The Precise Integration Time Domain (PITD) Method

— A Supplement to the Computational Electromagnetics

Xikui Ma[1] and Tianyu Dong[1,2]
maxikui@mail.xjtu.edu.cn tydong@mail.xjtu.edu.cn

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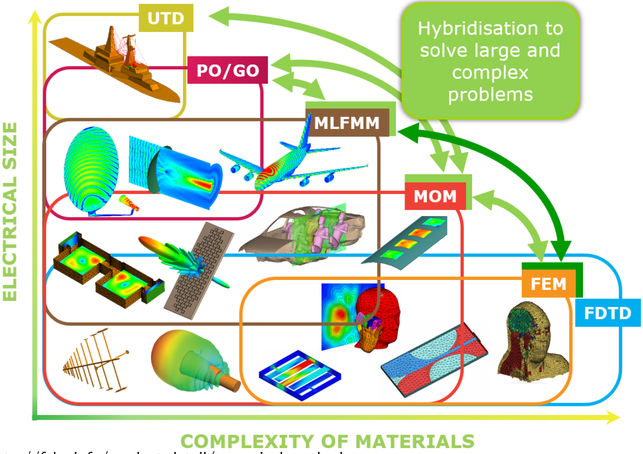
[1] SKLEI, School of Electrical Engineering, XJTU
[2] MSSV, School of Aerospace, XJTU

