Subsetix: Sparse 2D Geometry on GPU

From Set Algebra to AMR Simulation

Sébastien DUBOIS

HPC@Maths Team

December 2025

Outline

I. Context: GPU & Kokkos

Project Context — Towards Exascale

Background

- **Numpex Project**: French initiative pushing scientific computing to exascale
- **Samurai**: AMR library with unique sparse data structure (interval-based)
- **Challenge**: No prior GPU implementation of Samurai's core concepts

Objective

How can Samurai's strategy evolve for exascale?

- GPU acceleration (today's focus)
- Multi-node distribution (future work)

Approach

Proof of Concept Strategy

1. **Simplify** — Isolate core problems
2. **Prototype** — Build independent bricks
3. **Validate** — Test on real simulations
4. **Integrate** — Path back to Samurai

This work: GPU-native sparse 2D geometry as a standalone proof of concept

GPU Architecture — Massively Parallel

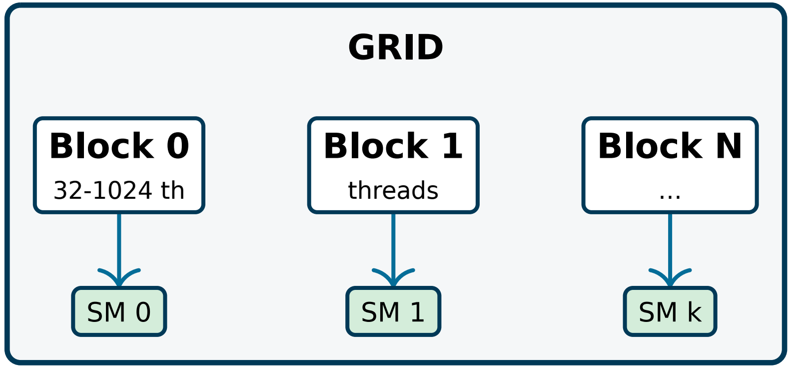
Execution Hierarchy

- **Warp** = 32 threads in **lockstep** (SIMT)
- **SM** = autonomous compute unit
- Multiple warps/SM → latency hiding

For Our Project

- **1 thread** = processes 1 Y row (or 1 cell)
- Thousands of rows → **saturate the GPU**

Execution Model



B200 vs EPYC 9965

	GPU B200	CPU EPYC 9965
Bandwidth	**8 TB/s**	576 GB/s
FP32	**90 TFlops**	14 TFlops

GPU: **14× more bandwidth** than CPU → ideal for large sparse meshes

Kokkos — Performance Portability

The Problem

- CUDA = NVIDIA only
- OpenMP = CPU only (limited GPU)
- HIP = AMD only
- Rewrite for each platform?

The Solution: Kokkos

```
// 1. COUNT – unknown result size
parallel_for(num_rows, KOKKOS_LAMBDA(int r) {
  counts[r] = count_intervals(r);
});
// 2. SCAN – compute offsets
exclusive_scan(counts, row_ptr);
// 3. FILL – parallel write
parallel_for(num_rows, KOKKOS_LAMBDA(int r) {
  fill_intervals(r, &out[row_ptr[r]]);
});
```

CUDA vs Kokkos

Native CUDA

```
double* d_data;
cudaMalloc(&d_data, n*8);

cudaMemcpy(d_data, h_data,
  n*8, HostToDevice);

kernel<<<B,T>>>(d_data, n);

cudaMemcpy(h_data, d_data,
  n*8, DeviceToHost);

cudaFree(d_data);
```

Kokkos

```
View<double*> data("d", n);
auto h = create_mirror_view(data);

deep_copy(data, h);

parallel_for(n, KOKKOS_LAMBDA(int
i){
  data(i) = compute(i);
});

deep_copy(h, data);
// Automatic cleanup (RAII)
```

