

# An Overture Overview

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[www.llnl.gov/casc/Overture](http://www.llnl.gov/casc/Overture)

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## Acknowledgements

### Supported by

Department of Energy, Office of Science

MICS Program: Mathematical, Information, and Computational Sciences

SciDAC: Scientific Discovery through Advanced Computing

TSTT: Terascale Simulation Tools and Technology Centre

APDEC: Applied Partial Differential Equations Centre

### Current Overture developers

Kyle Chand

Bill Henshaw

### Collaborators

Petri Fast (LLNL)

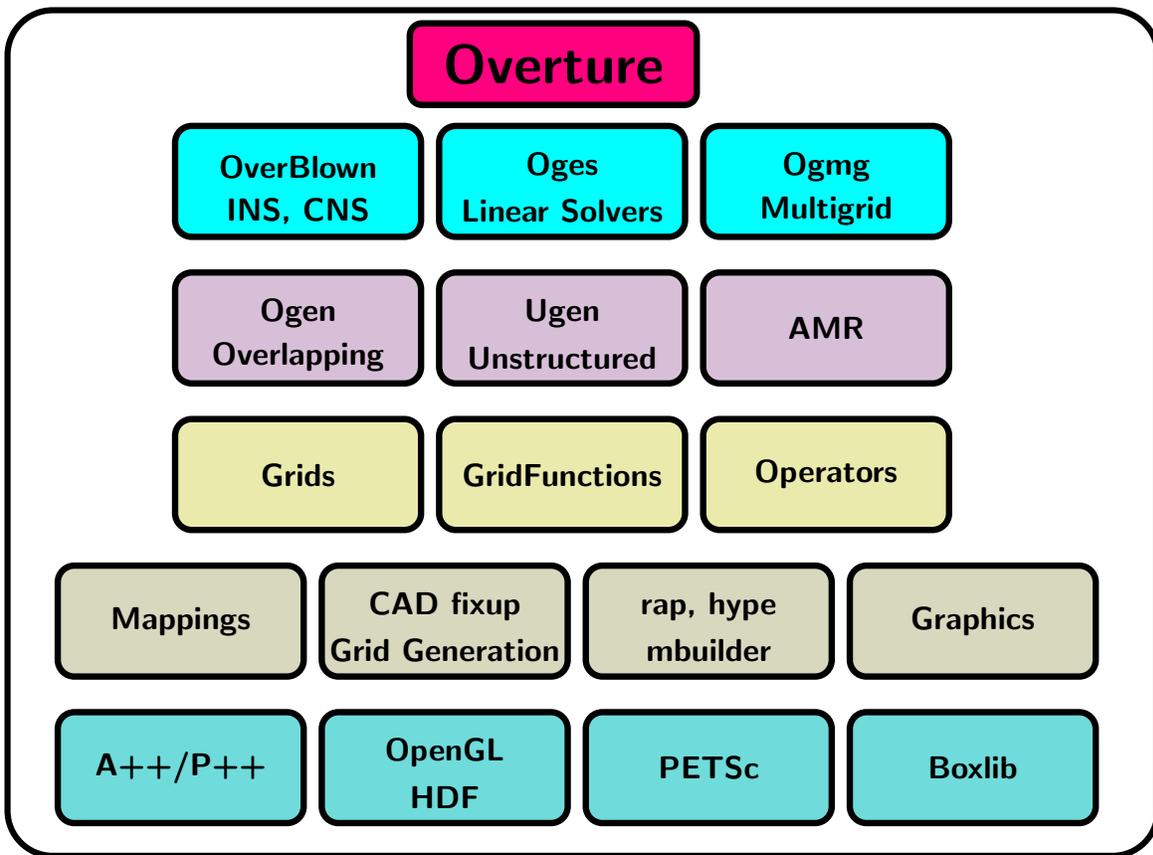
Don Schwendeman (RPI)

**Overture is a collection of C++ classes that can be used to solve partial differential equations on structured, overlapping and hybrid grids.**

