The Precise Integration Time Domain (PITD) Method
— A Supplement to the Computational Electromagnetics

Xikui Ma\textsuperscript{1} and Tianyu Dong\textsuperscript{1,2}
maxikui@mail.xjtu.edu.cn tydong@mail.xjtu.edu.cn

September 19, 2016
\textsuperscript{1} SKLEI, School of Electrical Engineering, XJTU
\textsuperscript{2} MSSV, School of Aerospace, XJTU
Outline

1. Overview

2. Methods
   - Introduction to PITD
   - Numerical dispersion and stability
   - Source and boundary conditions
   - Improved methods

3. Examples
   - Resonant cavity
   - Microstrip LPF
   - Small antenna

4. Outlooks
Overview

Methods

Examples

Outlook

CEM map

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

- **Birth of FDTD (Yee)**: 1965
- **Engquist-Majda ABC**
- **Mur ABC**
- **NTFF/RCS**
- **Coining of FDTD**
- **Liao ABC**
- **Nonlinear media/circuits**
- **Recursive convolution**
- **Dispersive dielectric**
- **Unstructured grid**
- **Contour path subcell model**
- **High-order FDTD (Gedney)**
- **CPML (Namiki; Zheng et al.)**
- **CFDTD (Mitra)**
- **PSTD (Liu)**
- **UPML (Sacks)**
- **PML (Berenger)**
- **PI technique to CEM (Ma)**
- **Nonlinear media/circuits**
- **Recursive convolution**
- **Dispersive dielectric**
- **Unstructured grid**
- **Contour path subcell model**
- **LOD-FDTD**
- **Metamaterial modeling (Hao & Mittra)**
- **Photonics & Nanotech. (Tafove et al.)**
- **3D-PITD (Ma)**
- **FDTD “Bible” (Tafove)**
- **Methods**
- **Examples**
- **Outlooks**

**Overview**

ICEF 2016 Xi’an — PITD
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
Overview  Methods  Examples  Outlooks

PITD timeline

PI technique for LTI ODEs (Zhong)  1990

PI technique for CEM (Ma)  1995

3D-PITD (Ma)  2000

Engquist-Madja & PML ABCs for PITD (Ma)

High order PITD (Ma)  2005

Leap-frog scheme (Ma); Lossy media (Ma)

Sub-domain PITD (Ma); Wavelet Galerkin PITD (Ma)  2010

Compact PITD (Ma); Split-step-scheme-based PITD (Ma)

Unified split-step PITD (Ma)

Hybrid PITD-FDTD Krylov subspace-based PITD

PITD monograph (Sci. Press, Ma)  2015

PITD in cylindrical coord. (Ma); Numerical dispersion analysis & stability condition (Chan)

Closed-surface criterion (Ma)
Maxwell’s equations

And God said:

\[
\frac{\partial \mathbf{E}}{\partial t} = \varepsilon^{-1} \cdot \nabla \times \mathbf{H},
\]

\[
\frac{\partial \mathbf{H}}{\partial t} = -\mu^{-1} \cdot \nabla \times \mathbf{E},
\]

and then there was light.

“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
Overview  Methods  Examples  Outlooks

**Updating equations / ODEs**

**FDTD**

\[
(R + F)X^{n+1} = (R - F)X^n + f^{n+1}
\]

\[
R = \frac{1}{2} \begin{bmatrix}
\frac{2}{\Delta t} D_\varepsilon & -K \\
-K^T & \frac{2}{\Delta t} D_\mu
\end{bmatrix}
\]

\[
F = \frac{1}{2} \begin{bmatrix}
D_\sigma_e & K \\
-K^T & D_\sigma_m
\end{bmatrix}
\]

where

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

- \(D_\varepsilon|\mu|\sigma_e|\sigma_m\) — diagonal matrices containing \(\varepsilon, \mu, \sigma_e, \sigma_m\) for each cell
- \(K\) — arises from the discretization of the curl operators
- \(f^{n+1}\) — sources