Single source code → compiles for OpenMP, CUDA, HIP, SYCL, Serial

II. Sparse Representation

Example: 2D Sparse Mesh with Intervals

“Smiley” Geometry :-)

```
       Y
       9│ . . . . . . . . . .    (empty)
       8│ . . . . . . . . . .    (empty)
       7│ . . ▓ ▓ . . ▓ ▓ . .    EYES
       6│ . . ▓ ▓ . . ▓ ▓ . .    EYES
       5│ . . . . . . . . . .    (HOLE)
       4│ . . . . . . . . . .    (HOLE)
       3│ . ▓ ▓ . . . . ▓ ▓ .    SMILE
       2│ . . ▓ ▓ . . ▓ ▓ . .    SMILE
       1│ . . . ▓ ▓ ▓ ▓ . . .    SMILE
       0│ . . . . . . . . . .    (empty)
        └──────────────────── X
          0 1 2 3 4 5 6 7 8 9
```

Sparse-CSR-like Representation

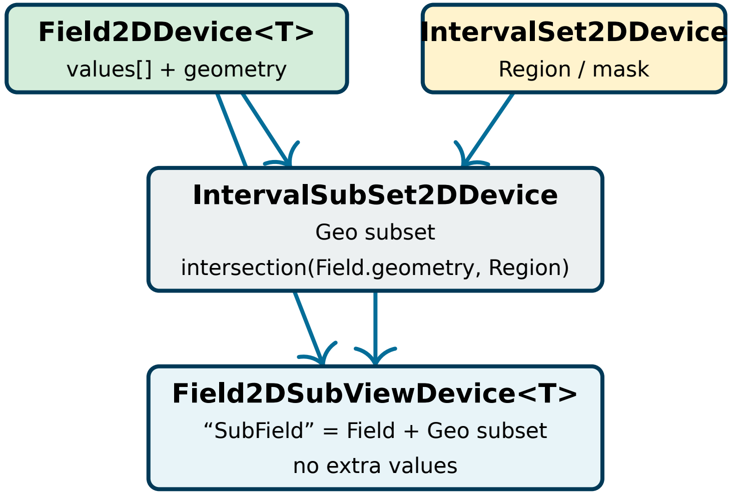
```
// 5 rows, HOLE Y=4,5
row_keys = [1, 2, 3, 6, 7]  // skips 4,5!
num_rows = 5

// Rows with 1 or 2 intervals
row_ptr = [0, 1, 3, 5, 7, 9]

intervals = [
  {3, 7},          // Y=1: smile bottom
  {2, 4}, {6, 8},// Y=2: smile thick
  {1, 3}, {7, 9},// Y=3: smile corners
  {2, 4}, {6, 8},// Y=6: EYES bottom
  {2, 4}, {6, 8},// Y=7: EYES top
]
num_intervals = 9

cell_offsets = [0,4,6,8,10,12,14,16,18,20]
total_cells = 20
```

Hole Y=4,5: row_keys jumps from 3 to 6

III. Data Structures

Overview — Device Structures

Core Types



Device-Side Grammar

- `Field2DDevice<T>` = field values + `IntervalSet2DDevice geometry`
- `IntervalSet2DDevice` (region) = mask / target cells
- `IntervalSubSet2DDevice` = geo subset = `geometry ∩ region`
- `Field2DSubViewDevice<T>` = “SubField” = `Field + IntervalSubSet2DDevice`

`Field2DSubViewDevice<T>` internally uses `IntervalSubSet2DDevice` to iterate only on active cells.

SubField: Usage Example

```
Field2DDevice<Real> rho(fluid_geo);      // Field

// Region = any IntervalSet2DDevice (BC, AMR, overlap)
IntervalSet2DDevice left_bc = make_box_device({0,2,0,ny});

// SubField = rho restricted to left_bc
Field2DSubViewDevice<Real> sub = make_subview(rho, left_bc);

// Apply operations only on this region
fill_subview_device(sub, rho_inlet);
apply_stencil_on_subview_device(sub, bc_stencil);
```

SubView Operations

- `fill_subview_device(sub, val)`
- `scale_subview_device(sub, alpha)`
- `copy_subview_device(dst, src)`
- `apply_stencil_on_subview_device(...)`

In `mach2_cylinder`, overlap/guard regions and AMR masks use exactly this SubField (SubView) + region mask design.

