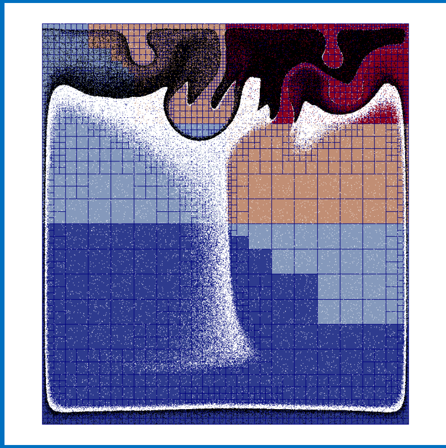
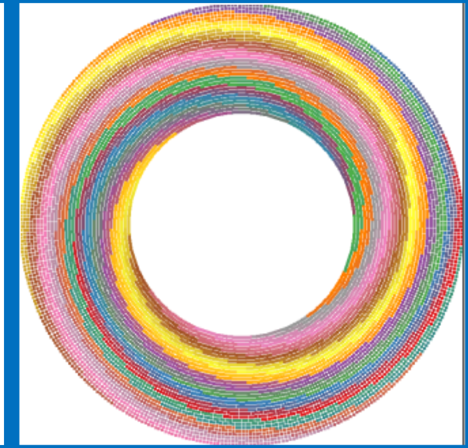
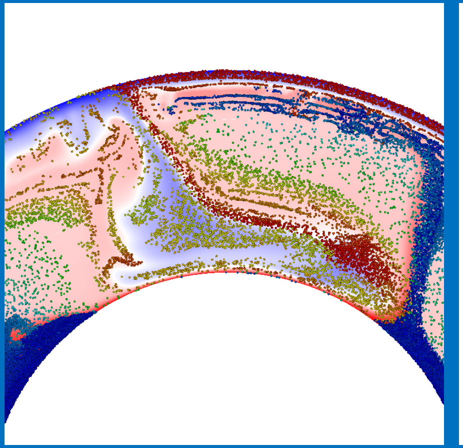
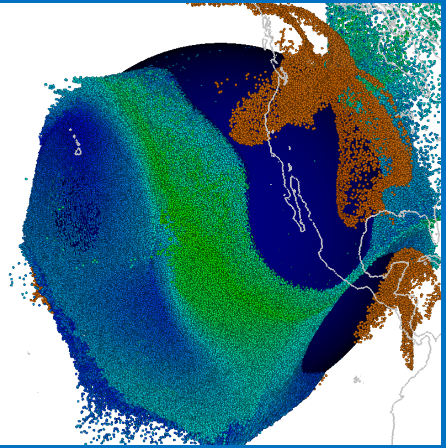
ACCURATELY UTILIZING PARTICLE-IN-CELL METHODS FOR ADAPTIVELY REFINED FINITE-ELEMENT MODELS









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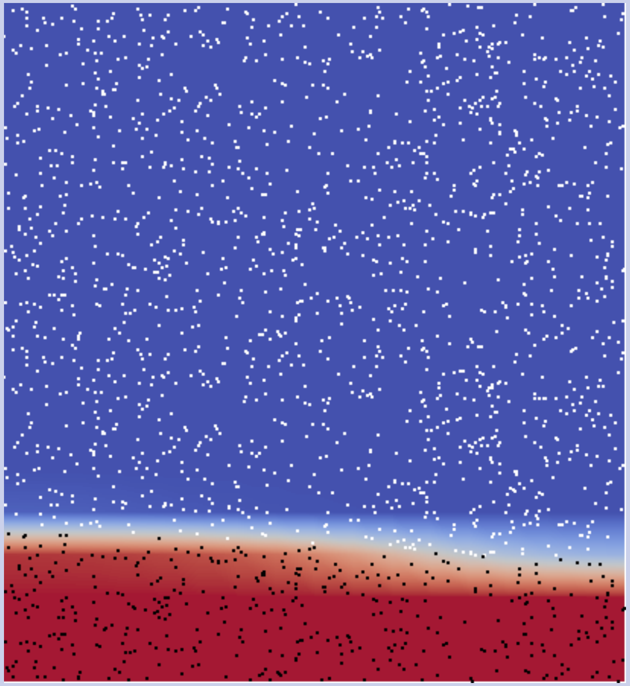
CONCEPTS OF PIC METHODS

$$-\nabla \cdot [2\eta \dot{\varepsilon}(\mathbf{u})] + \nabla p = \rho \mathbf{g} \qquad (1)$$

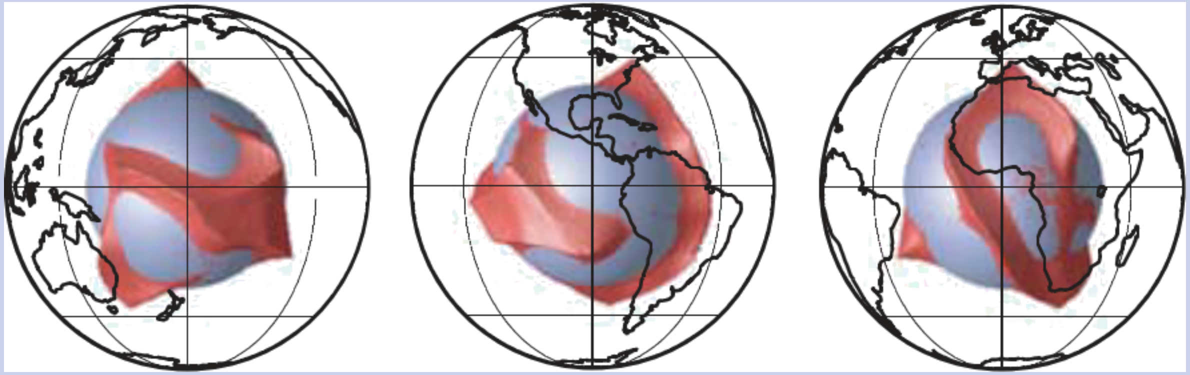
$$\nabla \cdot \mathbf{u} = 0 \qquad (2)$$

$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q - \nabla \cdot (D \nabla q) = 0 \qquad (3)$$

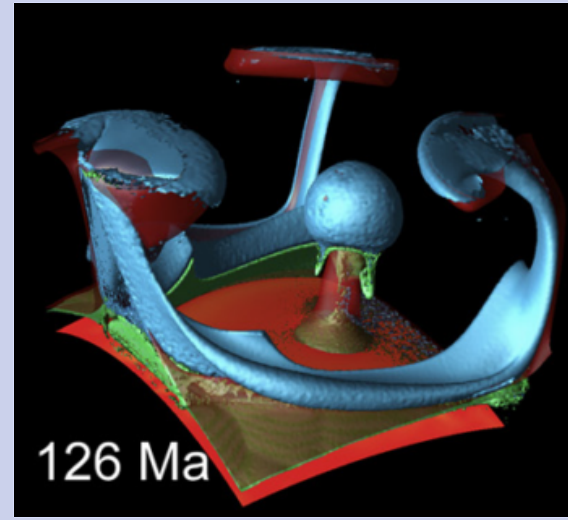


- Method to advect property on discrete particles (/tracers/markers)
- Transforms the PDE in (3) to a set of (non-coupled) ODE's
- Many variants and evolutions (e.g. Particle-in-cell, Evans & Harlow 1957; Marker-and-cell, Harlow & Welch 1965; Marker-in-cell, Gerya 2003; ...)

