Polynomial Inverse Mapping:

an acceleration strategy for modern Particle-in-Cell implementations

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August 31, 2021

Overview

PIC is a CFD technique (Evans & Harlow, 1957 [1]).

Modern algorithm (René Gasmöller et al., 2018 [2]):

- adaptive mesh refinement,
- parallel computations.

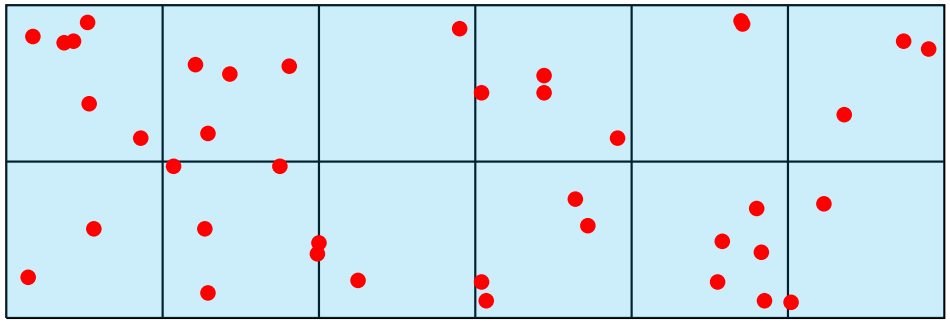
Our goal: speed up one of the main bottlenecks, i.e. $\forall K \in \mathcal{T}_h$ compute the inverse of

$$\Phi_K : \hat{K} \longmapsto K.$$

PIC concepts

PIC couples two viewpoint:

- discrete, using *particle*;
- continuous, mesh-based (*in-cell*).



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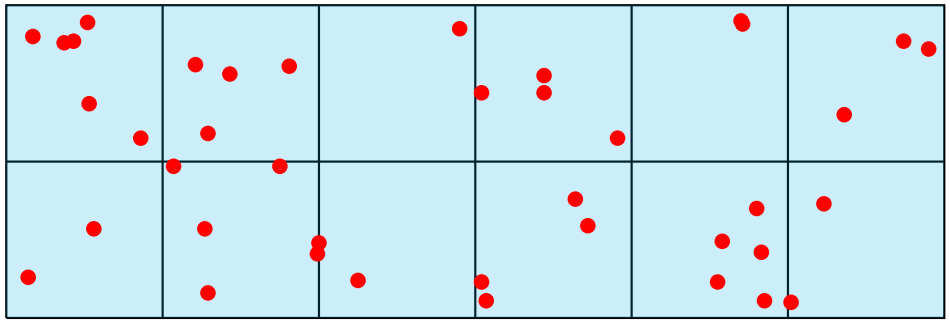

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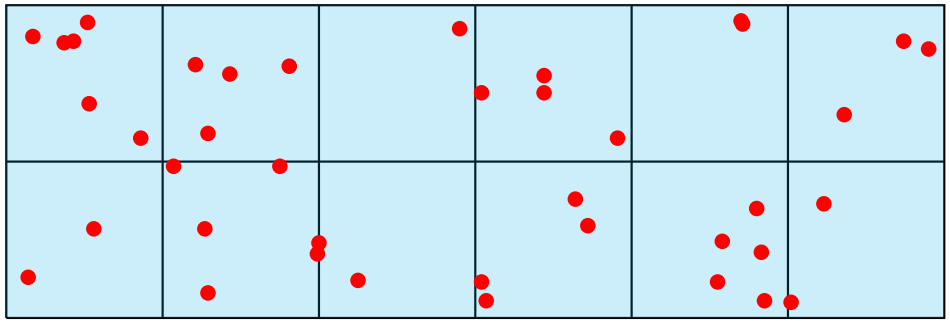

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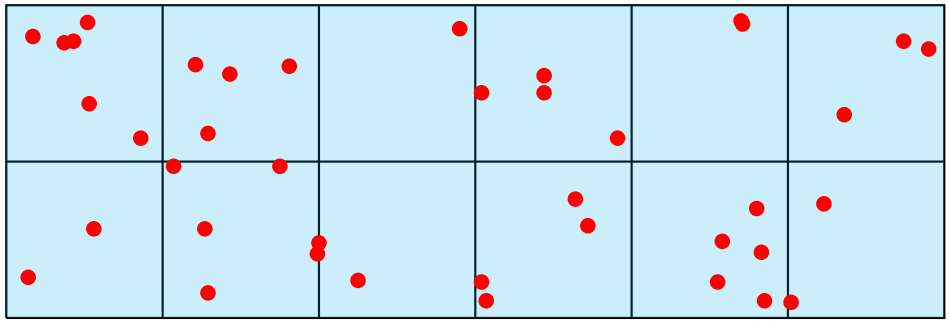

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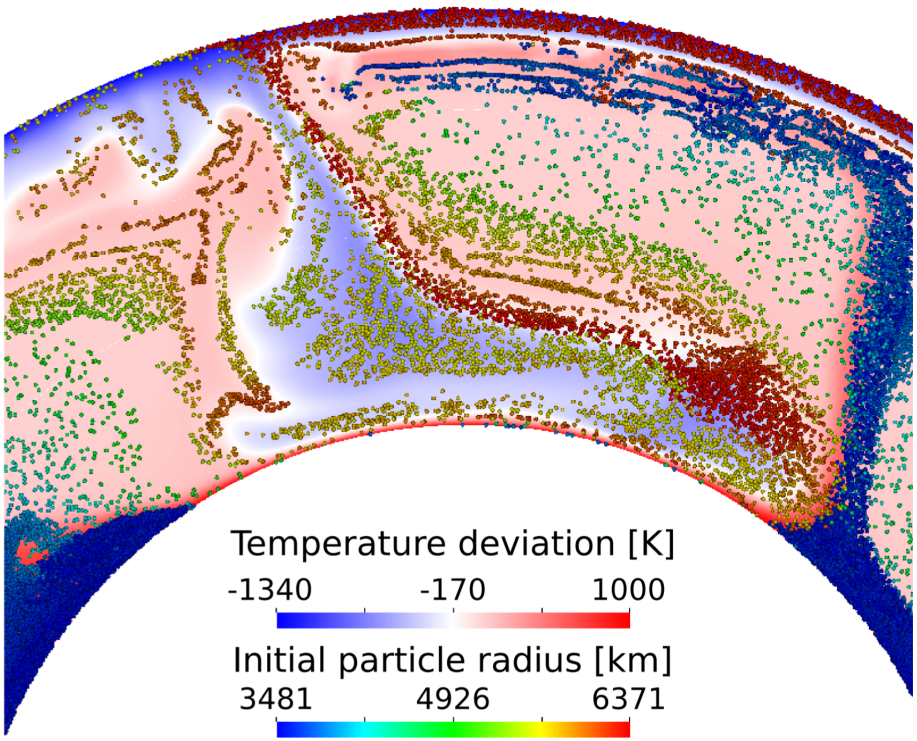
Get a set of (non-coupled) ODEs, i.e. the eq. of motion of each particle.

