Parallel Mesh Adaptation for Unsteady Blast Simulations on Cartesian Meshes

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Motivation

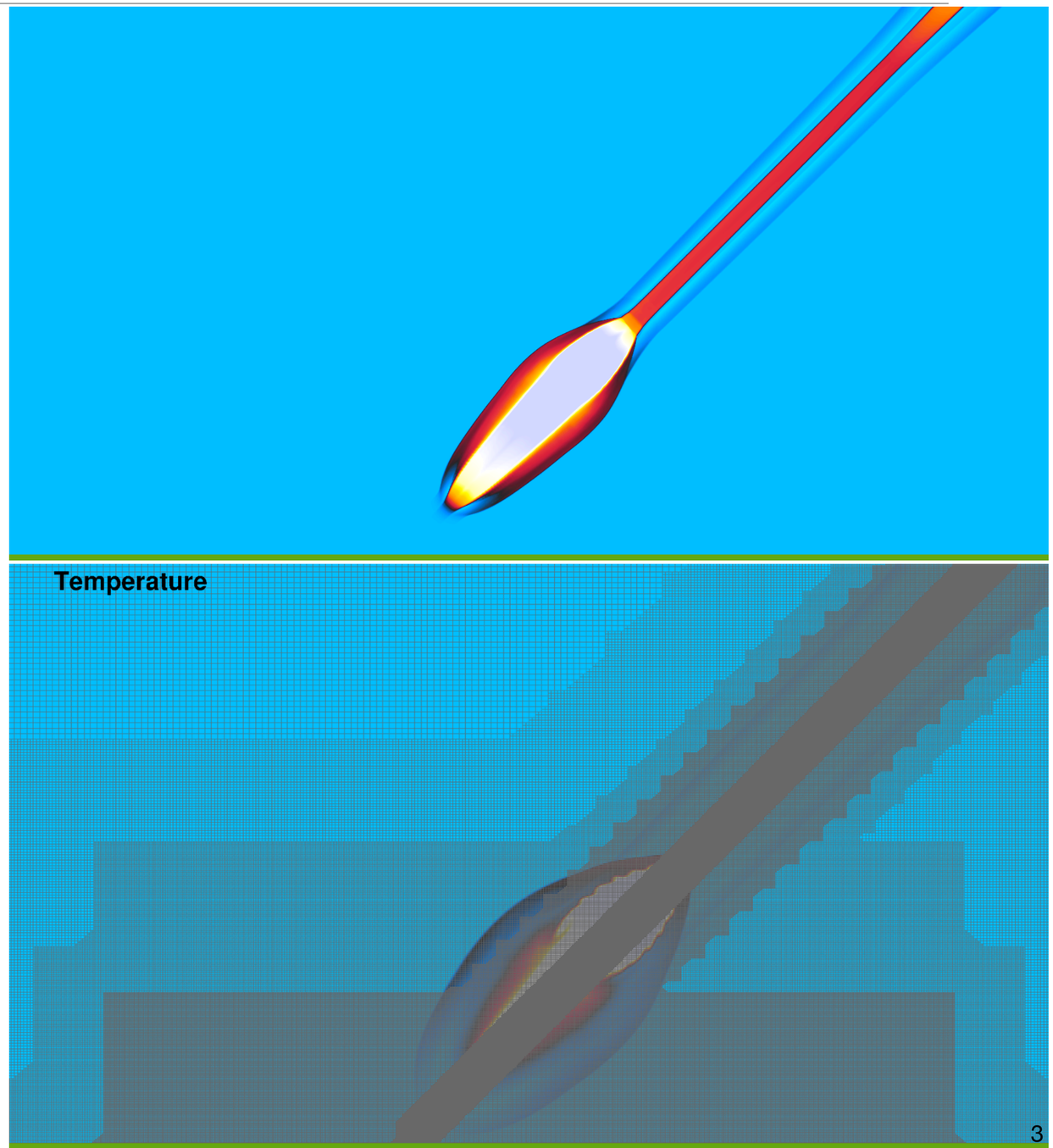


Image Credit: Alex Alishevskikh, / CC-BY 2.0 license

- Chelyabinsk, Russia, February 2013
  - Entry speed ~20 km/s
  - Energy ~520 kilotons of TNT (2.2 x 10^{15} Joules)
    - Equivalent to magnitude 7.0 earthquake
    - Roughly 25-35x higher yield than WWII nuclear weapons
  - Damaged ~7300 structures over 20,000 km^2 area

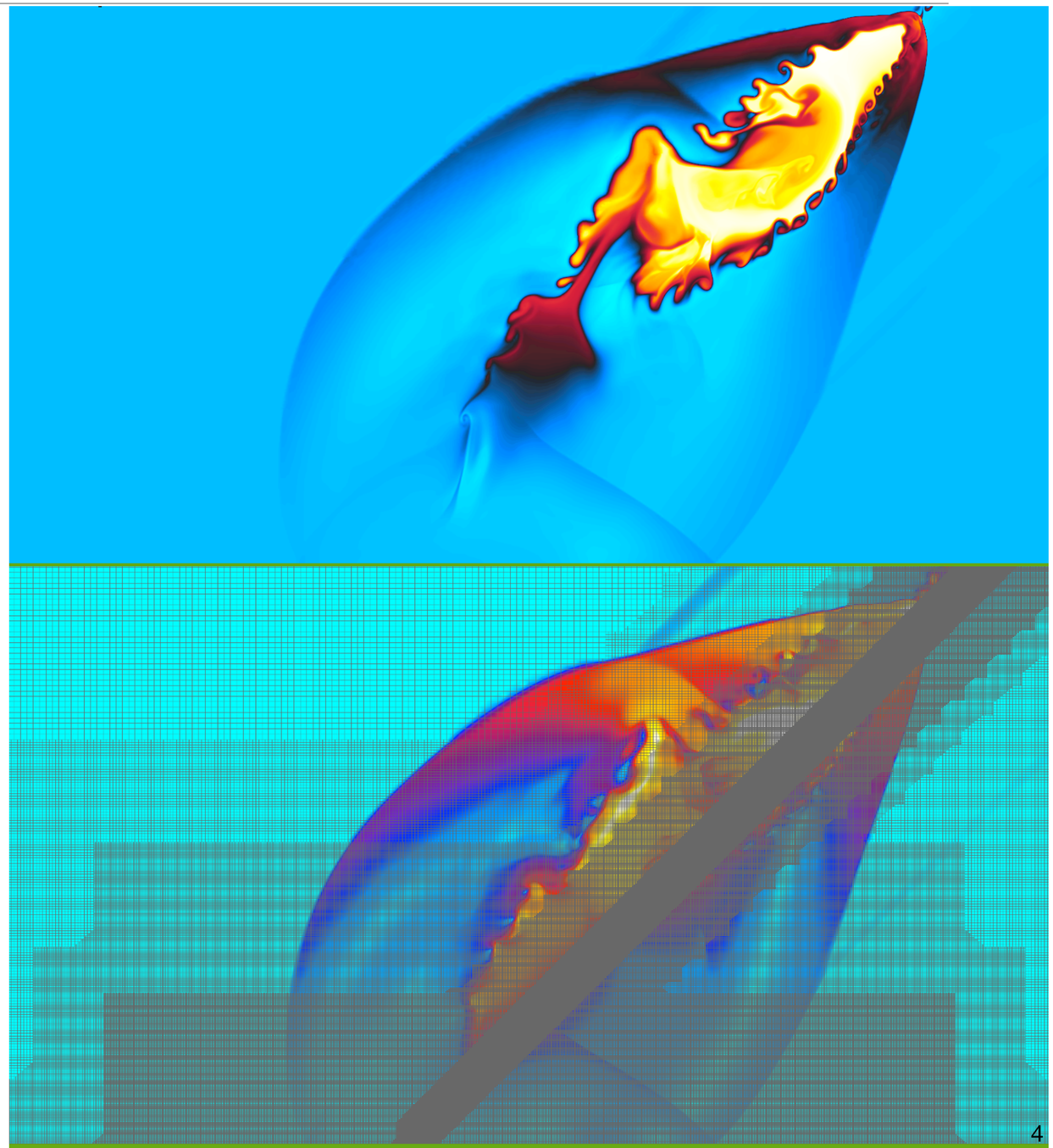
Motivation

- Unsteady blast simulations with Cart3D using a static mesh
  - Maintain high resolution near blast initiation (or entry corridor) and ground zero, (~8-16 m)
  - Lower resolution farther away (~1km)
  - Reduced accuracy far from ground zero increasing uncertainty in blast footprint
- Desire increased accuracy for blast footprint & interaction with terrain and structures - especially at late times far from ground zero
- Static mesh is a necessary compromise since it must resolve solution at all time steps
  - Setup requires “expert intervention” in order to obtain good resolution at reasonable cost
  - Danger of missing unexpected features



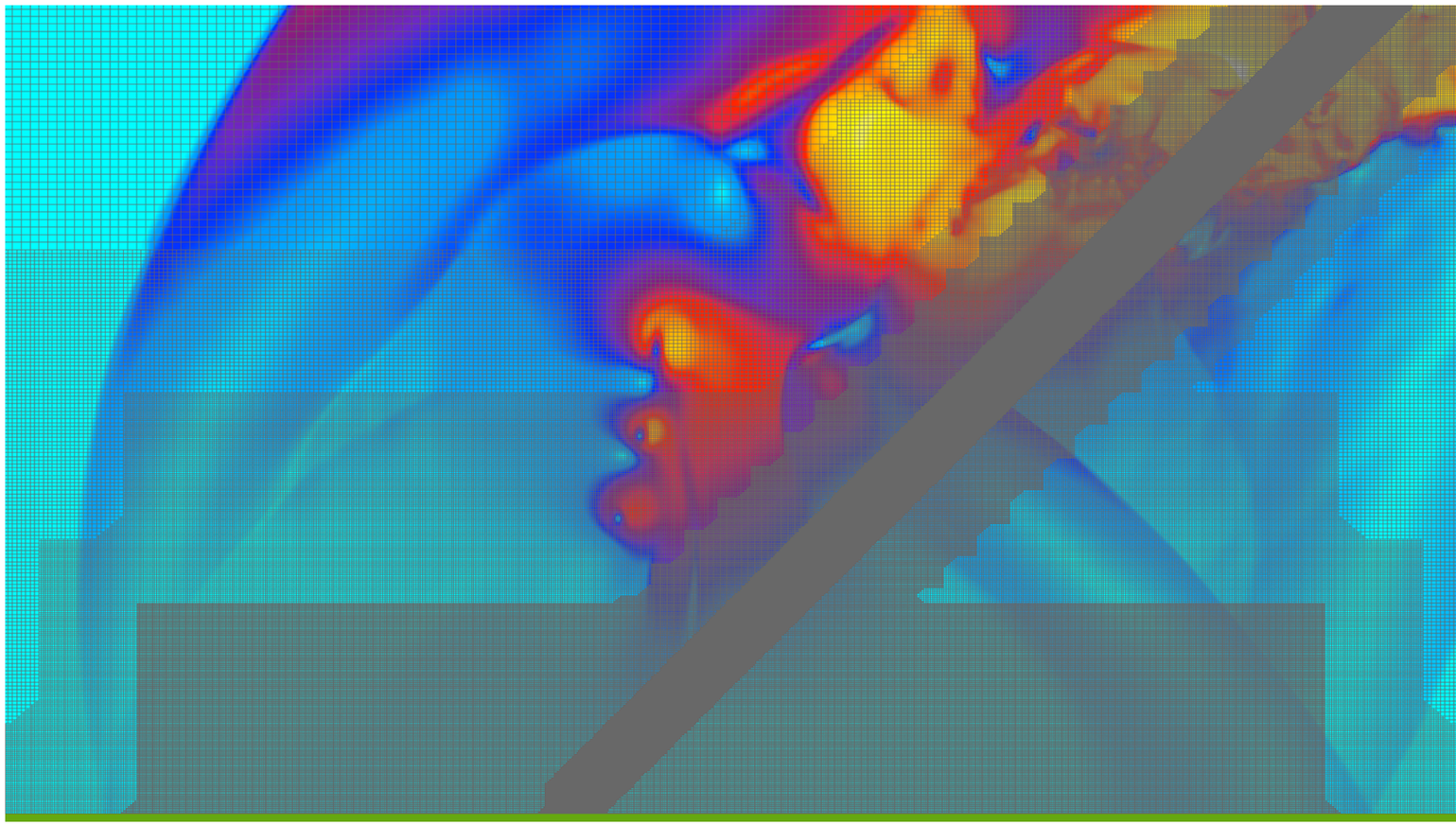
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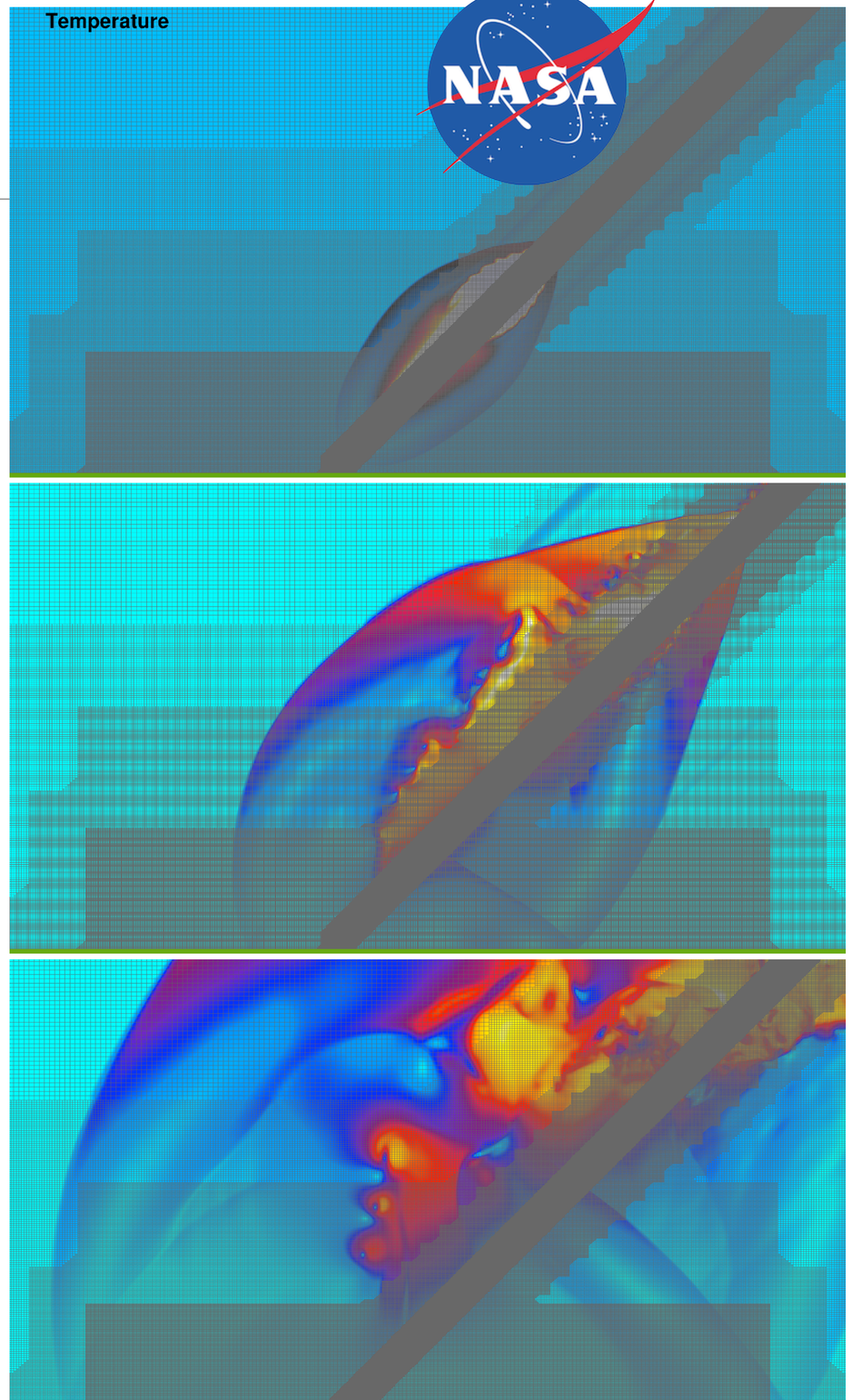
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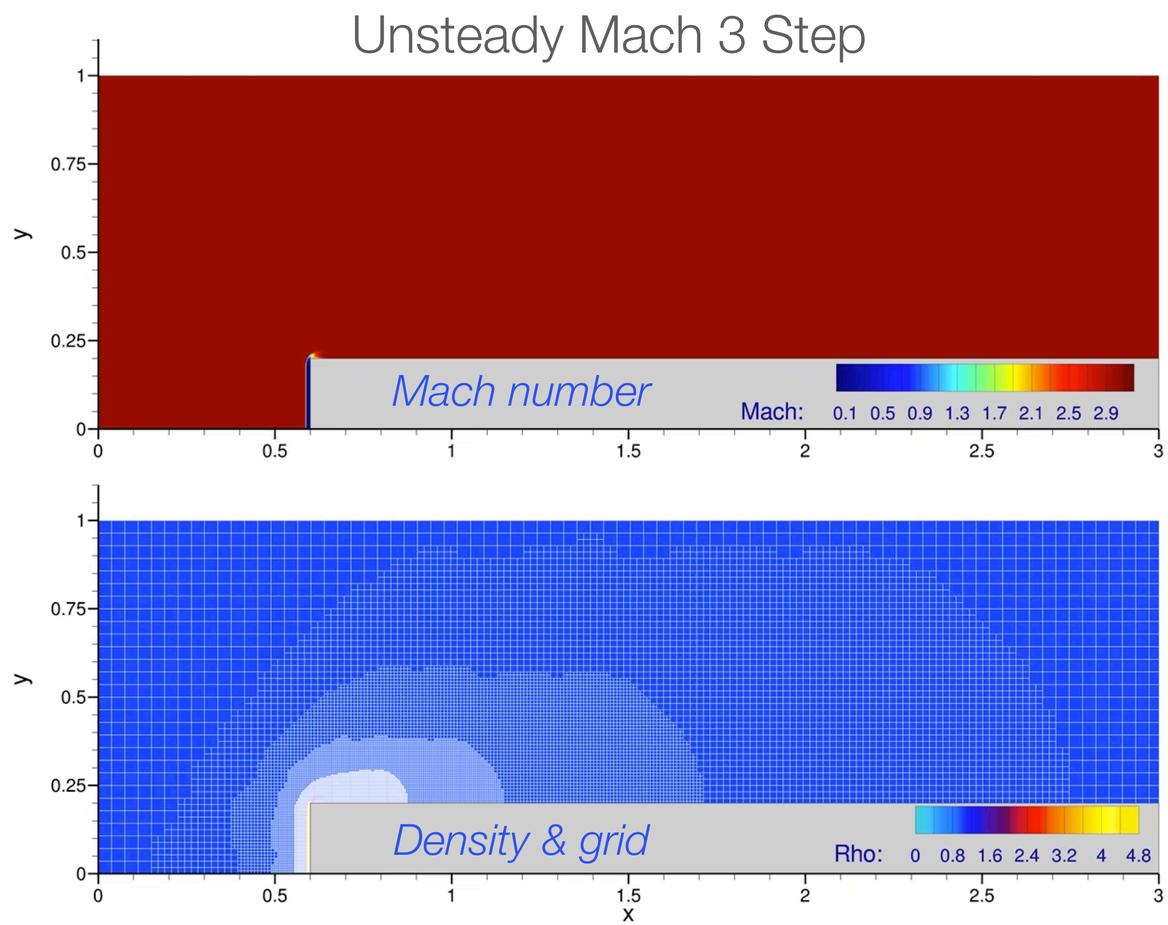
- Asteroid entry and blast propagation
  - Large spatial domain, over 200-400 km at 60-meter resolution results in billions of cells (10^9 - 10^{10})
  - Currently, 300 million cells takes ~12 hours on 16,000 cores
  - Large temporal domain (~10 minutes), high entry speed, and strong shocks result in tens of thousands of time steps ~O(10^4)
  - Cart3D package already has automatic output-based mesh adaptation for steady simulations
- Desire high-performance unsteady adaptive meshing capability
  - Minimize development time
  - Build capability leveraging software components already in use for steady problems
  - Build framework that can be extended to incorporate full unsteady adjoint when this becomes available & affordable

Adaptive meshing is the only affordable option



Motivation

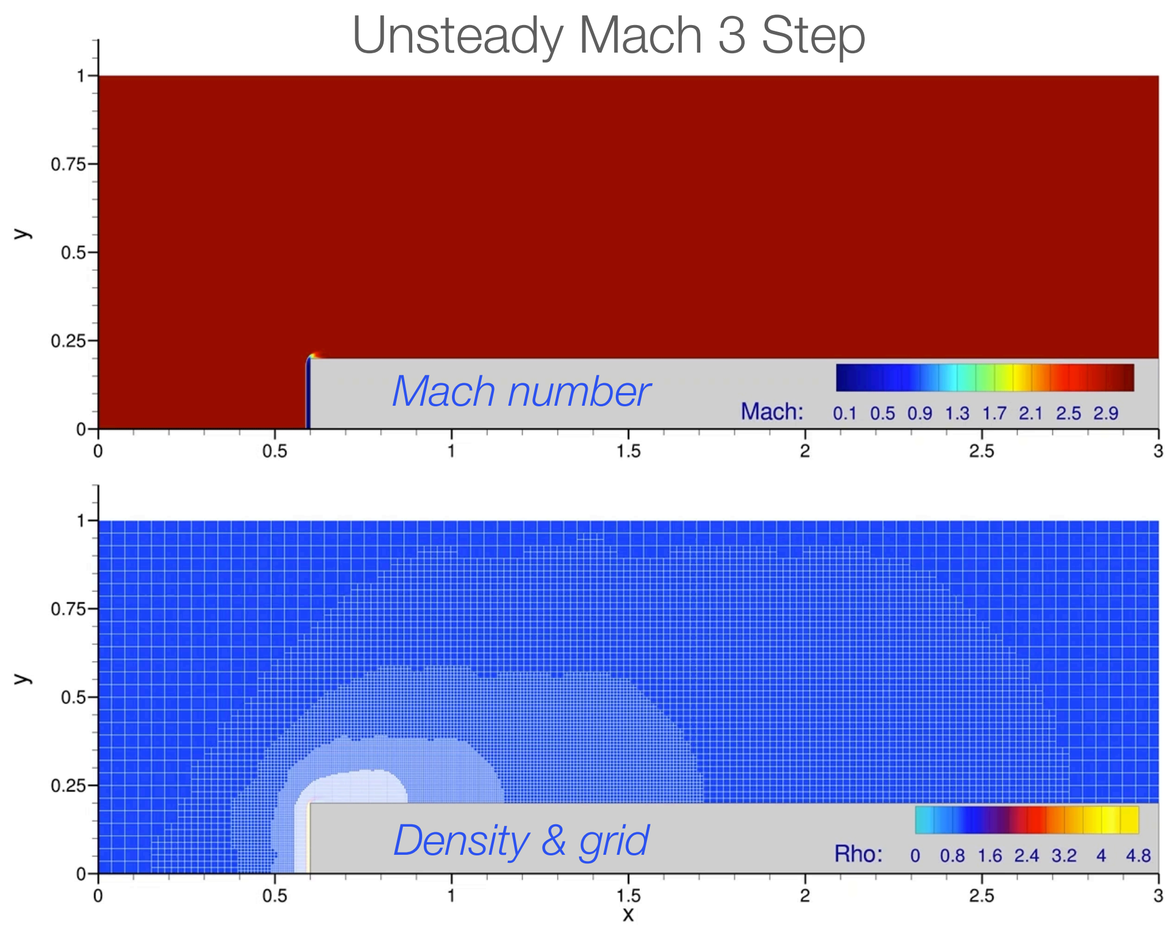
- Adaptation offers more efficient & robust approach since mesh is tailored to evolving solution
  - Less danger of missing unexpected physics
  - Automation reduces reliance on “expert” knowledge for setup
- Challenging to make unsteady mesh adaptation scale to massively parallel simulations
- *Single-pass*: Marching once through time domain
  - Results in one adaptation and remeshing/repartitioning operation at a time (sequential bottleneck)
  - May have to predict evolution of nonlinear flow features



- Emery, *JCP* 1968
- Woodward & Colella, *JCP* 1984

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  - May have to predict evolution of nonlinear flow features
- *Multiple-pass*: Sweep time domain multiple times
  - *A posteriori* meshing and adaptation can be parallelized
  - Multiple adapt cycles on successively refined meshes used to assess flow convergence and establish confidence in solution
  - Fixed-point based iteration (Alauzet et. al, 2003, 2007, 2011)



- Emery, *JCP* 1968
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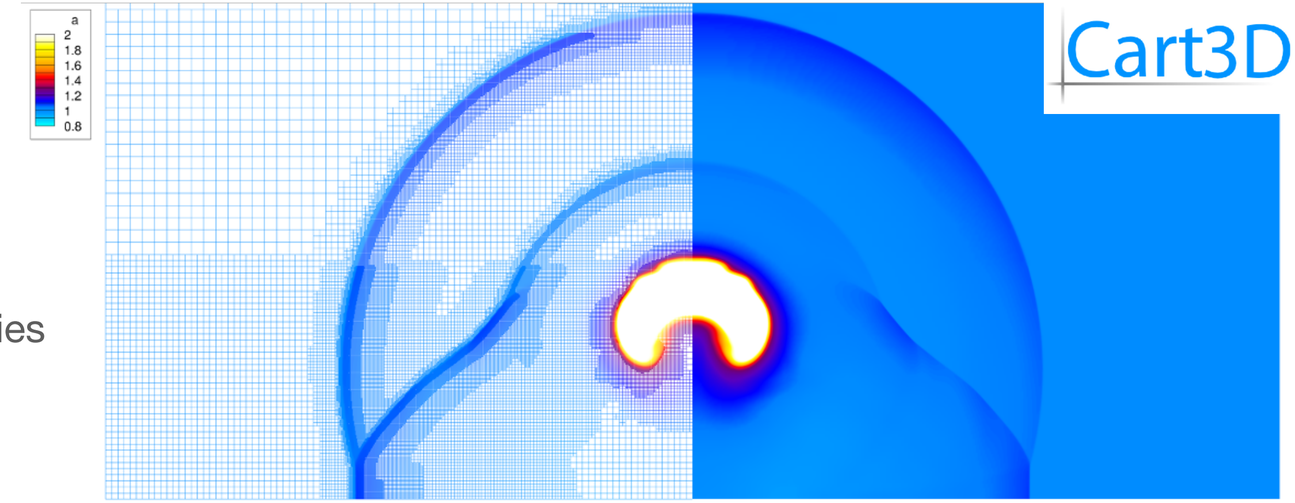
Parallelize mesh adaptation & repartitioning work

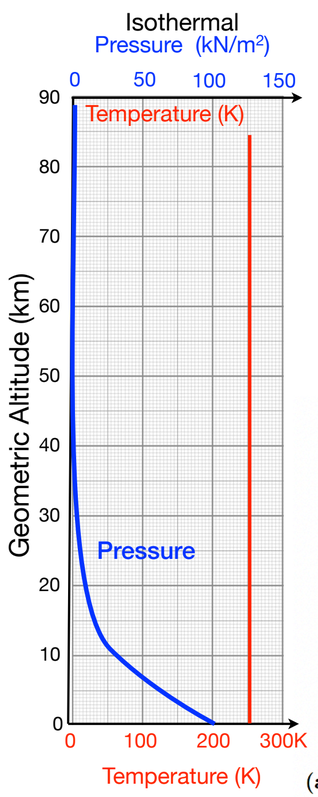
Outline

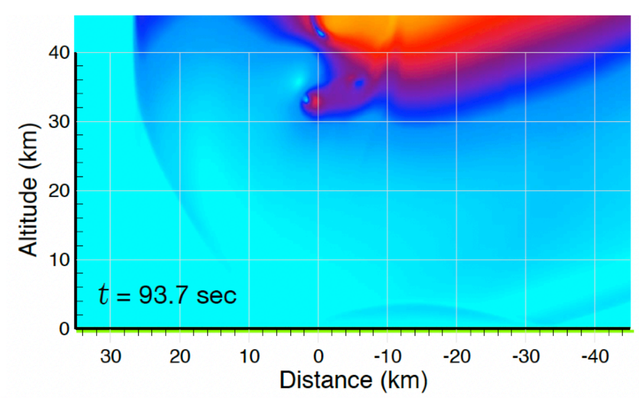
- Flow solver & methodology
- Parallel approach to unsteady mesh adaptation
- Example: Mach 3 step
- Results
  - 2D static airburst with buoyancy
  - 3D asteroid entry and blast propagation
- Summary

Cart3D Software Package

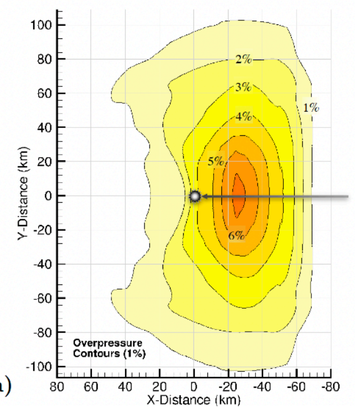
- Cart3D v1.5.9
  - Inviscid flow solver, multigrid acceleration
  - Domain decomposition, highly scalable
  - Multilevel Cartesian mesh with embedded cut-cell boundaries
  - Fully conservative finite-volume method
  - Dual-time stepping for time-dependent flow
  - Second-order in both spatial and temporal discretization
  - Unsteady simulations use feature-based mesh adaptation
- Atmosphere profile
  - Isothermal atmosphere model with scale height, H
  - $p(z) = p_0 e^{-z/H}$, $\rho(z) = \rho_0 e^{-z/H}$
  - Excellent agreement using isothermal atmosphere model in previous Chelyabinsk simulations
  - Aftosmis, M. J., Nemec, M., Mathias, D. L., and Berger, M. J., “Numerical Simulation of Bolide Entry with Ground Footprint Prediction,” 54th AIAA Aerospace Sciences Meeting, San Diego, CA, 2016. https://doi.org/10.2514/6.2016-0998.



