Pseudo-Spectral Analytical Time Domain and PICSAR coupling.

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PICSAR: Particle-In-Cell Scalable Ressources

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

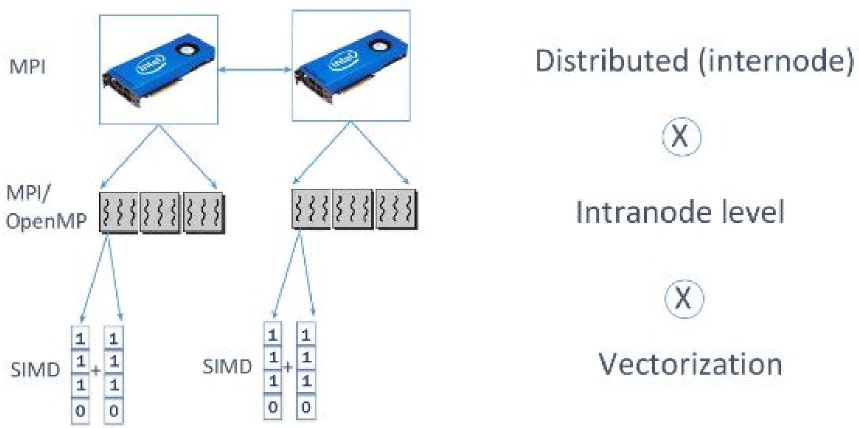
- Designed to bring highly optimized routines to other PIC codes.

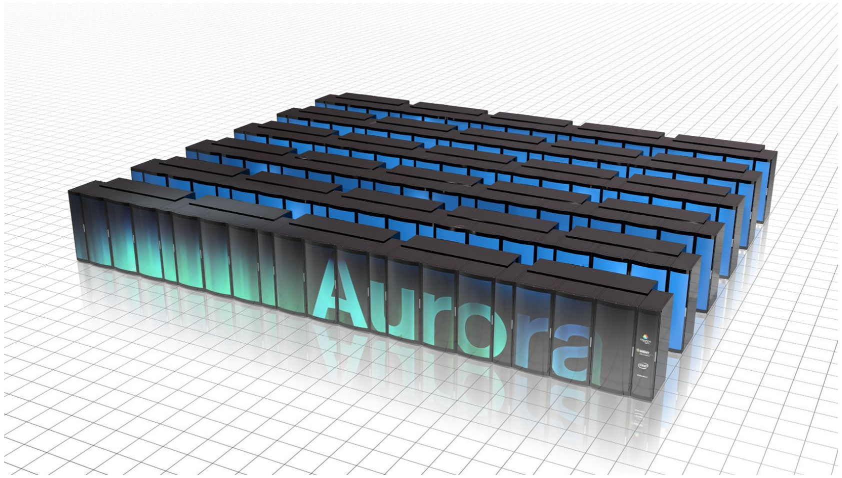
- Can also be used as a standalone framework to run HPC PIC simulations.

- https://picsar.net/

PICSAR: Particle-In-Cell Scalable Ressources

- PICSAR is designed to be ported to the next generation of supercomputers.





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Context And Challenges

❖ Many challenges arising in numerical plasma physics simulations:

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

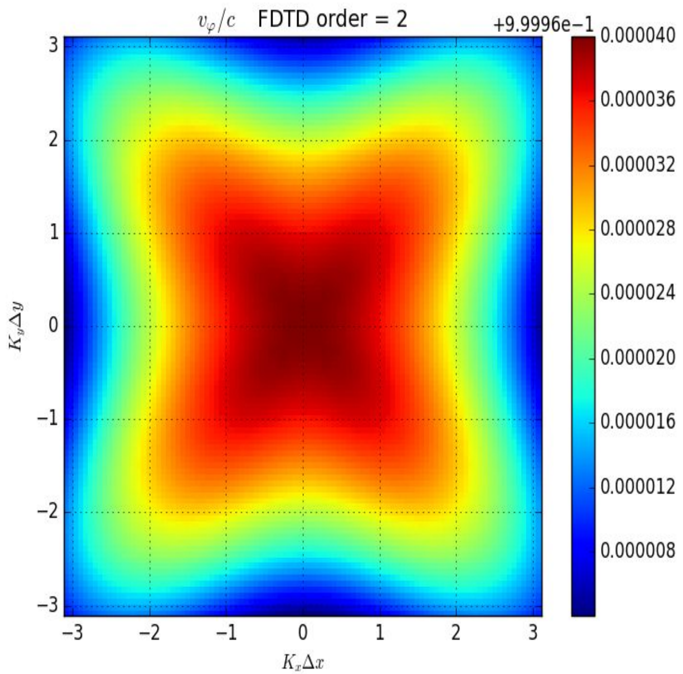
- Relativistic collisionless shocks in astrophysics simulations [6] .