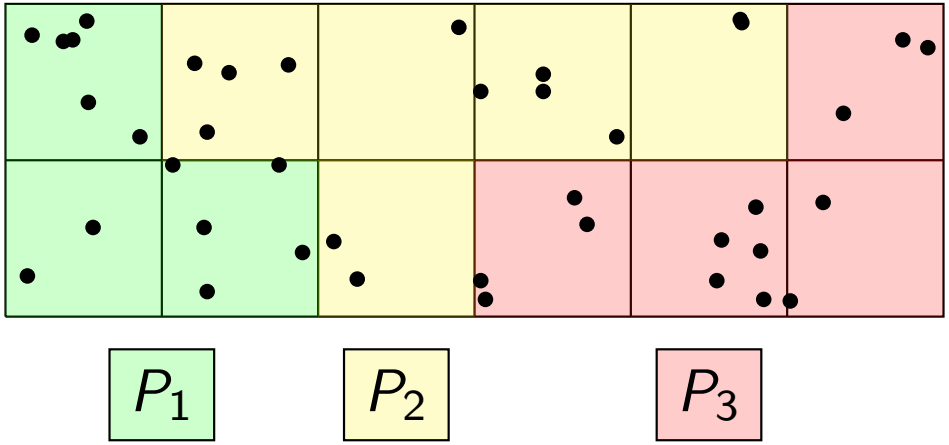
Advect particles along with the flow.

Why using particles

- Visualization of flows;
- tracking interfaces and origins;
- tracking history of material.



Data structures



For t fixed:

- each particle is inside one cell;
- the grid is fully distributed.

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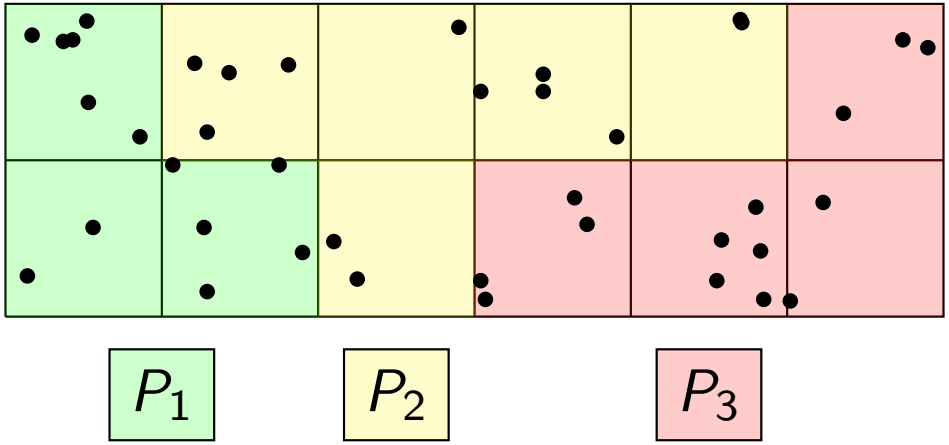


For t fixed:

- each particle is inside one cell;
- the grid is fully distributed.

For t moving forward:

- particles move and change cell;
- cells are redistributed (load balancing).

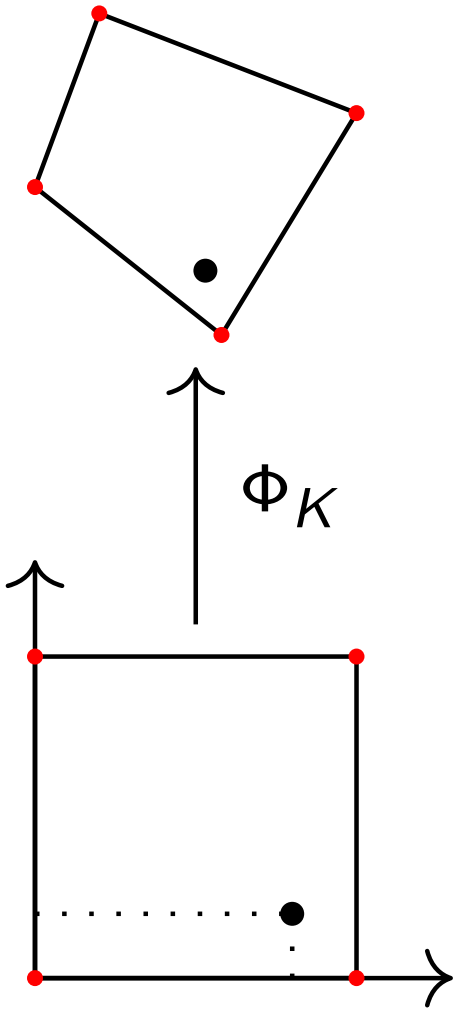
Data structures

C++ Particle object

```
template <int dim>
struct Particle
{
    ParticleId      p_id;
    CellId          cell_id;

    Point<dim>      location;
    Point<dim>      ref_location;

    double*         properties;
};
```



$$\text{ref_location} = \Phi_K^{-1}(\text{location}).$$

Is p inside K?

Suppose we know $p \in K_1 \cup \cdots \cup K_N$.

How do we find the only j s.t. $p \in K_j$?