IntervalSet2D — Complete CSR Structure

Sparse 2D geometry stored as **rows of X-intervals**, indexed by Y coordinate — similar to CSR matrix format.

C++ Definition

```
template<class MemorySpace>
struct IntervalSet2D {
  // Y coordinates of non-empty rows
  View<RowKey2D*> row_keys;  // [num_rows]

  // Index into intervals[] for each row
  View<size_t*> row_ptr;     // [num_rows + 1]

  // All intervals (contiguous)
  View<Interval*> intervals; // [num_intervals]

  // Linear cell offsets
  View<size_t*> cell_offsets;// [num_intervals]

  size_t total_cells;
  int num_rows;
  int num_intervals;
};
```

Basic Types

```
using Coord = std::int32_t;

struct Interval {
  Coord begin = 0;  // Inclusive
  Coord end = 0;    // Exclusive
};

struct RowKey2D {
  Coord y = 0;
};
```

Invariants

- `row_keys` sorted by increasing Y
- Intervals sorted by X within each row
- No overlap between intervals
- `row_ptr[r+1] - row_ptr[r]` = nb intervals row r

Field2D — Field on Sparse Geometry

Associates a **contiguous array of values** with each cell of an IntervalSet2D geometry.

Definition

```
template<class T, class MemorySpace>
struct Field2D {
  IntervalSet2D geometry;  // Geometry ref
  View<T*> values;         // [total_cells]
};
```

Memory Layout

```
Geometry:  ████ ░░ ████ ░░ ██████
values[]:  [v0 v1 | v2 v3 | v4 v5 v6]
            ↑       ↑       ↑
offsets:    0       2       4
```

Contiguous values → cache-friendly

Cell Access

```
// O(1) - interval index + x coordinate
T val = field.at(interval_idx, x);
```

Usage

```
Field2DDevice<double> rho(fluid_geo);
fill_field_device(rho, 1.0);
auto rho_host = to_host(rho);  // I/O
```

SubSet — Targeted Region Operations

Represents a **subset of the parent geometry** (intersection with a mask) — used by SubFields to restrict operations to specific cells.

Structure

```
struct IntervalSubSet2D {
  IntervalSet2D parent;  // ref to Field geo
  interval_indices[];    // which intervals
  x_begin[], x_end[];    // restricted range
  row_indices[];         // Y row in parent
  num_entries;
};
```

Usage

```
// Build subset (intersection)
build_interval_subset(
  field.geometry, mask, subset, &ctx);

// Operations on subset only
fill_on_subset(field, subset, 0.0);
```

1D Example: Intersection

```
Parent:  [==A==]   [==B==]   [==C==]
  idx:      0         1         2
         0     8  12    18  22    30

Mask:        [=======M=======]
             5              25

SubSet:      [=]   [==B==]   [=]
             5 8  12    18  22 25
              ↑       ↑       ↑
entry:        0       1       2
```

SubSet = references to Parent

```
entry | interval_idx | x_begin | x_end
------+--------------+---------+------
  0   |      0 (A)   |    5    |   8
  1   |      1 (B)   |   12    |  18
  2   |      2 (C)   |   22    |  25
```

No data copy — just indices + bounds

⚠ Structure too complex — needs simplification

Field2DSubView — View on Field + Region

Combines a Field with a target region for **localized operations**.

Structure

```
struct Field2DSubView<T> {
  Field2D<T> parent;        // ref to field
  IntervalSet2D region;     // where to operate
  IntervalSubSet2D subset;  // intersection
};
```

Lazy Pattern

```
// 1. Create (no computation)
Field2DSubViewDevice<T> sub = make_subview(field, region);
// sub.subset is empty

// 2. First op with ctx → triggers build
fill_subview_device(sub, 0.0, &ctx);
// sub.subset = field.geo ∩ region

// 3. Next ops reuse subset
scale_subview_device(sub, 2.0);  // fast!
fill_subview_device(sub, 1.0);   // fast!
```

Memory Mapping

```
Geometry:   [==A==]    [==B==]    [==C==]
               ↓          ↓          ↓
values[]:  [░░███|░░░░░████░|██░░░░░░]
              ↑          ↑       ↑
           entry 0    entry 1  entry 2
```

░ = skipped █ = accessed by SubSet

Workspace & AMR Support

Reusable buffer pool to avoid repeated GPU allocations, and multi-resolution grid structure for AMR.