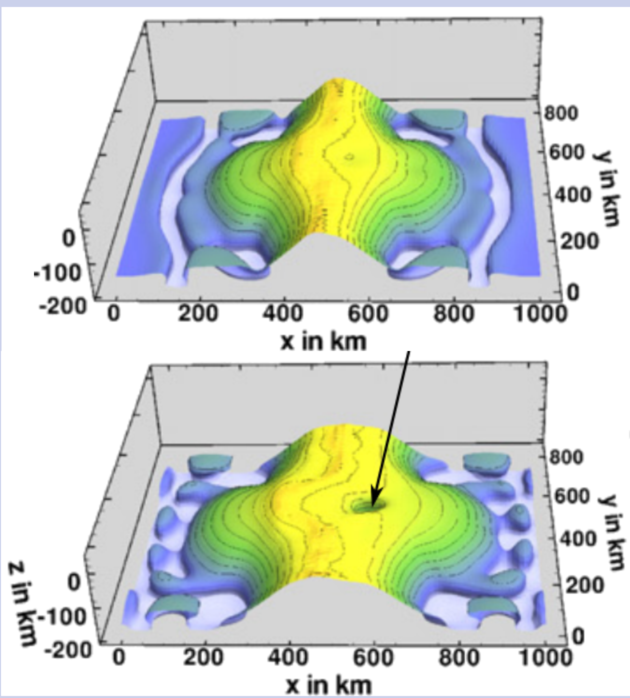
EXAMPLE APPLICATIONS IN GEODYNAMICS



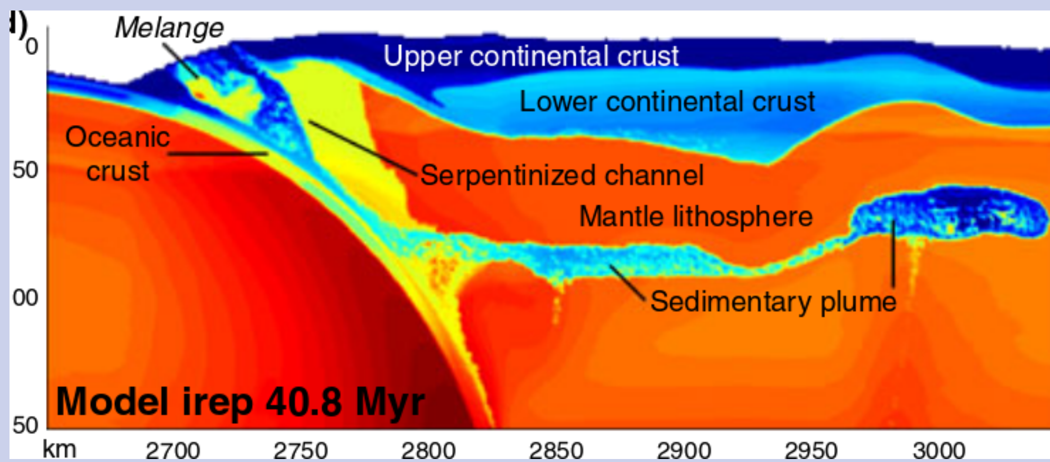
McNamara
& Zhong, 2005



Tackley, 2011



Brune et al., 2013



Gerya & Meilick, 2011

MODERN PARTICLE METHODS:

Challenges when applying Particle methods to modern finite-element codes:

- Quantifying accuracy and convergence behavior
- Load balancing strategies in adaptively refined meshes
- Geometry independent particle-cell search

ACCURACY: CONVERGENCE BEHAVIOR

Known from previous studies:

- Increasing the number of particles per cell converges towards a solution (known from other fields, geodynamics: Tackley & King, 2003)
- Particles do not decrease convergence rate for second order accurate methods if interpolation is accurate enough (Thielmann et al, 2014)
- Suggestion: Particles limit the accuracy of the velocity solution to at most second order (Thielmann et al, 2014)

Our goal:

- Quantify the influence of the particles on the accuracy of the solution, in particular in dependence of number of particles per cell (PPC)?
- Is it possible to increase the convergence rate above second order?

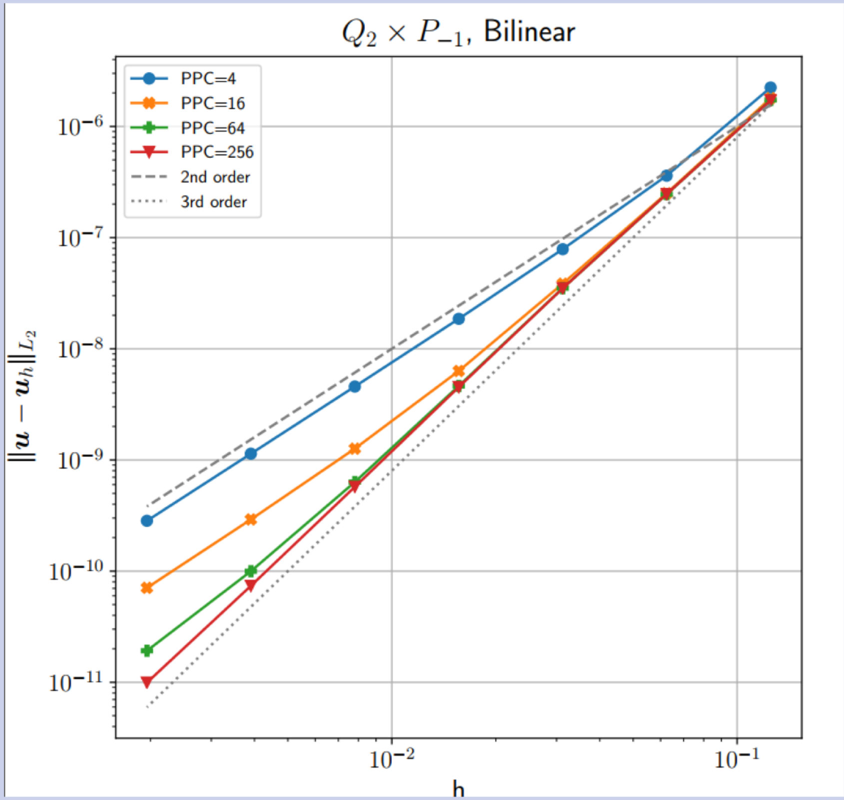
Our approach:

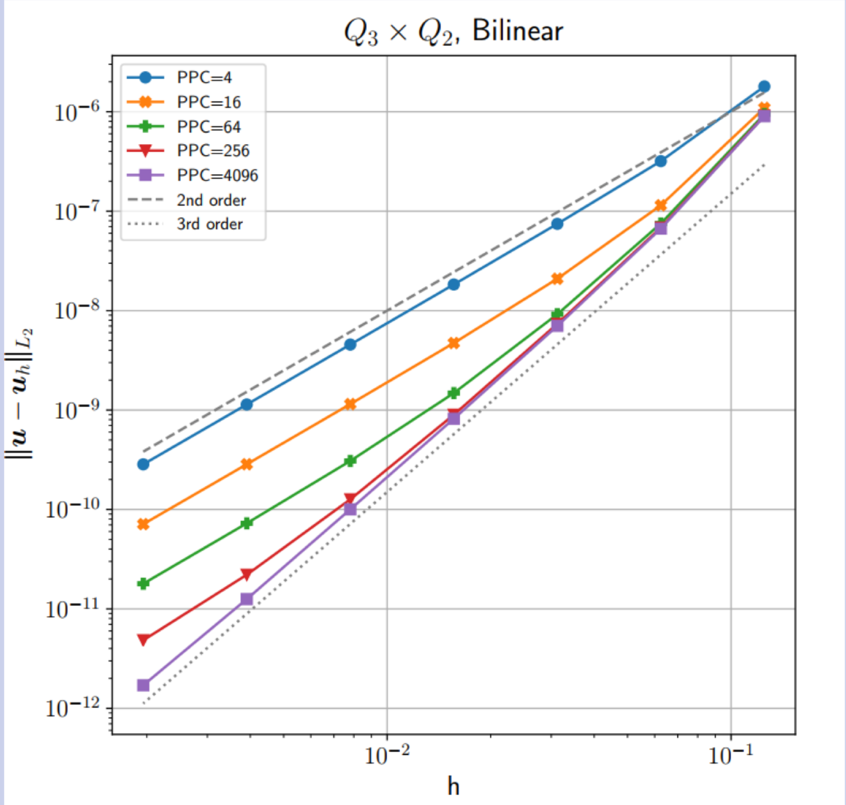
- Use existing instantaneous benchmarks and quantify accuracy for different FEs, different interpolation schemes, and different PPC
- Develop a theoretical understanding of the underlying error sources
- Develop a new time-dependent benchmark with analytical solution

ACCURACY: CONVERGENCE BEHAVIOR

Using the SolKz (Duretz et al., 2011) benchmark:

- For constant PPC: 2nd order velocity convergence (like Thielmann et al, 2014)
- For increasing PPC with resolution: 3rd order velocity convergence
- Even for a Q3xQ2 element: 3rd order convergence (expected: 4th order)

