A Computer Science Approach to Interface Dominated Fluid Problems

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The physics problem

- Turbulent flows with multifluid interfaces
  - Acceleration driven mixing
    - Inertial confinement fusion
    - Target design for high energy particle accelerators
  - Rapidly stirred flows
    - Chemical processing (e.g. fuel separation for spent nuclear reactor rods)
  - Turbulent combustion
    - Combustion in the engine of a Scramjet (M = 7 experimental aircraft)

The Applied Mathematics Problem

- Numerical methods for interfaces are usually low order and inaccurate.
- For problems dominated by interfaces or by approximate interfaces (steep gradients), the dominant error occurs at or near the interface
- Interface methods help a little
- Good interface methods help a lot
- Also need help from physics/engineering: models for unresolved turbulence below the grid scale.

The Program:
Construct good interface methods, Couple to good subgrid scale models

- This presentation: good interface methods
- This is a Computer Science problem
- Essential difficulties
  - Code organization to describe a general interface
  - Robust handling of intersection detection and recovery from self intersections
  - Higher order methods

The Solution

- Code organization: C++ and other modern paradigms are sufficient
- Self intersections: not too hard.
  - Hash list of triangles in blocks, linear algebra to detect collisions. O(n) algorithm, but still expensive.
- Intersection recovery
  - Extreme reliability is needed
    - Simulations on up to 8K cores, running for week+ time frames, require an extremely low error rate.
- Higher order accuracy
  - Seldom attempted; partially implemented in our programs

Intersection Recovery

- Combine a low order recovery algorithm with a more accurate geometry and propagation algorithm
  - Interface defined as triangulated surface
    - Accurate, but not robust for intersection resolution
    - Retriangulate periodically to assure uniform size and aspect ratios for triangles
  - Interface reconstructed from intersections with cell block edges
    - Typical of computer graphics routines
    - Robust and fast but not very accurate
- First is grid free, second is grid based

Hybrid solution

- Locally Grid Based (LGB)
  - Has high accuracy of grid free
  - Has robustness of grid based
  - Main idea: put intersecting region of interface in a rectangular solid formed out of mesh blocks
    - Use grid free outside
    - Use grid based inside
    - Inside region is small, integrated over space and time, so accuracy is dominated by grid free part (high)
    - All problems are inside, where robust algorithm is used, so LGB is robust
  - If several intersections, put such a bounding box outside of each.
  - If too many intersections and too much overlap of bounding boxes, restart time step with a smaller Delta t.
  - Existing time step restriction makes above reduction of time step unlikely

First Problem

- There is a gap between inside and outside surface. This must be filled in.
- Typically edge of inner and outer surface is a curve.
- Trace around points of inner and outer edge curves, adding one bond at a time to join the two.

Second Problem

- For parallel computation,
- Determination of inner and outer surface curve to be communicated between processors if necessory
- Choices of bonds to fill in gaps also to be communicated
- Impractical levels of communication

