A hierarchical framework for sparse-grid particle-in-cell method

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   - Method
   - Benefits and limitations
2. Hierarchical sparse-grid particle-in-cell
   - Principle
   - Approximation space
   - Error estimates
   - Spatially adaptive refinement
3. Numerical results
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Sparse-grid particle-in-cell

PIC methods

Principles (PIC)

- **Lagrangian** representation of the particle distribution by N particles in phase space
- **Eulerian** grid with mesh size h to discretize the field equation

Electrostatic, **collisionless** PIC scheme:

1. Particles evolve according to Newton's equations:

$$\frac{d\boldsymbol{x}_s}{dt} = \boldsymbol{v}_s, \qquad \frac{d\boldsymbol{v}_s}{dt} = (\boldsymbol{E} + \boldsymbol{v}_s \times \boldsymbol{B})\Big|_{\boldsymbol{x}=\boldsymbol{x}_s}$$

2. Charge density **approximated on the grid** by Monte–Carlo method:

$$\rho_h(\boldsymbol{x}) = \sum_{s=1}^{N} \frac{1}{N} W_h(\boldsymbol{x} - \boldsymbol{x}_s), \qquad W_h\text{: shape function} \approx \delta$$

3. Solve the Poisson equation on the grid using ρ_h as the source term and compute the electric field
4. Interpolate the electric field at the particle positions

Component grid framework

Main idea (SGCT-PIC)

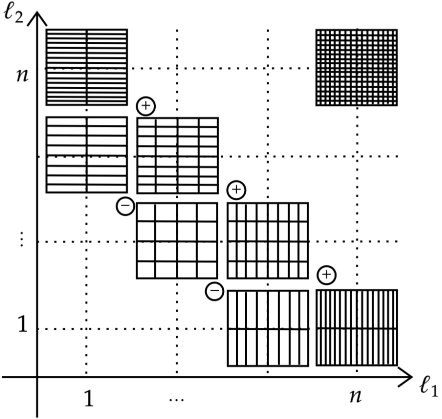
Cartesian full-grid is replaced by a set of **anisotropic component grids**

Component grids have **varying mesh sizes**

$$h_{\boldsymbol{\ell}} = (2^{-\ell_1}, \ldots, 2^{-\ell_d}), \quad \boldsymbol{\ell} \in \mathbb{N}^d$$

with level constraint

$$|\boldsymbol{\ell}|_1 = n+(d-1)-i, \quad i = 0, \ldots, d-1$$



Scheme

Scheme (SGCT-PIC)

1. On **each component grid**:
   - Accumulate charge density with Monte-Carlo method
   - Solve Poisson equation with FD, FEM or FFT
   - Compute electric field by differentiation
2. Interpolate electric field at particle positions using the **sparse-grid combination technique (SGCT)**
3. Advance particles using the standard PIC time integration

Benefits...

Benefits

- **Computational costs** (# mesh nodes and # particles) reduced to $\mathcal{O}(h^{-1}|\log h|^{d-1})$ vs $\mathcal{O}(h^{-d})$
- **Small** and **sparse** linear systems to solve
- Easy to implement and **parallelize**

... and limitations

Limitations

- **Projection/interpolation** operations has complexity in $\mathcal{O}(N|\log h|^{d-1})$ vs $\mathcal{O}(N)$
- **Restricting analysis framework**, based on Taylor expansions limited to $\mathcal{C}^q_{\mathrm{mix}}$ functions
- Large grid-based errors for solutions with **strong mixed derivatives**, require **spatially adaptive refinement**
- Framework not suited for adaptive refinement, requires **heavy implementation**[a]
- Framework limited to **rectangular geometries**

[a] [Obersteiner, Bungartz. *A generalized spatially adaptive sparse grid combination technique with dimension-wise refinement*. 2021]

An alternative **hierarchical** method to address these limitations?

