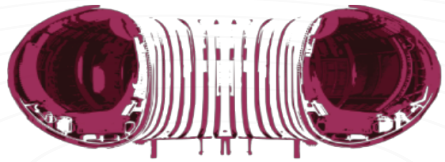

EFTC 2017

# The Particle-In-Fourier (PIF) Approach Applied to Gyrokinetic Simulations

European Fusion Theory Conference, Athens

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CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

# Outline



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1. Introduction
2. Model implementation
3. Precision of physical results
   - Linear simulations
   - Non-linear simulations
4. Numerical performance
5. Conclusion

# Motivation



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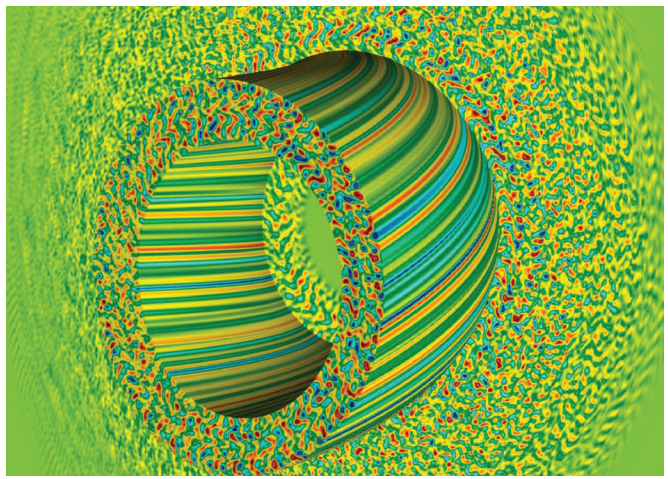
Legacy code ORB5 [Tran, 1999, Jolliet, 2009] includes 20 years of developments from tens of physicists.

How to adapt it to emerging supercomputing platforms?

- Develop a simplified test-bed embedding main kernels
- Modularize data structures for easier maintenance
- Optimize those kernels for different architectures (such as GPUs)
- Investigate alternative numerical models (PIF approach instead of PIC)

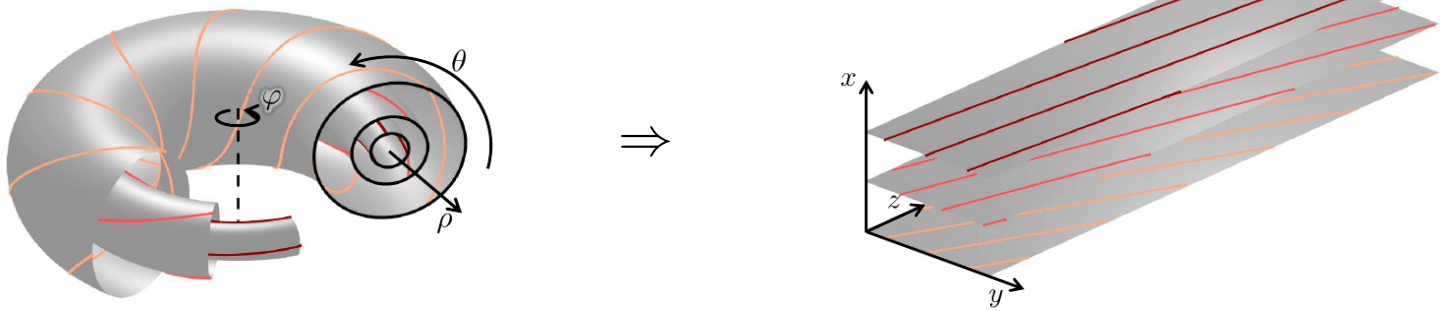


[Fasoli, 2016]

# GK-engine features



- Physics:
  - Gyrokinetic equations of particle motion
  - Slab geometry
  - Sheared magnetic field




  - Electrostatic, collisionless instabilities
  - Adiabatic electrons

- Numerics:
  - $\delta f$ representation of distribution function
  - Runge-Kutta of fourth order time integrator
  - Intra-node multi-threading with OpenMP or OpenACC
  - Inter-node MPI communication with domain decomposition and cloning

# Particle and field representations

- Marker discretization:

$$\delta f(\mathbf{R}, v_{/\!/}, \mu, t) = \sum_{p=1}^{N_p} \frac{m}{2\pi B^{\star}_{/\!/}} w_p(t) \delta\big(\mathbf{R} - \mathbf{R}_p(t)\big) \delta\big(v_{/\!/} - v_{/\!/p}(t)\big) \delta\big(\mu - \mu_p\big)$$

- B-spline field representation (PIC method):

$$\phi(x, y, z) = \sum_{i=1}^{N_x+p} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} \phi_{ijk} \Lambda_i(x) \Lambda_j(y) \Lambda_k(z)$$

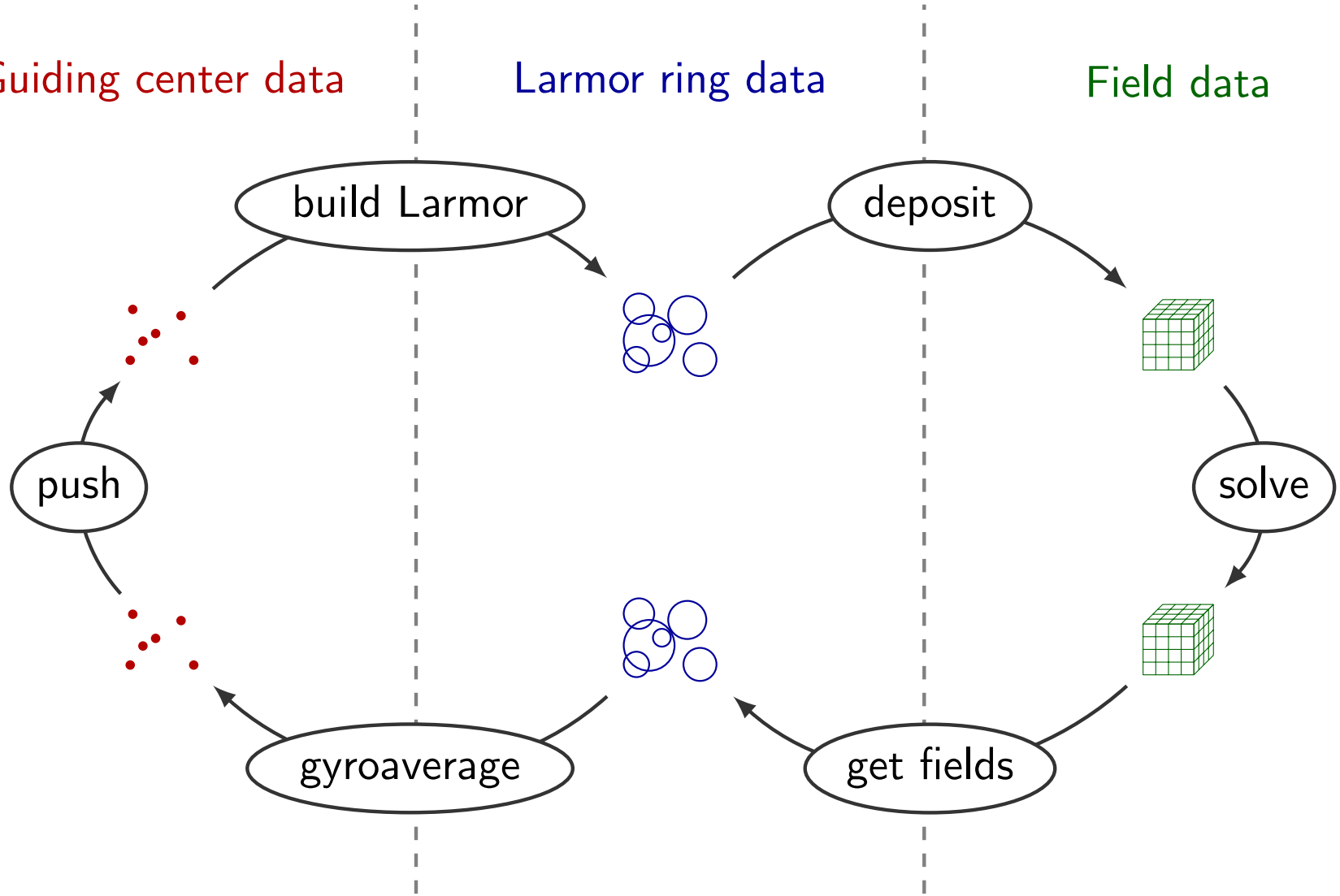
- Fourier mode field representation (PIF method):

$$\phi(x, y, z) = \sum_{i=1}^{N_x+p} \sum_{n=n_{\min}}^{n_{\max}} \sum_{m=-nq_i-\Delta m}^{-nq_i+\Delta m} \tilde{\phi}_{imn} \Lambda_i(x) e^{2\pi \mathrm{i}(my/L_y + nz/L_z)}$$

