An Overture Overview

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Current Overture developers

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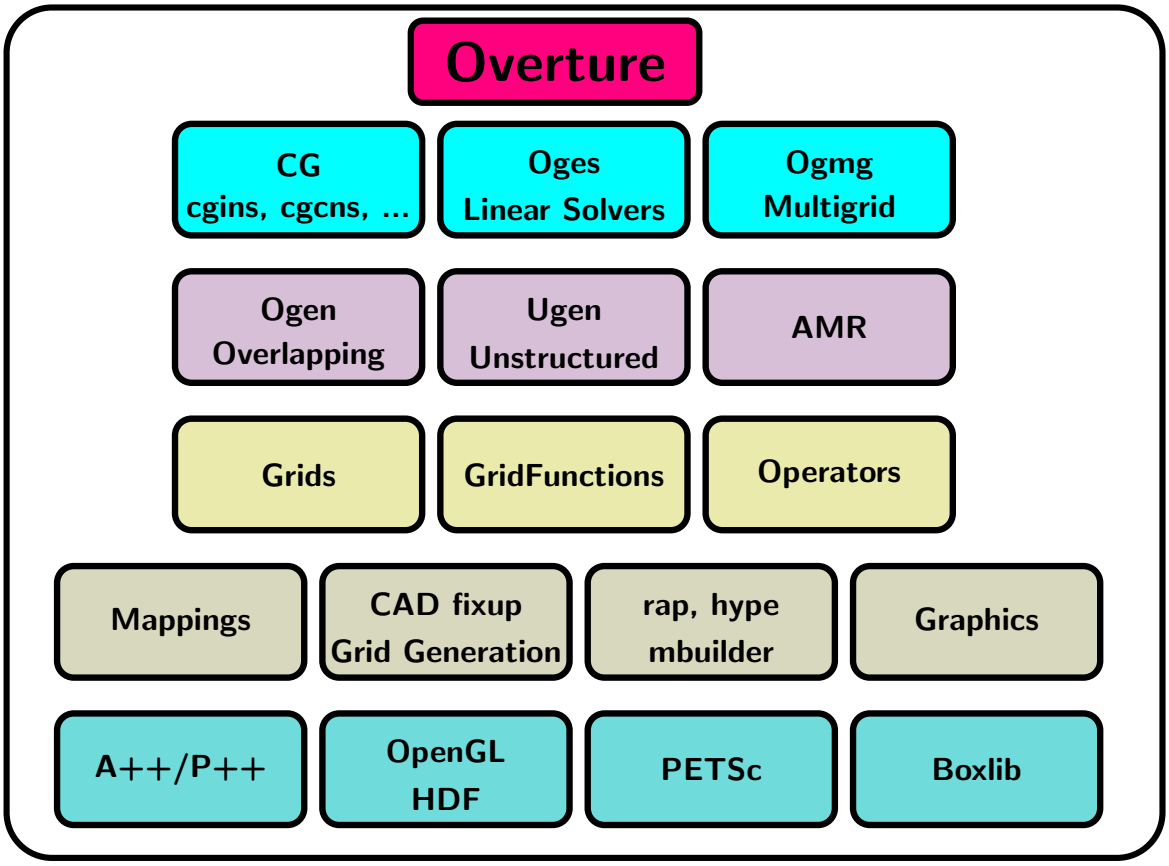
Collaborators

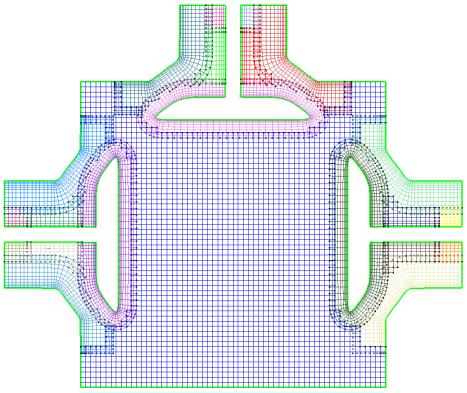
Don Schwendeman (RPI),
Tom Hagstrom (UNM),
Nikos Nikiforakis (U. Cambridge),
Jeff Banks (SNL)

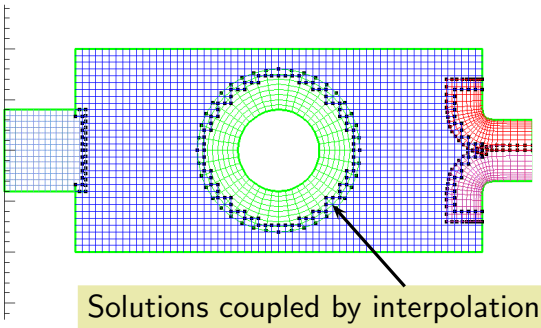
Overture is toolkit for solving partial differential equations on structured, overlapping and hybrid grids.

Key features:

- provides a high level C++ 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 (AMR).
- extensive grid generation capabilities.
- CAD fixup tools (for CAD from IGES files).
- interactive graphics and data base support (HDF).
- PDE solvers built upon Overture include: (*new* for version 22)
  - cgins: incompressible Navier-Stokes with heat transfer.
  - cgcns: compressible Navier-Stokes, reactive Euler equations.
  - cgmp: multi-physics solver.
  - cgmx: time domain Maxwell's equations solver.