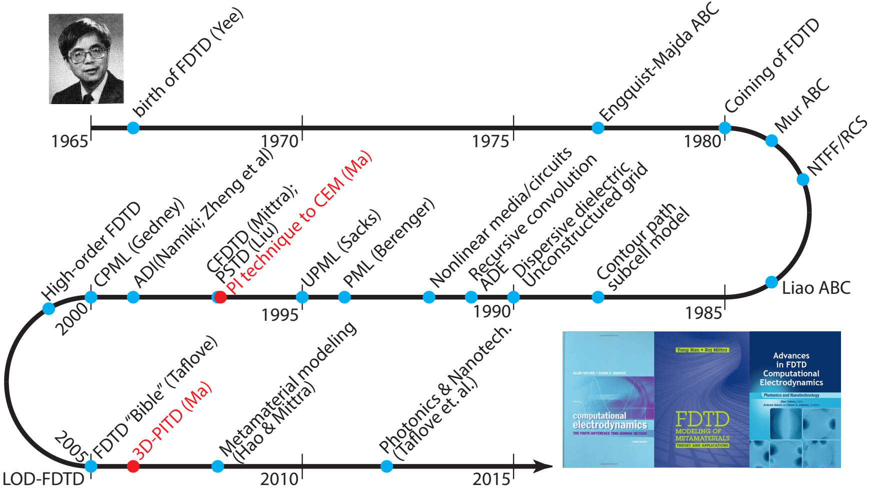
Outline

CEM map *



* source: http://feko.info/product-detail/numerical_methods

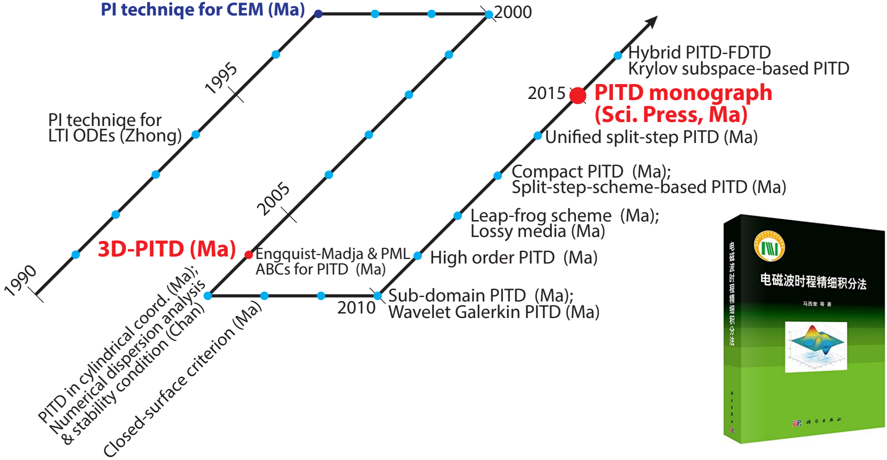
FDTD timeline



FDTD major technical paths

- ✔ Absorbing boundary conditions
  - Mur; Engquist-Majda; Berenger PML, UPML, CPML
- ✔ Numerical dispersion
  - High-order space differences; MRTD; PSTD
- ✔ Numerical stability
  - ADI techniques; **PITD**; One-step Chebyshev method
- ✔ Conforming grids
  - Locally/globally conforming; Stable hybrid FETD/FDTD
- ✔ Digital signal processing
  - Near-to-far-field transformation
- ✔ Dispersive and nonlinear materials
  - Isotropic/anisotropic dispersions; Nonlinear dispersions
- ✔ Multiphysics

PITD timeline

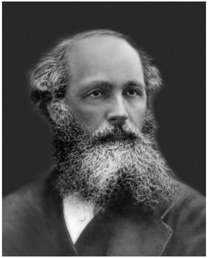


Maxwell's equations

And God said:

$$\begin{aligned}\frac{\partial \mathbf{E}}{\partial t} &= \varepsilon^{-1} \cdot \nabla \times \mathbf{H}, \\ \frac{\partial \mathbf{H}}{\partial t} &= -\mu^{-1} \cdot \nabla \times \mathbf{E},\end{aligned}$$

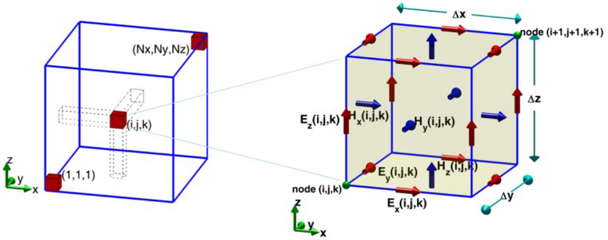
and then there was light.



J. C. Maxwell

"From a long view of the history of mankind the most significant event of the nineteenth century will be judged as Maxwell's discovery of the laws of electrodynamics." — Richard P. Feynman

Discretization and Yee cells



FDTD

- Finite difference in space
- Finite difference in time

PITD

- Finite difference in space
- ODEs in time

Updating equations / ODEs

FDTD

$$(\mathbf{R}+\mathbf{F})\mathbf{X}^{n+1} = (\mathbf{R}-\mathbf{F})\mathbf{X}^{n} + \mathbf{f}^{n+1}$$

$$\mathbf{R} = \frac{1}{2}\begin{bmatrix} \frac{2}{\Delta t}\mathbf{D}_{\epsilon} & -\mathbf{K} \\ -\mathbf{K}^{T} & \frac{2}{\Delta t}\mathbf{D}_{\mu} \end{bmatrix} \qquad \mathbf{F} = \frac{1}{2}\begin{bmatrix} \mathbf{D}_{\sigma_e} & \mathbf{K} \\ -\mathbf{K}^{T} & \mathbf{D}_{\sigma_m} \end{bmatrix}$$

where

$$\mathbf{X}^{n} = \begin{bmatrix} \mathbf{E}^{n} \\ \mathbf{H}^{n+1/2} \end{bmatrix}$$

- $\mathbf{D}_{\epsilon|\mu|\sigma_e|\sigma_m}$ — diagonal matrices containing $\epsilon, \mu, \sigma_e, \sigma_m$ for each cell
- $\mathbf{K}$ — arises from the discretization of the curl operators
- $\mathbf{f}^{n+1}$ — sources

E and **H** are **staggered** in time.

PITD

$$\frac{\mathrm{d}\mathbf{X}(t)}{\mathrm{d}t} = \mathbf{M}\mathbf{X}(t) + \mathbf{f}(t)$$

where

$$\mathbf{X}(t) = \begin{bmatrix} \mathbf{E}(t) \\ \mathbf{H}(t) \end{bmatrix}$$

- $\mathbf{M}$ — matrix containing material properties and the discretization of the curl operators
- $\mathbf{f}$ — sources

E and **H** are **non-staggered** in time.

