Performance evaluation of existing and new VoF simulation techniques: solving, interface treatment, and dynamic meshes.

9th OpenFOAM Workshop
23 June 2014 – Zagreb, Croatia

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Technology Process Consulting

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INTRODUCTION
AGENDA

- Investigate stability limits of explicit and semi-implicit MULES solvers.
- Evaluate curvature estimates of different discretization schemes
- Automatic mesh refinement (AMR)
  - Background
  - Distributed processor load balancing
  - Demo cases
- Next steps

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STABILITY AND BOUNDEDNESS

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STABILITY
IMPLICIT VS EXPLICIT

- Investigate stability limits of explicit and semi-implicit MULES
- Compare run times and changes in solution vs. time step size.
- Compare alpha field boundedness

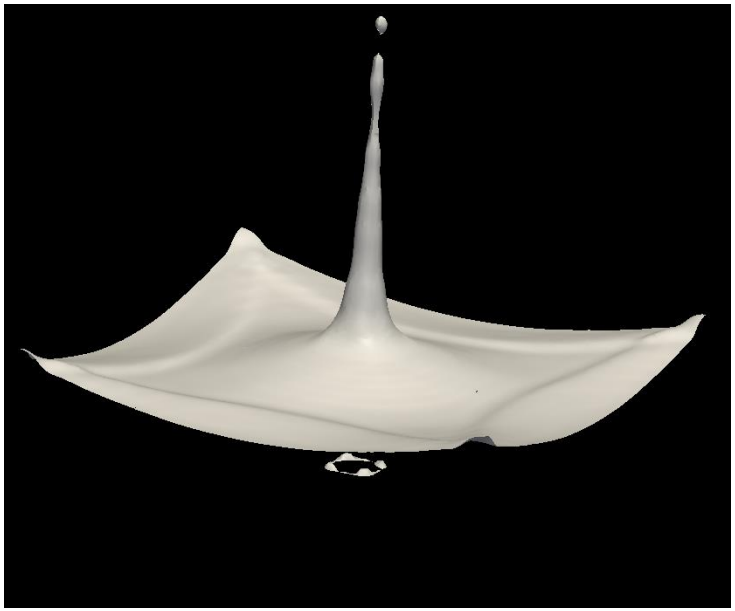
Case:

100x100x100 hex mesh

Material: air & water

20 cells / drop diameter

gravity driven



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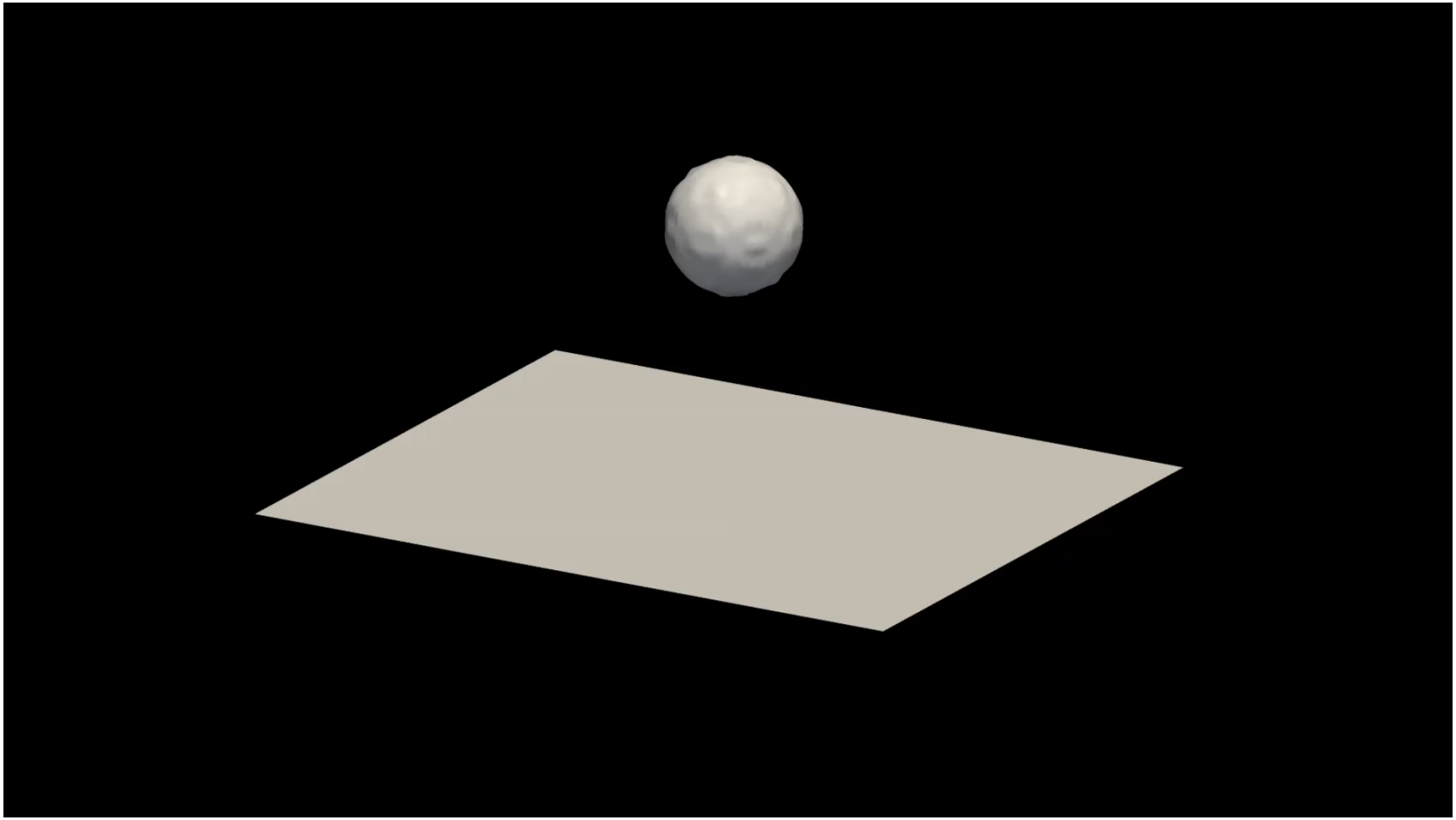
STABILITY
IMPLICIT VS EXPLICIT



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STABILITY
IMPLICIT VS EXPLICIT

	Implicit	Explicit
maxCo = maxAlphaCo	runTime [s]	
0.1	20579	17614
0.5	3627	3474
1	1995	Unstable
2	1175	Unstable
4	791	Unstable

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STABILITY
IMPLICIT RUNTIME

	Implicit
maxCo / maxAlphaCo	runTime [-]
0.1	26.01
0.5	4.59
1	2.52
2	1.49
4	1

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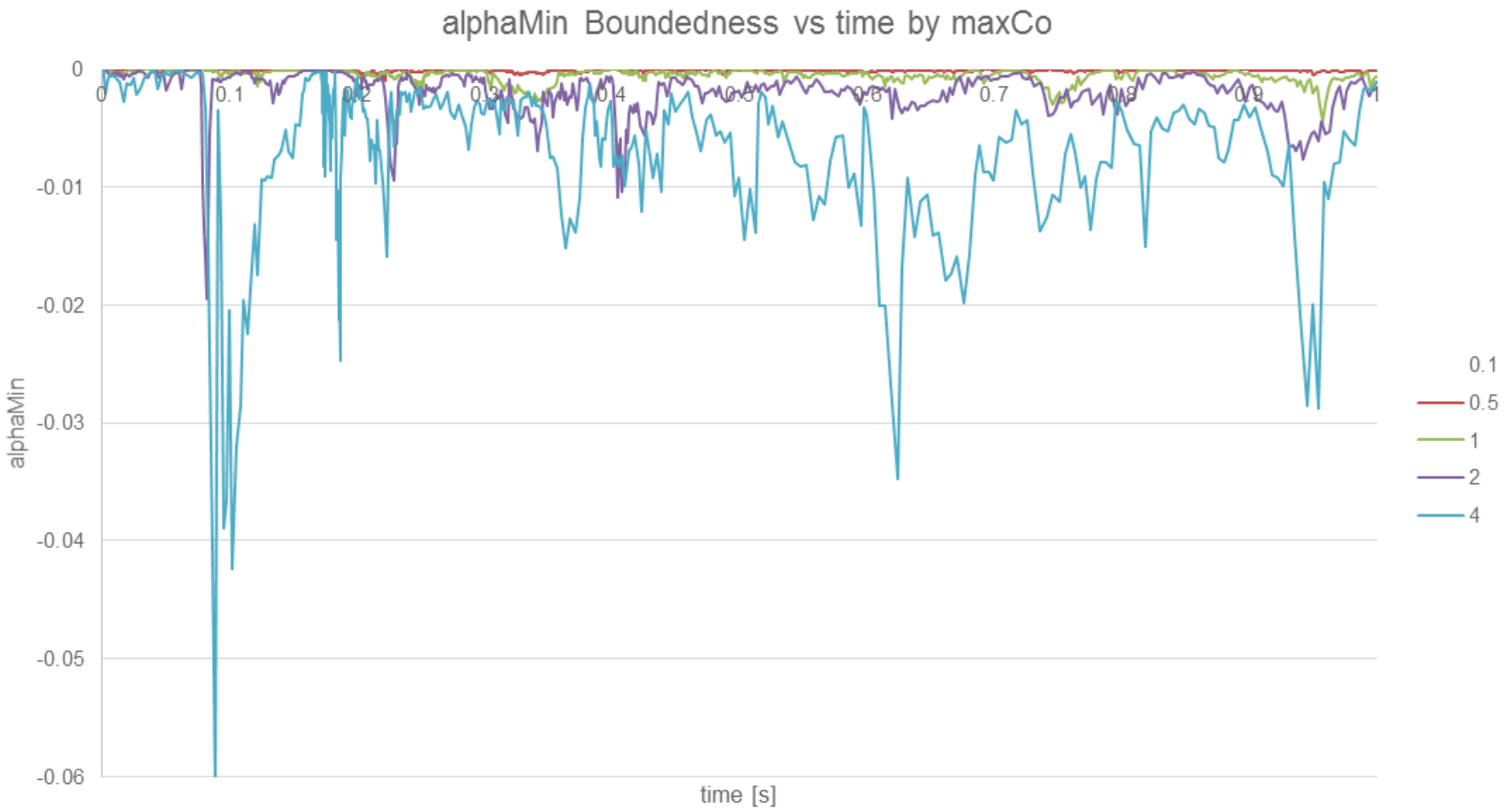
BOUNDEDNESS
IMPLICIT-MULES