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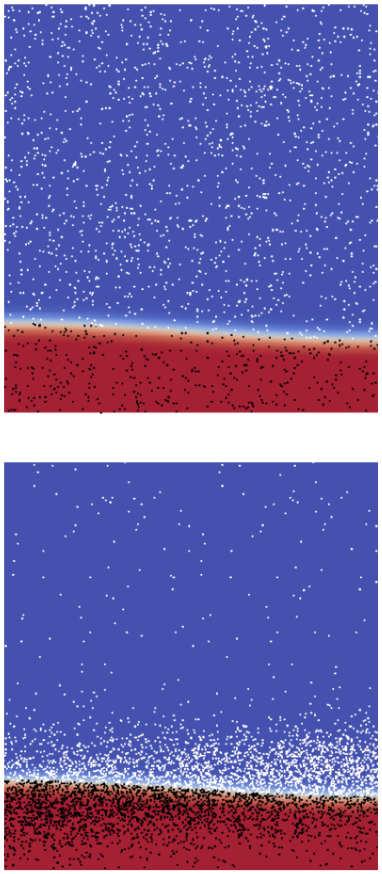
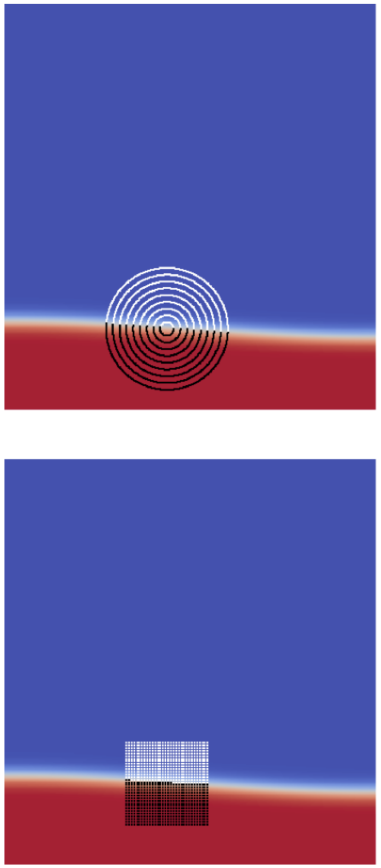
$$p \in K_j \iff \Phi_{K_j}^{-1}(p) \in \hat{K}.$$

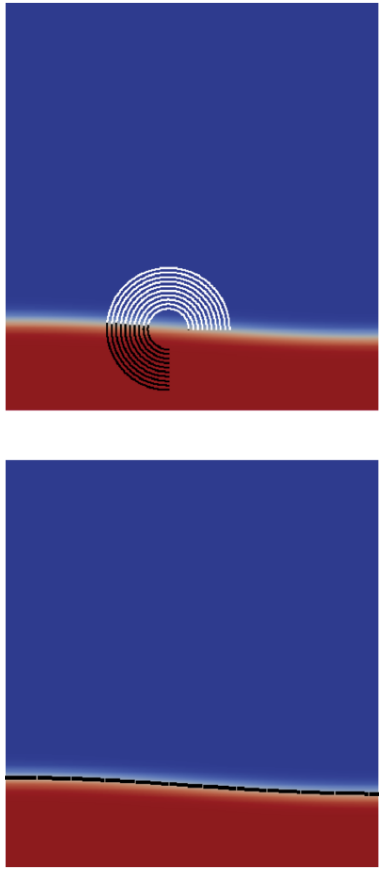
Particles generation



Statistical distribution



Regular distribution



User-defined pattern

Particles advection

$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{u}(\boldsymbol{x}, t).$$

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$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{u}_h(\boldsymbol{x}, t).$$

- FE approximation;

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$$\frac{d\boldsymbol{x}(t_n)}{dt} = \boldsymbol{u}_h(\boldsymbol{x}, t_n).$$

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- ODE integration scheme:
  - Forward Euler,
  - Runge-Kutta 2/4.

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Evaluation of $\boldsymbol{u}_h^n$ at arbitrary positions is required.

Particles advection

After the advection, we need to find the current cell for each particle.

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After the advection, we need to find the current cell for each particle.

There are four possibilities:

- in the same cell,
- in a locally owned cell,
- in a ghost cell,
- outside the subdomain known by the processor.

Mesh refinement

Two steps:

1. mesh locally refined or coarsened;
2. load balancing.

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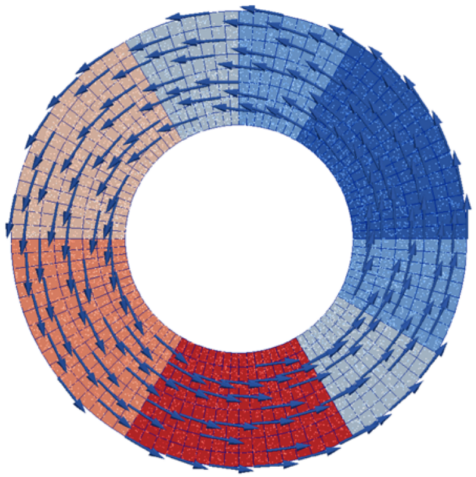
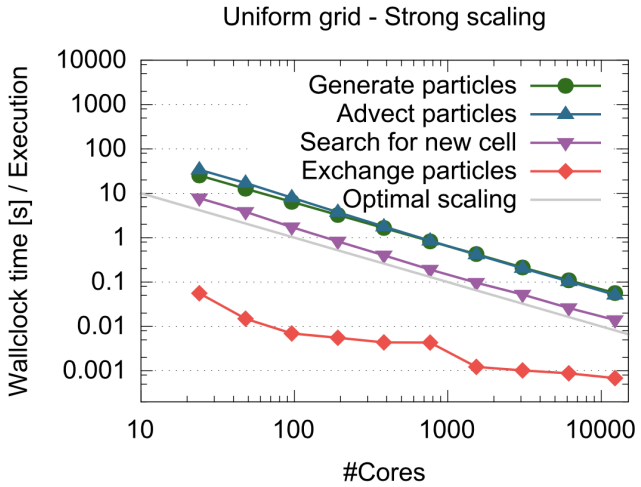
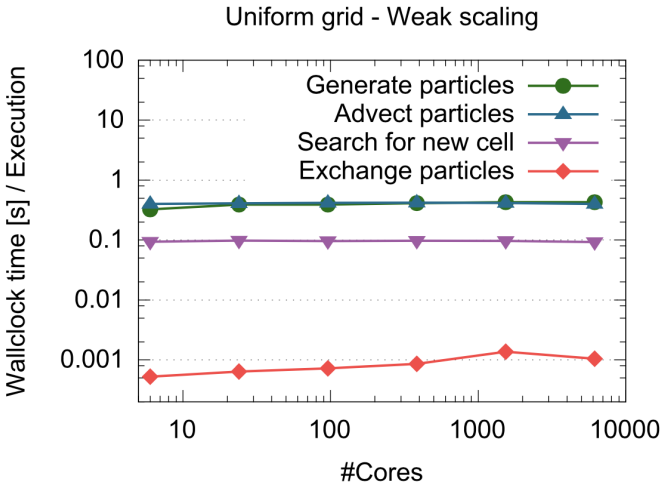
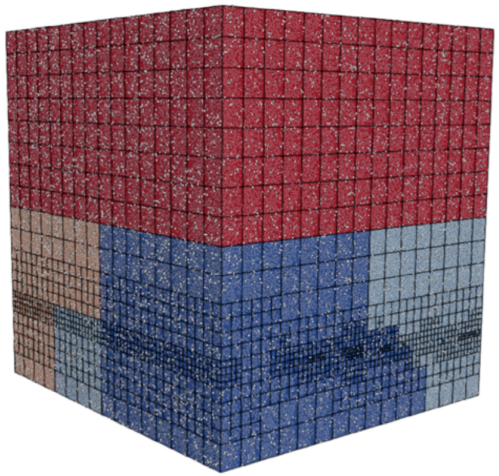
At the end of Step 1 we need to find current cell for each particle.