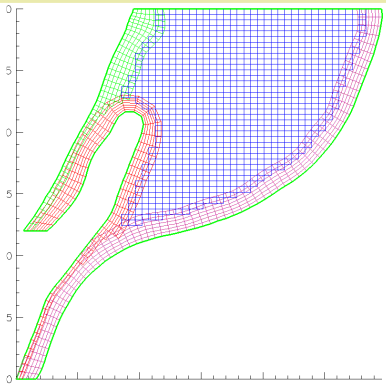


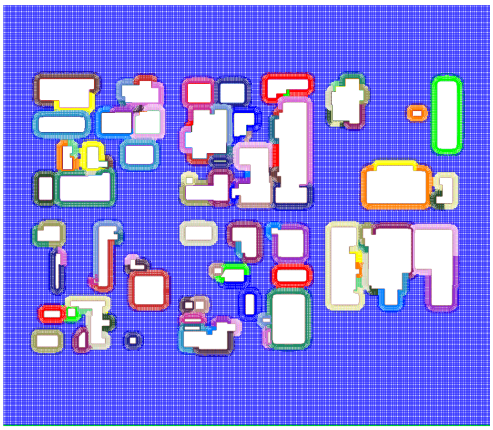




Solutions coupled by interpolation

Sample 2D overlapping grids





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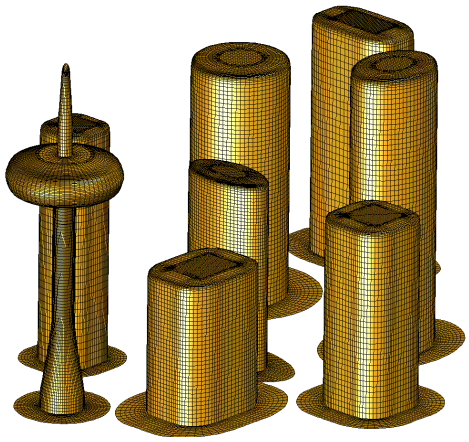
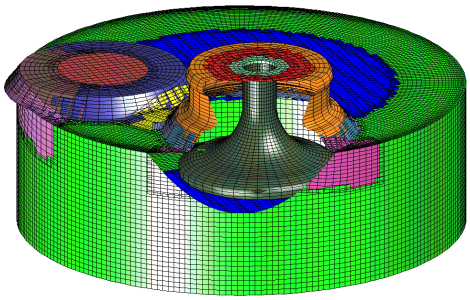
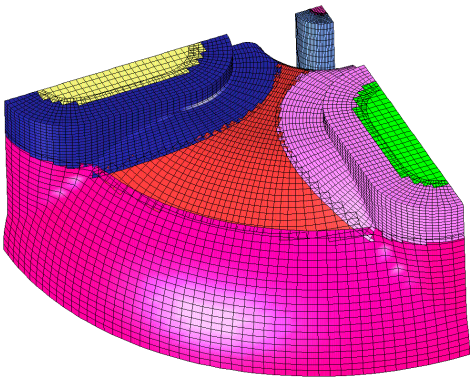
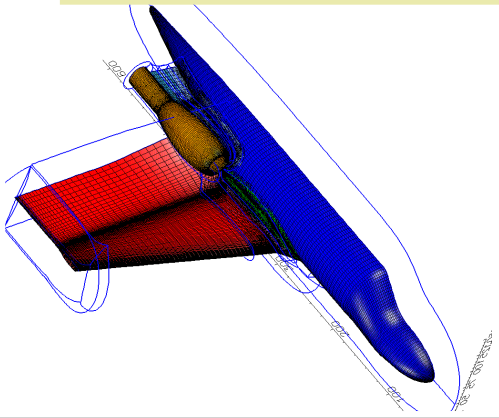