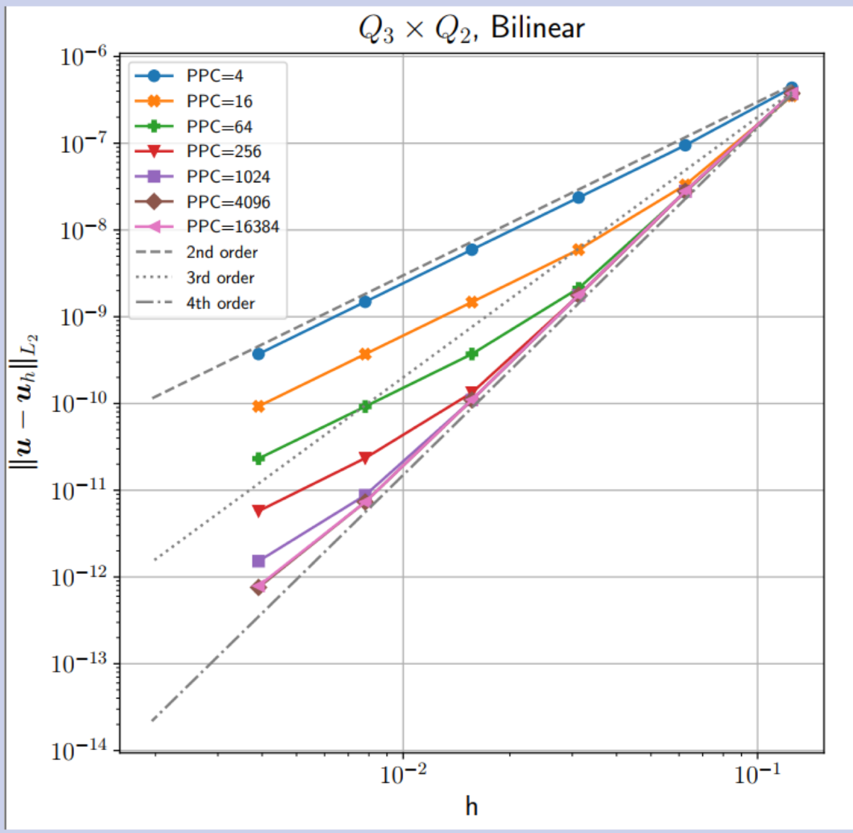


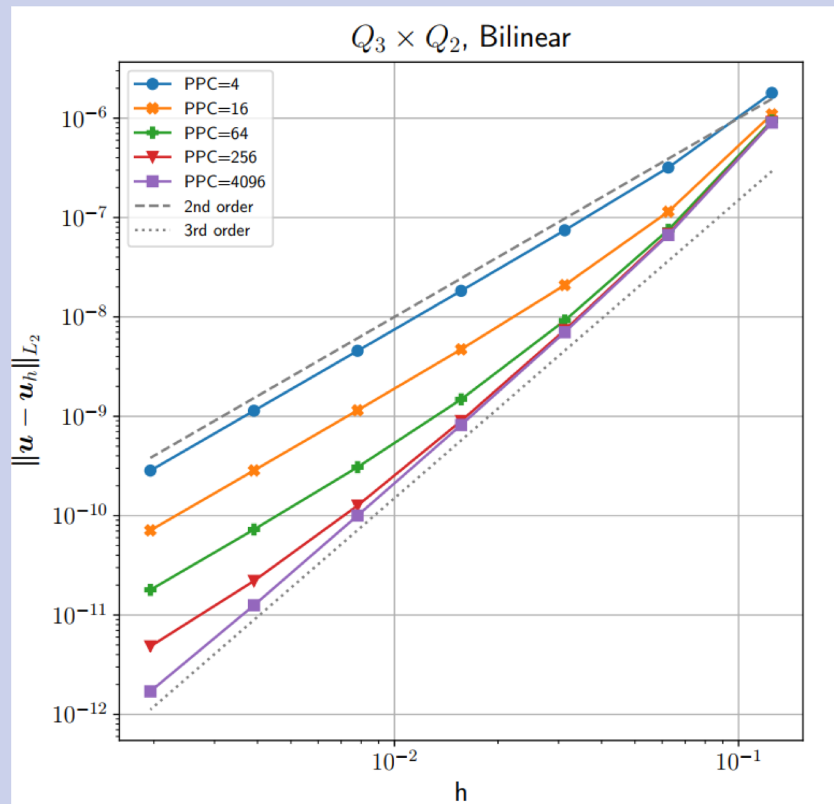


ACCURACY: CONVERGENCE BEHAVIOR

Using the SolKz benchmark:

- For an analytic viscosity: up to 4th order velocity convergence
- In general: Viscosity on particles limits convergence more strictly





ACCURACY: THEORETICAL ERROR

Total error = difference between continuous and discretized Stokes operator and properties:

(1) Error by density approximation
(2) Error by viscosity approximation
(3) Error by evaluation at particle locations
(4) Error by finite element approximation

$$
\begin{aligned}
\left(\eta_0 \|\nabla(\boldsymbol{u}-\boldsymbol{u}_h)\|_{L_2}^2 + \|p-p_h\|_{L_2}^2\right)^{1/2}
&= |||\mathcal{L}_\eta(\rho \boldsymbol{g}) - \mathcal{L}^h_{\eta_h}(\rho_h \boldsymbol{g})||| \\
&\le \underbrace{|||\mathcal{L}_\eta(\rho \boldsymbol{g}) - \mathcal{L}_\eta(P_h \rho\, \boldsymbol{g})|||}_{(1)} \\
&\quad + \underbrace{|||\mathcal{L}_\eta(P_h \rho\, \boldsymbol{g}) - \mathcal{L}_{P_h \eta}(P_h \rho \boldsymbol{g})|||}_{(2)} \\
&\quad + \underbrace{|||\mathcal{L}_{P_h \eta}(P_h \rho\, \boldsymbol{g}) - \mathcal{L}_{\eta_h}(\rho_h \boldsymbol{g})|||}_{(3)} \\
&\quad + \underbrace{|||\mathcal{L}_{\eta_h}(\rho_h \boldsymbol{g}) - \mathcal{L}^h_{\eta_h}(\rho_h \boldsymbol{g})|||}_{(4)}.
\end{aligned}
$$

ACCURACY: THEORETICAL ERROR

Velocity error:

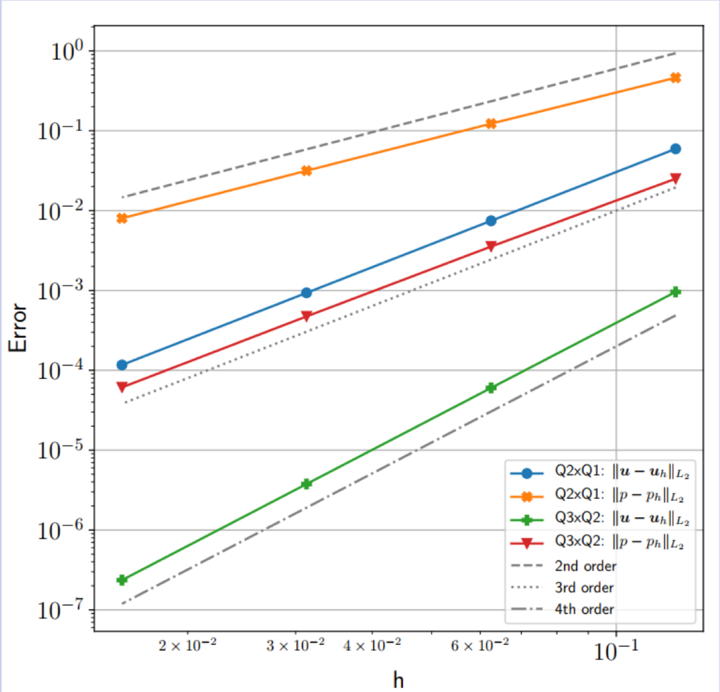
$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L_2} = \mathcal{O}(h^{r+2}) + \mathcal{O}(h^{r+1}) + \mathcal{O}(h\,E(h, PPC)) + \mathcal{O}(h^{k+1}).$$

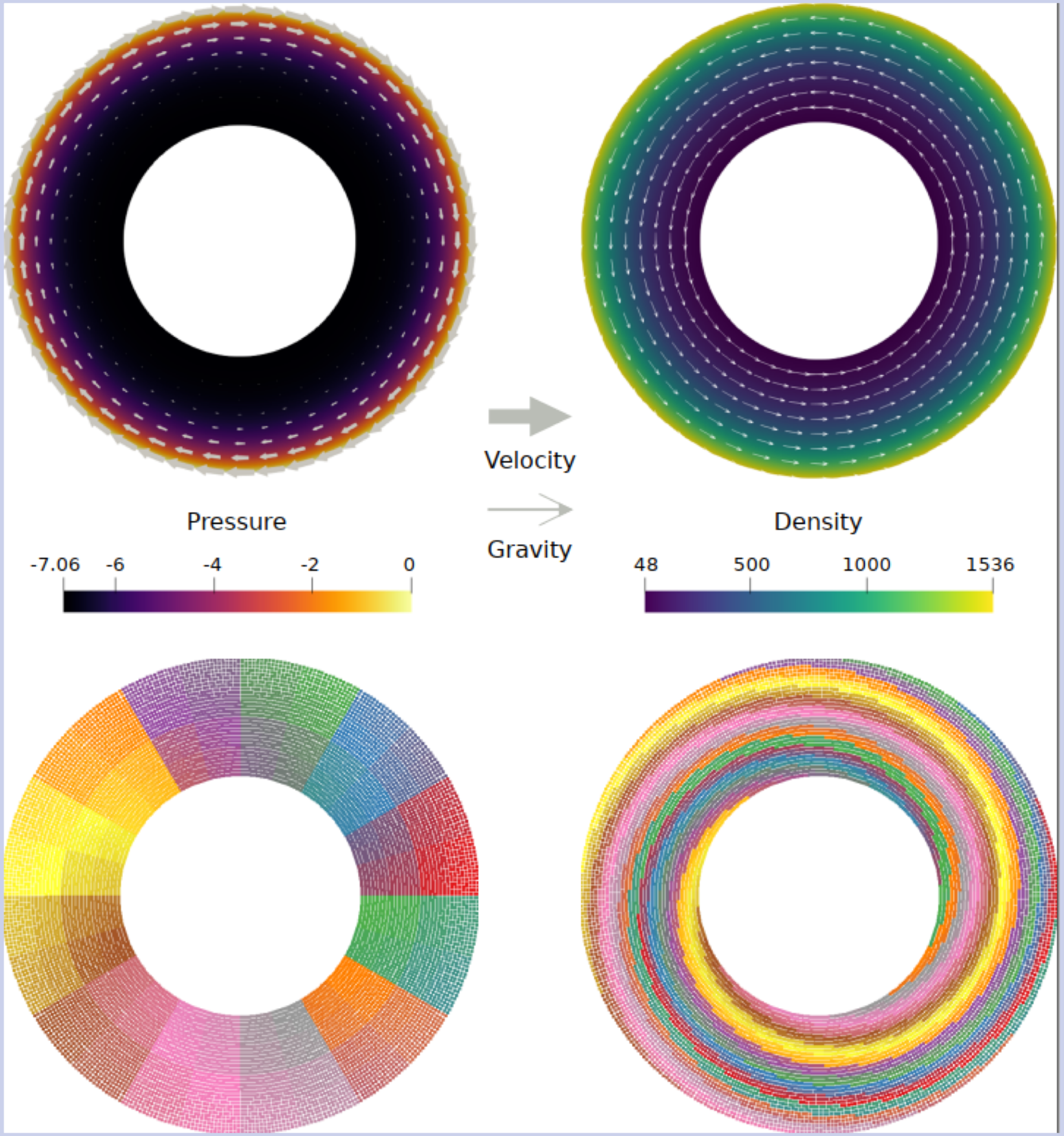
- The convergence order of the interpolation method (r) places an upper limit on the velocity accuracy, just like the choice of finite element degree (k)
- This upper limit depends on whether particles only carry density (r+2) or also viscosity (r+1)
- There is a hard to quantify term E that depends on PPC and h (we will experimentally try to estimate this term next)