**PITD**

\[
\frac{dX(t)}{dt} = MX(t) + f(t)
\]

where

\[
X(t) = \begin{bmatrix}
E(t) \\
H(t)
\end{bmatrix}
\]

- \(M\) — matrix containing material properties and the discretization of the curl operators
- \(f\) — sources

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

**E and H are non-staggered in time.**
Formal solution to $\frac{dX}{dt} = MX + f(t)$

- **Analytical form**

  $$X(t) = \exp(Mt)X(0) + \int_0^t \exp[M(t - s)]f(s)ds$$

- **Recursive form**

  $$X_{n+1} = TX_n + T^{n+1}\int_{t_n}^{t_{n+1}} \exp(-sM)f(s)ds$$

**Key points!**

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

2. $\int_{t_n}^{t_{n+1}} \exp(-sM)f(s)ds$
Ways to compute $e^{M\Delta t}$

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

*SIAM REVIEW
Vol. 20, No. 4, October 1978
© Society for Industrial and Applied Mathematics

NINETEEN DUBIOUS WAYS TO COMPUTE THE EXPONENTIAL OF A MATRIX*
CLEVE MOLER† AND CHARLES VAN LOAN‡

*SIAM REVIEW
Vol. 45, No. 1, pp. 3–49
© 2003 Society for Industrial and Applied Mathematics

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

Cleve Moler†
Charles Van Loan‡
PI technique to compute $T = e^{M\Delta t}$

1. scaling and squaring

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

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

$$e^{M\tau} = I + T_a \approx I + \left(M\tau\right) + \frac{(M\tau)^2}{2!} + \frac{(M\tau)^3}{3!} + \frac{(M\tau)^4}{4!}$$

3. compute $T = \left(e^{M\tau}\right)^\ell = \left(I + T_a\right)^\ell$ — to be contd.
PI technique to compute $T = e^{M\Delta t}$ (contd.)

3. compute $T = (e^{M\tau})^\ell = (I + T_a)^\ell$

$$T = (I + T_a)^{2N} = (I + T_a)^{2^{N-1}} \times (I + T_a)^{2^{N-1}} = ...$$

with $(I + T_a)^2 = I + 2T_a + T_a \times T_a$.

Pseudo code

```
do $i = 1, ..., N$
    $T_a \leftarrow 2T_a + T_a \times T_a$
end do

$T \leftarrow I + T_a$
```

The algorithm holds the computational precision.
(1) Analytical solution under the linear representation of \( f(t) \)

- 1\(^{st}\) order Taylor approximation of \( f(t) \), i.e.,
  \[
  f = f_0 + (t - t_n)f_1, \quad t \in (t_n, t_{n+1})
  \]

- Integrate \( T\int_{t_n}^{t_{n+1}} e^{-sM}f(s)ds \) analytically

- Recursive form for \( X_{n+1} \):
  \[
  X_{n+1} = T\left[ X_n + M^{-1}(f_0 + M^{-1}f_1) \right] \\
  - M^{-1}\left[ f_0 + M^{-1}f_1 + f_1\Delta t \right]
  \]

*compute \( M^{-1} \)? It is *noninvertible* generally!
Evaluating $T \int_{t_n}^{t_{n+1}} e^{-sM} f(s) ds \ & \text{the recursive formula (contd.)}$

(2) Recursive formula by using the Gaussian quadrature rule

- three-point Gaussian quadrature
- recursive form for $X_{n+1}$:

$$X_{n+1} = TX_n + \frac{5}{18} e^{\left(1+\sqrt{3/5}\right)M \Delta t/2} f \left[ t_n + \left(1 - \sqrt{3/5}\right) \Delta t/2 \right]$$

$$+ \frac{5}{18} e^{\left(1-\sqrt{3/5}\right)M \Delta t/2} f \left[ t_n + \left(1 + \sqrt{3/5}\right) \Delta t/2 \right]$$

$$+ \frac{8}{18} e^{M \Delta t/2} f \left( t_n + \Delta t/2 \right)$$
Remarks

\[ \frac{d\mathbf{X}}{dt} = \mathbf{M}\mathbf{X} + \mathbf{f}, \quad \mathbf{X} = [\mathbf{E}, \mathbf{H}]^T \]

