Parallel Particle-In-Cell (PIC) Codes

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Outline

- Motivation
- The Particle-In-Cell (PIC) Algorithm
- Parallelization and Performance Modeling for PIC
- Simulation and Performance Examples
- Conclusion

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Motivation

- It exists a continuous demand for

1. more computational resources to perform larger and more accurate simulations,
2. faster computations to perform more simulations in less time.

High Performance Computing provides a possibility to meet those requirements.

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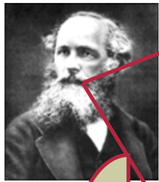
Physical Model



Maxwell Equations

$$\begin{aligned}\nabla \times \vec{E} &= -\frac{\partial}{\partial t}\vec{B}\\ \nabla \times \vec{H} &= \vec{J} + \frac{\partial \vec{D}}{\partial t}\\ \nabla \cdot \vec{D} &= \rho\\ \nabla \cdot \vec{B} &= 0\end{aligned}$$

$\vec{E}, \vec{B}$

coupled nonlinear equation system

$\vec{J}, \rho$

Newton-Lorentz Equations

$$\begin{aligned}\frac{\mathrm{d}\vec{p}_i}{\mathrm{d}t} &= q_i\left(\vec{E}(\vec{r}_i) + \frac{\vec{p}_i}{m_i} \times \vec{B}(\vec{r}_i)\right)\\ \frac{\mathrm{d}\vec{r}_i}{\mathrm{d}t} &= \frac{\vec{p}_i}{m_i}\end{aligned}$$

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Particle-In-Cell Algorithm

Advance fields
$\vec{E}^{(n)} \rightarrow \vec{E}^{(n+1)}$
$\vec{B}^{(n)} \rightarrow \vec{B}^{(n+1)}$.

Interpolate fields to particles (gather).

Push particles
$\vec{r}_i^{(n)} \rightarrow \vec{r}_i^{(n+1)}$
$\vec{p}_i^{(n)} \rightarrow \vec{p}_i^{(n+1)}$.

Extrapolate currents to grid (scatter).

Δt

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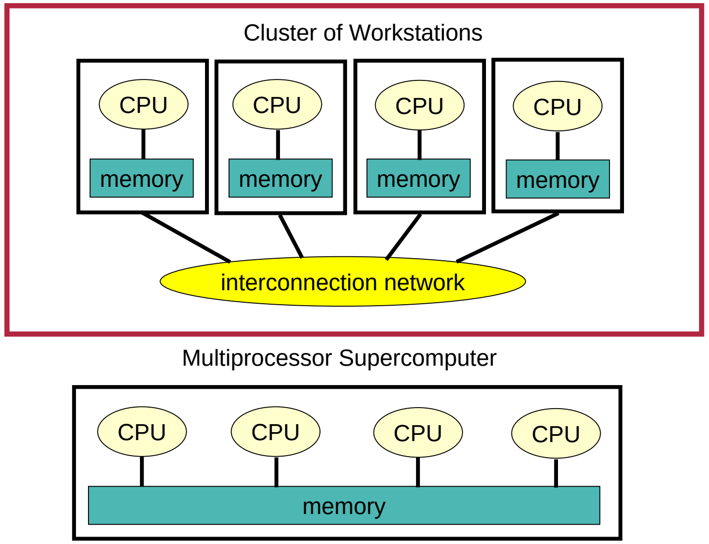
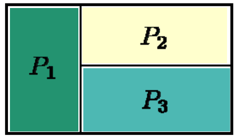
Computational Environment



Parallelization Strategies

- The Parallelization of the field solver requires a geometrical partitioning of the computational domain.