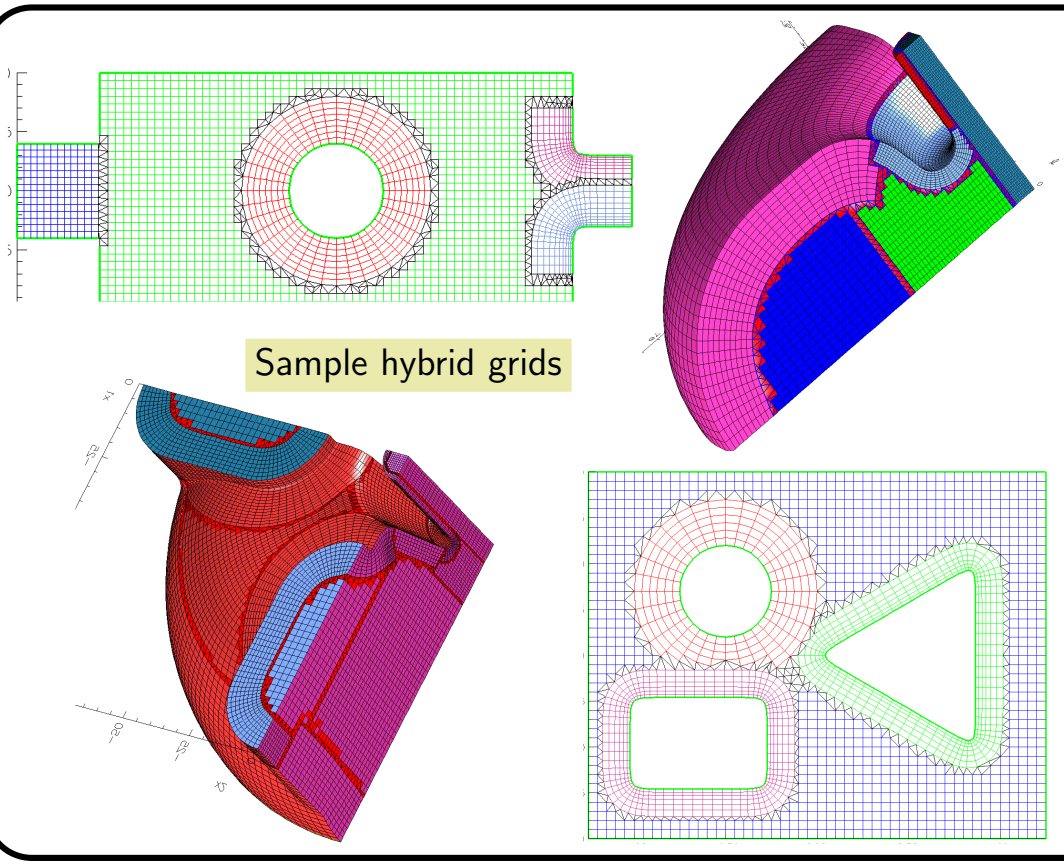
Sample 3D overlapping grids



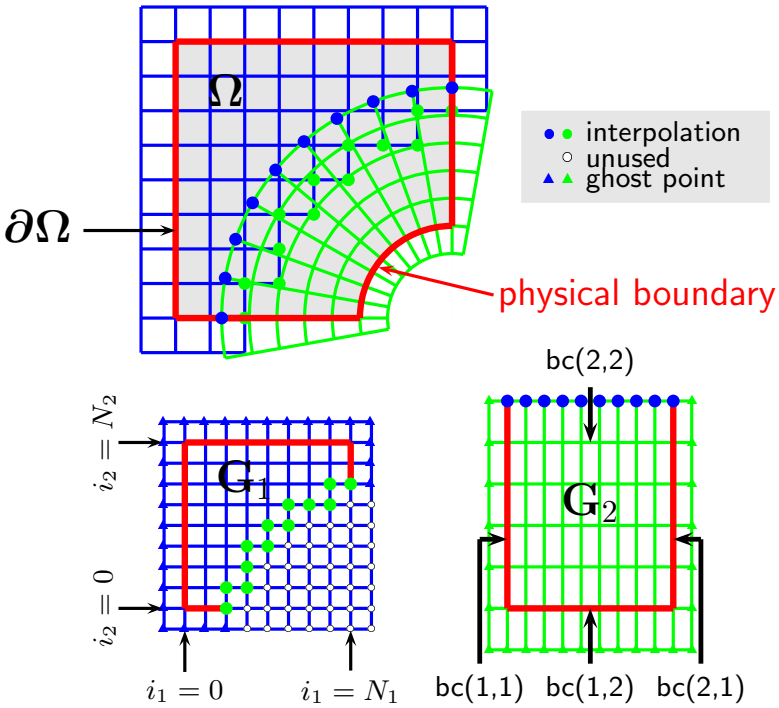


6

Sample hybrid grids



Components of an Overlapping Grid



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

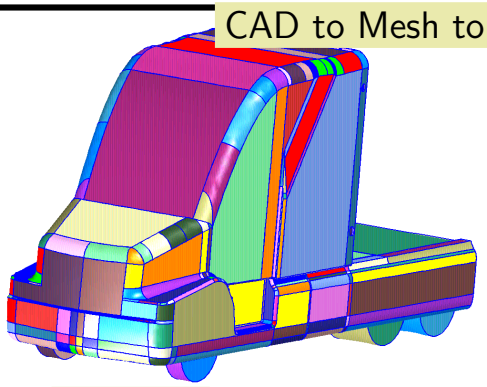
Solve $u_t + au_x + bu_y = \nu(u_{xx} + u_{yy})$

```
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();
}
```

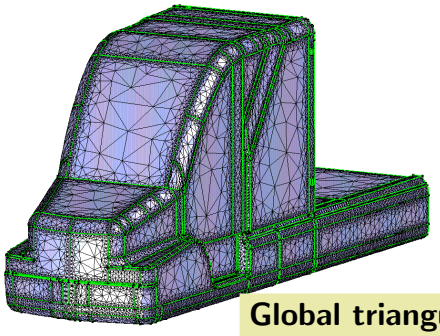

Current Projects with Overture

- Support for multi-physics problems, for example:
  - incompressible fluid flow coupled to solid heat transfer
  - compressible fluid flow coupled to solid mechanics
- Electromagnetics: time dependent Maxwell's equations.
- Parallel adaptive mesh refinement and parallel overlapping grid generation.
- Parallel multigrid algorithms for overlapping grids.
- High speed reactive flow with moving grids and AMR (Don Schwendeman (RPI))
- Compressible multiphase flows (Don Schwendeman (RPI))
- Compressible multi-material flows (Jeff Banks (SNL))
- Compressible axisymmetric flow with swirl (Kyle Chand)
- Compressible flow with ice formation (Graeme Leese, U. Cambridge).
- Einstein field equations (Philip Blakely, U. Cambridge)
- Flow on the surface of the eye (Kara Maki, U. Delaware).

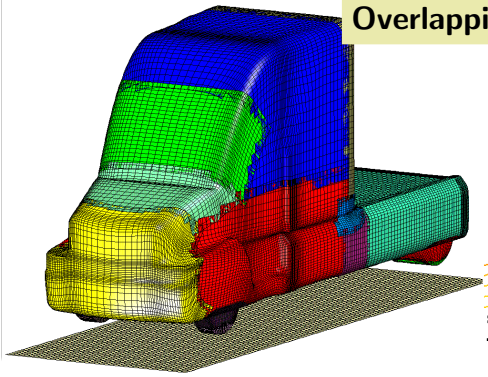
CAD to Mesh to Solution with Overture



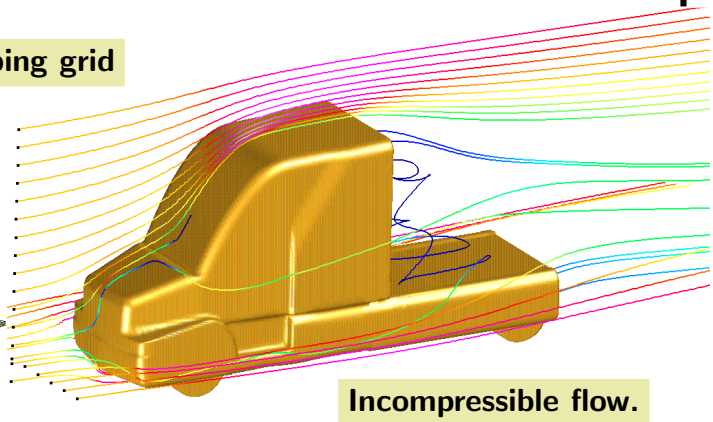
Cad fixup



Global triangulation

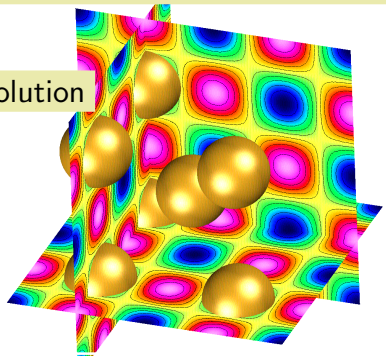


Overlapping grid

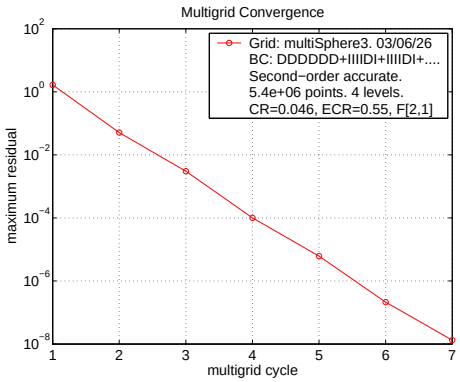


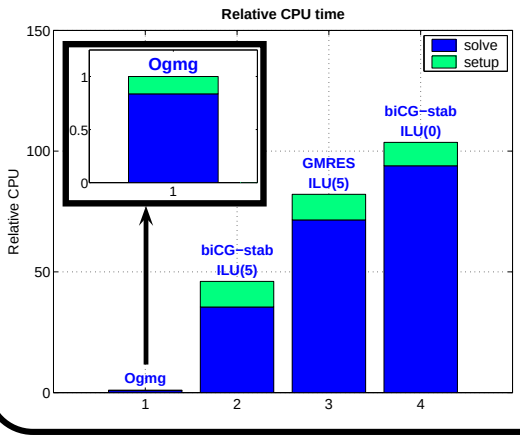
Incompressible flow.