- Field aligned $\Leftrightarrow$ $k_{/\!/} \sim 0$ $\Leftrightarrow$ $m + nq(x) \sim 0$

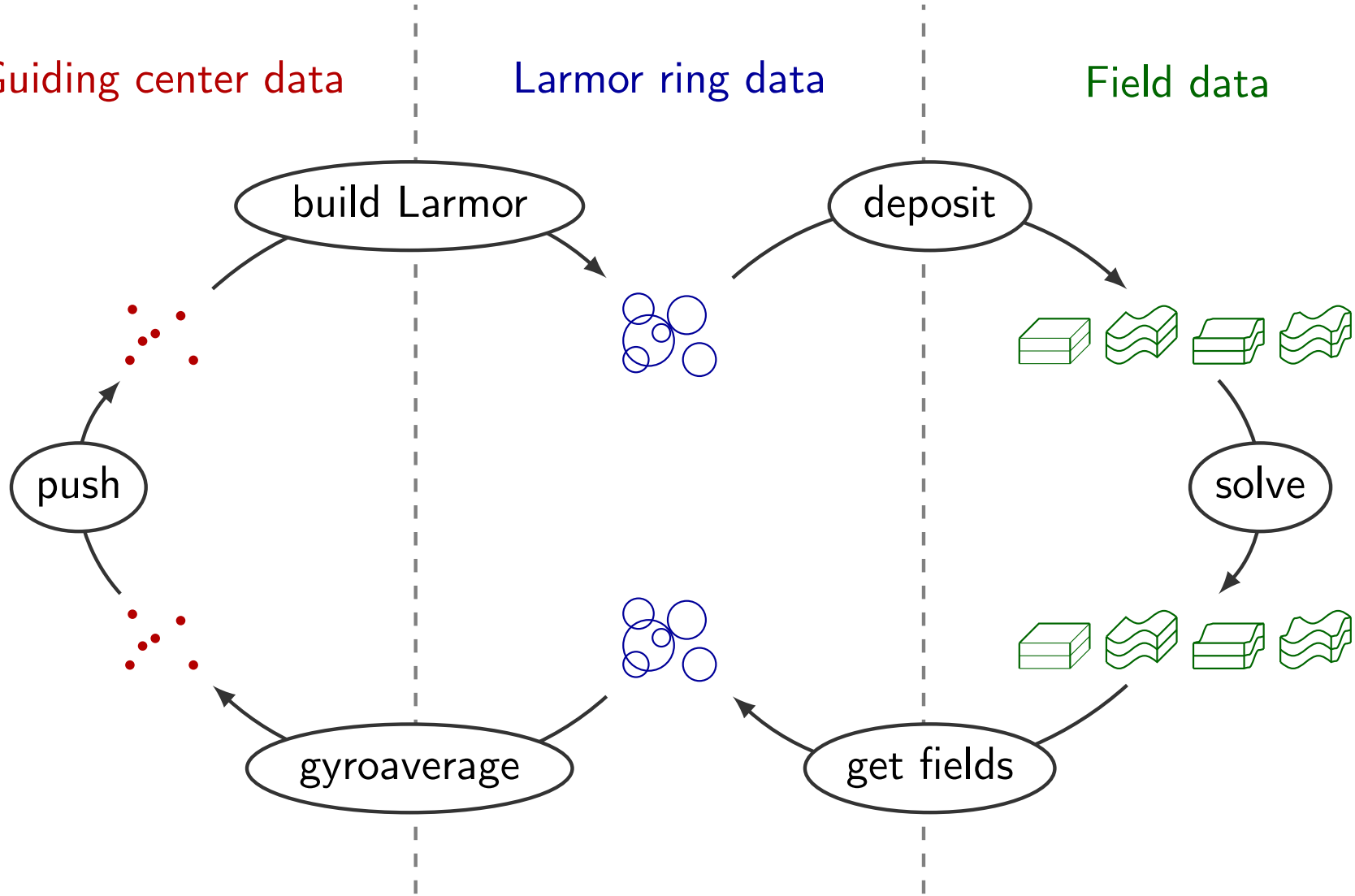
# Stages of a time step





# Stages of a time step

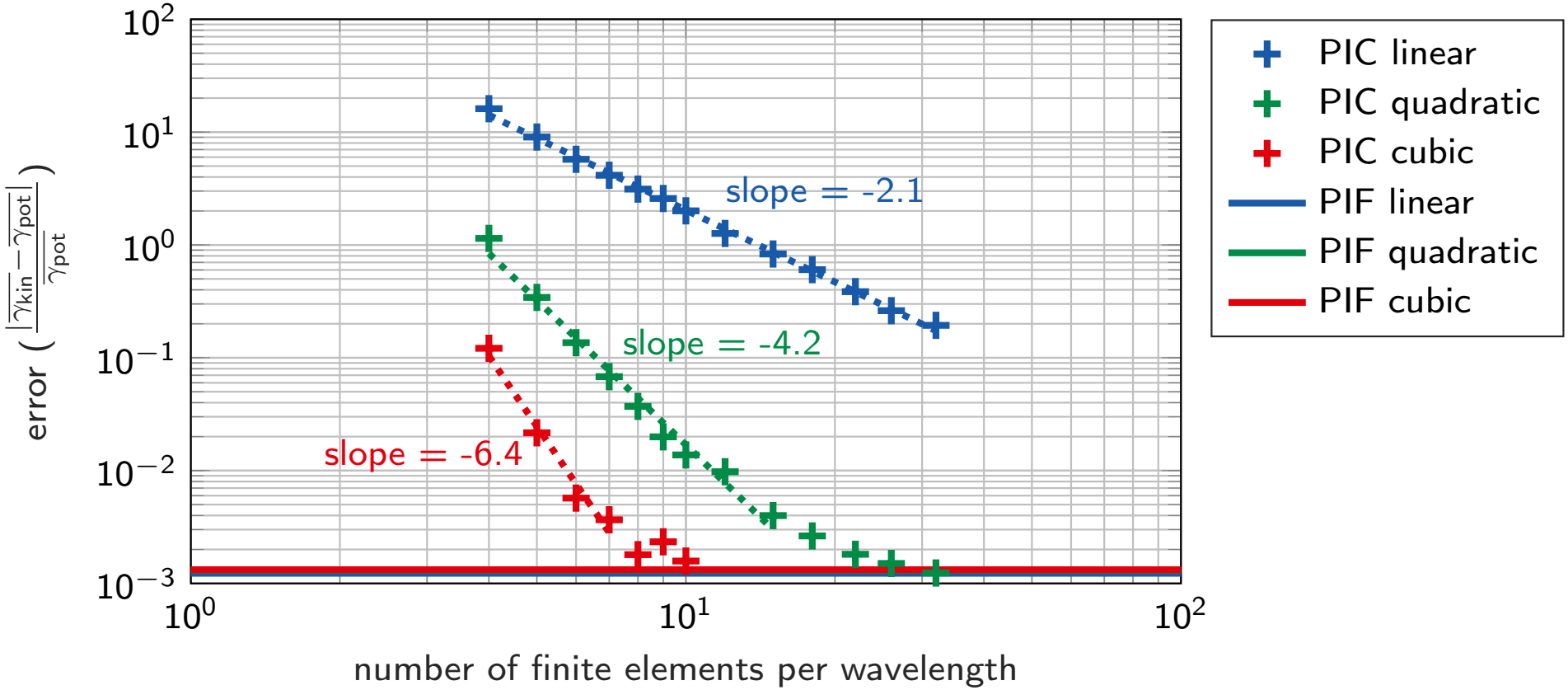




# Energy conservation



- Single Ion-Temperature-Gradient (ITG) mode $(m, n) = (-49, 35)$ (physical parameters from [Görler, 2016])
- Convergence with number of finite elements versus PIF:




- The saturation level depends on the other parameters.

