An Overture Overview

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Downloading Overture and the CG (Composite Grid) suite of PDE solvers.

Overture and CG are freely available from the web:

www.llnl.gov/CASC/Overture

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Current Overture developers

Kyle Chand
Bill Henshaw

Major Contributors

Don Schwendeman (RPI),
Jeff Banks (LLNL).

Overture: a toolkit for solving partial differential equations (PDEs) on overlapping grids.

Top three reasons for using Overture:

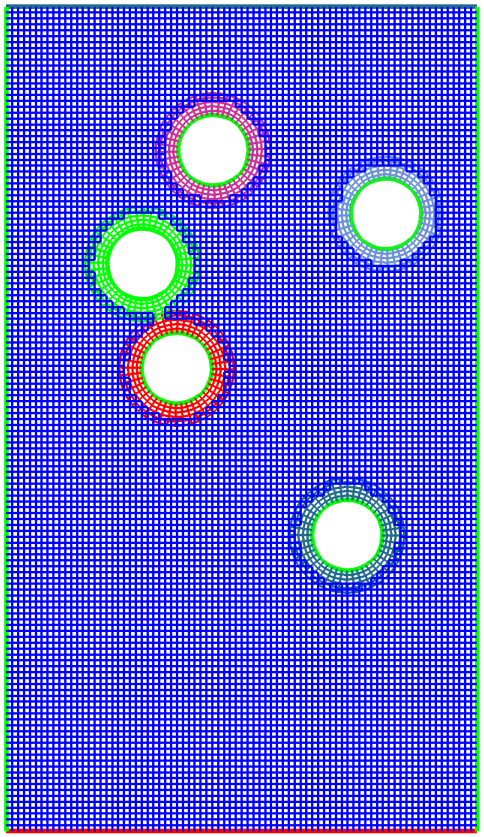
1. You need to efficiently solve a PDE on a complex geometry.
2. You need to solve a PDE on a moving geometry.
3. You need to generate an overlapping grid.

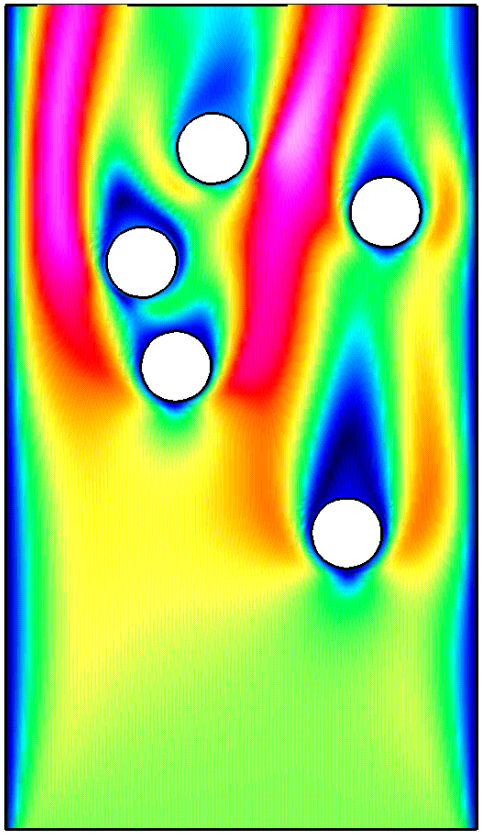
You can

- write your own PDE solver using the capabilities provided by Overture.
- use (or change) an existing PDE solver from the CG suite.

What are overlapping grids and why are they useful?

Overlapping grid: a set of structured grids that overlap.





- Overlapping grids can be rapidly generated as bodies move.
- High quality grids under large displacements.
- Cartesian grids for efficiency.
- Efficient for high-order accurate methods.

Key Features of Overture

- high level C++ interface for rapid prototyping of PDE solvers.
- built upon optimized C and fortran kernels.
- 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).