UnifiedCsrWorkspace

Pool of reusable buffers

```
struct UnifiedCsrWorkspace {
  View<int*> int_bufs_[5];        // indices, maps, flags
  View<size_t*> size_t_bufs_[2];  // row_ptr, counts
  View<RowKey2D*> row_key_bufs_[2]; // Y coords
  View<Interval*> interval_buf_0;   // X intervals

  auto get_int_buf(int id, size_t n) {
    if (n > int_bufs_[id].extent(0))
      Kokkos::resize(int_bufs_[id], n*1.5);
    return subview(int_bufs_[id], {0,n});
  }
};
```

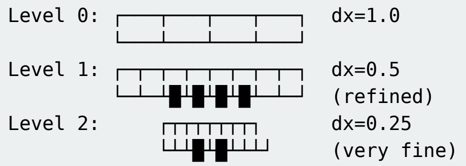
Avoids repeated GPU allocations
Crucial for chained operations

Note: Outputs must be pre-allocated
Use `allocate_interval_set_device()`

MultilevelGeo (AMR)

Multi-resolution grids

```
template<class MemorySpace>
struct MultilevelGeo {
  double origin_x, origin_y;
  double root_dx, root_dy;
  int num_active_levels;
  Array<GeoView, 16> levels;

  double dx_at(int level) {
    return root_dx / (1 << level);
  }
};
```



IV. Algorithms

Binary Search — O(log n) Lookups Everywhere

CSR structure requires binary search for row and interval lookups — efficient but suboptimal on GPU.

CSR Requires Sorted Data

All lookups rely on binary search:

1. Find row by Y coordinate

```
int find_row_by_y(row_keys, num_rows, y) {
  // Binary search in row_keys[]
  return lower_bound(row_keys, y);
}
```

O(log R) — R = number of rows

2. Find interval by X coordinate

```
int find_interval_by_x(intervals, begin, end, x) {
  // Binary search in intervals[begin..end]
  return lower_bound(intervals, x);
}
```

O(log I_{row}) — I = intervals in row

Combined: Cell Lookup

```
T& get(Coord x, Coord y) {
  // Step 1: find row
  int row = find_row_by_y(row_keys, y);
  // Step 2: find interval in row
  int iv = find_interval_by_x(
    intervals, row_ptr[row], row_ptr[row+1], x);
  // Step 3: compute offset
  return values[offsets[iv] + (x - intervals[iv].begin)];
}
```

Total: **O(log R + log I)**

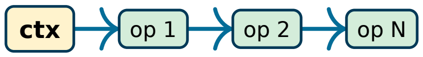
GPU: Binary search = suboptimal (future work)

Set Algebra — Binary Operations

Binary set operations (∪, ∩, \) combine geometries using a shared workspace to avoid repeated GPU allocations.

CsrSetAlgebraContext

```
struct CsrSetAlgebraContext {
  UnifiedCsrWorkspace workspace;
  // Pool of reusable GPU buffers:
  // - int_bufs_[5], size_t_bufs_[2]
  // - row_key_bufs_[2], interval_buf_
  // Auto-grows on demand, never shrinks
};
```



Same ctx reused → **zero allocations** after warmup

Complete Example

```
CsrSetAlgebraContext ctx;  // create once

auto domain = make_box_device({0,400,0,160});
auto obstacle = make_disk_device({80,80,20});

auto fluid = allocate_interval_set_device(
    domain.num_rows,
    domain.num_intervals + obstacle.num_intervals);

set_difference_device(domain, obstacle, fluid, ctx);
```