# Energy conservation



- Single Ion-Temperature-Gradient (ITG) mode $(m, n) = (-49, 35)$ (physical parameters from [Görler, 2016])
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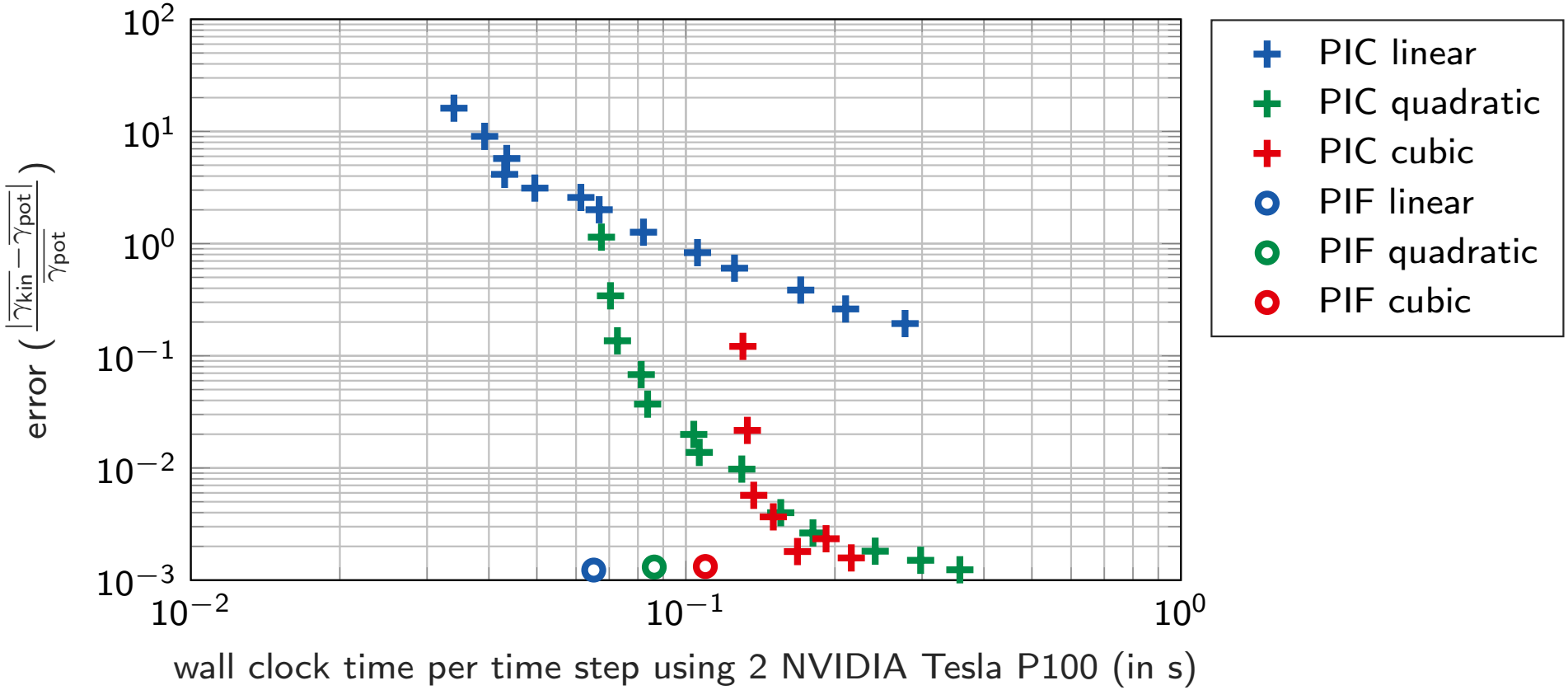
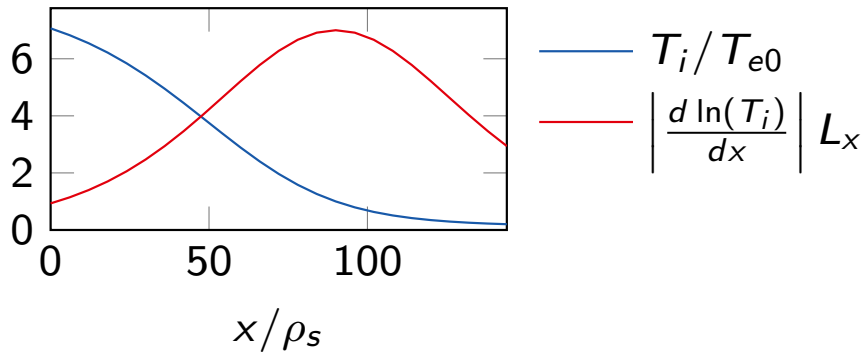



- The saturation level depends on the other parameters.

# ITG turbulence

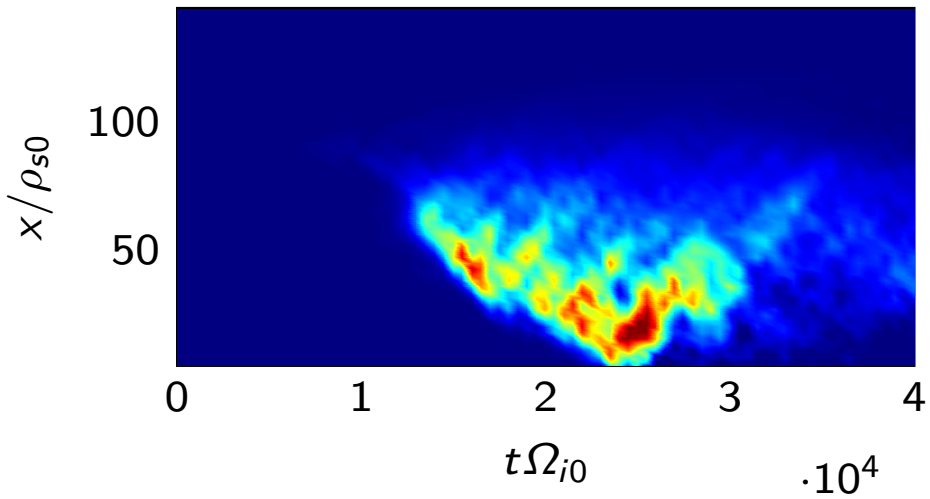


- ITG non-linear simulation

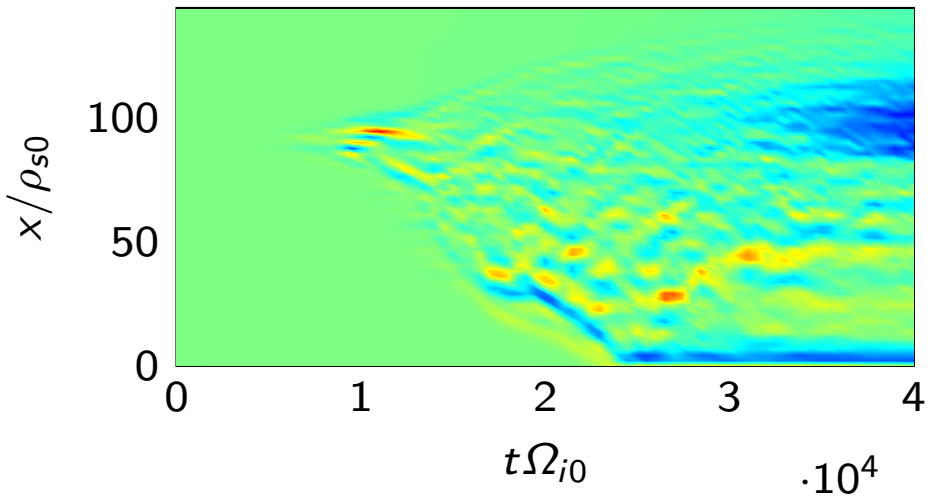



- Full Fourier spectrum (15 toroidal modes times 11 poloidal modes)
- PIC method:

Heat flux




Zonal flow shearing rate

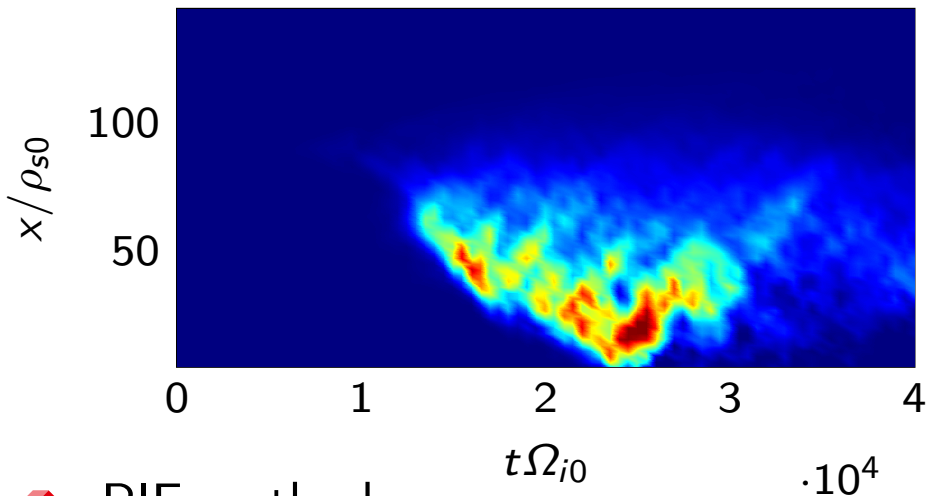


# ITG turbulence

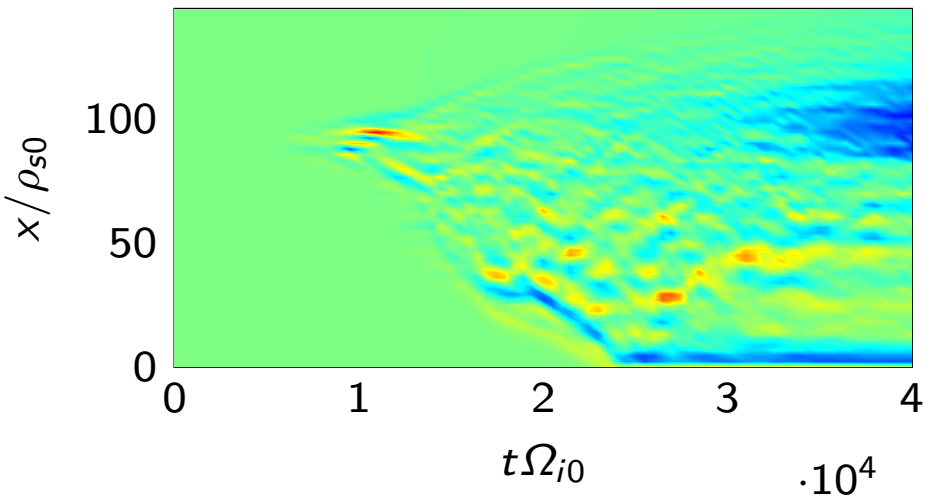


- PIC method:

Heat flux

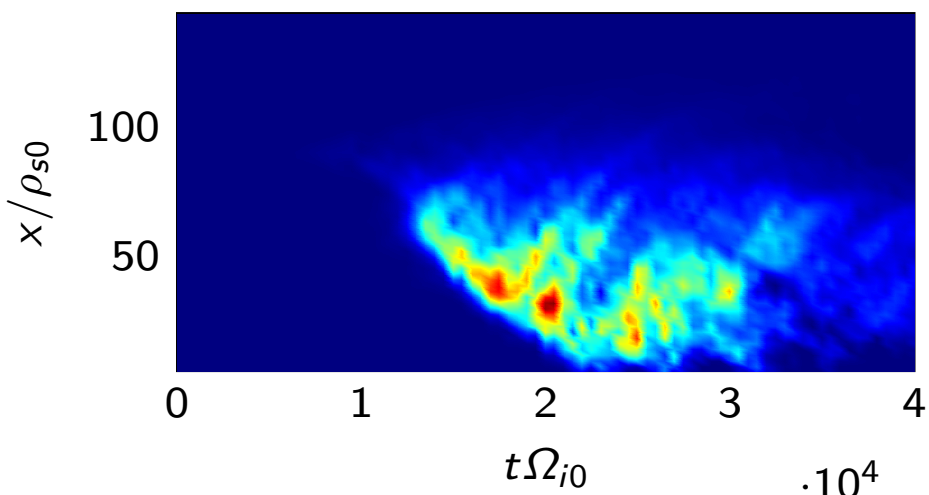



Zonal flow shearing rate

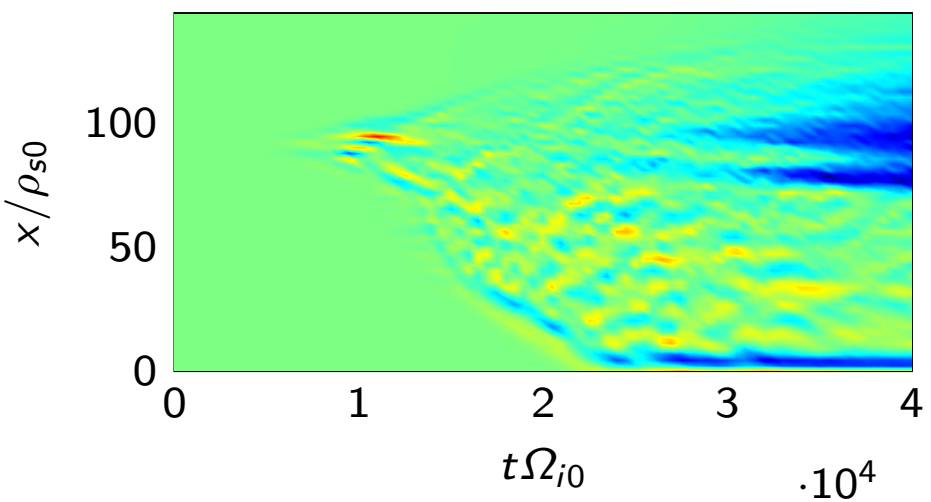



- PIF method:

Heat flux

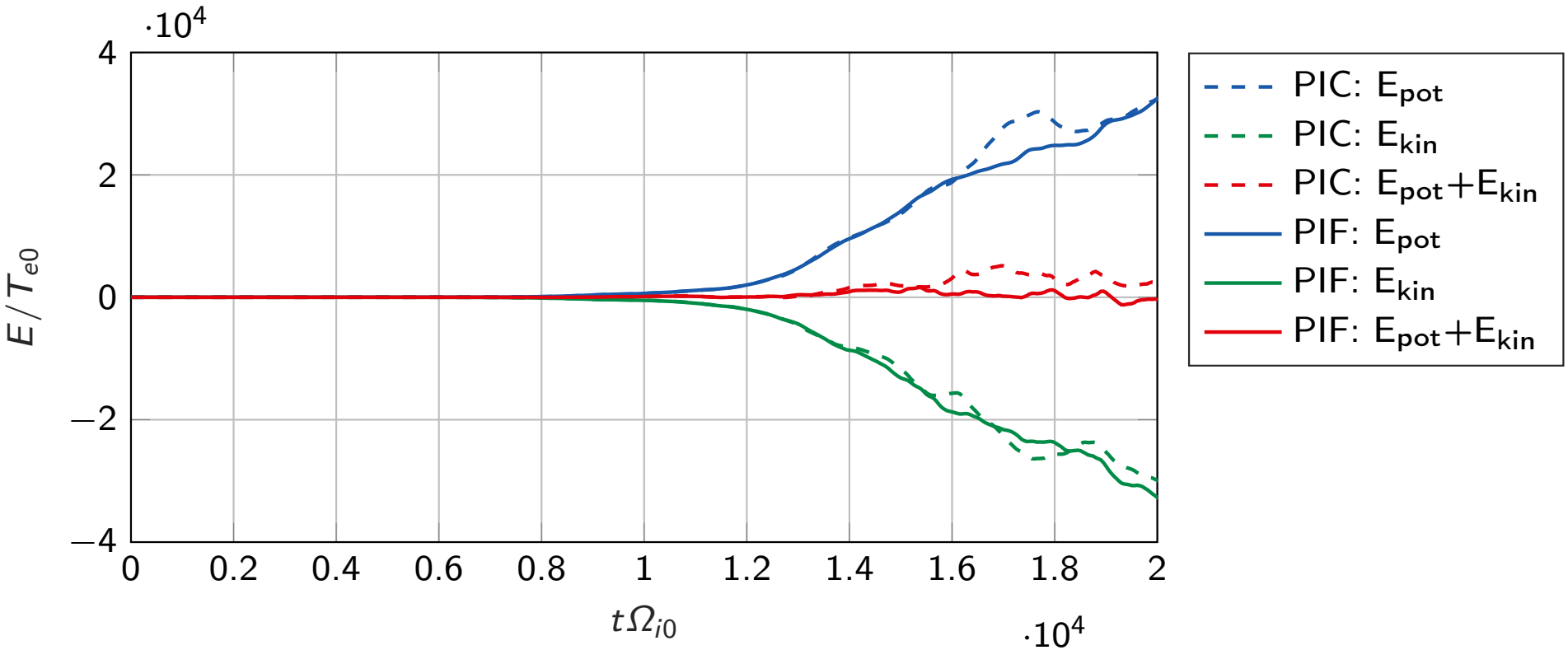



Zonal flow shearing rate



# Energy conservation

- Check energy conservation over time:




- Error with PIF method always lower than with PIC

# Scanning number of toroidal modes



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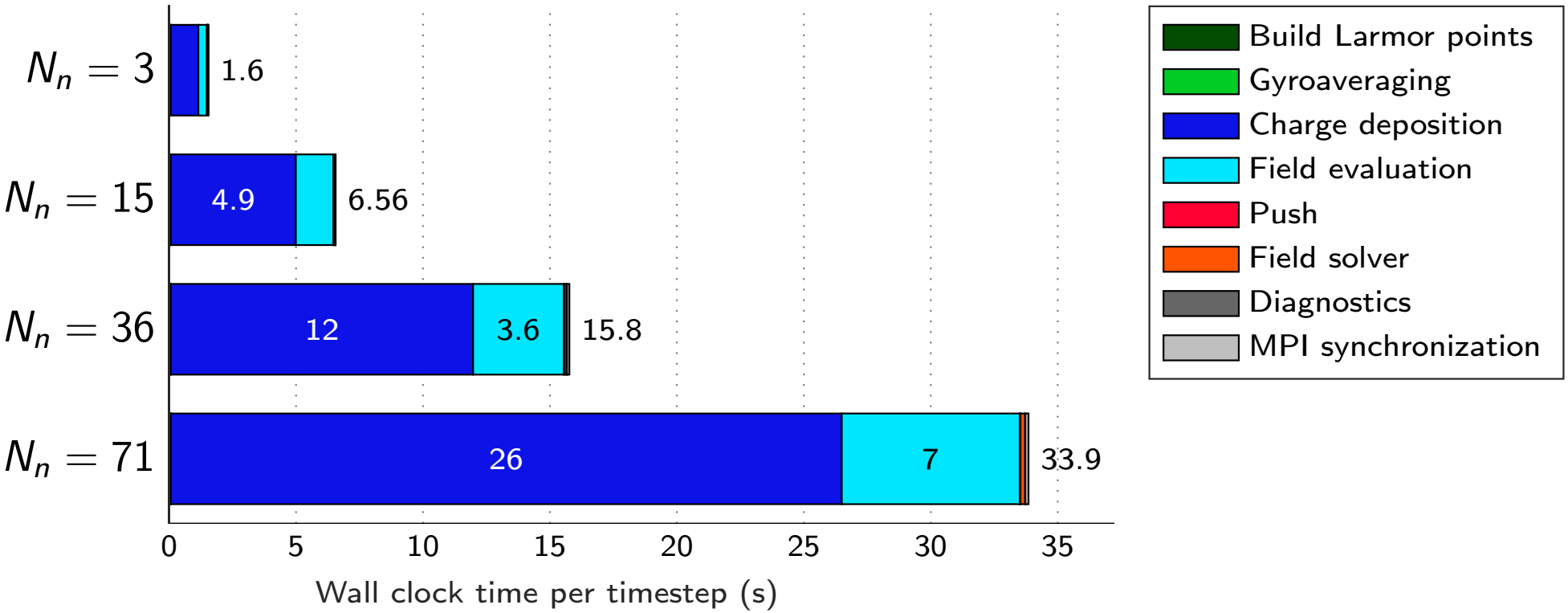
- PIF, 32 GPUs (NVIDIA Tesla P100), 128M particles, 128 radial cells, $N_m = 11$




- Wall clock time roughly proportional to $N_n$

# Parallel scaling of PIC on CPU



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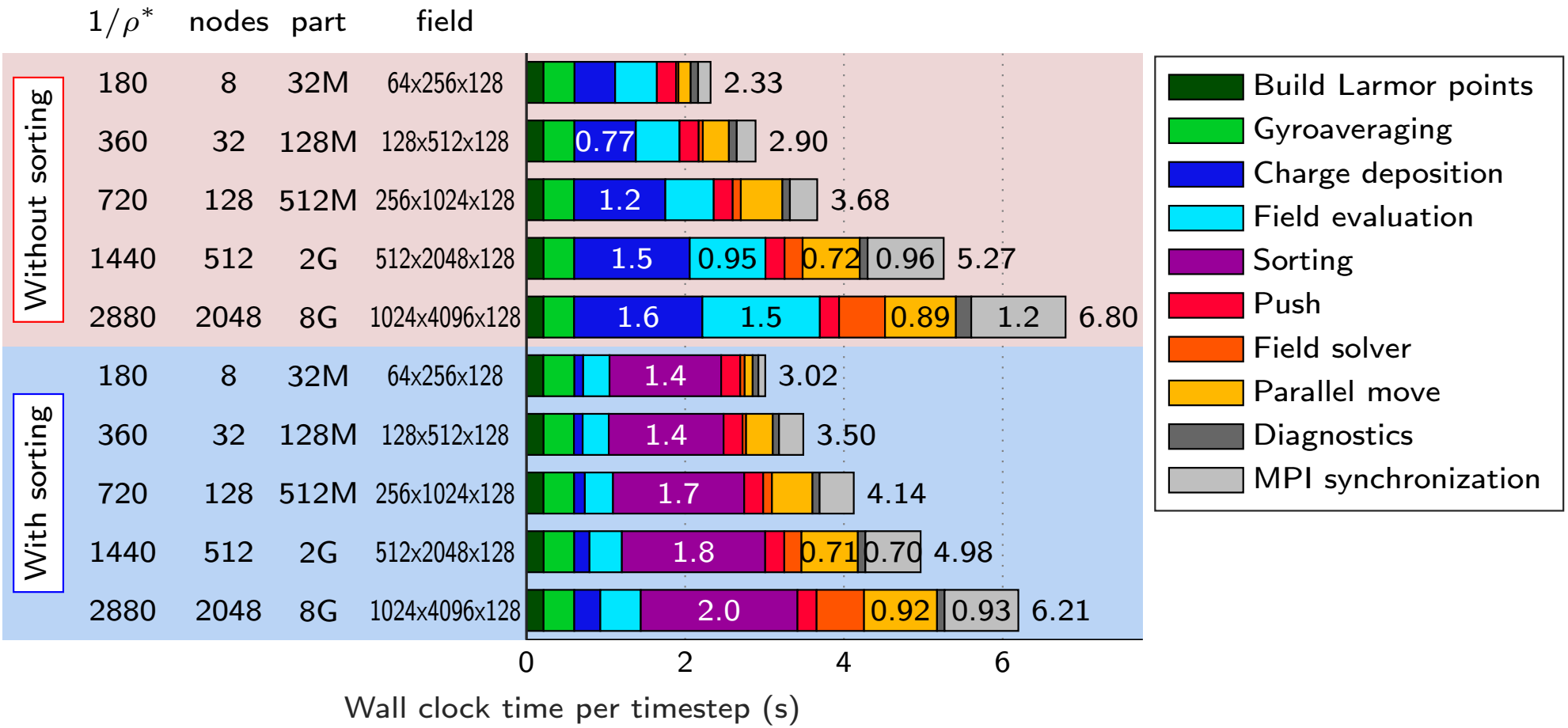
- $\rho^*$ scan, PIC, quad. splines, 12 OpenMP threads per node