Context And Challenges

❖ 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].

Pseudo-Spectral Solver for Maxwell Equations

❖ To tackle these milestones we need to modify the Maxwell Solver algorithm

$$\frac{\partial \hat{E}}{\partial t} = ic^2\vec{k} \wedge \hat{B} - c^2\mu_0\hat{J}$$

$$\frac{\partial \hat{B}}{\partial t} = -i\vec{k} \wedge \hat{E}$$

Pseudo-Spectral Solver for Maxwell Equations

❖ These equations can be integrated analytically in time, assuming a constant source during a timestep [3].

$$E^{n+1} = CE^n + iS\vec{k} \wedge B^n - \frac{S}{|k|}\hat{J}^{n+\frac{1}{2}} + \frac{\vec{k}}{|k^2|}((\frac{S}{dt|k|} - 1)\hat{\rho}^{n+1} - (\frac{S}{dt|k|} - C)\hat{\rho}^n)$$

(1)

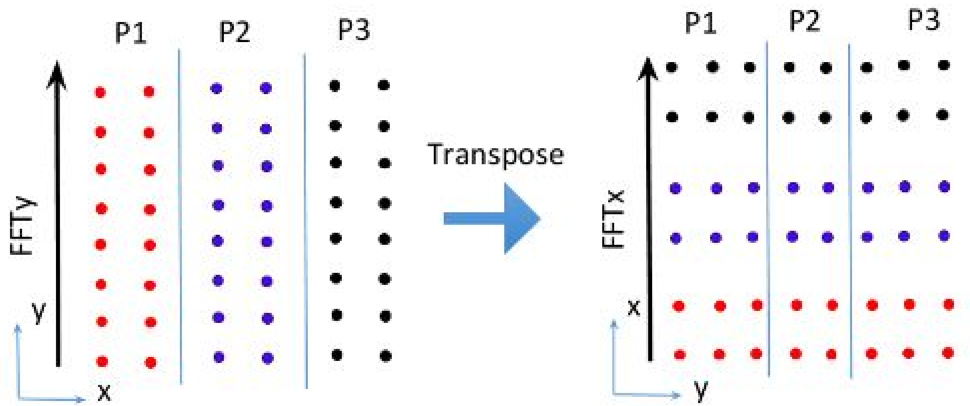
$$B^{n+1} = CB^n - iS\vec{k} \wedge E^n + i\frac{1-C}{|k|^2}\vec{k} \wedge \hat{J}^{n+\frac{1}{2}}$$

(2)

$$C = cos(|k|cdt) \qquad S = sin(|k|cdt)$$

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.



Pseudo-Spectral Solver for Maxwell Equations

- 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

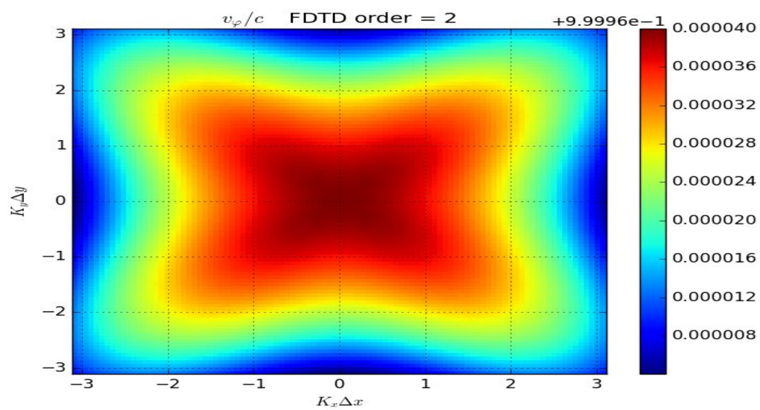
- This enables solving Maxwell's Equations locally with small numerical noise

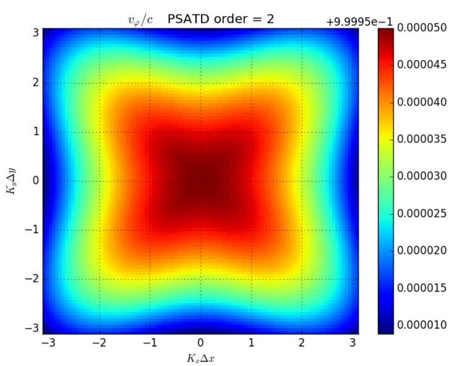
$$\vec{\nabla}_p \Leftrightarrow \vec{k}_p(k) = \frac{1}{dx}\sum_{i=1}^{p/2} 2c_i sin(2\pi ik/N)$$