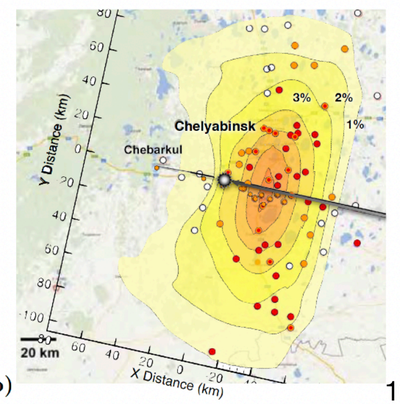




(a)



(b)

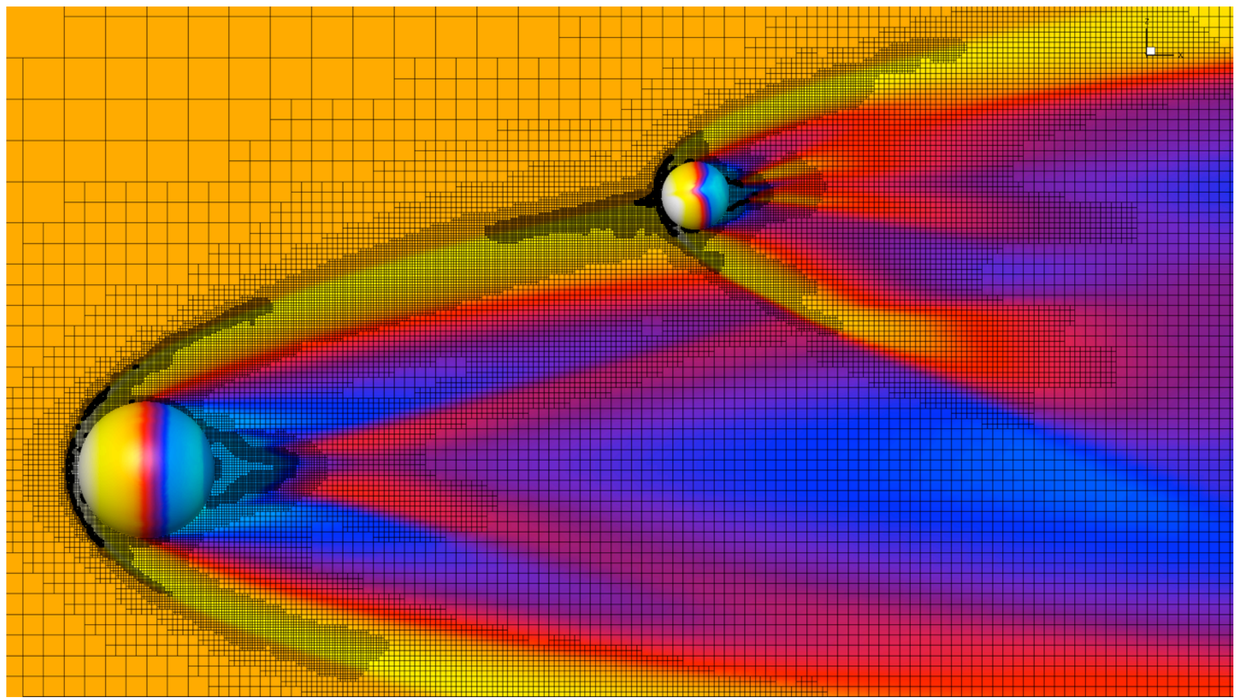


Adaptive Meshing for Steady Simulations

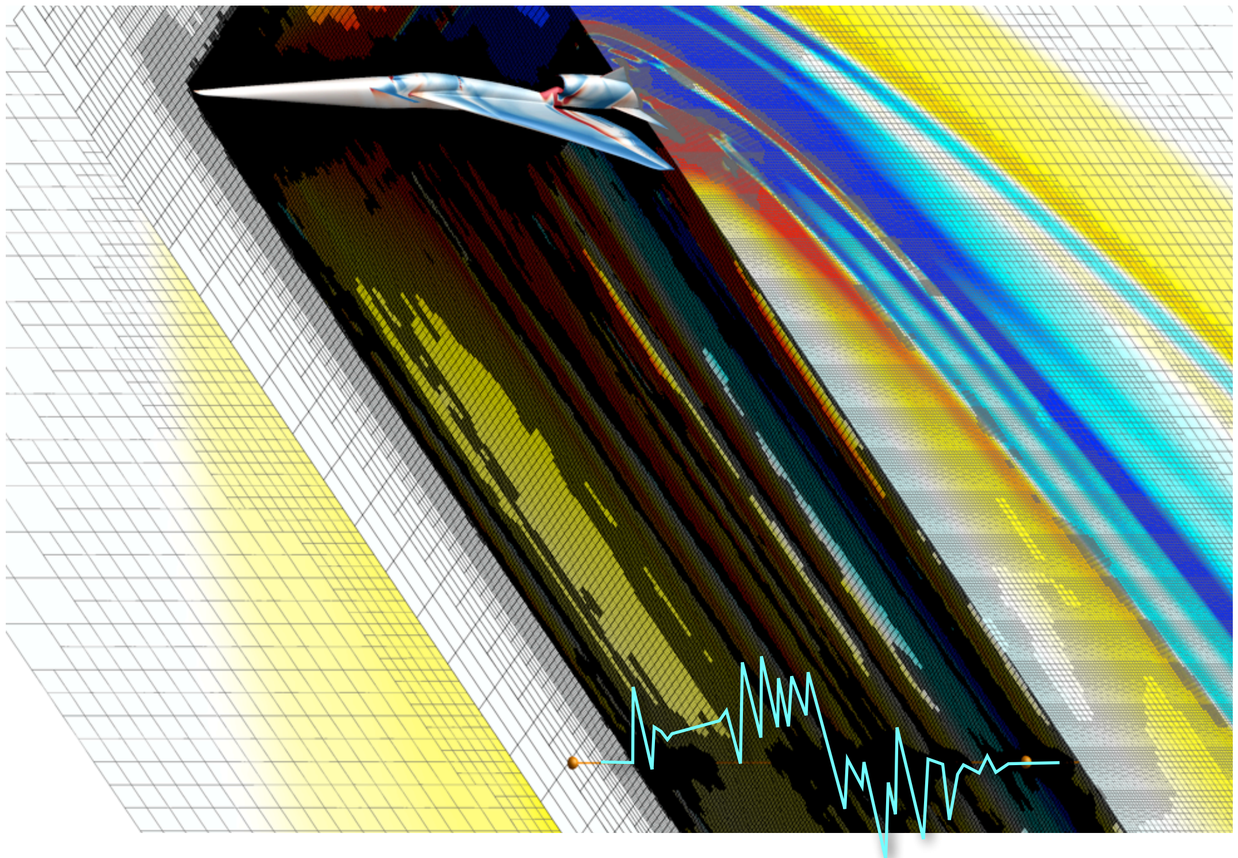
Current mesh adaptation suite typically use “output-based” mesh adaptation

- Use adjoint solution to automatically build a mesh that minimizes errors in engineering outputs, (lift, drag, etc..)
- Tailors mesh to minimize discretization error for these outputs
- Goal is to have each cell in the domain “work” equally hard
- Provably convergent and delivers verifiable error tolerances on engineering outputs†

Spheres in hypersonic flow



NASA X-59

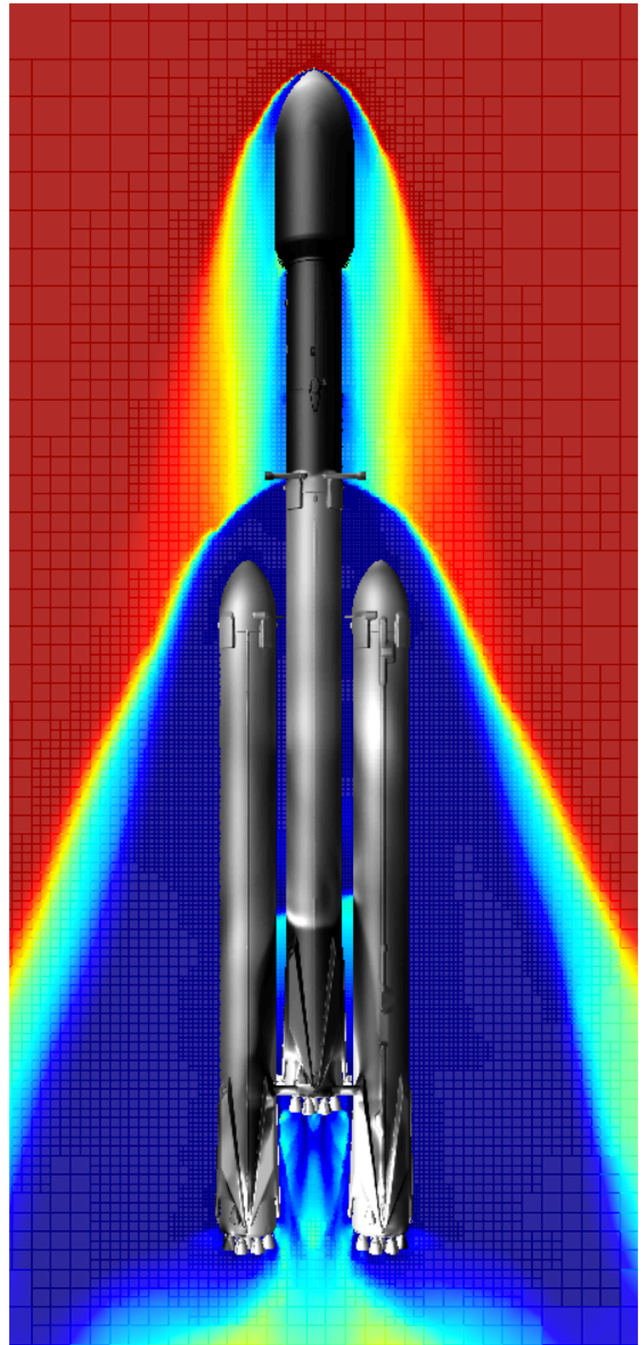


† Nemec, M., & Aftosmis M.J, NASA/TP-2016- 219422, Advances in Verification, Validation, and Uncertainty Quantification

Adaptive Meshing for Steady Simulations

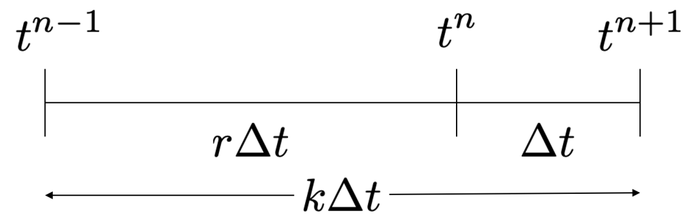
- Parallel software components - $O(N_{cells}/N_{procs})$ complexity
  - Parallel flow & adjoint solves
  - Parallel computation of output sensitivities
  - Parallel error estimation
- Scalar software components - $O(N_{cells})$ complexity
  - Mesh adaptation module
  - Solution injection
  - Repartitioner

Reuse as many software components as possible while maximizing parallel scalability



Physical Time Step Change

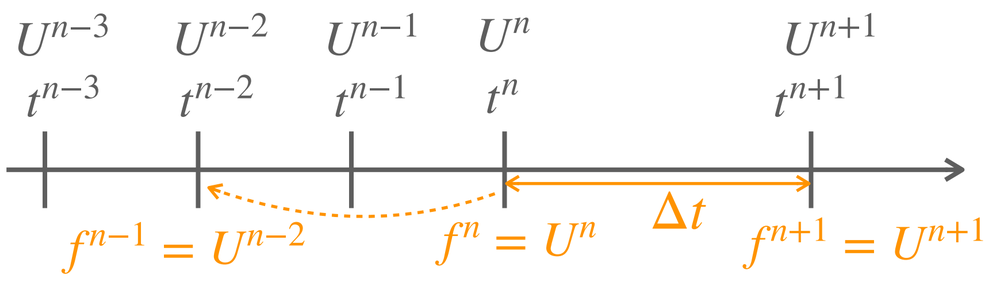
- Added capability to change physical time step size “on the fly”
- Second-order backward difference (BDF2) has a 3-point stencil
- Uniform time step BDF2: $\frac{df}{dt} \approx \frac{3f^{n+1} - 4f^{n} + f^{n-1}}{2\Delta t}$



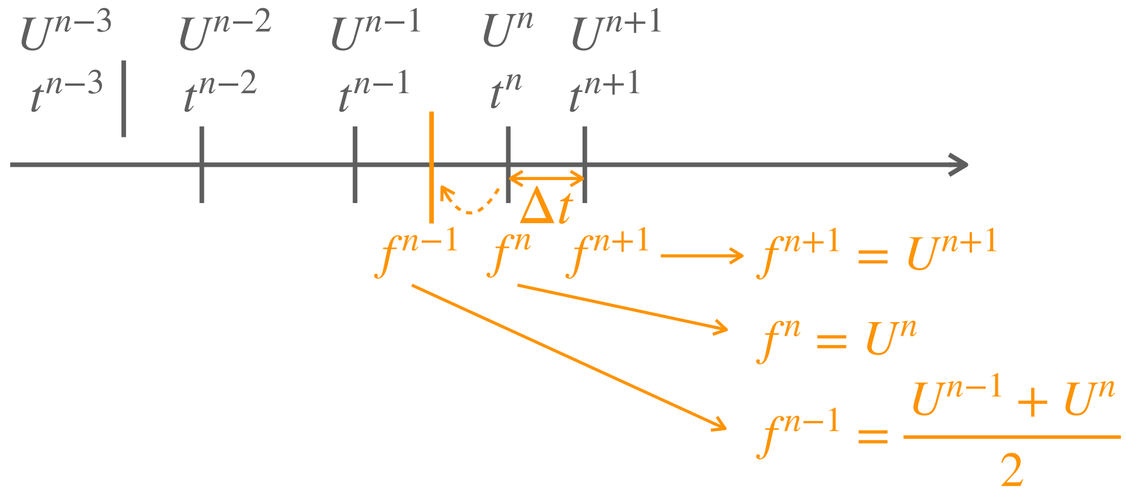
- Two options when changing time step size:

1. Adjust BDF2 coefficients for unequal time step in stencil: $\frac{df}{dt} \approx \frac{r(r+2)f^{n+1} - (r+1)^2 f^{n} + f^{n-1}}{r(r+1)\Delta t}$
2. *Use/construct a previous solution at appropriate time & retain uniform Δt coefficients*
   - and we choose to increase/decrease Δt by factor of 2

Increasing Δt: go back to U^{n-2}



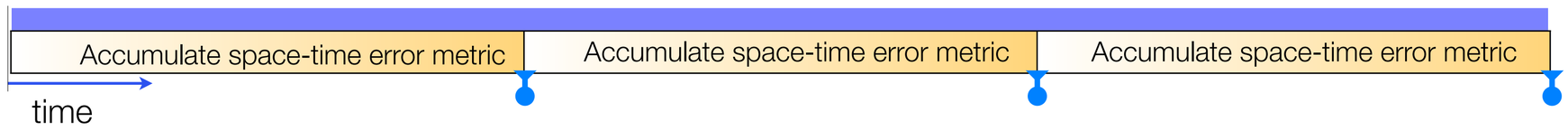
Decreasing Δt: interpolate solution to “$n - 1/2$ ”



An “All Parallel” Mesh Adaptation Approach

1. Coarse mesh parallel flow solve of entire unsteady scenario, drop *N* checkpoint files as we go

Initial mesh



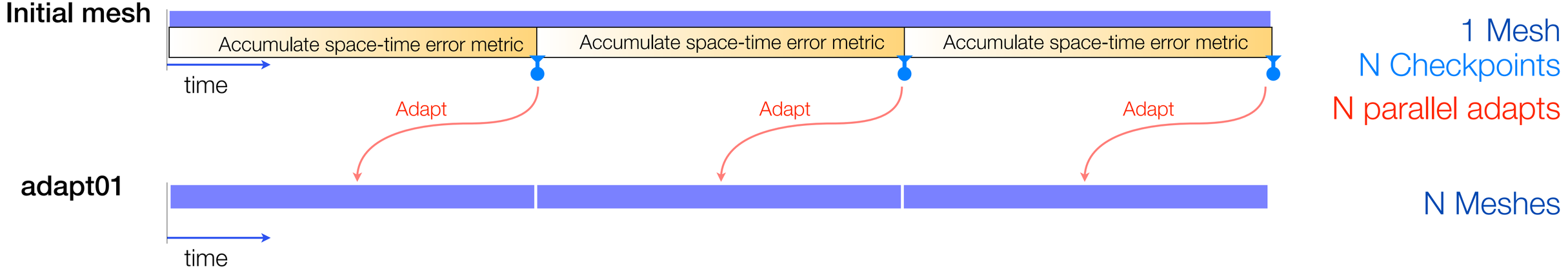
1 Mesh
N Checkpoints

An “All Parallel” Mesh Adaptation Approach

Fixed-point adaptation iterations

1. Coarse mesh parallel flow solve of entire unsteady scenario, drop *N* checkpoint files as we go

2. Parallel mesh adaptation: Run one mesh adaptation from each checkpoint file, no dependency. Creates *N* new meshes



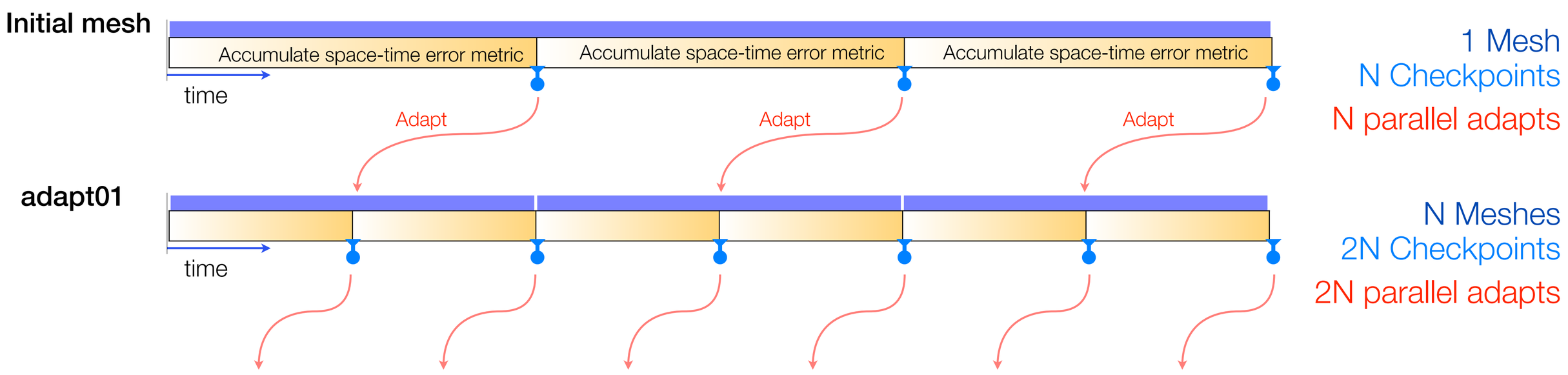
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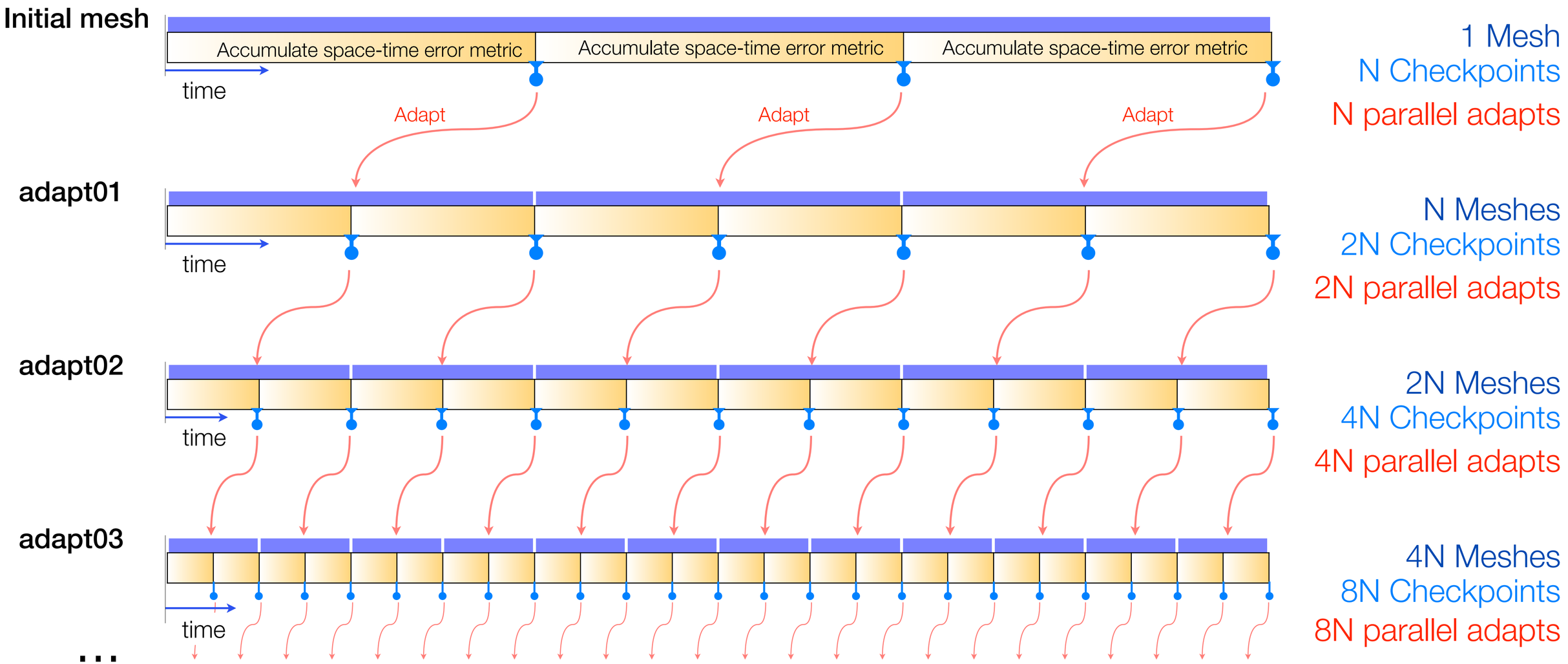
2. Parallel mesh adaptation: Run one mesh adaptation from each checkpoint file, no dependency. Creates *N* new meshes

3. Parallel flow solve: Start on first refined mesh. Halve the time step and run fully parallel, dropping new checkpoint files; transfer solution to next refined mesh & continue. Creates 2N checkpoint files.