**Key features:**

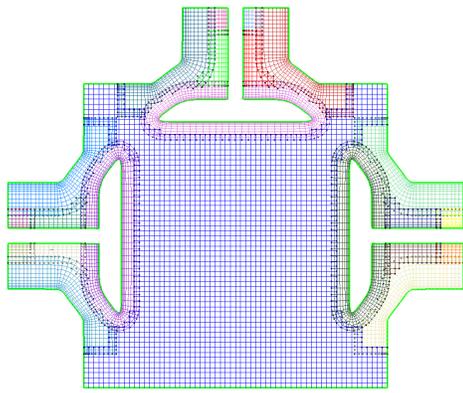
- provides a high level interface for rapid prototyping of PDE solvers.
- built upon optimized C and fortran kernels.
- provides a library of finite-difference operators: conservative and non-conservative, 2nd, 4th, 6th and 8th order accurate approximations.
- support for moving grids
- support for block structured adaptive mesh refinement
- extensive grid generation capabilities
- CAD fixup tools
- interactive graphics and data base support.
- PDE solvers built upon Overture include:
  - OverBlown: incompressible Navier-Stokes, compressible Navier-Stokes, reactive Euler equations.
  - Max: time domain Maxwell's equations solver: fourth-order accurate, parallel.

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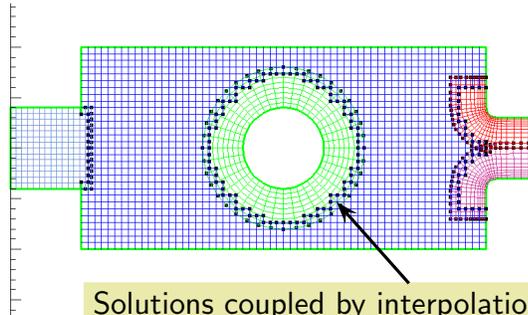
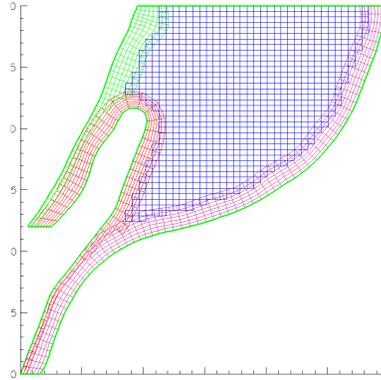


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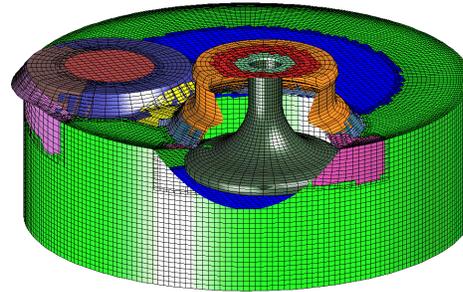
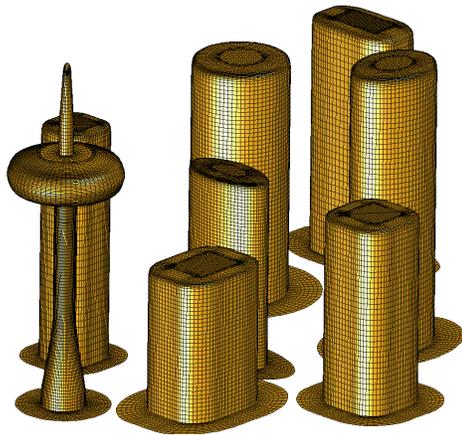
Sample 2D overlapping grids