Chaining with Buffer Reuse

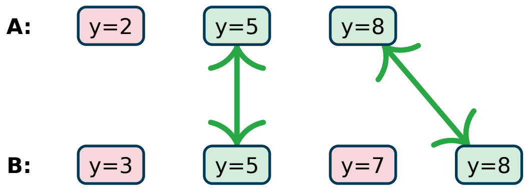
```
CsrSetAlgebraContext ctx;

// Pre-allocate output buffers ONCE
auto set1 = allocate_interval_set_device(512, 2048);
auto set2 = allocate_interval_set_device(512, 2048);

// Compute: set1 = A ∪ B
set_union_device(A, B, set1, ctx);

// Compute: set2 = set1 \ C
set_difference_device(set1, C, set2, ctx);

// ... use set2 (e.g., create Field2D on it) ...

// Later: reuse same buffers!
set_intersection_device(D, E, set1, ctx);  // set1 reused
set_union_device(set1, F, set2, ctx);      // set2 reused
```

Allocate once → reuse for entire simulation
ctx + set1 + set2: zero GPU malloc in hot loop

Intersection — How It Works

Intersection uses the **Count-Scan-Fill** pattern: count output intervals, compute offsets via prefix sum, then fill in parallel.

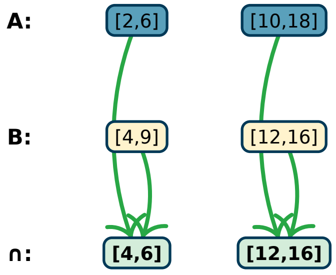
Phase 1: Row Mapping



Binary search: O(log n) per row

Phase 2: Interval Merge (per row)

Row y=5 — 2 intervals each



O(n+m) sweep — `max(begin), min(end)`

GPU Pattern: Count-Scan-Fill

Why? GPU threads can't dynamically allocate — output size must be known before parallel write.

1. COUNT — how many intervals per row?

```
row_counts[i] = count_intersect(A[i], B[i])
```

Parallel per row — don't write yet

2. SCAN — where does each row start?

```
row_ptr = exclusive_scan(row_counts)
```

Prefix sum → row_ptr[i] = write offset

3. FILL — write results at known offsets

```
fill_intersect(A[i], B[i], out, row_ptr[i])
```

Parallel per row — no conflicts!

Same pattern for **∪**, \, ⊕

Row Mapping — Why and How

GPU parallelization requires knowing output rows before processing — row mapping creates a correspondence table between output and input rows.

GPU Constraint

1 thread = 1 output row

We need to know output rows **before** parallel processing.

The Mapping Structure

```
struct RowMergeResult {
  row_keys[];    // Y coords of output rows
  row_index_a[]; // index in A (-1 if absent)
  row_index_b[]; // index in B (-1 if absent)
};
```

Usage in Parallel

```
parallel_for(num_rows_out, [&](int i) {
  int ia = row_index_a[i]; // -1 or valid
  int ib = row_index_b[i]; // -1 or valid

  intervals_a = (ia >= 0) ? A.row(ia) : ∅;
  intervals_b = (ib >= 0) ? B.row(ib) : ∅;

  merge(intervals_a, intervals_b, out[i]);
});
```

Each thread knows exactly what to read → **no conflicts**

Concrete Example: A ∪ B

A: y=2 y=5 y=8

B: y=3 y=5 y=8 y=9

i	y	idx_a	idx_b	Signification
0	2	0	−1	A[0] seul
1	3	−1	0	B[0] seul
2	5	1	1	A[1] ∪ B[1]
3	8	2	2	A[2] ∪ B[2]
4	9	−1	3	B[3] seul