Formal solution to $\frac{d\mathbf{X}}{dt} = \mathbf{MX} + \mathbf{f}(t)$

- Analytical form

$$\mathbf{X}(t) = \exp(\mathbf{M}t)X(0) + \int_0^t \exp[\mathbf{M}(t-s)]\mathbf{f}(s)\mathrm{d}s$$

- Recursive form

$$\mathbf{X}_{n+1} = \mathbf{T}\mathbf{X}_n + \mathbf{T}^{n+1}\boxed{\int_{t_n}^{t_{n+1}} \exp(-s\mathbf{M})\mathbf{f}(s)\mathrm{d}s}$$

2

1 $\boxed{\mathbf{T} = e^{\mathbf{M}\Delta t}}$

Key points!

Ways to compute $e^{\mathbf{M}\Delta t}$

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NINETEEN DUBIOUS WAYS TO COMPUTE THE EXPONENTIAL OF A MATRIX*

CLEVE MOLER† AND CHARLES VAN LOAN‡

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Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*

Cleve Moler†
Charles Van Loan‡

- Series methods
- ODE methods
- Polynomial methods
- Matrix decomposition methods
- Splitting methods
- Krylov space methods
- ...

PI technique to compute $\mathbf{T} = e^{\mathbf{M}\Delta t}$

N – preselected integer

1. scaling and squaring

$\tau = \Delta t/\ell$

$\ell = 2^N$

$$\mathbf{T} = e^{\mathbf{M}\Delta t} = \left(e^{\mathbf{M}\,\Delta t/\ell}\right)^{\ell} = \left(e^{\mathbf{M}\tau}\right)^{\ell}$$

2. series expansion of $e^{\mathbf{M}\tau}$

$$e^{\mathbf{M}\tau} = \mathbf{I} + \boxed{\mathbf{T}_a} \approx \mathbf{I} + \boxed{(\mathbf{M}\tau) + \frac{(\mathbf{M}\tau)^2}{2!} + \frac{(\mathbf{M}\tau)^3}{3!} + \frac{(\mathbf{M}\tau)^4}{4!}}$$

3. compute $\mathbf{T} = \left(e^{\mathbf{M}\tau}\right)^{\ell} = (\mathbf{I} + \mathbf{T}_a)^{\ell}$ — *to be contd.*

PI technique to compute $\mathbf{T} = e^{\mathbf{M}\Delta t}$ (contd.)

3. compute $\mathbf{T} = \left(e^{\mathbf{M}\tau}\right)^{\ell} = (\mathbf{I} + \mathbf{T}_a)^{\ell}$

$$\mathbf{T} = (\mathbf{I} + \mathbf{T}_a)^{2^N} = (\mathbf{I} + \mathbf{T}_a)^{2^{N-1}} \times (\mathbf{I} + \mathbf{T}_a)^{2^{N-1}} = \ldots$$

with $(\mathbf{I} + \mathbf{T}_a)^2 = \mathbf{I} + 2\mathbf{T}_a + \mathbf{T}_a \times \mathbf{T}_a$.

Pseudo code

do $i = 1, \ldots, N$

$\quad \mathbf{T}_a \leftarrow 2\mathbf{T}_a + \mathbf{T}_a \times \mathbf{T}_a$

end do

$\mathbf{T} \leftarrow \mathbf{I} + \mathbf{T}_a$

The algorithm holds the computational precision.

Evaluating $\mathbf{T}\int_{t_n}^{t_{n+1}} e^{-s\mathbf{M}}\mathbf{f}(s)\mathrm{d}s$ & the recursive formula

(1) Analytical solution under the linear representation of $\mathbf{f}(t)$

- 1^{st} order Taylor approximation of $\mathbf{f}(t)$, *i.e.*,

$$\mathbf{f} = \mathbf{f}_0 + (t - t_n)\mathbf{f}_1, \qquad t \in (t_n, t_{n+1})$$

- integrate $\mathbf{T}\int_{t_n}^{t_{n+1}} e^{-s\mathbf{M}}\mathbf{f}(s)\mathrm{d}s$ analytically
- recursive form for $\mathbf{X}_{n+1}$:

$$\begin{aligned}\mathbf{X}_{n+1} =& \mathbf{T}\left[\mathbf{X}_n + \mathbf{M}^{-1}(\mathbf{f}_0 + \mathbf{M}^{-1}\mathbf{f}_1)\right] \\ & - \mathbf{M}^{-1}\left[\mathbf{f}_0 + \mathbf{M}^{-1}\mathbf{f}_1 + \mathbf{f}_1\Delta t\right]\end{aligned}$$

compute $\mathbf{M}^{-1}$? It is *noninvertible* generally!