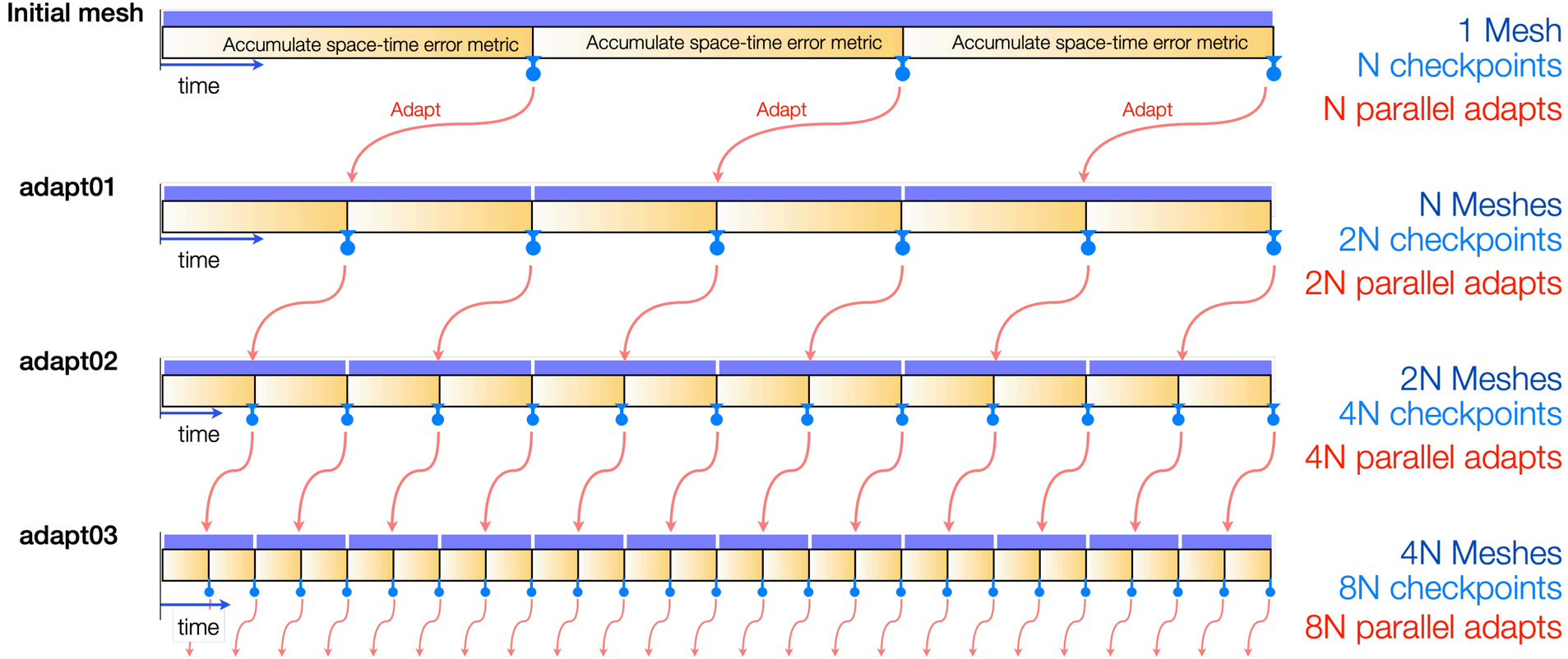
An “All Parallel” Mesh Adaptation Approach

Continue *ad nauseam....*



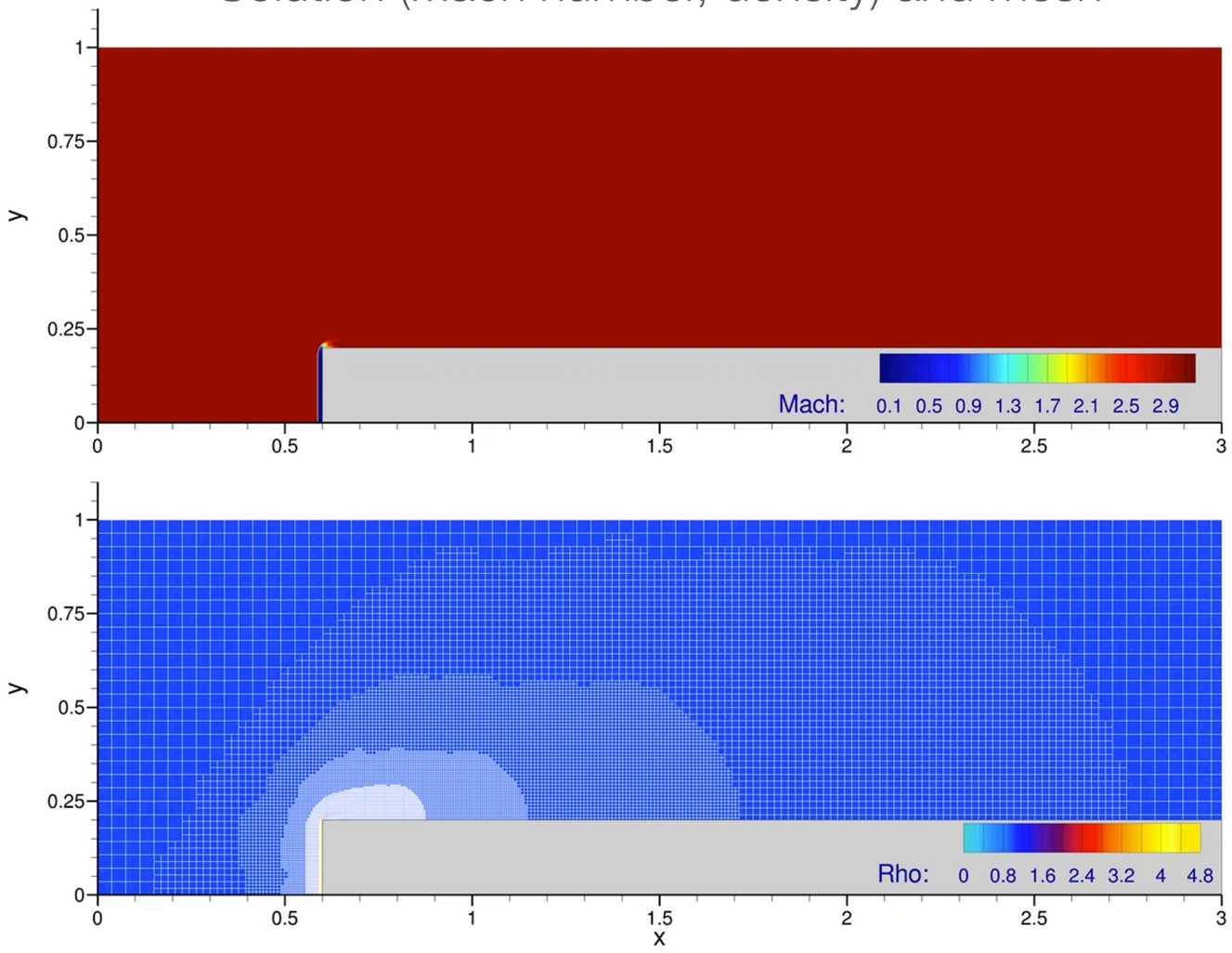
An “All Parallel” Mesh Adaptation Approach

- Multiple-pass approach based on fixed-point iteration
- “Spiral in” toward converged flow solution on successively refined meshes
- *A posteriori* error estimates allow mesh adaptation to be performed in parallel
- Time windows
  - Subdivide time domain, each spatial mesh adapts to solution over specific time window
  - User can control amount of mesh-work, flow computation, and solution-transfer overhead

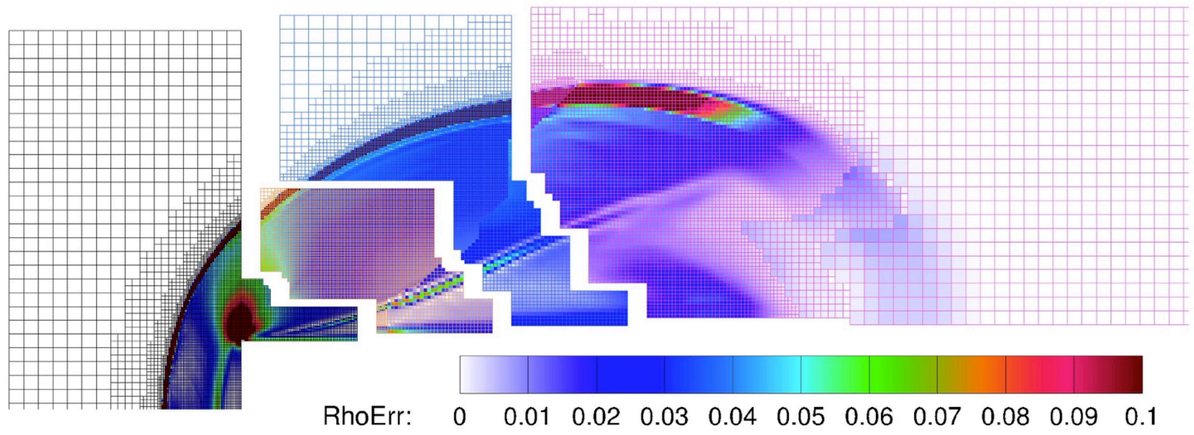


Example: Mach 3 Step

Solution (Mach number, density) and mesh

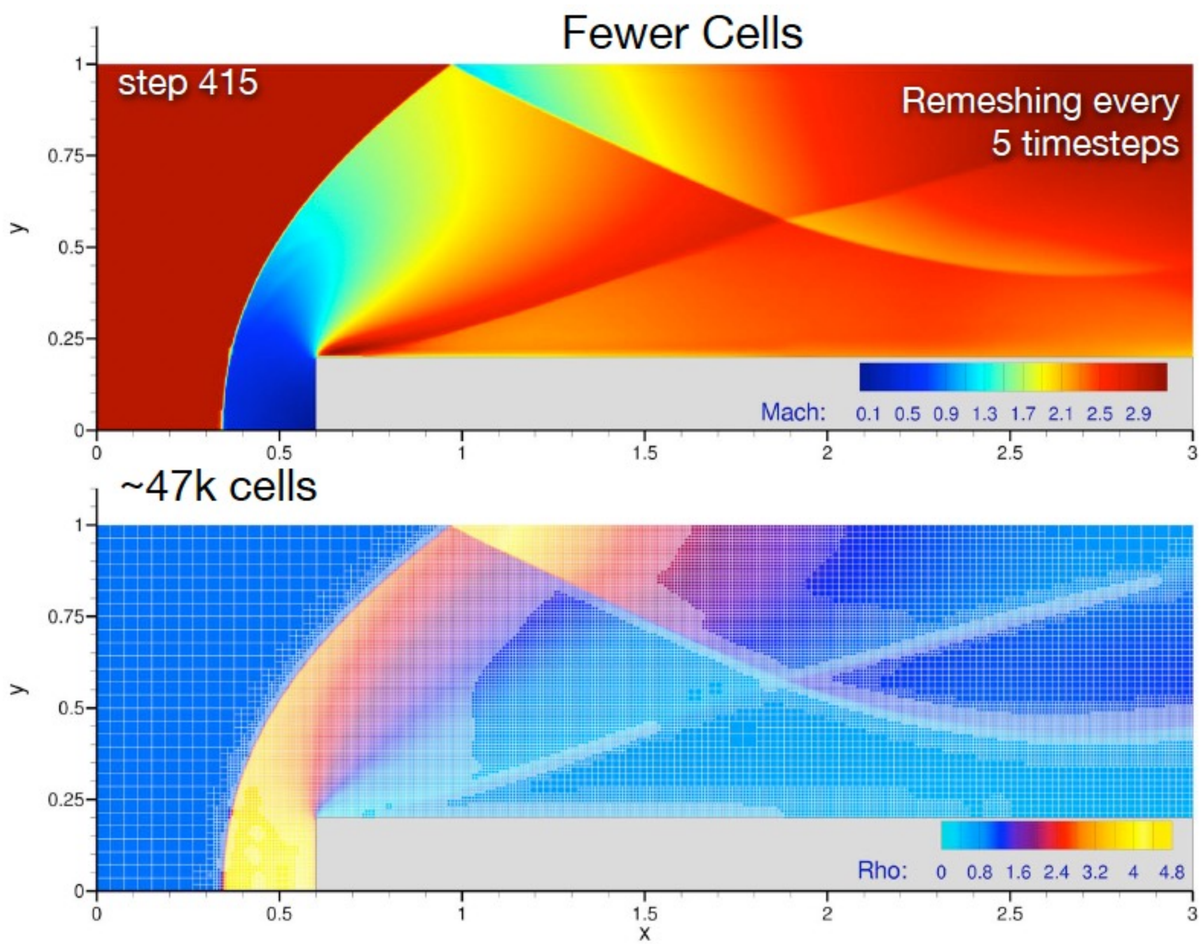


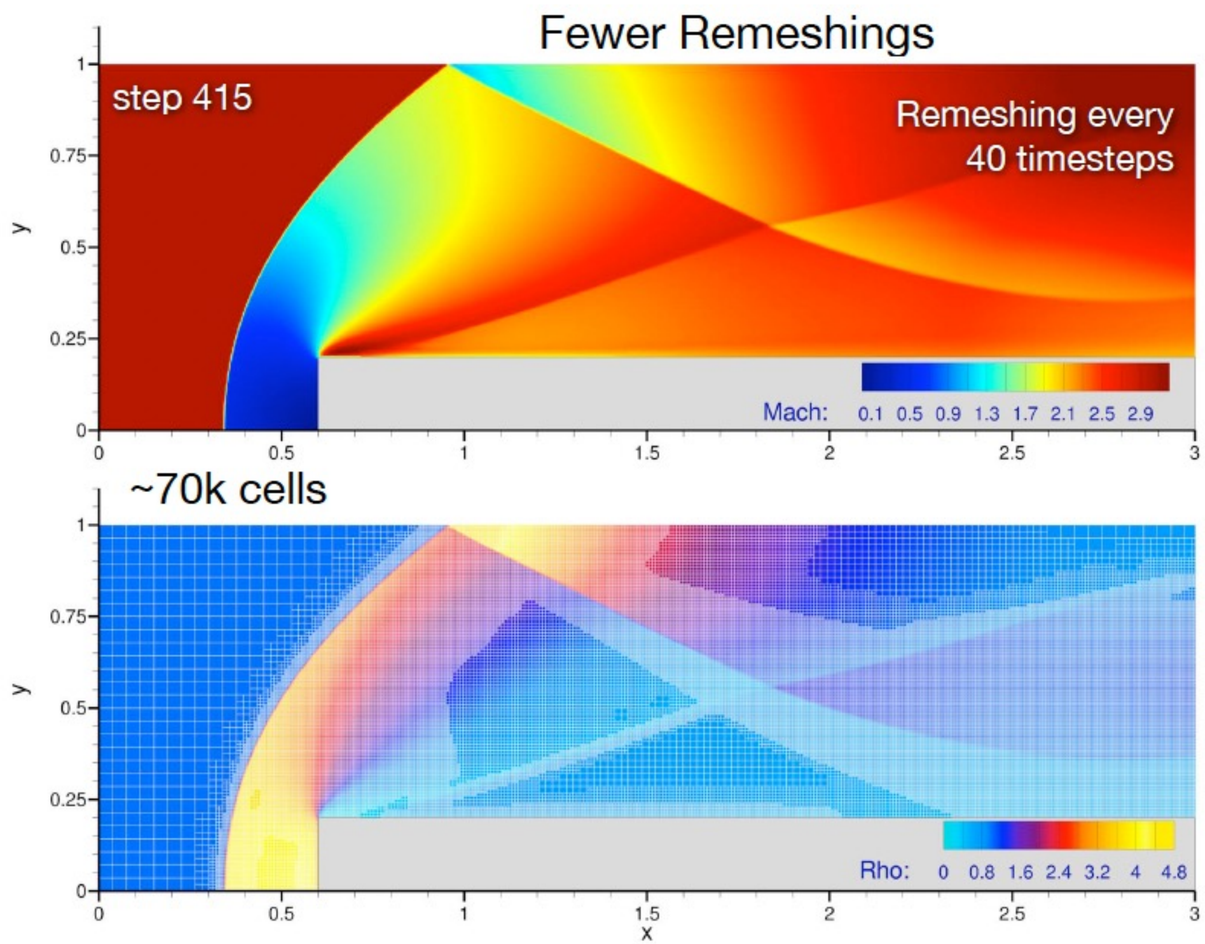
Error metric (density-based) and mesh partitioning



Effect of Remeshing Frequency

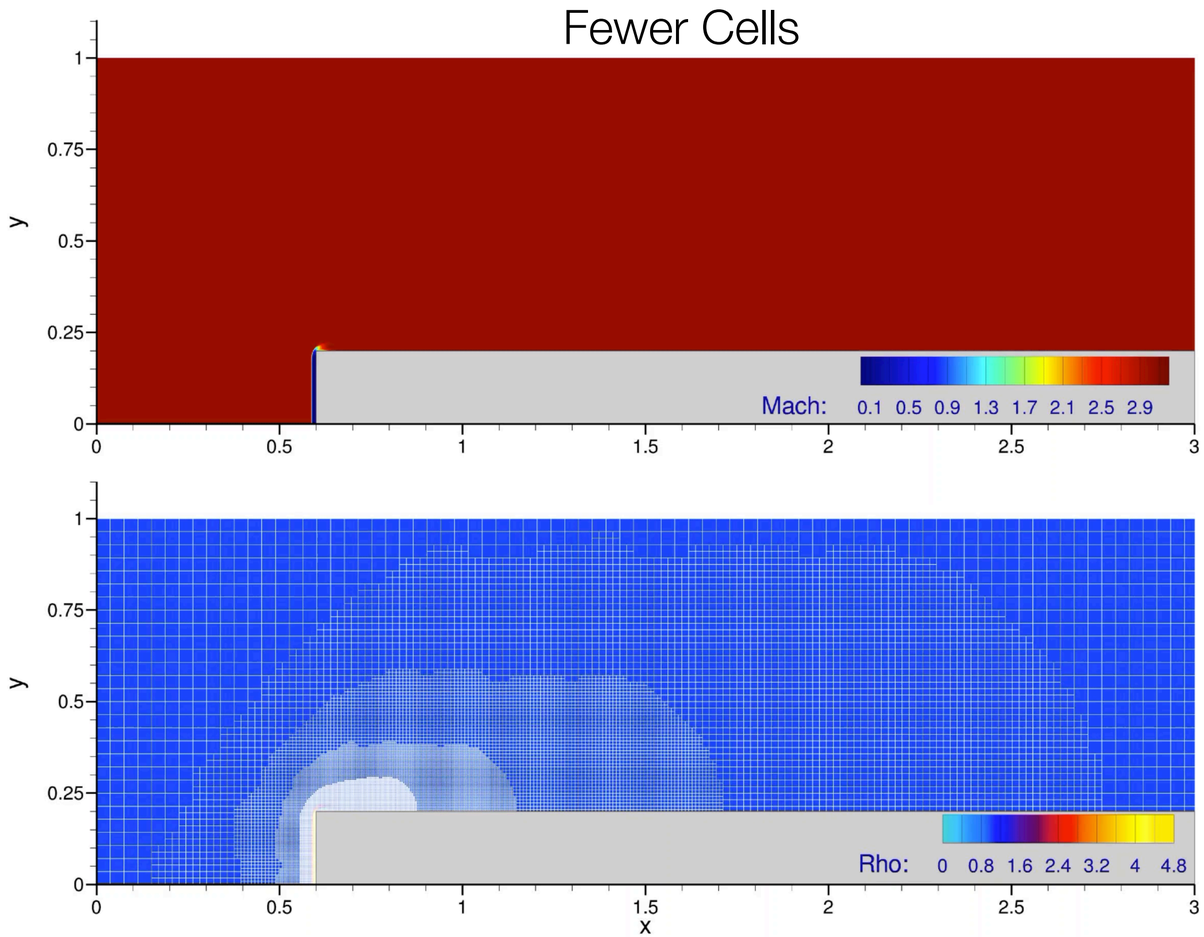
- User has control of time window size and remeshing frequency
  - Left: remeshing more often (every 5 time steps), fewer cells in each mesh, more meshing operations
  - Right: remeshing less often (every 40 time steps), more cells in each mesh, fewer meshing operations

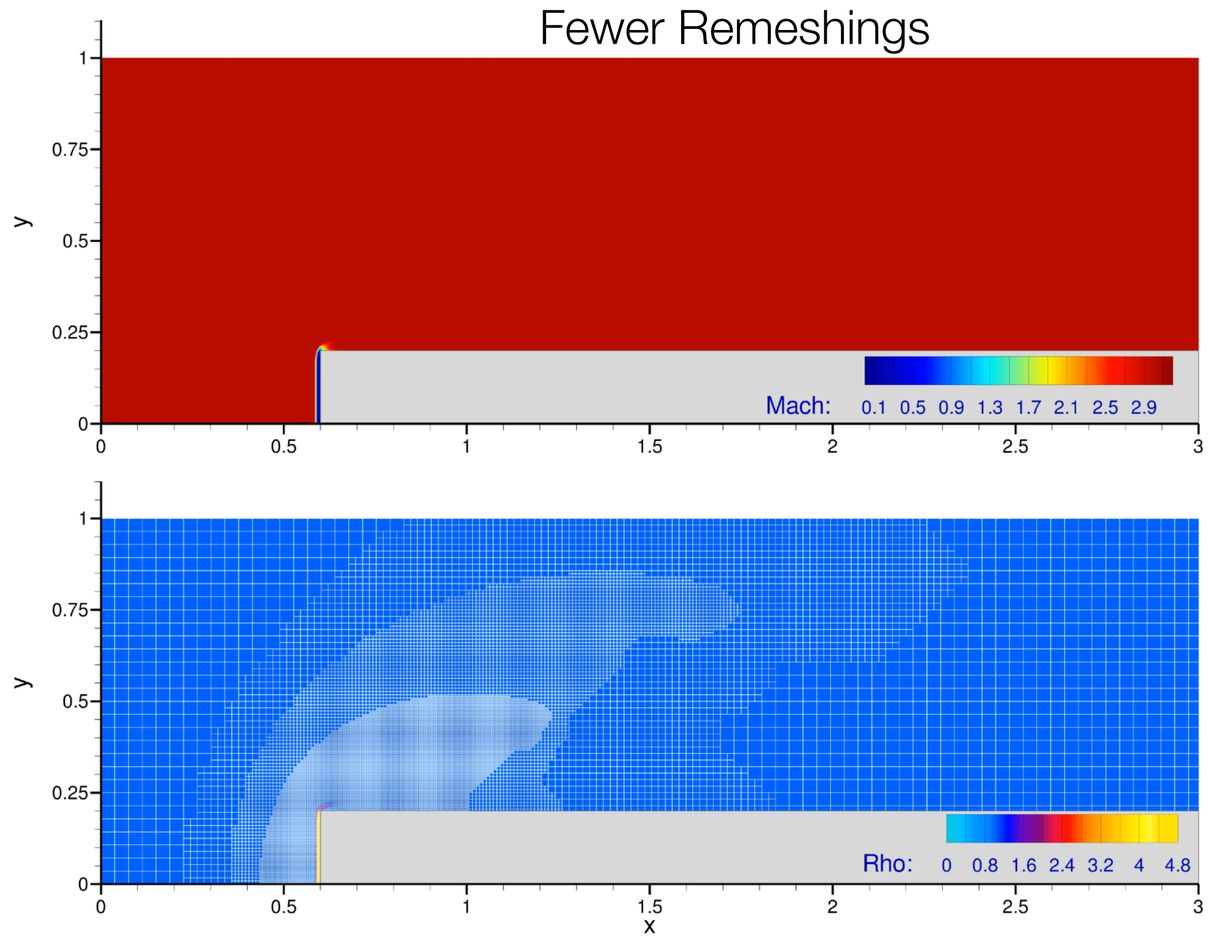




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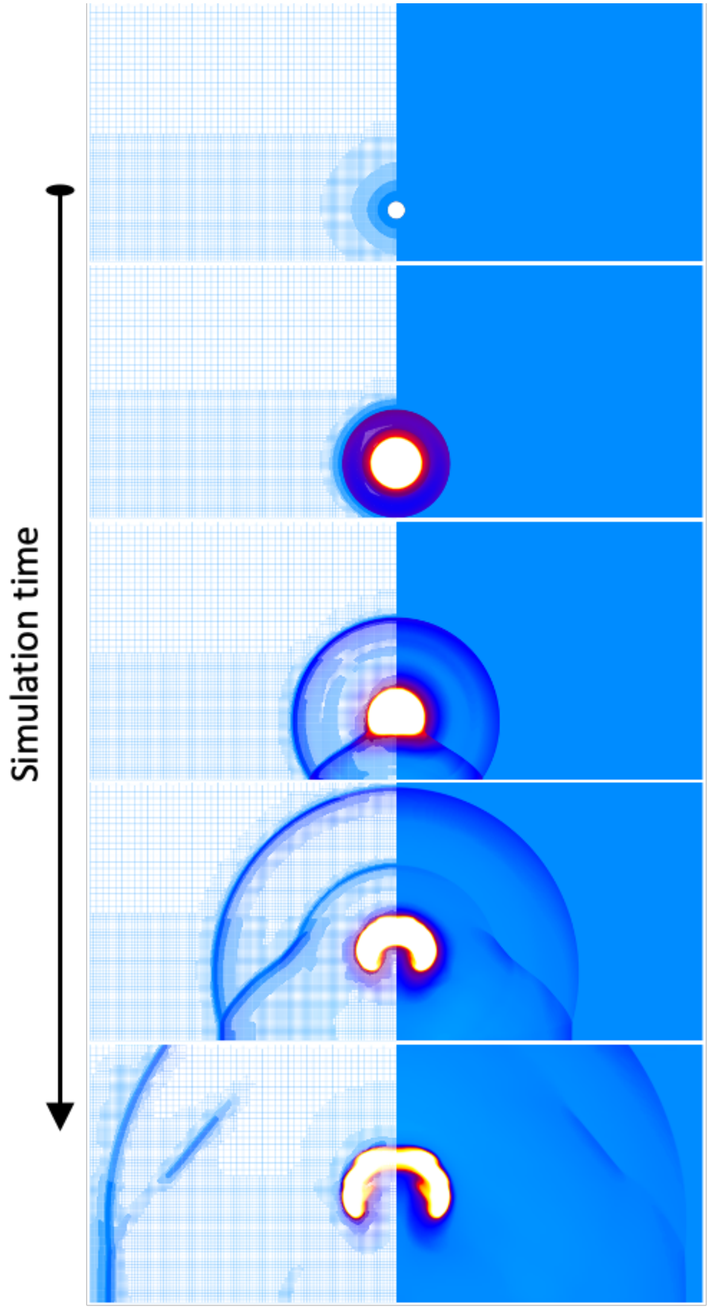
- User has control of time window size and remeshing frequency
  - Left: remeshing more often (every 5 time steps), fewer cells in each mesh, more meshing operations
  - Right: remeshing less often (every 40 time steps), more cells in each mesh, fewer meshing operations