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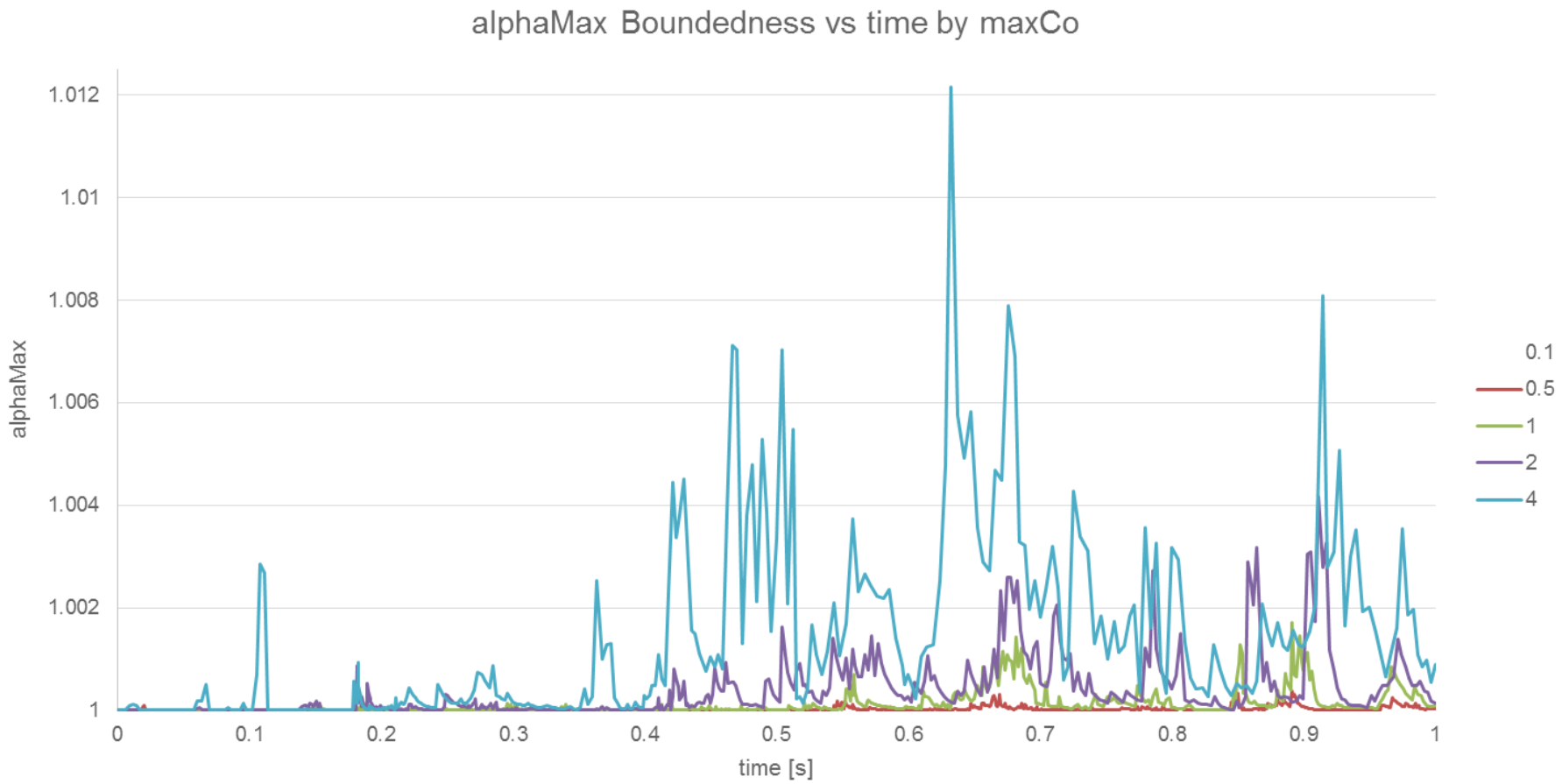
BOUNDEDNESS
IMPLICIT MULES



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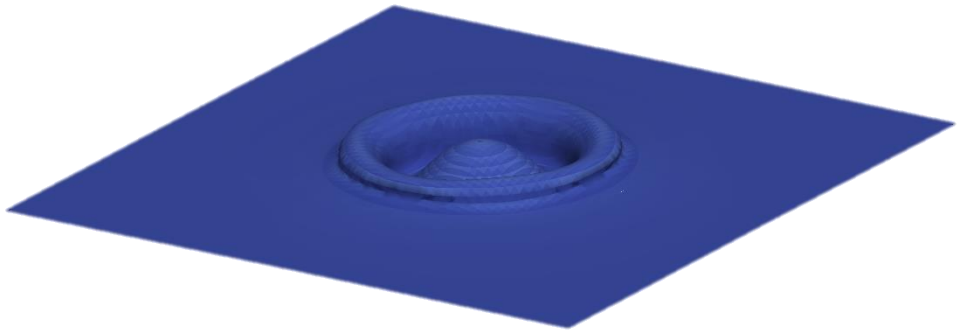
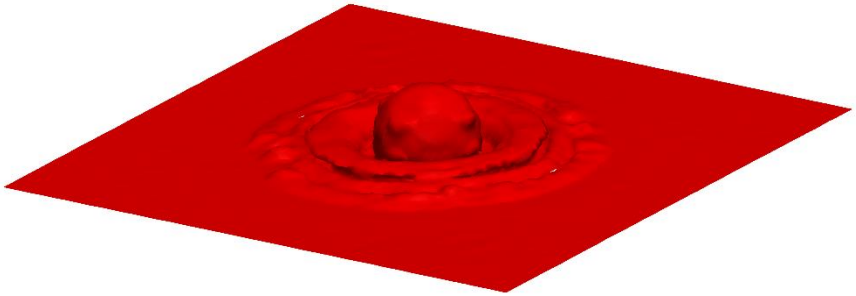
SOLUTION BY MAX COURANT NO.

t=0.1 [s]





maxCo=0.5

maxCo=4

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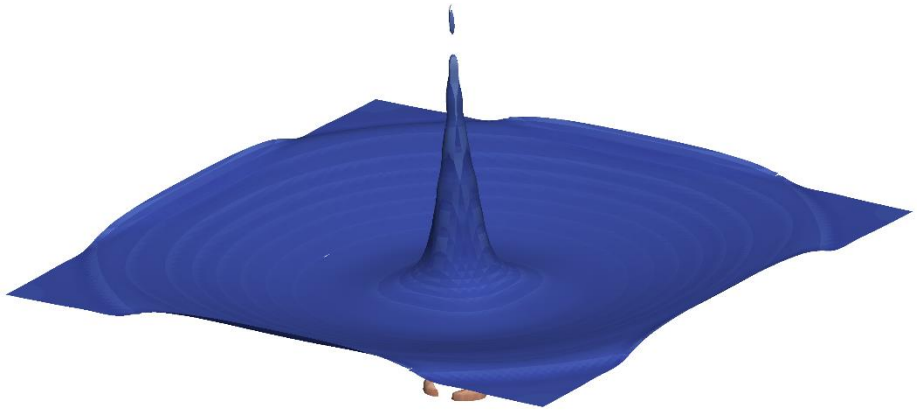
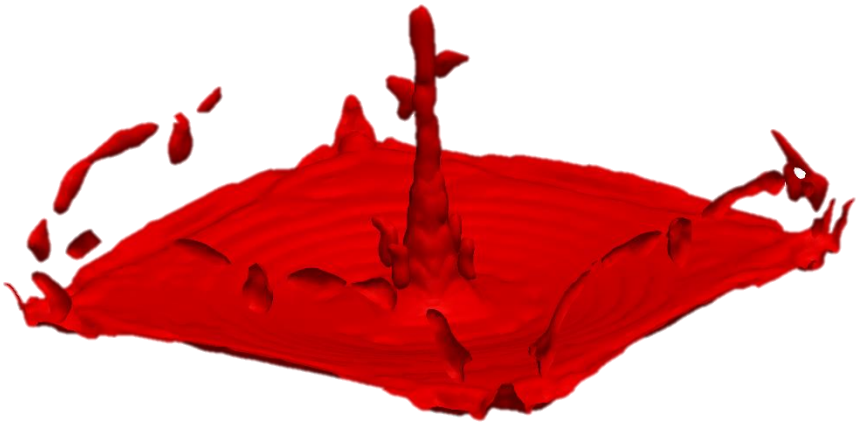
SOLUTION BY MAX COURANT NO.

t=0.2 [s]





maxCo=0.5

maxCo=4

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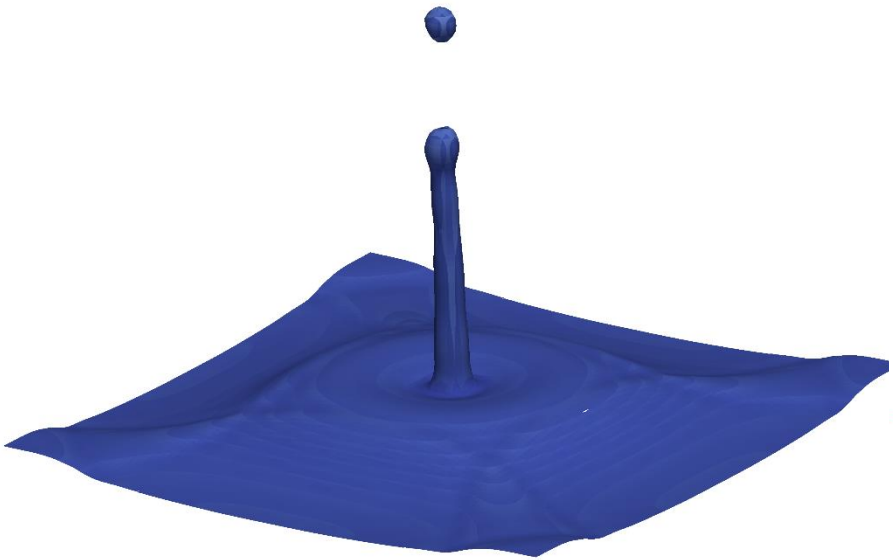
SOLUTION BY MAX COURANT NO.

