The mathematics that models wavefield physics in engineering applications - A voyage through the landscape of fundamentals

by

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Title and affiliation

Synopsis:

- System of wavefield equations in canonical form
- Field compatibility relations
- Constitutive relations in media with relaxation (absorption + dispersion)
- Spatial interface boundary conditions
- The initial-value problem and the time Laplace transformation (causality)
- Computational wavefield discretization
- The space-time integrated field equations + computational properties
- The 3D Perfectly Matched Embedding
- A simple application and benchmark problem

An intimate triangle

Mathematical methods:

- analytical
- computational

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Wavefield physics:

- acoustics
- elastodynamics
- electromagnetics

Engineering problems:

- formulation
- computation

Mathematics, (Wavefield) Physics, Engineering: An intimate triangle

Structure of any macroscopic physical configuration:

• BACKGROUND + CONTRAST **(Lorentz, 1916)**

Universal **BACKGROUND:**

- **empty universe** (homogeneous + isotropic) **(vacuum)**
- **observer** $\left\{\begin{array}{l}(N\text{-dimensional})\ \textbf{space}\\(1\text{-dimensional})\ \textbf{time}\end{array}\right\}$ decomposition
- capable of carrying **phenomena** satisfying **Lorentz-invariant** equations (**electromagnetics**, **gravitation (?)**)

CONTRAST:

- **matter** interacting with **phenomena in empty space** (**electromagnetics, gravitation (?)**) + carrying **material phenomena** (**acoustics**, **elastodynamics**)

Background and contrast in a macroscopic physical configuration

Each (macroscopic) FIELD is represented by:

FOUR FIELD QUANTITIES (FLDQ's):

- {**intensive FLDQ 1**, **intensive FLDQ 2**}
- {**extensive FLDQ 1**, **extensive FLDQ 2**}

PROPERTIES:

- **(intensive FLDQ 1) * (intensive FLDQ 2) =**
  - **area density of power flow**
- **(extensive FLDQ 1) * (extensive FLDQ 2) =**
  - **volume density of flow of momentum**

$\Longrightarrow$ **FLDQ = FLDQ**$(\boldsymbol{x}, t)$

with $\boldsymbol{x} = \{x_1, \ldots, x_N\} \in \mathbb{R}^N$ (**space**), $t \in \mathbb{R}$ (time)

Intensive and extensive field quantities in space-time

FIELD EQUATIONS

couple • **RATES OF CHANGE IN SPACE (∂_x) of intensive FLDQ's**

with • **RATES OF CHANGE IN TIME (∂_t) of extensive FLDQ's**

$\Longrightarrow$ **WAVE MOTION** $\Longleftarrow$

CANONICAL (TENSOR) FORM:

(Poincaré, 1905; Einstein, 1905; Minkowski, 1908)

- $\mathsf{D}(\boldsymbol{\partial_x})$ (**intensive FLDQ 1**) $+ \partial_t$ (**extensive FLDQ 2**) $= 0$
- $\mathsf{D}(\boldsymbol{\partial_x})$ (**intensive FLDQ 2**) $+ \partial_t$ (**extensive FLDQ 1**) $= 0$
- D: **array composed of unit tensors** (De Hoop, 1995, 2008)

• **COMPATIBILITY RELATIONS:** • $\partial_{x_1}\partial_{x_2}$ **(FLDQ)** $= \partial_{x_2}\partial_{x_1}$**(FLDQ)**

Field equations in canonical (tensor) form + compatibility relations

CONSTITUTIVE RELATIONS:

- **extensive FLDQ = CONSTITUTIVE OPERATOR (intensive FLDQ)**

CONSTITUTIVE OPERATOR:

- linear
- local $\Longrightarrow$ ~~**SPATIAL DISPERSION**~~ ($\Longrightarrow$ ~~**infinite wavespeed**~~)
- time-invariant
- active (field-independent) part (= external sources) +
  passive (field-dependent) part (= medium response)
- medium response = **instantaneous response** +
  (Boltzmann) relaxation (absorption + dispersion)

CONSTITUTIVE RELATIONS:

- **(extensive FLDQ 1,2)**$(\boldsymbol{x},t) =$

$$\underbrace{\textbf{(COEFF 1,2)}(\boldsymbol{x}) * \textbf{(intensive FLDQ 1,2)}(\boldsymbol{x},t)}_{\textbf{instantaneous response}} +$$

$$\underbrace{\int_{\boldsymbol{\tau}=0}^{\infty} \textbf{(RELAXF 1,2)}(\boldsymbol{x},\boldsymbol{\tau}) * \textbf{(intensive FLDQ 1,2)}(\boldsymbol{x},t-\boldsymbol{\tau})\mathrm{d}\boldsymbol{\tau}}_{\textbf{Boltzmann relaxation}}$$

- **BOLTZMANN RELAXATION** (Boltzmann, 1876) $\Longrightarrow$ **CAUSALITY**

Constitutive relations (canonical form)