ACCURACY: NEW BENCHMARK

New benchmark: Circular flow

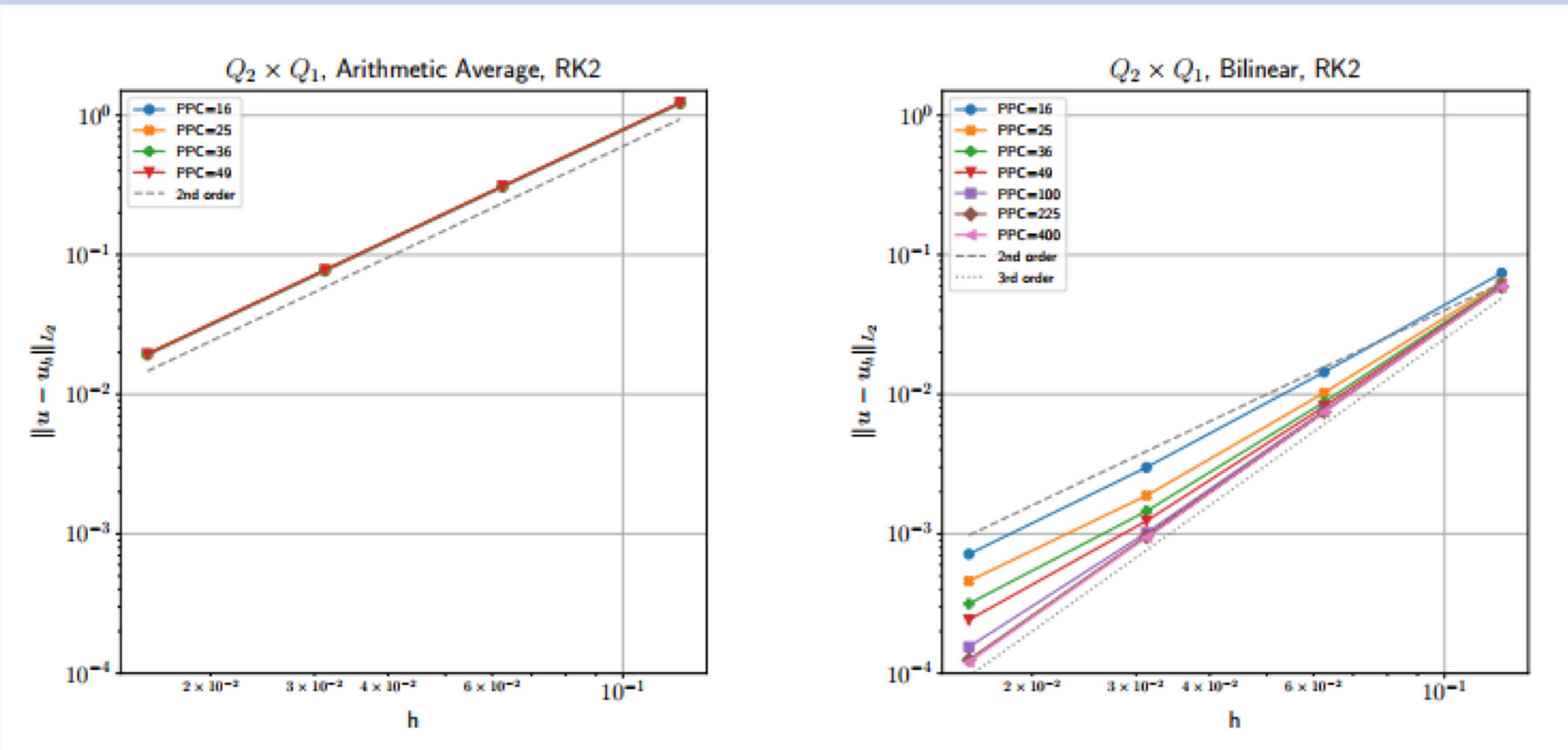
- Analytical solution: Time independent
- Numerical solution : Time dependent error
- Pure FE method reaches design convergence





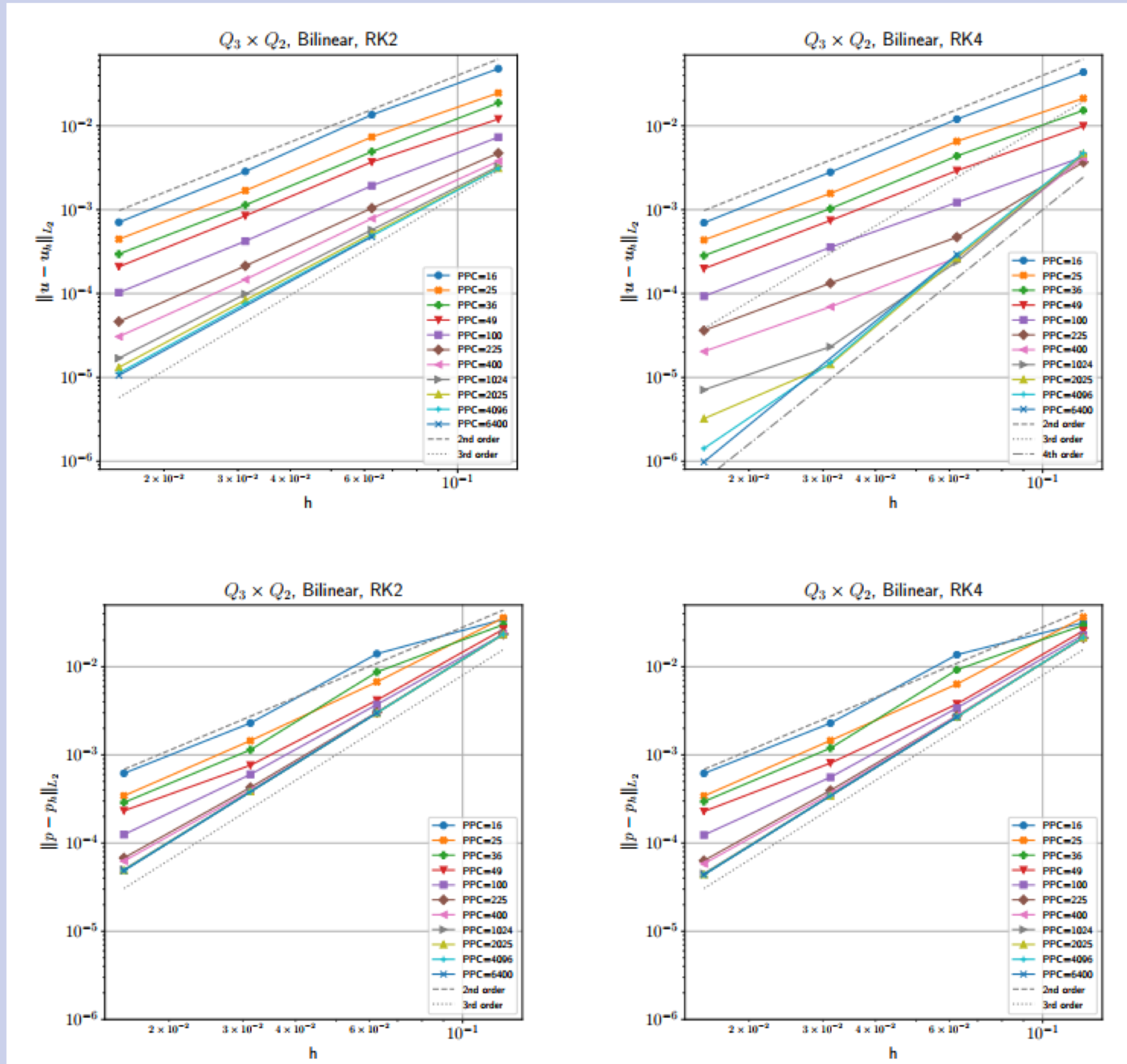
ACCURACY: CONVERGENCE BEHAVIOR

A comparison of different interpolation methods (arithmetic average vs bilinear least squares approximation) shows expected results:



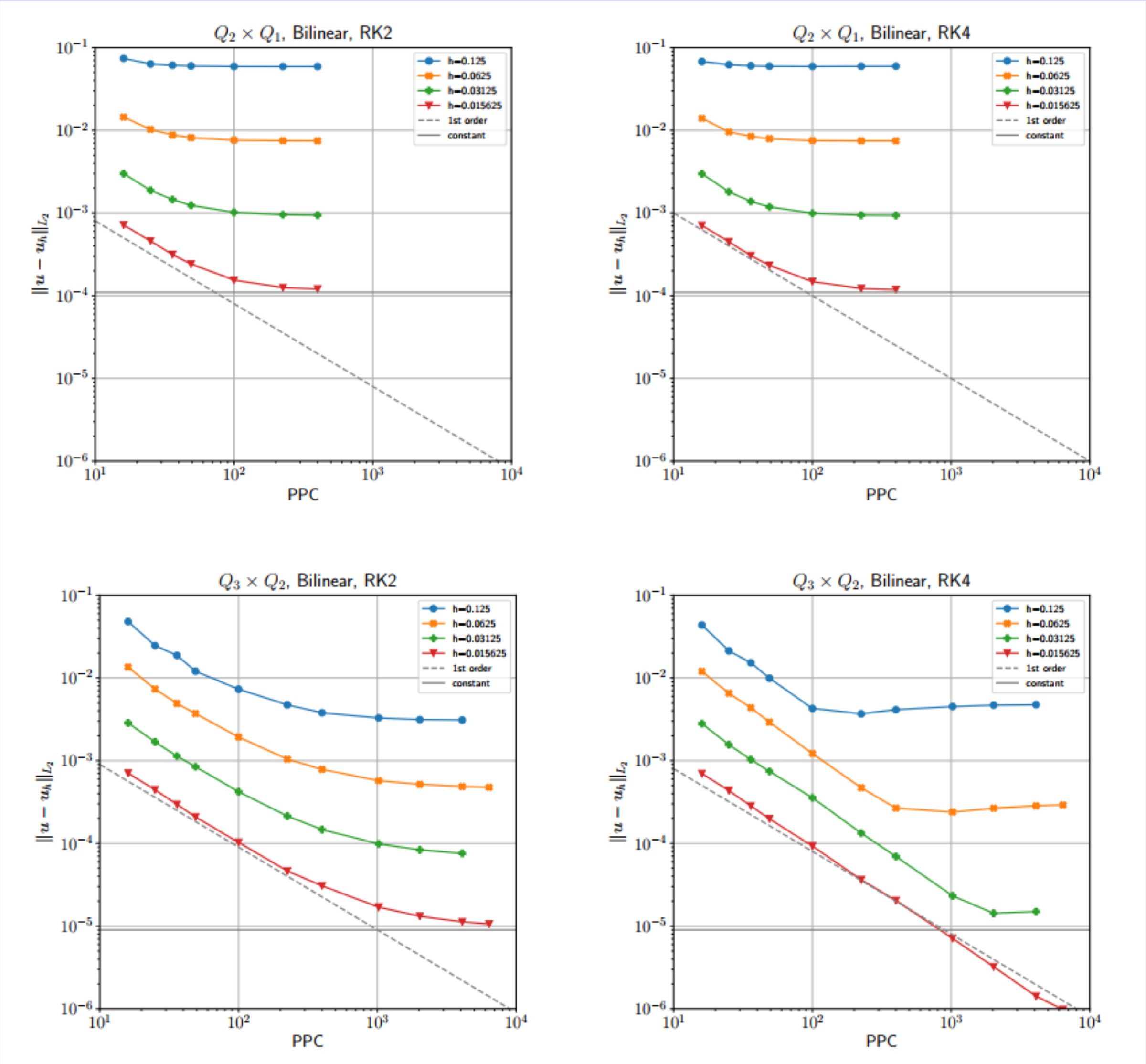
ACCURACY: CONVERGENCE BEHAVIOR

- Particle advection scheme also limits the accuracy, but only for higher order elements
- Q2xQ1 element shows optimal convergence with RK2 integrator
- Q3xQ2 requires higher order (e.g. RK4)



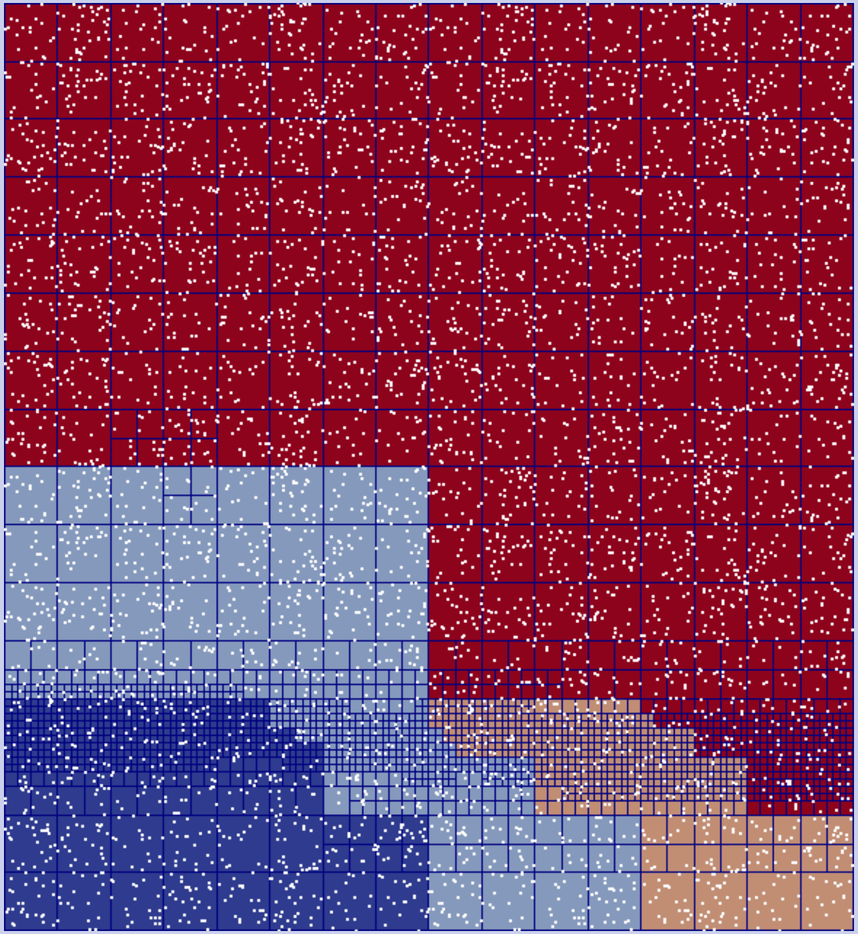
ACCURACY: CONVERGENCE BEHAVIOR

- Results for FE order, interpolation and advection scheme shows: E(h,PPC)~1/PPC
- Thus for optimal convergence (Q2Q1): PPC ~h (Q3Q2): PPC ~h^2
- For typical resolutions PPC <= 100 in 2D (<= 1000 in 3D)
- Scalability?



SCALABILITY: LOAD BALANCING

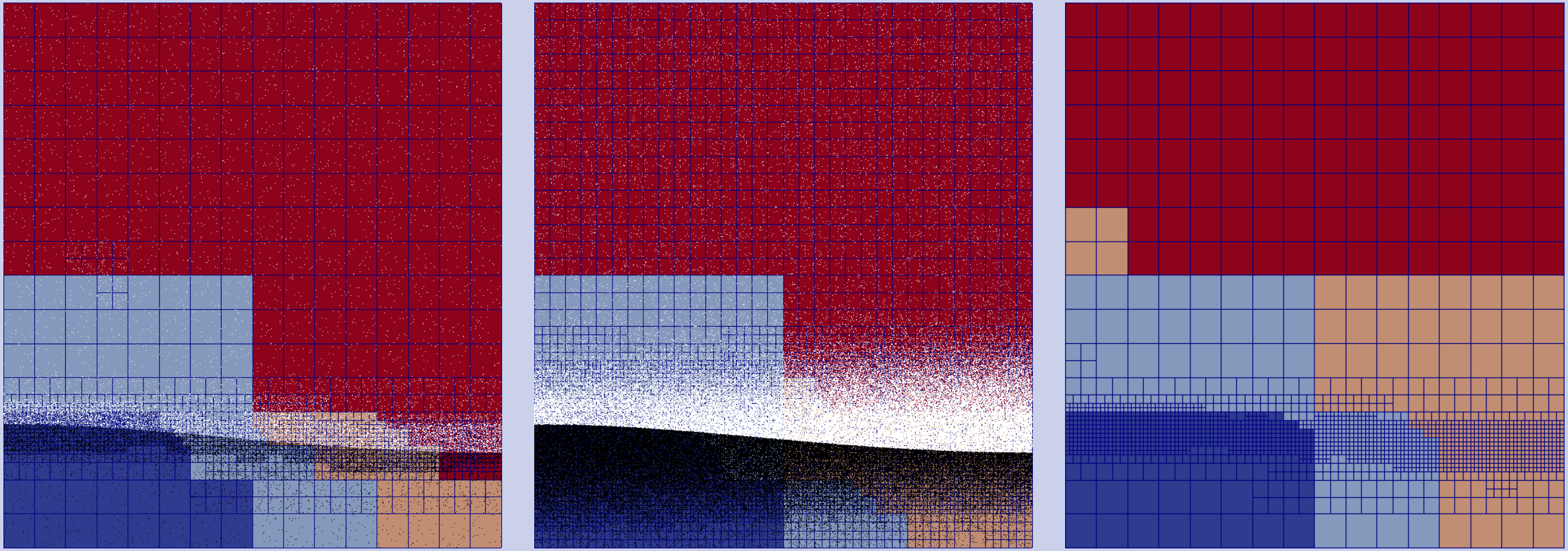
How to balance particle and cell work for adaptive meshes?