Overture

Oges
Linear Solvers

Ogmg
Multigrid

Ogen
Overlapping

Ugen
Unstructured

AMR

Grids

GridFunctions

Operators

Mappings

CAD fixup
Grid generation

rap, hype
mbuilder

Graphics

A++/P++
array class

OpenGL
HDF

PETSc

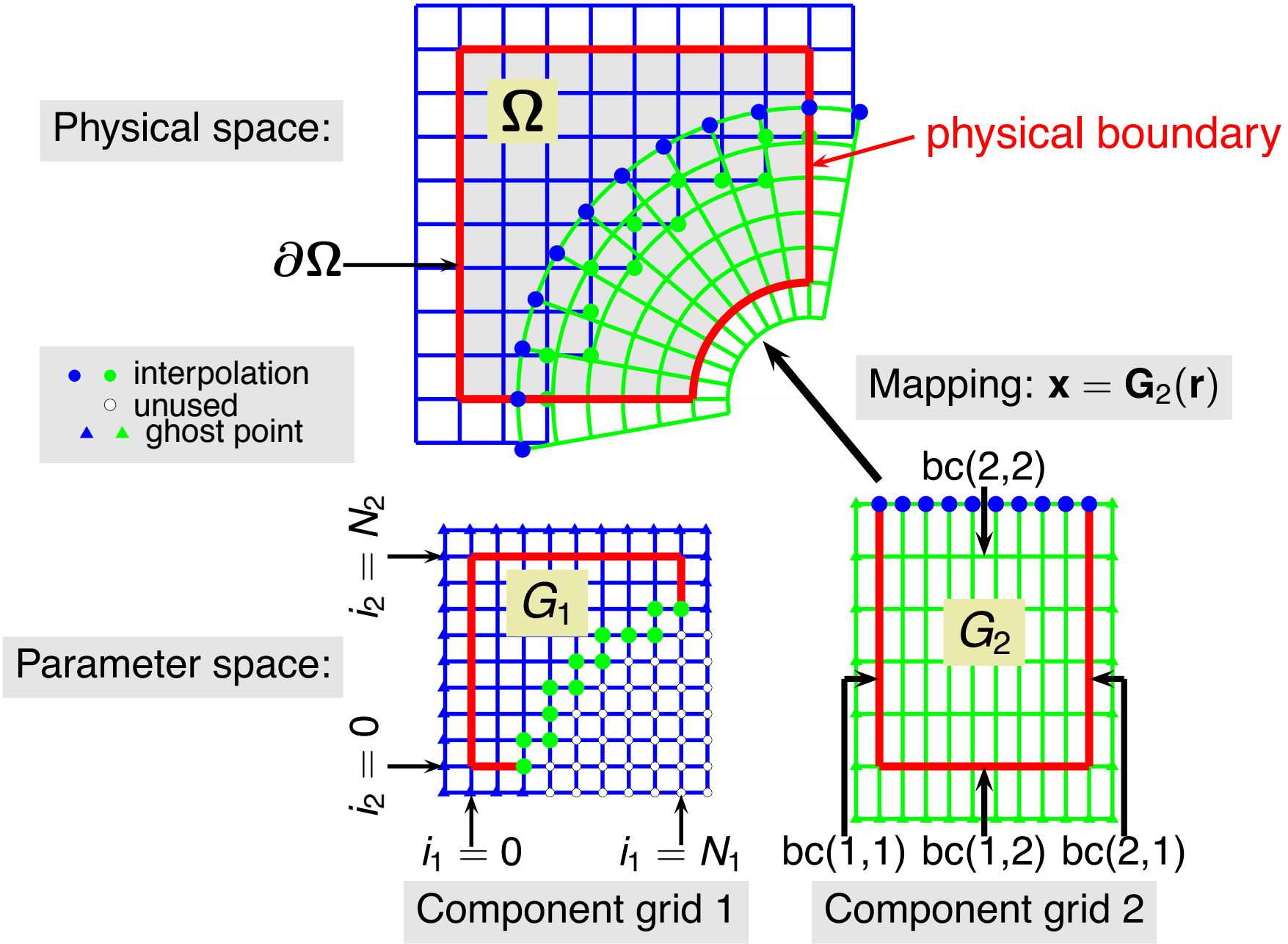
Boxlib

CG: Composite Grid PDE solvers built with Overture

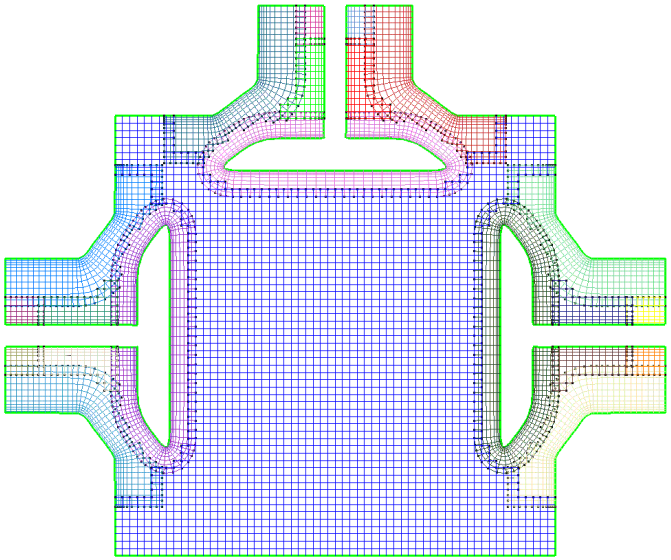
Different PDE solvers in the CG suite:

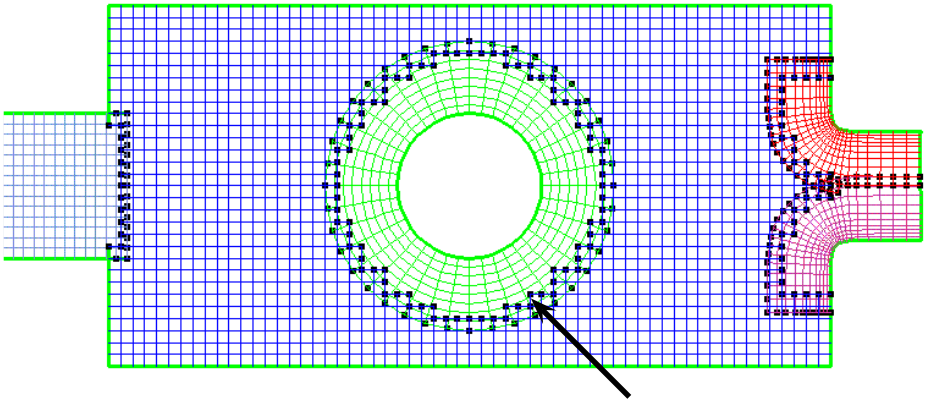
- cgad: advection diffusion equations.
- cgins: incompressible Navier-Stokes with heat transfer.
- cgcns: compressible Navier-Stokes, reactive Euler equations.
- cgmp: multi-physics solver (e.g. conjugate heat transfer).
- cgmx: time domain Maxwell's equations solver.
- cgsm: elastic wave equation (linear elasticity).