t=0.3 [s]



maxCo=0.5

maxCo=4

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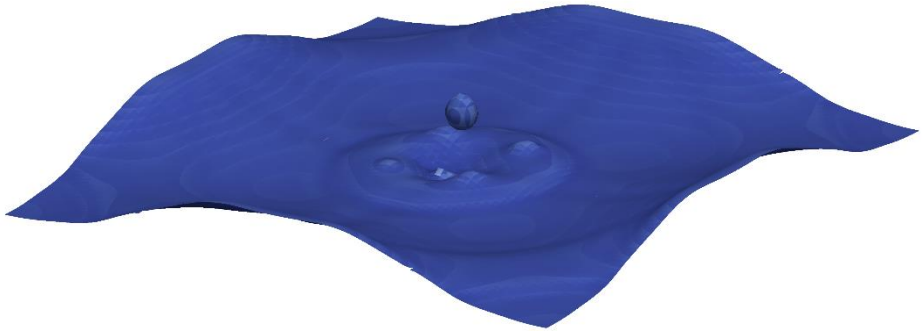
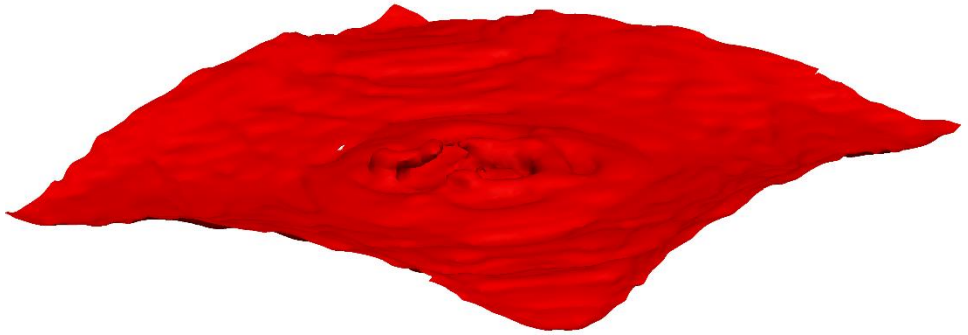
SOLUTION
BY MAX COURANT NO.

t=0.4 [s]





maxCo=0.5

maxCo=4

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SOLUTION BY MAX COURANT NO.

t=0.5 [s]

maxCo=0.5

maxCo=4

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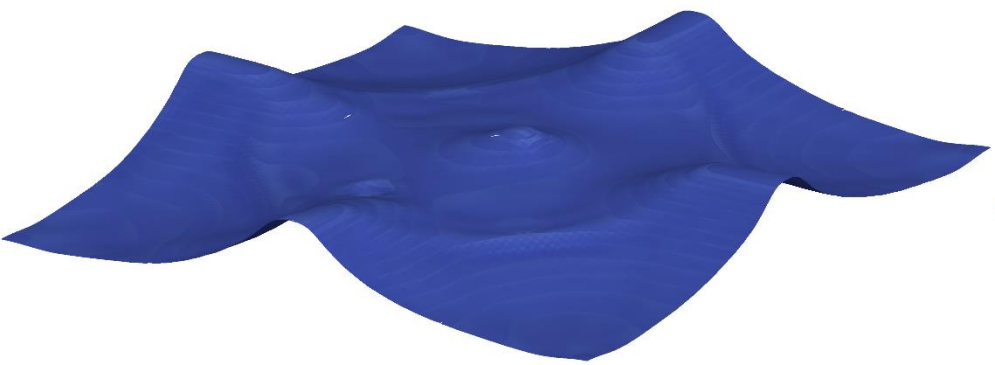
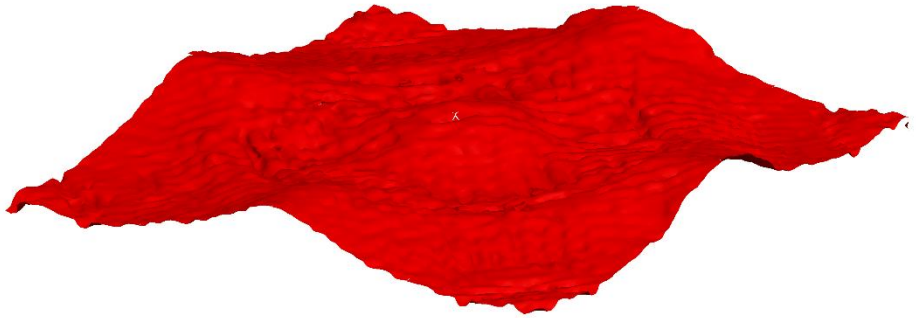
SOLUTION BY MAX COURANT NO.

t=0.6 [s]





maxCo=0.5

maxCo=4

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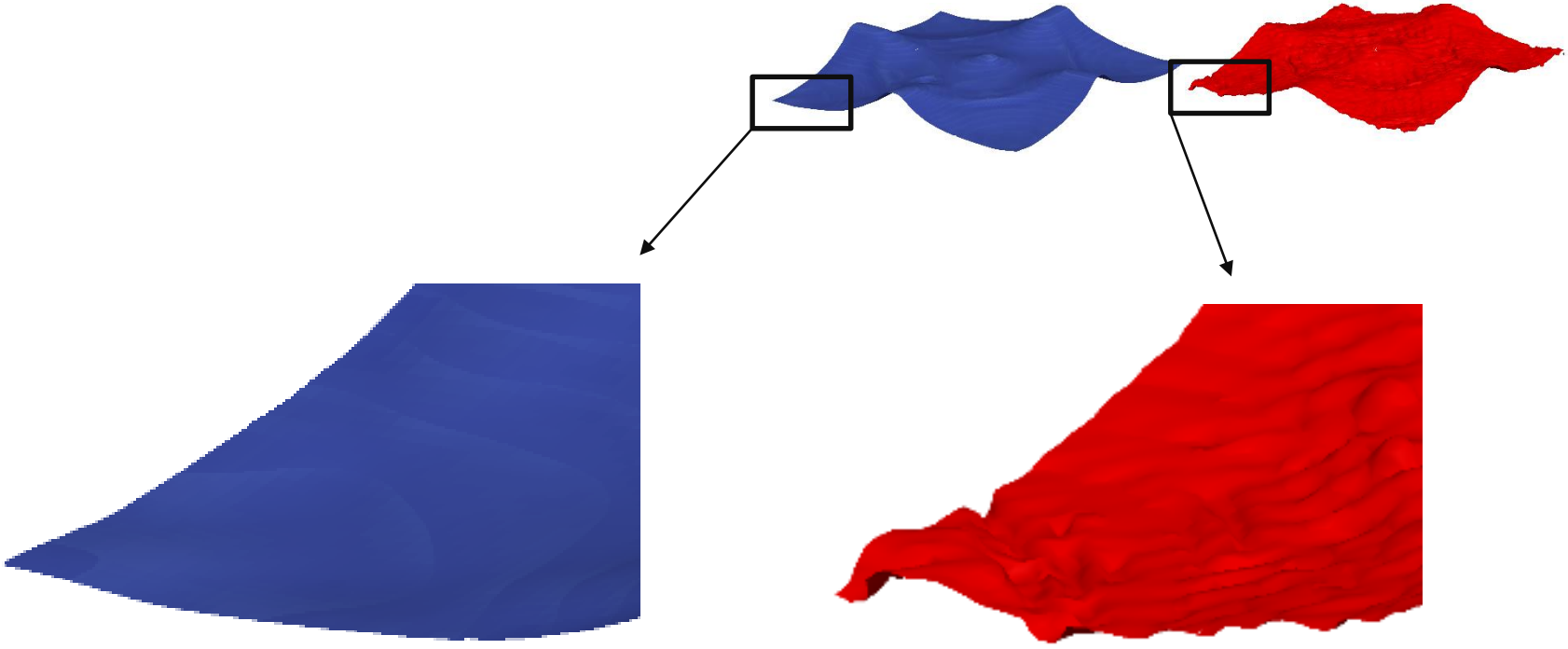
SOLUTION BY MAX COURANT NO.

t=0.6 [s]



maxCo=0.5

maxCo=4

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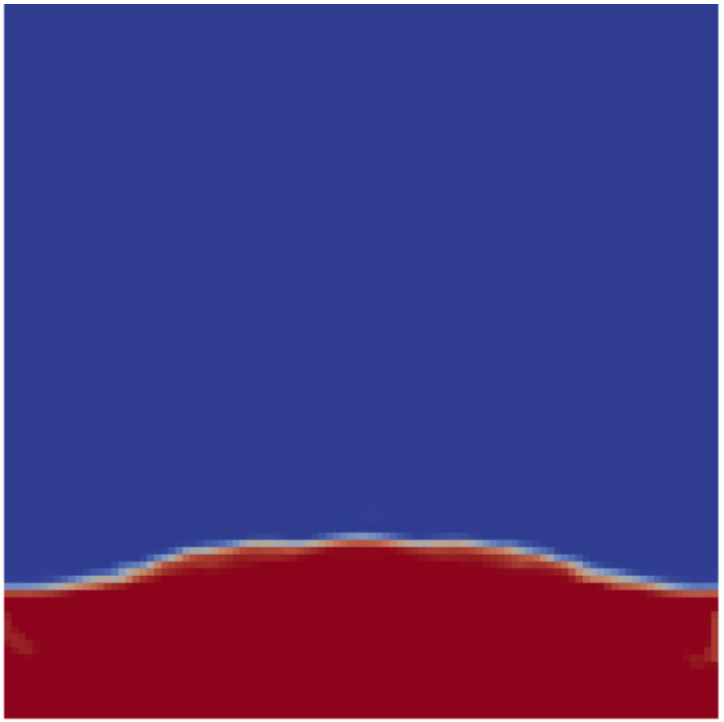
SOLUTION BY MAX COURANT NO.