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



solution

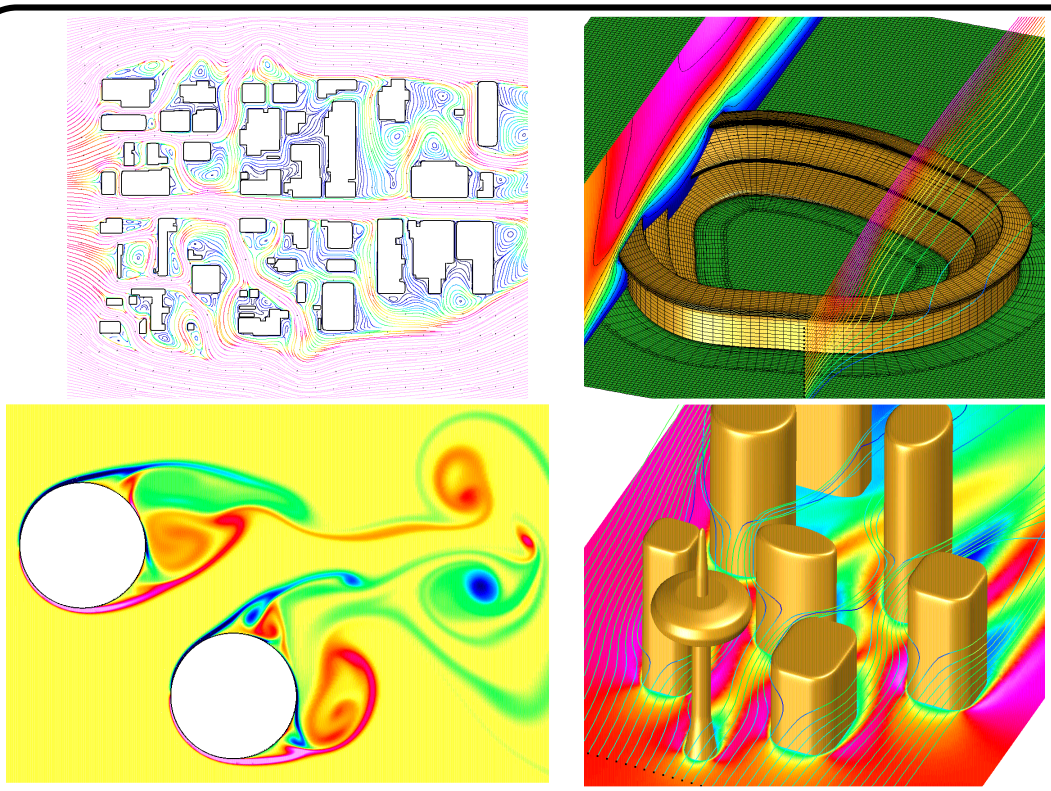




Mesh independent convergence rates

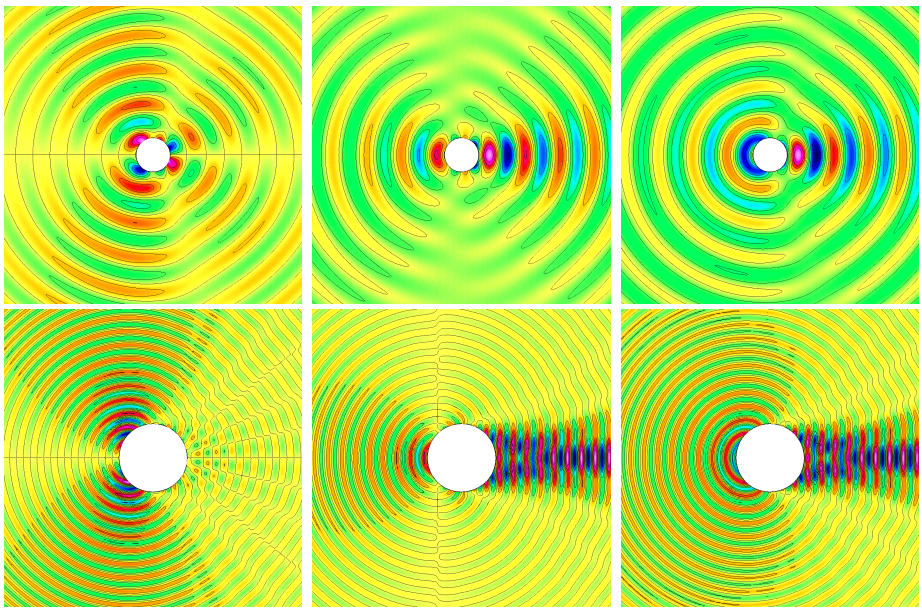
New adaptive MG for overlapping grids.

In comparison to Krylov solvers multigrid is an order of magnitude faster and uses an order of magnitude less storage



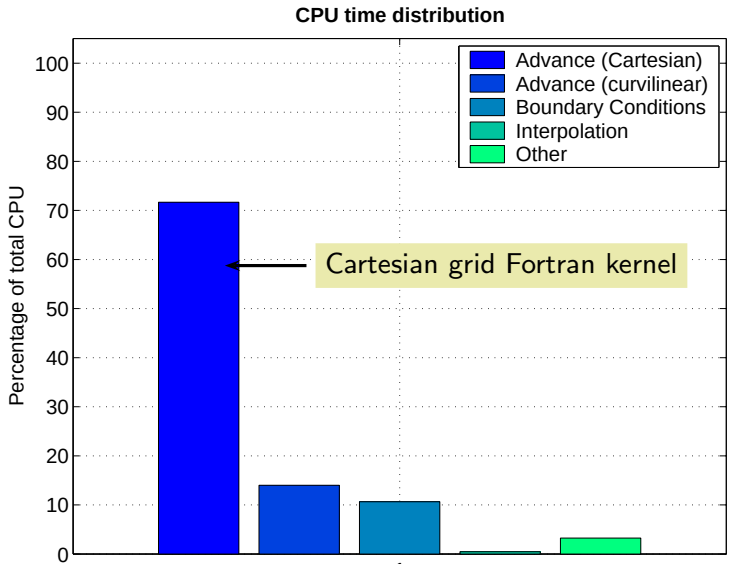
Incompressible flow computations with cgins.