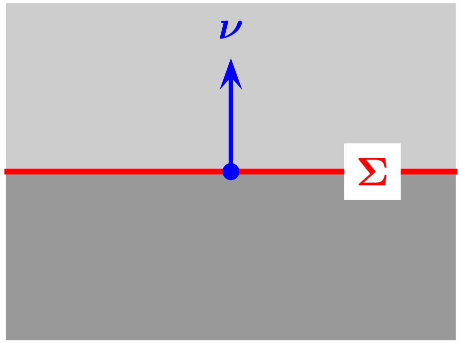
(PASSIVE) INTERFACE BOUNDARY CONDITIONS:

- Across passive interface Σ between two different media

NO JUMPS ALLOWED in certain FLDQ's: WHICH ONES?

- **DECOMPOSITION OF: ∂_x about $x \in \Sigma$:**

- $$\partial_x = \underbrace{\nu(\nu\cdot\partial_x)}_{\text{normal to } \Sigma} + \underbrace{[\partial_x - \nu(\nu\cdot\partial_x)]}_{\text{tangential to } \Sigma}$$



CONTINUITY CONDITIONS:

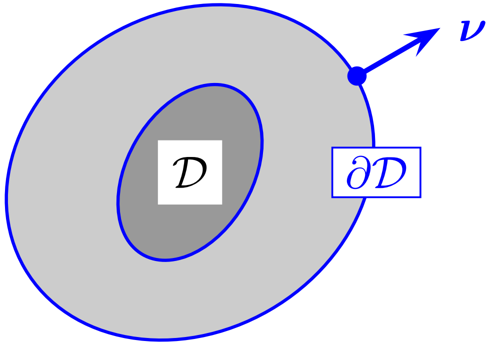
- $\mathsf{D}(\nu)$**(intensive FLDQ 1,2)**$\big|_{-}^{+} = 0$

Spatial interface boundary conditions

INITIAL-VALUE PROBLEM FIELD EQUATIONS: $(t \in \mathbb{R}; t_0 \leq t < \infty)$

• UNIQUENESS DATA:

• **Field on bounded support $\mathcal{D} \subset \mathbb{R}^N$**



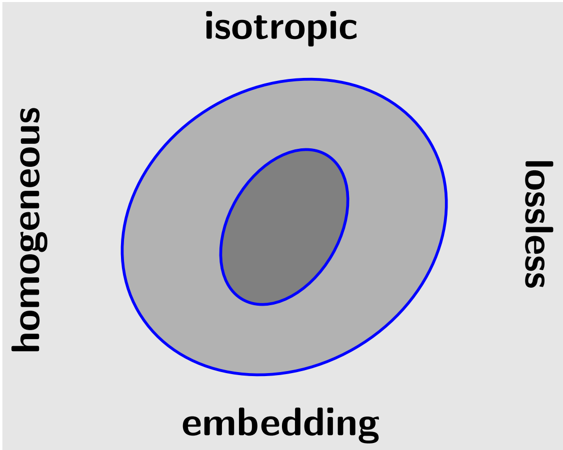
- **Initial field values: FLDQ's**$(\boldsymbol{x}, t_0)$ for $\boldsymbol{x} \in \mathcal{D}$
- **FIELD EQUATIONS** for $\boldsymbol{x} \in \mathcal{D};\ t_0 < t < \infty$
- **BOUNDARY VALUES:**
  - D$(\boldsymbol{\nu})$**(intensive FLDQ 1)**$(\boldsymbol{x}, t)$ for $\boldsymbol{x} \in \partial\mathcal{D},\ t_0 \leq t < \infty$ **OR**
  - D$(\boldsymbol{\nu})$**(intensive FLDQ 2)**$(\boldsymbol{x}, t)$ for $\boldsymbol{x} \in \partial\mathcal{D},\ t_0 \leq t < \infty$

Time evolution of field (physics) = Initial-value problem field equations (mathematics) (1)

INITIAL-VALUE PROBLEM FIELD EQUATIONS: $(t \in \mathbb{R}; t_0 \leq t < \infty)$

• UNIQUENESS DATA:

- **Field on unbounded support** $\mathbb{R}^N$



- **Initial field values: FLDQ's**$(\boldsymbol{x}, t_0)$ for $\boldsymbol{x} \in \mathbb{R}^N$
- **FIELD EQUATIONS** for $\boldsymbol{x} \in \mathbb{R}^N;\ t_0 < t < \infty$
- **OUTGOING WAVES in homogeneous, isotropic, lossless embedding**