−1 = ligne absente dans ce set
Le mapping est construit par recherche binaire

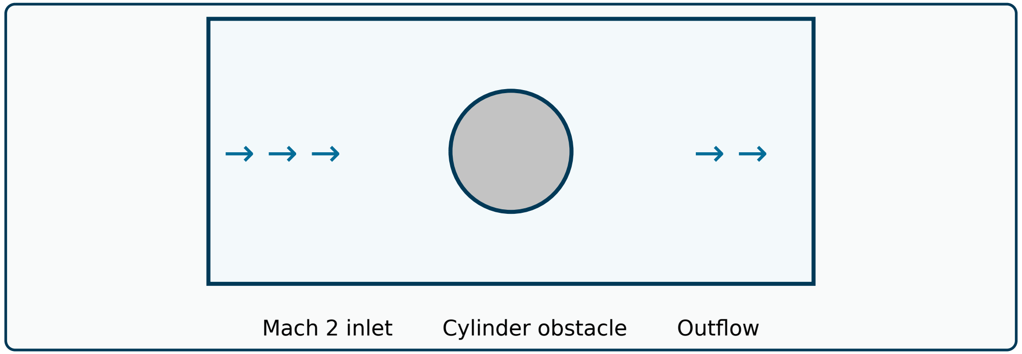
Op	Mapping
A ∩ B	Garde les y communs
A ∪ B	Fusionne tous les y
A \ B	Garde les y de A

V. Demo

Mach2 Cylinder — Problem & Setup

Physical Problem

Supersonic flow around a cylinder — classic CFD benchmark for shock capturing.



Boundary Conditions

- **Left**: Supersonic inlet (Mach 2, fixed state)
- **Right**: Supersonic outlet (extrapolation)
- **Top/Bottom**: Reflective walls (slip)
- **Cylinder**: Solid wall (reflective)

Numerical Method

- **Equations**: 2D Euler (compressible, inviscid)
- **Variables**: ρ, ρu, ρv, E (density, momentum, energy)
- **Scheme**: 1st order finite volume, Rusanov flux
- **Gas**: Ideal gas, $\gamma = 1.4$

Adaptive Mesh Refinement

- **4 levels** of refinement (factor 2 per level)
- **Criterion**: Density gradient magnitude
- **Dynamic**: Regrid every step
- **Guard zones**: Smooth transitions between levels

Sparse geometry: only fluid cells stored & computed

Bow shock forms in front of cylinder
AMR refines automatically near discontinuity

Mach2 Cylinder — Subsetix Usage

1. Fluid Geometry

```
auto domain = make_box_device({0, nx, 0, ny});
auto obstacle = make_disk_device({cx, cy, radius});
auto fluid = allocate_interval_set_device(...);
set_difference_device(domain, obstacle, fluid, ctx);
```

`fluid = domain \ obstacle`

2. Refinement Mask (detect shock)

```
IntervalSet2DDevice interior;
shrink_device(fluid, 1, 1, interior, ctx);

Field2DDevice<Real> indicator(interior);
apply_csr_stencil_on_set_device(
    indicator, rho, interior, GradientStencil{});

auto mask = threshold_field(indicator, thresh);
```

`shrink → stencil → threshold`

3. Coarse Active (exclude fine level)

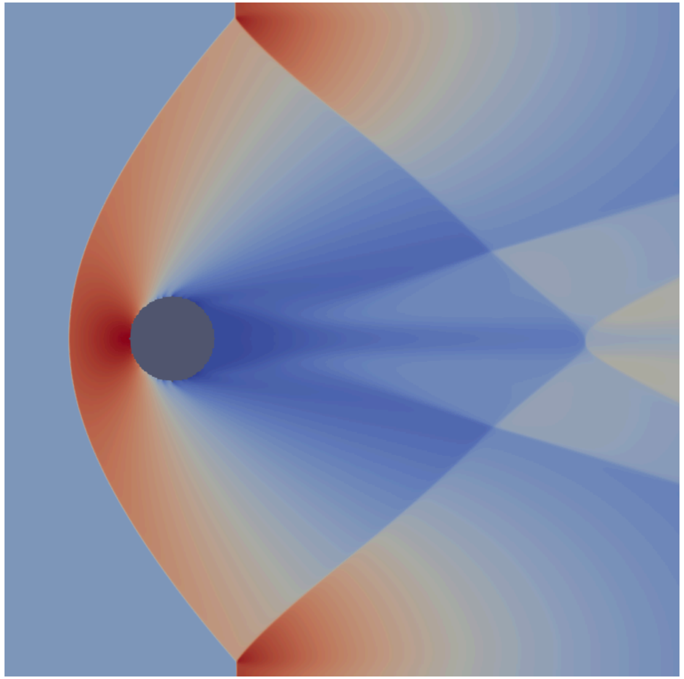
```
IntervalSet2DDevice fine_proj;
project_level_down_device(fine_geo, fine_proj, ctx);

auto coarse_active = allocate_interval_set_device(...);
set_difference_device(coarse_geo, fine_proj,
                      coarse_active, ctx);
```