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 $ka = 5/2$

Performance of overlapping grid codes can approach that of Cartesian grid codes.

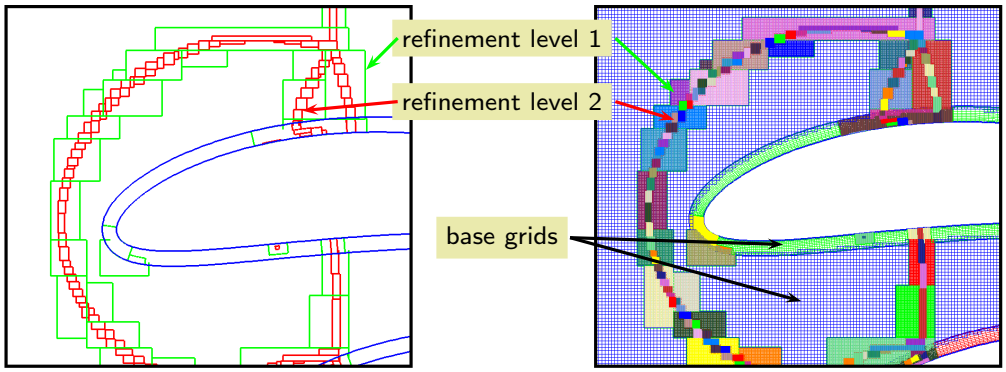


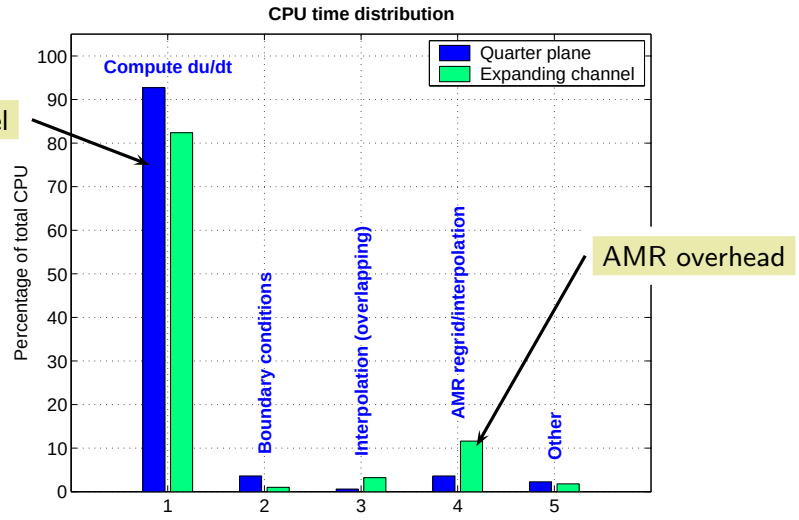
Performance of the Maxwell solver (serial).

Two-dimensions, 3.8 million grid-points.

Block Structured Adaptive Mesh Refinement and Overlapping Grids

- ♢ Refinement patches are generated in the parameter space of each component grid (base grid).
- ♢ Refinement patches are organized in a hierarchy of *refinement levels*.
- ♢ Error estimators determine where refinement is needed.
- ♢ AMR grid generation (Berger-Rigoutsos algorithm) builds refinement patches based on the error estimate.
- ♢ refinement grids may interpolate from refinement grids of different base grids.
- ♢ The key issue is efficiency.





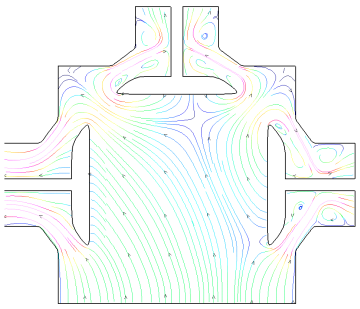
	Quarter plane	Expanding channel
time steps	12418	21030
seconds per step	14.94	13.96
grids (min,ave,max)	(2, 57, 353)	(5, 274, 588)
points (min,ave,max)	(2.0e5, 9.2e5, 1.9e6)	(1.2e5, 6.4e5, 1.3e6)

Overlapping grid AMR performance on two detonation problems.

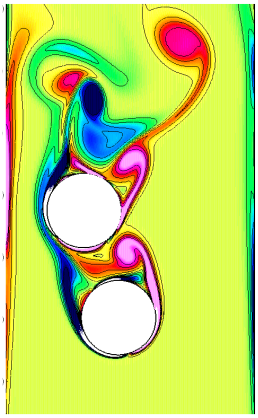
17

Moving Overlapping Grids

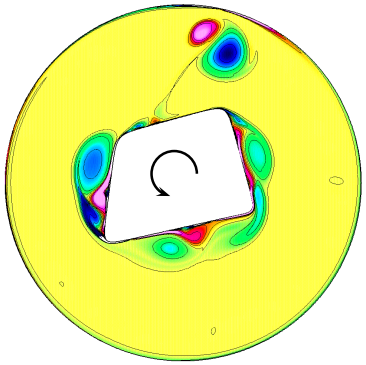
- ♢ Boundary fitted component grids are used to discretize each moving body.
- ♢ Grids move at each time step according to some governing equations.
- ♢ Overlapping connectivity information is updated by Ogen (interpolation points, discretization points, unused points).
- ♢ Solution values at **exposed points** are interpolated at previous time levels.
- ♢ Issue: Detection and treatment of collisions – elastic/in-elastic collisions
- ♢ Issue: Bodies that get very close – how should the grids interpolate



Moving valves (INS)