INITIAL-VALUE PROBLEM FIELD EQUATIONS: $(t \in \mathbb{R}; t_0 \leq t < \infty)$

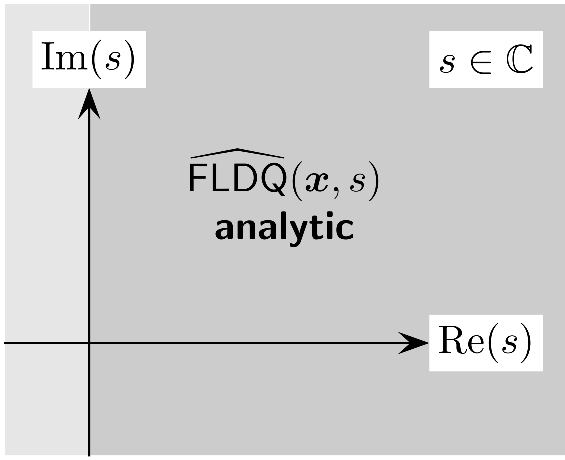
• MATHEMATICAL PROOF:

• Via shifted time Laplace transformation: (De Hoop, 2003, 2004)

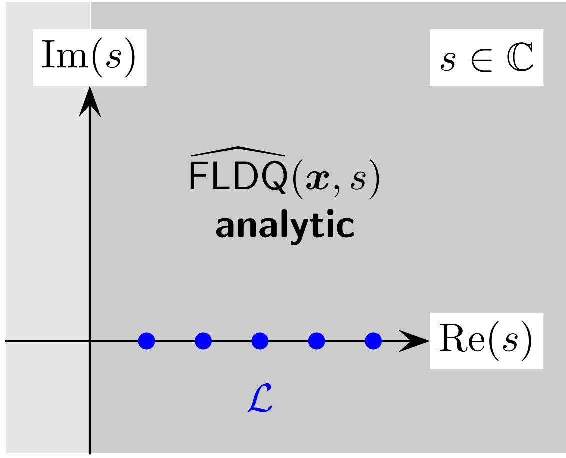
• $\widehat{\text{FLDQ}}(\boldsymbol{x}, s) = \int_{t=t_0}^{\infty} \exp(-st)\text{FLDQ}(\boldsymbol{x}, t)\text{d}t$

for $s \in \mathbb{C}, \text{Re}(s) > 0$

• $\partial_t \text{FLDQ}(\boldsymbol{x}, t) \longmapsto s\,\widehat{\text{FLDQ}}(\boldsymbol{x}, s) - \underbrace{\text{FLDQ}(\boldsymbol{x}, t_0)}_{\text{initial value}}$



INVERSE TIME LAPLACE TRANSFORMATION: $(t \in \mathbb{R}; 0 \leq t < \infty)$



- **use of Lerch's uniqueness theorem:**
  - $\{\widehat{\text{FLDQ}}(\boldsymbol{x}, s)|_{s \in \mathcal{L}}\} \overset{\text{1-to-1}}{\longmapsto} \text{FLDQ}(\boldsymbol{x}, t)H(t)$
  - $\mathcal{L} = \{s \in \mathbb{C}; \text{Im}(s) = 0, \text{Re}(s) = \boldsymbol{s_0 + nh}, s_0 > 0, h > 0, n = 0, 1, 2, 3, \ldots\}$
- **via INSPECTION** (Tables of Laplace Transforms)
- **use of Schouten-Van der Pol theorem:** (Schouten, 1934; Van der Pol, 1934)
  - **For** $\exp[-\hat{\Phi}(\boldsymbol{x}, s)\tau] \longmapsto \Psi(\boldsymbol{x}, t, \tau)H(t)$
  - $\widehat{\text{FLDQ}}[\boldsymbol{x}, \hat{\Phi}(\boldsymbol{x}, s)] \longmapsto \left[\int_{\tau=0}^{\infty} \Psi(\boldsymbol{x}, t, \tau)\text{FLDQ}(\boldsymbol{x}, \tau)\text{d}\tau\right] H(t)$

WAVEFIELD COMPUTATION

- Select (bounded) **spatial domain of computation** $[\mathcal{D}] \subset \mathbb{R}^N$
- Select (bounded) **time window of computation** $[\mathcal{T}] \subset \mathbb{R}$
- Construct (unbounded) **Perfectly Matched Embedding (PME)** $[\mathcal{D}]^\infty = \mathbb{R}^N \backslash [\mathcal{D}]$ **via time-dependent orthogonal Cartesian coordinate stretching** (De Hoop, Remis, Van den Berg, 2007)
- **Terminate PME with periodic boundary conditions** (De Hoop, Remis, Van den Berg, 2007)
- **Discretize** $[\mathcal{D}]$ **into union of adjacent simplices**
- **Discretize** $[\mathcal{T}]$ **into union of successive intervals**

