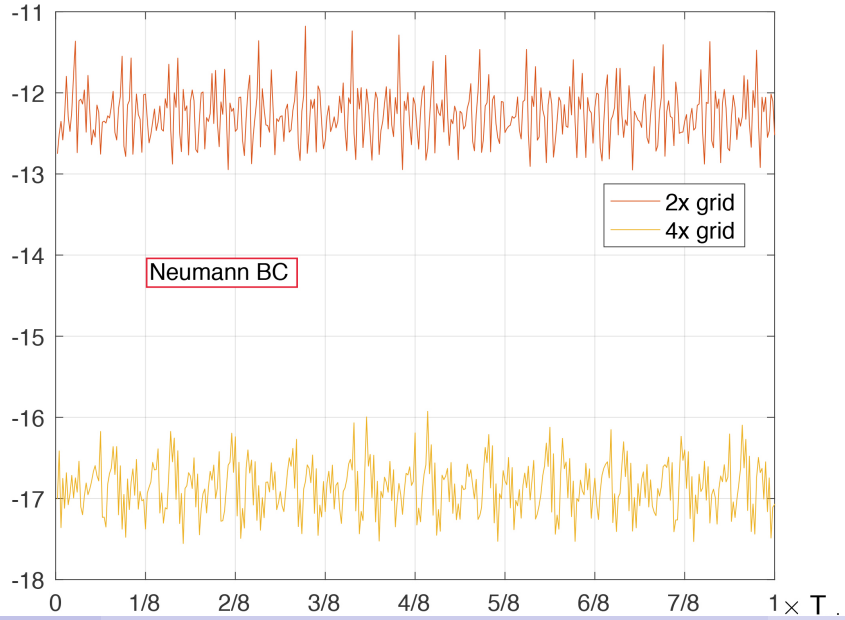
Cumulative mean error.

- A volumetric scheme terminated with PML allows to compute the solution over long times.
- MDP+lacunae fix the long-time error growth.