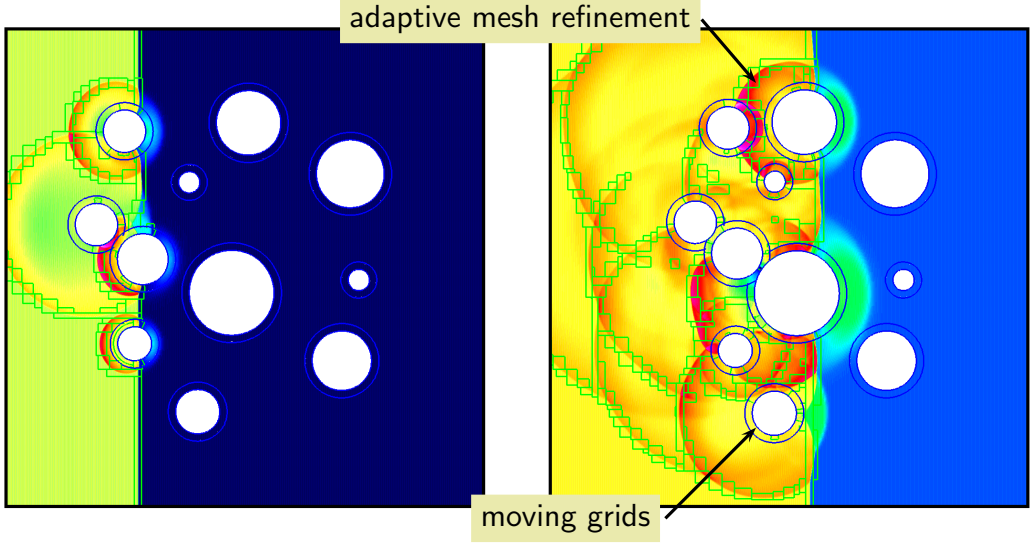
Falling cylinders (INS)



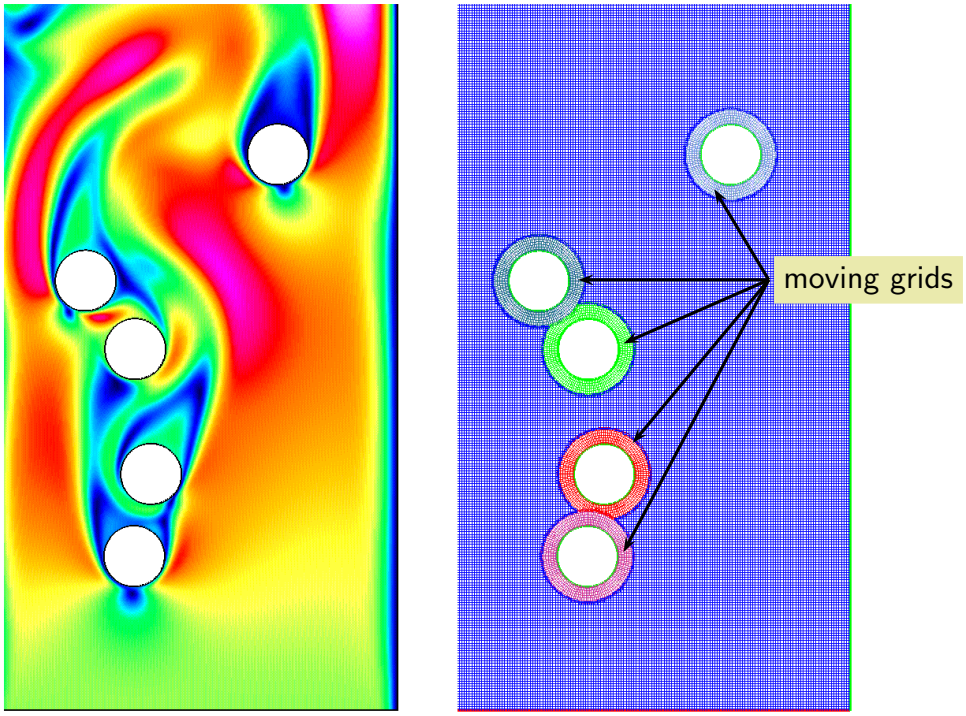
Rotating body (INS)

18

Moving geometry and AMR

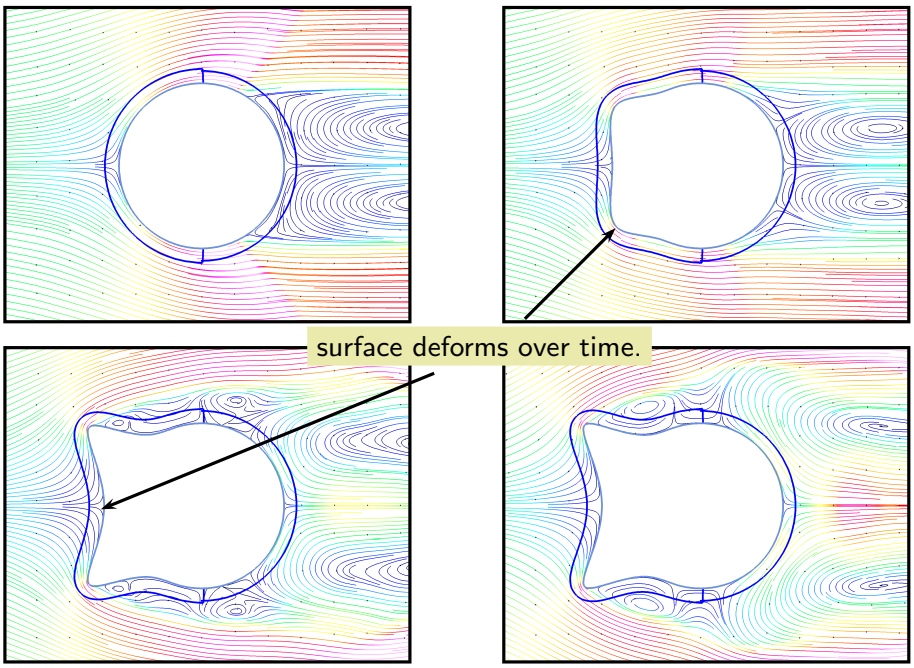


A shock hitting a collection of cylinders (density).