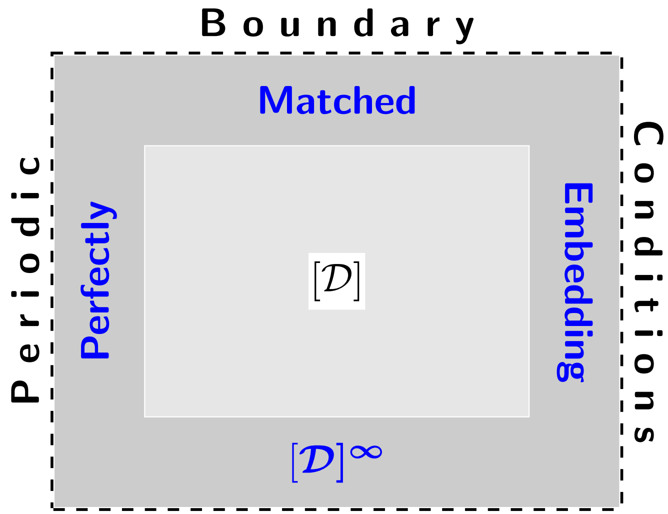
WAVEFIELD COMPUTATION

- **Discretize** FLDQ$(\boldsymbol{x}, t)$ **using:**
  - **piecewise linear interpolation on spatial grid**
  - **piecewise linear interpolation on temporal grid**
  - **nodal values of CONTINUOUS field components as (nodal, edge, face) expansion coefficients**
- **Substitute discretized field in space-time integrated field equations**
- **Compute integrations via simplicial ('trapezoidal') rule**
- **Discretize constitutive relations (piecewise constant in $[\mathcal{D}]$)**
- **Solve system of equations in space-time expansion coefficients**

Wavefield computation (2)

CONSTRUCTION OF PERFECTLY MATCHED EMBEDDING (PME)

- **Time Laplace-transform Cartesian coordinate stretching:**



- $\partial_{x_n} \longmapsto \partial_{\hat{X}_n} = \dfrac{1}{\hat{\chi}_n(x_n, s)}\partial_{x_n} \Longrightarrow$

$$\hat{X}_n(x_n, s) = \int_{\xi_n = a_n}^{x_n} \hat{\chi}_n(\xi_n, s)\mathrm{d}\xi_n$$

$$(n = 1, \ldots, N)$$

- $\{\hat{\chi}_n(x_n, s); n = 1, \ldots, N\}$ **analytic** for $s \in \mathbb{C}, \mathrm{Re}(s) > 0$, $\boldsymbol{x} \in [\mathcal{D}]^\infty$
- $\{\hat{\chi}_n(x_n, s); n = 1, \ldots, N\} > 0$ for $s \in \mathbb{C}, \mathrm{Re}(s) > 0, \mathrm{Im}(s) = 0$, $\boldsymbol{x} \in [\mathcal{D}]^\infty$
- $\{\hat{\chi}_n(x_n, s); n = 1, \ldots, N\} = 1$ for $\boldsymbol{x} \in [\mathcal{D}]$ $\Longrightarrow$ **field unchanged in** $[\mathcal{D}]$

Boundary Conditions $\Longrightarrow$ spurious field (De Hoop, Remis, Van den Berg, 2007)

THE SPACE-TIME INTEGRATED FIELD EQUATIONS

- **Apply operators**
  - $\int_{\boldsymbol{x}\in\mathcal{D}} \dots \mathrm{d}V$ and
  - $\int_{t\in\mathcal{T}} \dots \mathrm{d}t$ **to** **FIELD EQUATIONS**
- **Use**
- $\int_{\boldsymbol{x}\in\mathcal{D}} \mathsf{D}(\boldsymbol{\partial_x})[\textbf{intensive}\ \text{FLDQ}(\boldsymbol{x},t)]\mathrm{d}V = \int_{\boldsymbol{x}\in\partial\mathcal{D}} \mathsf{D}(\boldsymbol{\nu})[\textbf{intensive}\ \text{FLDQ}(\boldsymbol{x},t)]\mathrm{d}A$

  (Gauss in $\mathbb{R}^N$)

  - $\int_{t\in\mathcal{T}} \partial_t[\textbf{extensive}\ \text{FLDQ}(\boldsymbol{x},t)]\mathrm{d}t = [\textbf{extensive}\ \text{FLDQ}(\boldsymbol{x},t)]\Big|_{t\in\partial\mathcal{T}}$

    (Gauss in $\mathbb{R}$)

$\Longrightarrow$ **In RHS's only continuous quantities occur**

THE SIMPLICIAL INTEGRATION RULE

- **Simplicial integration rule in $\mathbb{R}^{N}$ (= trapezoidal rule in $\mathbb{R}$):**

Let $\Sigma^N \subset \mathbb{R}^N = N$**-simplex on vertices** $\{\boldsymbol{x}(0), \ldots, \boldsymbol{x}(N)\}$, then

- $$\int_{\boldsymbol{x}\in\Sigma^N} [\textbf{discretized } \text{FLDQ}(\boldsymbol{x}, t)]\mathrm{d}V \simeq$$
  $$\frac{V^N}{N+1}\Big[\text{FLDQ}[(\boldsymbol{x}(0), t)] + \ldots + \text{FLDQ}[(\boldsymbol{x}(N), t)]\Big]$$
- $V^N =$ **volume of** Σ^N