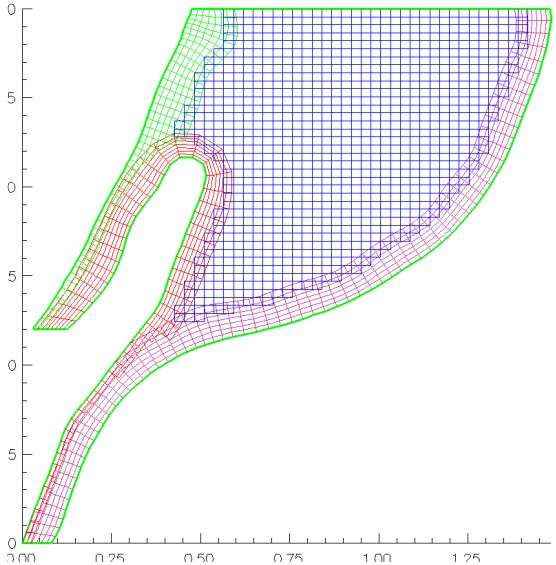
Components of an Overlapping Grid



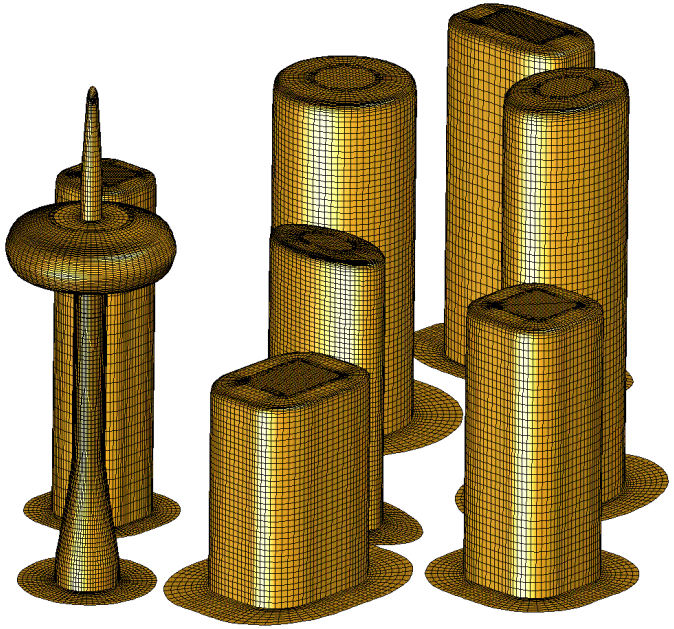
Ogen can be used to build 2D overlapping grids:

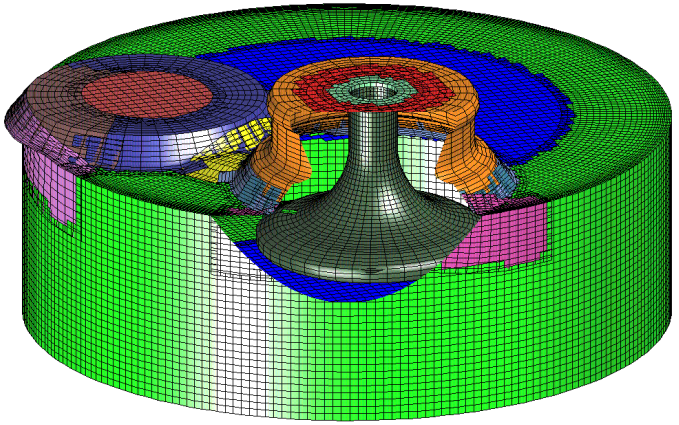


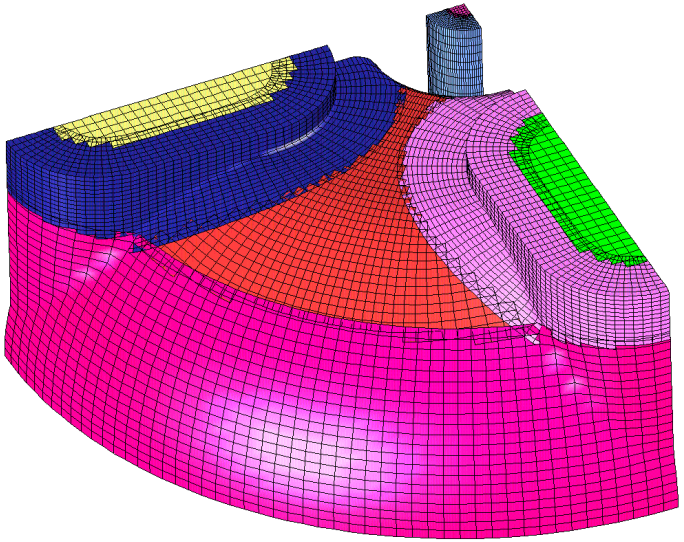


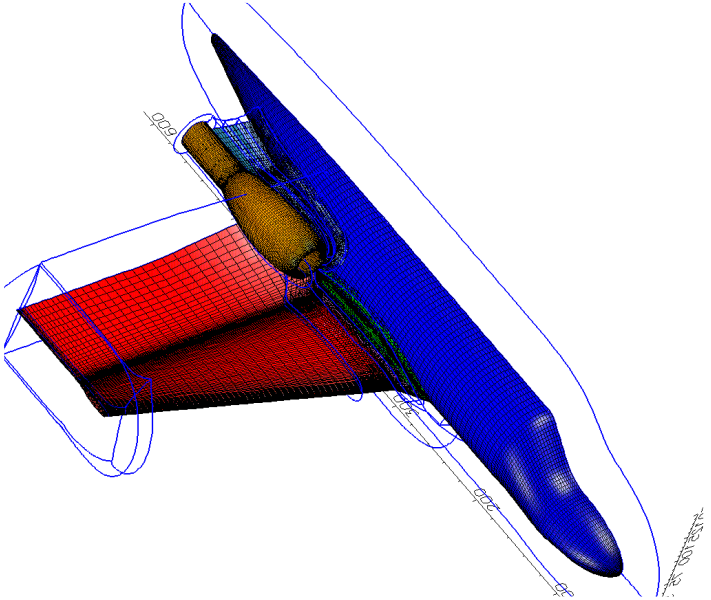


Ogen can be used to build 3D overlapping grids:









Overture supports a high-level C++ interface

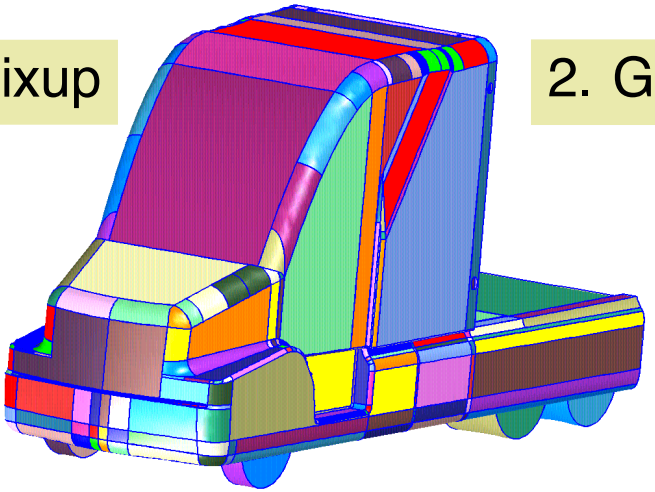
But is built upon mainly Fortran kernels.