`coarse_active = coarse \ project(fine)`

Même `ctx` pour toutes les opérations
→ **zéro allocation GPU** après warmup

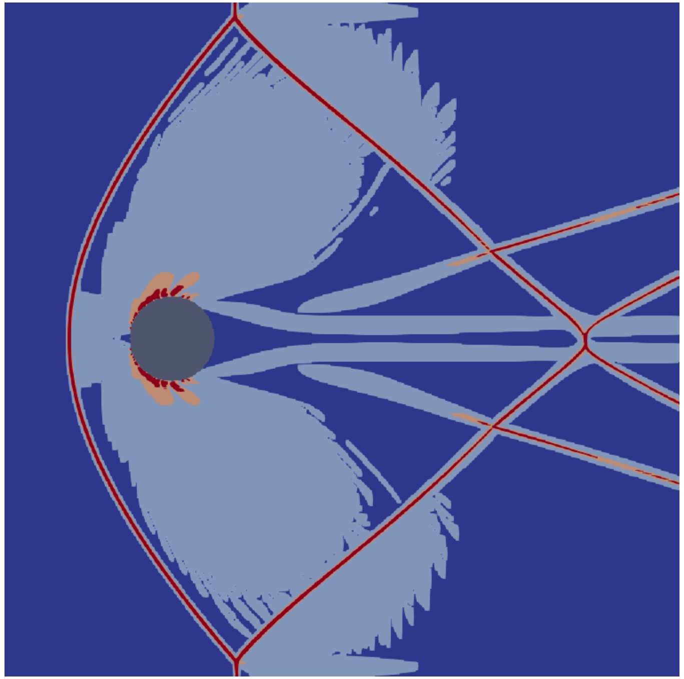
Mach2 Cylinder — Visual Results

Density Field



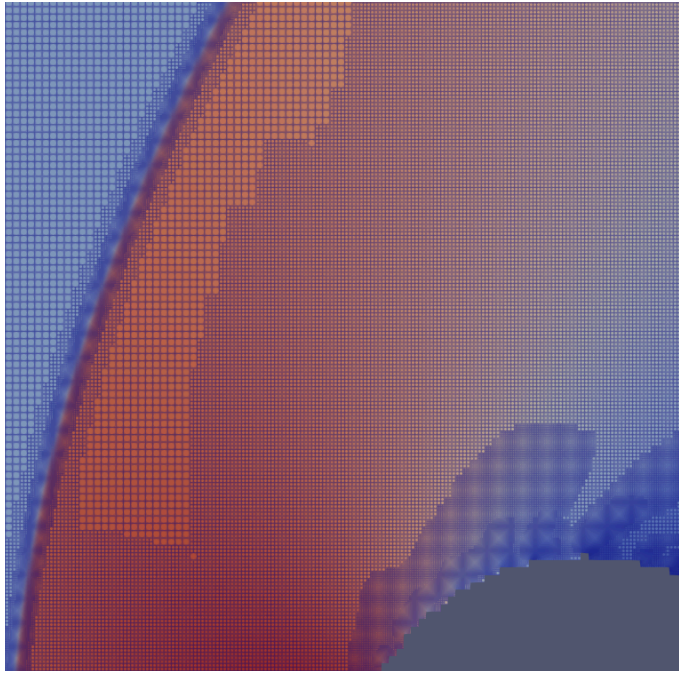
Bow shock in front of cylinder
Colormap: blue (low) → red (high)