Falling cylinders in an incompressible flow

Modeling Deforming Geometry with Overlapping Grids

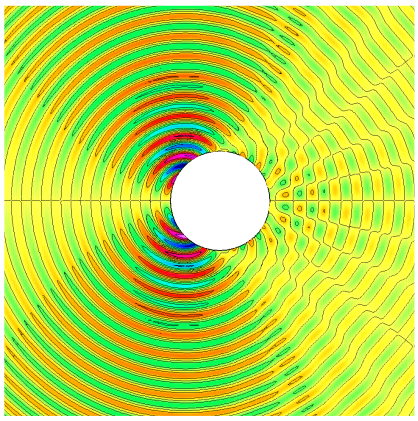


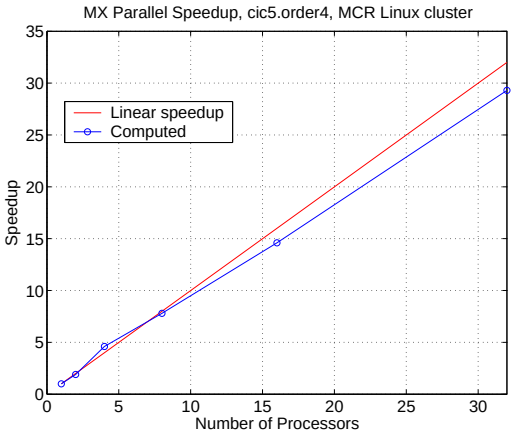
Streamlines of a compressible flow around a deforming boundary.

The model for distributed parallel computing in Overture

- ♢ Grids can be distributed across one or more processors.
- ♢ Distributed parallel arrays using P++ (K. Brislawn, B. Miller, D. Quinlan)
- ♢ P++ uses Multiblock PARTI (A. Sussman, G. Agrawal, J. Saltz) for block structured communication with MPI (ghost boundary updates, copies between different distributed arrays)
- ♢ A special parallel overlapping grid interpolation routine is used for overlapping grid interpolation.

Parallel scaling of the Maxwell solver



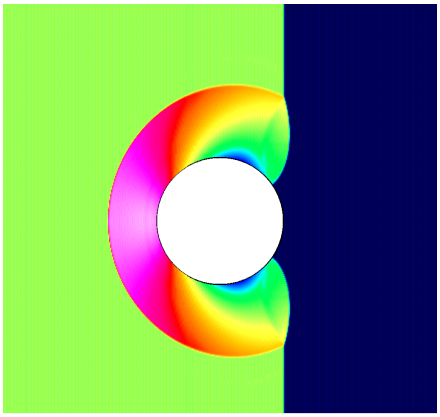


Fourth-order accurate

2D scattering from a cylinder

Fixed size problem, 3.8 million grid-points

Solving the Euler equations, parallel results



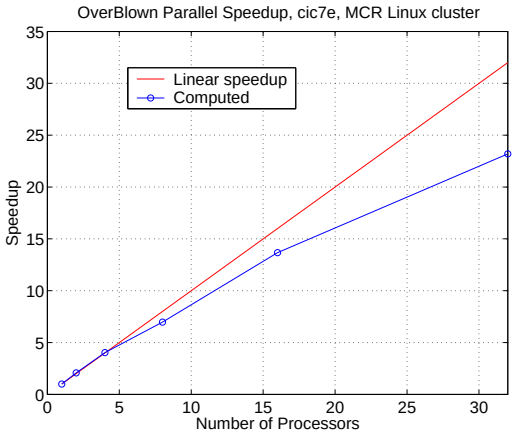
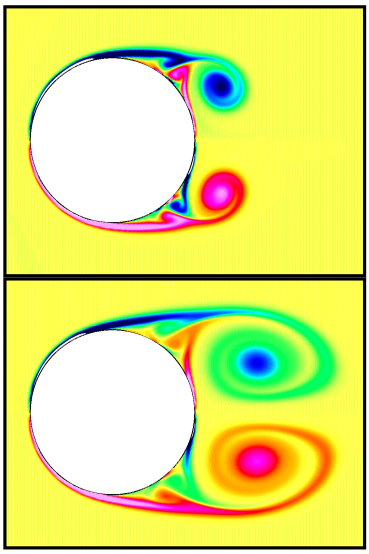


Figure 1: Left: the computation of a shock hitting a cylinder (density). Right: parallel speedup for this problem, keeping the problem size fixed (4 Million grid points), on a linux cluster (Xeon processors).

Incompressible Navier-Stokes, parallel results



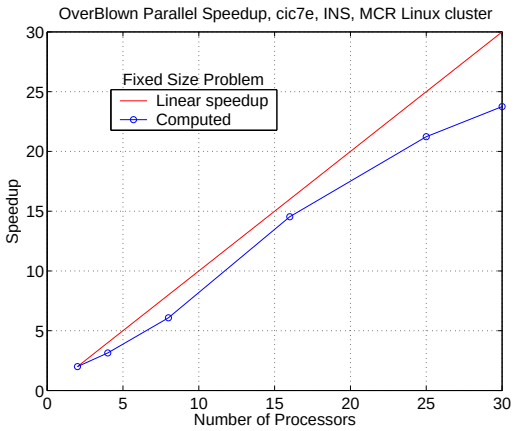
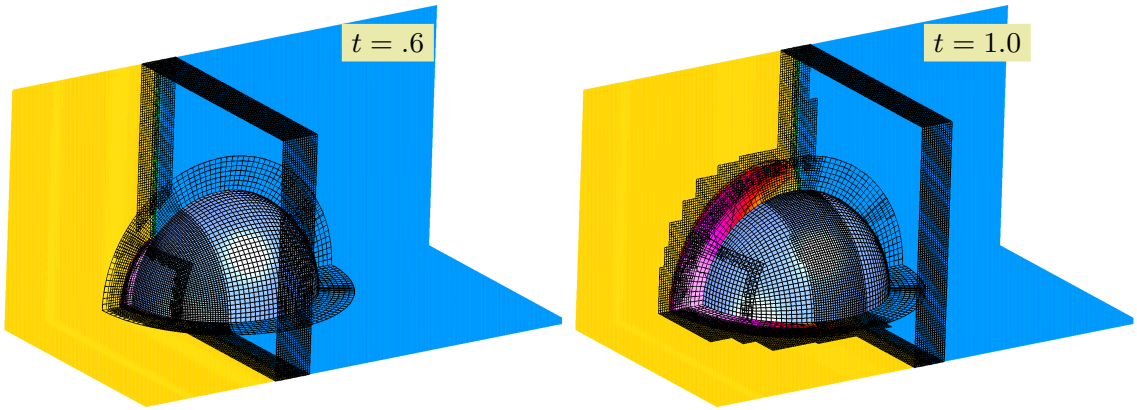