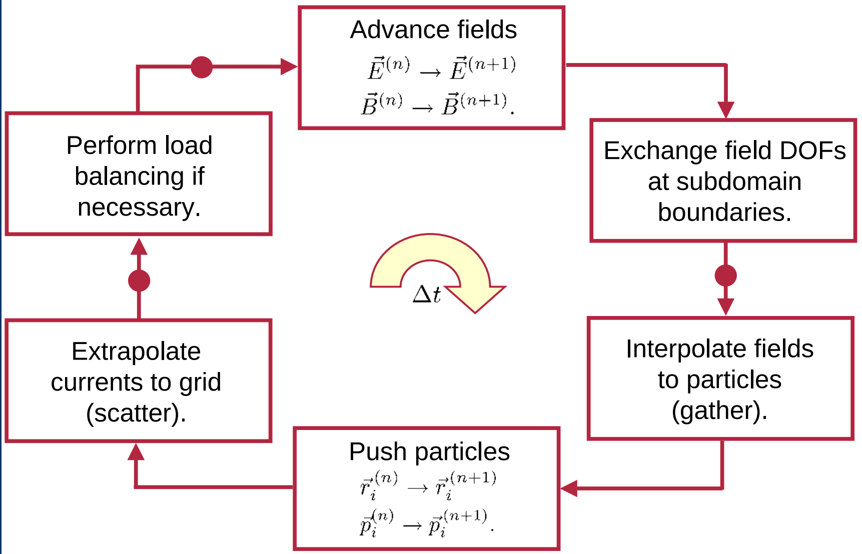


- Assignment of particles to processors is critical for simulation efficiency.

coupled assignment:
+ local gather/scatter phases
- imbalanced load

uncoupled assignment:
+ balanced load
- nonlocal gather/scatter phases

Particle-In-Cell Algorithm



Performance Modeling

- How should the particles be assigned to the available processors?

Objective Function

$$\text{minimize} \quad F := \sum_{i_T=1}^{N_T} \Bigg(\max_{i_\pi} \left\{ w_F^{(i_\pi)}(i_T) + w_B^{(i_\pi)}(i_T) \right\} + \max_{i_\pi} \left\{ w_{GS}^{(i_\pi)}(i_T) + w_P^{(i_\pi)}(i_T) \right\} + \max_{i_\pi} \left\{ w_M^{(i_\pi)}(i_T) \right\} \Bigg)$$

N_T - total number of timesteps

$w_{\dots}^{(i_\pi)}(i_T)$ - Time needed by processor i_π to complete phase ... in time step i_T .

Performance Modeling

$$F := \sum_{i_T=1}^{N_T} \Big(\cancel{\max_{i_\pi} \left\{ w_F^{(i_\pi)}(i_T) + w_B^{(i_\pi)}(i_T) \right\}}$$
$$+ \max_{i_\pi} \left\{ w_{GS}^{(i_\pi)}(i_T) + w_P^{(i_\pi)}(i_T) \right\}$$
$$+ \cancel{\max_{i_\pi} \left\{ w_M^{(i_\pi)}(i_T) \right\}} \Big)$$

- Assumptions:
  - Field solver is ideally balanced.
  - Migration costs are neglected.

Performance Modeling

$$F = \sum_{i_T=1}^{N_T} \max_{i_\pi} \left\{ w_{GS}^{(i_\pi)}(i_T) + w_P^{(i_\pi)}(i_T) \right\}$$

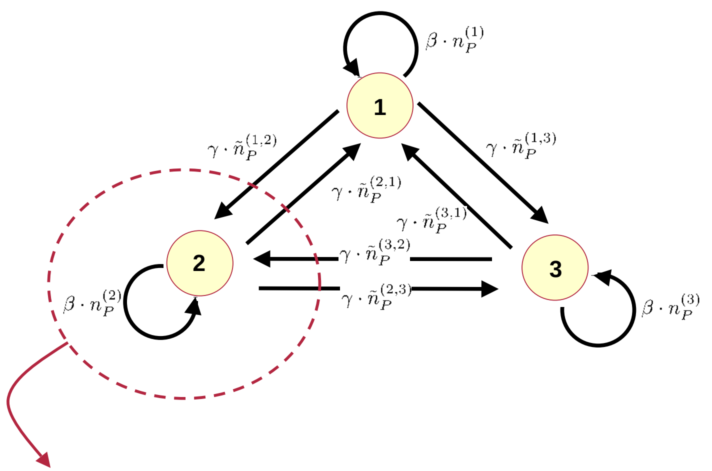
$$w_P^{(i_\pi)}(i_T) := \beta \cdot n_P^{(i_\pi)}(i_T)$$

$$w_{GS}^{(i_\pi)}(i_T) := \gamma \cdot \sum_{\substack{j_\pi = 1 \\ j_\pi \neq i_\pi}}^{N_\pi} \left(\tilde{n}_P^{(i_\pi, j_\pi)}(i_T) + \tilde{n}_P^{(j_\pi, i_\pi)}(i_T) \right)$$

- Assumptions:
  - Field solver is ideally balanced.
  - Migration costs are neglected.
  - For the particle pusher and the gather/scatter costs a linear dependency is assumed.
  - Computational environment is a homogeneous cluster.