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

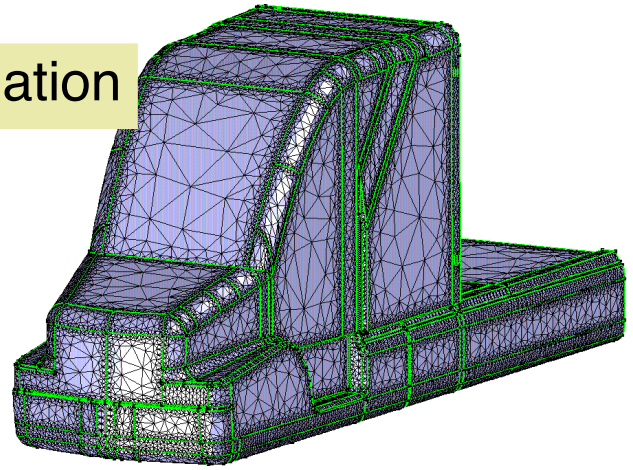
```
CompositeGrid cg; // create a composite grid
getFromADataBaseFile(cg,"myGrid.hdf");
floatCompositeGridFunction u(cg); // create a grid function
u=1.;
CompositeGridOperators op(cg); // operators
u.setOperators(op);
float t=0, dt=.005, a=1., b=1., nu=.1;
for( int step=0; step<100; step++ )
{
   u+=dt*( -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();
}
```

From CAD to Mesh to Solution with Overture

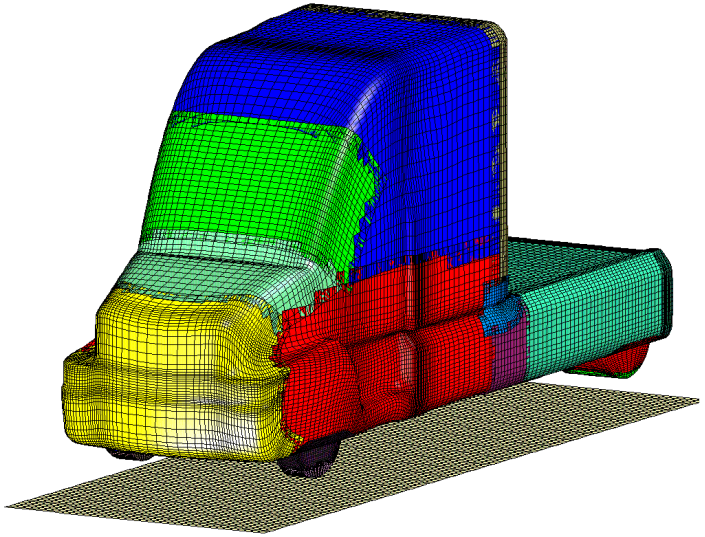
1. Cad fixup



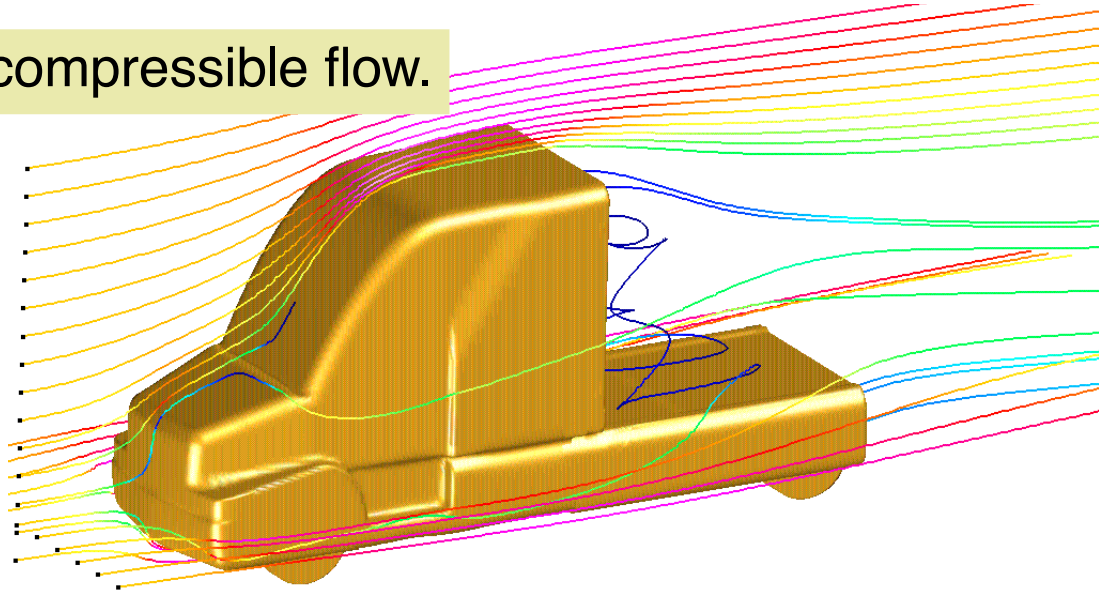
2. Global triangulation



3. Overlapping grid



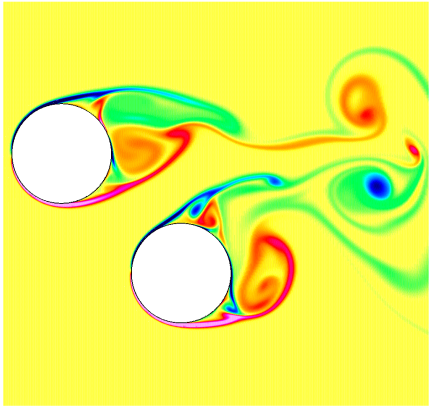
4. Incompressible flow.