AMR Levels



Automatic refinement zones
near the shock front

Mesh Zoom



Multi-level AMR resolution
near the bow shock

4 AMR levels (9–12) — Automatic refinement based on density gradient

Status & Future Work

Done

Complete set algebra
- Union, intersection, difference
- Morphology (expand, shrink)
- Threshold, projection

Complete AMR pipeline
- Multi-level geometry management
- Refinement mask computation
- Restrict / prolong operations
- Dynamic regridding every step

Future Work

Refine algorithms
- Optimize binary search on GPU
- Reduce kernel launch overhead
- Better load balancing

3D extension
- IntervalSet3D with Z-slices
- Same CSR structure per slice

CUDA Streams
- Overlap operations
- Maximize GPU occupancy
- Hide memory transfer latency

Thank You!

Questions?

Key Points

- CSR interval representation
- Count-Scan-Fill pattern
- Kokkos parallelism (CPU/GPU)
- Workspace for memory reuse
- Multi-level AMR (Mach2)

Contact

Sébastien DUBOIS
HPC@Maths Team

Code: `include/subsetix/`
Demo: `examples/mach2_cylinder/`

Appendices

Appendix A: Project Evolution

Implementation History

Version	Description	Performance	Status
v1	CPU only, Sparse CSR + Workspaces First sequential implementation	Faster than baseline	✓ Stable
v2	Multithreaded **Tiled** Sparse CSR OpenMP and TBB backends Tiling for locality	Excellent on large mesh	⚠ Complex Likely bugs
v3	CUDA only GPU set algebra Proof of concept	**Fastest**	✓ PoC validated
v4	**Kokkos** (current version) Non-tiled Sparse CSR OpenMP + CUDA portability	Slower than v2/v3	✓✓ **Reliable** Verified

Lessons Learned

- **Tiling** improves locality but greatly increases complexity
- Native CUDA faster but less portable
- Kokkos = best **reliability/portability** tradeoff

Final Choice: Kokkos

- **Single** code for CPU and GPU
- Simplified maintenance
- Easy testing and verification
- Active ecosystem (Sandia, Trilinos)

Appendix B: Why Kokkos?

Comparison with Native CUDA

Aspect	CUDA	Kokkos
Portability	NVIDIA only	**Multi-vendor**
Syntax	<<<>>>	**C++ standard**
Memory	cudaMalloc	**View<T*>**
CPU Debug	Difficult	**Easy (Serial)**
Maintenance	Duplicated code	**Single code**
Performance	**Optimal**	90-95%

Supported Backends

- **OpenMP**: CPU multi-thread
- **CUDA**: NVIDIA GPU
- **HIP**: AMD GPU
- **SYCL**: Intel GPU
- **Serial**: debug and tests

Benefits for This Project

1. Faster Development
Debug on CPU (Serial/OpenMP), deploy on GPU

2. Reliable Tests
Same code tested on CPU and GPU
No hidden “GPU-only” bugs

3. Std Algorithms
`transform`, `reduce`, `scan`, `copy`...
Familiar API, platform-optimized

4. Ecosystem
Trilinos, ArborX, Cabana...
Sandia National Labs support

Appendix C: Development Methodology

Models Used

- **Claude 4.5 Opus** (Anthropic)
- **Claude 4.5 Sonnet** (Anthropic)
- **gpt-5.1-codex-max** (OpenAI)

Work Pattern

PLAN
Architecture & interfaces
Alternatives

↓

QUESTION
Impl details
Edge cases

↓

IMPLEMENTATION
Code generation
Review & iteration

Observed Benefits

- **Rapid exploration** of designs
- Generated inline documentation
- Automatically suggested tests
- Assisted refactoring

Points of Attention

- Systematic code verification
- LLMs can hallucinate APIs
- Always compile and test
- Maintain **architectural control**

LLM = **accelerator**, not replacement
Human expertise remains essential