(De Hoop, 1995, 2008)

UNIT TENSORS IN WAVEFIELD PHYSICS

Symmetrical unit tensor of rank two: (Kronecker tensor)

- $\delta_{i,p} = 1$ for $i = p$, $\delta_{i,p} = 0$ for $i \neq p$

Unit tensors of rank four:

- $\Delta_{i,j,p,q} = \delta_{i,p}\delta_{j,q}$ **(reproduction)**
- $\Delta^{-}_{i,j,p,q} = (1/2)(\Delta_{i,j,p,q} - \Delta_{i,j,q,p})$ **(electromagnetics)**
- $\Delta^{+}_{i,j,p,q} = (1/2)(\Delta_{i,j,p,q} + \Delta_{i,j,q,p})$ **(elastodynamics)**
- $\Delta^{\delta}_{i,j,p,q} = (1/N)\delta_{i,j}\delta_{p,q}$ **(acoustics)**
- $\Delta^{\Delta}_{i,j,p,q} = \Delta_{i,j,p,q} - \Delta^{\delta}_{i,j,p,q}$ **(elastodynamics)**
- $\Delta^{\Delta,+}_{i,j,p,q} = \Delta^{+}_{i,j,p,q} - \Delta^{\delta}_{i,j,p,q}$ **(elastodynamics)**

(De Hoop, 1995, 2008)

TEST PULSES IN TIME FOR BENCHMARKING:

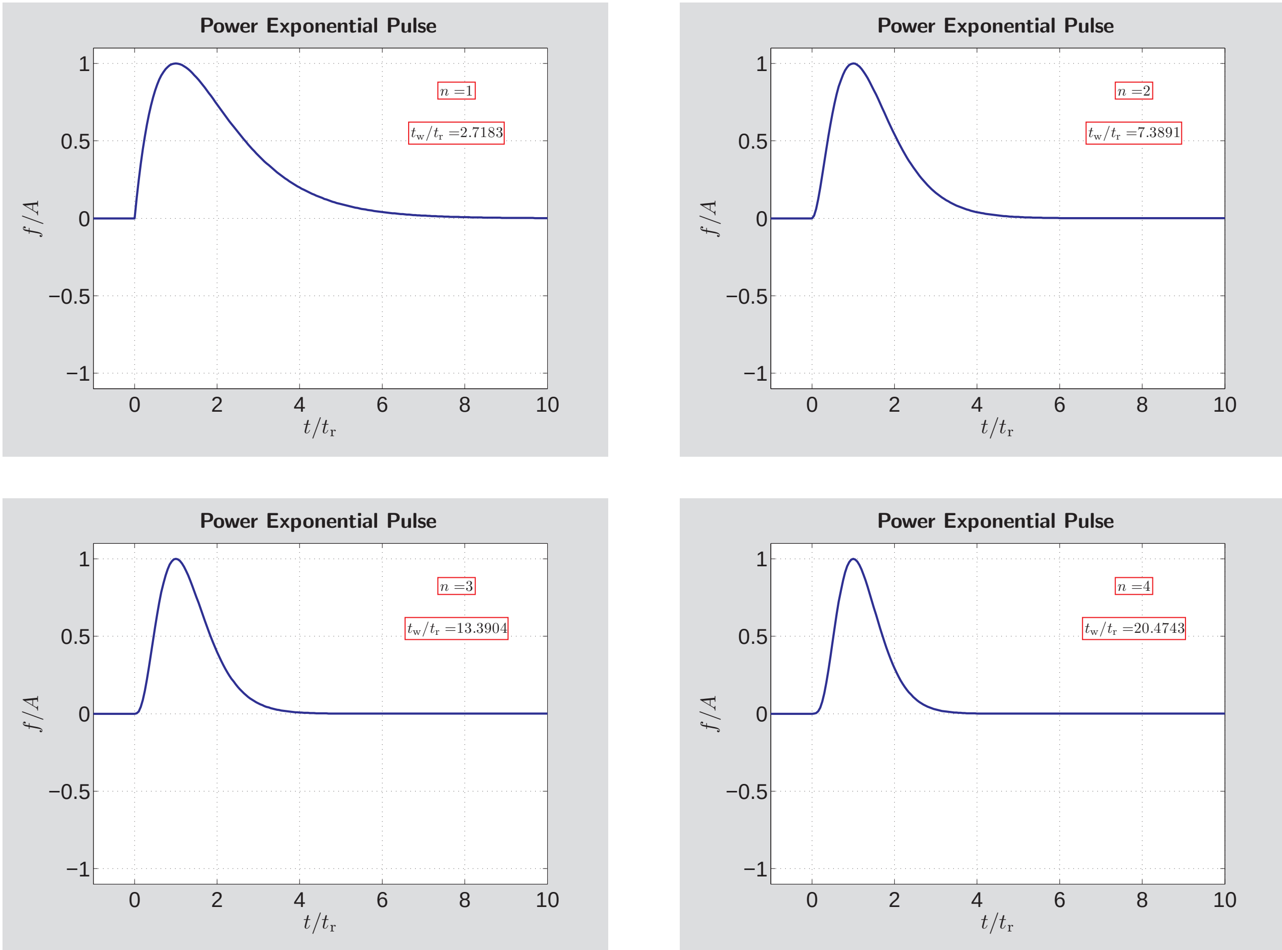
The unipolar pulse:

- $f(t) \geq 0$ for $t \geq 0$
- $\partial_t f(t)|_{t=t_\mathrm{r}} = 0 \Longrightarrow t_\mathrm{r}$ **(pulse rise time)**
- $A = f(t_\mathrm{r})$ **(pulse amplitude)**
- $t_\mathrm{w} = \dfrac{1}{A}\displaystyle\int_{t=0}^{\infty} f(t)\mathrm{d}t$ **(pulse time width)**

The power exponential pulse:

- $f(t) = A\left(\dfrac{t}{t_\mathrm{r}}\right)^n \exp\left[-n\left(\dfrac{t}{t_\mathrm{r}} - 1\right)\right] H(t)$ for $n = 1, 2, 3, \ldots$
- $t_\mathrm{w} = \dfrac{n!}{n^{n+1}}\exp(n)t_\mathrm{r}$
- $\hat{f}(s) = A\dfrac{n!}{(s + n/t_\mathrm{r})^{n+1}}\dfrac{\exp(n)}{t_\mathrm{r}^n}$ for $s \in \mathbb{C}, \mathrm{Re}(s) > 0$

POWER EXPONENTIAL PULSES:

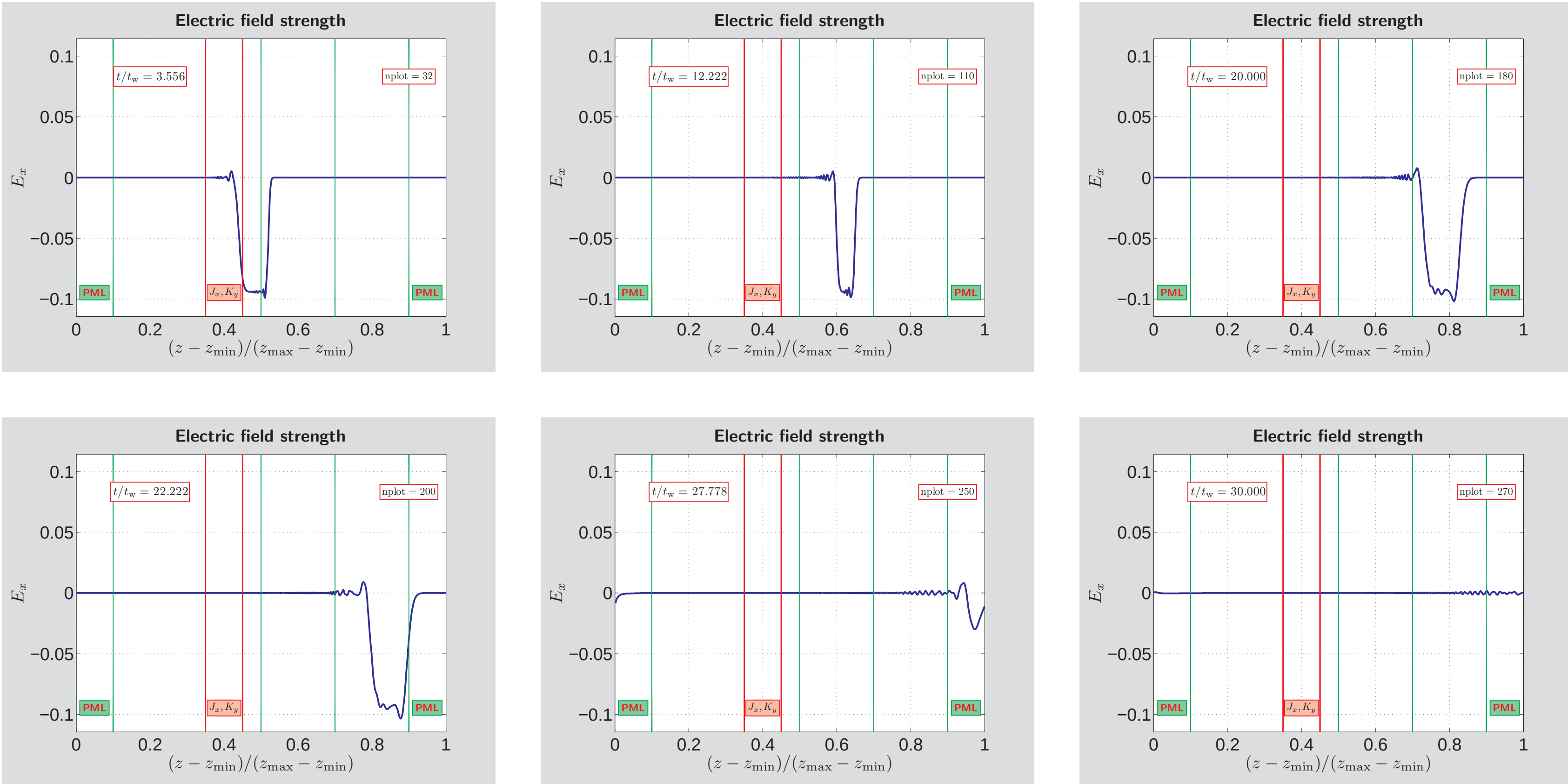