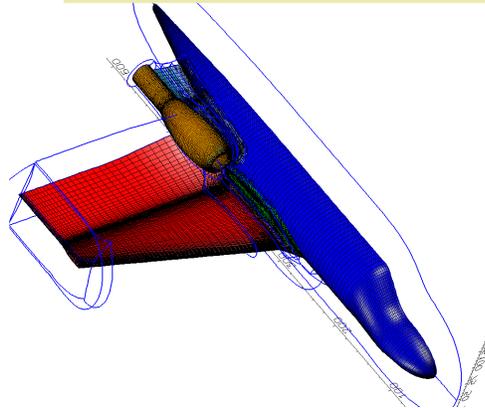
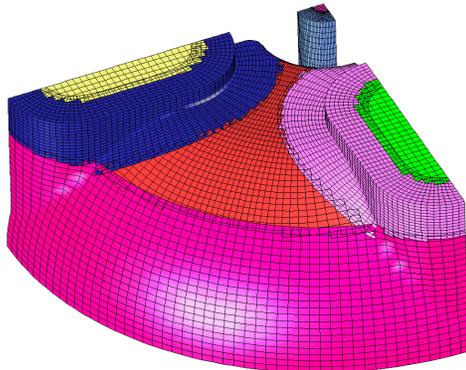
Solutions coupled by interpolation



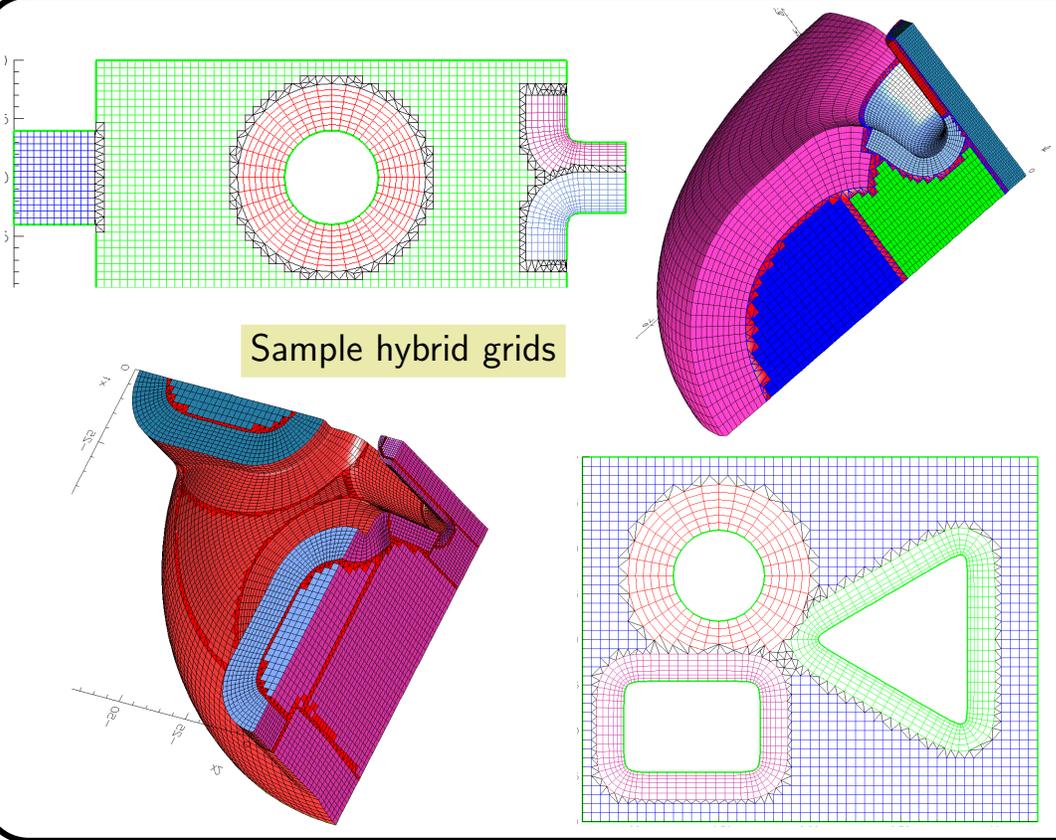
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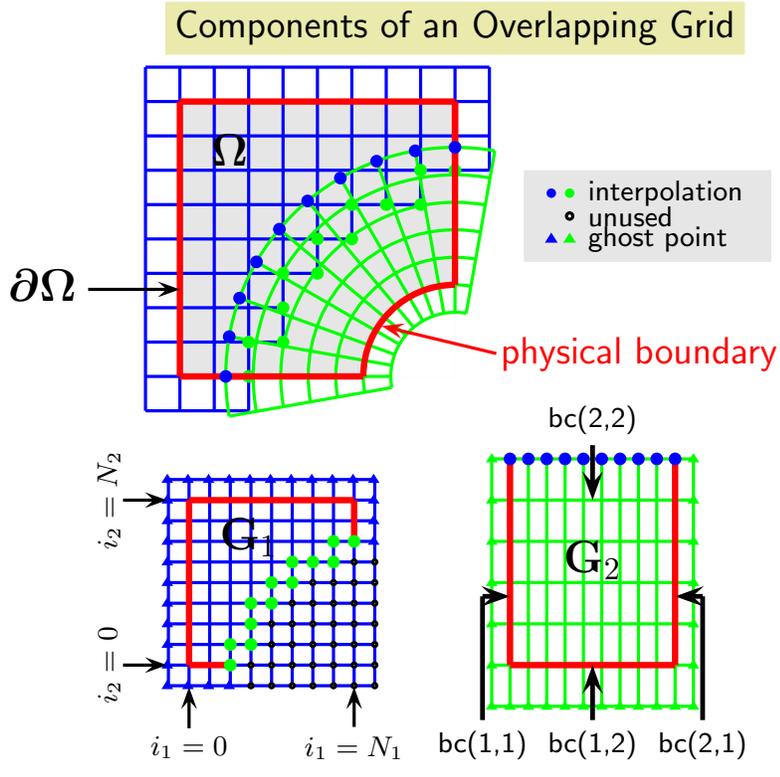
Sample 3D overlapping grids