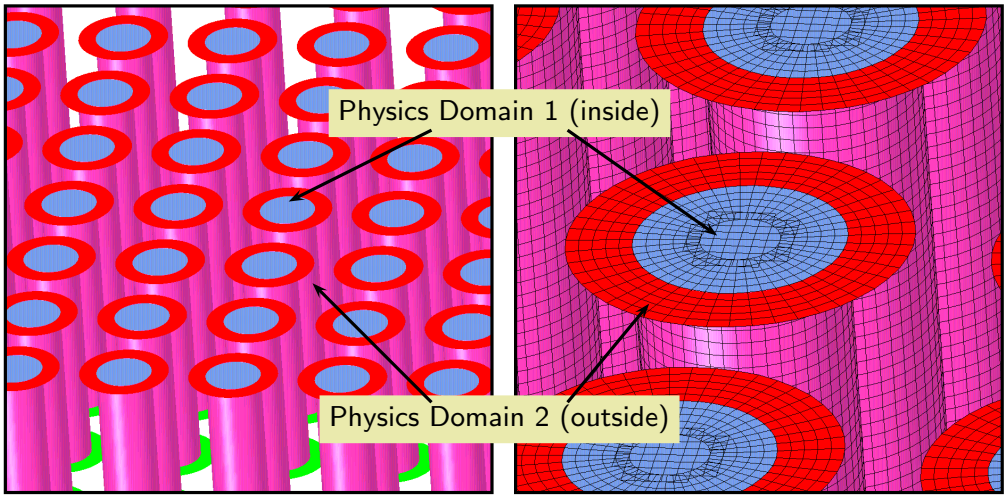
Figure 2: Left: impulsively started cylinder in an incompressible flow (vorticity). Right: parallel speedup keeping the problem size fixed (4 Million grid points), on a linux cluster (Xeon processors). The pressure equation is solved with algebraic multigrid (Hypre).

Parallel Adaptive Mesh Refinement on Overlapping Grids



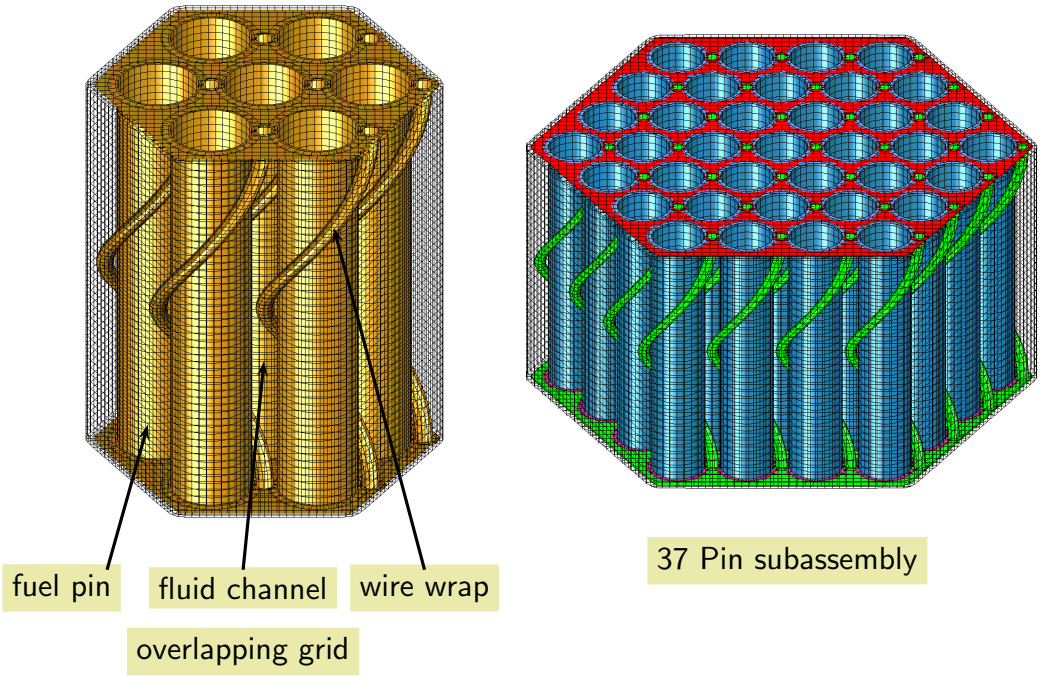
A shock hitting a sphere.

Multi-Physics and Multi-Material Applications

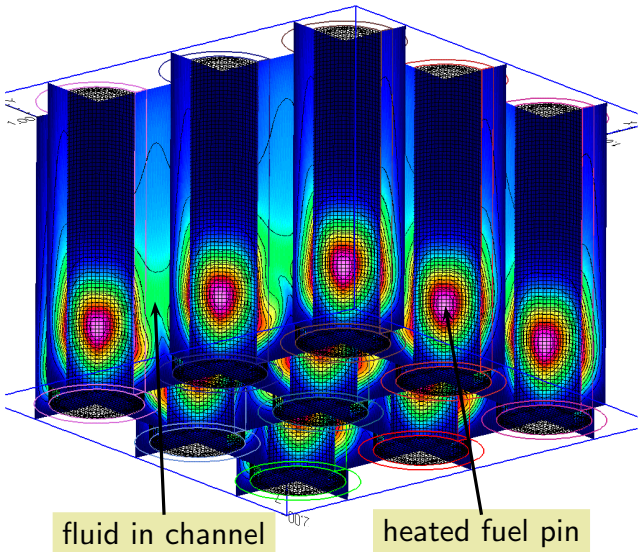


An overlapping grid for a lattice of cylinders modeling a photonic bad gap device (Maxwell's equations) or a heat exchanger (fluid-flow solid-heat transfer).

Subassembly Grids for Pins with Wire Wraps

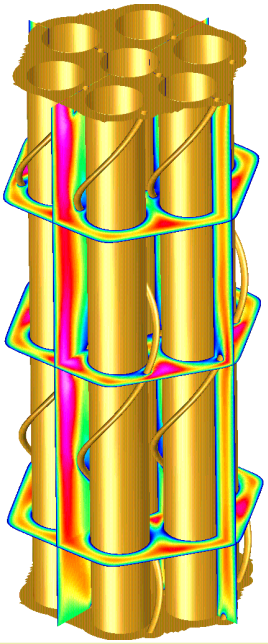


Subassembly Thermal-Hydraulics Flow



fluid-solid conjugate heat transfer

flow



T-H flow, 7 pins with wires