Load Graph

- The workload can be illustrated by a directed graph.

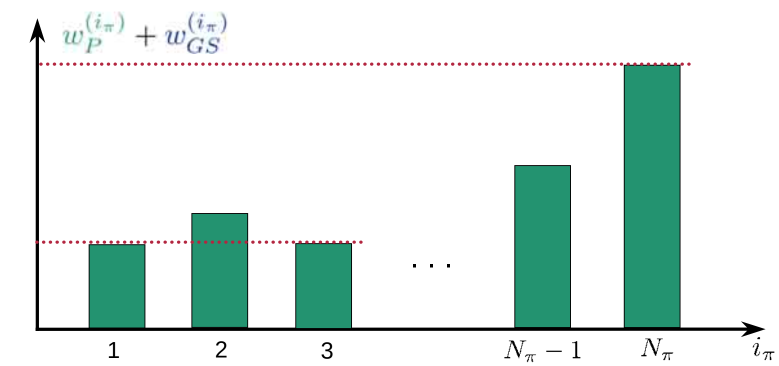


$$w_P^{(2)} + w_{GS}^{(2)} = \beta \cdot n_P^{(2)} + \gamma \cdot \left(\tilde{n}_P^{(1,2)} + \tilde{n}_P^{(2,1)} + \tilde{n}_P^{(2,3)} + \tilde{n}_P^{(3,2)} \right)$$

Optimization Procedure

First case $\gamma > \beta$ **:**

It is optimal to choose the coupled assignment and accept the unbalanced load for the particle pusher.



Optimization Procedure

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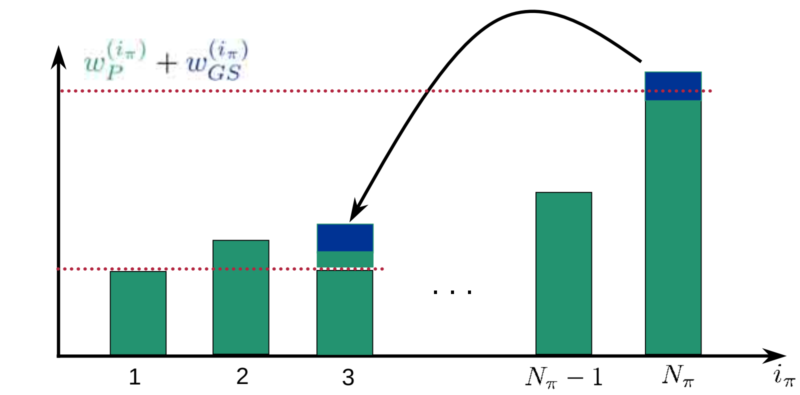

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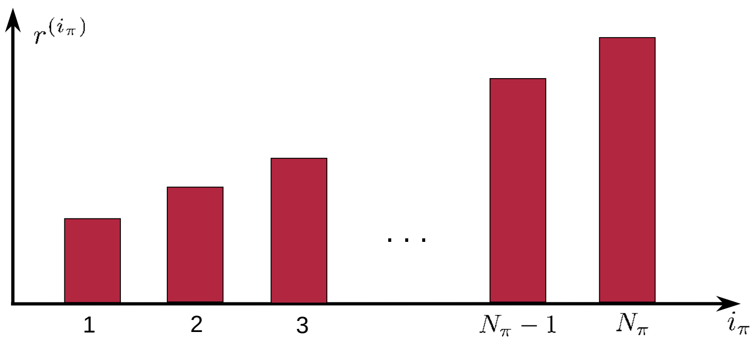
Optimization Procedure

Second case $\gamma \leq \beta$**:**

1. Sort processes such that

$$r^{(i_\pi)} \leq r^{(j_\pi)} \quad \forall i_\pi, j_\pi \in [1, .., N_\pi] : i_\pi < j_\pi,$$

where $r^{(i_\pi)}$ describes the number of particles depending on field DOFs from processor i_π .