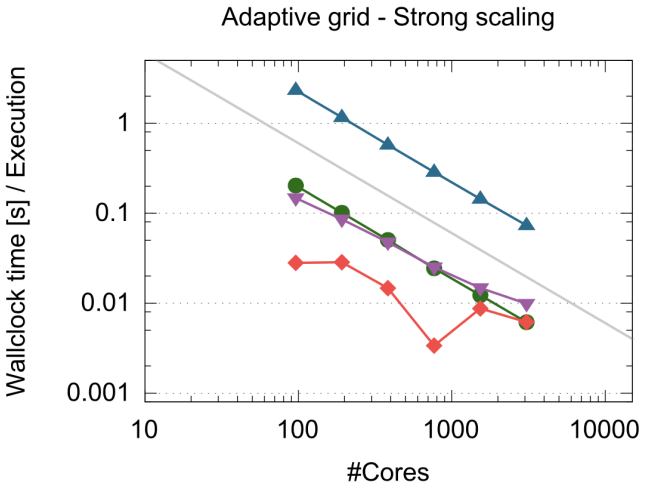
Scalability

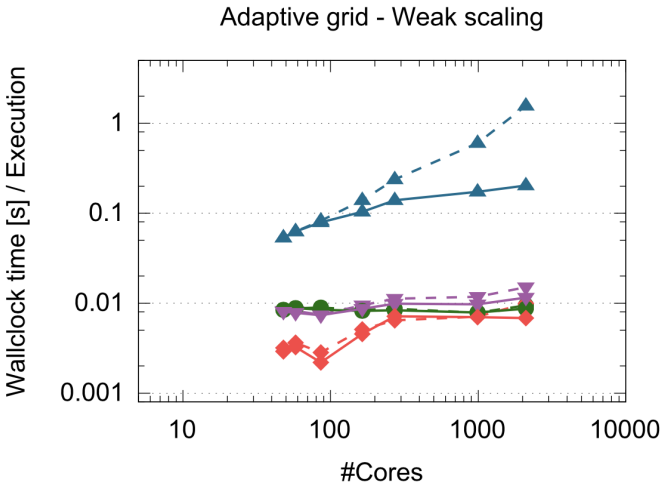












The inverse map problem

How do we compute $\Phi_K^{-1}(\boldsymbol{x})$?

- K hypercube $\longrightarrow$ Φ_K affine $\longrightarrow$ $\Phi_K^{-1}(\boldsymbol{x})$ trivial.
- K not hypercube $\longrightarrow$ Φ_K higher order polynomial $\longrightarrow$ $\Phi_K^{-1}(\boldsymbol{x})$?

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Newton-Raphson algorithm

- start ($i = 0$) from an *initial guess* $\boldsymbol{\alpha}^{(0)} \in \hat{K}$.
- **while** ($|\Phi_K(\boldsymbol{\alpha}^{(i)}) - \boldsymbol{x}| > \epsilon$):
  - $\boldsymbol{\alpha}^{(i+1)} = \boldsymbol{\alpha}^{(i)} - \mathbf{J}_{\Phi_K}^{-1}(\boldsymbol{\alpha}^{(i)}) \cdot (\Phi_K(\boldsymbol{\alpha}^{(i)}) - \boldsymbol{x})$,
  - i += 1;

Polynomial Inverse Mapping

We would like to:

- define Φ_K^{-1} not as an iteration but as a direct (polynomial) map

$$\Psi_K : K \longmapsto \hat{K},$$

  where possibly $\deg(\Phi_K) \neq \deg(\Psi_K)$;

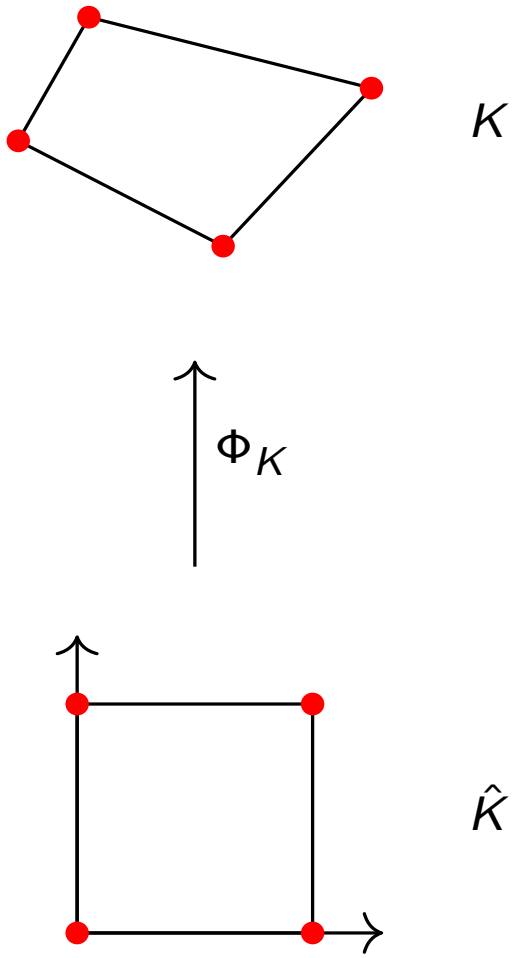
- exploit the off-line VS on-line paradigm.