Power Exponential pulses

1D EM TD benchmark problem:

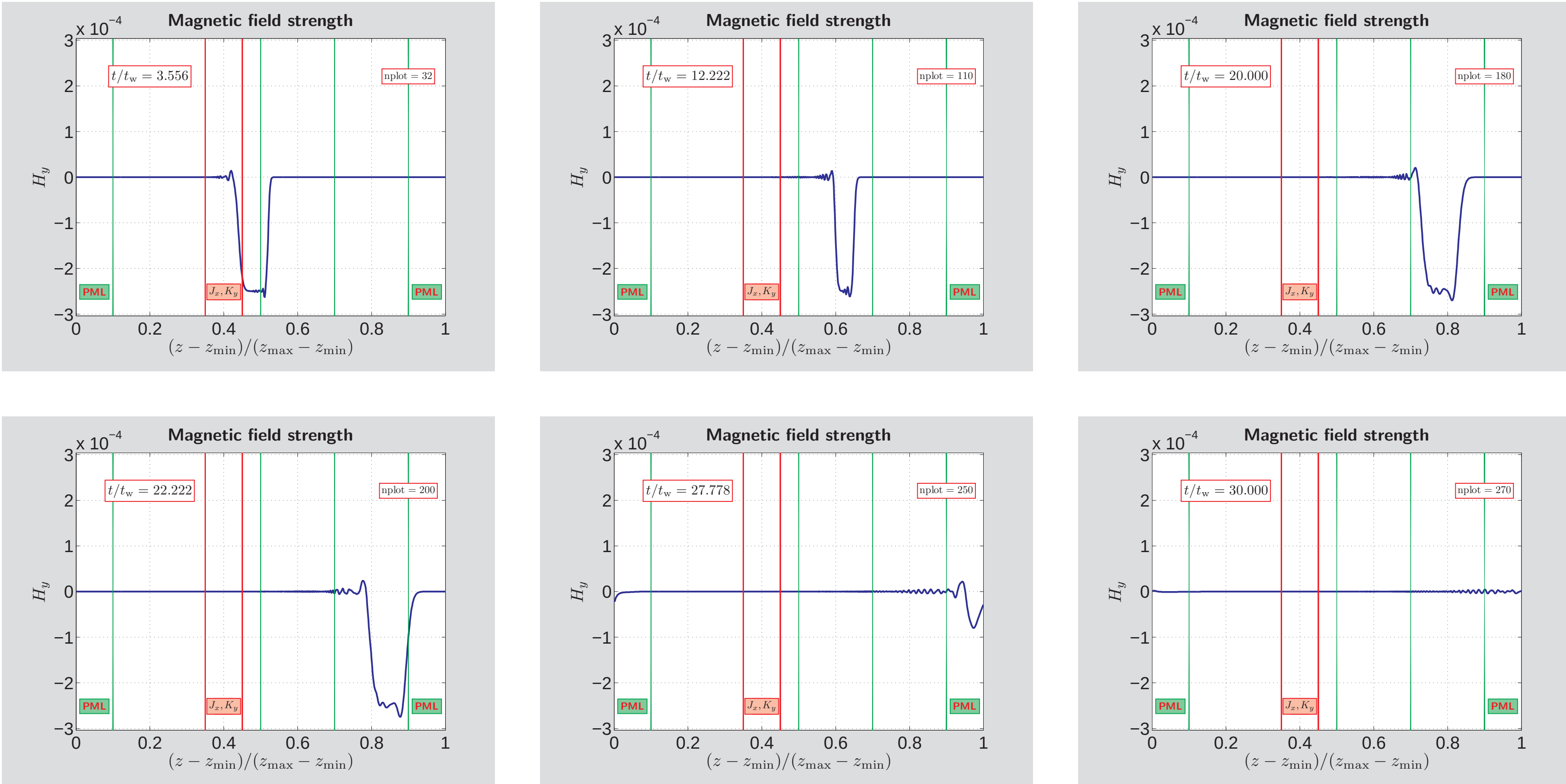
- **Electric-/Magnetic-current source excitation** $\Longrightarrow$ One-sided field
- **Propagation across slab with contrasting wave speed, no contrast in wave impedance** $\Longrightarrow$ Pulse narrowing in space, no reflection
- **Absorptive PML-padding with jump discontinuity at interface** $\Longrightarrow$ Absorption, no reflection
- **Periodic boundary condition** $\Longrightarrow$ Uniformity in PML absorption
- **Discretization data**
  - $\Delta z =$ (spatial pulse width)$/10$
  - $\Delta t =$ (pulse time width)$/9$
  - $N_{\text{cells}} = 681$
  - $\Gamma_{\text{period}} = 6.17$