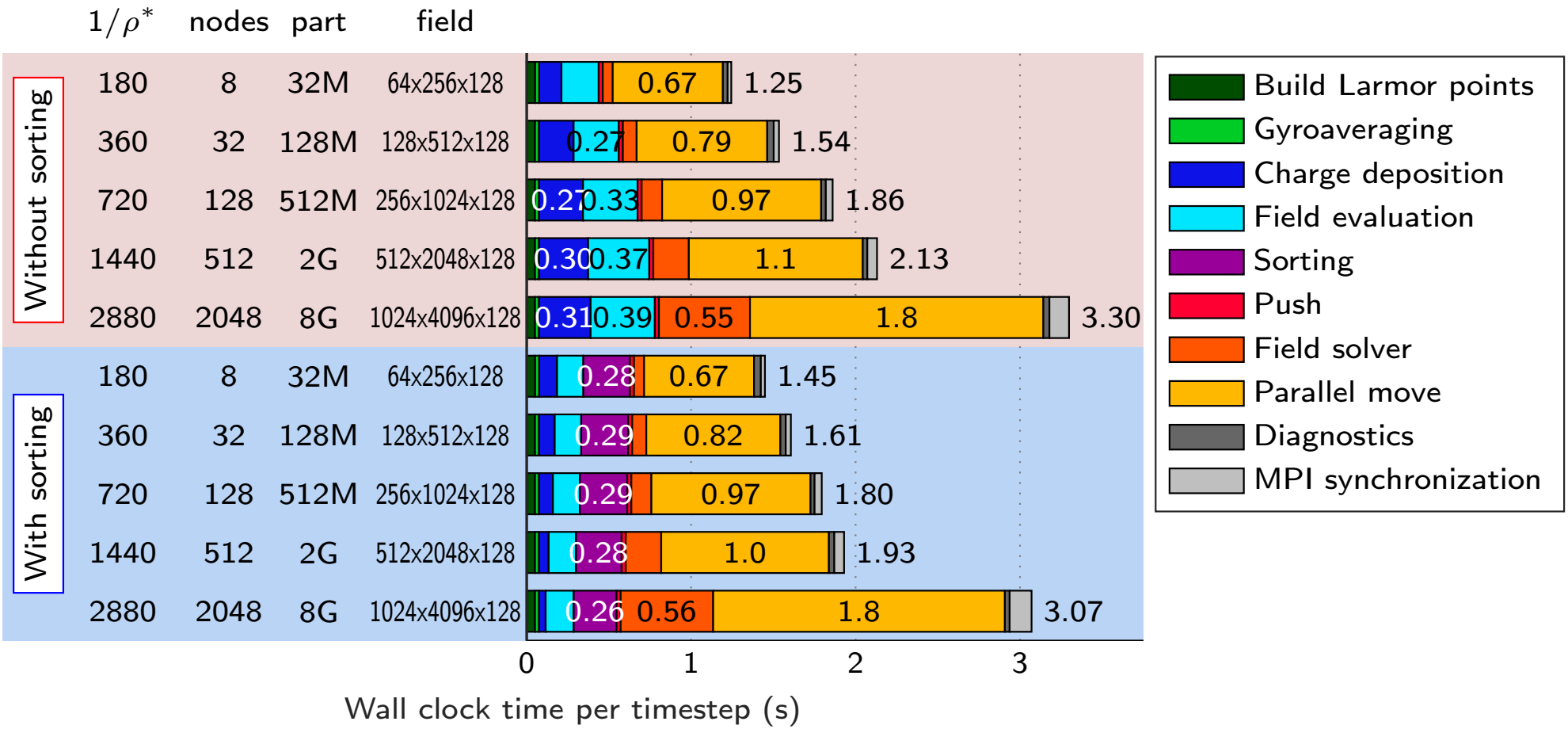



- Number of particle per cell decreases with system size ⇒ sorting can help

# Parallel scaling of PIC on GPU



- $\rho^*$ scan, PIC, quad. splines, 1 GPU per node




- Parallel communication becomes the bottleneck

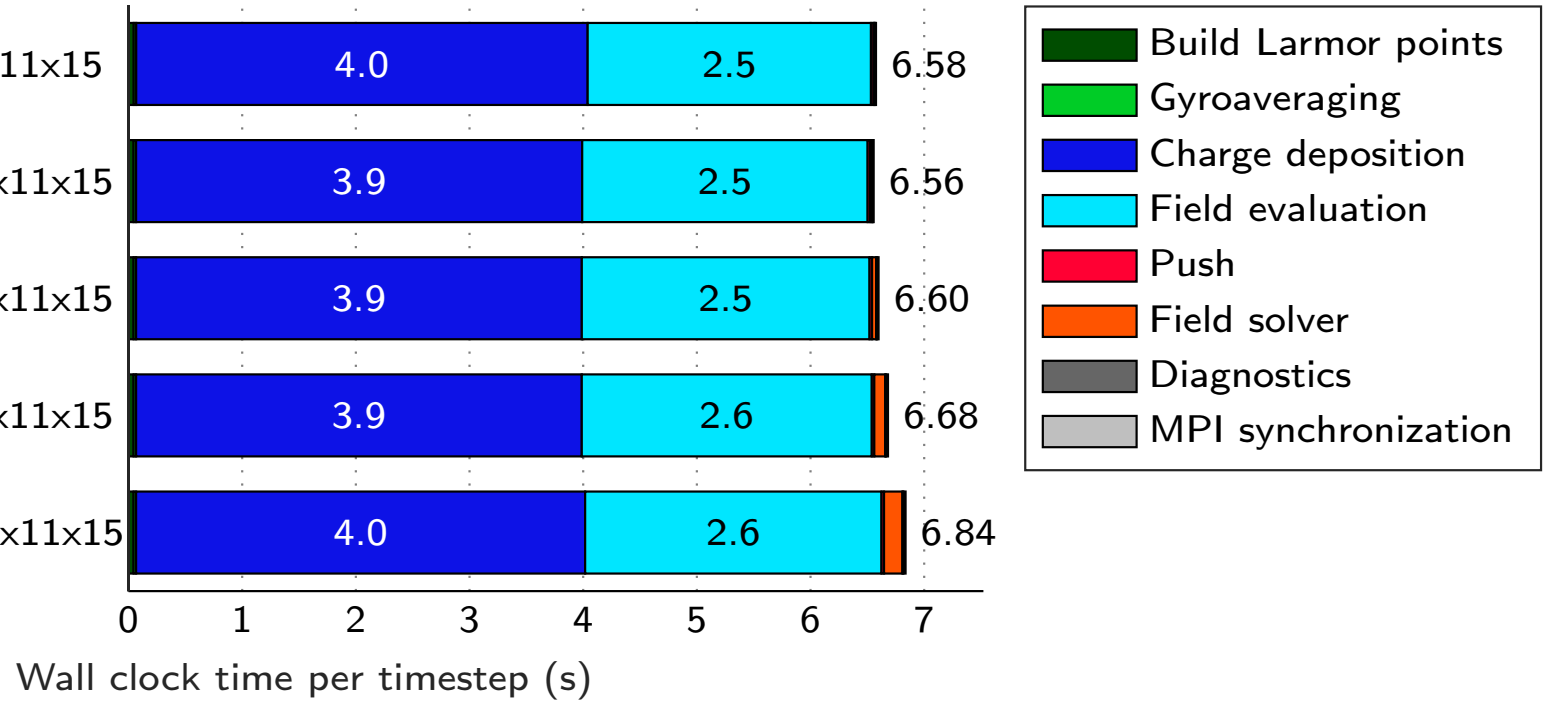
# Parallel scaling of PIF on GPU





- $\rho^*$ scan, PIF, quadratic splines, 1 GPU per node

| $1/\rho^*$ | nodes | part | field |
|---|---|---|---|
| 180 | 8 | 32M | 64x11x15 |
| 360 | 32 | 128M | 128x11x15 |
| 720 | 128 | 512M | 256x11x15 |
| 1440 | 512 | 2G | 512x11x15 |
| 2880 | 2048 | 8G | 1024x11x15 |




- Non-scalable part is negligible

# Conclusion





- What to take home:
  - **CPU or GPU**: GPU is 2-4 times faster than CPU for PIC (on Piz Daint machine), and essential for PIF.
  - **Spline order**: choice for best time-to-solution depends on required precision.
  - **PIC or PIF**: PIF is more precise than PIC, but can be slower if many Fourier modes are kept.
- Future work:
  - Make ORB5 run on GPU, and see if PIF approach can be used to study mode-to-mode coupling.