The off-line part

Given $m \in \mathbb{N}$ (the *inverse map degree*) and given $\mathcal{T}_h$,

$\forall K \in \mathcal{T}_h$:

- find the bounding box $\mathcal{BB}_K$;
- define the support points of order m on $\mathcal{BB}_K$;
- find their pre-images using Newton (and store them).



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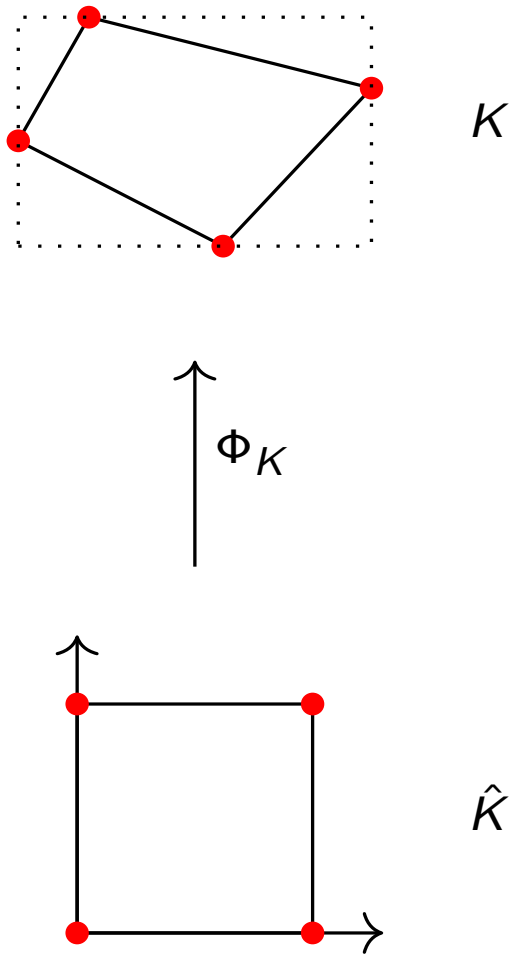

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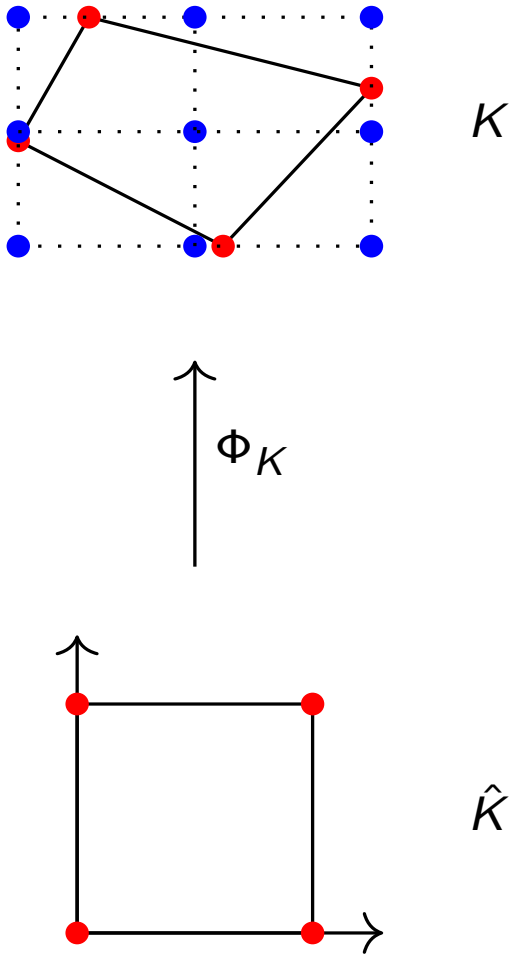

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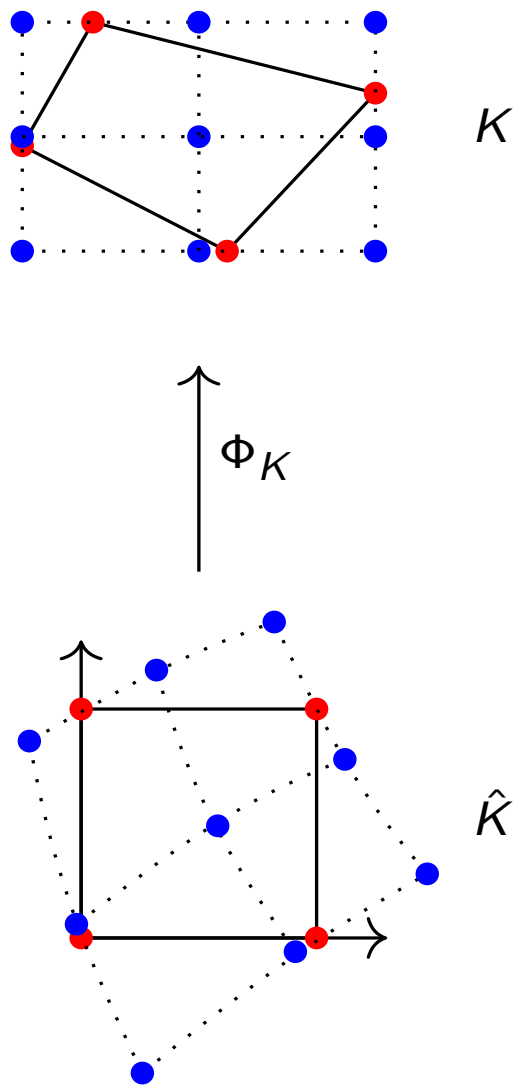