Hierarchical sparse-grid particle-in-cell

Variational framework

Principles

1. **Galerkin projection** of the Monte–Carlo estimator of the charge density onto $V_h(\Omega)$:

$$\Pi_h \rho_N = \Pi_h \left(\frac{1}{N} \sum_{s=1}^{N} \delta(\cdot - \boldsymbol{x}_s) \right)$$

2. **Variational Galerkin formulation** of the field equation:

$$(\nabla \Phi_h, \nabla \varphi_h)_{L^2(\Omega)} = (\Pi_h \rho_N, \varphi_h)_{L^2(\Omega)}, \qquad \forall \varphi_h \in V_h(\Omega)$$

- Requires the definition of an **approximation space**:

$$V_h(\Omega) \subset H^q(\Omega)$$

that **well approximate** the solution space and **minimize statistical noise**

Method

- Choose a **basis** of the space:

$$V_h(\Omega) = \mathrm{span}\{\varphi_{h,j} \mid \forall j\}$$

Scheme (HSG-PIC)

1. **Solve the variational formulation** of Poisson equation using Galerkin method:

$$\sum_i \Phi_i \underbrace{(\nabla\varphi_{h,i}, \nabla\varphi_{h,j})_{L^2(\Omega)}}_{\text{stiffness matrix}} = \underbrace{\frac{1}{N}\sum_{s=1}^{N}\varphi_{h,j}(\boldsymbol{x}_s)}_{\substack{\text{weak form of}\\ \text{Galerkin projection}}}, \quad \forall j$$

2. **Interpolate electric field** at particle positions by evaluating the potential **gradient**
3. Advance particles using the standard PIC time integration

...How to choose a good approximation space?

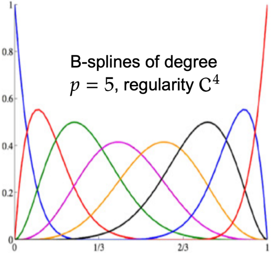
Approximation space

Construction (approximation space)

1. Define **univariate B-spline** space
2. Extend to d-dimensional space using **tensor products**
3. Construct **hierarchical** basis representation
4. **Select levels** according to full-grid/sparse-grid/etc. rule

1. **Univariate** space of **B-splines** of degree p and regularity $\mathcal{C}^{p-1}$:

$$S_h([0,1]) := \left\{ u \in H^p([0,1]) \;\middle|\; u|_{(hj,\, h(j+1))} \in \mathbb{P}^p, \quad \forall j \right\}$$



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2. Tensor-product space with **varying mesh sizes**:

$$S_{h_{\boldsymbol{\ell}}}(\Omega) := \bigotimes_{i=1}^{d} S_{h_{\ell_i}}([0,1])$$

same degree p in each dimension, but varying h_{ℓ_i}

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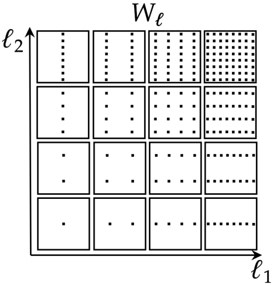
3. Construct **hierarchical** basis representation
4. **Select levels** according to full-grid/sparse-grid/etc. rule

3. **Hierarchical subspace** decomposition via direct sum of hierarchical increments:

$$S_{h_{\ell}}(\Omega) = \bigoplus_{\boldsymbol{k} \leq \boldsymbol{\ell}} \underbrace{S_{h_{\boldsymbol{k}}}(\Omega) \Big/ \bigoplus_{i=1}^{d} S_{h_{\boldsymbol{k}-\boldsymbol{e}_i}}(\Omega)}_{W_{h_{\boldsymbol{k}}}(\Omega)}$$



Approximation space

Construction (approximation space)

1. Define **univariate B-spline** space
2. Extend to d-dimensional space using **tensor products**
3. Construct **hierarchical** basis representation
4. **Select levels** according to full-grid/sparse-grid/etc. rule

4. Approximation space constructed by *a priori* **selection of levels**:

$$V_h(\Omega) := \bigoplus_{\ell \in ?} W_{h_\ell}(\Omega)$$

Different choices of approximation spaces depending on the level selection rule, such as...

Full-grid space

- Approximate **regular Sobolev space**

$$V_{h,p}^{(\infty)}(\Omega) \subset \mathrm{H}^p(\Omega)$$

with **best** asymptotic error in L^2 norm:

$$\min_{u_h \in V_{h,p}^{(\infty)}(\Omega)} \|u_h - u\|_{L^2(\Omega)} \lesssim h^{p+1} \|u\|_{H^p(\Omega)}$$