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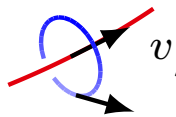
  Intercode comparison of gyrokinetic global electromagnetic modes
  *Physics of Plasmas*, 23(7), 072503, 2016

# Vlasov-Maxwell system of equations



- Distribution function:

$$f = f_0(\mathbf{R}, v_{/\!/}, \mu) + \delta f(\mathbf{R}, v_{/\!/}, \mu, t)$$




- Vlasov:

$$\frac{df}{dt} = 0 \quad \Rightarrow \quad \frac{d\,\delta f}{dt} = -\frac{d\mathbf{R}}{dt} \cdot \frac{\partial f_0}{\partial \mathbf{R}} - \frac{dv_{/\!/}}{dt} \frac{\partial f_0}{\partial v_{/\!/}}$$

- Equations of motion:

$$\frac{d\mathbf{R}}{dt} = \underbrace{v_{/\!/}\mathbf{b}}_{\text{parallel motion}} + \underbrace{\frac{\mu}{eB^\star_{/\!/}}\mathbf{b} \wedge \boldsymbol{\nabla} B}_{\boldsymbol{\nabla} B \text{ drift}} + \underbrace{\frac{1}{B^\star_{/\!/}}\mathbf{b} \wedge \boldsymbol{\nabla}\langle\phi\rangle}_{\mathbf{E}\wedge\mathbf{B} \text{ drift}}$$

$$\frac{dv_{/\!/}}{dt} = -\frac{e}{m}\mathbf{b} \cdot \boldsymbol{\nabla}\langle\phi\rangle$$

$$\frac{d\mu}{dt} = 0$$

- Quasi-neutrality equation:

$$\int \frac{n_0 e}{T_e}(\phi - \bar{\phi})\eta \; d^3\mathbf{x} + \int \frac{m}{eB^2} n_0 \boldsymbol{\nabla}_\perp \phi \cdot \boldsymbol{\nabla}_\perp \eta \; d^3\mathbf{x} = \int \delta f \langle\eta\rangle \; d^3\mathbf{x} \; d^3\mathbf{v}$$

# Power balance



- Balance equation $\frac{d\mathcal{E}_{\text{pot}}}{dt} = -\frac{d\mathcal{E}_{\text{kin}}}{dt}$
  - Potential energy $\mathcal{E}_{\text{pot}} = \int \frac{1}{2} e\langle\phi\rangle f \; d^3\mathbf{x} \; d^3\mathbf{v}$
  - Kinetic energy $\mathcal{E}_{\text{kin}} = \int \left(\frac{1}{2} m v_{/\!/}^2 + \mu B\right) f \; d^3\mathbf{x} \; d^3\mathbf{v}$
- Linear growth rate
  - $\gamma_{\text{pot}} = \frac{1}{2} \frac{d \ln(\mathcal{E}_{\text{pot}})}{dt}$ computed by finite difference in time
  - $\gamma_{\text{kin}} = \frac{-1}{2\mathcal{E}_{\text{pot}}} \frac{d\mathcal{E}_{\text{kin}}}{dt}$ computed instantaneously at each timestep

# Exponential computation



**Algorithm 1** Explicit method

**for** $n \in [n_{\min}, n_{\max}]$ **do**
  einz = $\exp(2\pi \mathrm{i} n z / L_z)$
  **for** $m \in [-nq - \Delta m, -nq + \Delta m]$ **do**
    eimy = $\exp(2\pi \mathrm{i} m y / L_y)$
    ... = ...$\times$ eimy $\times$ einz
  **end for**
**end for**

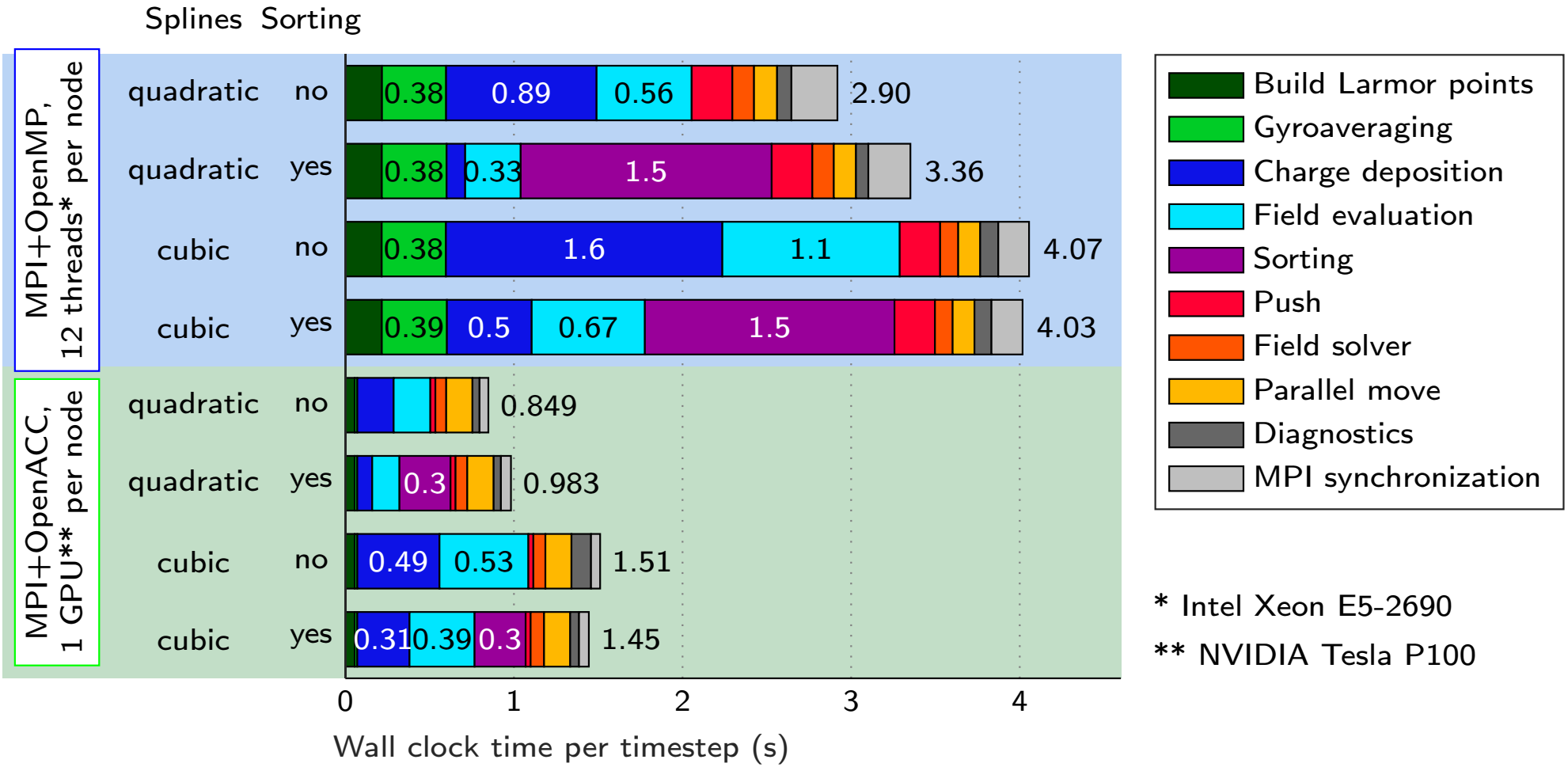
**Algorithm 2** Prefactor method

eiz = $\exp(2\pi \mathrm{i} z / L_z)$
einz = eiz^$n_{\min}$
**for** $n \in [n_{\min}, n_{\max}]$ **do**
  eiy = $\exp(2\pi \mathrm{i} y / L_y)$
  eimy = eiy^$(-nq - \Delta m)$
  **for** $m \in [-nq - \Delta m, -nq + \Delta m]$ **do**
    ... = ...$\times$ eimy $\times$ einz
    eimy = eimy $\times$ eiy
  **end for**
  einz = einz $\times$ eiz
**end for**