2D Static Airburst with Buoyancy

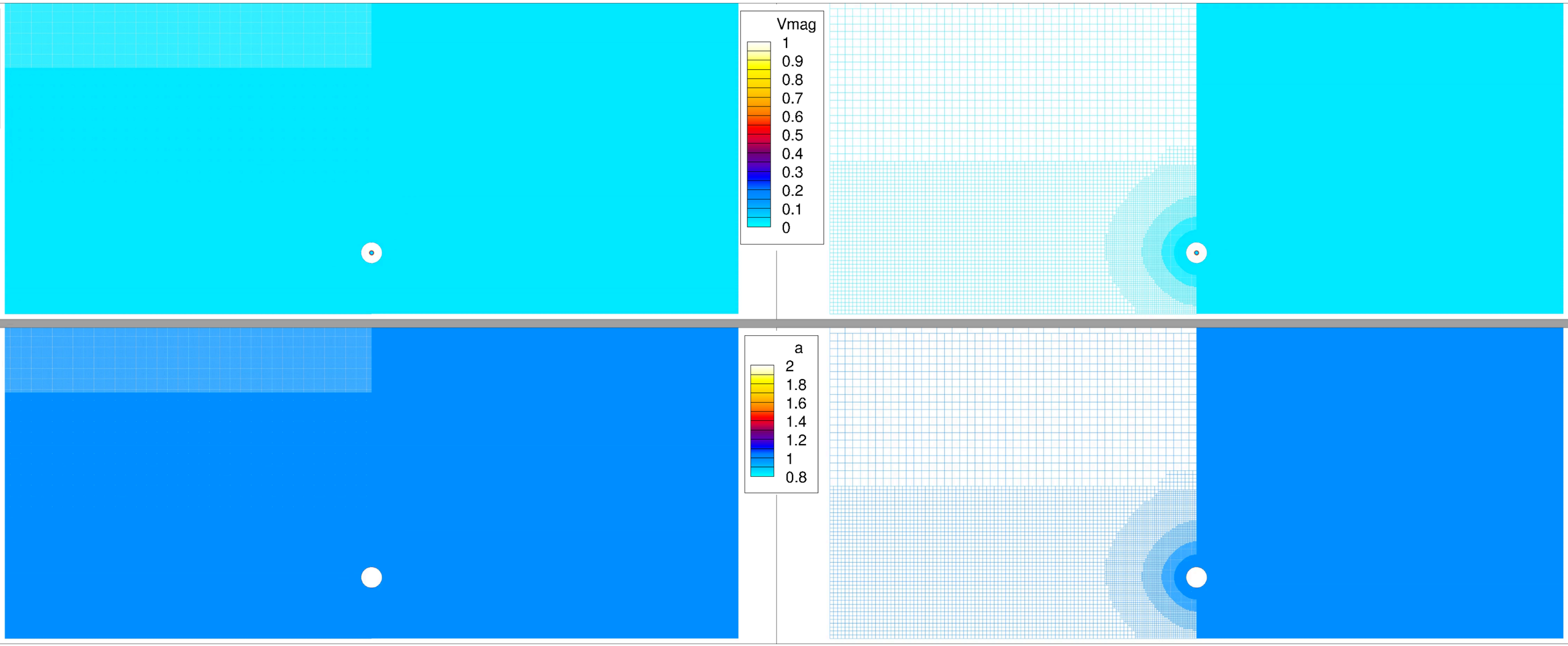
- Blast: radius 0.4 km, altitude 4.0 km, $p/p_\infty = 70$, $T/T_\infty = 30$
- Compare:
  - 5 adaptation cycles, finest meshes ~100-250k cells
  - "*Unaffordable"* static fine mesh (5 ref. levels everywhere), 4.2 million cells
- Results:
  - Solution snapshots and mesh adaptation
  - Ground overpressure convergence and error estimate
  - Mesh size evolution over time
  - Computational cost and scalability study



Solution on Fixed & Adaptive Meshes

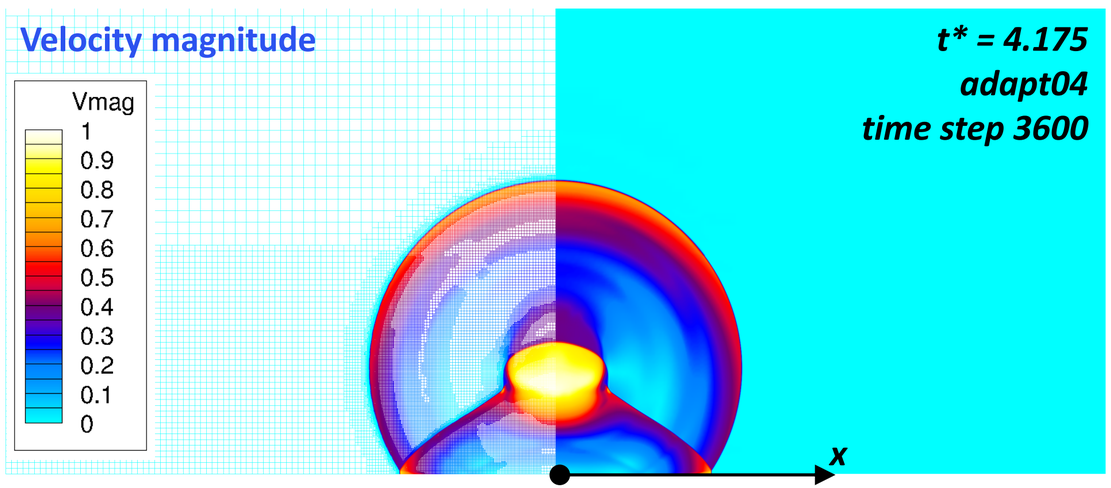
"*Unaffordable*" Static Fine Mesh

Final Adapt Cycle

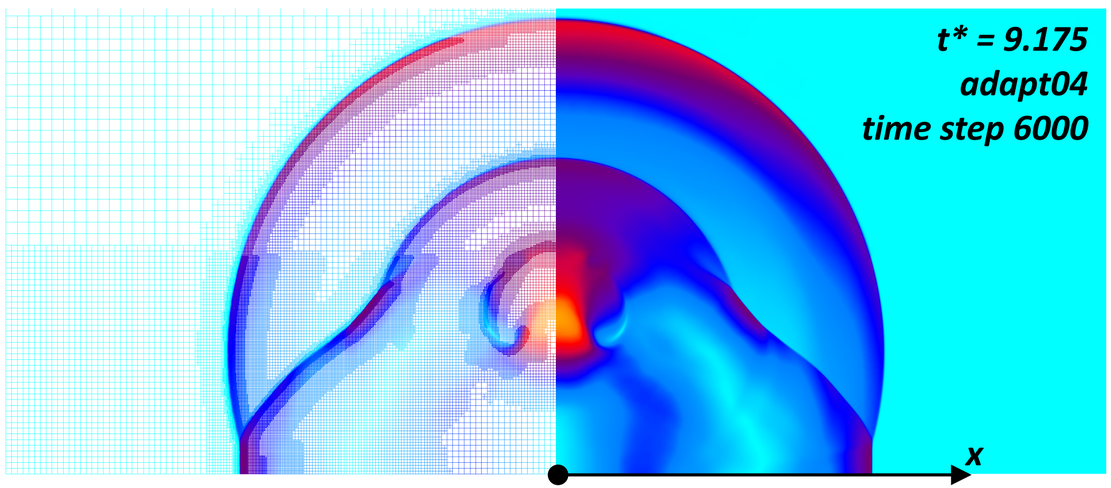


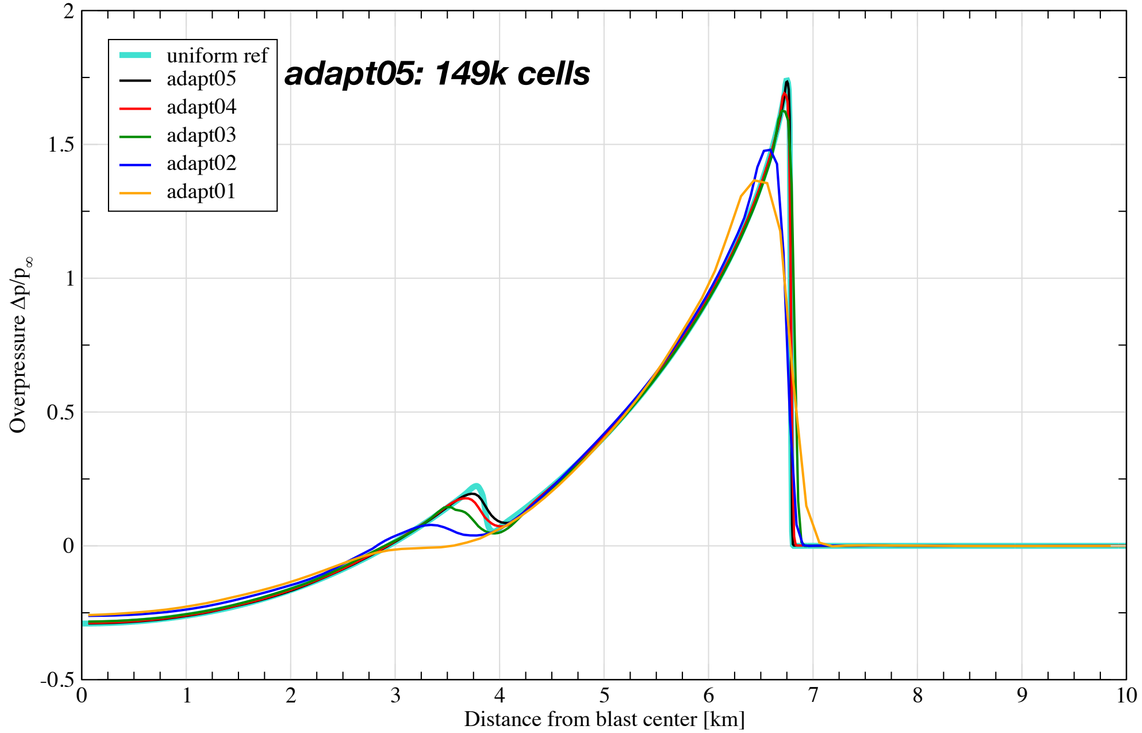
Ground Overpressure Convergence

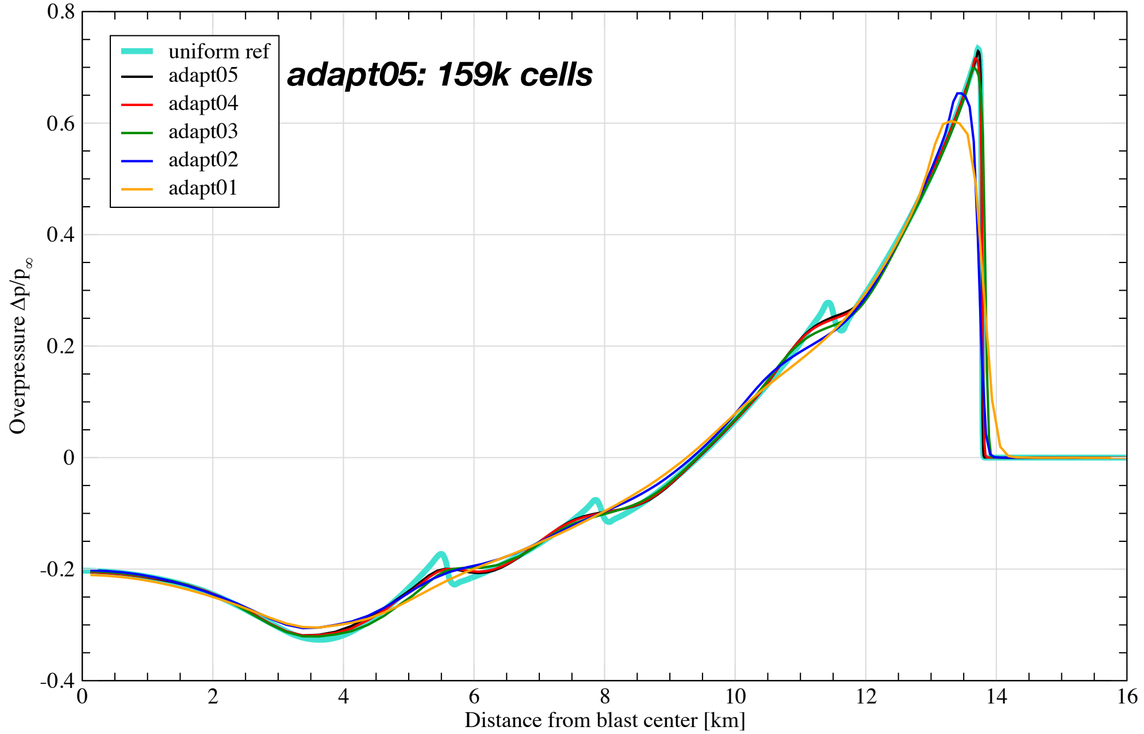
Early time



Later time

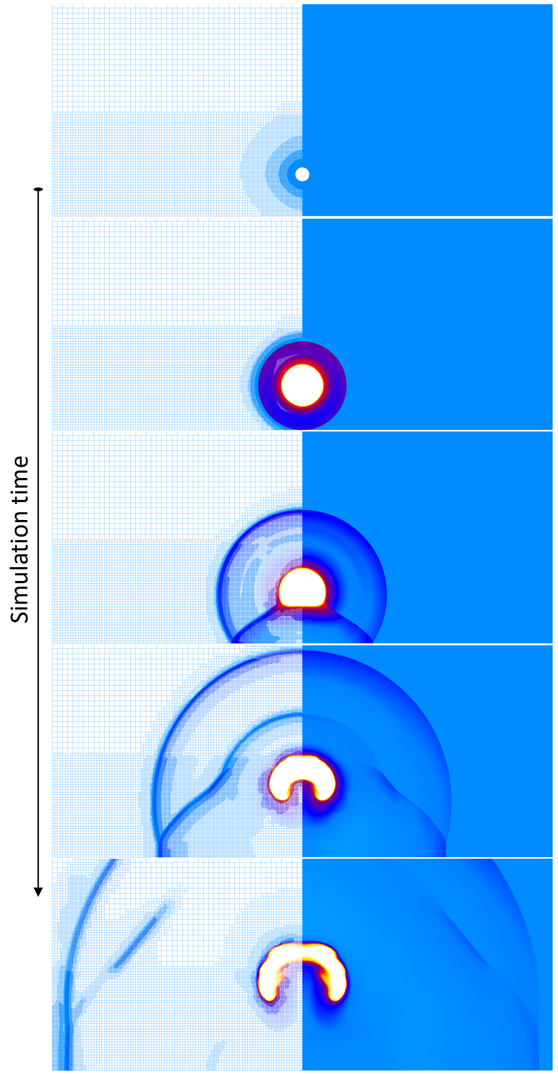


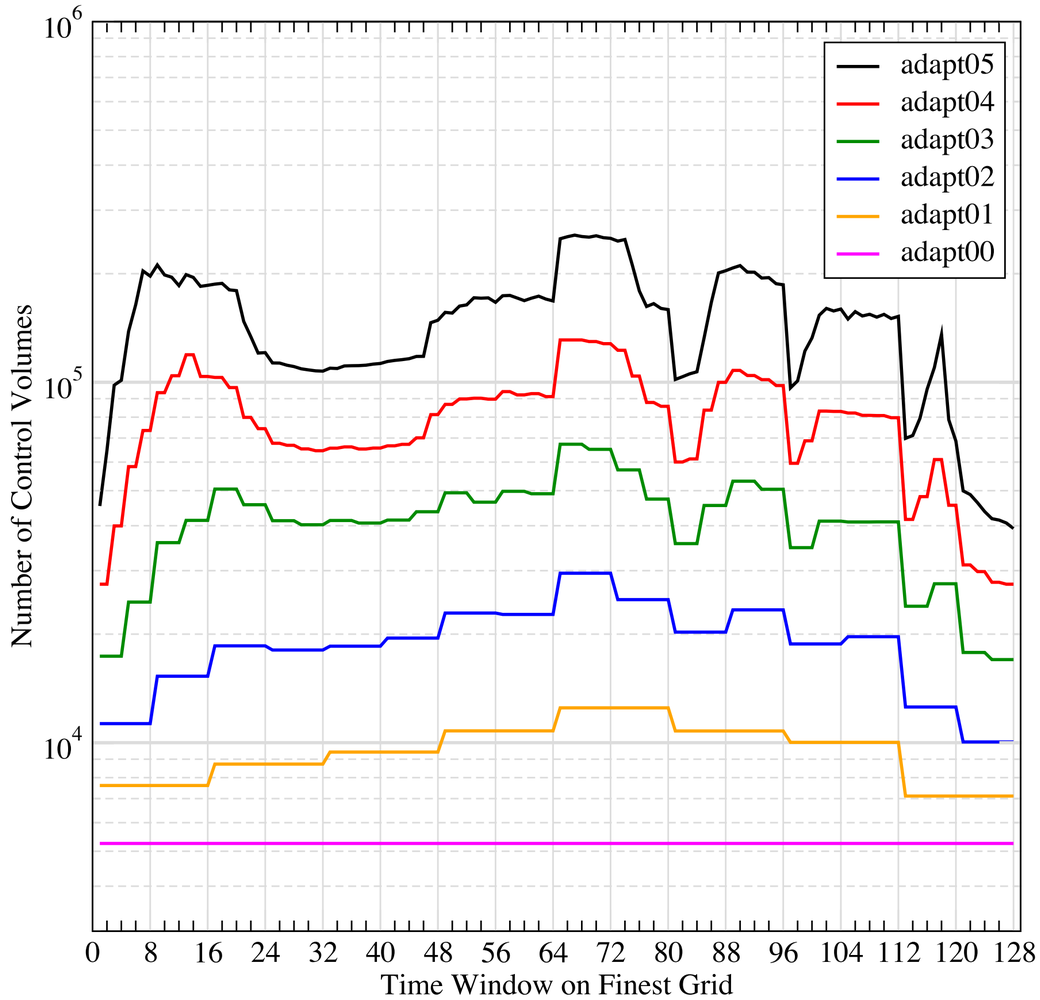




Cell Count Evolution

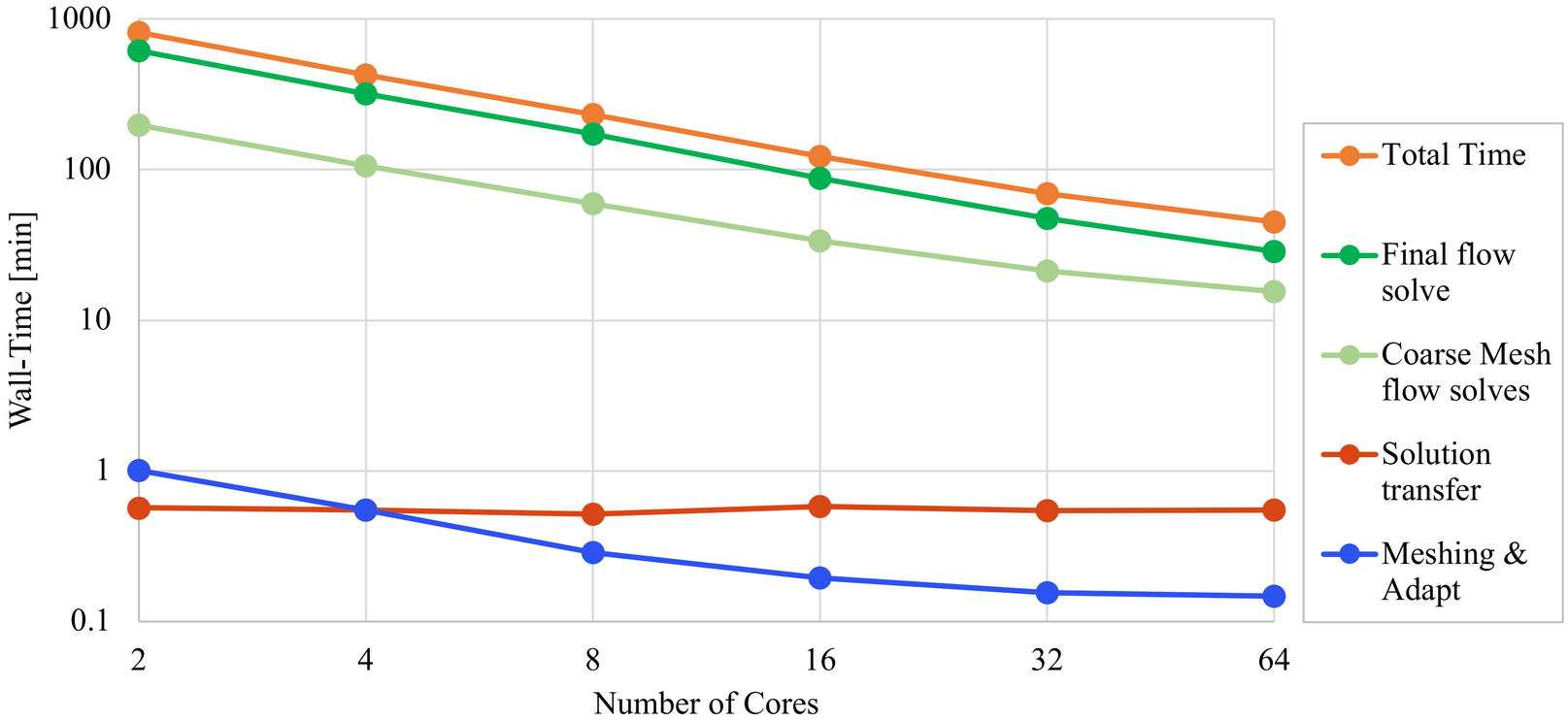
- Mesh growth rates are reasonable, factor of ~2 or less
- Initial mesh: 5k cells
- Final adapt cycle
  - Average cell count 148k
  - Max cell count 256k
- Fixed mesh: 4.2M cells (off the top of the figure)
- Time windows
  - Adapt cycle 1: 8 windows
  - Adapt cycle 5: 128 windows
  - 150 time steps per window (all adapt cycles)

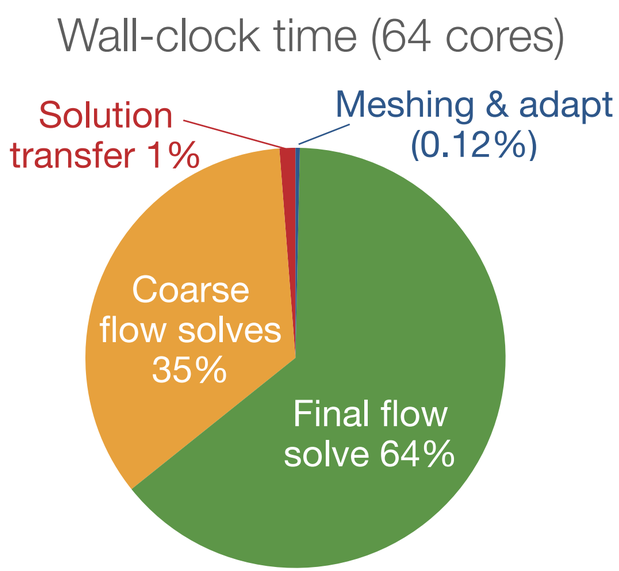




Computational Cost and Parallel Scaling

- Flow solve is highly scalable and dominates both wall-time and computational cost, even in this 2D simulation
- Early adapt cycles have smaller number of time windows, not enough mesh-work to fully take advantage of 32 & 64 cores
- Solution transfer cost is essentially constant for a given mesh size but can be controlled by choosing number of time windows

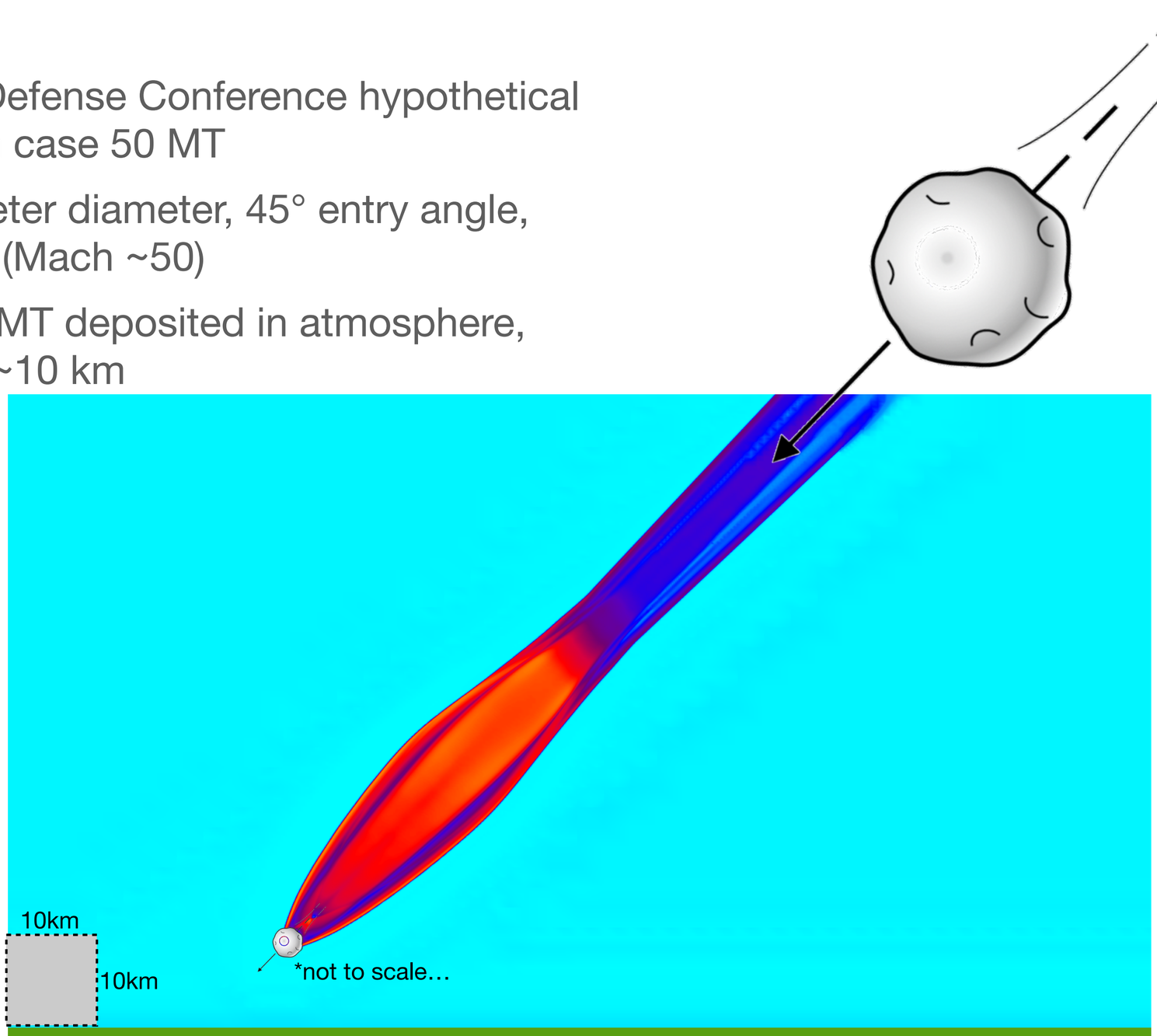




Meshing and adaptation is performed in parallel, shows excellent scalability

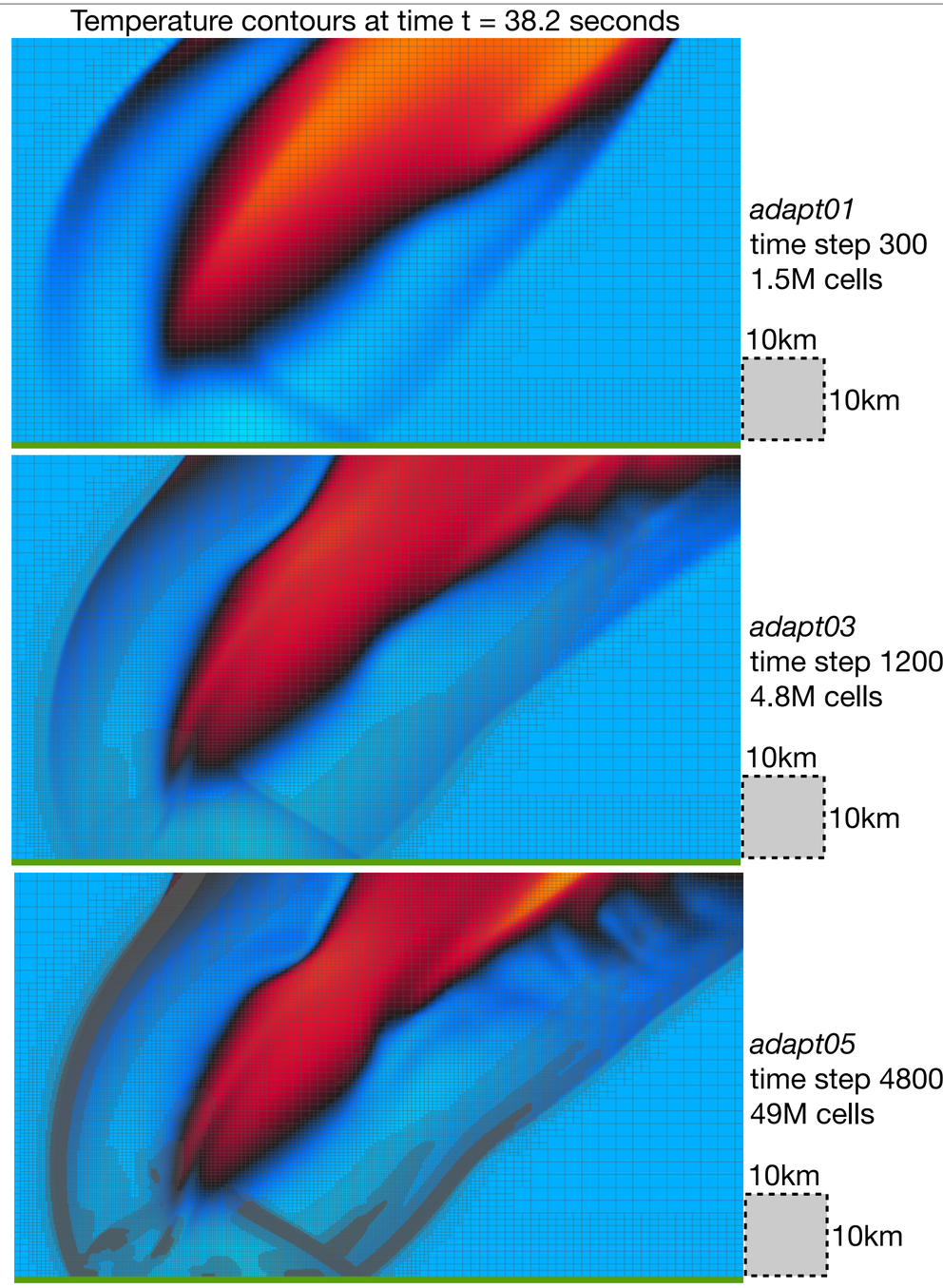
3D Asteroid Entry & Blast Propagation

- 2021 Planetary Defense Conference hypothetical exercise, median case 50 MT
- Asteroid: 120-meter diameter, 45° entry angle, 15 km/s velocity (Mach ~50)
- Essentially all 50MT deposited in atmosphere, airburst altitude ~10 km