Evaluating $\mathbf{T}\int_{t_n}^{t_{n+1}} e^{-s\mathbf{M}}\mathbf{f}(s)ds$ & the recursive formula (contd.)

(2) Recursive formula by using the Gaussian quadrature rule

- three-point Gaussian quadrature
- recursive form for $\mathbf{X}_{n+1}$:

$$
\begin{aligned}
\mathbf{X}_{n+1} = \mathbf{T}\mathbf{X}_n &+ \frac{5}{18} e^{\left(1+\sqrt{3/5}\right)\mathbf{M}\Delta t/2}\mathbf{f}\left[t_n + \left(1-\sqrt{3/5}\right)\Delta t/2\right] \\
&+ \frac{5}{18} e^{\left(1-\sqrt{3/5}\right)\mathbf{M}\Delta t/2}\mathbf{f}\left[t_n + \left(1+\sqrt{3/5}\right)\Delta t/2\right] \\
&+ \frac{8}{18} e^{\mathbf{M}\Delta t/2}\mathbf{f}\left(t_n + \Delta t/2\right)
\end{aligned}
$$

Remarks

$$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = \mathbf{MX} + \mathbf{f}, \quad \mathbf{X} = [\mathbf{E}, \mathbf{H}]^T$$

1. finite difference in space, but differential in time
2. scaling and squaring for $\exp(\mathbf{M}\Delta t)$
3. $\mathbf{T}_a \leftarrow 2\mathbf{T}_a + \mathbf{T}_a \times \mathbf{T}_a$ to guarantee the computational precision
4. Gaussian quadrature for the excitation term
5. non-staggered **E** and **H** in time

Precise Integration

Numerical stability condition

FDTD CFL criteria: $\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}} = \dfrac{1}{c\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}+\frac{1}{(\Delta z)^2}}}$

PITD

Stability conditions vary for different orders of Taylor approximation:

- $1^{\text{st}}/2^{\text{nd}}$-order: unstable;
- 3^{rd}-order: $\Delta t < \sqrt{3}/2\,\ell\,\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}} = \sqrt{3}/2\,2^N\,\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}}$
- 4^{th}-order: $\Delta t < \sqrt{2}\ell\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}} = 2^{N+1/2}\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}}$
- 5^{th}-order: $\frac{\sqrt{2}(15-\sqrt{65})}{4\sqrt{15-\sqrt{65}}}\ell\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}} < \Delta t < \frac{\sqrt{2}(15+\sqrt{65})}{4\sqrt{15+\sqrt{65}}}\ell\Delta t^{\text{FDTD}}_{\substack{\text{upper}\\\text{bound}}}$

Almost **unconditionally** stable for large N.

Numerical dispersion analysis

FDTD numerical dispersion relation:

$$W_t^2/c^2 = W_x^2 + W_y^2 + W_z^2,$$

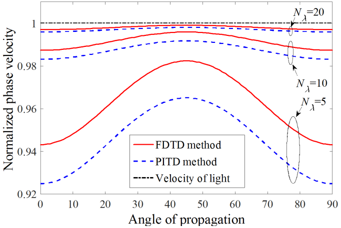
where $W_{x|y|z} = \frac{\sin(\tilde{k}_{x|y|z}\Delta x|y|z/2)}{\Delta x|y|z/2}$, $W_t = \frac{\sin(\omega\Delta t/2)}{\Delta t/2}$.