- Partitioning of domain by number of cells per process
- For uniform particle density large imbalance in particle work
- Imbalance grows with number of mesh levels
  - ➢ Limited scalability

SCALABILITY: LOAD BALANCING

Particle Management: Variable Distribution: Balanced Repartition:



Particle Management:

- Introduce particle population management
- Remove/add particles according to mesh
- Adds diffusion to particle properties

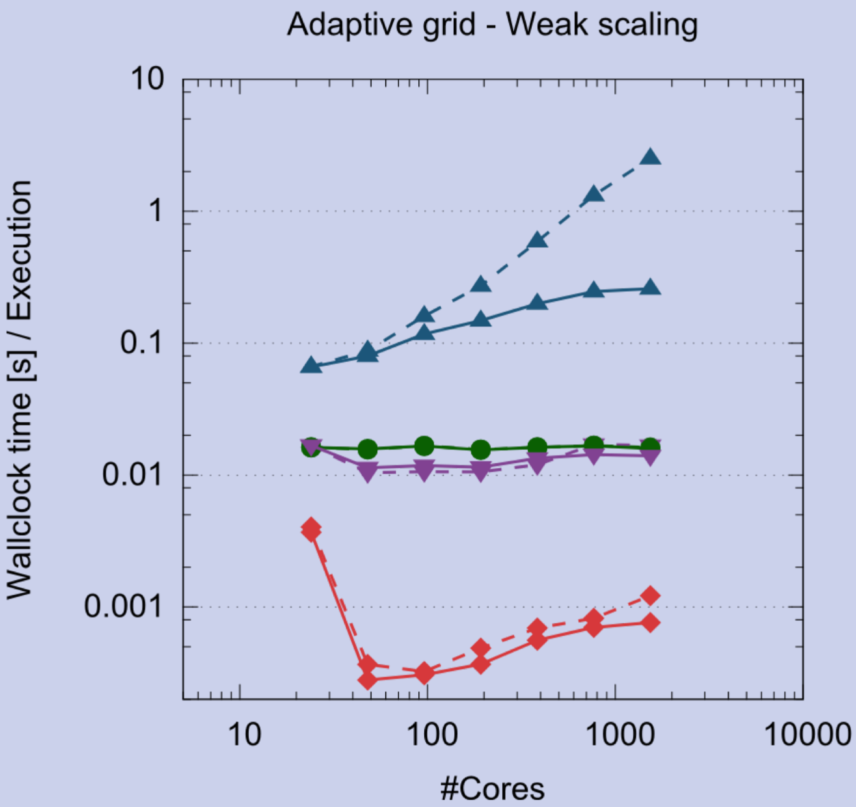
Variable Distribution:

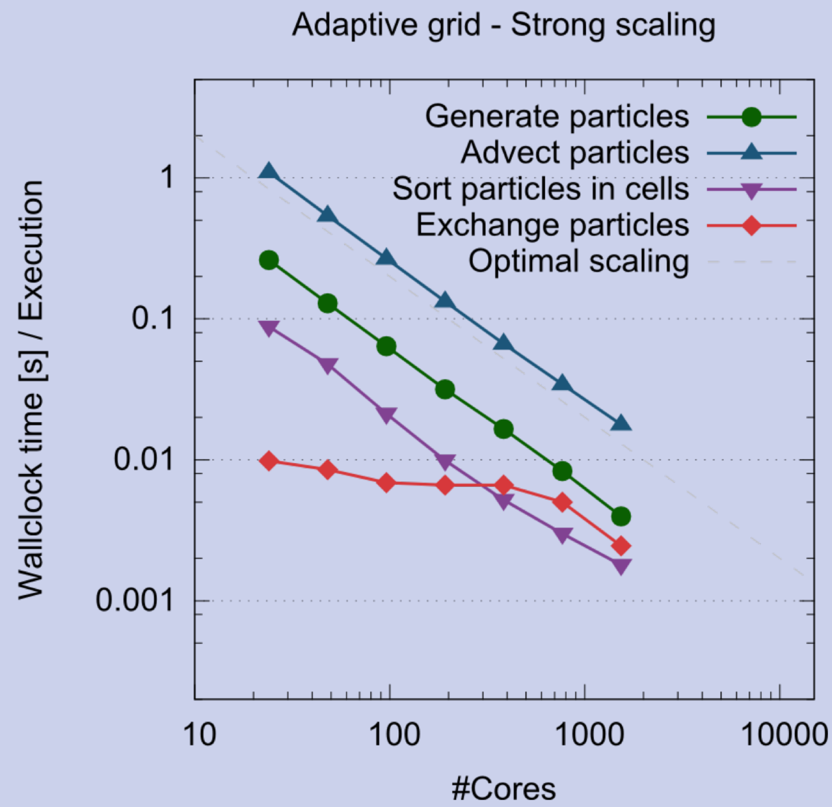
- Generate variable particle distribution
- Adjust mesh according to particles
- Requires a known region of interest

Balanced Repartition:

- Adjust parallel partition of mesh
- Retains identical solution
- Reaches reasonable scalability

SCALABILITY: LOAD BALANCING

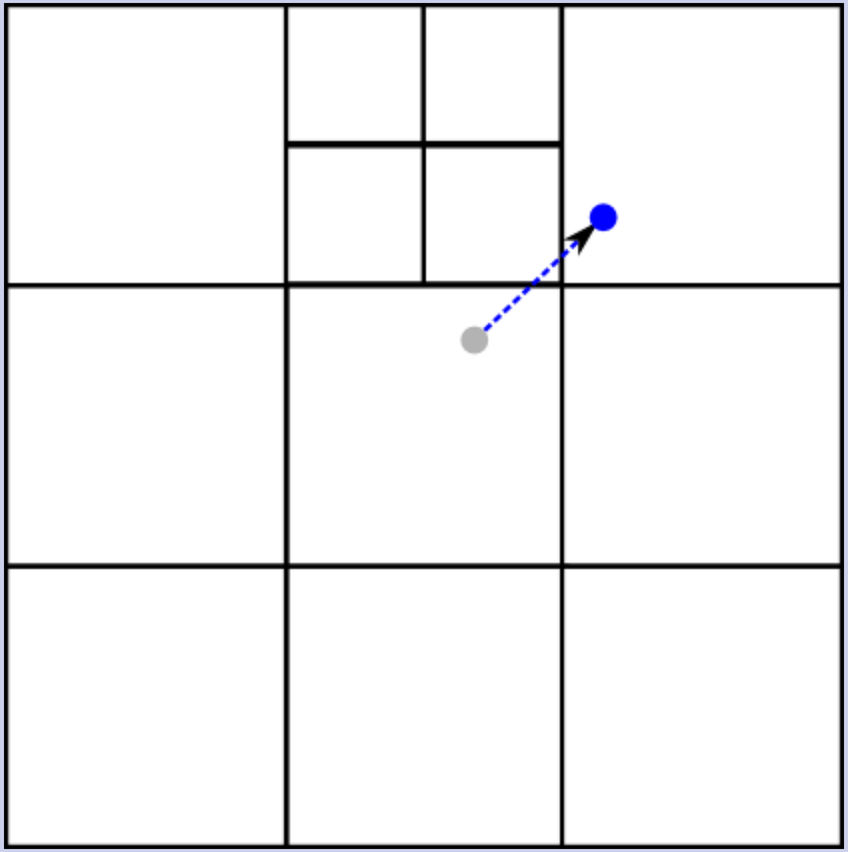




- Weak scaling dependent on load balancing technique
- Optimal strong scalability independent of technique

EFFICIENCY: GEOMETRY INDEPENDENT

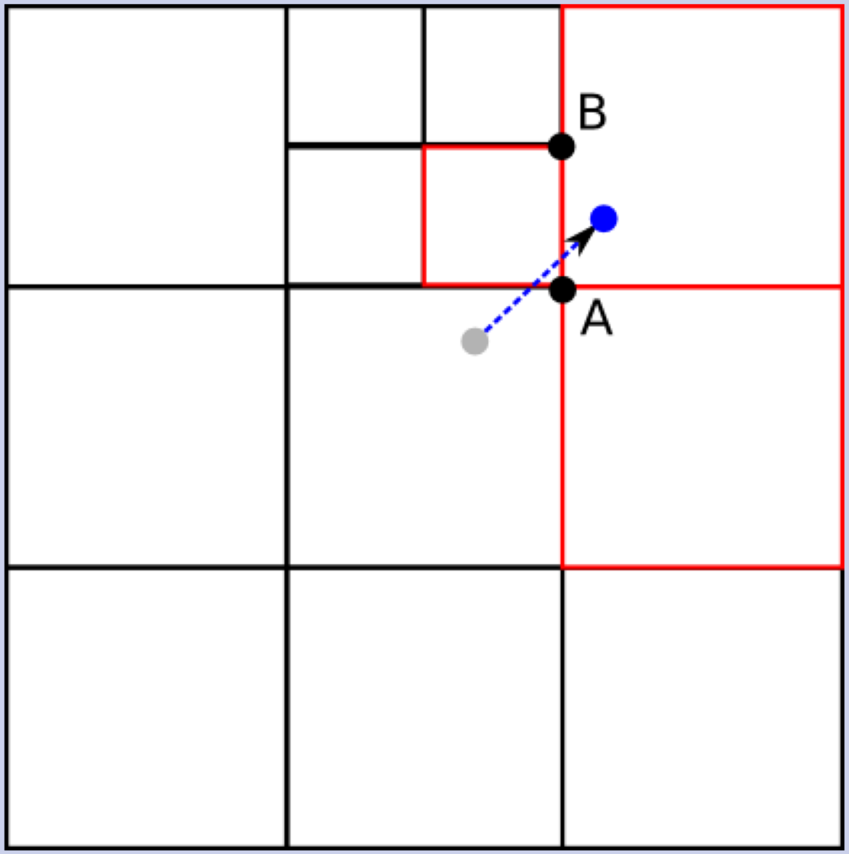
Which cell did a certain particle move to?