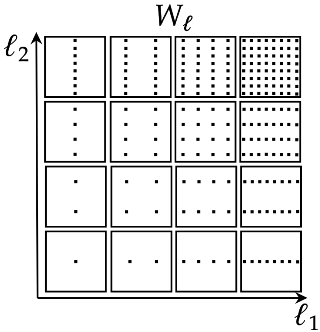
- Selection of **all levels**:

$$|\boldsymbol{\ell}|_\infty \leq n$$

- Complexity/noise with **exponential dimension** dependence:

$$|V_{h,p}^{(\infty)}(\Omega)| = \mathcal{O}(h^{-d})$$

$$\mathrm{Var}[\cdot]^{1/2} = \mathcal{O}\left(\sqrt{1/(Nh^d)}\right)$$



Sparse-grid space

- Approximate **mixed Sobolev space**

$$V^{(1)}_{h,p}(\Omega) \subset \mathrm{H}^p_{\mathrm{mix}}(\Omega) \subset \mathrm{H}^p(\Omega)$$

with **close to best** asymptotic error in L^2 norm:

$$\min_{u_h \in V^{(1)}_{h,p}(\Omega)} \|u_h - u\|_{L^2(\Omega)} \lesssim h^{p+1} |\log h|^{d-1} \|u\|_{H^p_{\mathrm{mix}}(\Omega)}$$

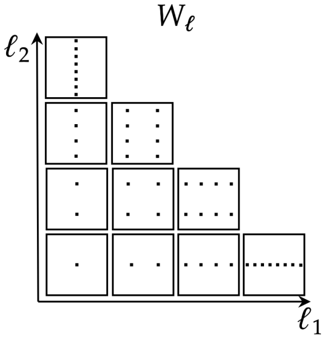
- Selection of **lower-diagonal levels**:

$$|\boldsymbol{\ell}|_1 \leq n$$

- Complexity/noise with **weak (log) exponential dimension** dependence:

$$|V^{(1)}_{h,p}(\Omega)| = \mathcal{O}(h^{-1} |\log h|^{d-1})$$

$$\mathrm{Var}[\cdot]^{1/2} = \mathcal{O}\left(\sqrt{|\log h|^{d-1}/(Nh)}\right)$$



Energy-based sparse-grid space

- Approximate **mixed Sobolev space**

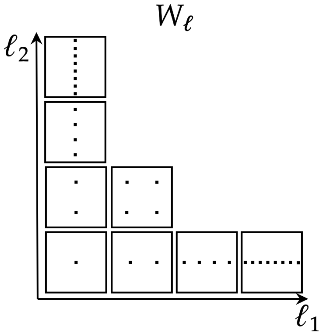
$$V_{h,p}^{(E)}(\Omega) \subset \mathrm{H}^p_{\mathrm{mix}}(\Omega) \subset \mathrm{H}^p(\Omega)$$

with **best** asymptotic error in H^1 norm:

$$\min_{u_h \in V_{h,p}^{(E)}(\Omega)} \|u_h - u\|_{H^1(\Omega)} \lesssim h^p \|u\|_{H^p_{\mathrm{mix}}(\Omega)}$$

- Penalization of uniform discretizations:

$$|\boldsymbol{\ell}|_1 - \frac{1}{5}\left|\log\left(\sum_{i=1}^{d} h_{\ell_i}^2\right)\right| \leq n - \frac{1}{5}|\log(h^2)|$$



- Complexity/noise **without dimension** dependence:

$$|V_{h,p}^{(E)}(\Omega)| = \mathcal{O}(h^{-1})$$

$$\mathrm{Var}[\cdot]^{1/2} = \mathcal{O}\left(\sqrt{1/(Nh)}\right)$$

Error estimates

Theorem (charge density)

If f is **sufficiently smooth** (in $H^{p+1}_{\mathrm{mix}}(\Omega)$), then

$$\|\mathrm{bias}[\Pi_h^{(1)}\rho_N]\|_{L^2(\Omega)} \lesssim h^{p+1}|\log h|^{d-1}\|\rho\|_{H^{p+1}_{\mathrm{mix}}(\Omega)}$$

and, for $(\star) = (1)$ or (E),

$$\left\|\mathrm{Var}[\Pi_h^{(\star)}\rho_N]^{1/2}\right\|_{L^1(\Omega)} \lesssim \sqrt{\frac{|\log h|^{d-1}}{Nh}}$$

Compared to high-order SGCT-PIC:

- **Less restricting** regularity assumptions ($\mathcal{C}^{p+1}_{\mathrm{mix}} \subset H^{p+1}_{\mathrm{mix}}$)
- **Same** asymptotic convergence rates/complexity
- Numerical experiments[1] show statistical error in $\mathcal{O}(\sqrt{(Nh)^{-1}})$ for energy-based space

[1] in 2d

Error estimates

Assuming linear B-splines[2],

Theorem (electric field)

If f is **sufficiently smooth** (in $H^2_{\mathrm{mix}}(\Omega)$) then

$$\sum_{i=1}^{d} \|\mathrm{bias}[(\nabla \Phi_h^{(\star)})_i]\|_{L^2(\Omega)} \lesssim h\|\rho\|_{H^2_{\mathrm{mix}}(\Omega)},$$

with $(\star) = (1), (\infty)$, or (E).