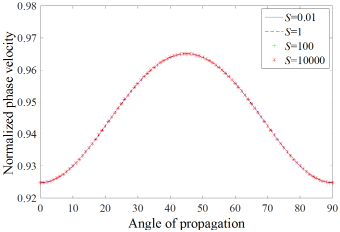
PITD

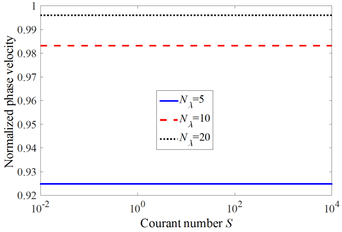
$$\tan^2\left(\frac{\omega\Delta t}{\ell}\right) = \frac{\left(\Lambda_{\mathrm{PITD}} - \Lambda_{\mathrm{PITD}}^3/3!\right)^2}{1 + \Lambda_{\mathrm{PITD}}^2/2! - \Lambda_{\mathrm{PITD}}^4/4!}$$

where $\Lambda_{\mathrm{PITD}} = \frac{c\Delta t}{\ell}\sqrt{W_x^2 + W_y^2 + W_z^2}$.

Numerical dispersion analysis (contd.)







- numerical dispersion is slightly worse than that of FDTD
- independent of the time step
- dense griding improves the accuracy

Source and boundary conditions

Source conditions

- Hard sources
- Plane waves & TS/SF technique
- ...

Boundary conditions

- Engquist-Majda ABC
- PMLs
- ...

“它山之石，可以攻玉。” —《诗经·小雅·鹤鸣》

“Stones from other hills may serve to polish the jade of this one.”

— Classic of Poetry ▪ Lesser Court Hymns ▪ Singing of Cranes

Remarks

Characteristics of the PITD method:

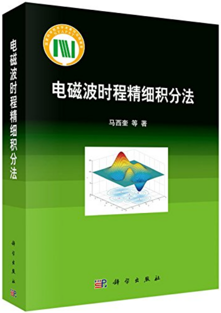
- ✓ preselected N determines the upper bound of Δt^{PITD}
- ✓ $\Delta t^{\mathrm{PITD}}_{\substack{\mathrm{upper}\\ \mathrm{bound}}} >> \Delta t^{\mathrm{FDTD}}_{\substack{\mathrm{upper}\\ \mathrm{bound}}}$
- ✓ slight worse numerical dispersion compared with that of the FDTD method
- ✓ numerical dispersion can be independent of Δt
- ✓ technique paths of the FDTD method can be learned

"Stones from other hills may serve to polish the jade of this one."

— Classic of Poetry ▪ Lesser Court Hymns ▪ Singing of Cranes

Improved methods

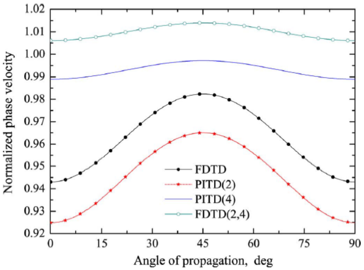
- Fourth-order PITD [PITD(4)] method
- Wavelet Galerkin PITD (WG-PITD) method
- Leapfrog PITD (L-PITD) method
- Compact PITD (CPITD) method
- Hybrid PITD-FDTD method
- Krylov subspace method
- ...

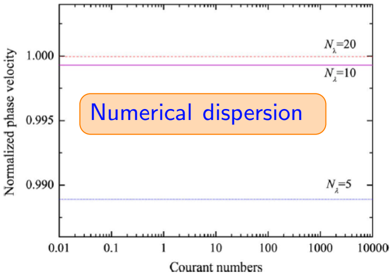


Improved methods — PITD(4) [1]

4^{th}-order spatial difference scheme is used as:

$$\frac{\partial u_i}{\partial x} = \frac{1}{\Delta x}\left[\frac{1}{24}\left(u_{i-3/2} - u_{i+3/2}\right) - \frac{27}{24}\left(u_{i-1/2} - u_{i+1/2}\right)\right] + O\left[(\Delta x)^4\right]$$





[1] IEEE T-AP, **59**(4), 2011: 1311-1320.