3D Asteroid Entry & Blast Propagation

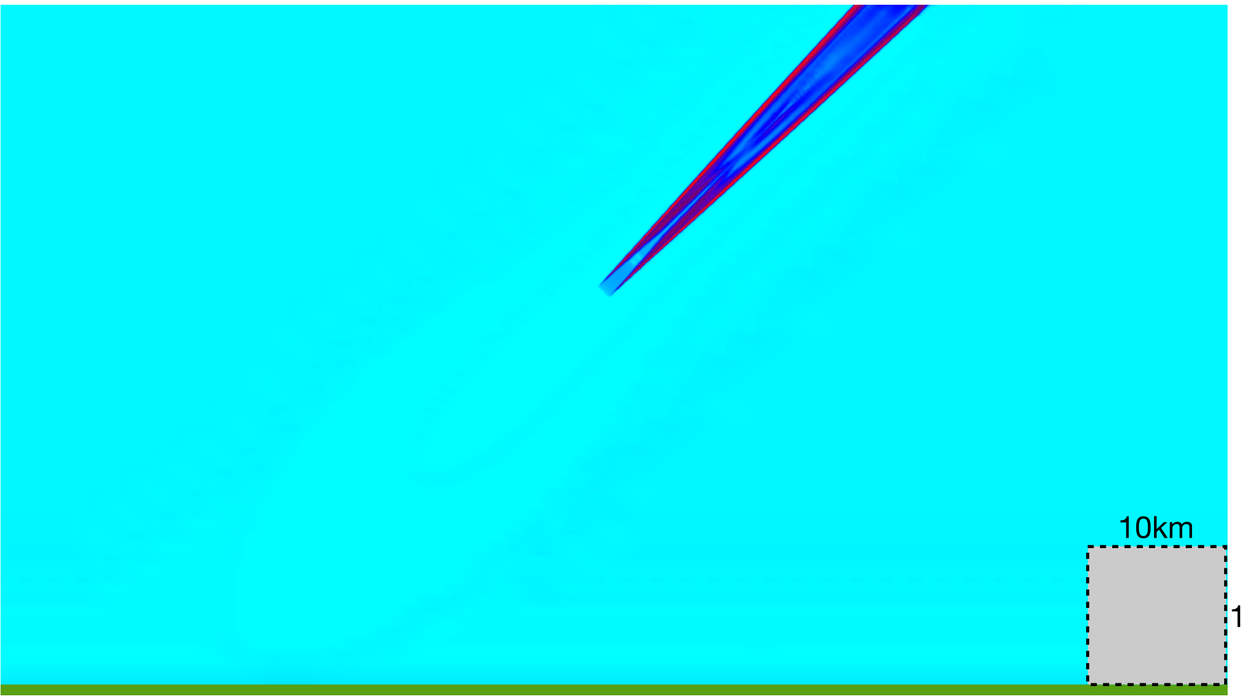
- 2021 Planetary Defense Conference hypothetical exercise, median case 50 MT
- Asteroid: 120-meter diameter, 45° entry angle, 15 km/s velocity (Mach ~50)
- Essentially all 50MT deposited in atmosphere, airburst altitude ~10 km
- Simulate blast spreading for over 7 minutes and distances ~150 km from blast center
- Results:
  - Solution snapshots and mesh adaptation
  - Comparison of fixed mesh and adaptive mesh
  - Ground overpressure convergence and error estimate
  - Blast footprints
  - Mesh size evolution over time
  - Computational cost



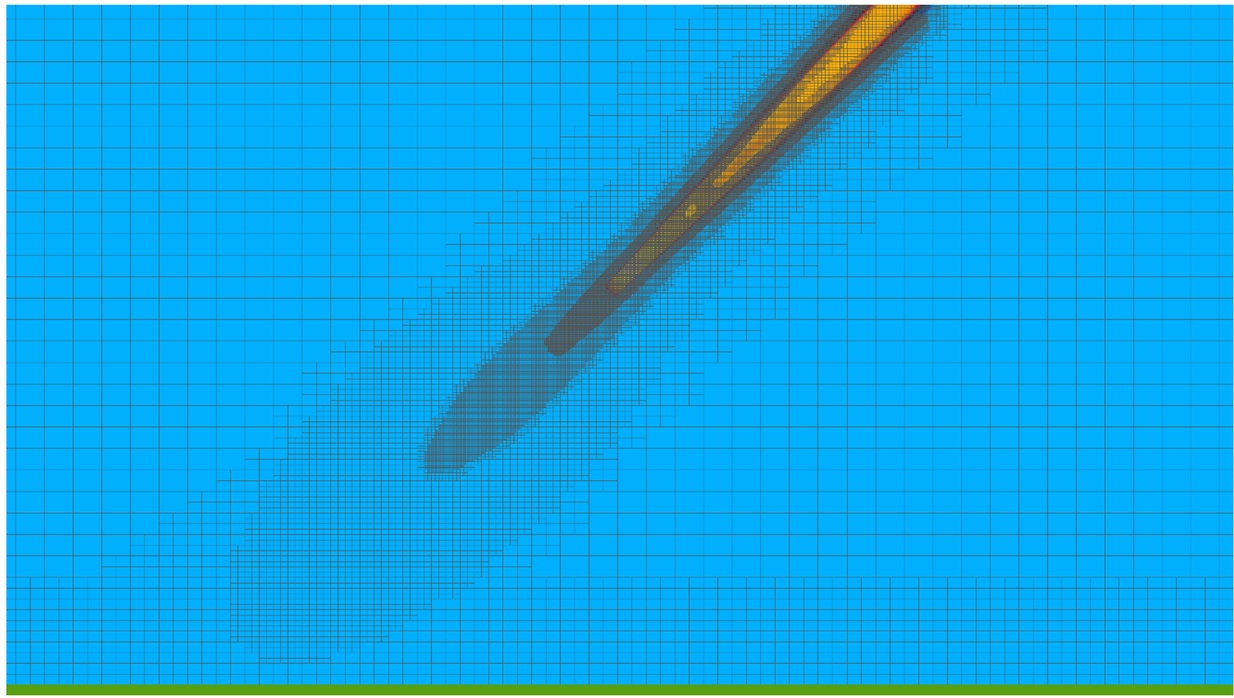
Solution Progression Through Time

adapt05
time = 2.0 s
time step 500
2.4M cells

Mach Number



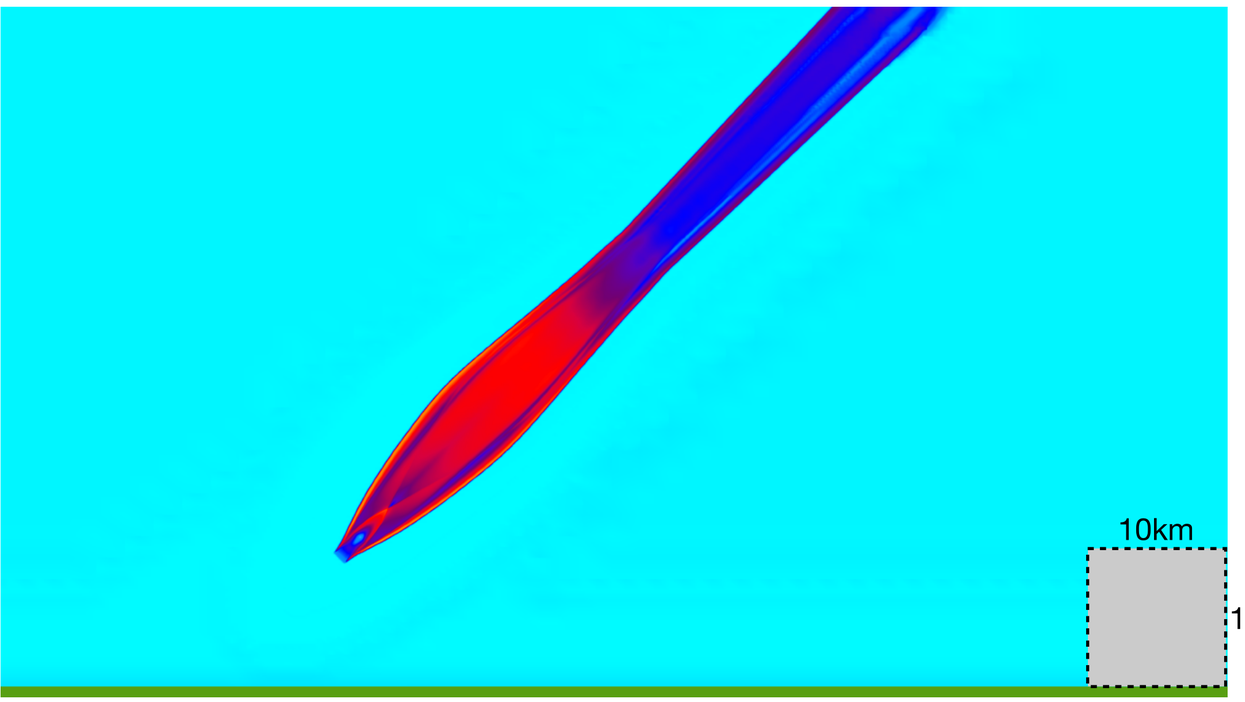
Temperature



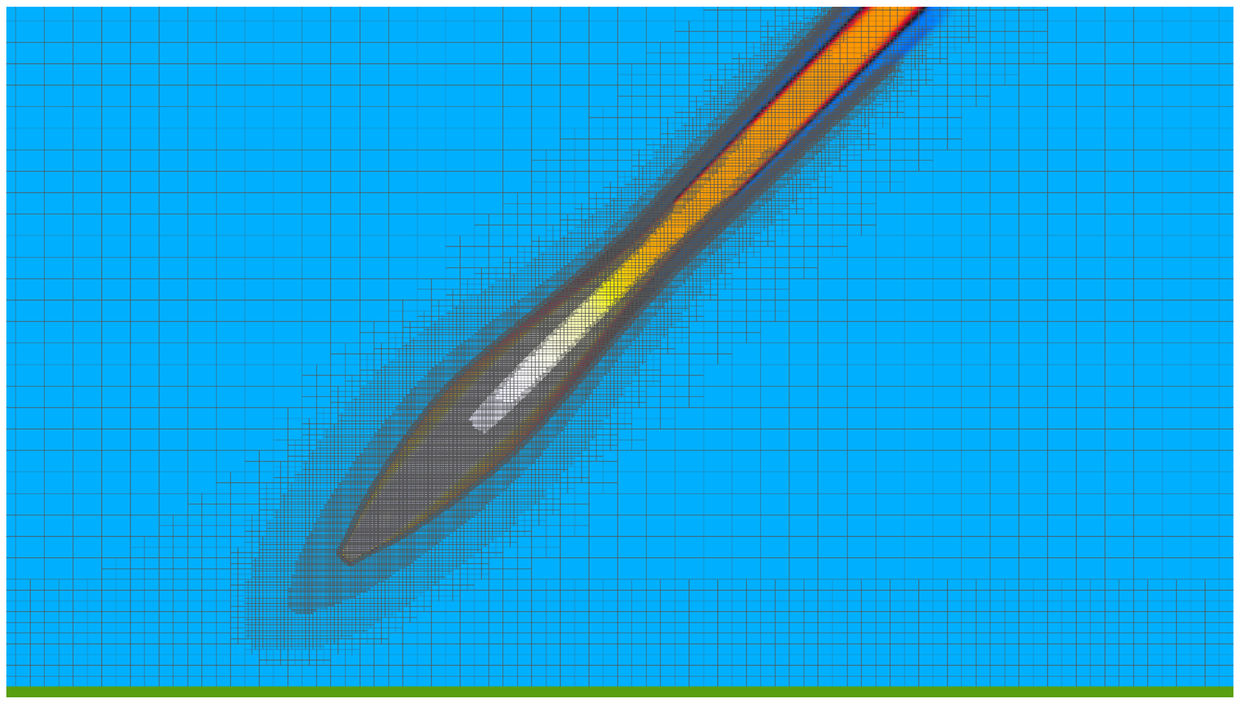
Solution Progression Through Time

adapt05
time = 4.0 s
time step 1000
4.7M cells

Mach Number



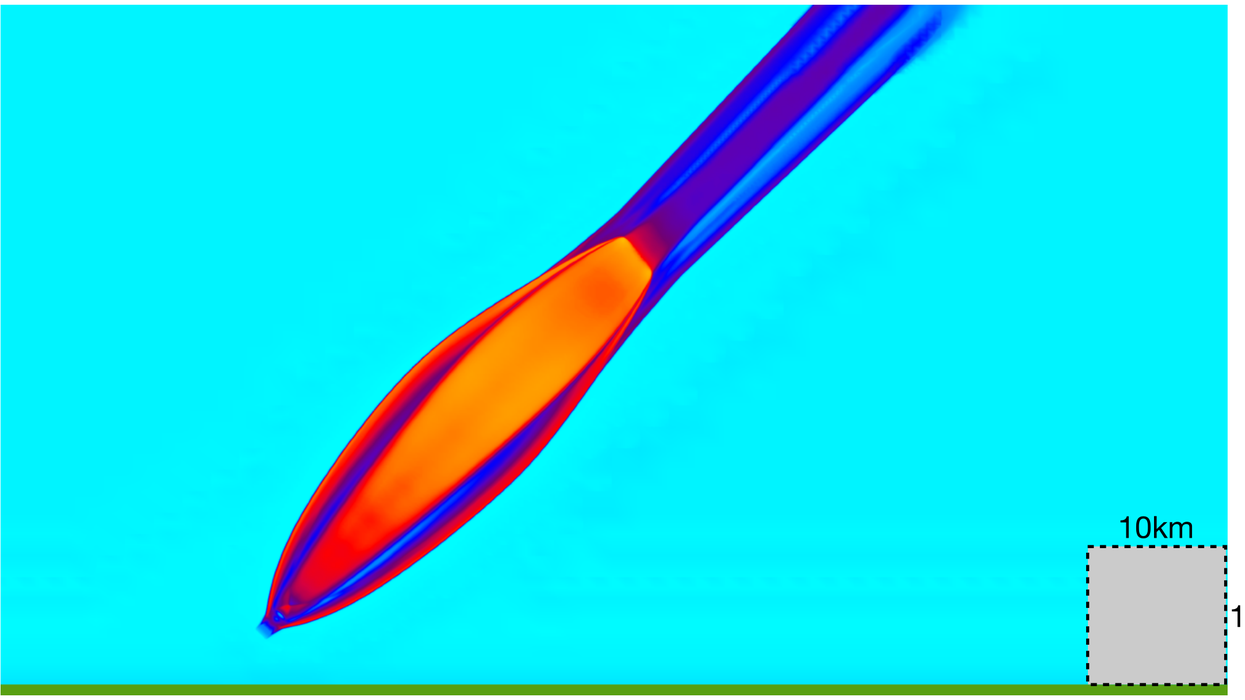
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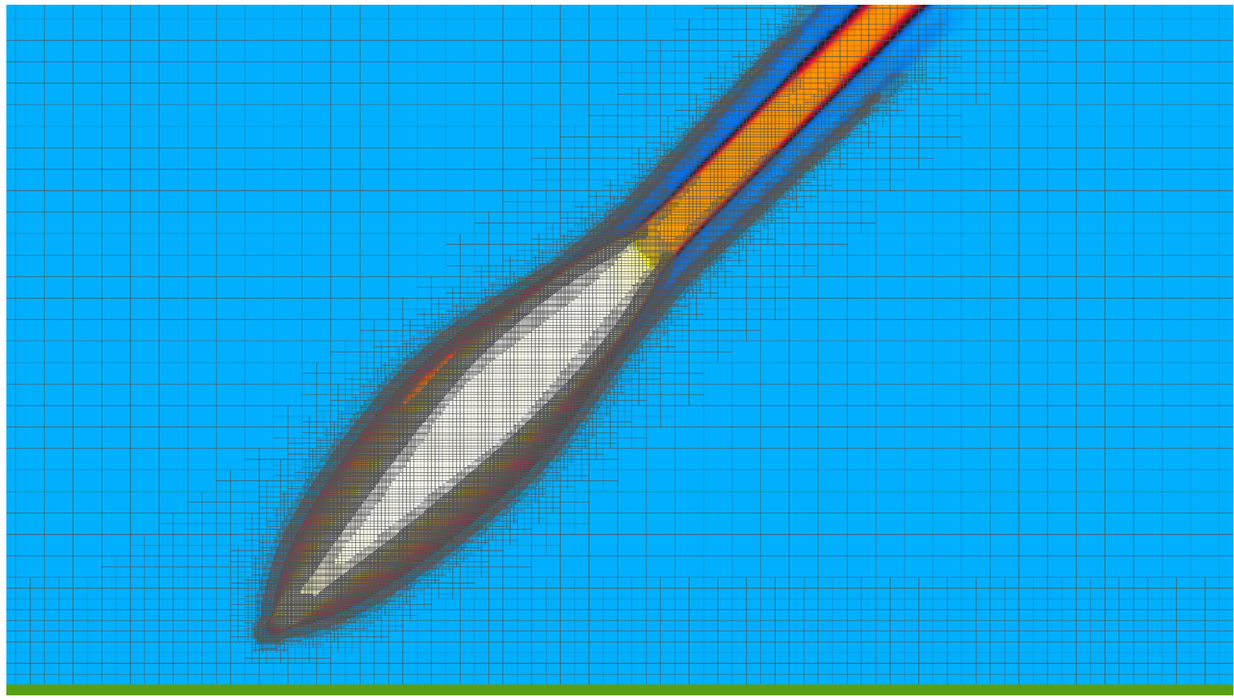
Solution Progression Through Time