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## Overture supports a high-level C++ interface (but is built mainly upon Fortran kernels):

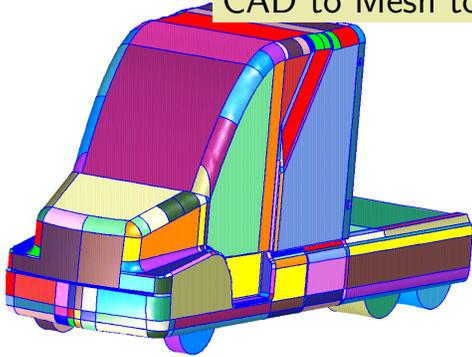
Solve  $u_t + au_x + bu_y = \nu(u_{xx} + u_{yy})$

```
CompositeGrid cg; // create a composite grid
getFromADatabaseFile(cg,"myGrid.hdf");
floatCompositeGridFunction u(cg); // create a grid function
u=1.;
CompositeGridOperators op(cg); // operators
u.setOperators(op);
float t=0, dt=.005, a=1., b=1., nu=.1;
for( int step=0; step<100; step++ )
{
    u+=dt*( -a*u.x()-b*u.y()+nu*(u.xx()+u.yy()) ); // forward Euler
    t+=dt;
    u.interpolate();
    u.applyBoundaryCondition(0,dirichlet,allBoundaries,0.);
    u.finishBoundaryConditions();
}
```