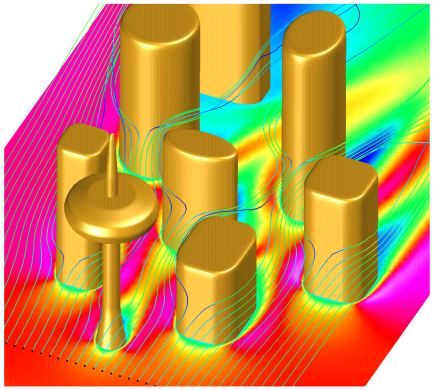


Overture is used by research groups worldwide

- Blood flow in veins with blood clot filters. (Mike Singer, LLNL).
- Pitching airfoils and micro-air vehicles (Yongsheng Lian, U. of Louisville)
- Relativistic hydrodynamics and Einstein field equations (Philip Blakely, Nikos Nikiforakis, U. Cambridge).
- Compressible flow/ice-formation (Graeme Leese, U. Cambridge).
- Tear films and droplets (Rich Braun U. Delaware, Kara Maki UMN).
- High-order accurate subsonic/transonic aero-acoustics (Phillipe Lafon, CNRS, EDF, France).
- Low Reynolds flow for pitching airfoils (D. Chandar, R. Yapalparvi, M. Damodaran, NTU, Singapore).
- Incompressible flow in pumps (J.P. Potanza, Shell Oil, Houston).
- High-order accurate, compact Hermite-Taylor schemes (Tom Hagstrom, SMU, Dallas).

Cgins: incompressible Navier-Stokes solver.



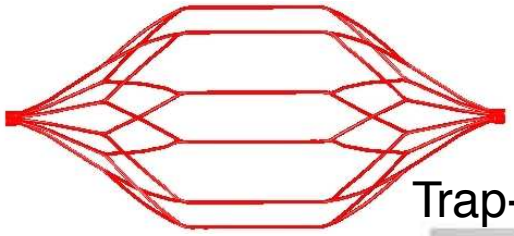


- 2nd-order and 4th-order accurate (DNS).
- support for moving rigid-bodies (not parallel yet).
- heat transfer (Boussinesq approximation).
- semi-implicit (time accurate), pseudo steady-state (efficient line solver), full implicit.

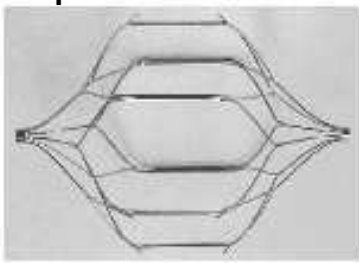
- WDH., *A Fourth-Order Accurate Method for the Incompressible Navier-Stokes Equations on Overlapping Grids*, J. Comput. Phys, **113**, no. 1, (1994) 13–25.