adapt05
time = 6.0 s
time step 1500
9.0M cells

Mach Number



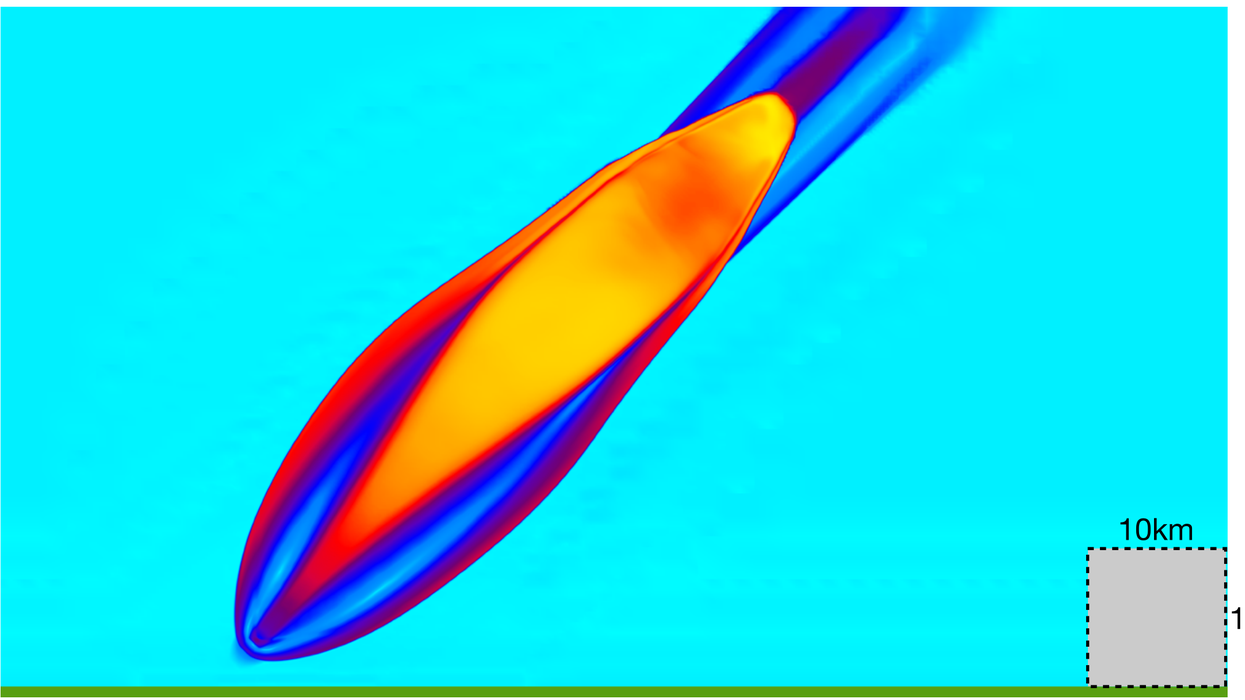
Temperature



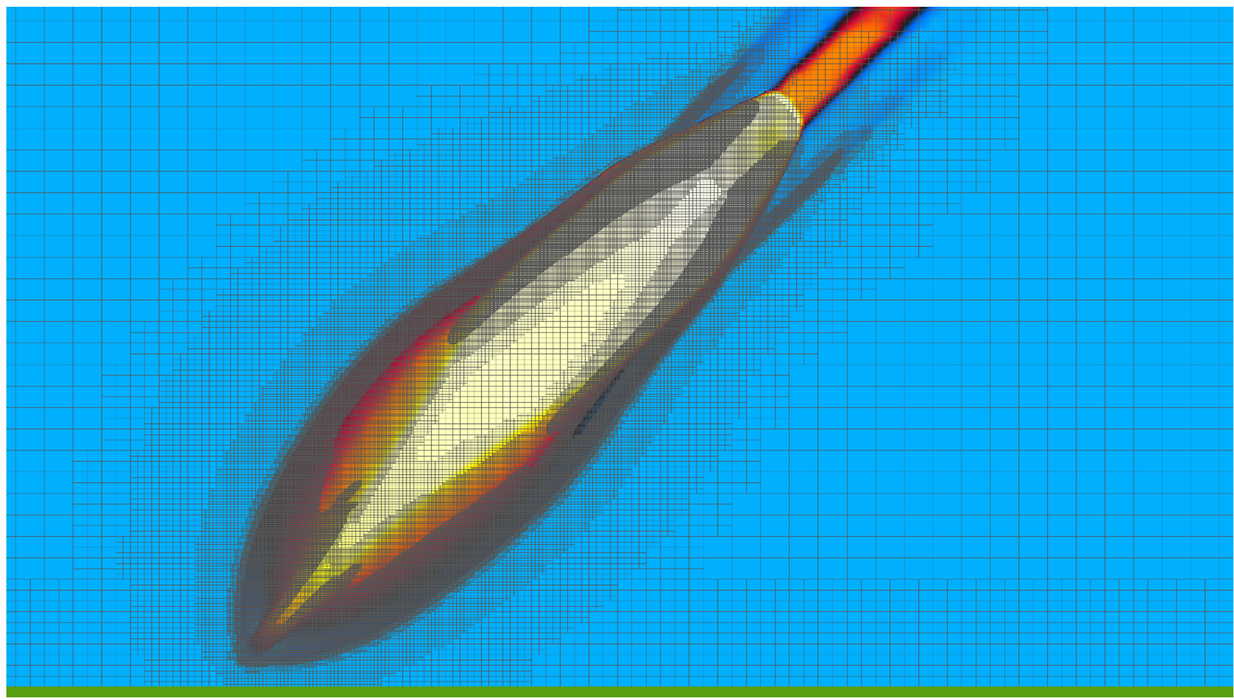
Solution Progression Through Time

adapt05
time = 9.6 s
time step 2000
17M cells

Mach Number



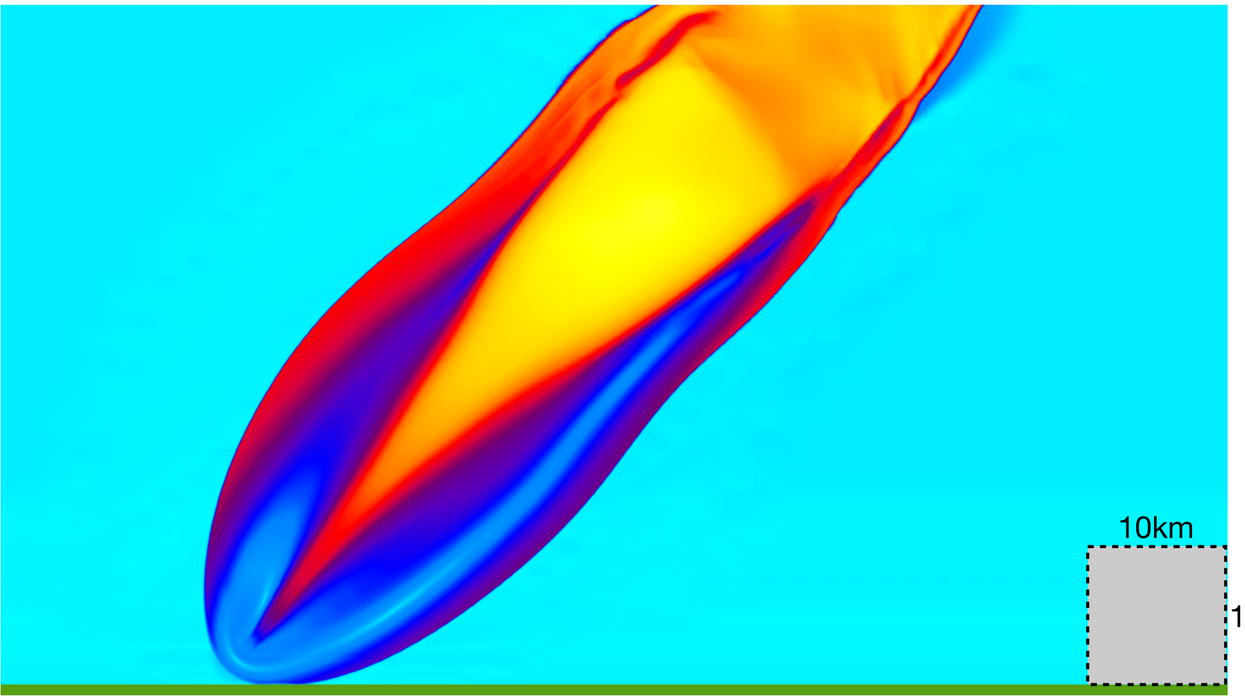
Temperature



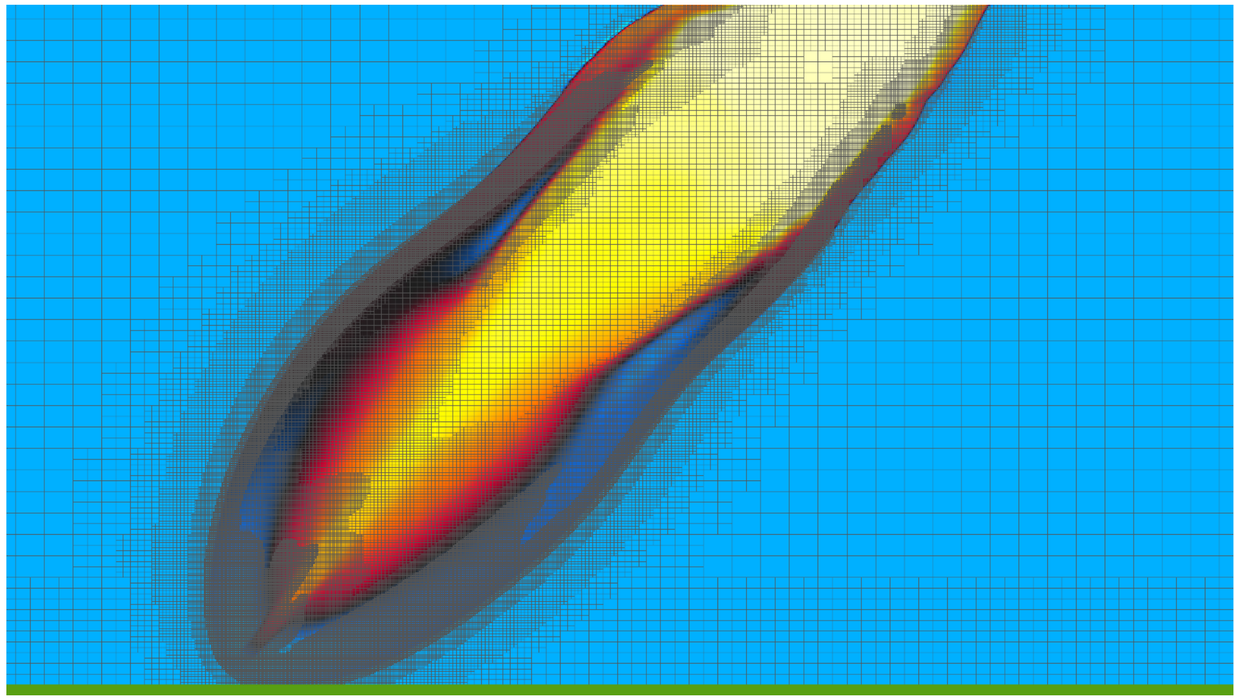
Solution Progression Through Time

adapt05
time = 14.3 s
time step 2600
24M cells

Mach Number



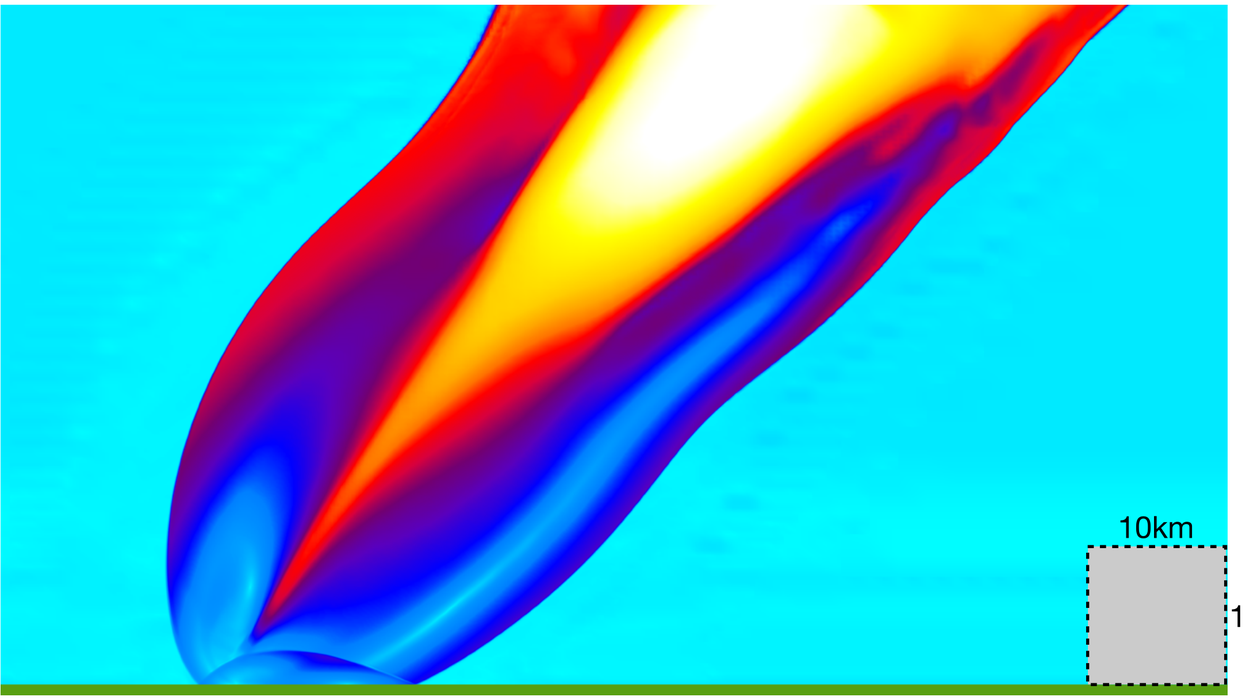
Temperature



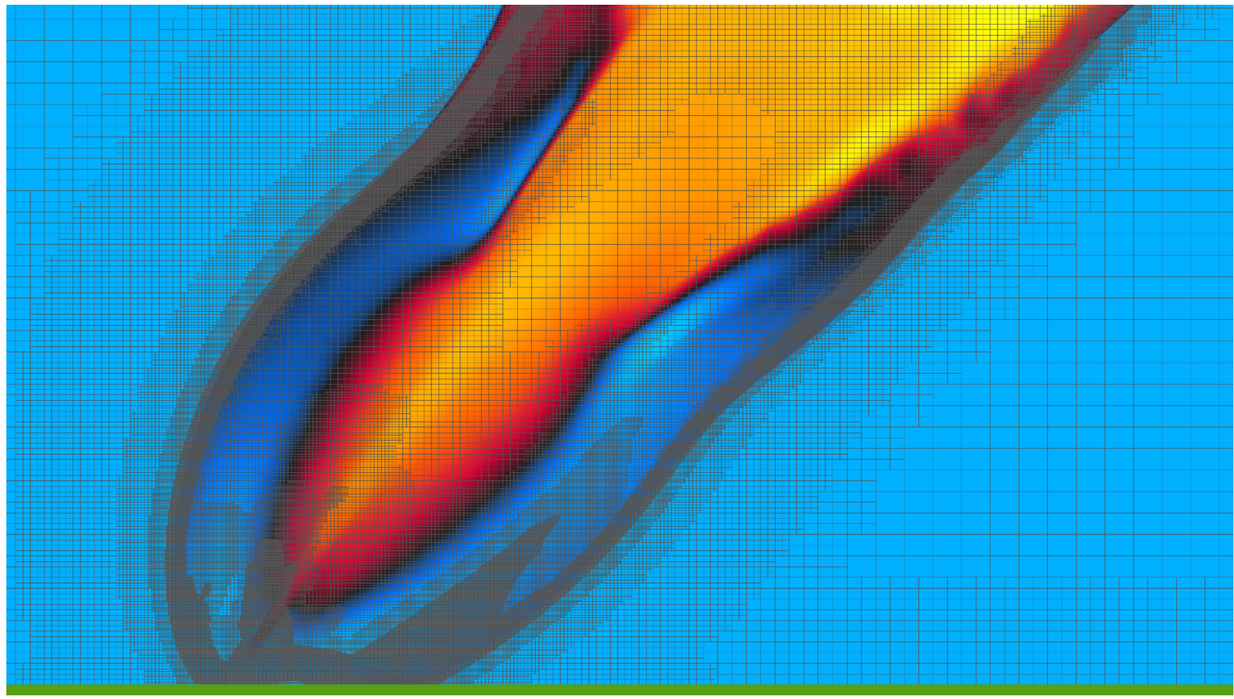
Solution Progression Through Time

adapt05
time = 20.7 s
time step 3400
37M cells

Mach Number



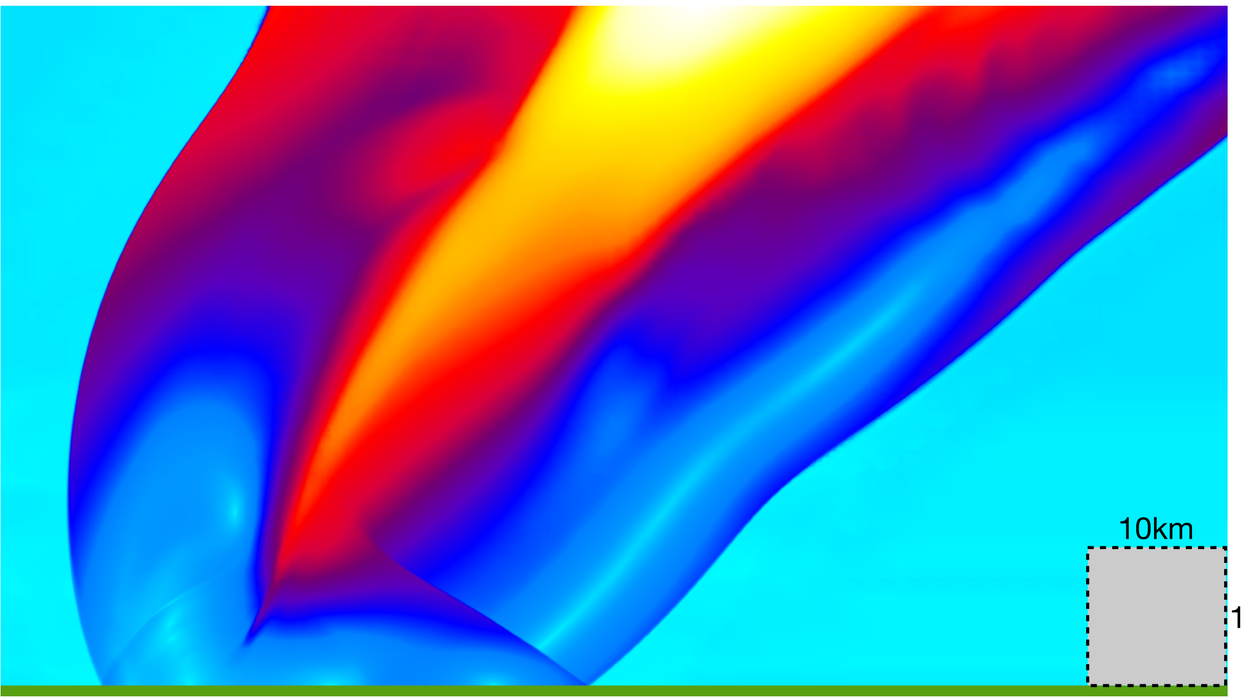
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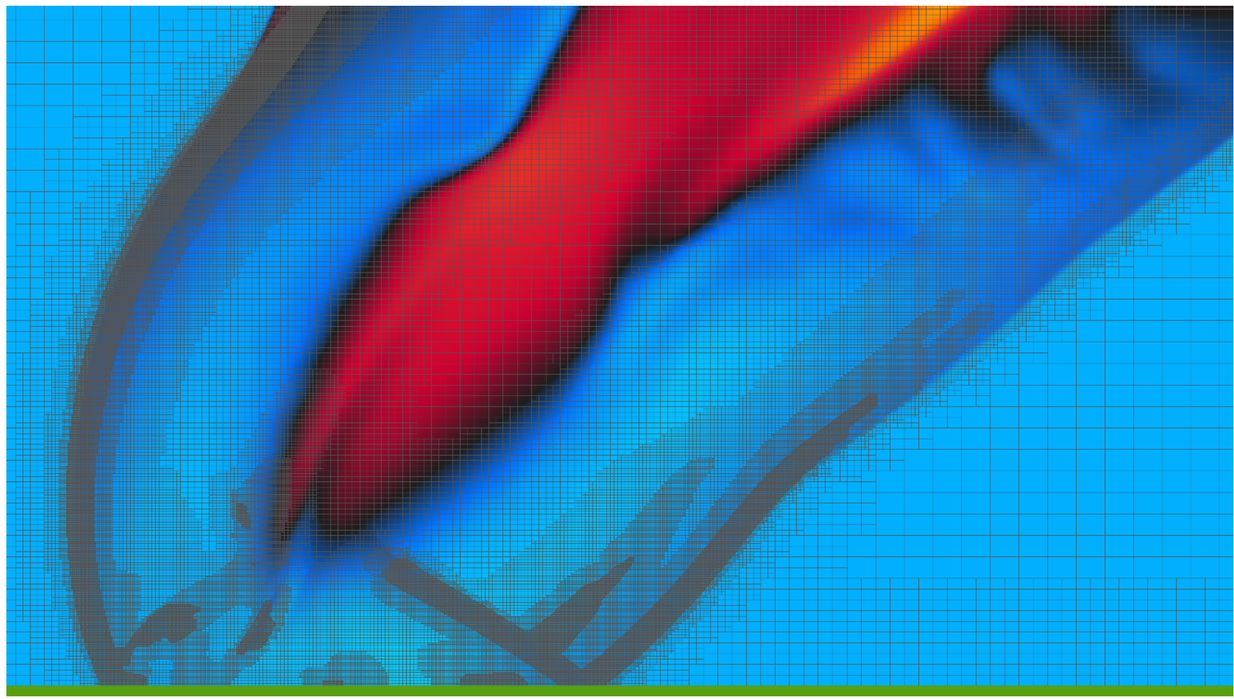
Solution Progression Through Time