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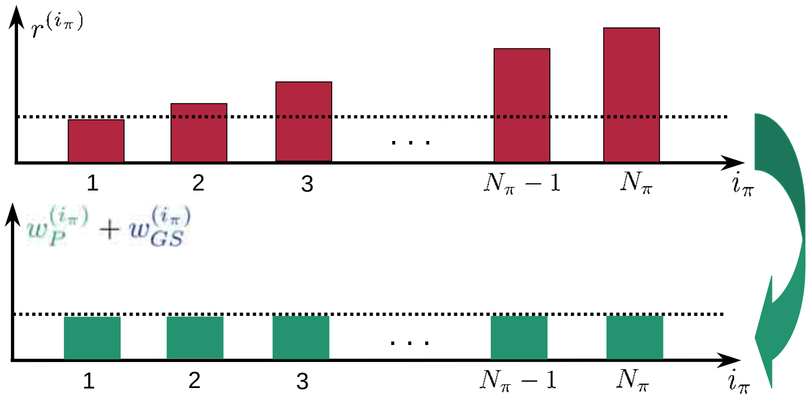
Optimization Procedure

Second case $\gamma \leq \beta$**:**

2. Assign the first $N_\pi \cdot r^{(1)}$ particles to the processors such that the particles depend only on local field DOFs.



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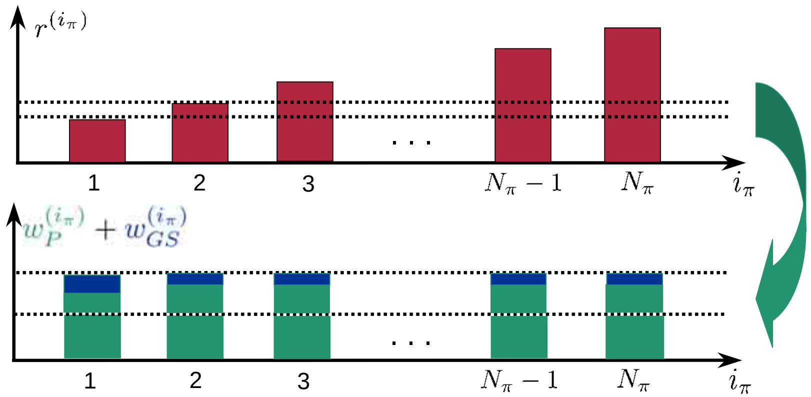
Optimization Procedure

Second case $\gamma \leq \beta$**:**

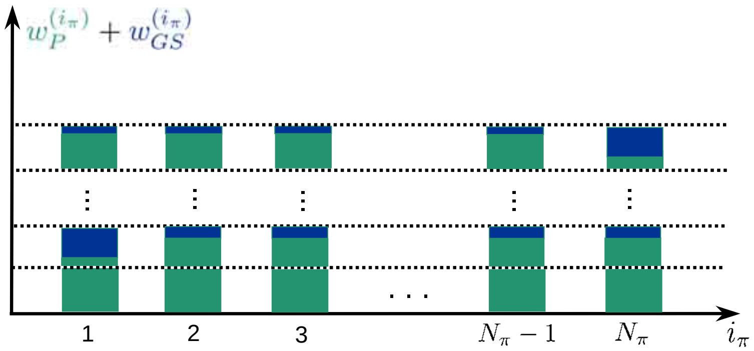
3. Assign $(N_\pi - 1) \cdot (r^{(2)} - r^{(1)})$ particles requiring field DOFs possessed by processors $2, .., N_\pi$. Preserve a balanced load.



Optimization Procedure

Second case $\gamma \leq \beta$:

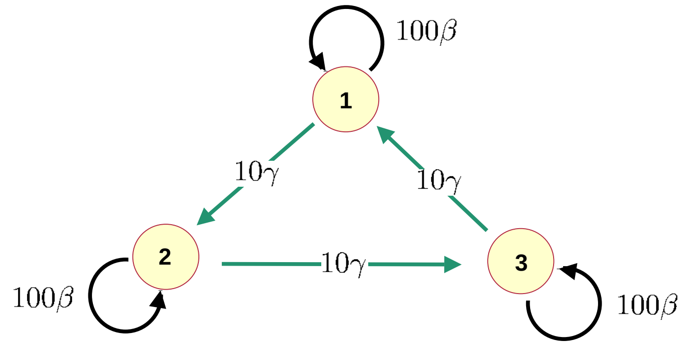
4. In the i^{th} step assign $(N_\pi - i)\cdot(r^{(i+1)} - r^{(i)})$ particles depending on field DOFs from processors $i+1, .., N_\pi$. Again, preserve a balanced load.



Optimization Procedure

- Is this the optimal solution in terms of the model?

➡ Yes, it is. For all suboptimal strategies the Load Graph isn‘t load balanced or contains circles.