t=0.2 [s]

Interface diffusion

maxCo=0.5



maxCo=4

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CURVATURE ESTIMATION

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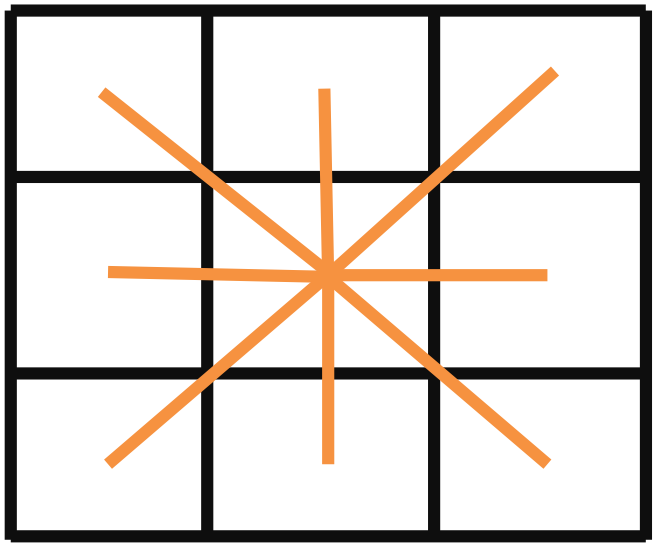
INTERPOLATION
CURVATURE ACCURACY

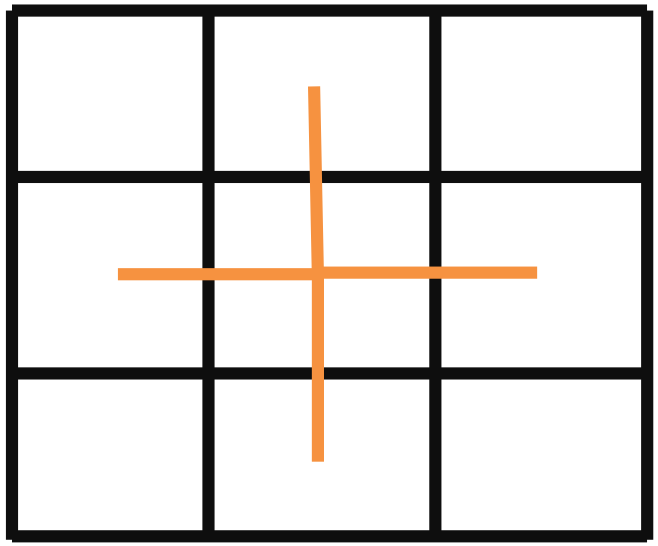
pointCellsLeastSquares

Constructs larger interpolation stencil by including point connected cell neighbours

$$\hat{n} = \frac{\nabla\gamma}{|\nabla\gamma|}$$

Gauss linear





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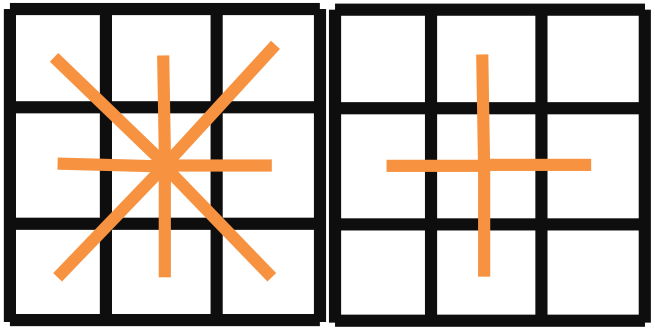
INTERPOLATION
CURVATURE ACCURACY

Test procedure:

1. Initialize droplet
2. Wait until droplet stabilizes
3. Write cell-centered K field
4. Create alpha=0.5 isoSurface
5. Interpolate K onto surface
6. Compute curvature error



Case:

- 100x100x100 uniform block mesh
- 20 cells / drop diameter
- Initial spherical alpha=1 field

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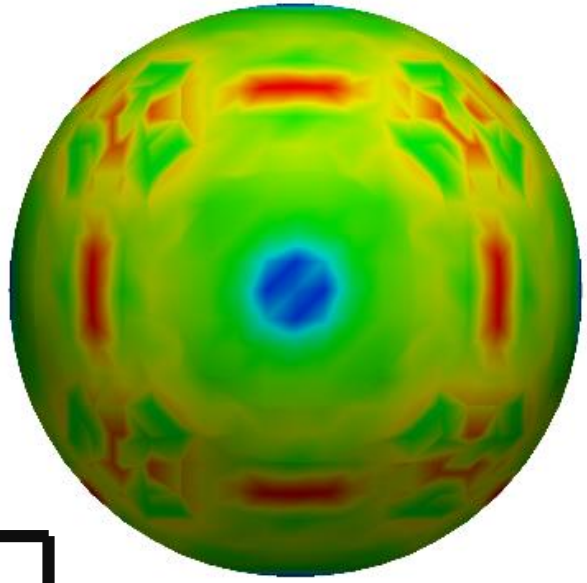
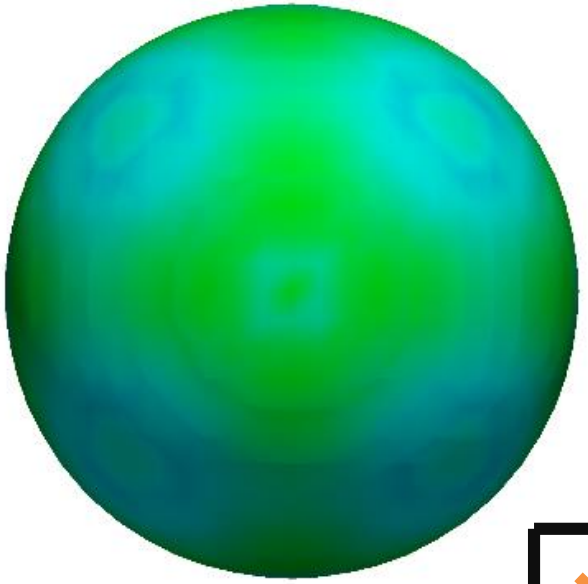
INTERPOLATION
CURVATURE % ERROR

Gauss linear

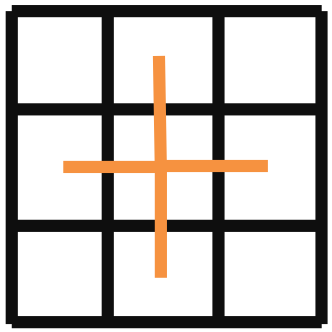
pointCellsLeastSquares

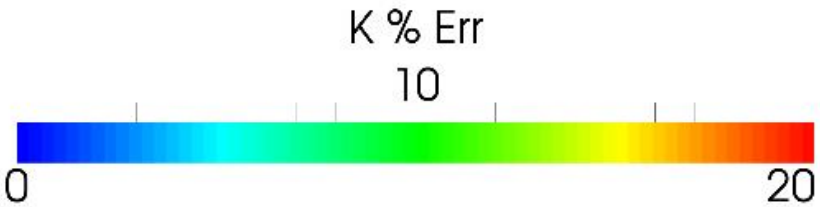
Run time: 2036

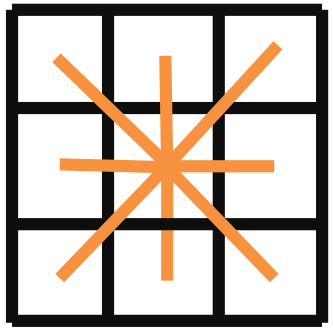




Run time: 2261







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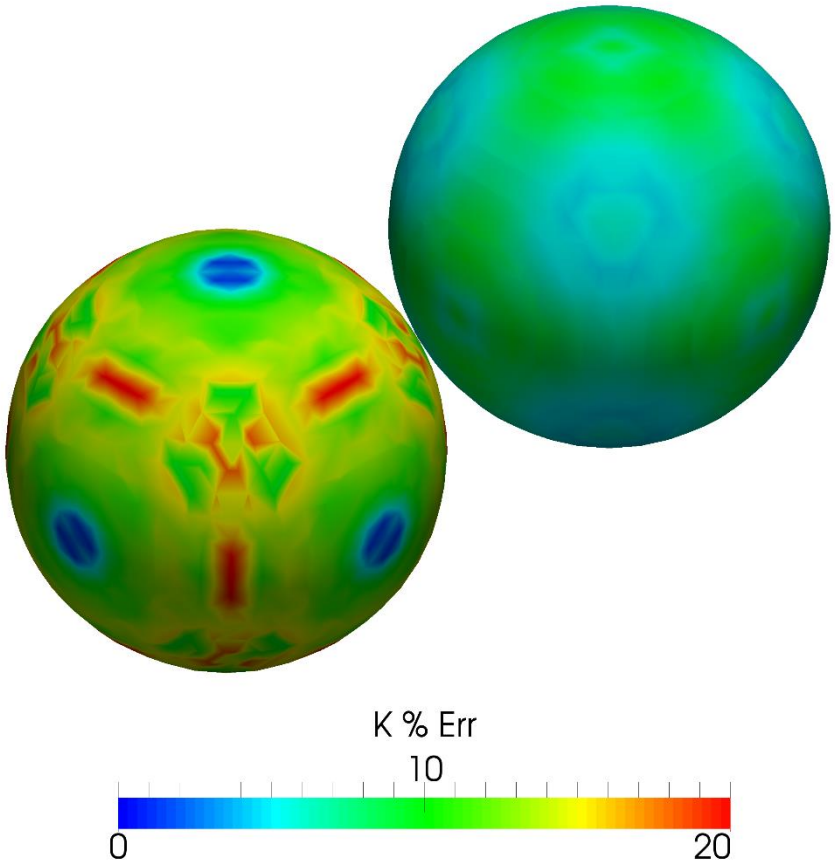
INTERPOLATION
CURVATURE % ERROR