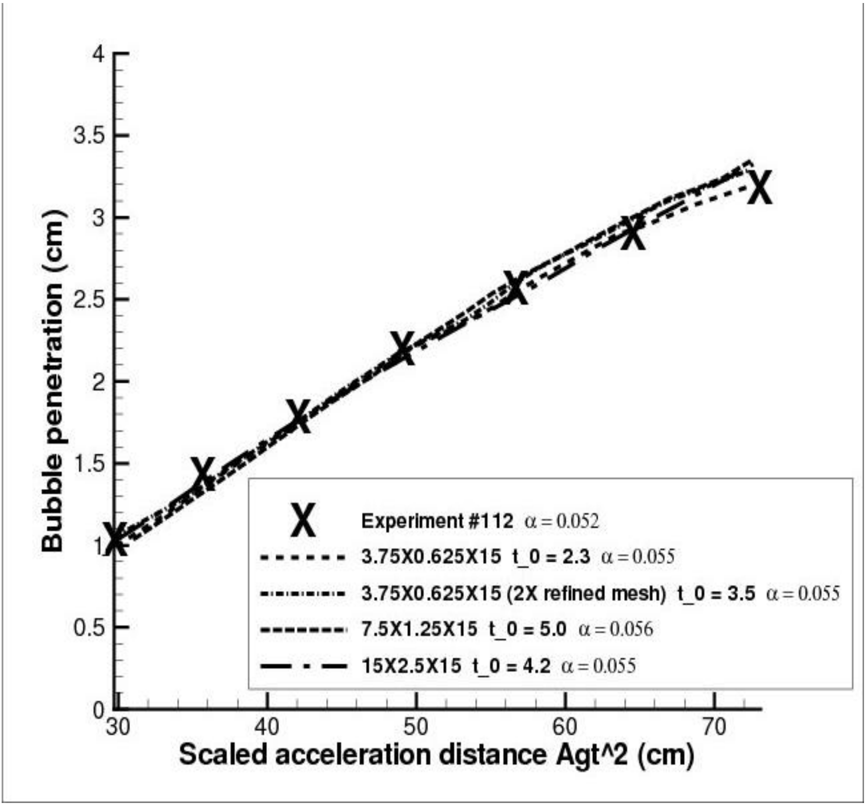
Solution of Second Problem

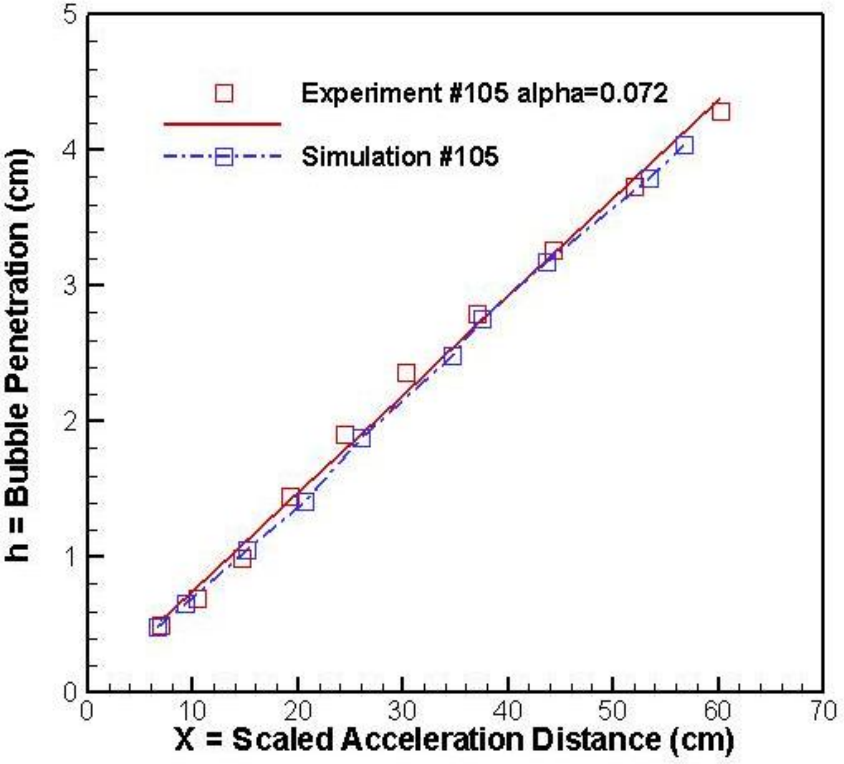
- If possible, increase the buffer size of duplicate shared information at the boundary of parallel processing domains
- If not possible, move entire inside-outside geometry to a single processor
  - Solve locally
  - Communicate solution to location needed
- Solution is currently under test with 8K cores running at ANL, for week+ simulation.

The Payoff: Quality Solutions

- Rayleigh-Taylor fluid mixing
  - Controversial problem with a 60 year history, and generally persistent failure to achieve simulation agreement with experiment.
  - Heavy fluid (water) over light fluid (air), accelerated (by gravity): flat surface is unstable
    - Bubbles of light fluid penetrate into the heavy fluid
    - Distance h = bubble penetration distance
    - Compared to a scaled acceleration distance Agt^2
      - Define alpha = h/Agt^2