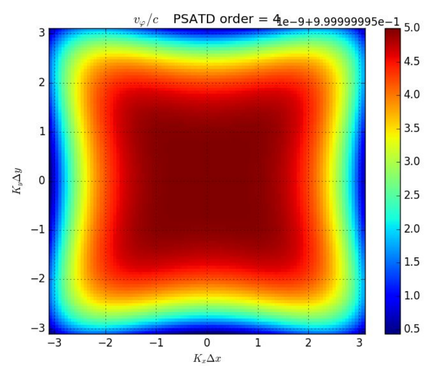
Ci : Fornberg coefficients

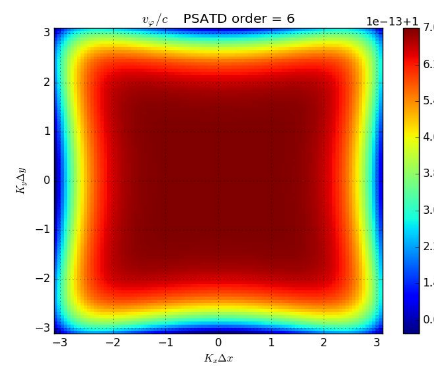
PSATD dispersion

- With high but finite order stencil, Finite order PSATD solver is nearly dispersion free.



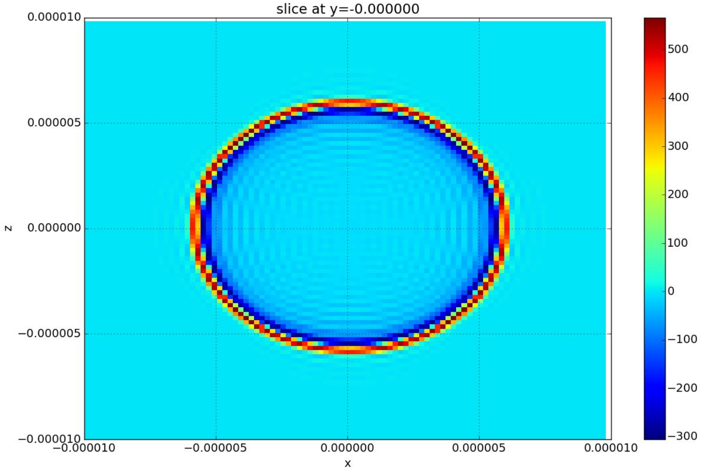


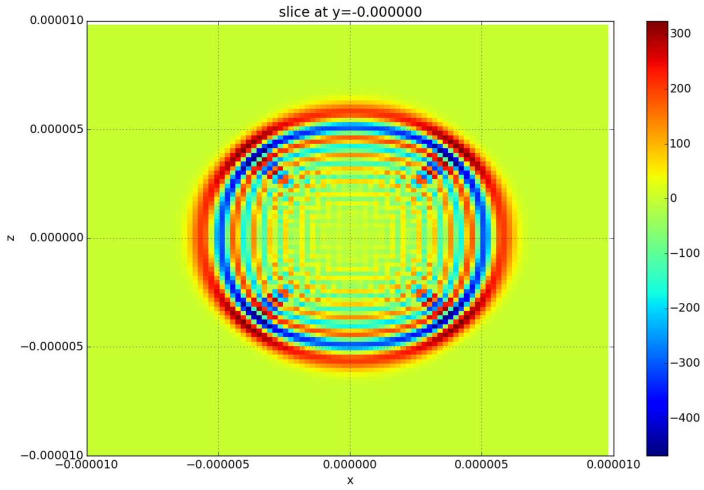




PSATD dispersion

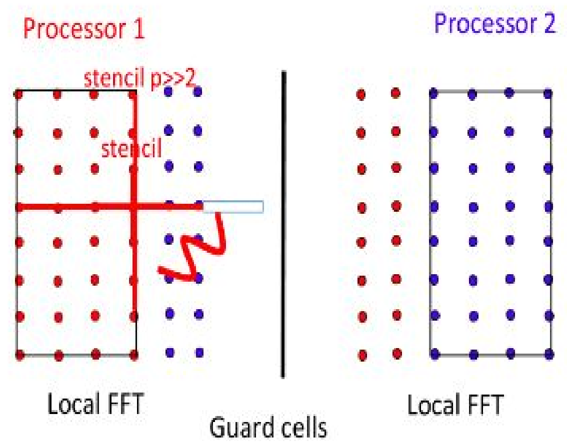
- Comparison between FDTD solver and PSATD-order 16 in vaccum





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]