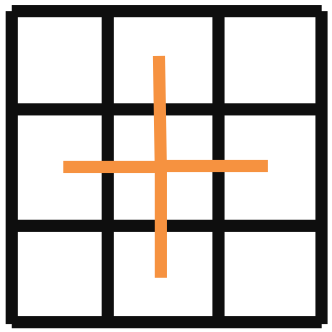
Gauss linear

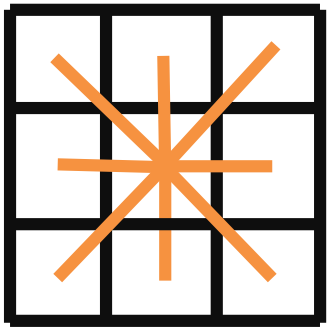
Normalized
run time: 1



pointCellsLeastSquares

Normalized
run time: 1.11





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AUTOMATIC REFINEMENT AND PARALLEL LOAD BALANCING

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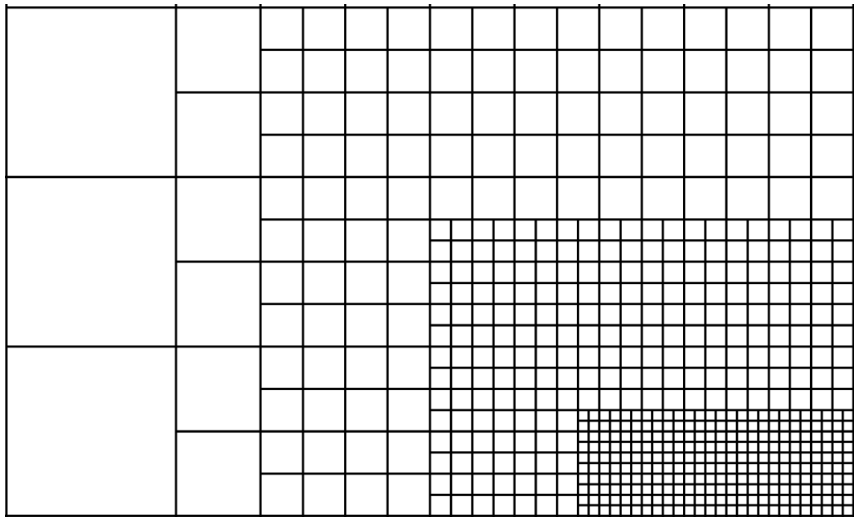
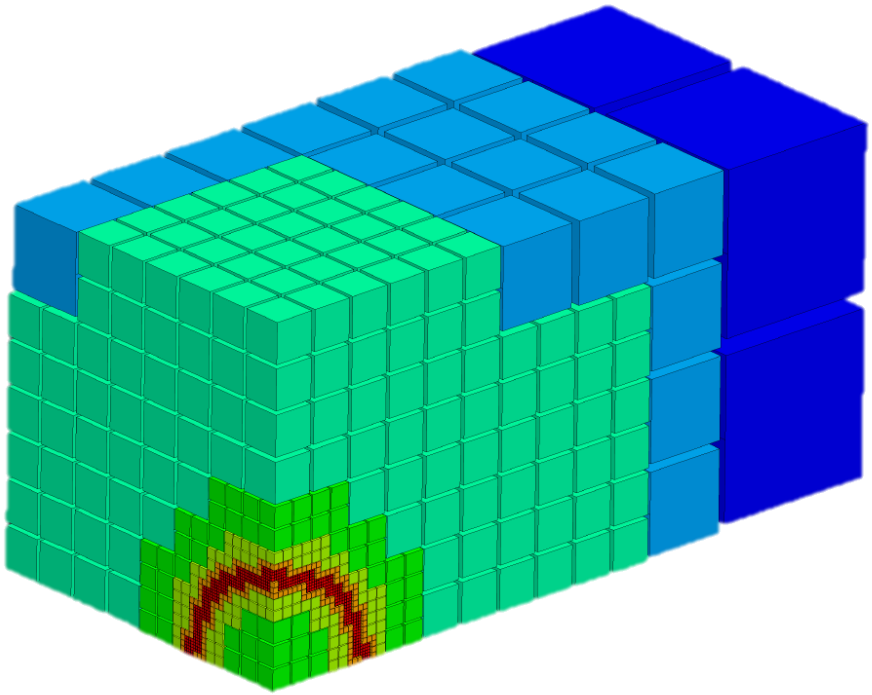
DYNAMIC REFINEMENT

QUAD – HEX BASED



Quadtree – 2D



Octree – 3D

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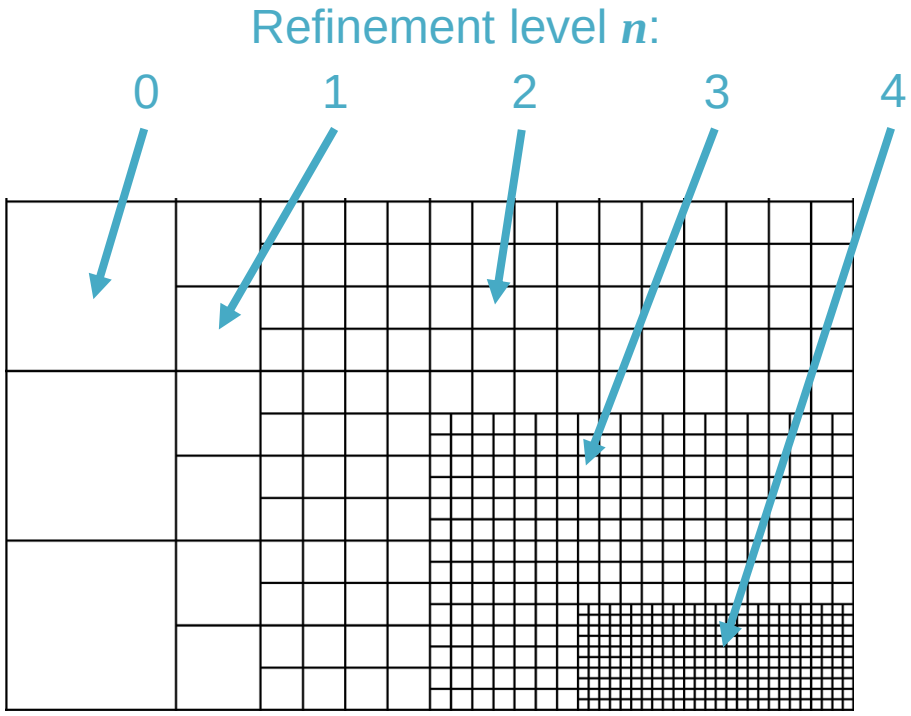
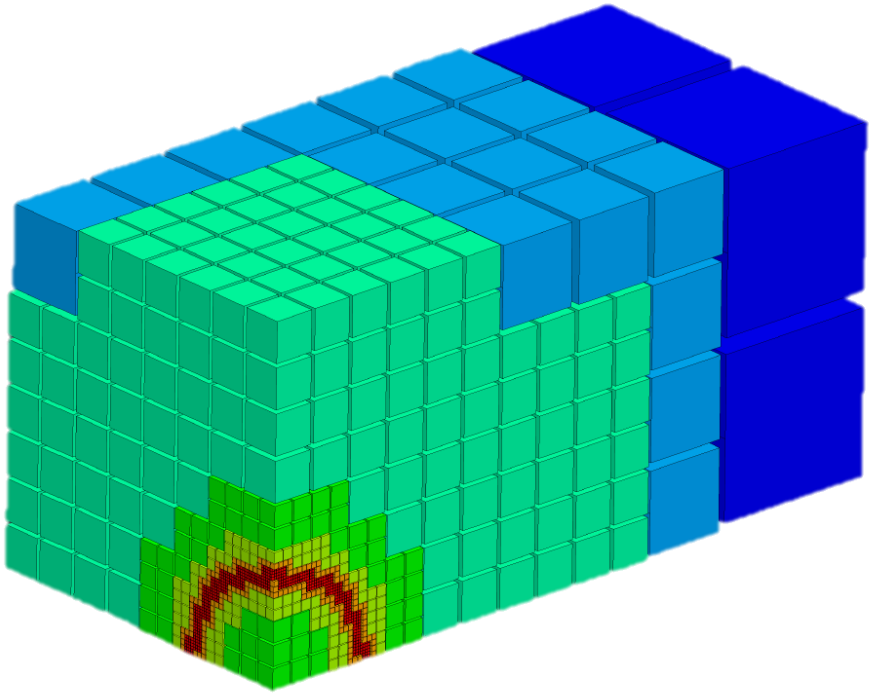
DYNAMIC REFINEMENT
QUAD – HEX BASED