adapt05
time = 38.2 s
time step 4800
49M cells

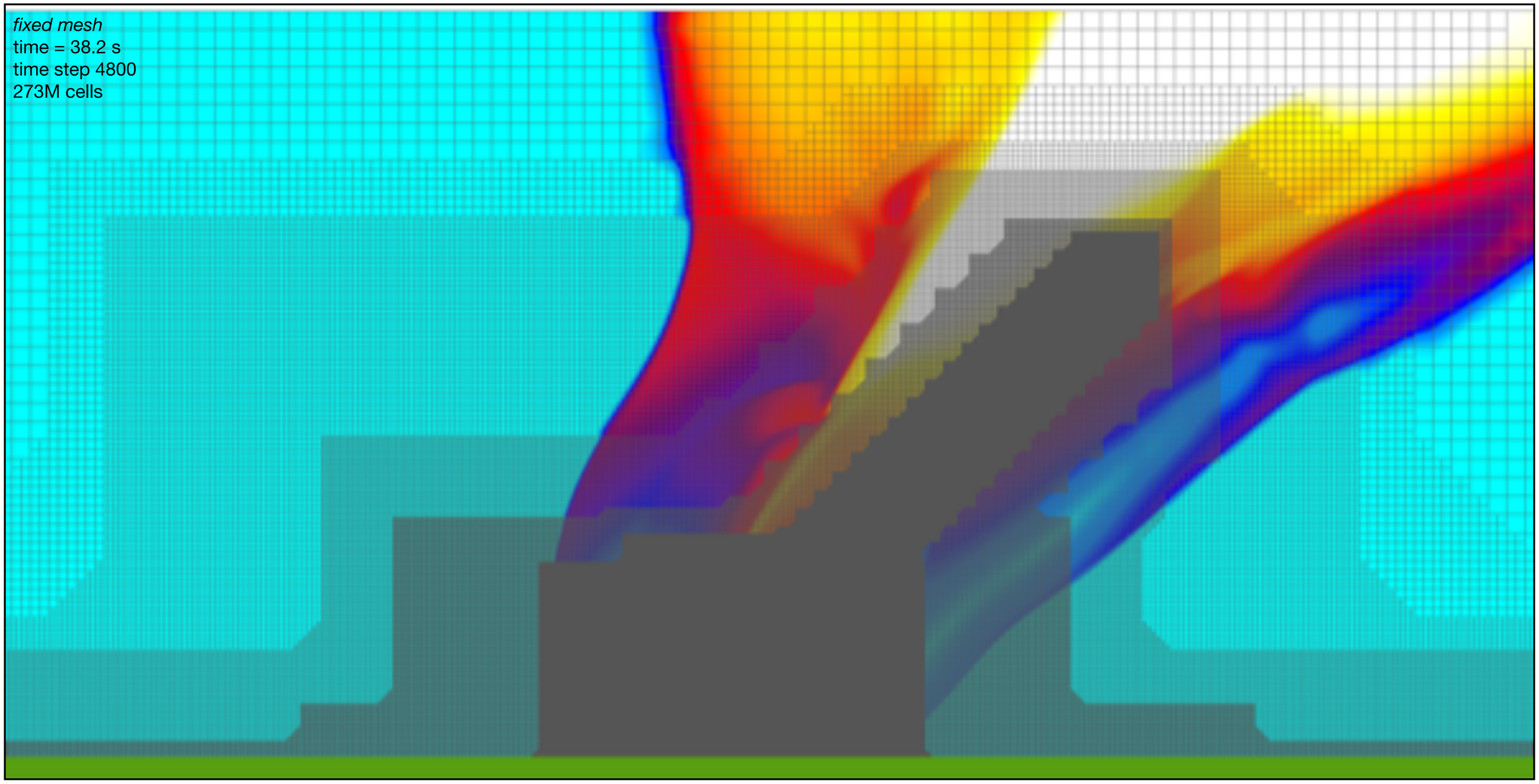
Mach Number



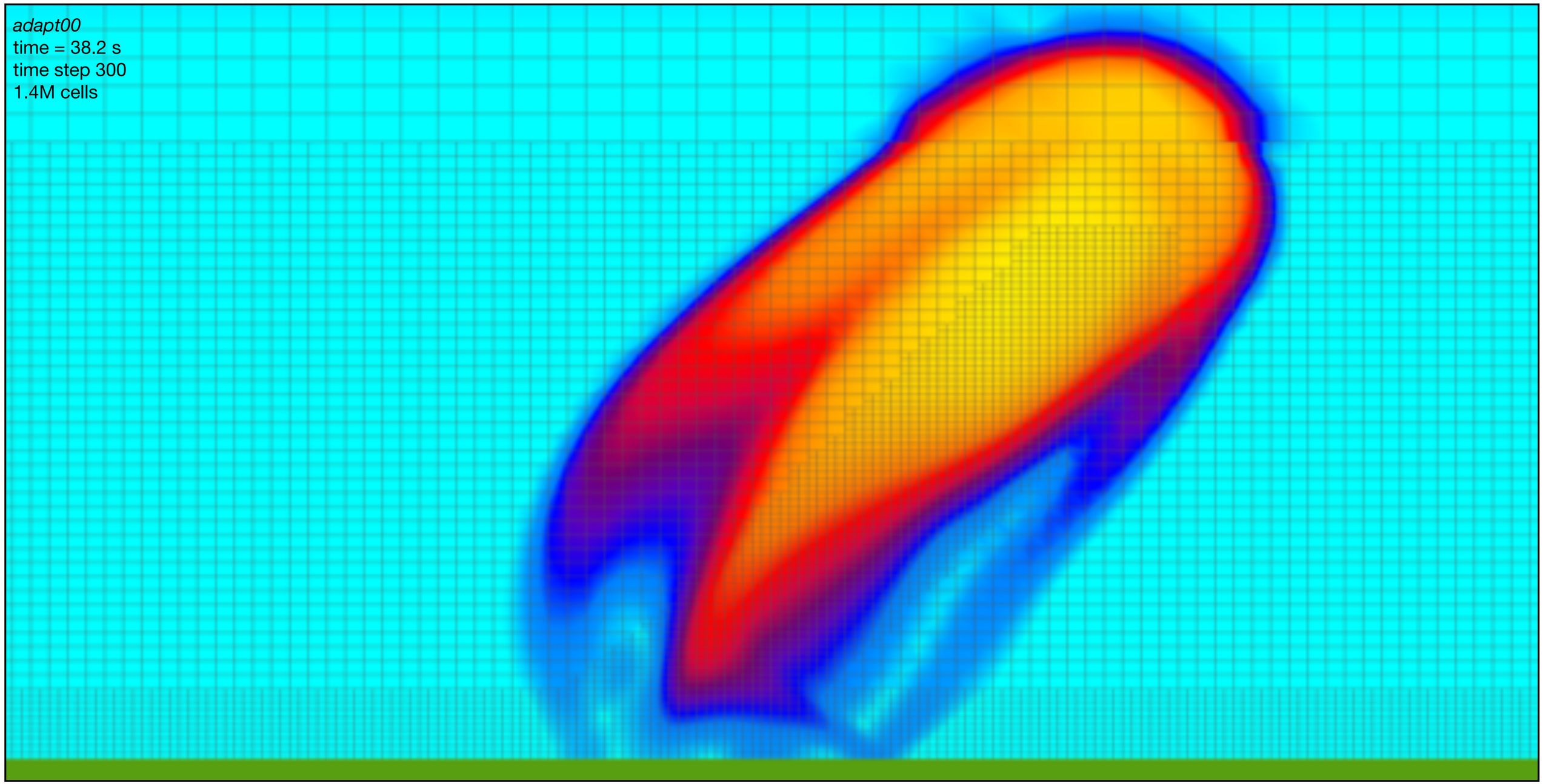
Temperature



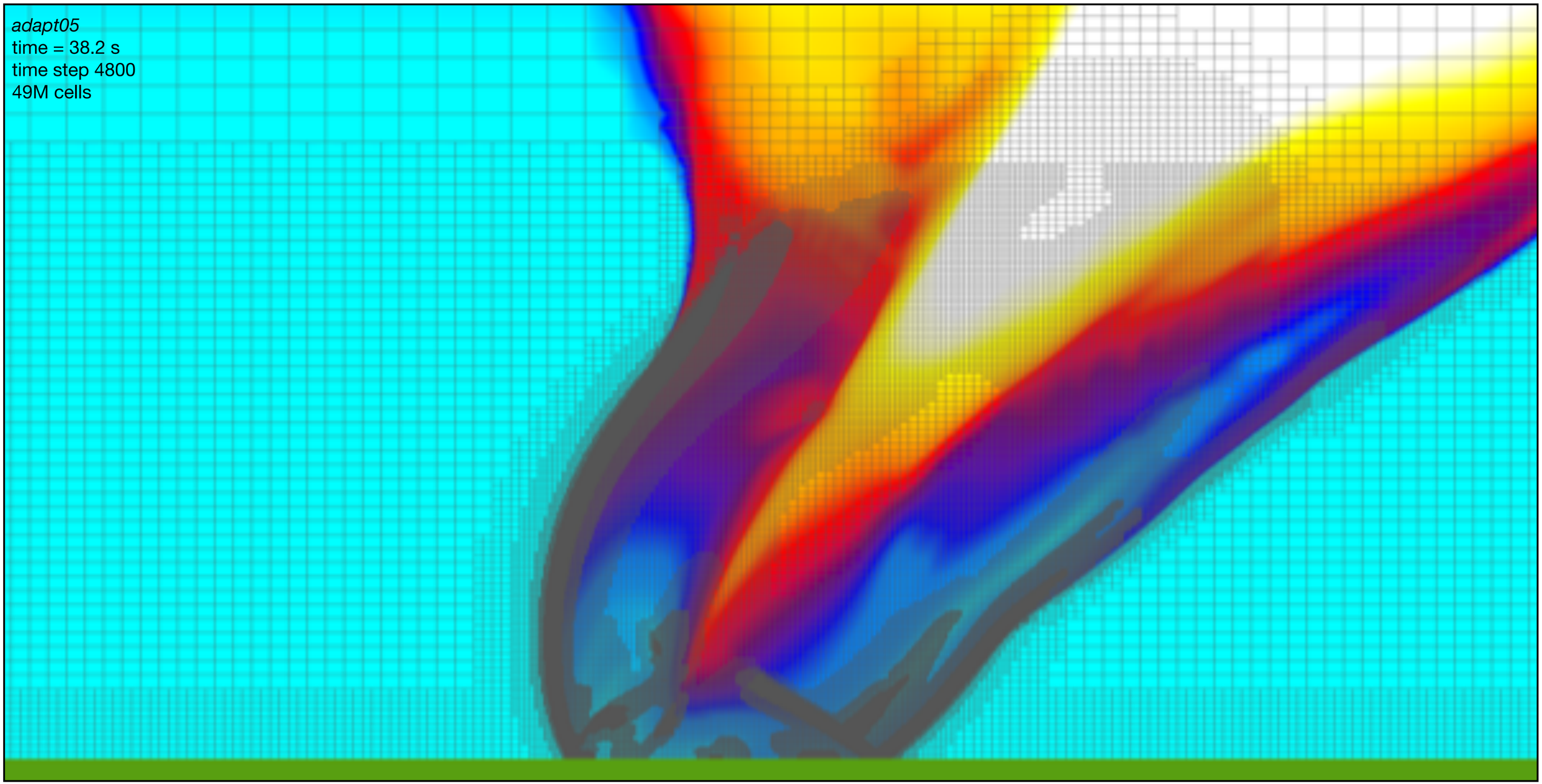
Fixed Mesh vs Adaptive Meshes



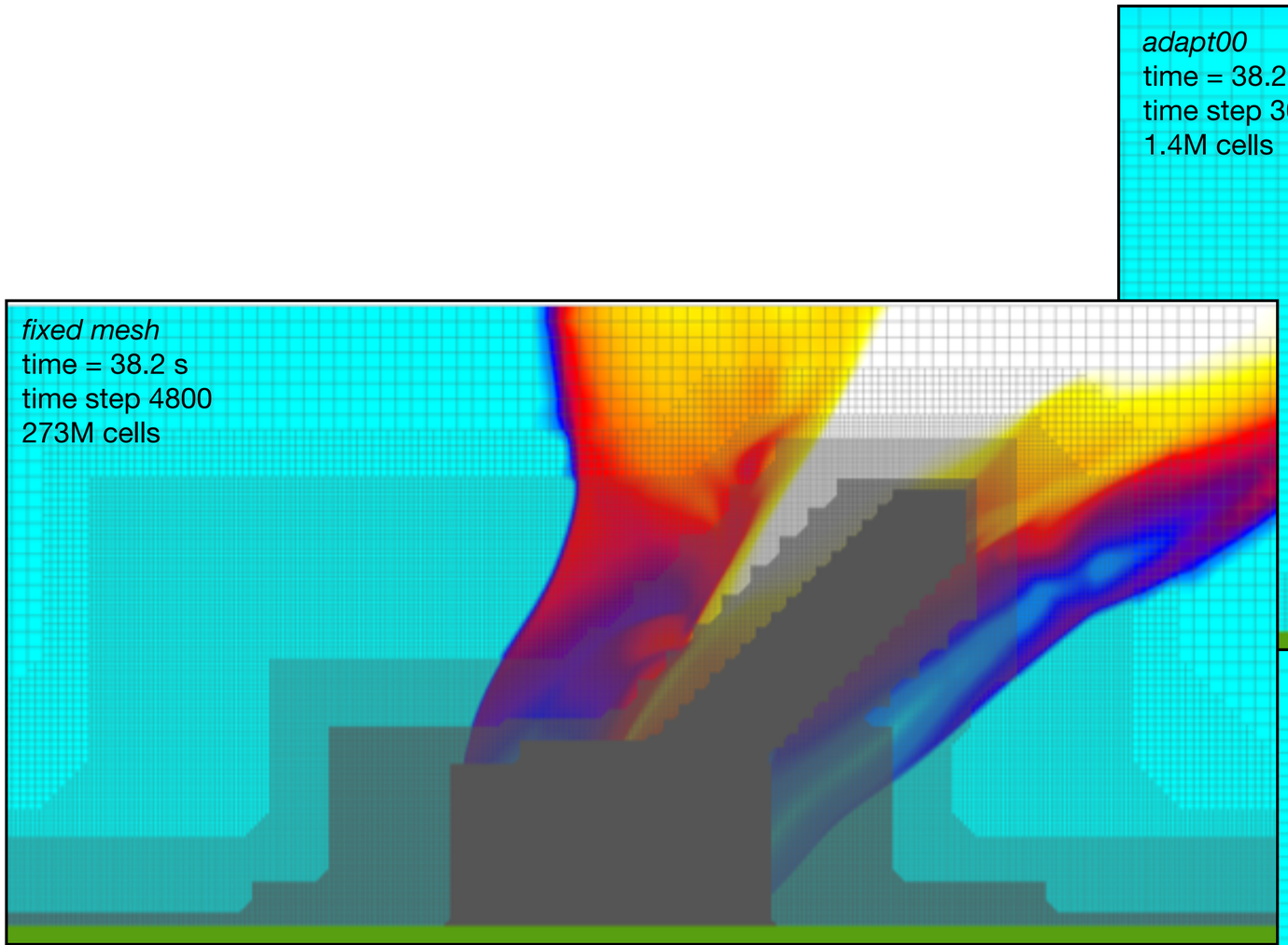
Fixed Mesh vs Adaptive Meshes

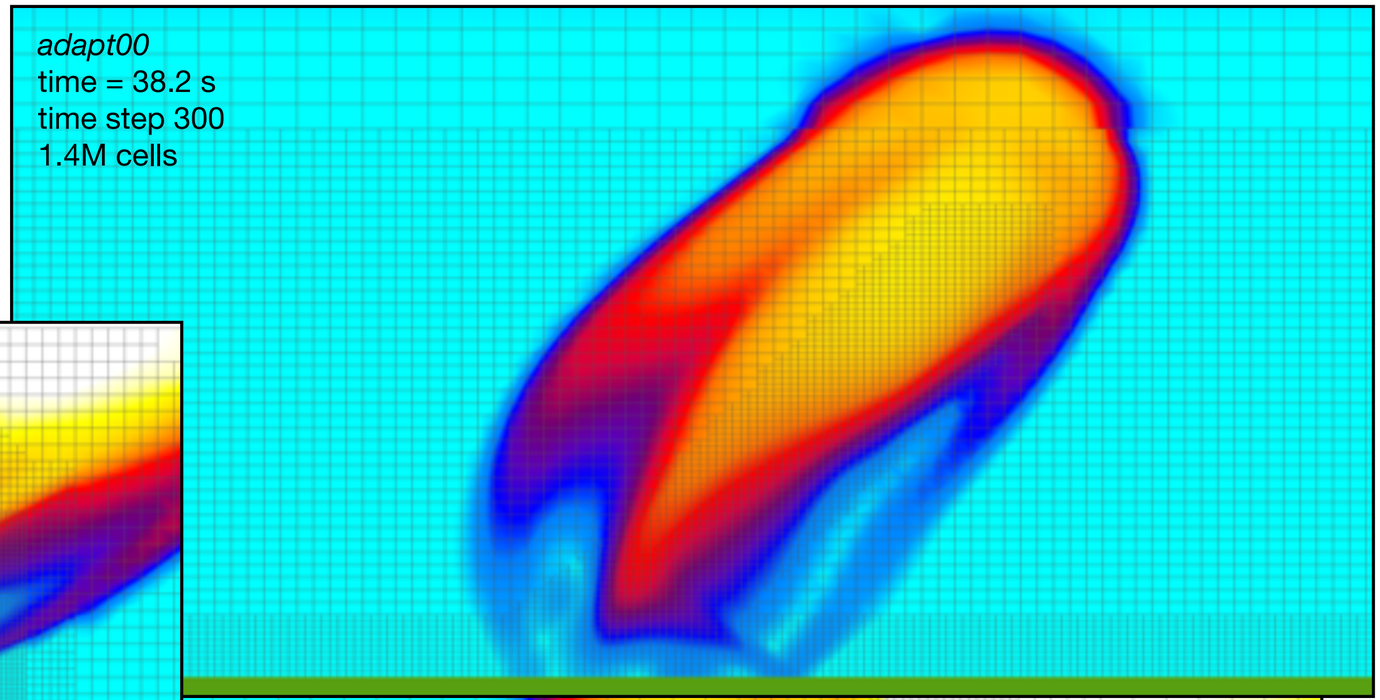


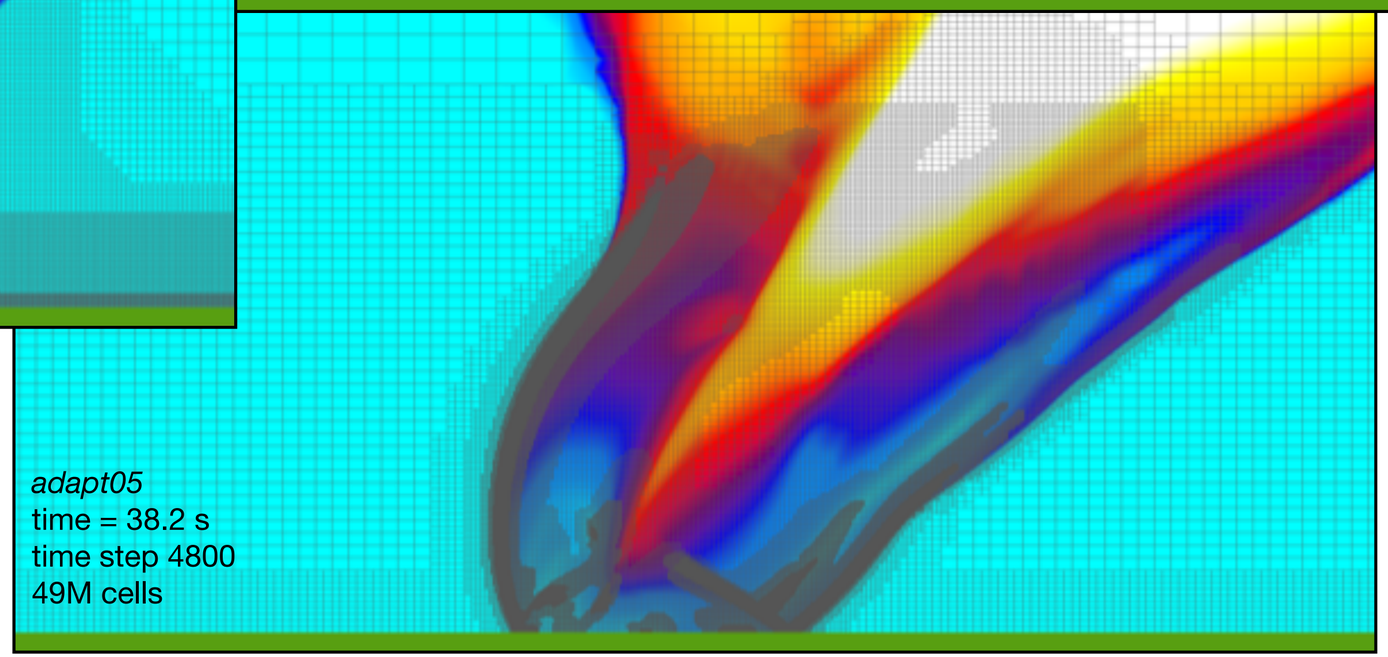
Fixed Mesh vs Adaptive Meshes



Fixed Mesh vs Adaptive Meshes

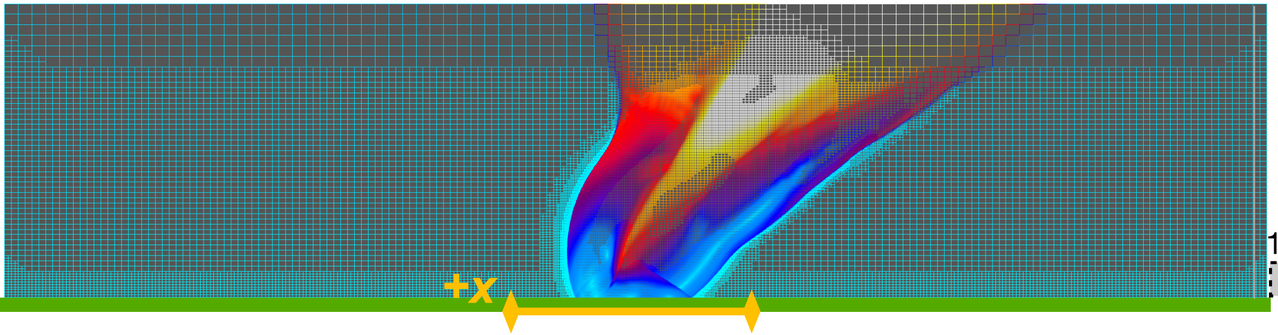


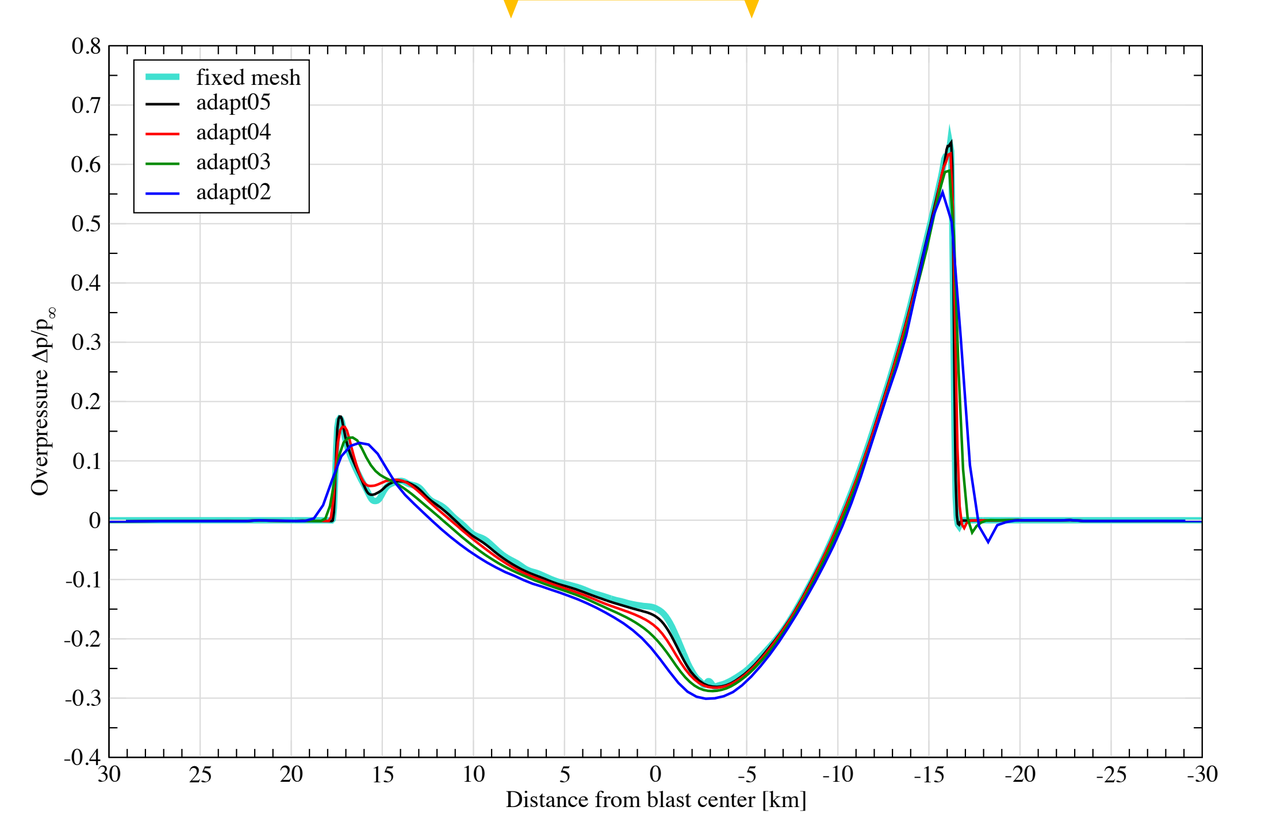




Ground Overpressure Convergence

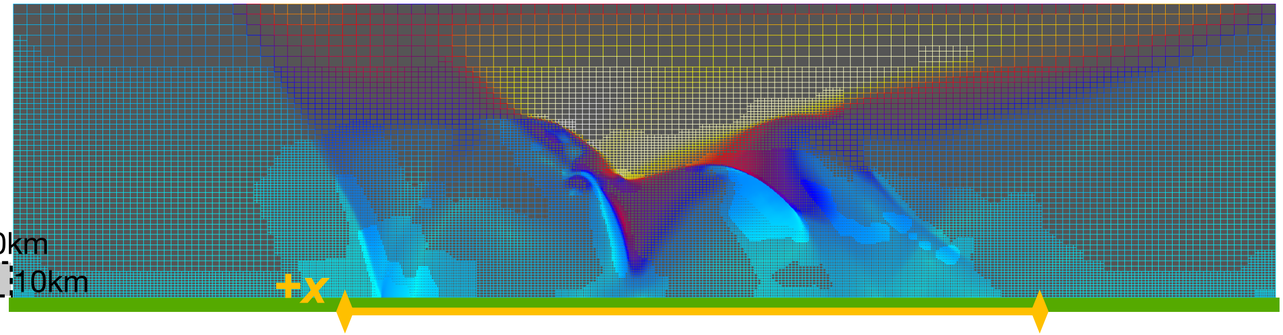
Early time, t = 38.2 s (49M cells)

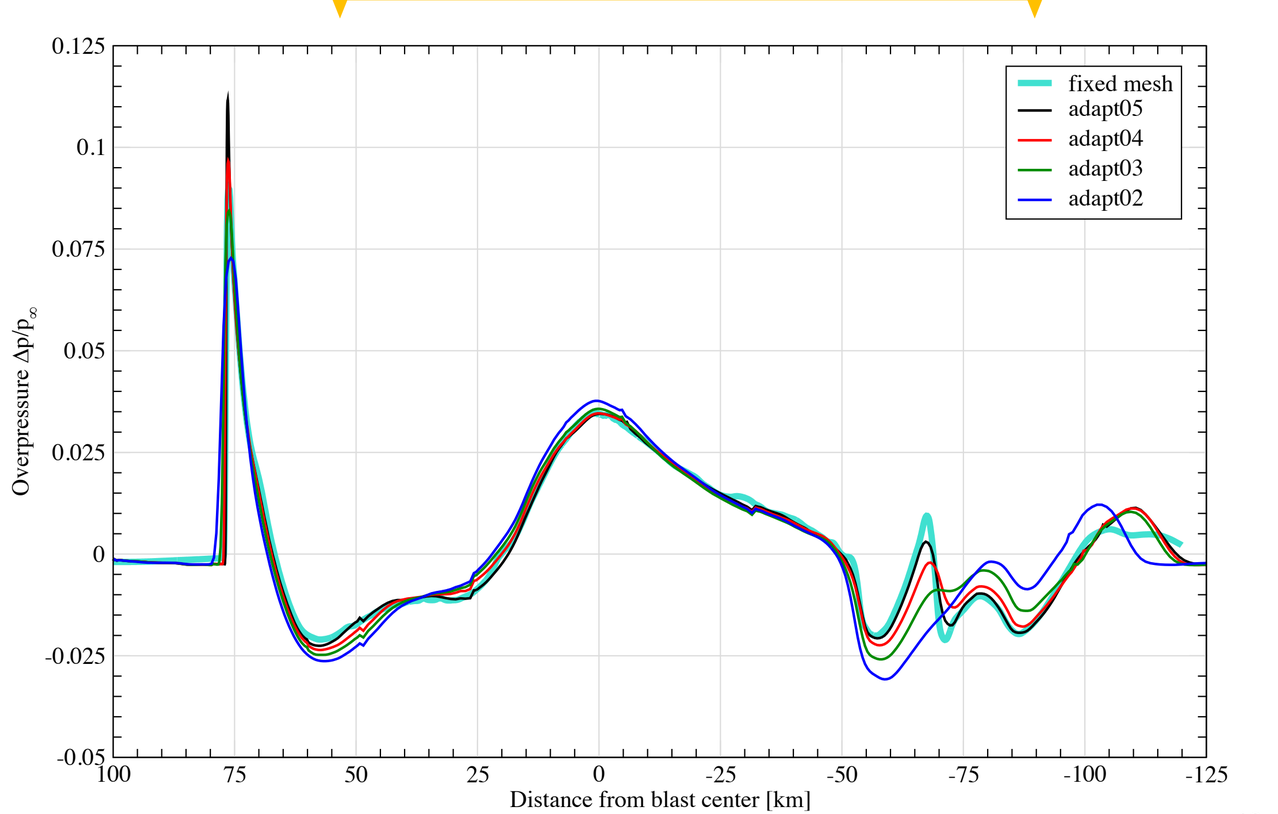




10km
10km

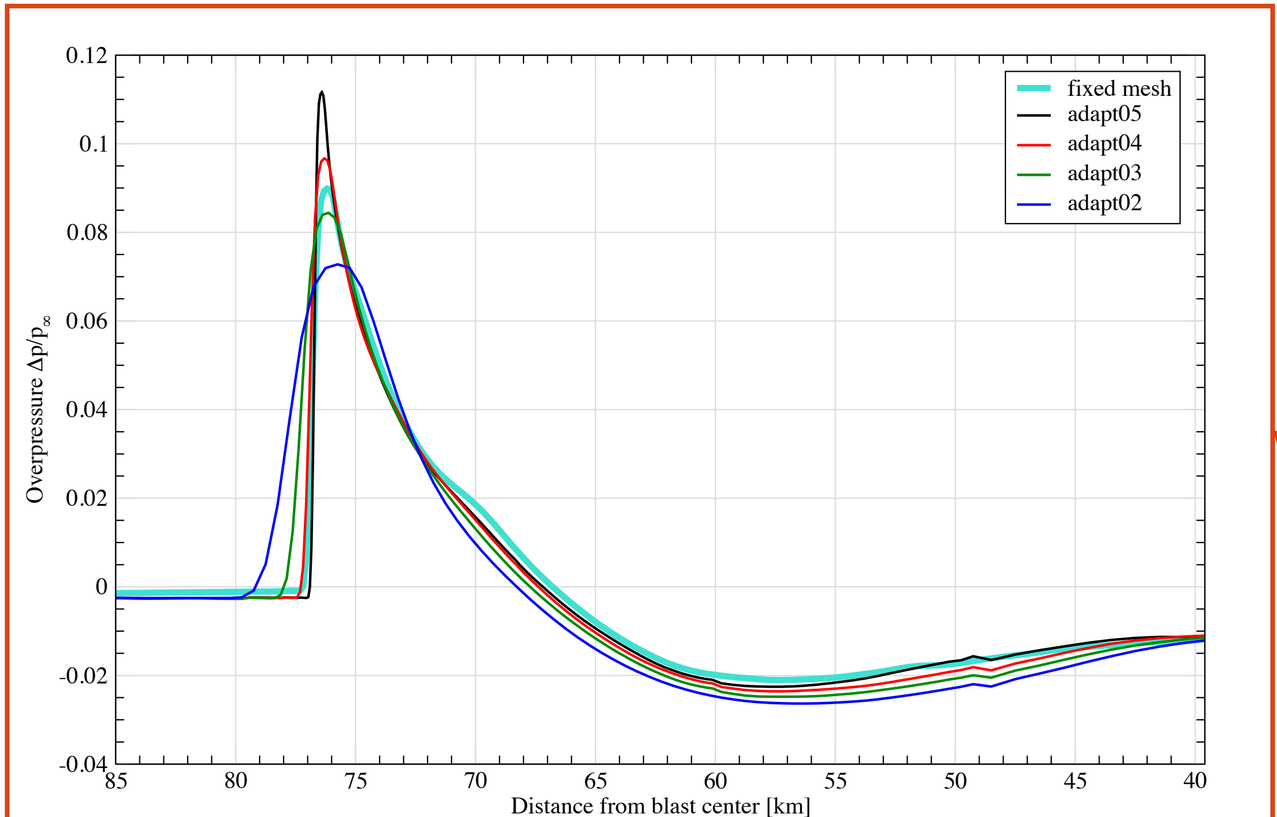
Later time, t = 211 s (145M cells)



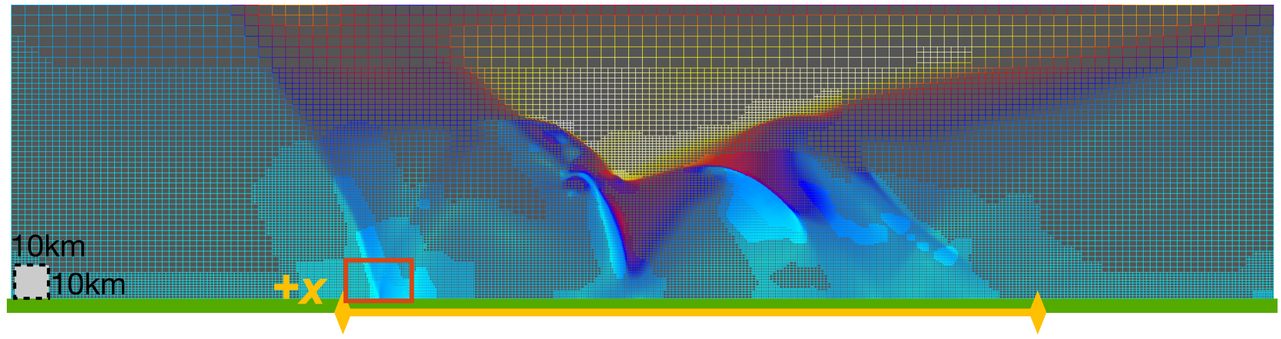


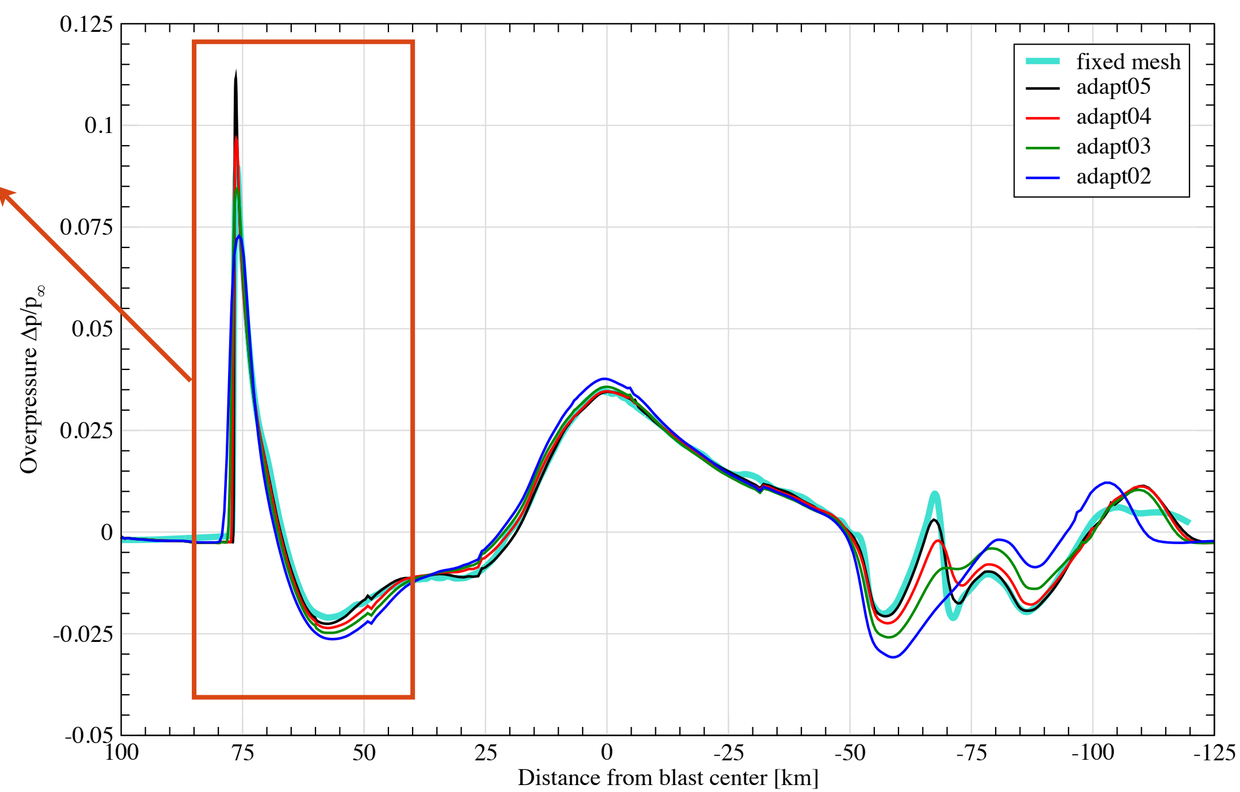
Ground Overpressure Convergence

- Downrange shock
  - Adaptation cycles 4 & 5 predict higher overpressure peak than fixed mesh