- Same asymptotic convergence rate **for all spaces**
- Numerical experiments **confirm rate** of $\mathcal{O}(h^p)$ for degree p splines
- Compared to SGCT-PIC estimates in $\mathcal{O}(h^{p+1}|\log h|^{d-1})$
- Statistical error estimates are not sharp

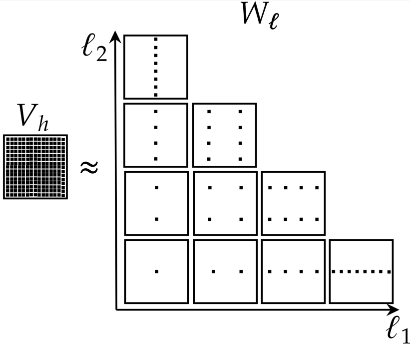
[2] it is a technical proof assumption

Spatially adaptive refinement

Principle

Mesh with **only basis functions** or subspaces that **contribute most** to the solution.

- Different granularities:
  1. **No adaptivity** or *a priori* selection: sparse-grid mesh is based on **mixed-derivative smoothness**



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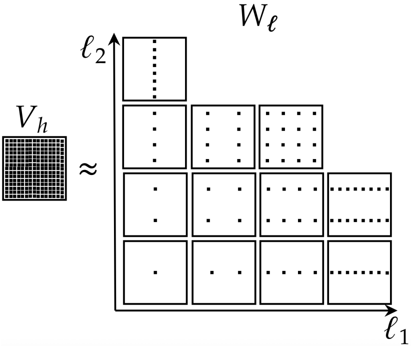
- Different granularities:
  2. **Subspace adaptivity**: selection of **hierarchical subspaces** that contribute the most



Spatially adaptive refinement

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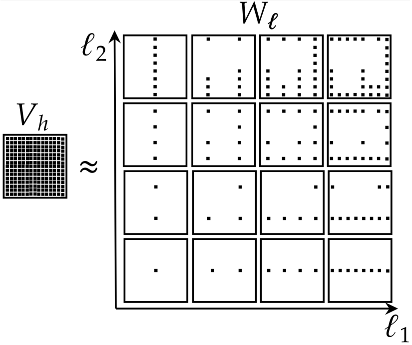
  3. **Spatial adaptivity**: selection of **basis functions** that contribute the most



Method

- Hierarchical surpluses are related to the **second-order derivatives** of the solution[3]:

$$|\alpha_{\boldsymbol{\ell},\boldsymbol{j}}| = \left| \int_\Omega \varphi_{\boldsymbol{\ell},\boldsymbol{j}} \cdot D^2 f \, d\boldsymbol{x} \right| \lesssim h_{\boldsymbol{\ell}} \| D^2 f \|_{\mathrm{L}^2(\Omega)}$$

- Nodes are selected by iteratively **expanding the space** with hierarchical subspaces, checking an **admissibility condition**
- **Admissibility criterion**: for a tolerance $\alpha > 0$

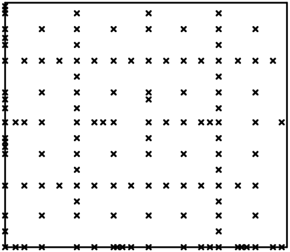
$$\text{If } \; |\alpha_{\boldsymbol{\ell},\boldsymbol{j}}| \geq \alpha h_{\boldsymbol{\ell}} \; \text{ then select node } \boldsymbol{j}$$

- Hierarchical surpluses are obtained by solving augmented linear systems, **eliminating unknowns** from previously selected subspaces with static condensation
- Mesh is **updated** periodically every τ iterations

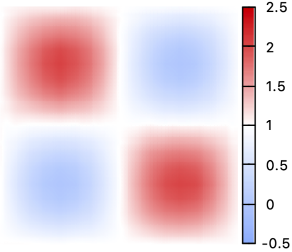
[3] [Bungartz, Griebel. *Sparse grids*. 2004]

Numerical results

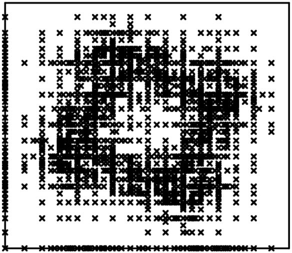
Examples of adaptive grid and approximation