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 \( \mathbf{E} \) and \( \mathbf{H} \) in time

Precise Integration
Numerical stability condition

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

PITD

Stability conditions vary for different orders of Taylor approximation:

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

Almost unconditionally stable for large \( N \).
Numerical dispersion analysis

FDTD numerical dispersion relation:

\[ \frac{W_t^2}{c^2} = W_x^2 + W_y^2 + W_z^2, \]

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

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

where \( \Lambda_{\text{PITD}} = \frac{c\Delta t}{\ell} \sqrt{W_x^2 + W_y^2 + W_z^2}. \)
Numerical dispersion analysis (contd.)

- numerical dispersion is slightly worse than that of FDTD
- independent of the time step
- dense gridding 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 $\Delta t^{\text{PITD}}$
- $\Delta t_{\text{upper bound}}^{\text{PITD}} > > \Delta t_{\text{upper bound}}^{\text{FDTD}}$
- slight worse numerical dispersion compared with that of the FDTD method
- numerical dispersion can be independent of $\Delta t$
- 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
- ...

Overview  Methods  Examples  Outlooks
Improved methods — PITD(4) \(^1\)

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

\(^1\)IEEE T-AP, 59(4), 2011: 1311-1320.
Improved methods — WG-PITD method

Discretization form of Maxwell equation(s) in space:

\[
\frac{d}{dt} E_{x|l+1/2,m,n} = -\frac{\sigma_{l+1/2,m,n}}{\varepsilon_{l+1/2,m,n}} E_{x|l+1/2,m,n} + \sum_i a_i \left[ \frac{H_{z|l+1/2,m+i+1/2,n}}{\varepsilon_{l+1/2,m,n} \Delta y} - \frac{H_{y|l+1/2,m,n+i+1/2}}{\varepsilon_{l+1/2,m,n} \Delta z} \right]
\]

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

Numerical dispersion

\[S_{11}\text{-parameter}\]

\(^2\)IEEE MWCL, 20(12), 2010: 651-653
Improved methods — Hybrid PITD-FDTD method

How to handle multiscale problems with fine geometrical features?

- Subgridding in FDTD — $\Delta t$ depends on $\Delta x_{\text{min}}$
- PITD — need to compute $e^{M\Delta t}$, but $\Delta t$ can be relaxed

$^3$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:

\[ X_{n+1} = e^{M\Delta t}X_n + \sum_i \alpha_i e^{M\beta_i\Delta t}f(t_n + \gamma_i\Delta t) \]

<table>
<thead>
<tr>
<th>number of nonzero elements</th>
<th>Denseness</th>
<th>Memory cost (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(M)</td>
<td>1558</td>
<td>0.0039</td>
</tr>
<tr>
<td>(e^{M\Delta t})</td>
<td>370482</td>
<td>0.9334</td>
</tr>
</tbody>
</table>

Evaluate \(e^{M\Delta t}\) explicitly? \(\times\) → Estimate \(e^{M\Delta t}v\) directly. \(\checkmark\)

⁴Please refer to OC2-6 (Tue. 08:30-10:00, Function Room 3, 3F)
Improved methods — Krylov space method\(^4\) (contd.)