Flow past a blood-clot filter using cgins

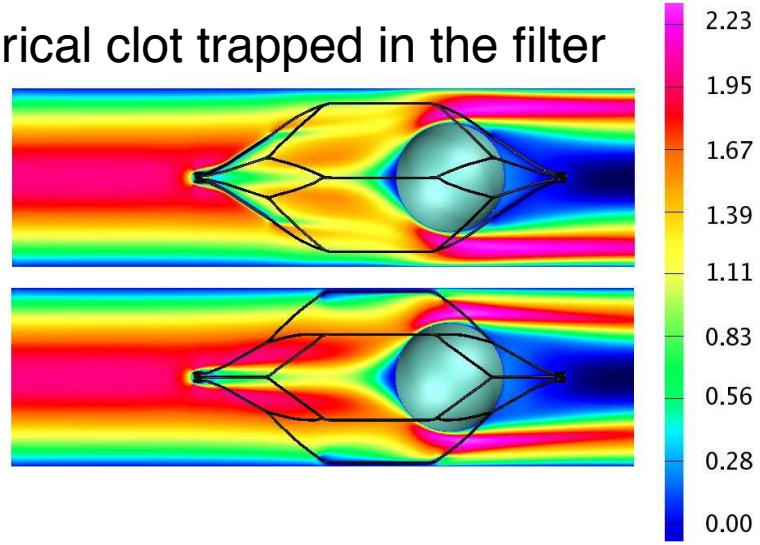
Overlapping grid for the filter



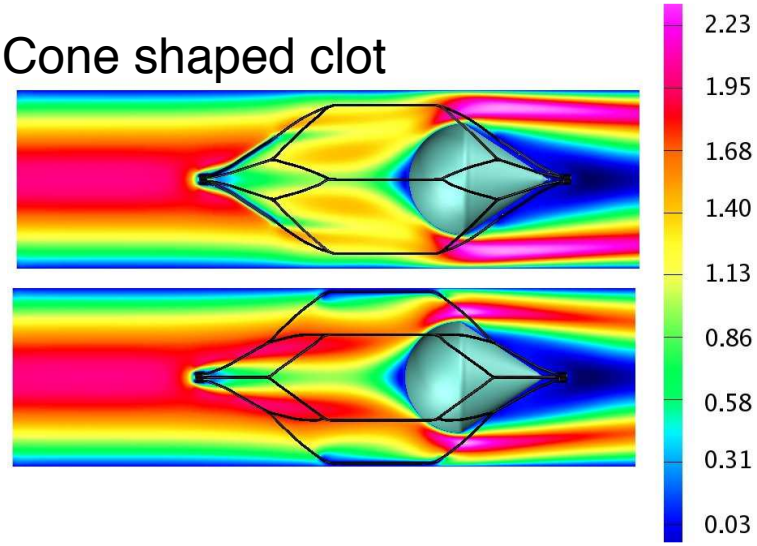
Trap-ease wire filter



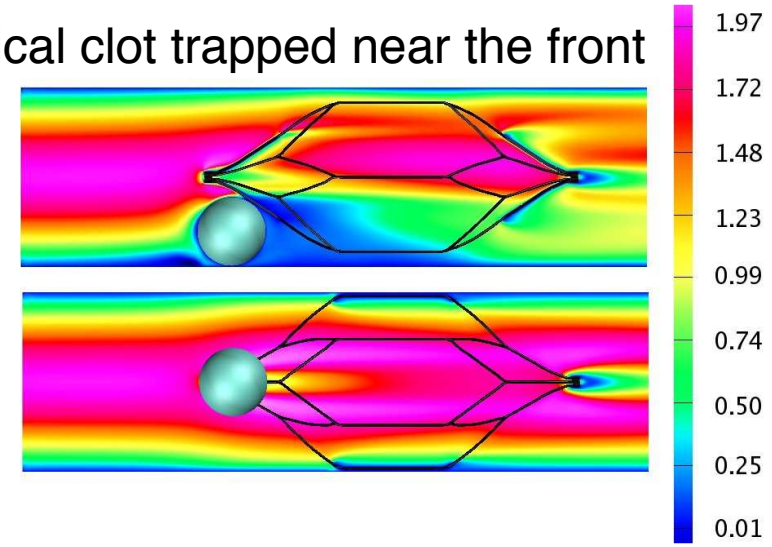
Spherical clot trapped in the filter



Cone shaped clot

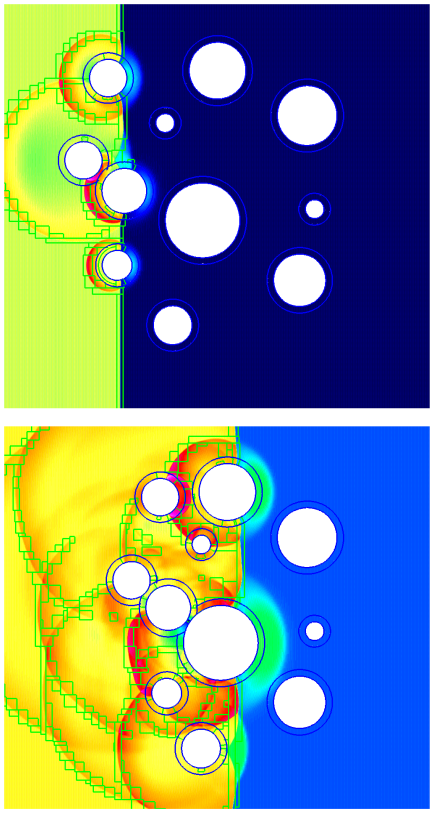


Spherical clot trapped near the front



M.A. Singer, WDH, S.L. Wang, *Computational Modeling of Blood Flow in the Trapease Inferior Vena Cava Filter*, Journal of Vascular and Interventional Radiology, **20**, 2009.

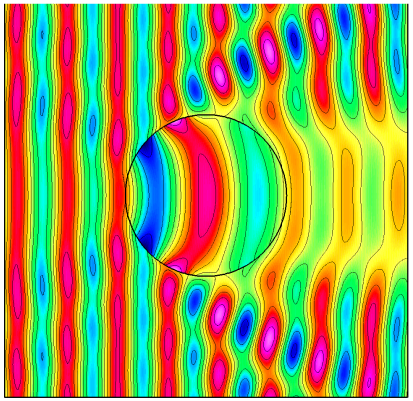
Cgcns: compressible N-S and reactive-Euler.

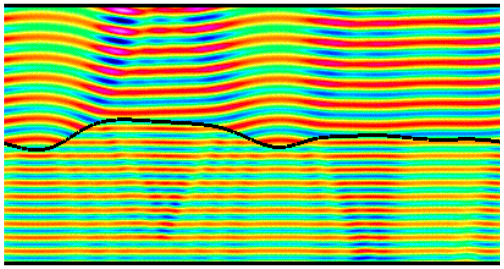


- reactive and non-reactive Euler equations, Don Schwendeman (RPI).
- compressible Navier-Stokes.
- multi-fluid formulation, Jeff Banks (LLNL).
- adaptive mesh refinement and moving grids.

- WDH., D. W. Schwendeman, *Parallel Computation of Three-Dimensional Flows using Overlapping Grids with Adaptive Mesh Refinement*, J. Comp. Phys. **227** (2008).
- WDH., DWS, *Moving Overlapping Grids with Adaptive Mesh Refinement for High-Speed Reactive and Nonreactive Flow*, J. Comp. Phys. **216** (2005).
- WDH., DWS, An adaptive numerical scheme for high-speed reactive flow on overlapping grids, J. Comp. Phys. **191** (2003).

Cgmx: electromagnetics solver.





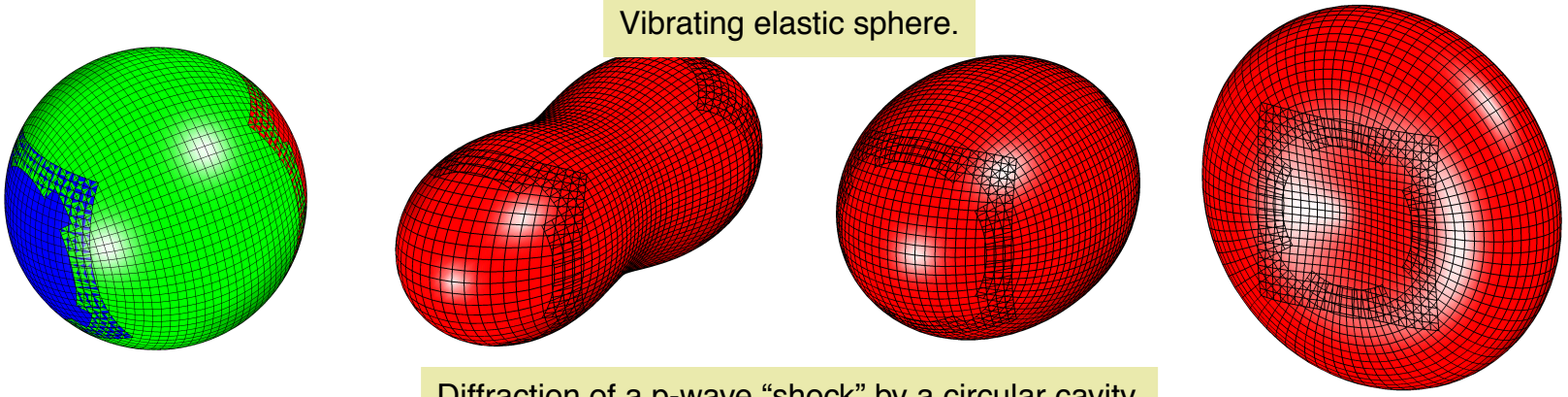
- fourth-order accurate, 2D, 3D.
- Efficient time-stepping with the modified-equation approach
- High-order accurate symmetric difference approximations.
- High-order-accurate *centered* boundary and interface conditions.