Quadtree – 2D

$$\Delta x = \frac{baseSize}{2^n}$$

Octree – 3D

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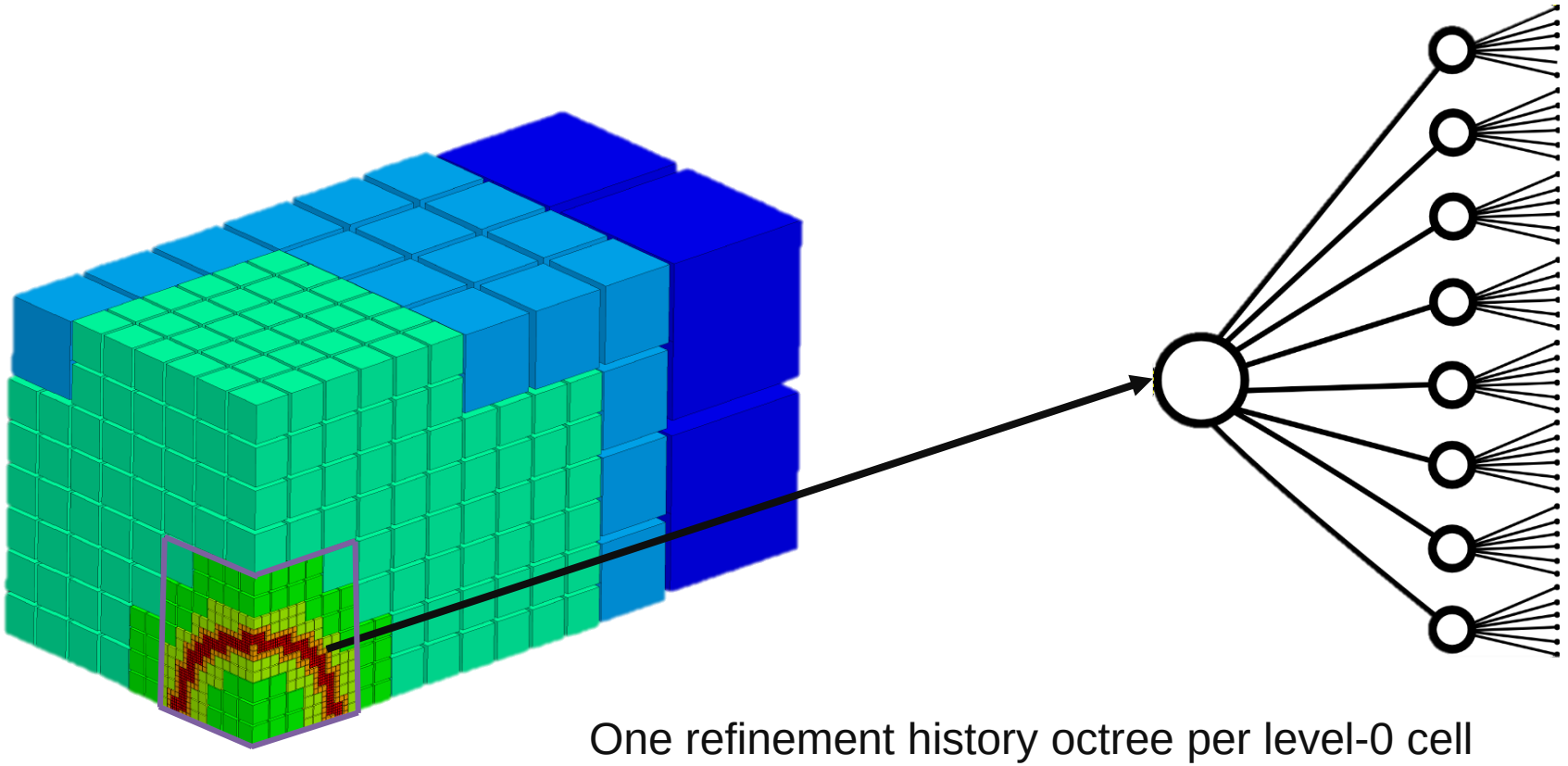
DYNAMIC REFINEMENT

OCTREE REFINEMENT HISTORY



One refinement history octree per level-0 cell
Contains data required for de-refinement
Cannot split octree during load balancing

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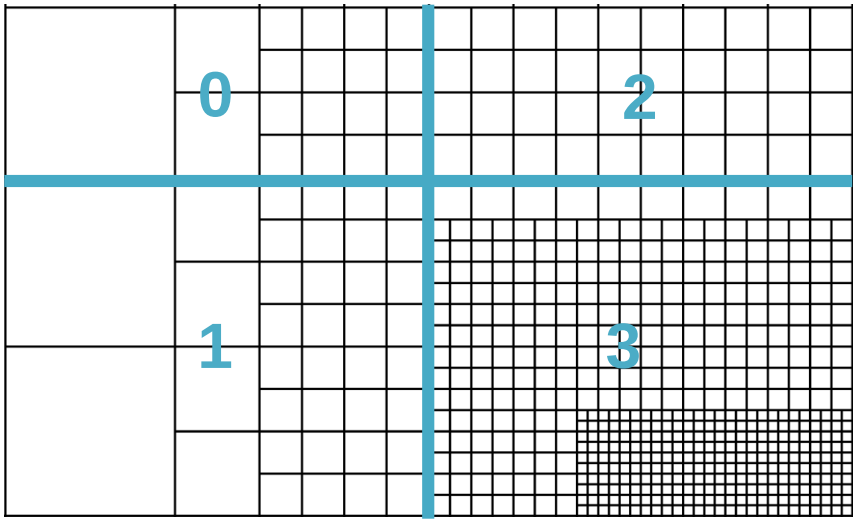
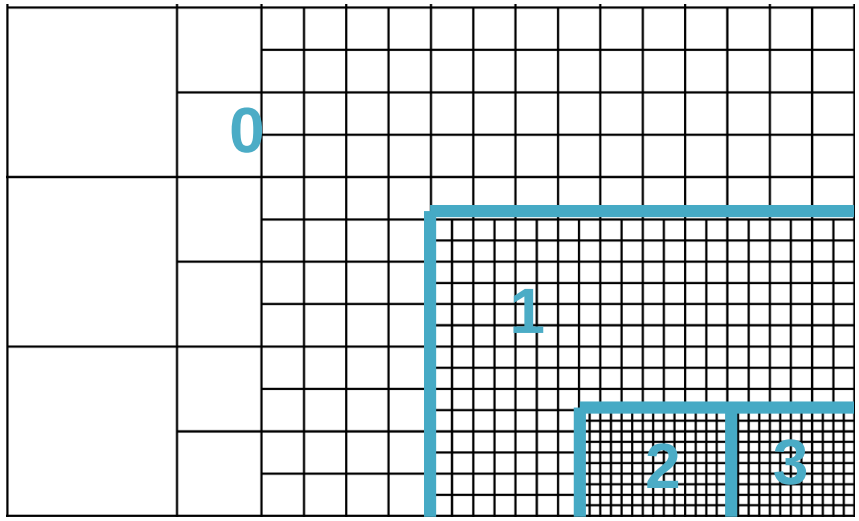
DYNAMIC REFINEMENT
PTSCOTCH - GRAPH PARTITIONER



Poor processor balance



Better processor balance

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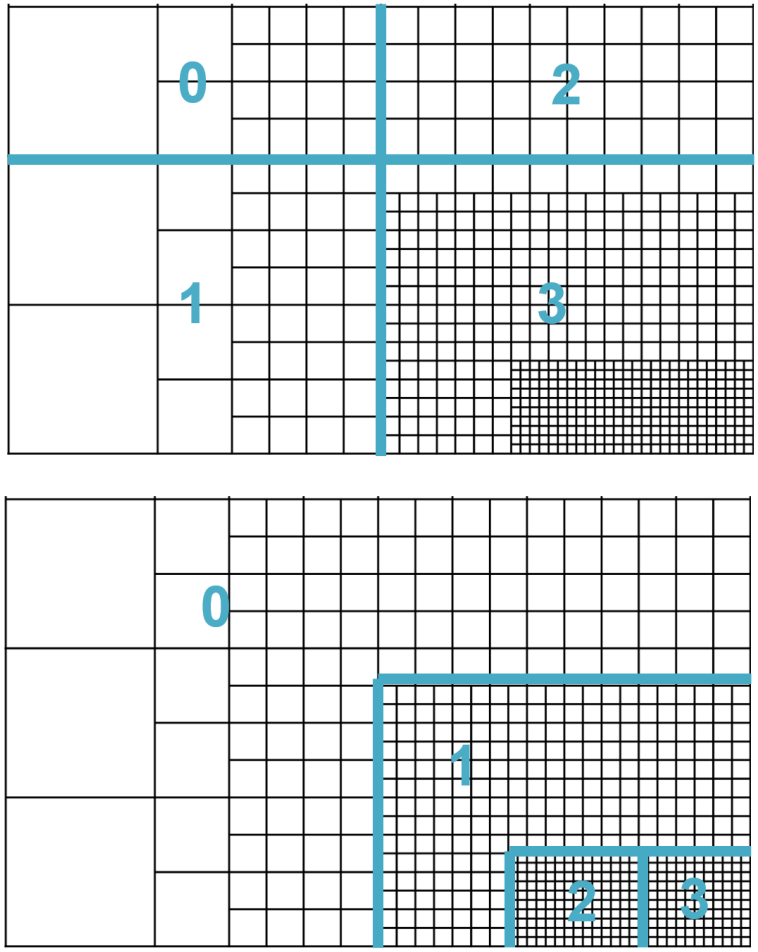
LOAD BALANCING

PTSCOTCH - GRAPH PARTITIONER



PT-Scotch

\+

Constrain to keep octrees

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DYNAMIC REFINEMENT

CONFIG: GRADIENT / CURL / REGION DRIVEN

```
refinementControls
{
    enableRefinementControl  true;

    gradients
    (
        alpha.water     (1000.0 10)
    );

    curls
    (
        U    (0.5 1)
    );

    regions
    (
            boxToCell
        {
            minLevel 1;

            box (-1 -1 -1)(1 1 1);
        }

    );
}
```

```
dynamicRefineFvMeshCoeffs
{
    enableBalancing true;
    allowableImbalance 0.15;

    // How often to refine
    refineInterval  2;

    // Field to be refinement on
    field           internalRefinementField;

    // Refine field inbetween lower..upper
    lowerRefineLevel 0.3;
    upperRefineLevel 1e200;

    // If value < unrefineLevel unrefine
    unrefineLevel   0.05;

    // Have slower than 2:1 refinement
    nBufferLayers   1;

    // Refine cells only up to maxRefinement levels
    maxRefinement   5;

    // Stop refinement if maxCells reached
    maxCells        10000000;
```