**Direct estimation of** \(e^{M\Delta t}v\)

1. \(m\)\(^{th}\)-order Krylov subspace: \(K^m(M, v) = \text{span}(v, Mv, \ldots, M^{m-1}v)\)

2. Arnoldi process
   - \(V_m = [v_1, v_2, \ldots, v_m]^T\) — orthogonal basis of \(K^m\)
   - \(H_m \approx V_m^T MV_m\) — matrix generated during the Arnoldi process

3. \(e^{M\Delta t}v \approx V_m e^{H_m \Delta t} V_m^T v = V_m e^{H_m \Delta t} e_1, \quad e_1 = [1, 0, 0, \ldots, 0]^T \in \mathbb{R}^{m \times 1}\)

<table>
<thead>
<tr>
<th>Method</th>
<th>CPU time (s)</th>
<th>Memory cost (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Krylov-PITD</td>
<td>23.78</td>
<td>0.30</td>
</tr>
<tr>
<td>FDTD</td>
<td>137.28</td>
<td>1.34</td>
</tr>
</tbody>
</table>

\(^4\)Please refer to OC2-6 (Tue. 08:30-10:00, Function Room 3, 3F)
Rectangular cavity

<table>
<thead>
<tr>
<th>$f_{\text{ana.}}$ (GHz)</th>
<th>FDTD scheme $\Delta t = 1$ ps</th>
<th>ADI-FDTD scheme $\Delta t = 60$ ps</th>
<th>PITD scheme $\Delta t = 60$ ps</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$f$ (GHz)</td>
<td>rel. err.</td>
<td>$f$ (GHz)</td>
</tr>
<tr>
<td>3.125</td>
<td>2.983</td>
<td>4.54%</td>
<td>2.900</td>
</tr>
<tr>
<td>4.881</td>
<td>4.750</td>
<td>2.68%</td>
<td>4.650</td>
</tr>
<tr>
<td>5.340</td>
<td>5.450</td>
<td>2.06%</td>
<td>5.580</td>
</tr>
<tr>
<td>7.289</td>
<td>7.333</td>
<td>0.60%</td>
<td>6.817</td>
</tr>
<tr>
<td>7.529</td>
<td>7.567</td>
<td>0.51%</td>
<td>7.000</td>
</tr>
</tbody>
</table>

- 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

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

<table>
<thead>
<tr>
<th>Method</th>
<th>$\Delta x$</th>
<th>$\Delta y$</th>
<th>$\Delta z$</th>
<th>$\Delta t$</th>
<th>Memory</th>
<th>CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDTD</td>
<td>0.41 mm</td>
<td>0.26 mm</td>
<td>0.42 mm</td>
<td>0.441 ps</td>
<td>24.44 MB</td>
<td>1024 s</td>
</tr>
<tr>
<td>L-PITD</td>
<td>0.41 mm</td>
<td>0.26 mm</td>
<td>0.42 mm</td>
<td>0.884 ps</td>
<td>248.4 MB</td>
<td>851 s</td>
</tr>
</tbody>
</table>

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

Small antenna

Comparison between the FDTD method and the Krylov-PITD method

<table>
<thead>
<tr>
<th></th>
<th>CPU time (s)</th>
<th>Memory cost (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Krylov-PITD</td>
<td>23.78</td>
<td>0.30</td>
</tr>
<tr>
<td>FDTD</td>
<td>137.28</td>
<td>1.34</td>
</tr>
</tbody>
</table>

ICEF 2016 Xi’an — PITD
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

Acknowledgements

Dr. Jinquan Zhao, Mr. Min Tang, Ms. Mei Yang, Dr. Xintai Zhao, Dr. Gang Sun, Dr. Zhongming Bai, Dr. Qi Liu and Dr. Zhen Kang are kindly acknowledged.

References

- IEEE MWCL, 2007, 17(7): 471
- PIER, 2007, 69: 201
- IEEE T-MTT, 2008, 56(12): 2859
- IEEE T-MTT, 2012, 60(9): 2723
- COMPEL, 2013, 33(1/2): 85
- IEEE T-MTT, 2013, 61(7): 2535
- IEEE MWCL, 2016, 26(2): 83
Thank you!
Q & A.
Our **Group for Advanced Electrical Technologies (GAET)** is seeking for highly self-motivated students with the solid scientific strength in one of the following areas:

- Electromagnetics (theory and computation)
- Metamaterials and plasmonics (graphene plasmonics)
- Wireless power transfer
- Power electronics