Two comparisons: experiments vs. simulations

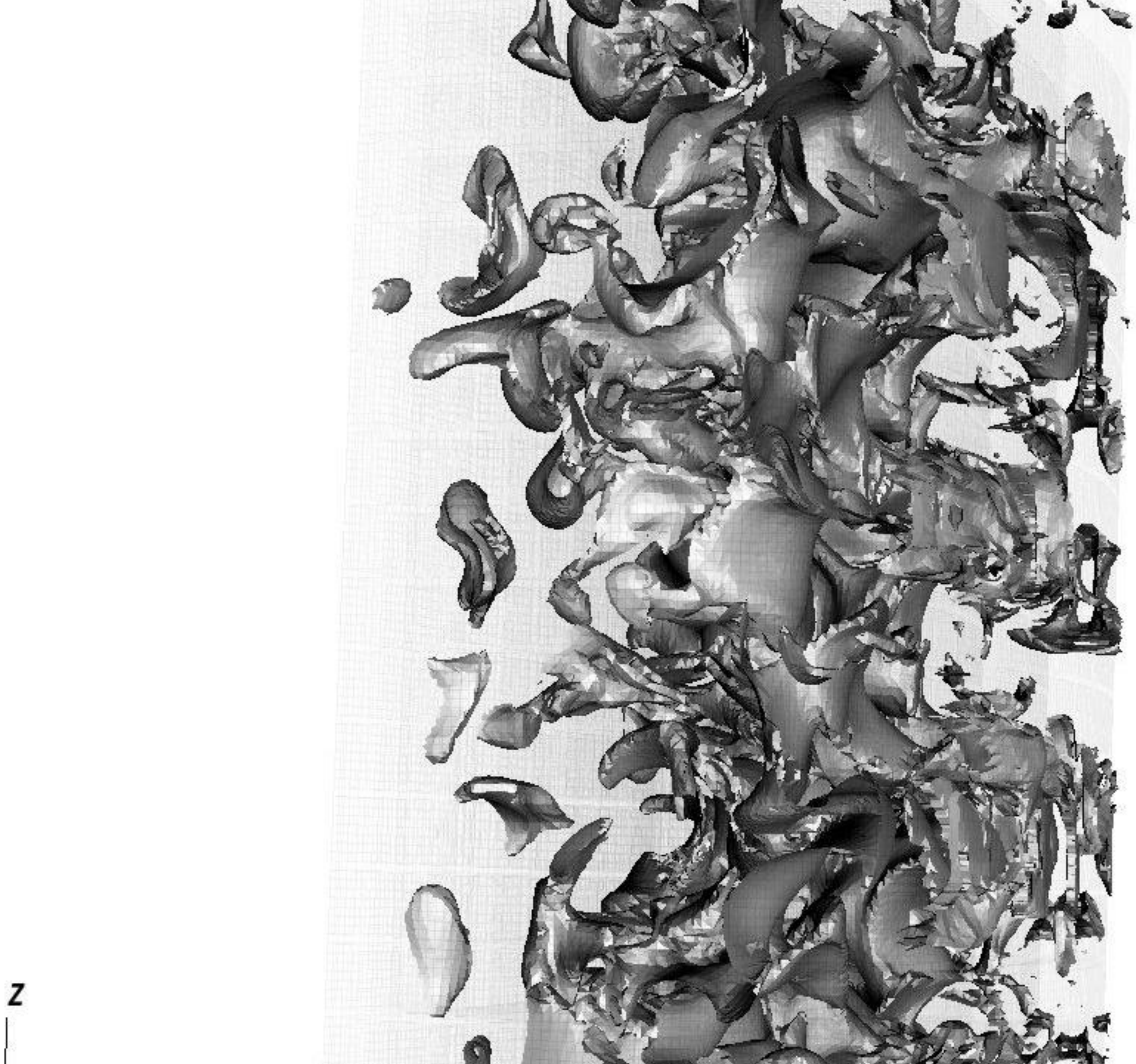




Simulations by Hunkyung Lim and Tulin Kaman. Performed on NYBlue.

Summary Results

- Six simulations compared to experiments
  - Nearly perfect agreement with experiment in all cases
  - Multiple physical processes and parameters
    - Immiscible
      - Variable surface tension (Weber number)
    - Miscible
      - variable rates of mass diffusion (Schmidt number)
    - High and moderate Reynolds number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