• WDH., *A High-Order Accurate Parallel Solver for Maxwell's Equations on Overlapping Grids*, SIAM J. Scientific Computing, **28**, no. 5, (2006).

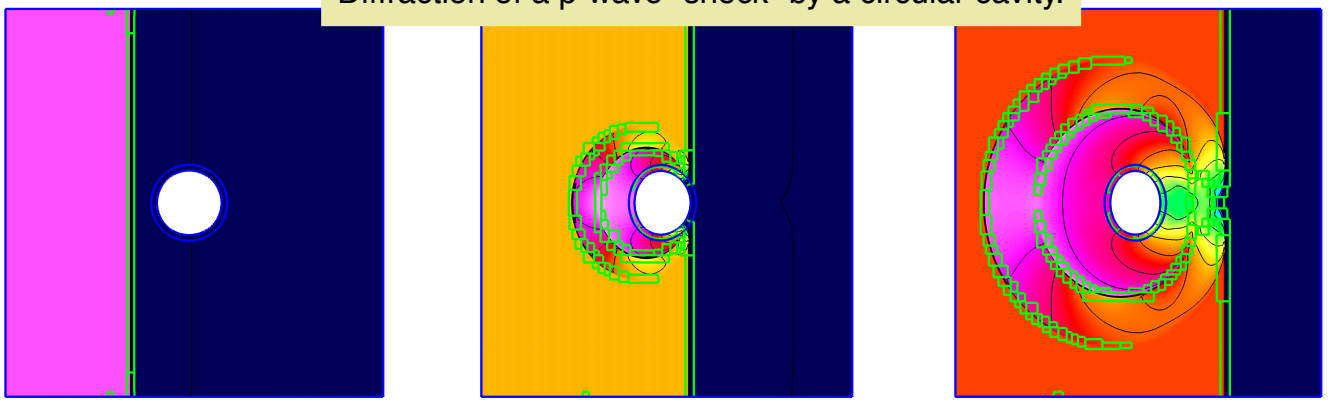
Cgsm: solve the elastic wave equation.

- linear elasticity on overlapping grids, with adaptive mesh refinement,
- conservative finite difference scheme for the second-order system,
- upwind Godunov scheme for the first-order-system.

Vibrating elastic sphere.



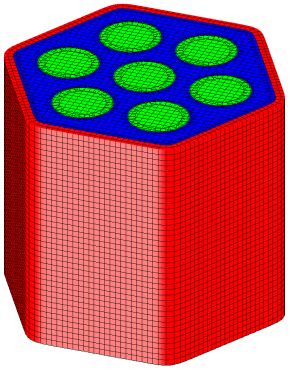
Diffraction of a p-wave “shock” by a circular cavity.

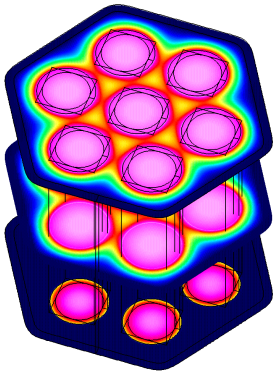


- D. Appelö, J.W. Banks , WDH, D.W. Schwendeman, *Numerical Methods for Solid Mechanics on Overlapping Grids: Linear Elasticity*, LLNL-JRNL-422223, submitted.

Cgmp: a multi-domain multi-physics solver.

Conjugate heat transfer: coupling incompressible flow to heat conduction in solids.