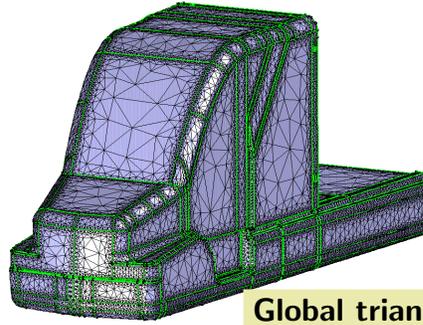
## Current Projects with Overture

- ◇ Hybrid (unstructured) grid generation and algorithms (Kyle Chand)
  - ◇ the overlap region is replaced by an unstructured grid (advancing front algorithm).
  - ◇ a stabilized DSI scheme for Maxwell's equations on hybrid grids.
- ◇ Deforming boundaries in incompressible flow (Petri Fast).
- ◇ Multigrid solvers for elliptic problems on overlapping grids.
  - ◇ robust coarsening and adaptive smoothing techniques.
  - ◇ second- and fourth-order accurate, Dirichlet and Neumann boundary conditions.
- ◇ Incompressible Navier-Stokes solvers for overlapping grids.
  - ◇ fourth-order accurate time accurate solver.
  - ◇ line-implicit pseudo-steady state solver.
- ◇ High speed reactive flow and adaptive mesh refinement (with Don Schwendeman (RPI))
- ◇ An overlapping grid solver for the time dependent Maxwell's equations.
  - ◇ fourth-order accurate, parallel

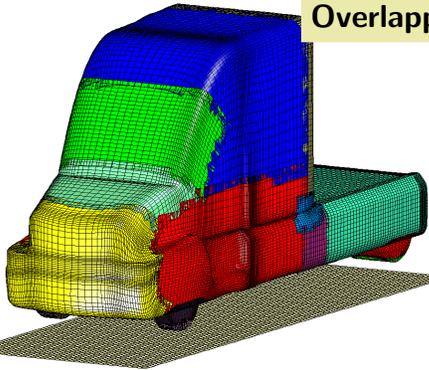
# CAD to Mesh to Solution with Overture



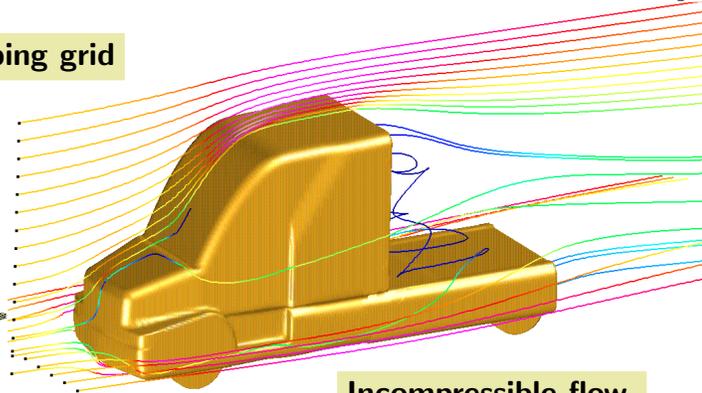
Cad fixup



Global triangulation



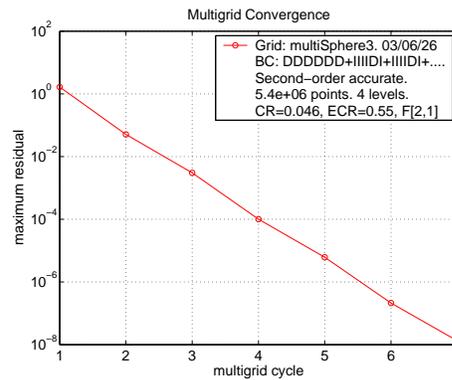
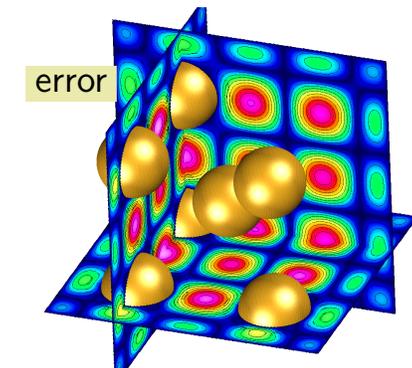
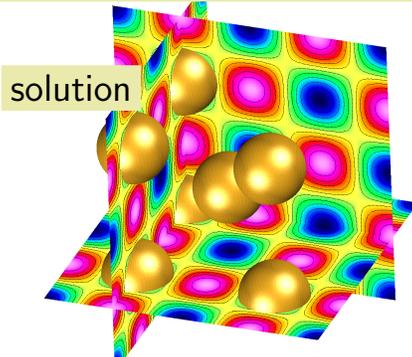
Overlapping grid