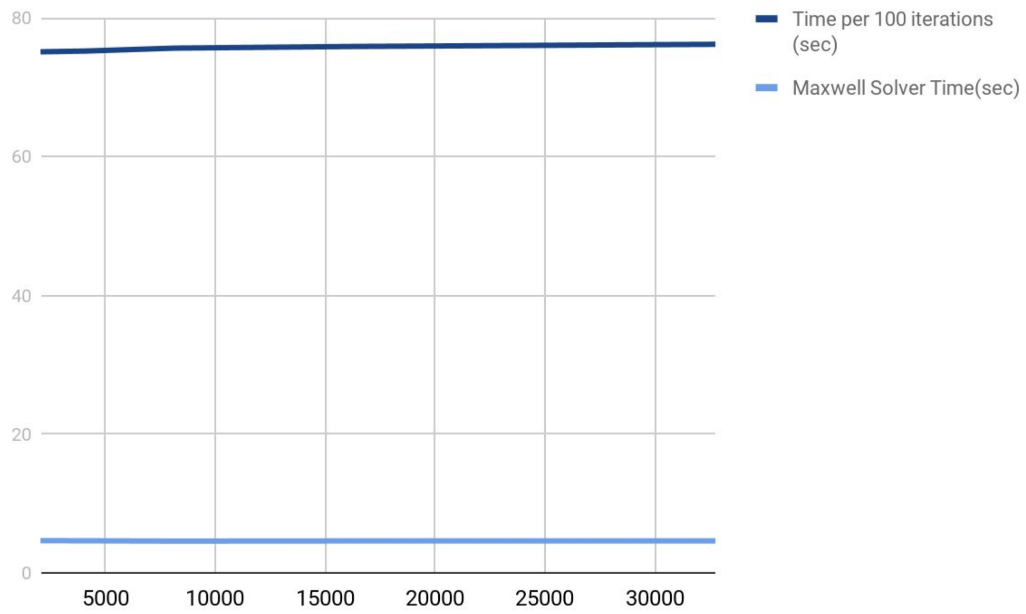


Pseudo-Spectral Solver for Maxwell Equations

- 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



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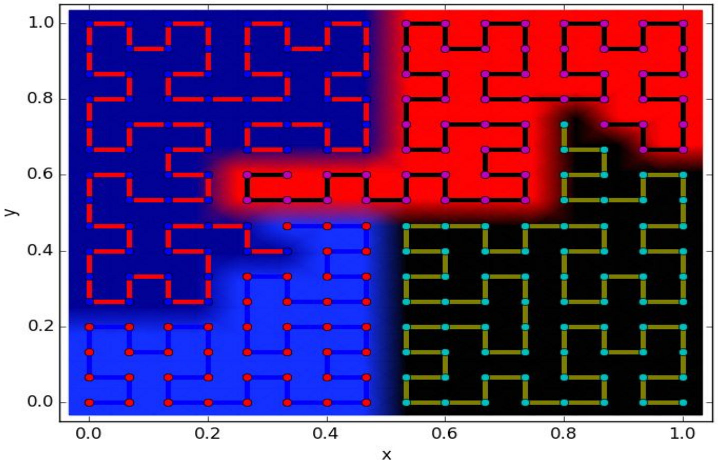
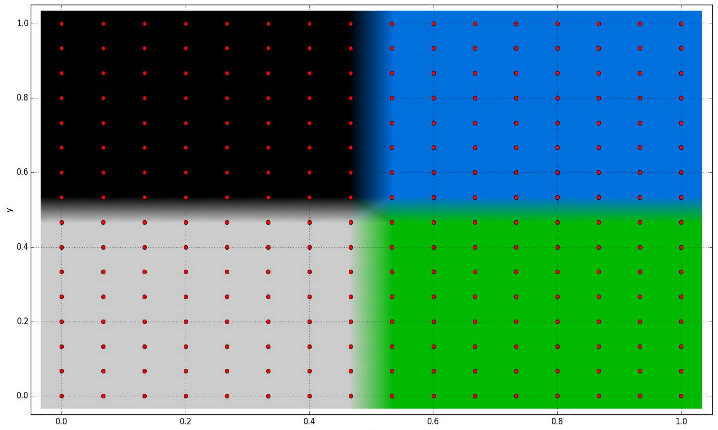
Smilei-PICSAR coupling

- 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.





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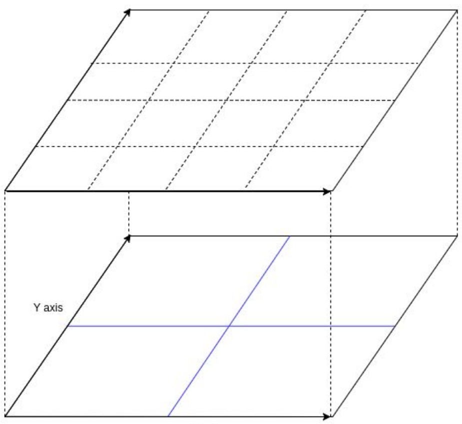
Pseudo-Spectral Solver for Maxwell Equations

- ❖ 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.

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