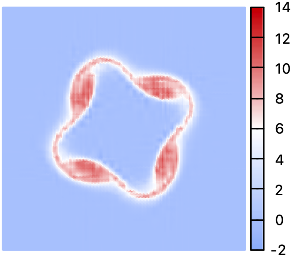
129/256 mesh nodes



$n = 6$, offset $= 0$



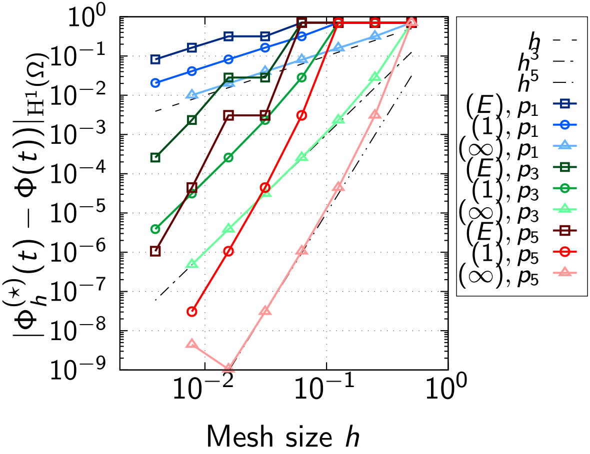
1,745/12,288 mesh nodes



$n = 8$, offset $= 4$

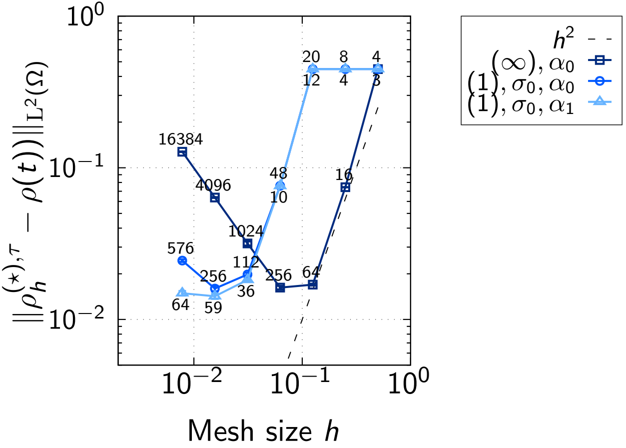
Grid-based error convergence for smooth solution

- **Without noise** (projection of exact density)
- Linear (p_1), cubic (p_3) and quintic (p_5) B-splines
- **No adaptivity**
- **No offset**



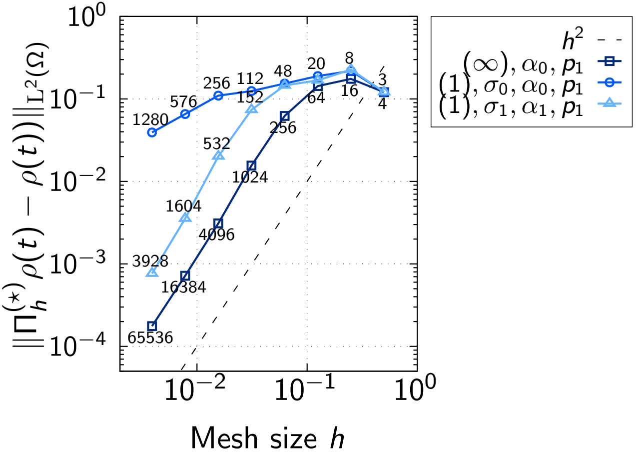
Global error convergence for smooth solution

- $N = 1{,}000{,}000$ particles
- Admissibility tolerance $\alpha_0 = 0$, $\alpha_1 = 10^{-3}$
- **No offset**



Grid-based error convergence for diocotron instability

- **Without noise** (projection of exact density)
- Admissibility tolerance $\alpha_0 = 0$, $\alpha_1 = 10^{-3}$
- **Offset** $\sigma_0 = 0$, $\sigma_1 = 4$