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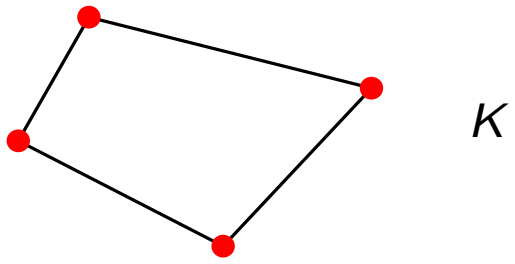

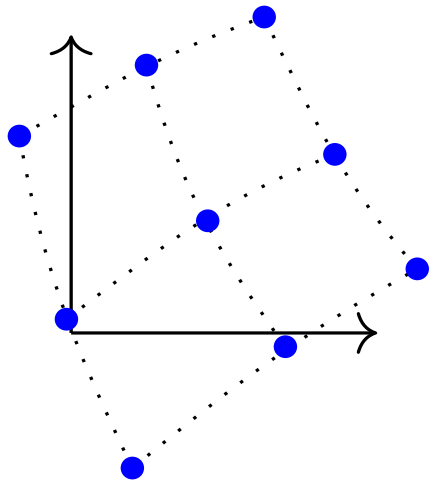

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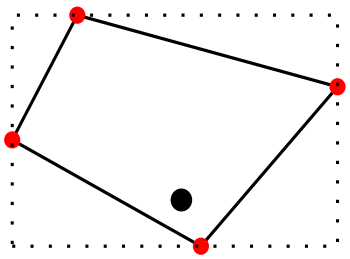

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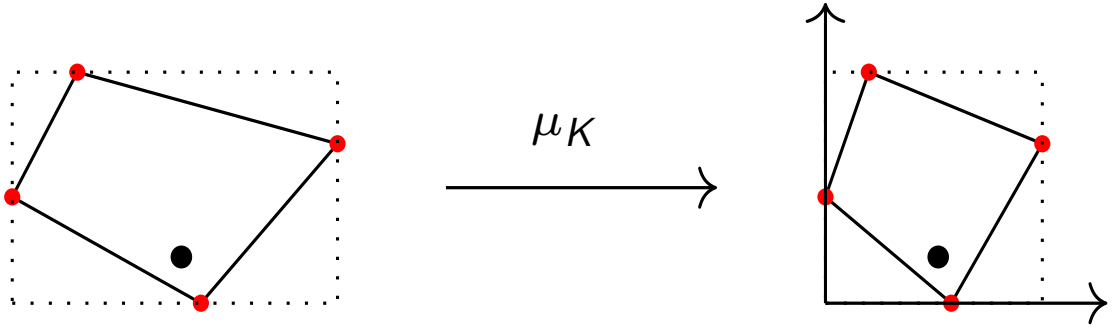

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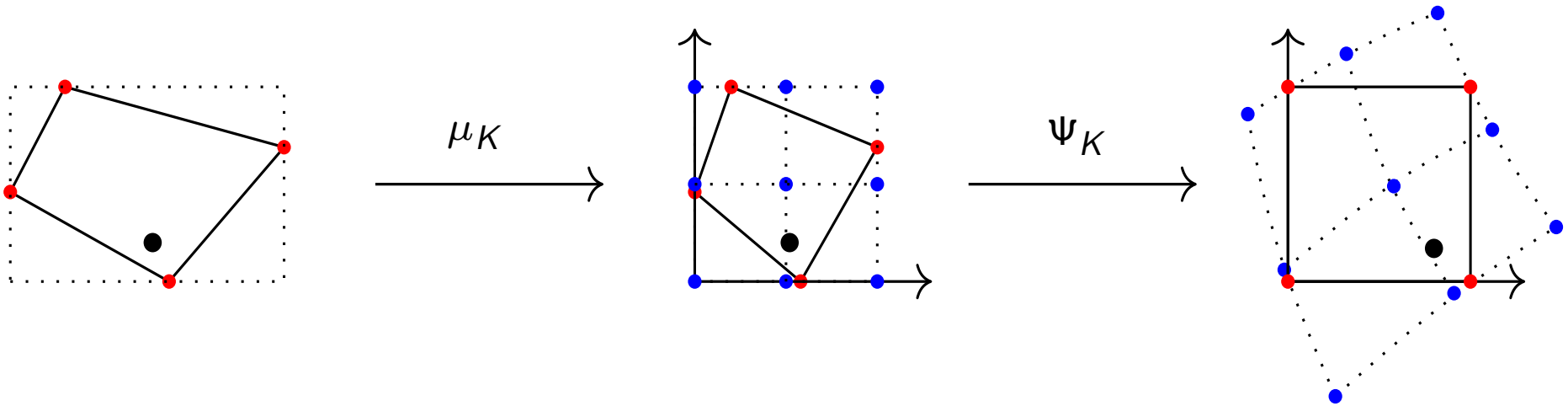

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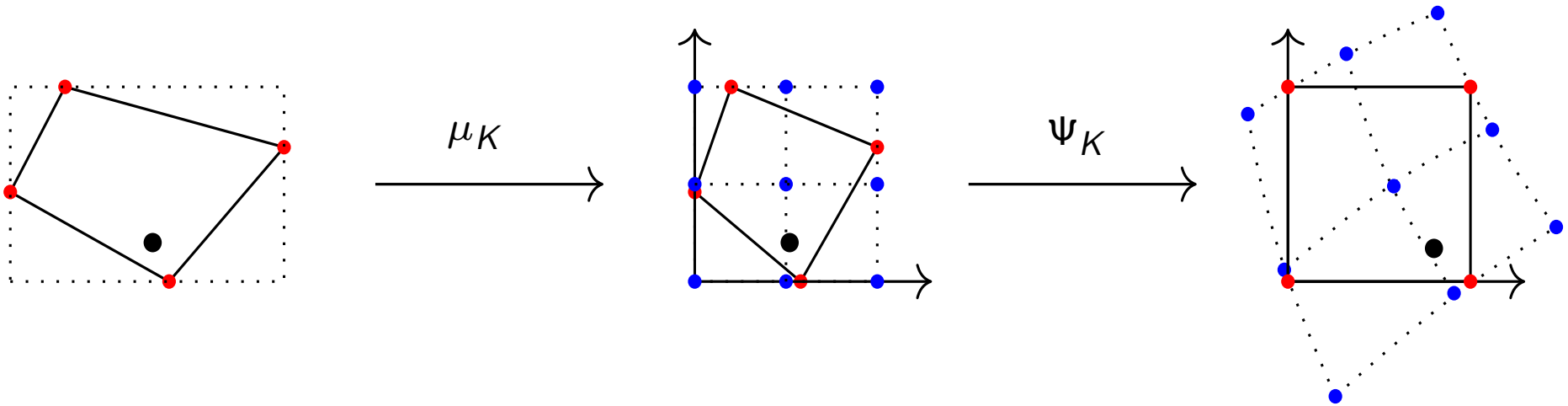
Ψ_K is the polynomial function that maps blue dots to blue dots.