Optimization Procedure

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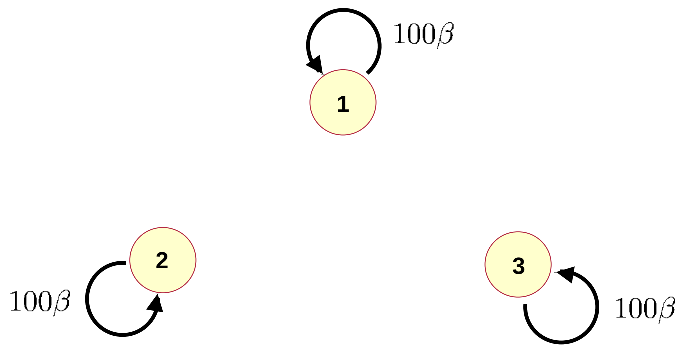
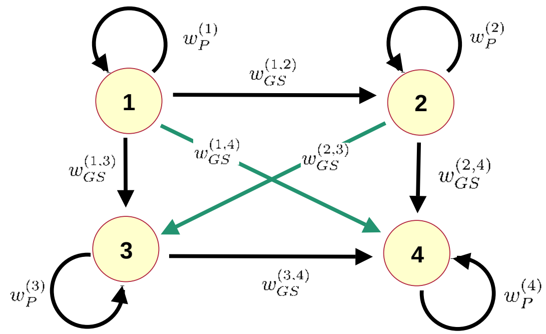


Optimization Procedure

- Is this the optimal solution in terms of the model?

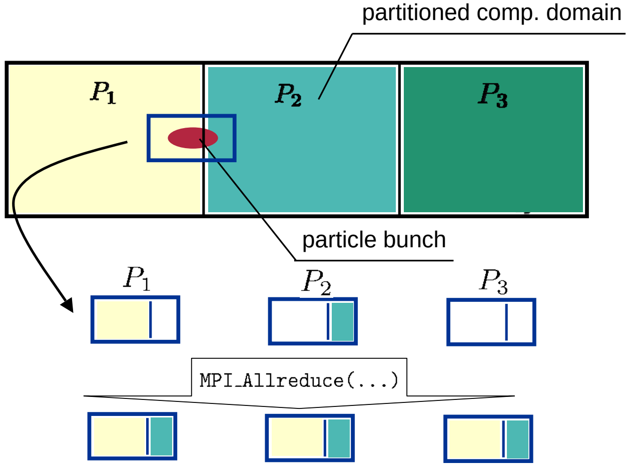
➡ Yes, it is. For all suboptimal strategies the Load Graph contains circles or isn‘t load balanced.

- But, the optimum is not unique for more than 2 processors.



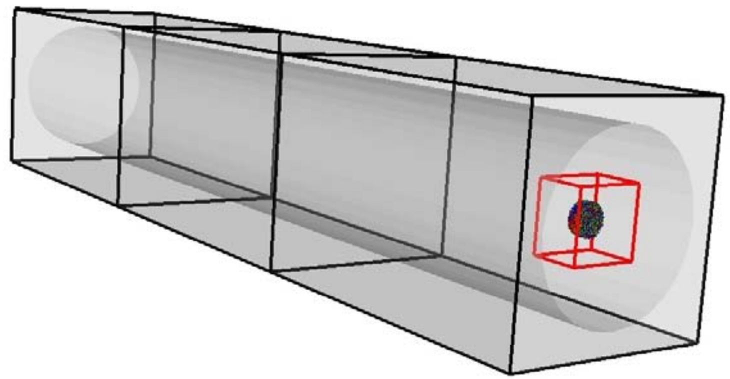
Adaptive Bounding Box

- Data exchange can be simplified for simulations with a very localized particle distribution.



Adaptive Bounding Box

- The Bounding Box is adaptively changed depending on the particle distribution.



Adaptive Bounding Box

- Communication costs can be approximated by

$$w_{GS} = \kappa \cdot N_{\text{bunch}} \cdot \log(N_\pi).$$

- The parallel speedup can be predicted by the expression

$$\hat{S}_{N_\pi} = \frac{1}{\frac{1}{N_\pi} + \frac{\kappa \cdot N_{\text{bunch}}}{\alpha \cdot N_C + \beta \cdot N_P} \cdot \log(N_\pi)}.$$

→ The algorithm is communication bound. Good performance results can only be expected for a fast interconnection network.