- Independent of geometry
- Dynamically changing mesh
- Only assumptions:
  - Quadrilateral cells
  - Hierarchical refinement
  - CFL timestep

EFFICIENCY: GEOMETRY INDEPENDENT

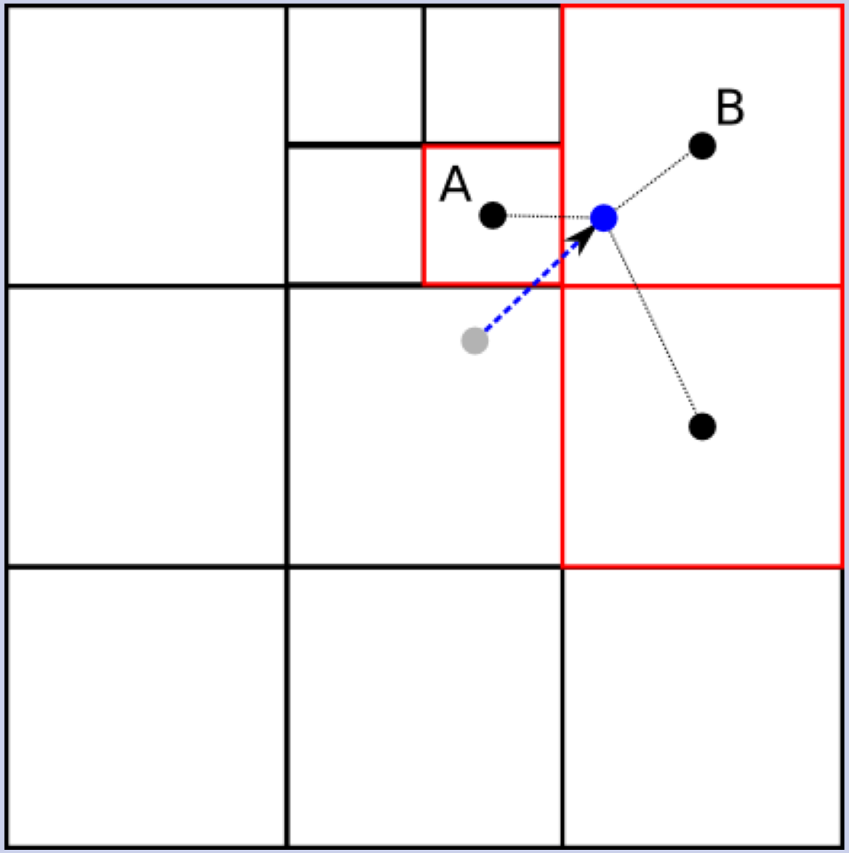
Which cell did a certain particle move to?



- Cell checks are expensive
- Check neighbors of old cell
- Check closest vertex
- Can we reduce the number of cell checks? Sort the neighbor cells?

EFFICIENCY: GEOMETRY INDEPENDENT

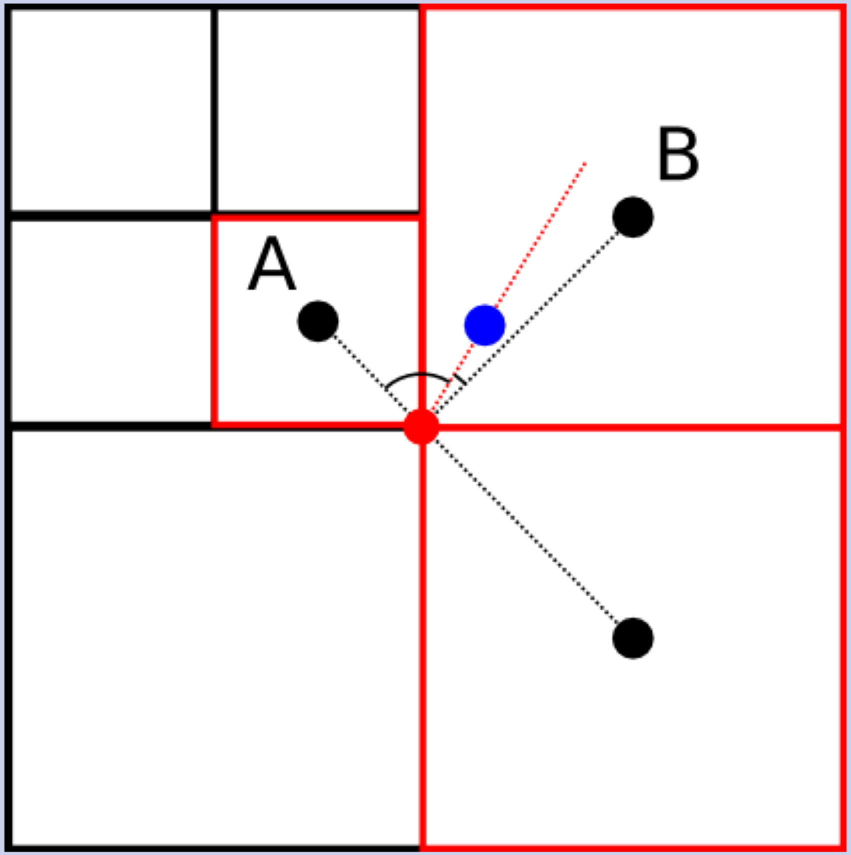
Which cell did a certain particle move to?



- Sort cells by distance to particle
- Find particle in first try for many cases
- Unreliable in adaptive meshes

EFFICIENCY: GEOMETRY INDEPENDENT

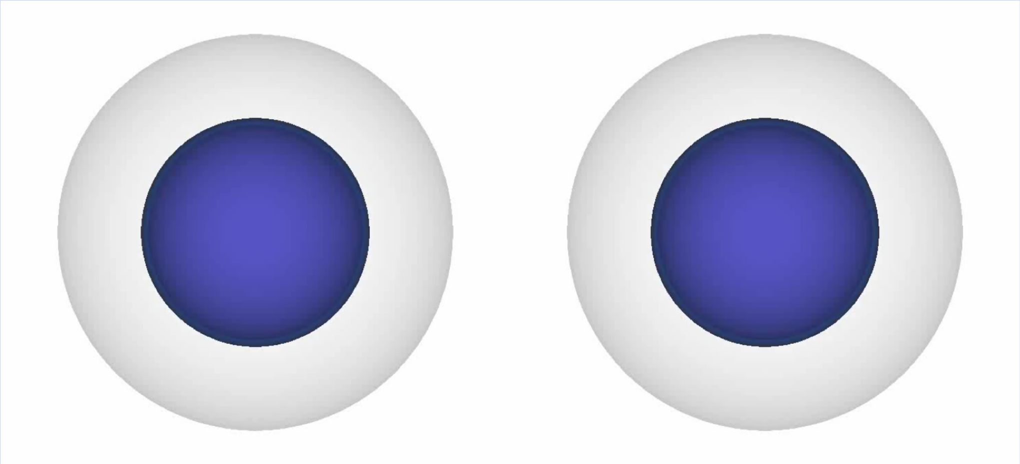
Which cell did a certain particle move to?