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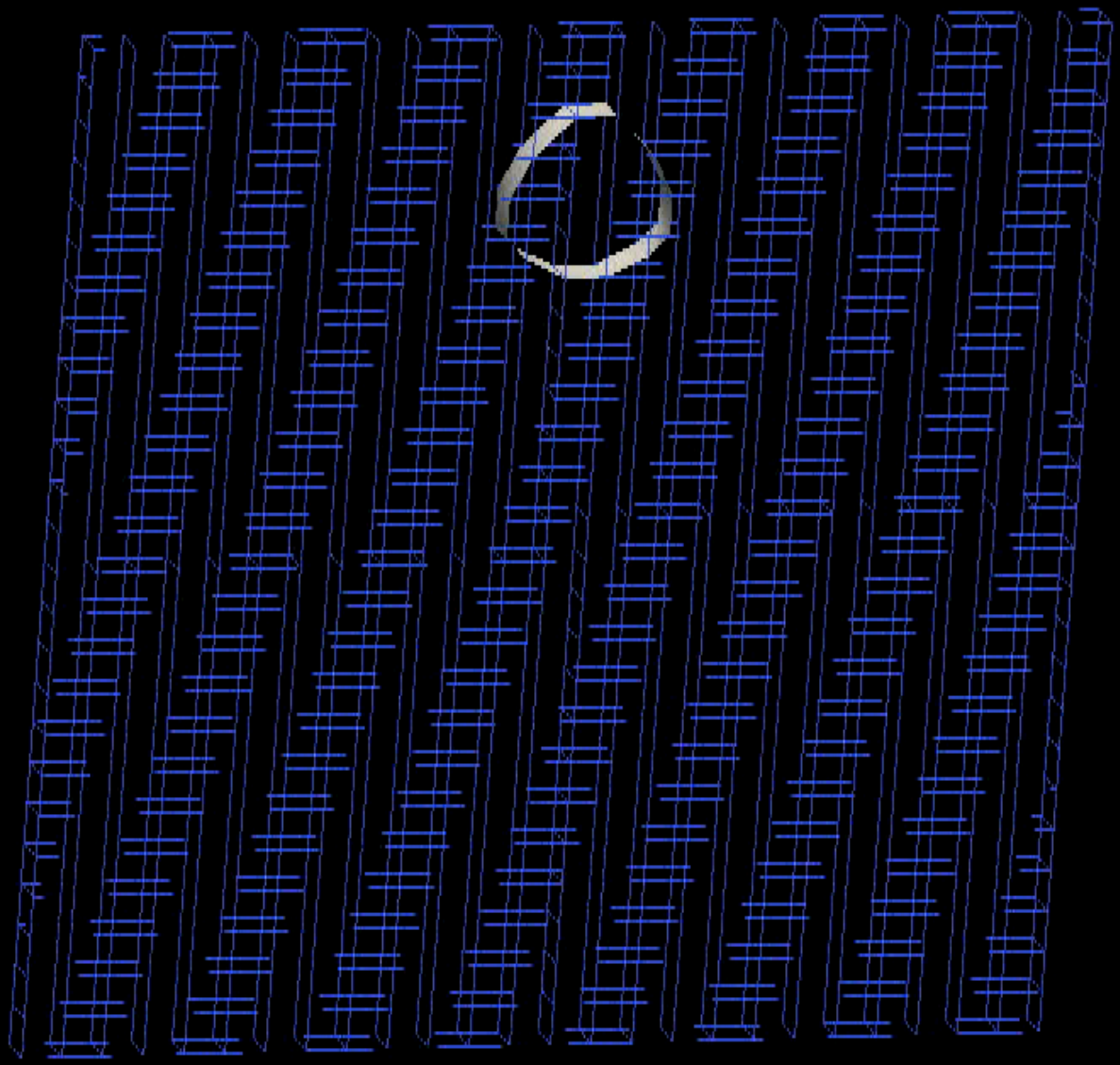

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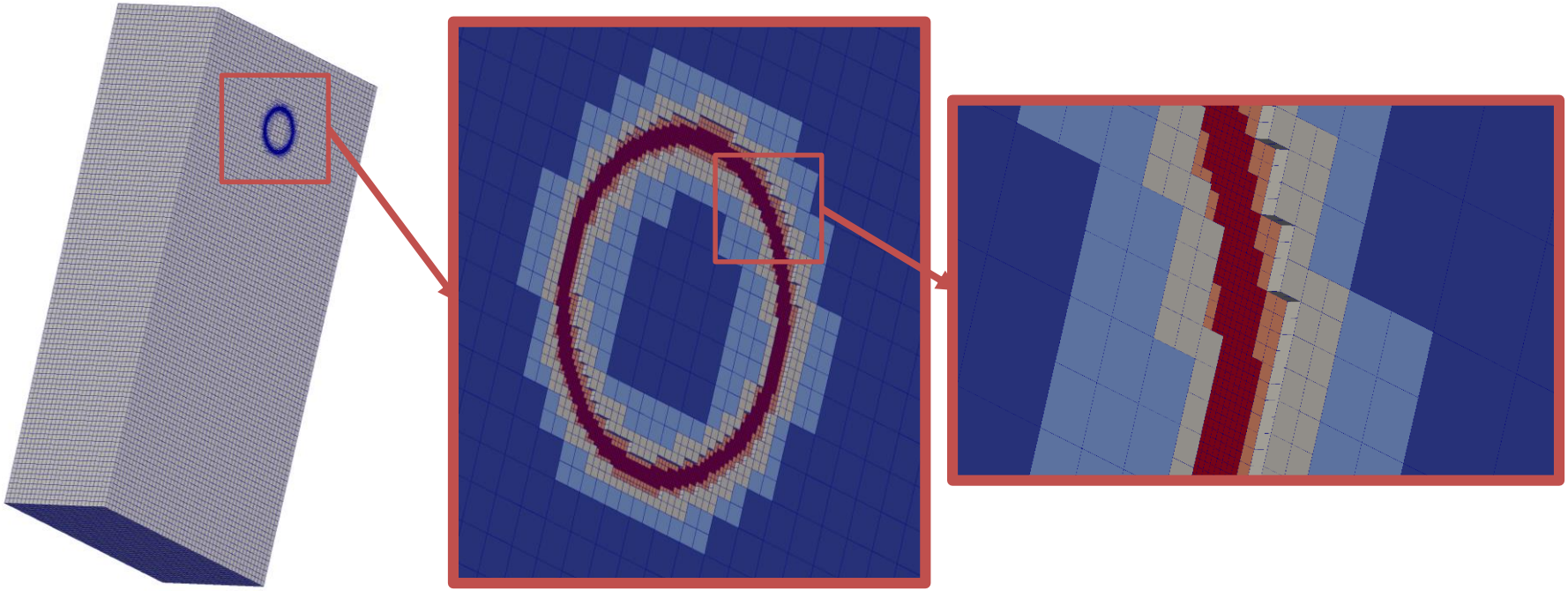
DYNAMIC REFINEMENT

LARGE SCALE CASE



Eo	196.875
Oh_d	6.32E-01
Oh_c	2.00E-01
Vis ratio	10
Density ratio	10

Gravity driven droplet acceleration / breakup
Max 5 levels of refinement
Equivalent to ~1.2 billion cells of uniform mesh size
Actual max mesh size = ~3.5 million

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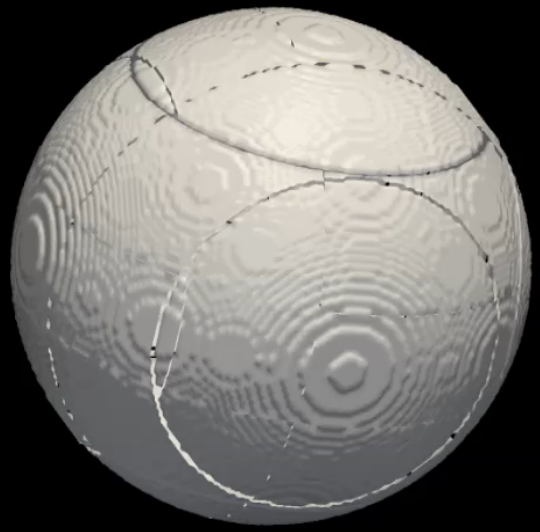

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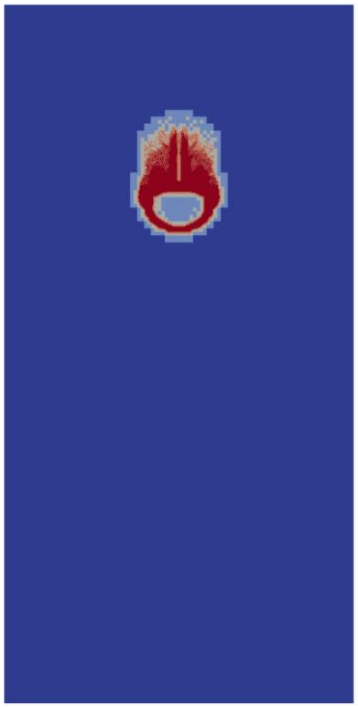
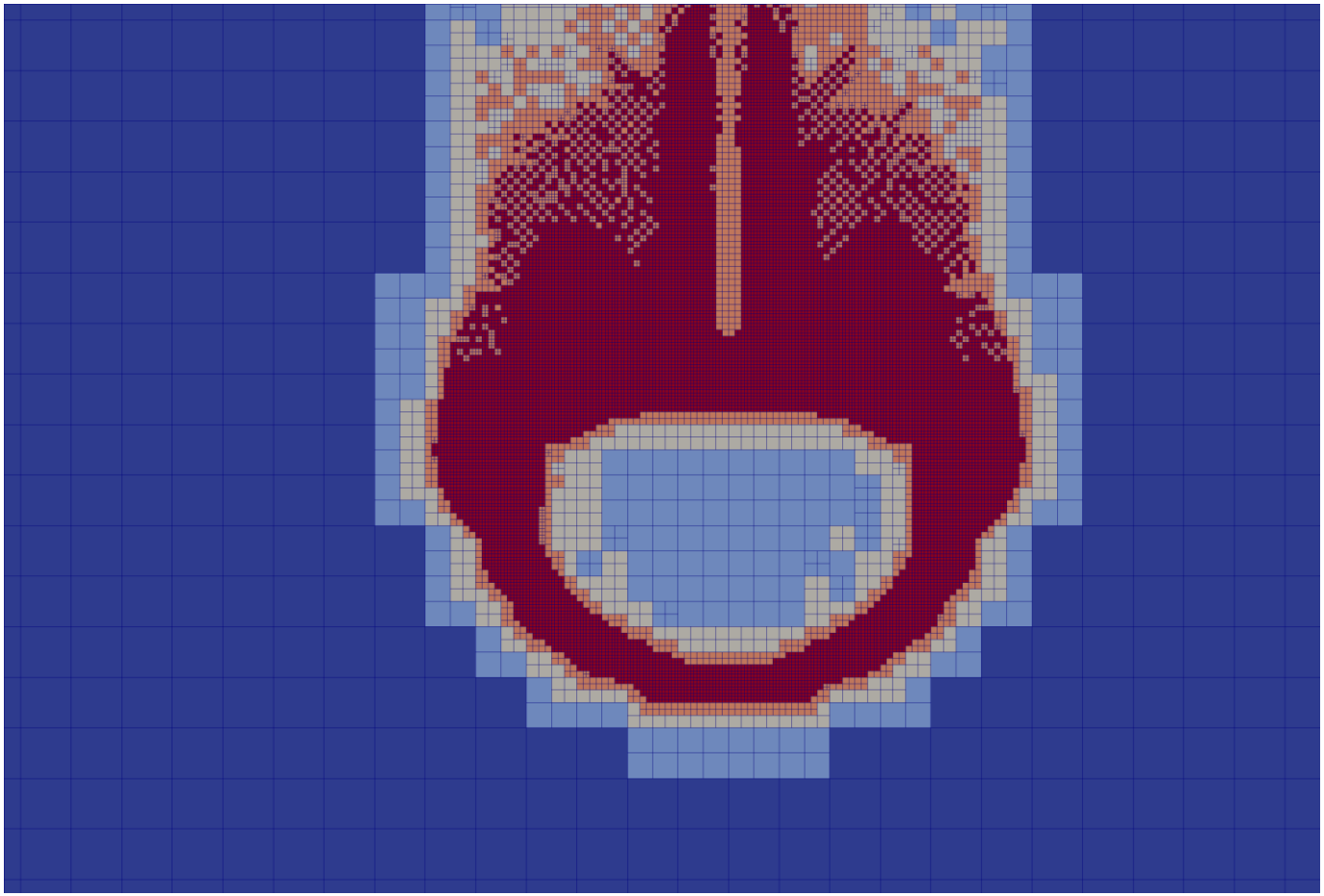
DYNAMIC REFINEMENT