# Sorting particles in grid cells



- PIC, 32 nodes, 128M particles, $128 \times 512 \times 128$ grid cells




* Intel Xeon E5-2690

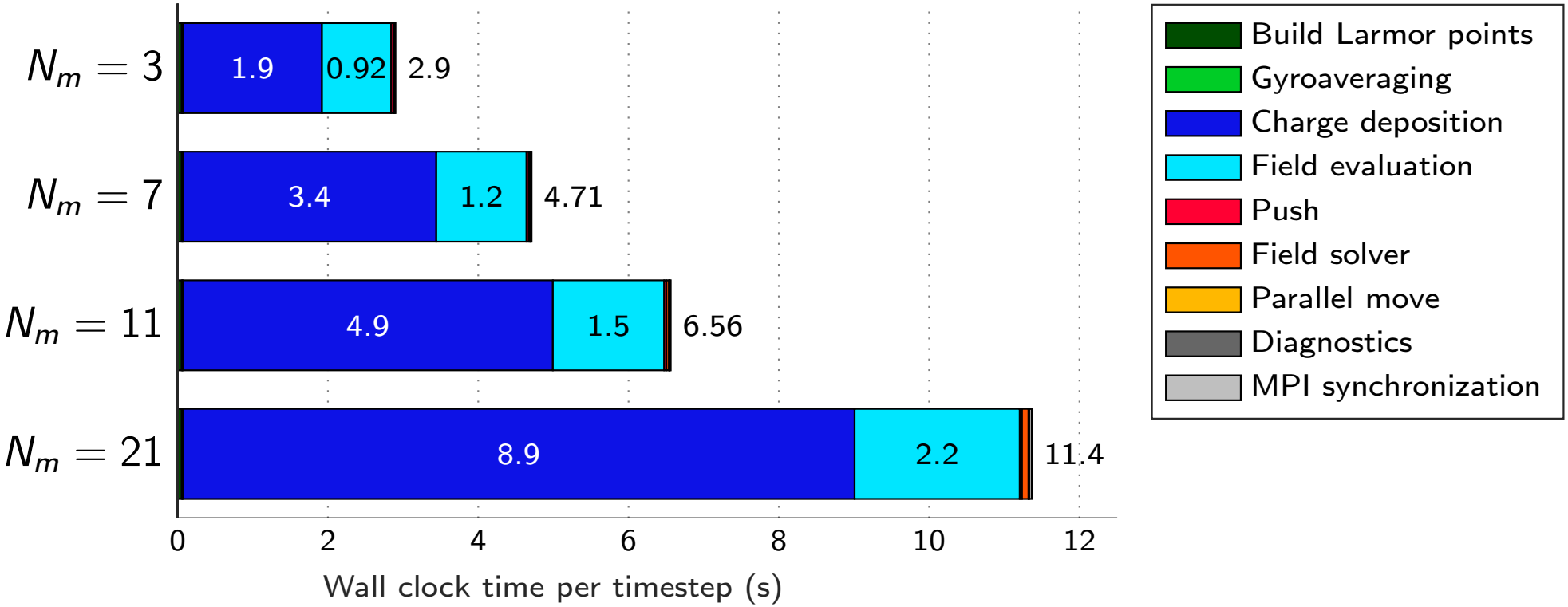
** NVIDIA Tesla P100

- Sorting interesting for cubic splines, not for quadratic
- GPU** up to 3.5 times faster than CPU*

# Scanning number of poloidal modes



- PIF, 32 nodes, 128M particles, 128 radial cells, $N_n = 15$

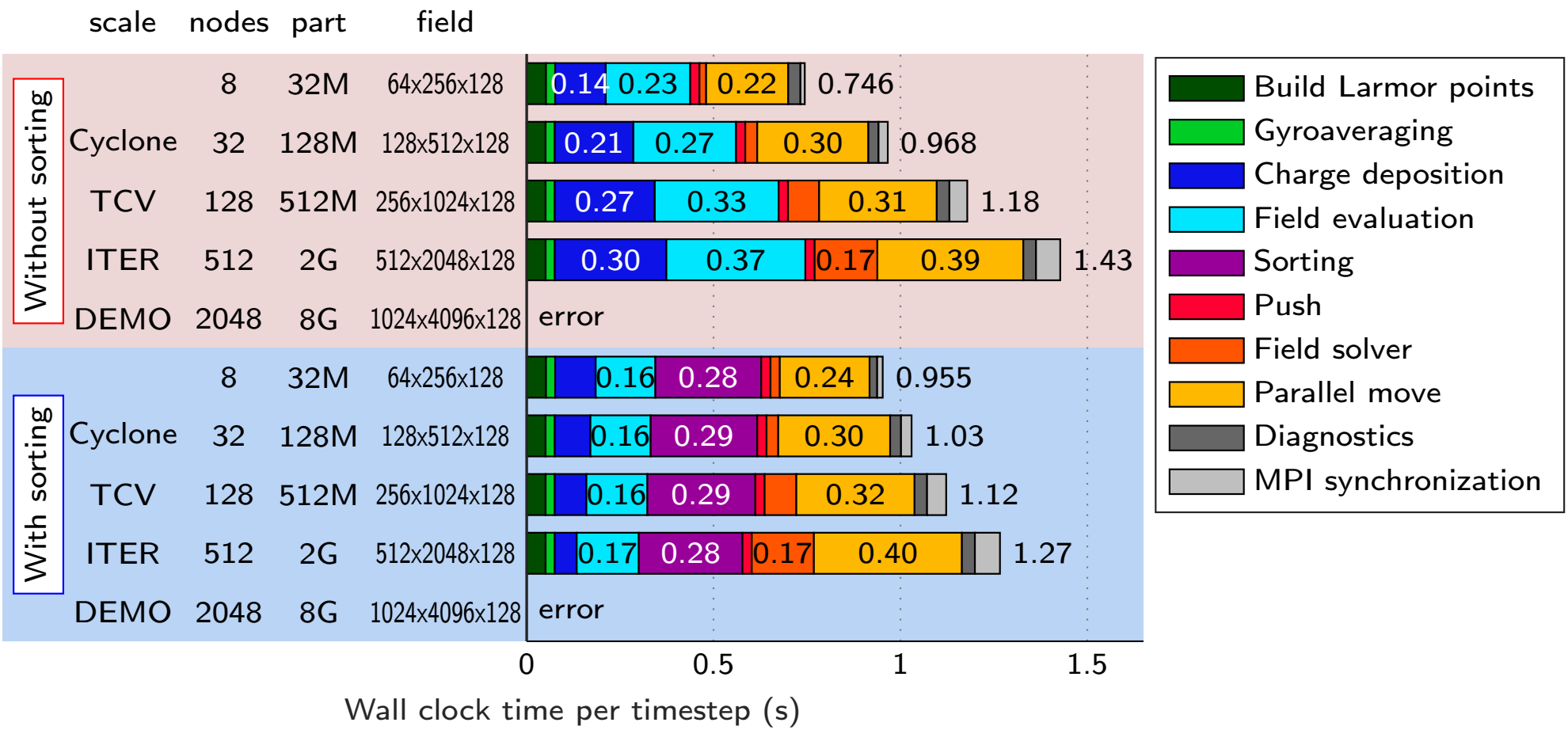



- Wall clock time scales less than linearly with $N_m$ because exponential is computed with prefactor successive multiplications.

# Parallel scalability of PIC on GPU



- $\rho^*$ scan, PIC, quad. splines, 1 GPU per node
- Using GPU_DIRECT to skip CPU memory writing




- GPU_DIRECT is numerically very efficient, but unfortunately buggy.