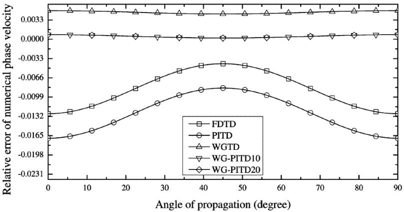
Improved methods — WG-PITD method [2]

Discretization form of Maxwell equation(s) in space:

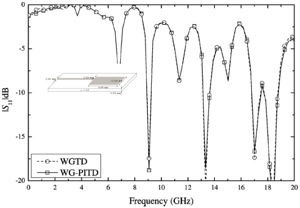
$$\frac{\mathrm{d}\ E_x|_{l+1/2,m,n}}{\mathrm{d}t} = -\frac{\sigma|_{l+1/2,m,n}}{\varepsilon|_{l+1/2,m,n}} E_x|_{l+1/2,m,n} + \sum_i a_i \left[\frac{H_z|_{l+1/2,m+i+1/2,n}}{\varepsilon|_{l+1/2,m,n}\,\Delta y} - \frac{H_y|_{l+1/2,m,n+i+1/2}}{\varepsilon|_{l+1/2,m,n}\,\Delta z} \right]$$

where $a_i = \int_{-\infty}^{\infty} \frac{\mathrm{d}\phi_{1/2}(x)}{\mathrm{d}x} \phi_{-i}(x)\mathrm{d}x.$

Numerical dispersion



S_{11}-parameter



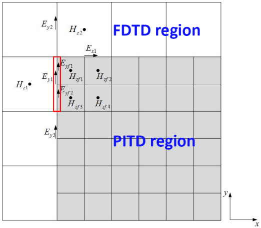
[2] IEEE MWCL, **20**(12), 2010: 651-653

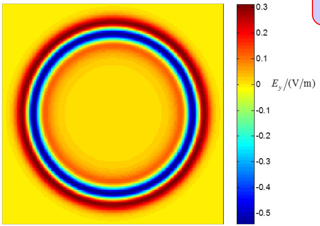
Improved methods — Hybrid PITD-FDTD method [3]

How to handle multiscale problems with fine geometrical features?

- Subgriding in FDTD — Δt depends on Δx_{min}
- PITD — need to compute $e^{\mathbf{M}\Delta t}$, but Δt can be relaxed

Hybriding





[3]Please refer to PA-11 (Mon. 14:00-15:30, Function Room 2, 2F)

Improved methods — Krylov space method [4]

Recursive form of the PITD method:

$$\mathbf{X}_{n+1} = e^{\mathbf{M}\Delta t}\mathbf{X}_n + \sum_i \alpha_i e^{\mathbf{M}\beta_i\Delta t}\mathbf{f}(t_n + \gamma_i \Delta t)$$

	number of nonzero elements	Denseness	Memory cost (MB)
$\mathbf{M}$	1558	0.0039	0.003
$e^{\mathbf{M}\Delta t}$	370482	0.9334	0.76

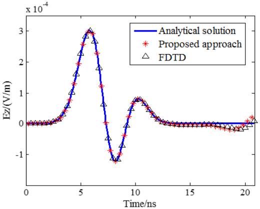
Evaluate $e^{\mathbf{M}\Delta t}$ explicitly? ✗ $\longrightarrow$ Estimate $e^{\mathbf{M}\Delta t}\mathbf{v}$ directly. ✓

[4] Please refer to OC2-6 (Tue. 08:30-10:00, Function Room 3, 3F)

Improved methods — Krylov space method [4] (contd.)

Direct estimation of $e^{\mathbf{M}\Delta t}\mathbf{v}$

1. m^{th}-order Krylov subspace: $K^m(\mathbf{M}, \mathbf{v}) = \text{span}(\mathbf{v}, \mathbf{Mv}, \ldots, \mathbf{M}^{m-1}\mathbf{v})$
2. Arnoldi process
   - $\mathbf{V}_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]^T$ – orthogonal basis of K^m
   - $\mathbf{H}_m \approx \mathbf{V}_m^T\mathbf{M}\mathbf{V}_m$ – matrix generated during the Arnoldi process
3. $e^{\mathbf{M}\Delta t}\mathbf{v} \approx \mathbf{V}_m e^{\mathbf{H}_m\Delta t}\mathbf{V}_m^T\mathbf{v} = \mathbf{V}_m e^{\mathbf{H}_m\Delta t}\mathbf{e}_1, \quad \mathbf{e}_1 = [1, 0, 0, \ldots, 0]^T \in \mathbb{R}^{m\times 1}$