1D EM TD benchmark problem (Electric field):



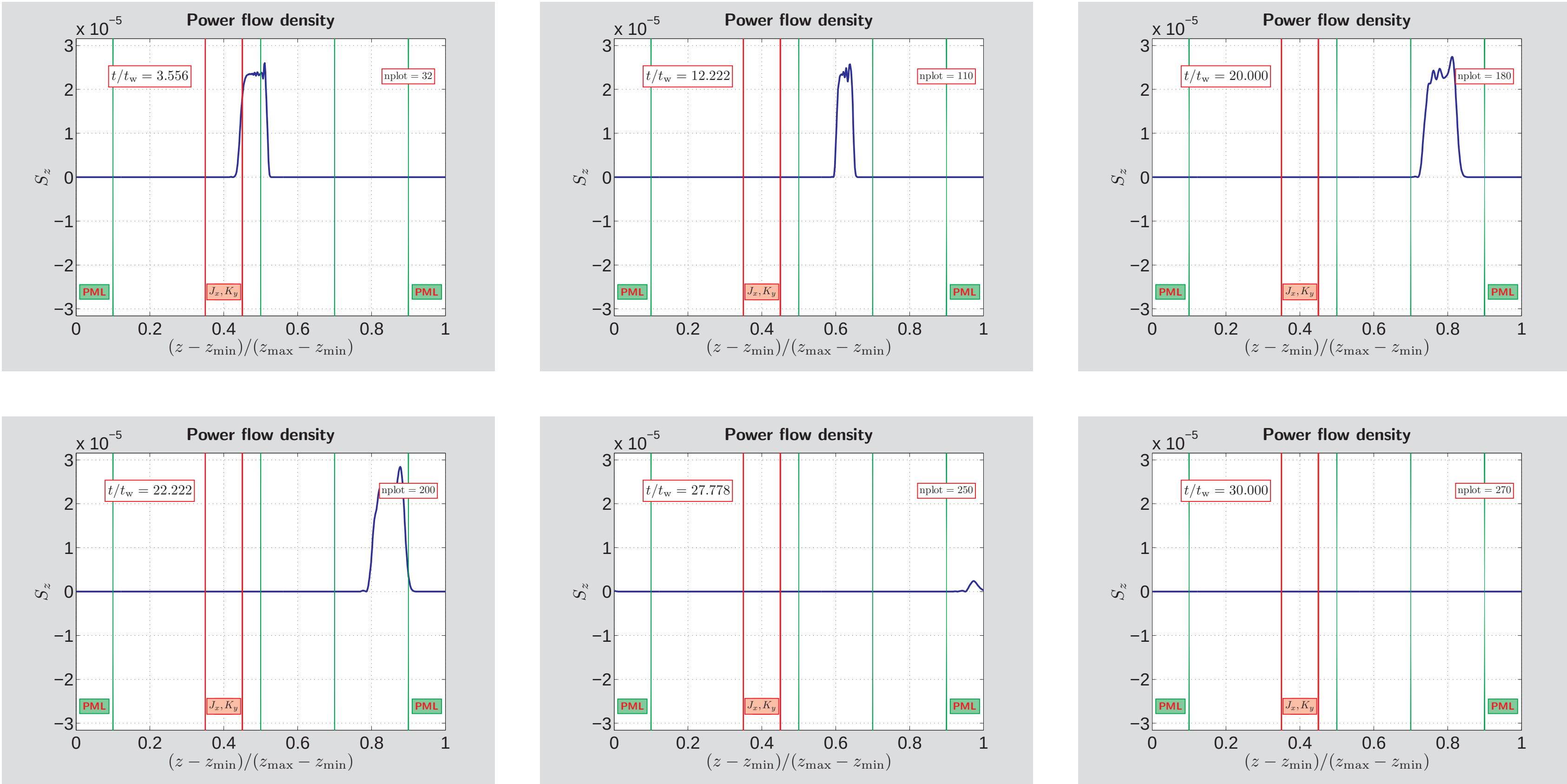
1D EM TD benchmark problem (Electric field)

1D EM TD benchmark problem (Magnetic field):



1D EM TD benchmark problem (Magnetic field)

1D EM TD benchmark problem (Poynting vector):



1D EM TD benchmark problem (Poynting vector)