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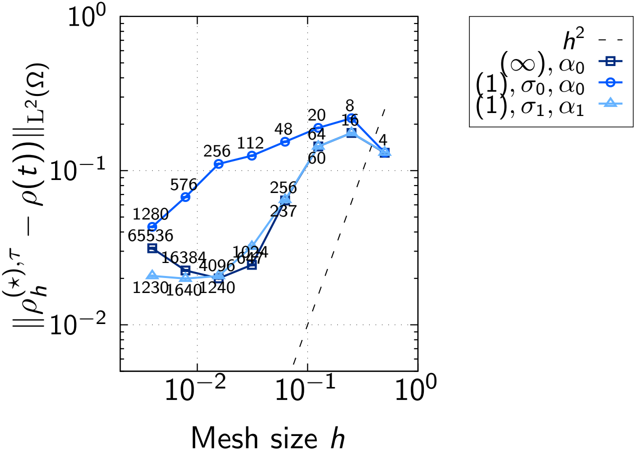
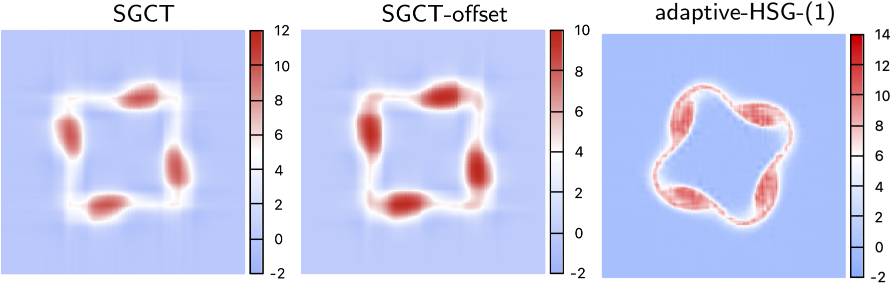


Comparison of accuracy

- **Similar complexity** of about 10^3 mesh nodes[4] and 588,800 particles,



SGCT	SGCT-offset	adaptive-HSG-(1)
$n = 7$, $\sigma = 0$	$n = 6$, $\sigma = 1$	$n = 8$, $\sigma = 4$
2,560 mesh nodes	1,792 mesh nodes	1,745 mesh nodes

- SGCT-offset with $n = 8$, $\sigma = 4$ would require 45,056 mesh nodes

[4] grid updated every 50 time steps

Comparison of performance

- Costs to reach an L^2 error of $\varepsilon = 0.01$ for smooth solution

Method	Parameters		Complexity		Time per iteration [s]				
	h	p	N	$\lvert V_h \rvert$	Total	Proj.	Interp.	Push	Grid ref.
STD-PIC	2^{-6}	1	28,672,000	4,096	4.08	1.67	0.08	1.90	$\times$
SGCT-PIC	2^{-7}	1	17,920,000	2,560	15.1	13.3	0.63	1.17	$\times$
SGCT-PIC	2^{-6}	3	3,264,000	1,088	2.89	2.48	0.28	0.20	$\times$
HSG-(1)	2^{-6}	1	2,816,000	256	0.94	0.49	0.24	0.18	$\times$
HSG-(E)	2^{-6}	3	1,920,000	160	1.99	1.21	0.69	0.12	$\times$
adapt-HSG-(1)	2^{-6}	1	1,620,000	120	0.62	0.29	0.15	0.10	0.07[5]

Speed-up

adapt-HSG-(1) compared to:

- STD-PIC: 6.5$\times$ faster with 18$\times$ fewer particles
- SGCT-PIC: 24$\times$ faster with 11$\times$ fewer particles
- High-order SGCT-PIC: 4.6$\times$ faster with 2$\times$ fewer particles

[5] Grid updated every 15 time steps

Conclusions

Conclusions

- **Larger complexity reduction** in 3d configurations:

$$\mathcal{O}(h^{-d}) \text{ reduced to } \mathcal{O}(h^{-1}|\log h|^{d-1}) \quad \text{or} \quad \mathcal{O}(h^{-1})$$

- A framework that allows: **adaptive refinement**, **general geometries**, and **weaker regularity assumptions**
- Python/C++ implementation available at: https://gitlab.inria.fr/cguillet/sg-pic

Perspectives

Research directions:

- Natural extensions: **3d geometries**, **non-periodic boundary conditions** and **electromagnetic regime** with Maxwell equations
- Extension to more **general geometries** using the **isogeometric analysis** framework, *i.e.*, B-spline–based **geometric mappings**
- **Variable-accuracy**: finer granularity (e.g. block low-rank compression, mixed precision) instead of truncation of subspaces or basis functions
- **Multilevel Monte-Carlo method**[6] to achieve accuracy of fine time discretization $\Delta t \ll \omega_p^{-1}$ at computational costs comparable to $\Delta t = \omega_p^{-1}$

[6] Code prototype at https://gitlab.inria.fr/cguillet/sg-pic/-/tree/multilevel-MC