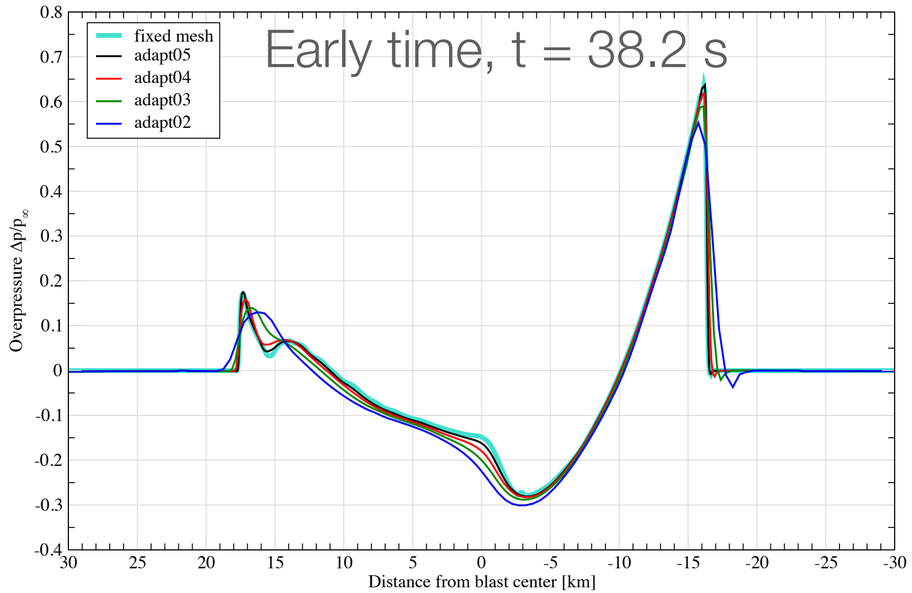
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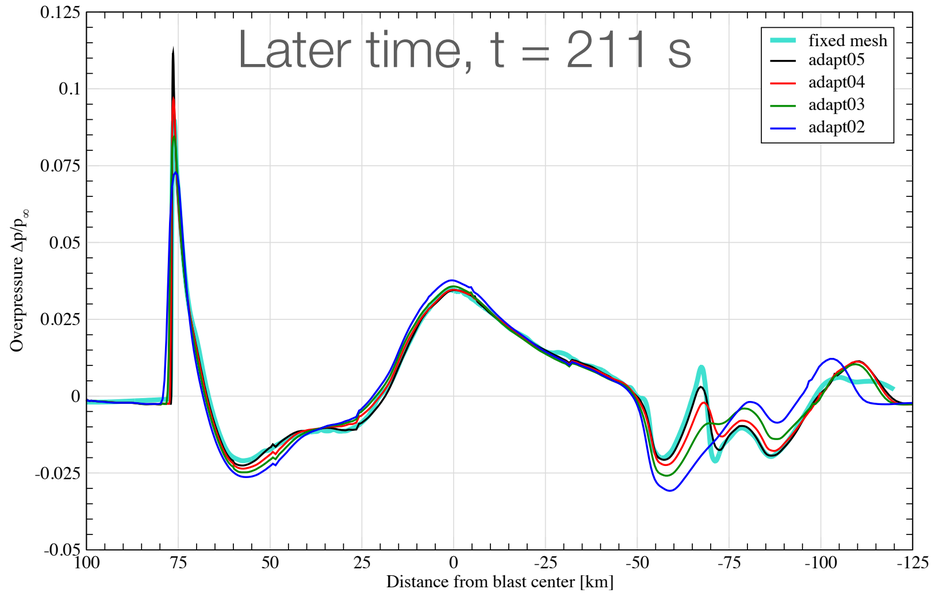


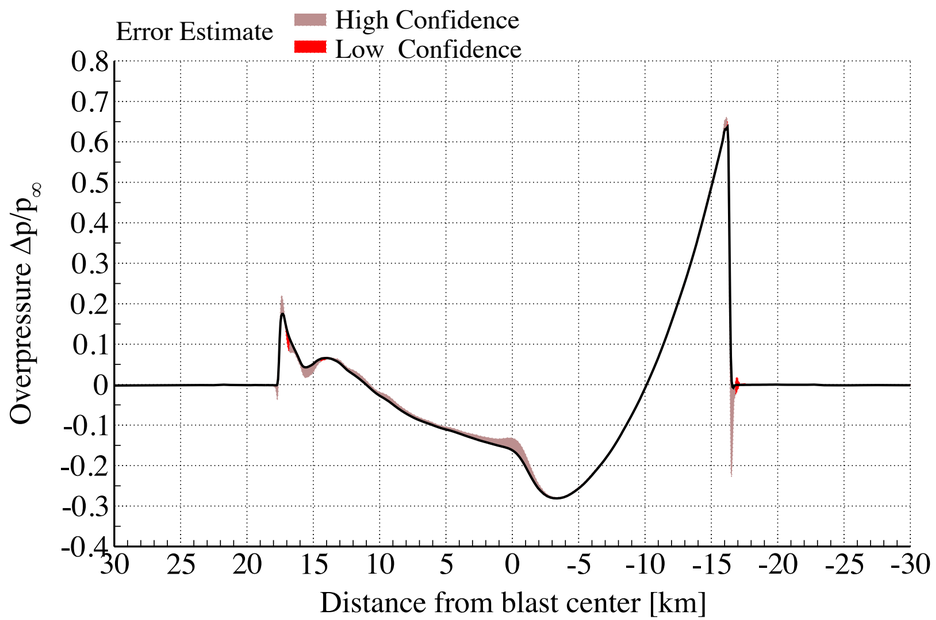


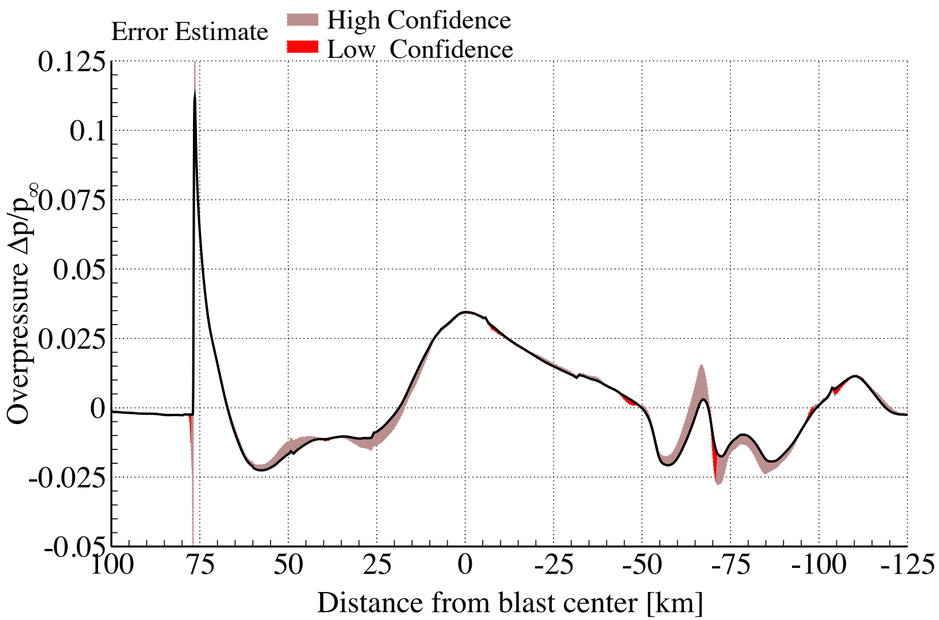
Ground Overpressure Error Estimate

- Richardson-based error estimate on finest 3 adaptive meshes



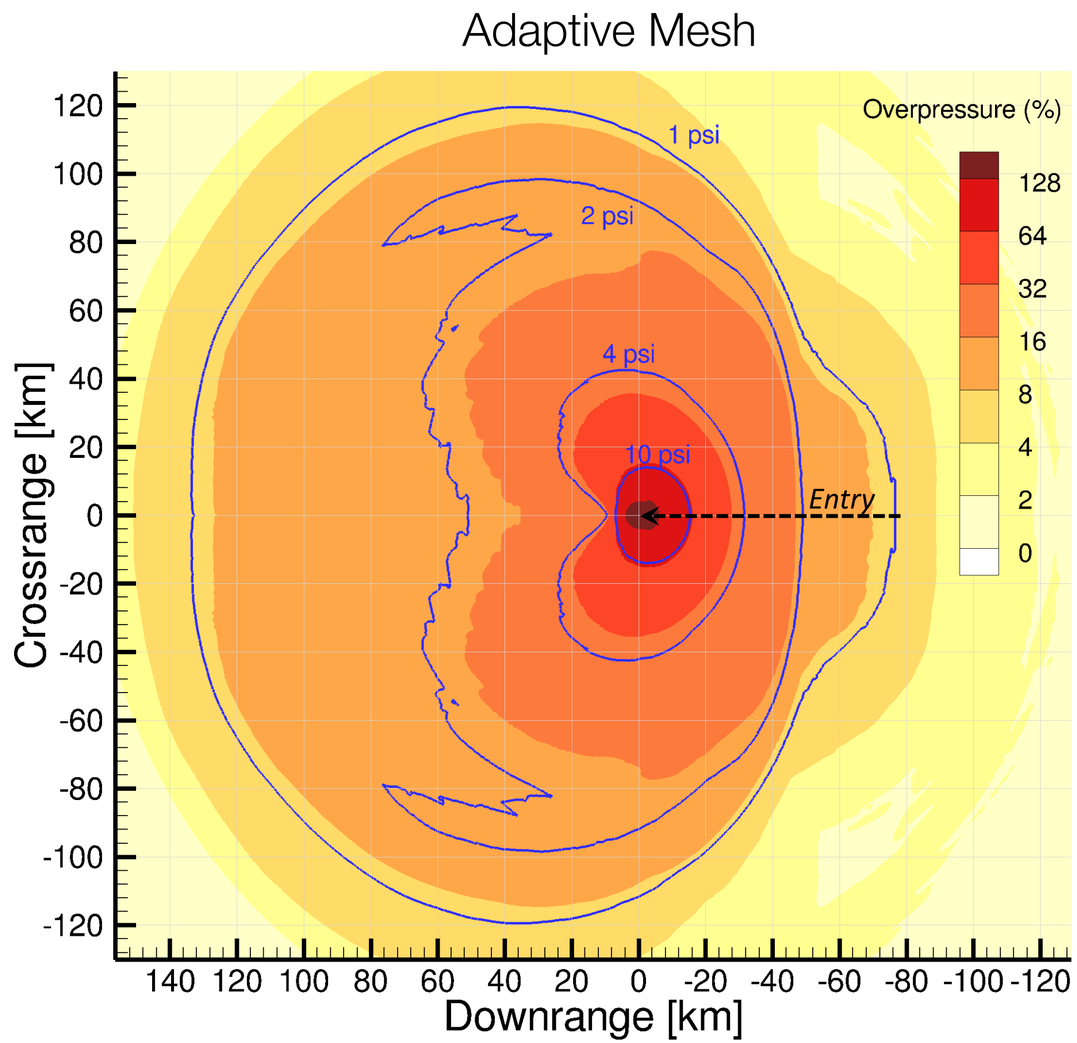






Blast Footprints

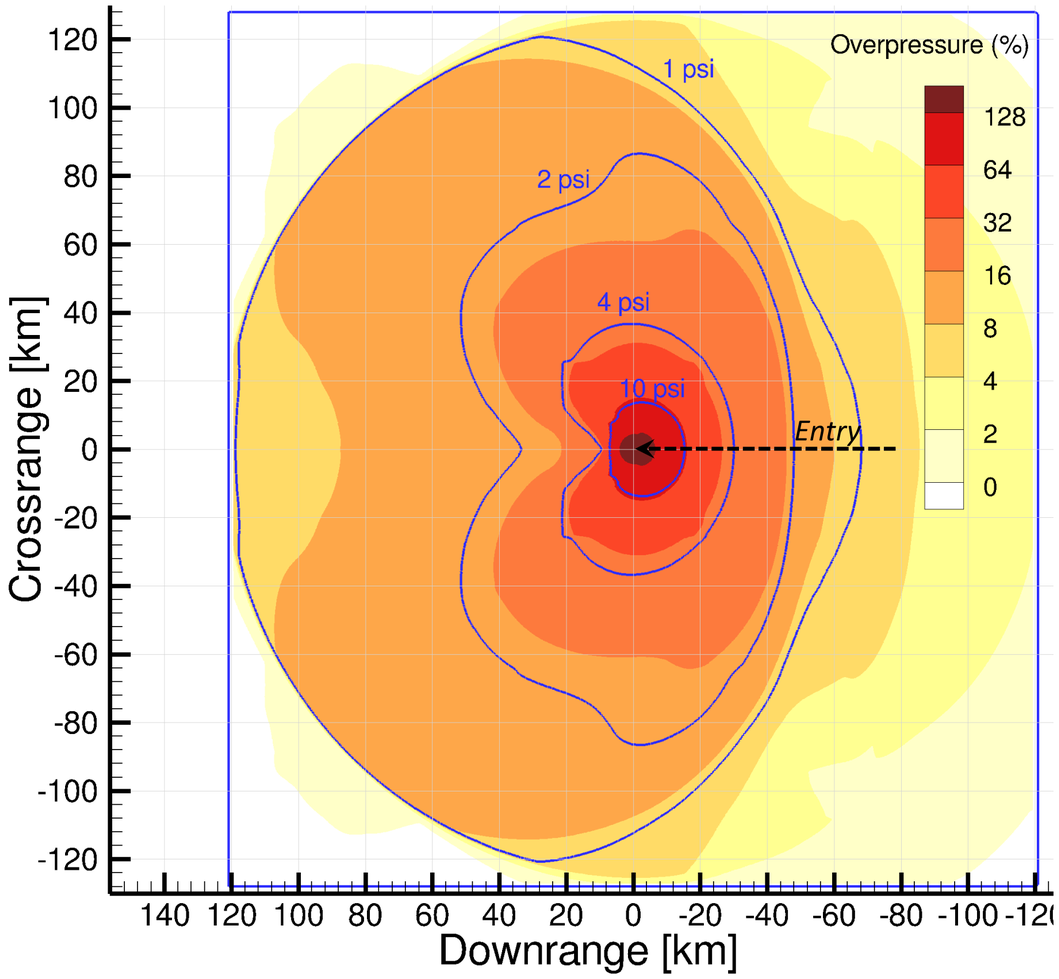
- Max ground overpressure over entire simulation



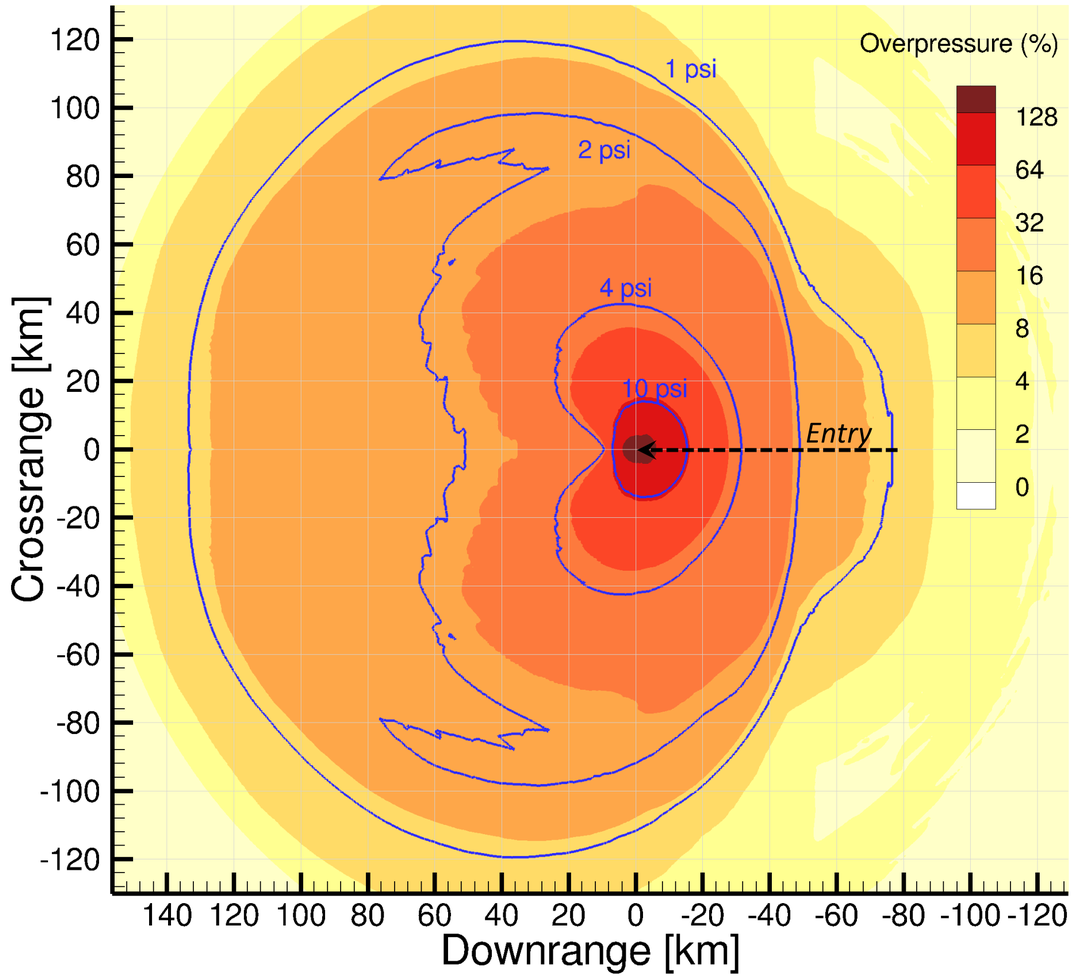
Blast Footprints

- Max ground overpressure over entire simulation
- Adaptive mesh carries overpressure levels to farther distances, especially 2 and 4 psi
- Note: fixed mesh domain is smaller and shock reaches the boundary, so ignore 1 psi contour downrange

Fixed Mesh

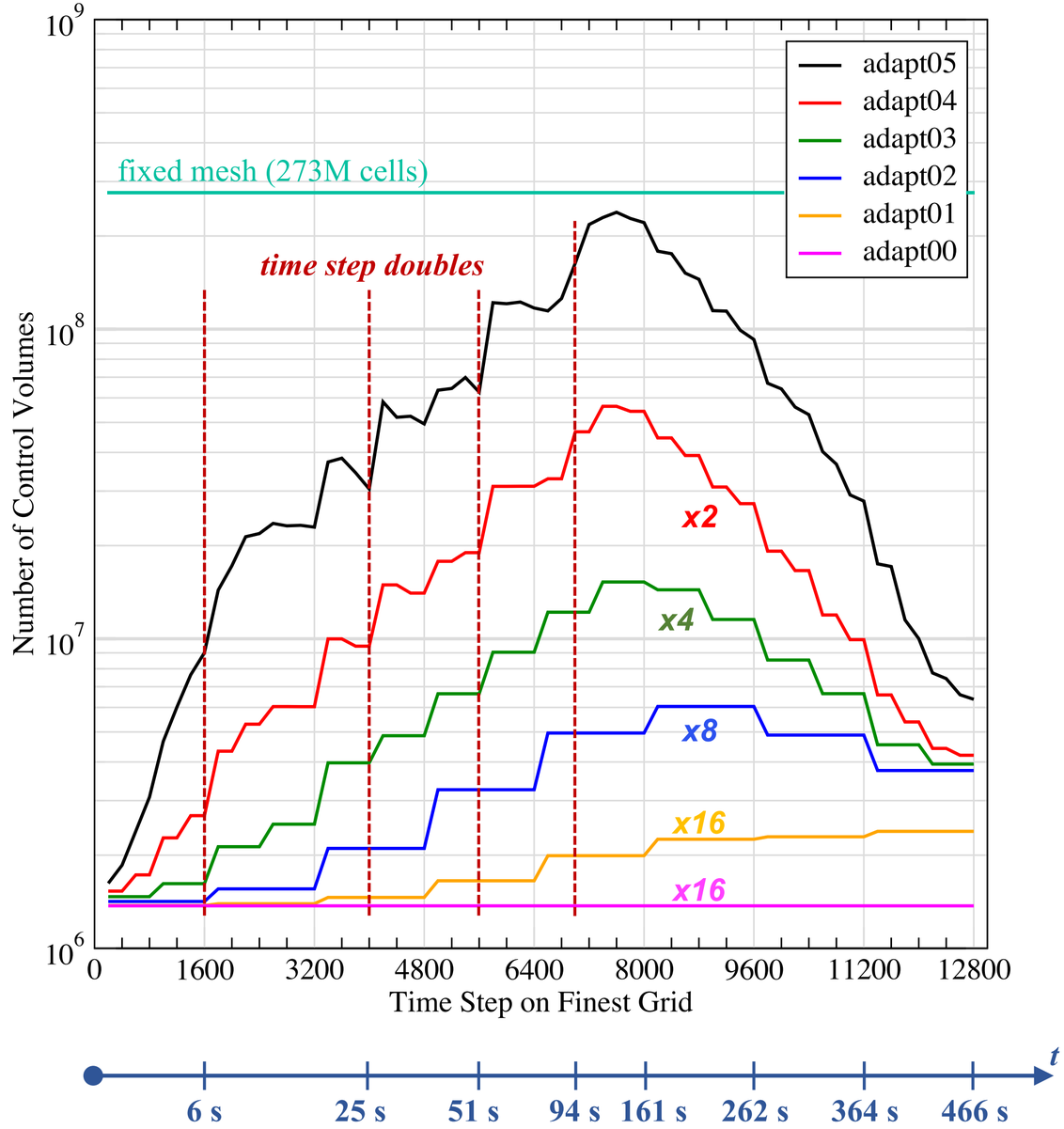


Adaptive Mesh



Mesh Size & Time Steps

- Cell count evolves over time and adaptation cycles
  - Mesh sizes increase as blast is strong and spreading
  - Eventually, shocks weaken and fewer cells are refined even as blast continues to spread
- Coarse grid time steps and windows scaled to line up with finest grid (200 time steps per window)
- Physical time step increased 2x at 4 points in time
  - Blast spreads and max wave speed decreases
  - Increase physical time step to advance more efficiently
  - Stretched time axis below figure

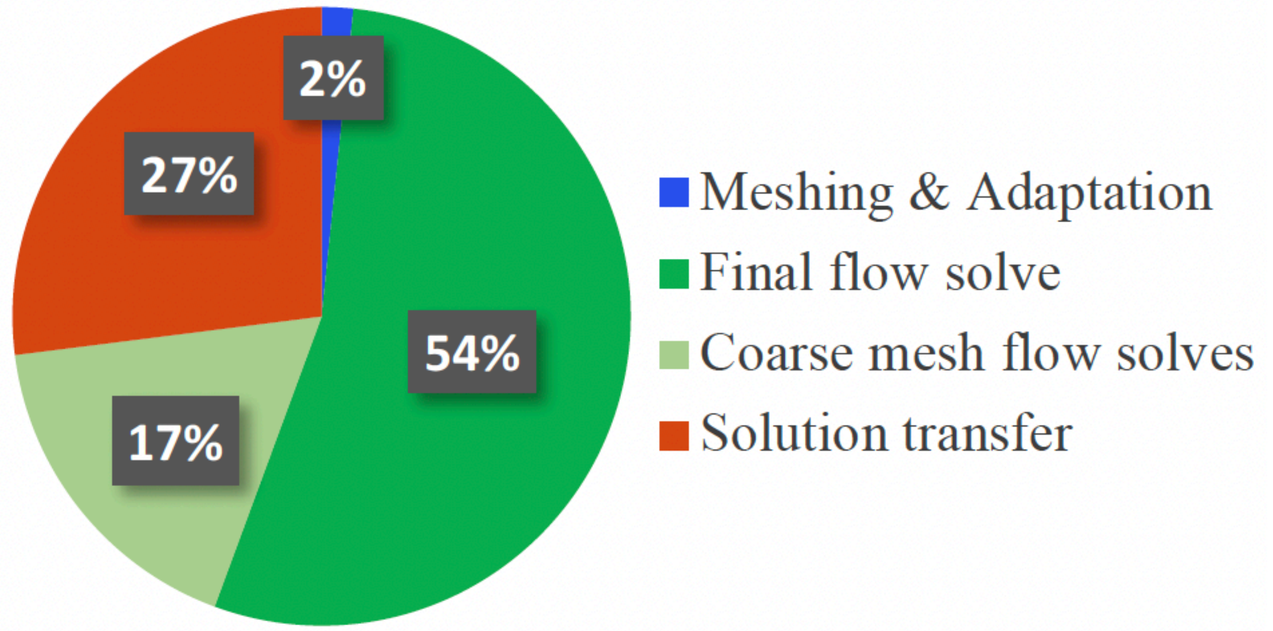


Computational Cost

- Run on NASA Aitken cluster, total of 4000 Cascade Lake cores (100 nodes with 40 cores each)
- Over half of the total wall-clock time is spent on final flow solve
- Solution transfer does use a very fast single-pass algorithm, but current implementation relies on serial file I/O
- Final adaptation cycle has 64 time windows, so mesh work is always completely parallelized
- All meshing, partitioning, and adaptation work is less than 2% of total simulation time

Wall-clock time and computational cost of 3D asteroid entry case

	Fixed Mesh	Parallel Adaptation
Meshing & adaptation [min]	17.6	9.9
Final flow solve [min]	605.6	325.9
Coarse mesh flow solves [min]	–	104.9
Solution transfer [min]	–	162.9
Total wall-clock time [min]	623.2	603.6
Total computational time [cpu-hr]	41.5k	40.2k



Summary

- Demonstrated scalable, massively parallel multi-pass algorithm for unsteady simulations with adaptive meshing
- Number of time windows can be chosen to control the relative cost of mesh work, flow computation, and solution transfer overhead
- In general, need enough mesh work (number of time windows) to utilize all cores/nodes
- Solution transfer remains serial process, computational cost does not depend on number of cores
- Demonstrated solution convergence and accuracy
- 3D Asteroid Entry & Blast Propagation
  - Adaptation results in finer mesh resolution where and *when* it is needed
  - Multiple adaptation cycles provide assessment of flow convergence and error estimate
  - Greater confidence in blast overpressure footprints, especially at lower psi levels
  - Majority of runtime spent on fine-grid flow computation
  - Less than 2% of run time spent on all meshing and adaptation mechanics

Takeaways: Adaptation makes unaffordable simulations affordable.
Multi-pass method parallelizes mesh adaptation work and is scalable.

Acknowledgments

- Thanks to Marsha Berger for many discussions about mesh adaptation strategies, space-time error estimation, unsteady time stepping, and temporal accuracy

- This work was supported by the NASA Ames Research Center contract NNA16BD60 through the Science Mission Directorate's Planetary Defense Coordination Office and the Asteroid Threat Assessment Project

- NASA Advanced Supercomputing Division for providing computing resources

- Science & Technology Corp. for supporting Wade Spurlock's involvement and travel