The on-line part



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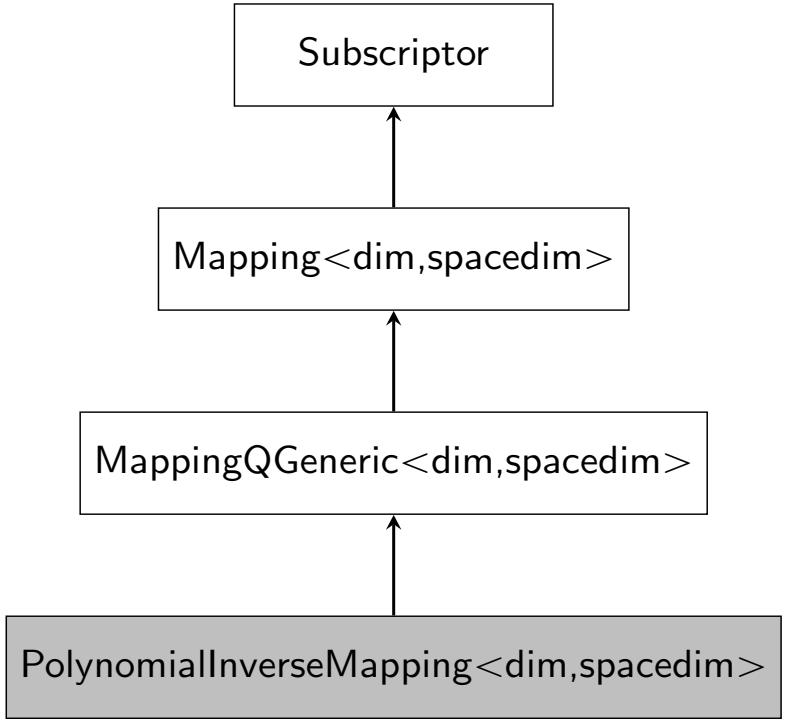
Ψ_K is the polynomial function that maps blue dots to blue dots.

$\Longrightarrow$ if $\Psi_K(q) \in \hat{K}$ then $p \in K$, i.e. $\Phi_K^{-1} \doteq \Psi_K \circ \mu_K$.

PIM class: derivation in deal.ii

"[$\cdots$] This flexibility is conveniently mapped onto implementations in object-oriented programming languages by defining interface classes for each step. Concrete algorithms can then be implemented in the form of derived classes."



PIM class: public member functions

- Constructor

```
PolynomialInverseMapping(int forward_degree, int inverse_degree);
```

- Off-line part

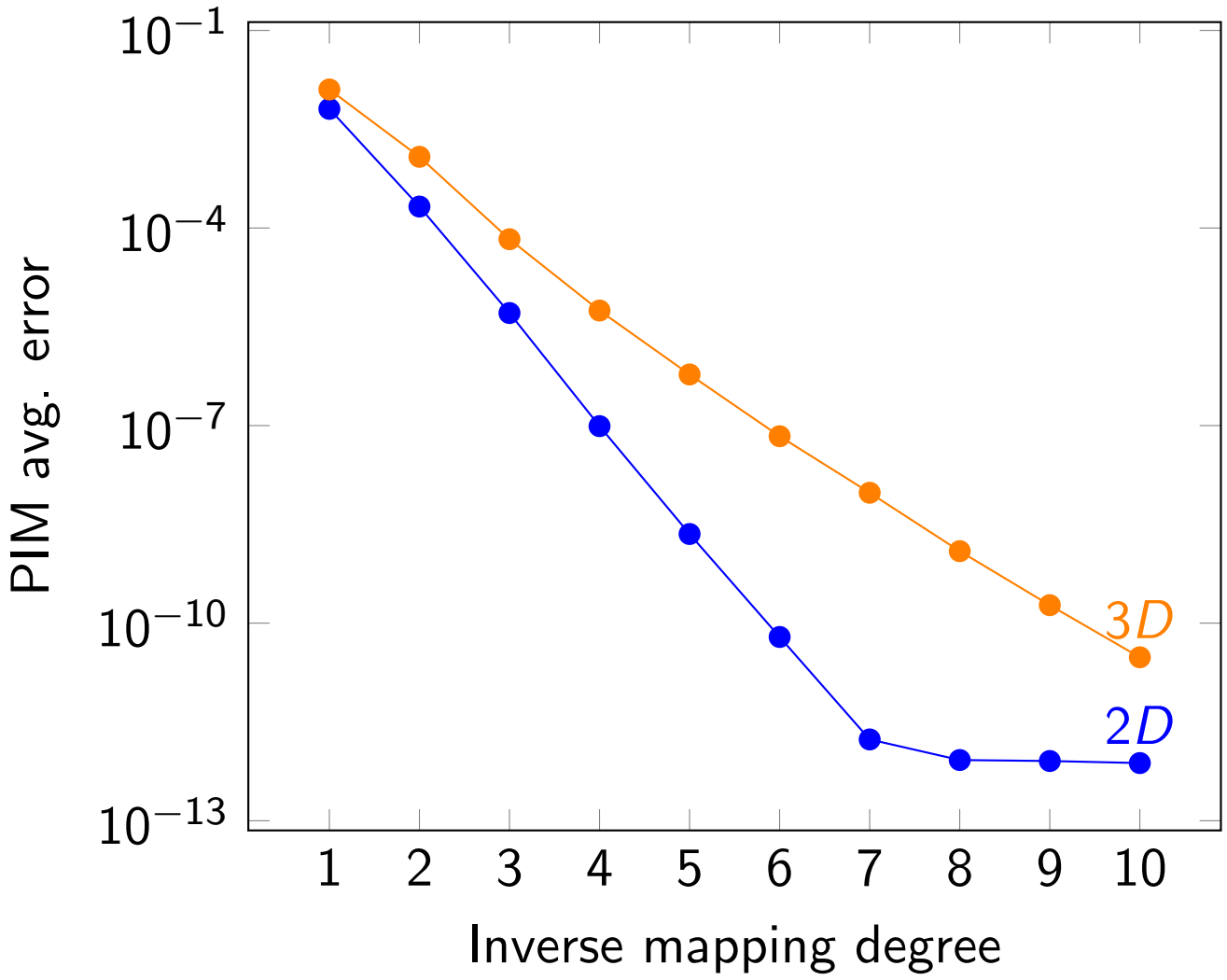
```
void initialize(const Triangulation<dim> &tria);
```