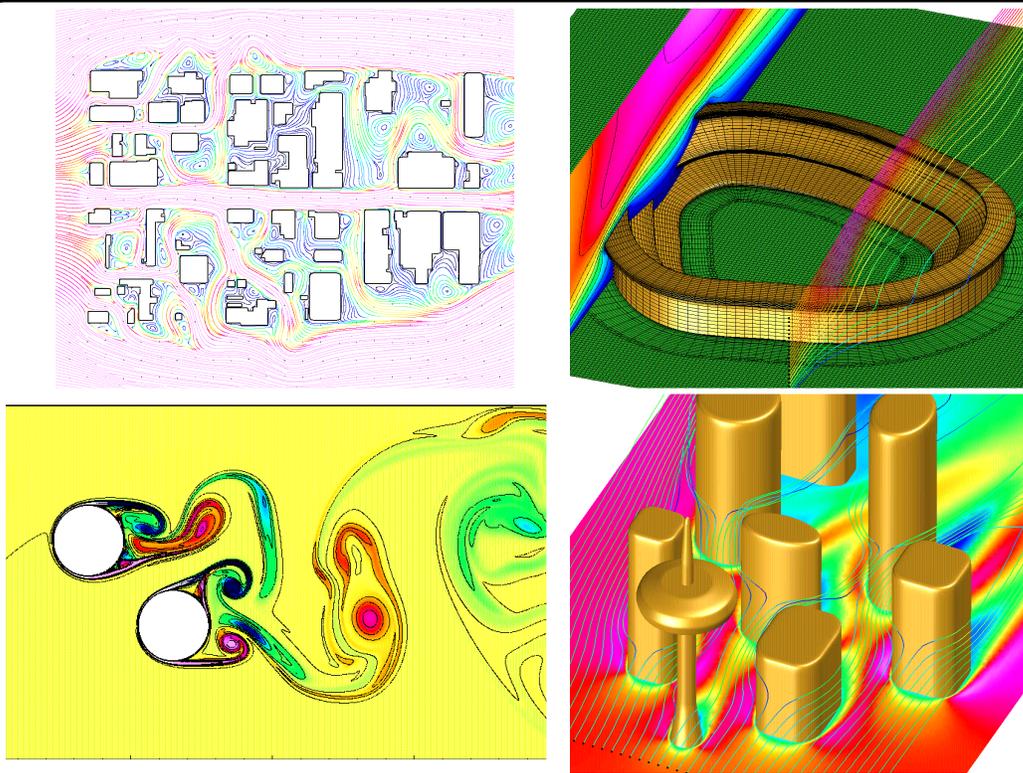
Incompressible flow.

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# Multigrid solution to Poisson's equation, 5.4 million grid points