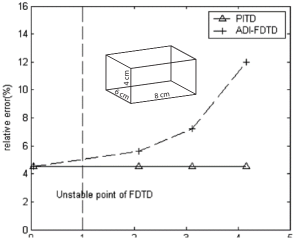
	CPU time (s)	Memory cost (MB)
Krylov-PITD	23.78	0.30
FDTD	137.28	1.34

[4] Please refer to OC2-6 (Tue. 08:30-10:00, Function Room 3, 3F)

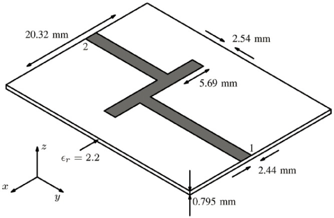
Rectangular cavity

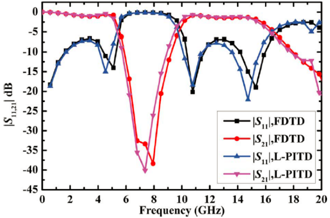
$f_{\text{ana.}}$ (GHz)	FDTD scheme $\Delta t = 1$ ps		ADI-FDTD scheme $\Delta t = 60$ ps		PITD scheme $\Delta t = 60$ ps	
	f (GHz)	rel. err.	f (GHz)	rel. err.	f (GHz)	rel. err.
3.125	2.983	4.54%	2.900	7.20%	2.983	4.54%
4.881	4.750	2.68%	4.650	4.73%	4.750	2.68%
5.340	5.450	2.06%	5.580	4.49%	5.450	2.06%
7.289	7.333	0.60%	6.817	6.92%	7.333	0.60%
7.529	7.567	0.51%	7.000	7.03%	7.567	0.51%

- relative error increases as the time-step increases for the ADI-FDTD method
- relative error is independent of the time step for the PITD method



Microstrip low pass filter [5]





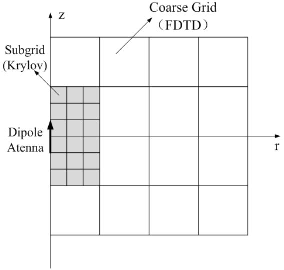
Comparison between the FDTD method and the L-PITD (Leapfrog PITD) method †

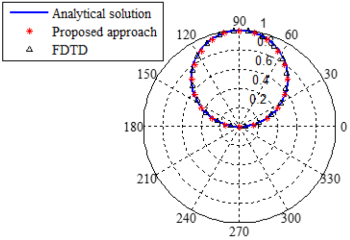
	Δx	Δy	Δz	Δt	memory	CPU time
FDTD	0.41 mm	0.26 mm	0.42 mm	0.441 ps	24.44 MB	1024 s
L-PITD	0.41 mm	0.26 mm	0.42 mm	0.884 ps	248.4 MB	851 s

† Simulations were performed on Intel® Core™ Duo CPU T8100 2.10 GHz PC.

[5] IEEE MWCL, 22(6), 2012: 294 – 296.

Small antenna





Comparison between the FDTD method and the Krylov-PITD method

	CPU time (s)	Memory cost (MB)
Krylov-PITD	23.78	0.30
FDTD	137.28	1.34

Remarks

- ✔ almost unconditionally stable
- ✔ relative large time step size can be used
- ✔ PI technique maintains the computational precision
- ✔ relative error independent of the time-step
- ✔ hybrid PITD-FDTD technique suitable for multiscale problems
- ✔ memory cost can be relaxed by using the Kyrlov space method

"瑕不掩瑜。" —《礼记·聘义》

"One flaw cannot obscure the splendor of the jade."

— Book of Rites ▪ Meaning of Interchange of Missions twixt Different Courts

Outlook

Future work :

- Sub-domain technique
- Parallel computing technique
- Extend to complex materials

Future prospects :

- Nanophotonics and nanoplasmonics. Ultimately, combination of quantum and classical electrodynamics
- Multiphysics

Acknowledgements & References

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Q & A.

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