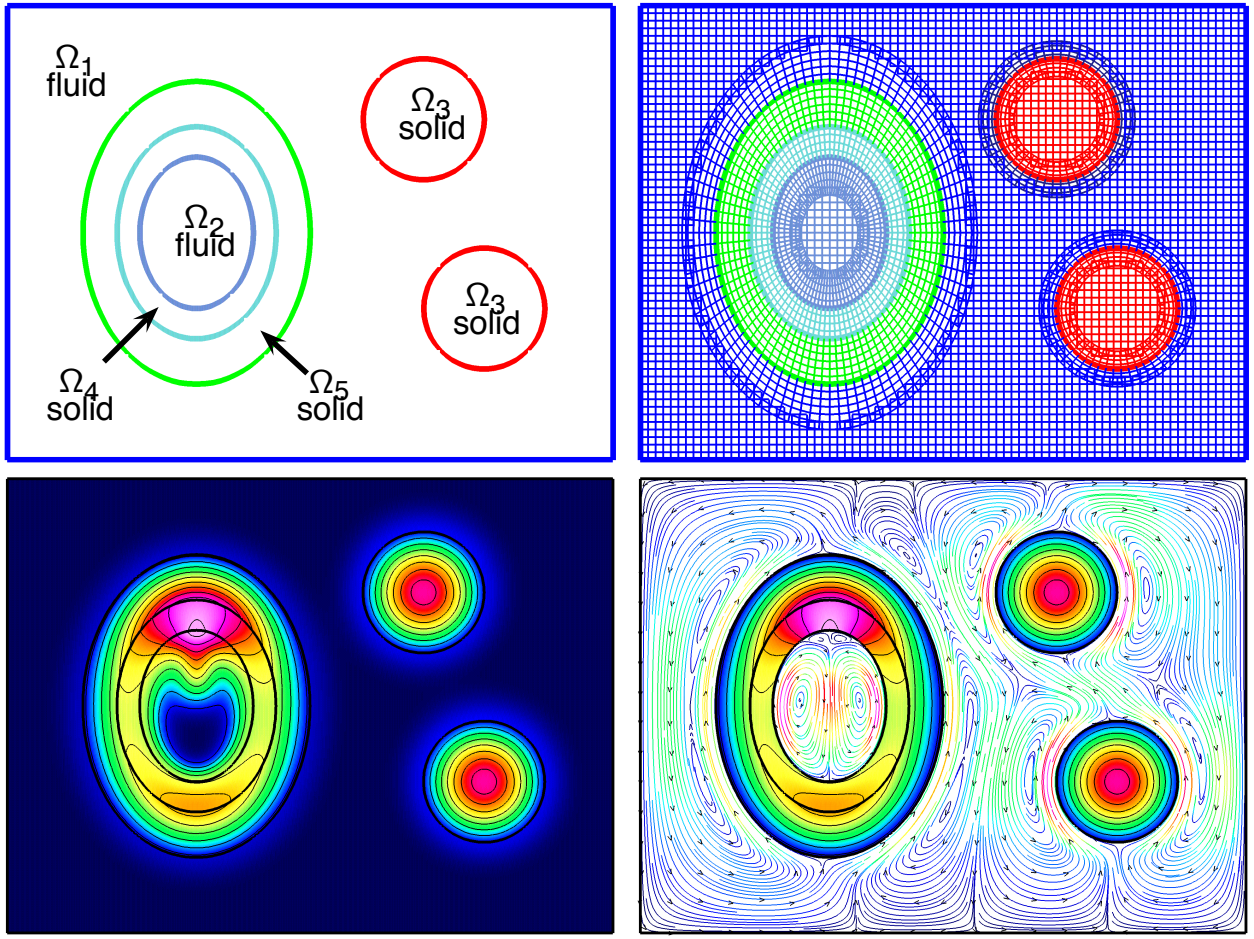




- overlapping grids for each fluid or solid domain,
- a partitioned solution algorithm (separate physics solvers in each sub-domain),
- (cgins) incompressible Navier-Stokes equations (with Boussinesq approximation) for fluid domains,
- (cgad) heat equation for solid domains,
- a key issue is interface coupling.

- WDH., K. K. Chand, *A Composite Grid Solver for Conjugate Heat Transfer in Fluid-Structure Systems*, J. Comput. Phys, 2009.

The multi-domain composite grid approach



The fluid and solid sub-domains, overlapping grids and solution (temperature and streamlines) to a CHT problem. Solvers: cgins (fluid sub-domains), cgad (solid sub-domains), cgmp (coupled problem).

Deforming composite grids (DCG) for Fluid-Structure Interactions (FSI)

Goal: To perform coupled simulations of compressible fluids and deforming solids.

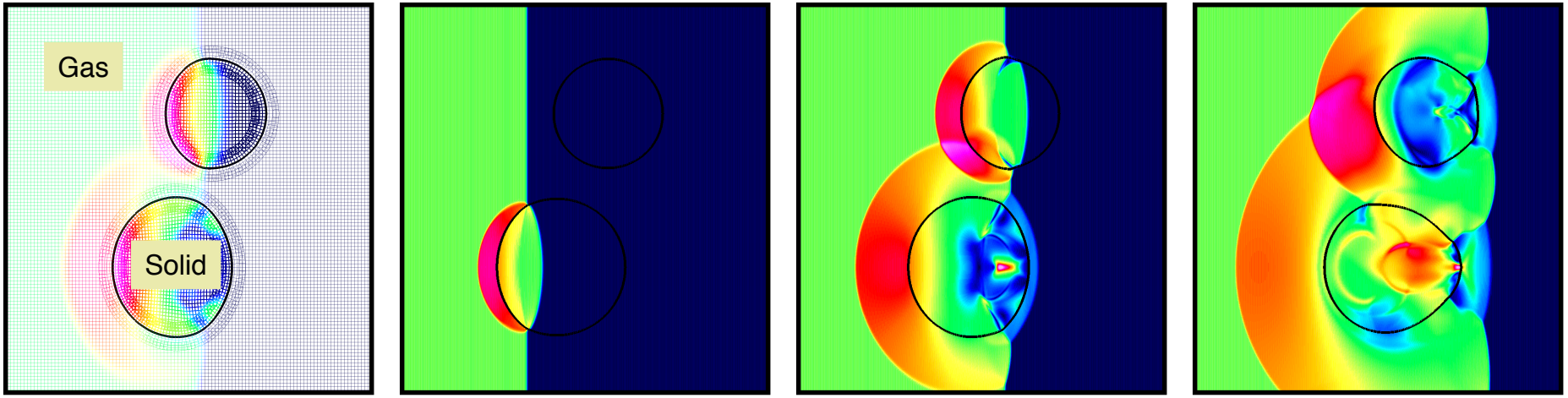
A mixed Eulerian-Lagrangian approach:

- Fluids: general moving coordinate system with overlapping grids.
- Solids : fixed reference frame with overlapping-grids (later: unstructured-grids, or beam/plate models).
- Boundary fitted deforming grids for fluid-solid interfaces.

Strengths of the approach:

- maintains high quality grids for large deformations/displacements.
- efficient structured grid methods (AMR) optimized for Cartesian grids.

A sample FSI-DCG simulation



Mach 2 shock in a gas hitting two elastic cylinders.

- Solve Euler equations in the fluid domains on moving grids.
- Solve equations of linear elasticity in the solid domains.
- Fluid grids at the interface deform over time (hyperbolic grid generator).
- Adaptive mesh refinement (in progress).

Summary.

- Overture: a toolkit for solving PDEs on overlapping grids.
- CG : a suite of PDE solvers for overlapping grids.

www.llnl.gov/CASC/Overture