- On-line part

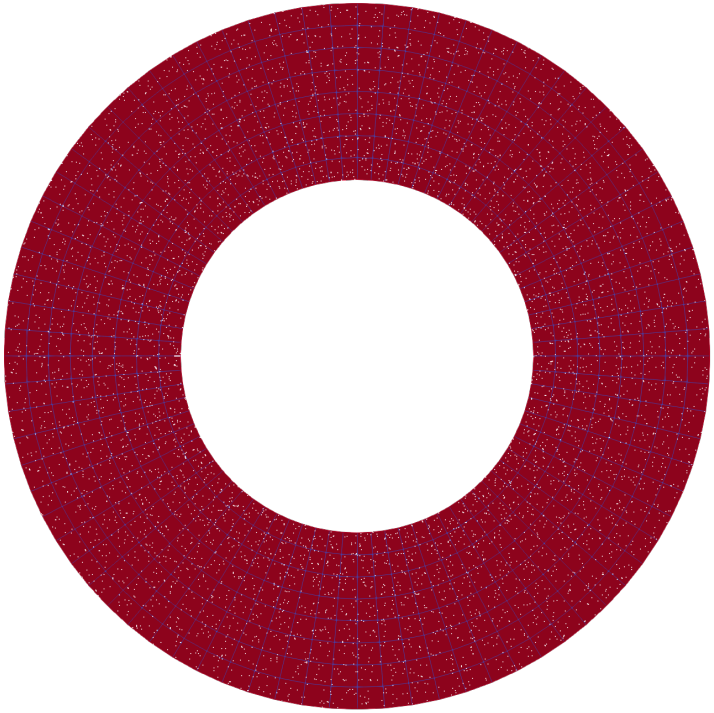
```
virtual
Point<dim> transform_real_to_unit_cell(
            const typename Triangulation<dim>::cell_iterator &cell,
            const Point<dim> &p
            ) const override;
```

PIM class: results (1)

Newton avg. error $\sim 10^{-13}$.



PIM class: results (2)

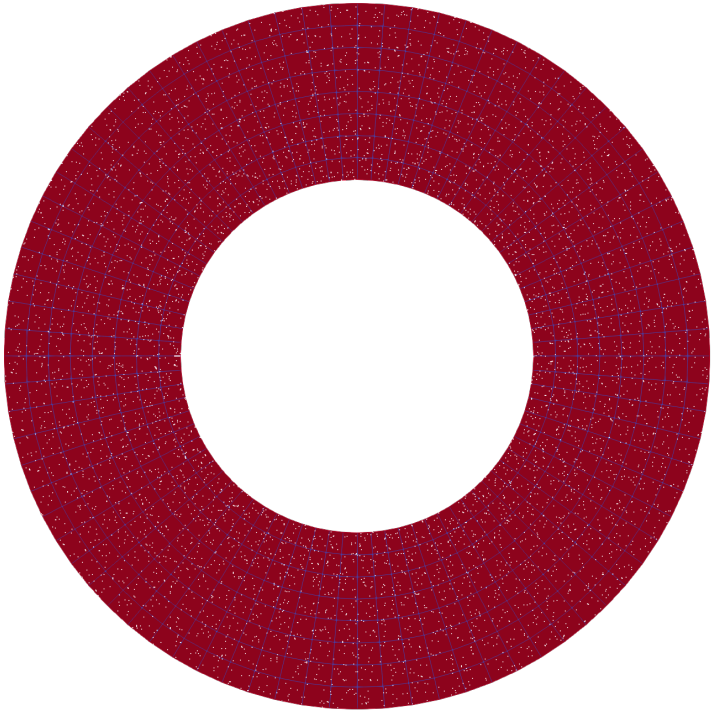


- Forward degree = 2,
- Inverse degree = 3.

Total CPU time elapsed since start : 0.509s.

(1) Newton: 0.0618s (12%),
(2) OFF-line: 0.134s (26%),
(3) IN-line: 0.122s (24%).

PIM class: results (3)



- Forward degree = 3,
- Inverse degree = 2.

Total CPU time elapsed since start : 0.518s.

(1) Newton: 0.0879s (17%),
(2) OFF-line: 0.133s (26%),
(3) IN-line: 0.0862s (17%).

Recap and conclusions

- PIC is a flexible and scalable method for modern CFD simulations.
- Polynomial Inverse Mapping algorithm (PIM) is an attempt to speed up one of the main bottleneck of PIC.
- Unfortunately, PIM is not working good as expected.

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FUTURE WORKS

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- Unfortunately, PIM is not working good as expected.

FUTURE WORKS

- Check for slow parts of the code and try to improve them.
- Try to exploit the last result we showed.

References

1. M. W. Evans, F. H. Harlow, and E. Bromberg. The particle-in-cell method for hydrodynamic calculations.Technical report, Los Alamos National Lab NM, 195

2. R. Gassmöller, H. Lokavarapu, E. Heien, E. G. Puckett, and W. Bangerth. Flexible and scalable particle-in-cell methods with adaptive mesh refinement for geodynamic computations. Geochemistry, Geophysics, Geosystems, 19(9):3596–3604, Sept. 2018

Thanks for your attention