Fourth order scheme: Grid convergence







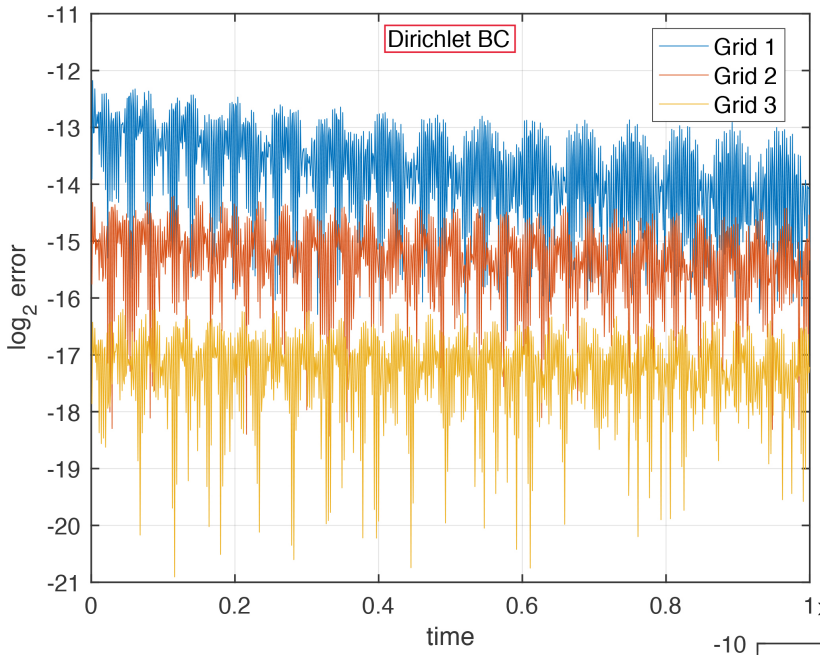
Fourth order scheme: Error

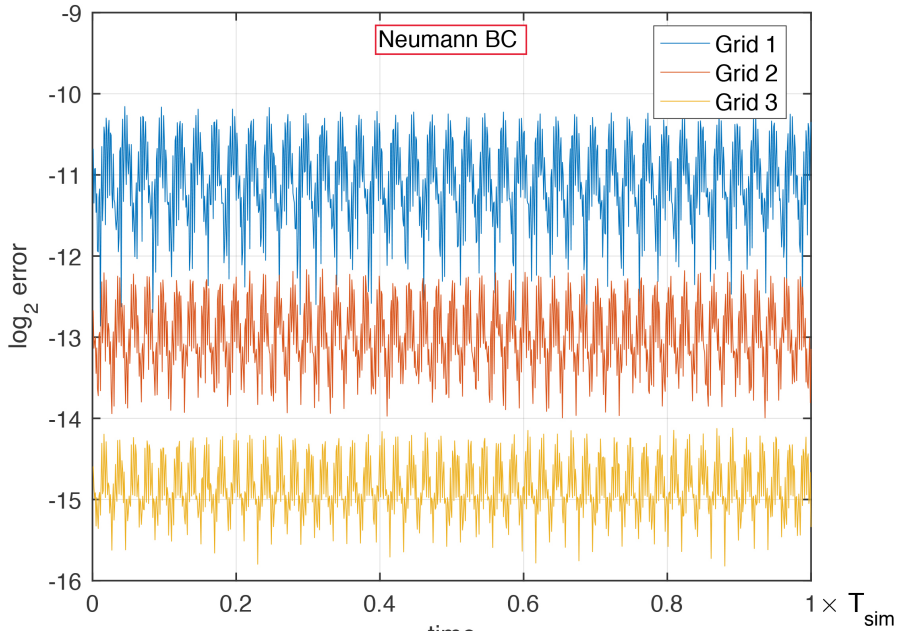
Grid	Dirichlet		Neumann		Mixed	
	Mean error	Rate	Mean error	Rate	Mean error	Rate
2x	6.52×10^{-5}	-	2.09×10^{-4}	-	2.86×10^{-4}	-
4x	2.44×10^{-6}	26	8.60×10^{-6}	24	1.31×10^{-5}	21

Actual values of the error and convergence rates.

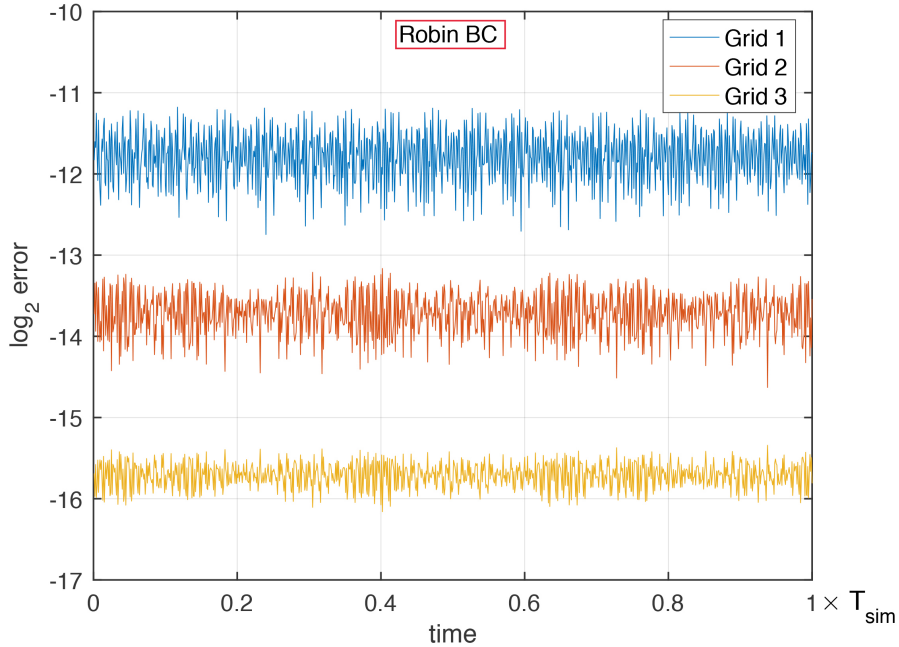
- Compared to the second order scheme:
  - Convergence rates are higher (expected);
  - Specific values of the error are lower on respective grids.

Second order scheme: Interior problem





- This formulation includes an inhomogeneous initial condition.



Future work

- More sophisticated geometries/shapes;
- Interfaces, transmission/scattering problems;
- Systems.