LARGE SCALE CASE – CELL LEVEL





Eo	196.875
Oh_d	6.32E-01
Oh_c	2.00E-01
Vis ratio	10
Density ratio	10

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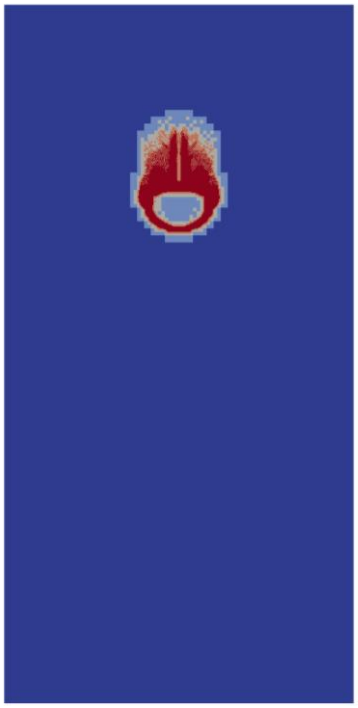
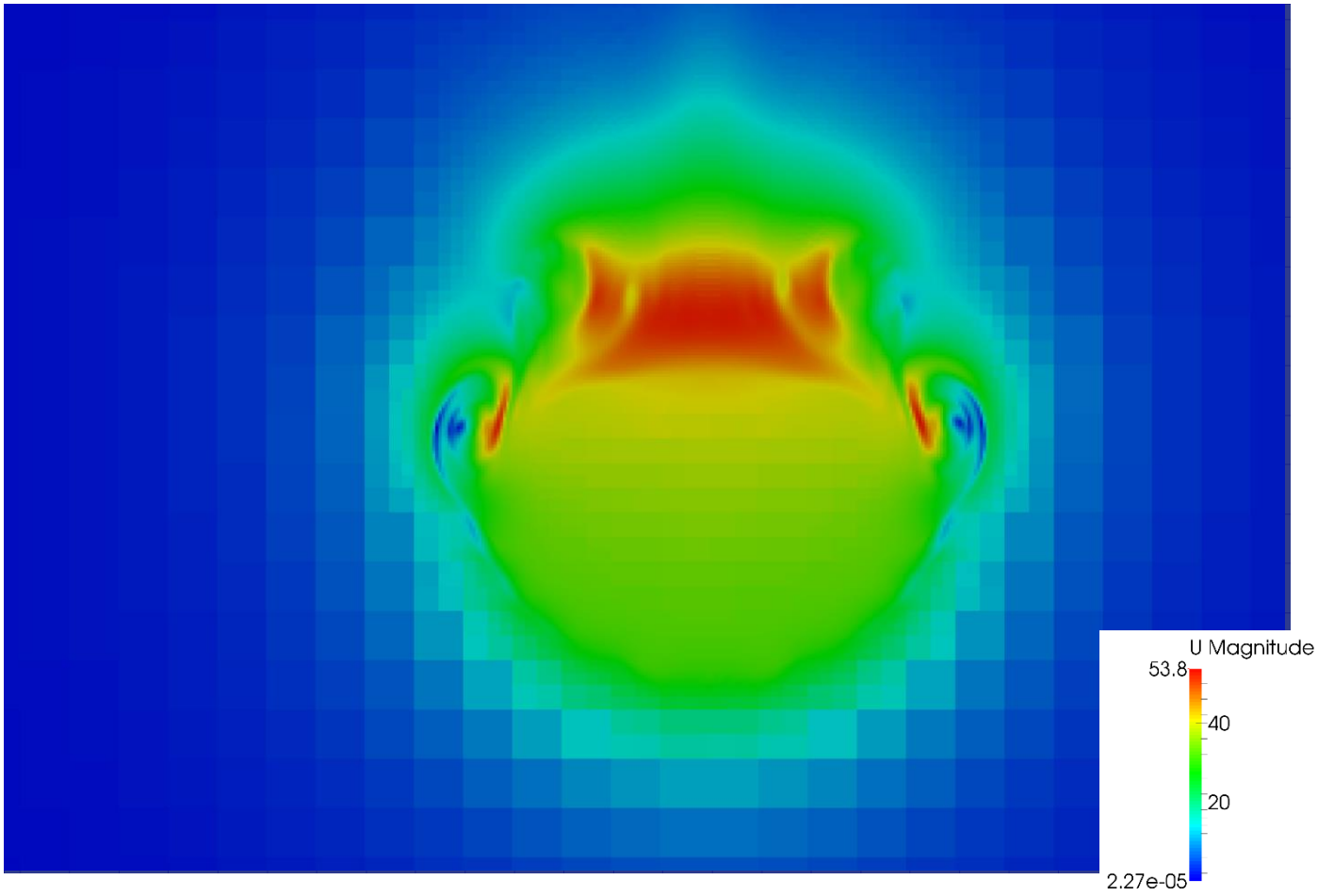
DYNAMIC REFINEMENT

LARGE SCALE CASE – MAG(U)





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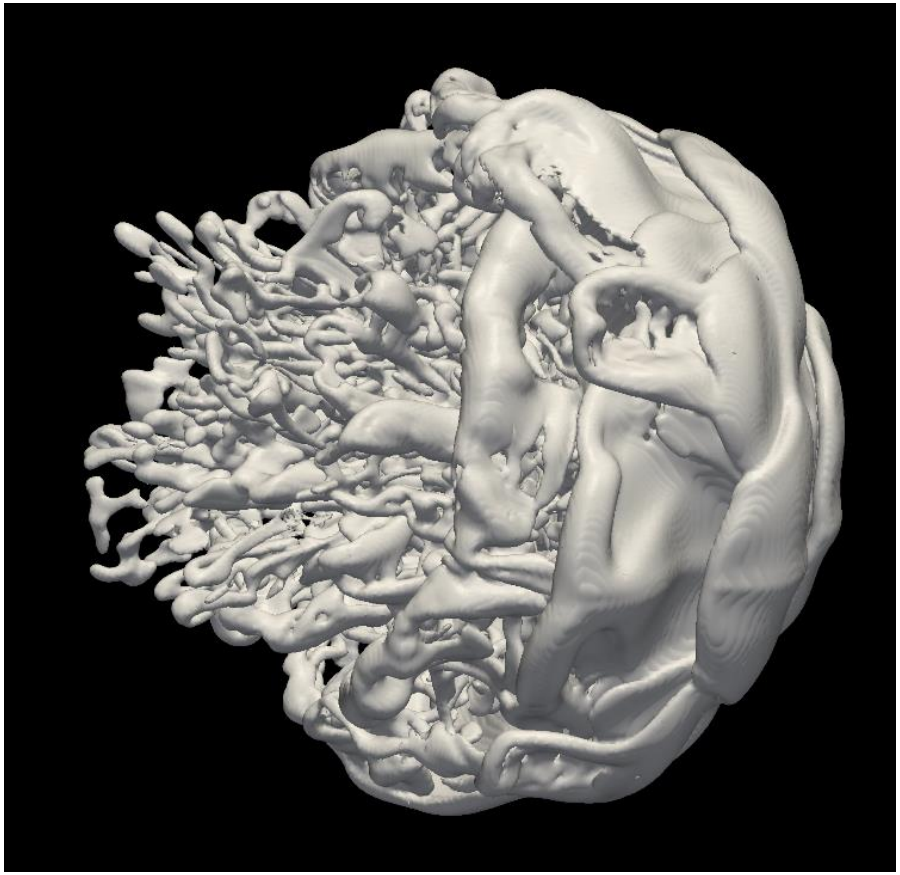
NEXT STEPS

- Incorporate error estimation
- Fix additional memory issues with PT-Scotch
- Extend to operate within non-hexahedral meshes (ex: hex-core within polyhedral)
- Apply immersed boundary / moving immersed boundary methods
- Optimize for run time: re-meshing frequency, allowable imbalance.



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THANK YOU
COLLABORATORS

Collaborators / Advisors:

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THANK YOU

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