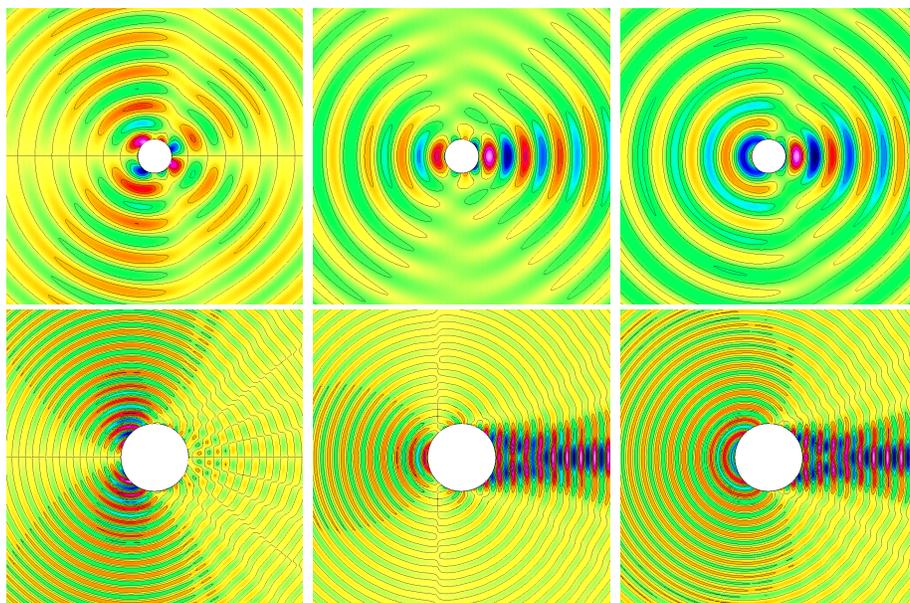


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Incompressible flow computations with OverBlown.

A Parallel 4th-order accurate solver for the time-dependent Maxwell equations

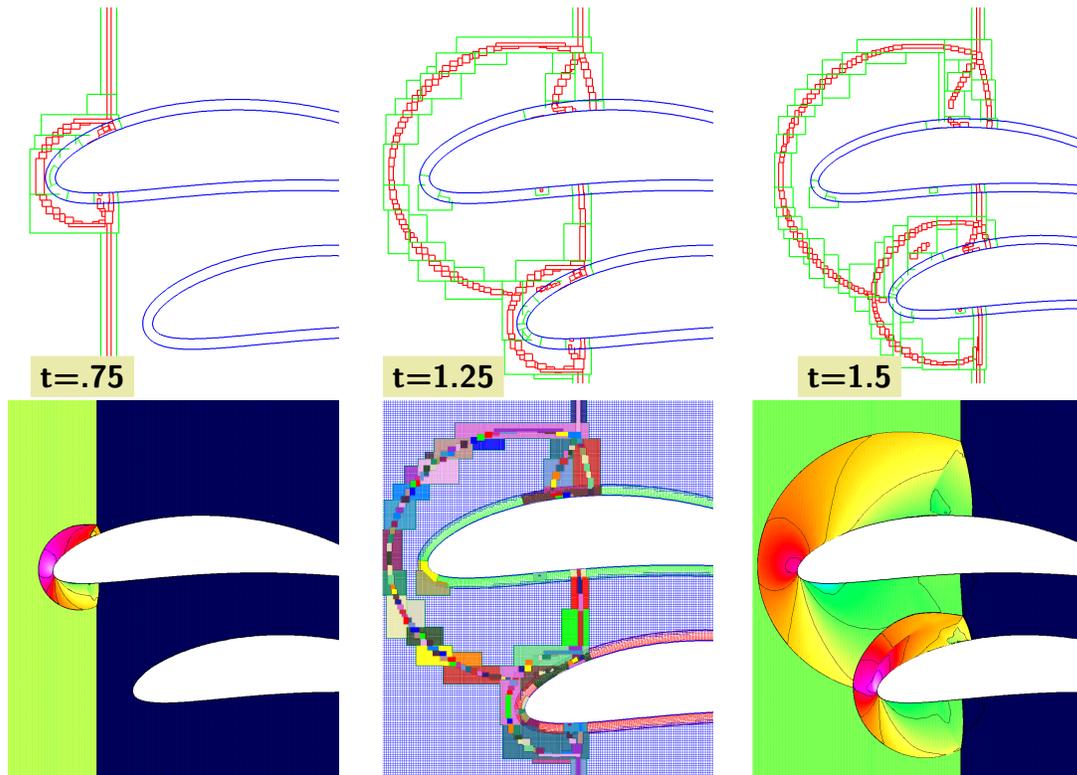


Scattering of a plane wave by a cylinder. Top: scattered field  $E_x$ ,  $E_y$  and  $H_z$  for  $ka = 1/2$ .