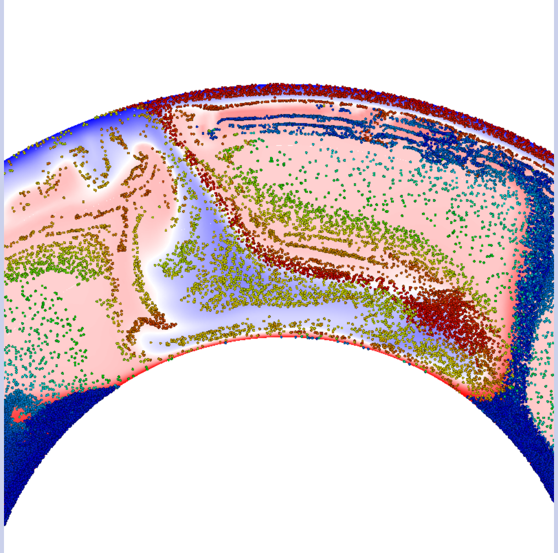


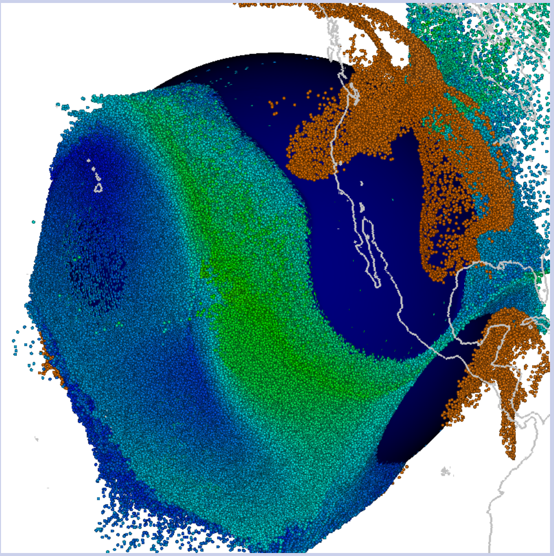
- Sort cells by angle between vertex–particle and vertex–center
- Find particle in first try for (nearly) all cases

- Reduce work by a factor of 10 compared to checking all neighbors
- Independent of geometry and mesh adaptivity

APPLICATIONS







- Large scale mantle convection:
    - Track deformation of material
    - Track origin of material
    - Track composition of material

CONCLUSIONS

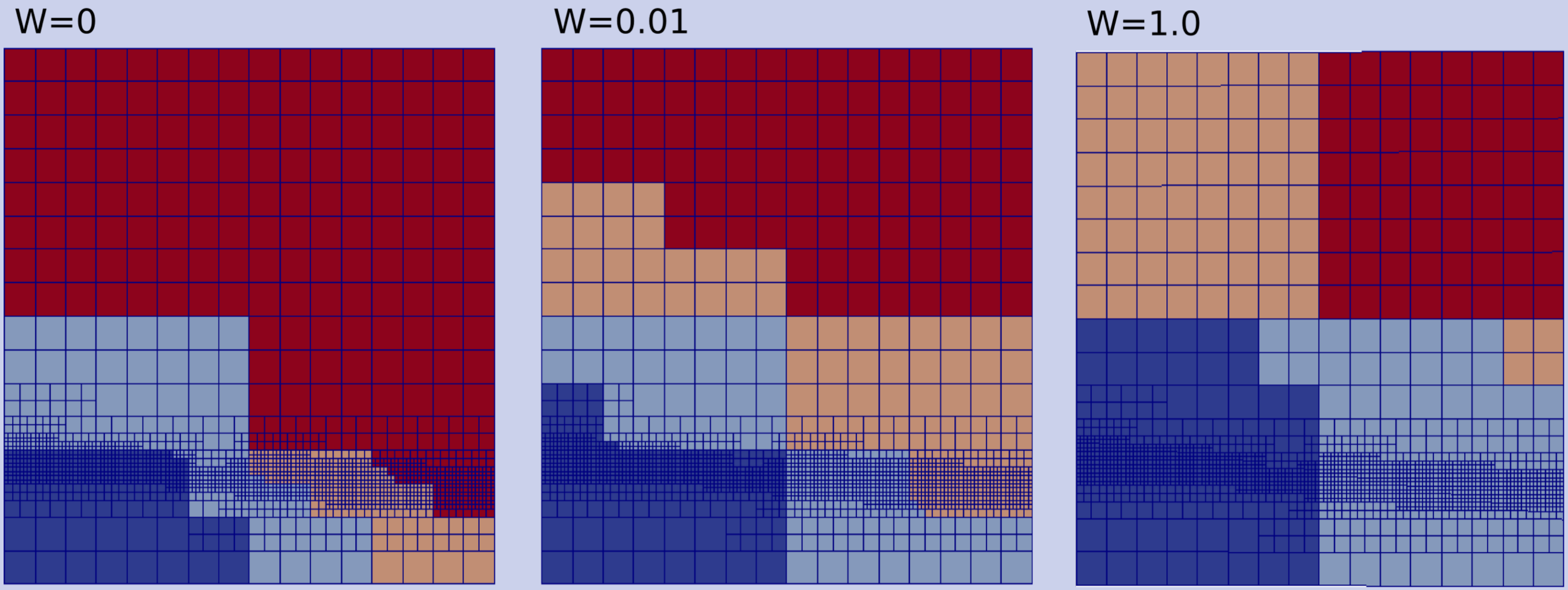
- We present hybrid particle-mesh methods for use in arbitrary geometries and adaptively refined meshes
- *Convergence rate* of hybrid PIC-FE methods depends on FE method, interpolation scheme and PPC. PPC needs to increase with mesh resolution to reach higher order accuracy (not scalable).
- *Balanced repartition* load balancing achieves reasonable weak scalability without affecting the solution up to thousands of processes.
- *Angle minimization* sorting reaches optimal complexity in arbitrary geometries.

References:

- Gassmöller, et al. "Flexible and Scalable Particle-in-Cell Methods With Adaptive Mesh Refinement for Geodynamic Computations." G*eochem. Geophys. Geosys.* 19.9 (2018): 3596-3604.
- Gassmöller, et al. "Evaluating the Accuracy of Hybrid Finite Element/Particle-In-Cell Methods for Modeling Incompressible Stokes Flow" 2019, submitted.

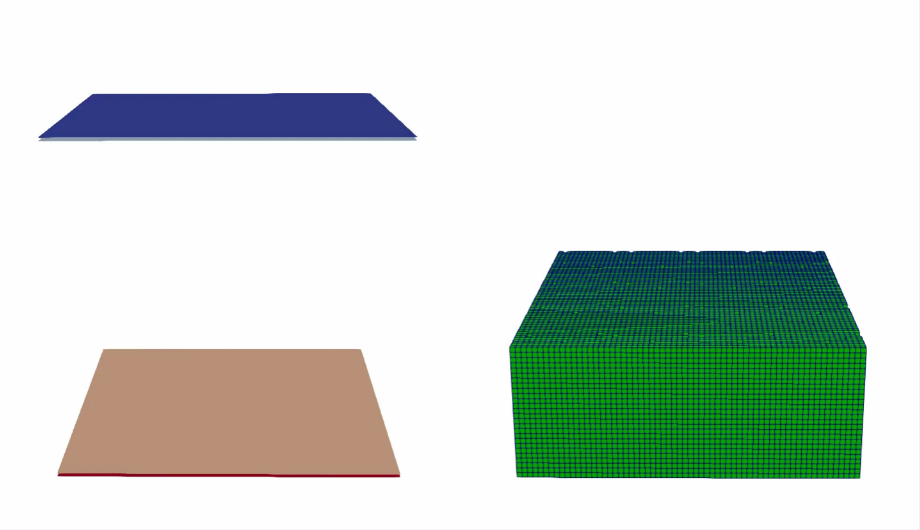
- *Code and benchmarks: https://github.com/geodynamics/aspect*

3. SCALABILITY: LOAD BALANCING

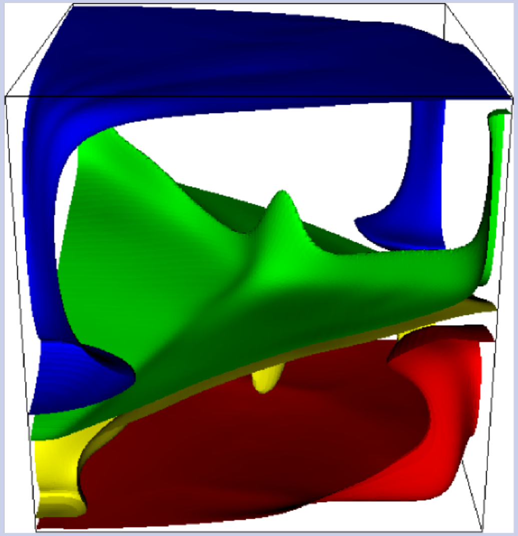


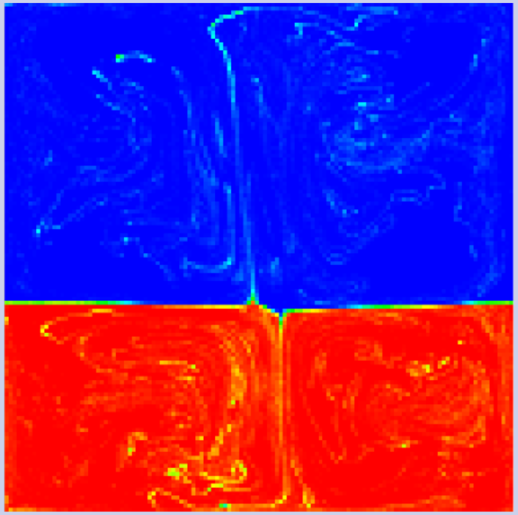
- Balance an appropriate sum of cells and particles
- Weight W determines the importance to balance particles
- Optimal W depends on the particle work
- Increased balancing of particles decreases balancing of cells

APPLICATIONS



After Tackley & King, 2003





- Entrainment benchmarks:
    - Compare field methods and particles
    - Measure entrainment and convergence of PIC methods