Pseudo-Spectral Analytical Time Domain and PICSAR coupling.

H. Kallala

SMILEI training workshop
November 6-7, 2017
Maison de la Simulation
Table of content

1. Introducing PICSAR

2. Pseudo-Spectral method for Maxwell Equations

3. Coupling with Smilei

4. Hybrid Pseudo-Spectral Algorithm
PICSAR: Particle-In-Cell Scalable Resources

- Initially developed at LBNL
  - Now developed at LBNL and CEA Saclay.

- Designed to bring highly optimized routines to other PIC codes.

- Can also be used as a standalone framework to run HPC PIC simulations.

- https://picsar.net/
PICSAR is designed to be ported to the next generation of supercomputers.
Table of content

1. Introduction to PICSAR

2. Pseudo-Spectral method for Maxwell Equations

3. Coupling with Smilei

4. Hybrid Pseudo-Spectral Algorithm
Context And Challenges

❖ Many challenges arising in numerical plasma physics simulations:

• Recent advances in laser technology (PetaWatt laser project) and UHI physics.

• Relativistic collisionless shocks in astrophysics simulations [6].
These intense regimes of interaction may be challenging to model with standard PIC codes:

- High order Harmonics subject to important numerical dispersion.

- Numerical Cherenkov Effect (NCE) in relativistic simulations [1].

Different solutions in FDTD case solver include digital filtering and modifying dispersion relation [2].
To tackle these milestones we need to modify the Maxwell Solver algorithm.

\[
\begin{align*}
\frac{\partial \hat{E}}{\partial t} &= ic^2 \hat{k} \wedge \hat{B} - c^2 \mu_0 \hat{J} \\
\frac{\partial \hat{B}}{\partial t} &= -i \hat{k} \wedge \hat{E}
\end{align*}
\]
These equations can be integrated analytically in time, assuming a constant source during a timestep [3].

\[
E^{n+1} = CE^n + iSk \wedge B^n - \frac{S}{|k|} \hat{j}^{n+\frac{1}{2}} + \frac{k}{|k|^2} \left(\left(\frac{S}{dt|k|} - 1\right) \hat{\rho}^{n+1} - \left(\frac{S}{dt|k|} - C\right) \hat{\rho}^n\right)
\]

(1)

\[
B^{n+1} = CB^n - iSk \wedge E^n + i\frac{1-C}{|k|^2} \hat{k} \wedge \hat{j}^{n+\frac{1}{2}}
\]

(2)

\[
C' = \cos(|k|c dt) \quad S = \sin(|k|c dt)
\]
Pseudo-Spectral Solver for Maxwell Equations

- PSATD is totally dispersion free.
- No Courant–Friedrichs–Lewy condition on timestep.
- PSATD is poorly scalable due to large communications involved in multi-task FFT computation.
A novel approach has been proposed by Ji Vay et al by using finite but high order stencil derivative [3].

The derivative operator in spectral space can be approximated by its finite difference equivalent in an arbitrary order $p$ instead of infinite order derivative.

This enables solving Maxwell’s Equations locally with small numerical noise.

$$\mathbf{\hat{\nabla}}_p \Leftrightarrow \mathbf{\hat{k}}_p(k) = \frac{1}{dx} \sum_{i=1}^{p/2} 2c_i \sin(2\pi ik/N)$$

Ci : Fornberg coefficients
• With high but finite order stencil, Finite order PSATD solver is nearly dispersion free.
• Comparison between FDTD solver and PSATD-order 16 in vacuum
Pseudo-Spectral Solver for Maxwell Equations

• How does this work?

• Far from the board, spatial derivative is equivalent to its finite difference high order counterpart.

• Near the board, the stencil is truncated, introducing a spurious error acting as a source in ghost region [4]

• Truncation error decreases very quickly for high order stencil with reasonably few ghost cells p>>ng/2 [4]
Pseudo-Spectral Solver for Maxwell Equations

- Using finite order PSATD allows performing local Maxwell solve more accurately than FDTD or infinite order PSATD.
- Very high order solvers can be used with few ghost cells.
- Numerical dispersion and NCE are mitigated [5]
- Allowing scaling within fft-based solvers.
PSATD Scalability

- Weak Scaling:
  - Theta machine (ALCF)
  - KNL architecture
  - 64*64*64 cells per Mpi Task
  - 32 threads per Mpi Task
Table of content

1. Introduction to PICSAR

2. Pseudo-Spectral method for Maxwell Equations

3. Coupling with Smilei

4. Hybrid Pseudo-Spectral Algorithm
Smilei-PICSAR coupling

- Take advantage of optimized tools from PICSAR.
- Collaboration between open-source PIC codes projects.
- The PSATD solver is called from PICSAR and uses FFTW 3.3.4 or Intel MKL to perform FFTs.
Smilei-PICSAR coupling: Issues

- Parallelism issues due to different MPI-parallelization paradigms:
  - Hilbert curve based domain decomposition is unfit with spectral methods (need for a cartesian domain decomposition)
  - Extra array copies and communications are needed.
Table of content

1. Introduction to PICSAR

2. Pseudo-Spectral method for Maxwell Equations

3. Coupling with Smilei

4. Group communications and Scaling
Another approach exploiting multilevel parallelism is under investigation:

- 2-level domain decomposition:
  - First level: Coarse Decomposition
    - Large subdomain containing many mpi-tasks
  - Second level: Fine Decomposition
    - Small subdomain containing one mpi-task
- Performing multi-task FFT under each coarse domain using FFTW_MPI
Pseudo-Spectral Solver for Maxwell Equations

• Extra-Communications between adjacent groups

• Different ghost cell sizes for Fields related and Particles related computations.
  
  • Larger communication for Field when using high order solver
  
  • Particle Ghost cell size = Interpolation order + 1
Pseudo-Spectral Solver for Maxwell Equations

• Decrease errors due to stencil truncation in Maxwell Solve.[4]

• Spurious MPI-ALLTOALL communications are avoided by using “FFTW-MPI_Transpose” plans, to improves scalability.

• But can lead to particle load unbalance within each MPI domain.
Conclusion

- Smilei can call PSATD solver from PICSAR in future release.
- Collaboration between Open Source PIC codes.
- Hybrid Pseudo spectral Solver can be added later in Smilei.