Bottom: scattered field  $E_x$ ,  $E_y$  and  $H_z$  for  $ka = 5/2$

## Adaptive overlapping grids

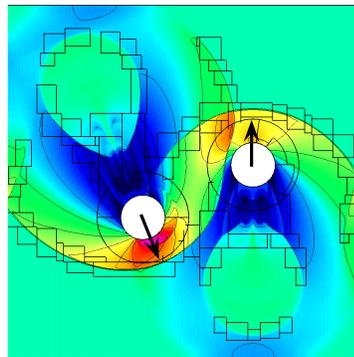
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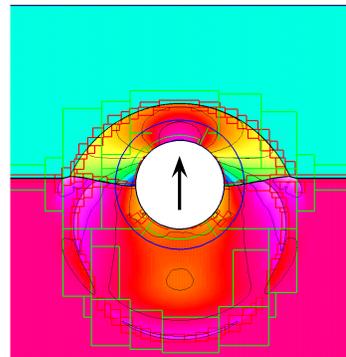
## Current work: moving geometry and AMR

- ◇ Refinement grids move with the corresponding base grid.
- ◇ The AMR regrid step is performed at the start of the step, followed by the grid movement.

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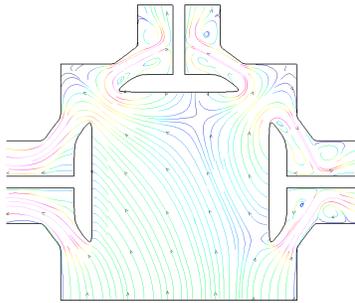
Moving cylinders (Euler)



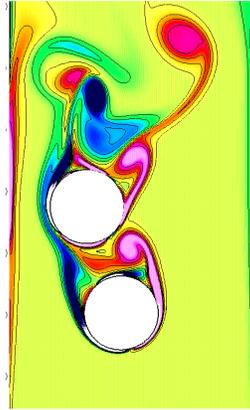
Cylinder moved by a shock (Euler)

## Current work: moving geometry

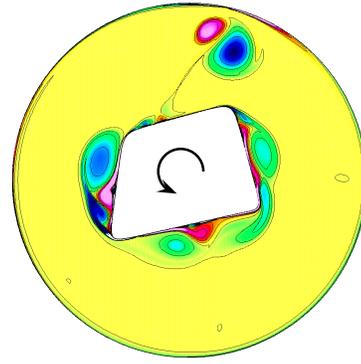
- ◇ The governing equations are written in the moving coordinate system
- ◇ Support for (1) specified motion, (2) rigid-body motion with forces and torques determined from the flow.
- ◇ The grids are moved at every time step and the interpolation points are recomputed.



Moving valves (INS)



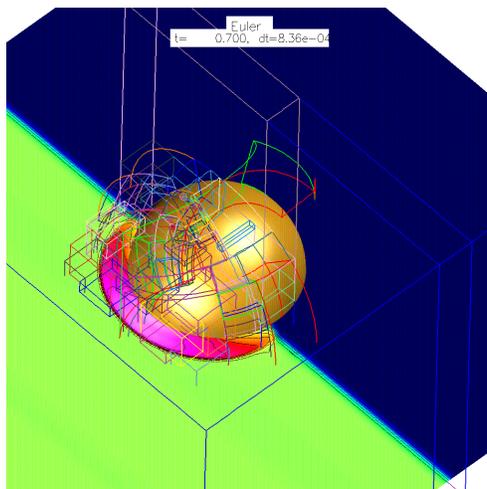
Falling cylinders (INS)



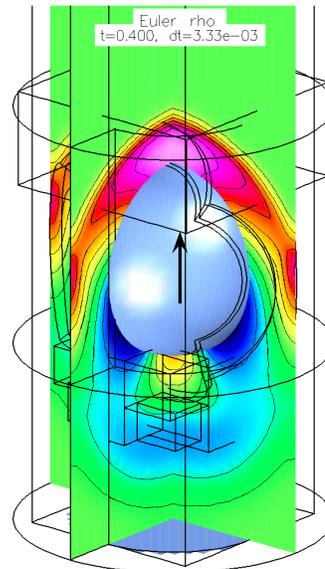
Rotating body (INS)

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## Current work: three-dimensions



Shock hitting a sphere (Euler)



Sphere moving in a tube with AMR (Euler)

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