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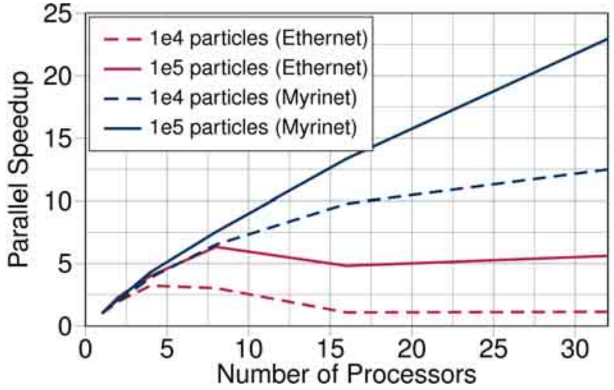
Benchmark Results

- Benchmark: electron bunch traveling within an ideally conducting tube (5 million grid points).



➡ The performance of the algorithm is not satisfactory for a cluster with a slow interconnection network.

Benchmark Results

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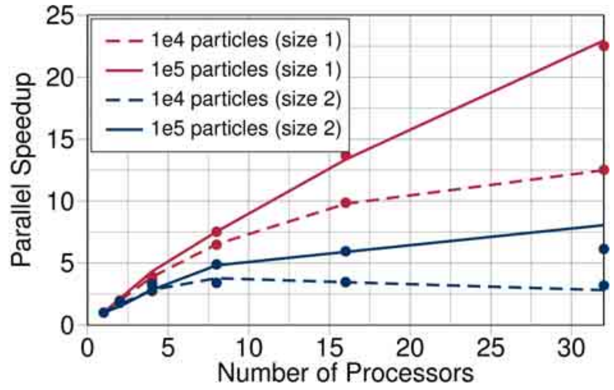
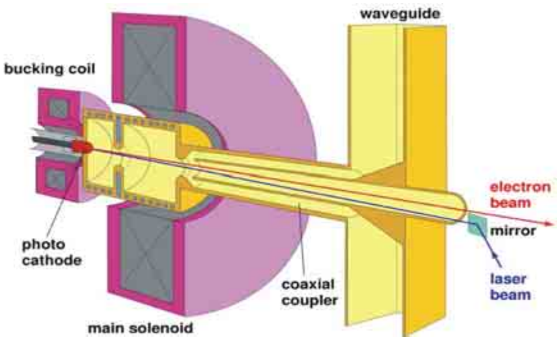


➡ The predicted speedup is in good agreement with the results obtained on the compute cluster.

PITZ-Injector

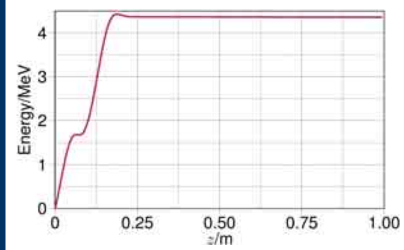


Bunch rms-radius: $\sigma_x = \sigma_y \approx 0.5 - 3.75\text{mm};\ \sigma_z \approx 2.5\text{mm}$

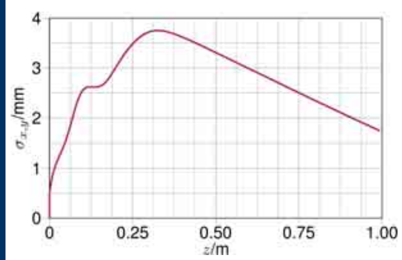
Geometry dimensions: $0.2\text{m} \times 0.2\text{m} \times 1.0\text{m}$

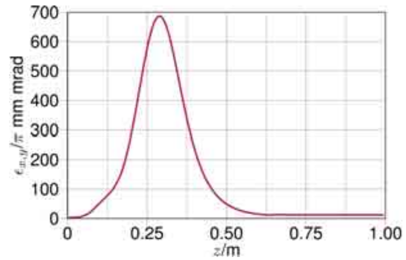
➡ **Multiscale problem: requires a high amount of computational resources.**

Results



- Fully 3D simulation using 300 million grid points and 250,000 particles.





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Conclusion

- Performance modeling has shown to be helpful for the construction and analysis of parallelization schemes.
- The Adaptive Bounding Box approach is well suited for the simulation of problems with very localized particle distributions.
- The Adaptive Bounding Box approach scales good on a high speed interconnection network.