An Overture Overview

Bill Henshaw

Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
Livermore, CA

Tenth DOE ACTS Workshop,
Berkeley California, 2009

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

Acknowledgments.

Supported by

Department of Energy, Office of Science

MICS Program: Mathematical, Information, and Computational Sciences

LLNL: Laboratory Directed Research and Development (LDRD) program

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:

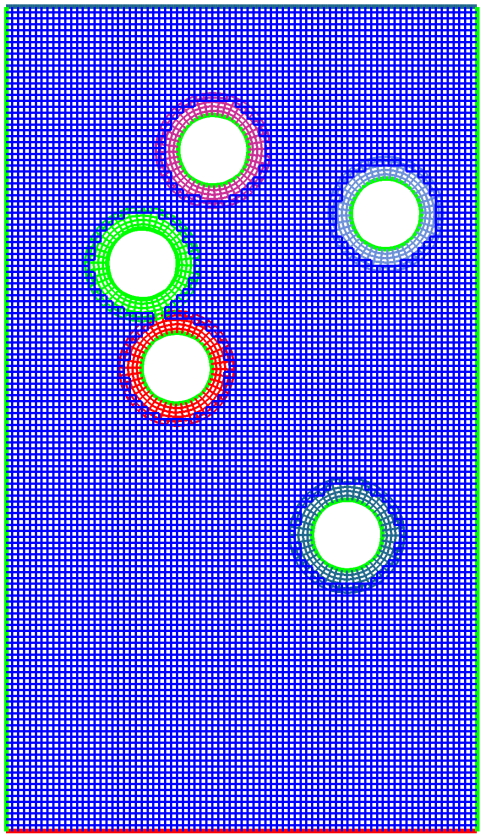
1. You need to efficiently solve a PDE on a complex geometry.
2. You need to solve a PDE on a moving geometry.
3. You need to generate an overlapping grid.

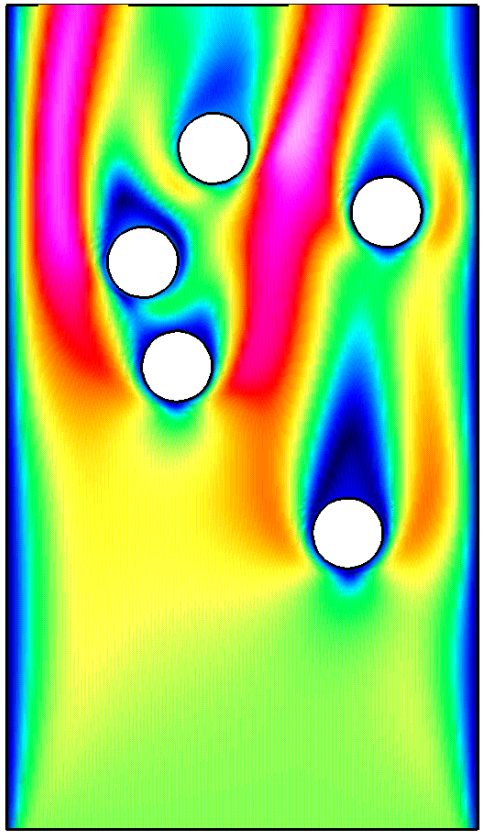
You can

- 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.

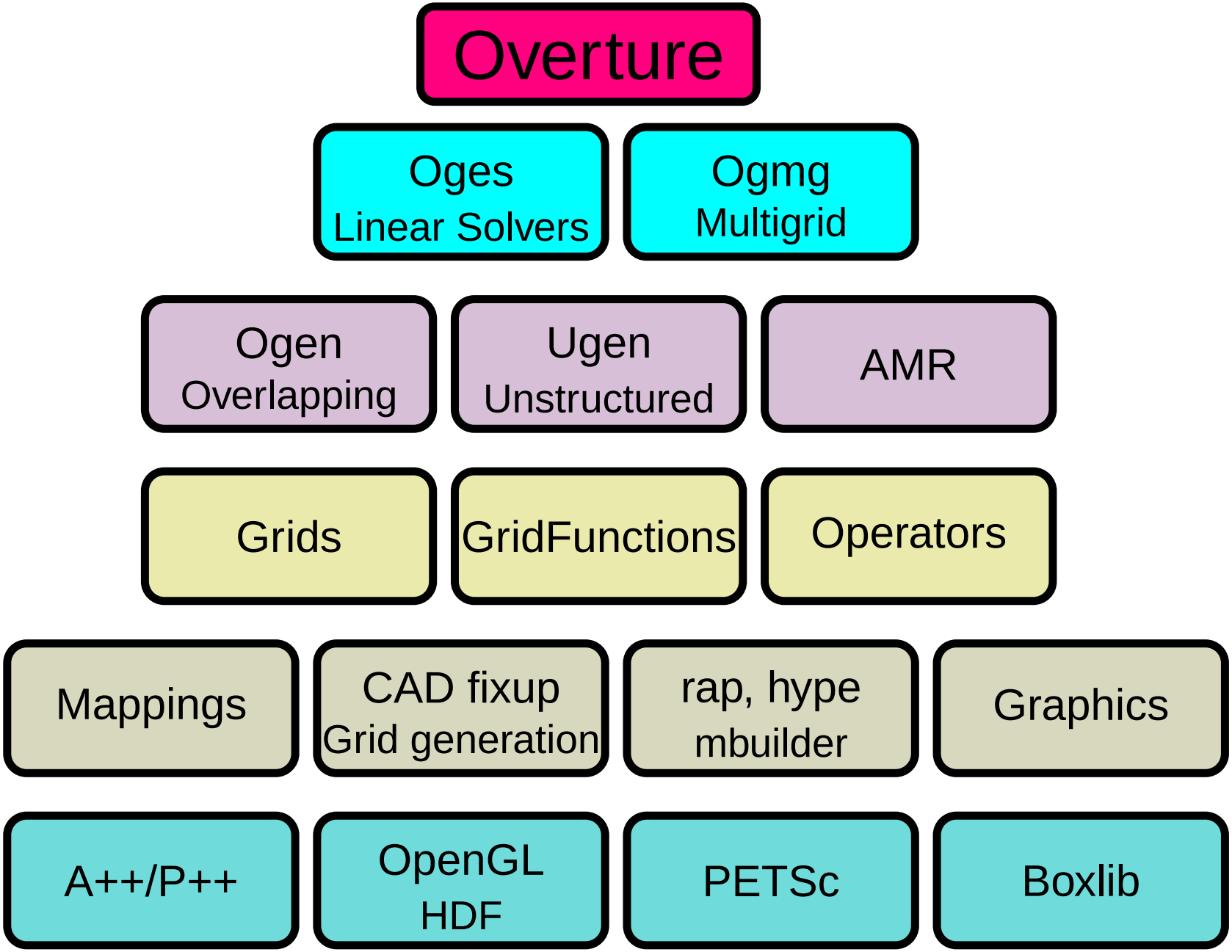




- Overlapping grids can be rapidly generated as bodies move.
- High quality grids under large displacements.
- Cartesian grids for efficiency.
- Efficient for high-order accurate methods.

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++
OpenGL
HDF
PETSc
Boxlib

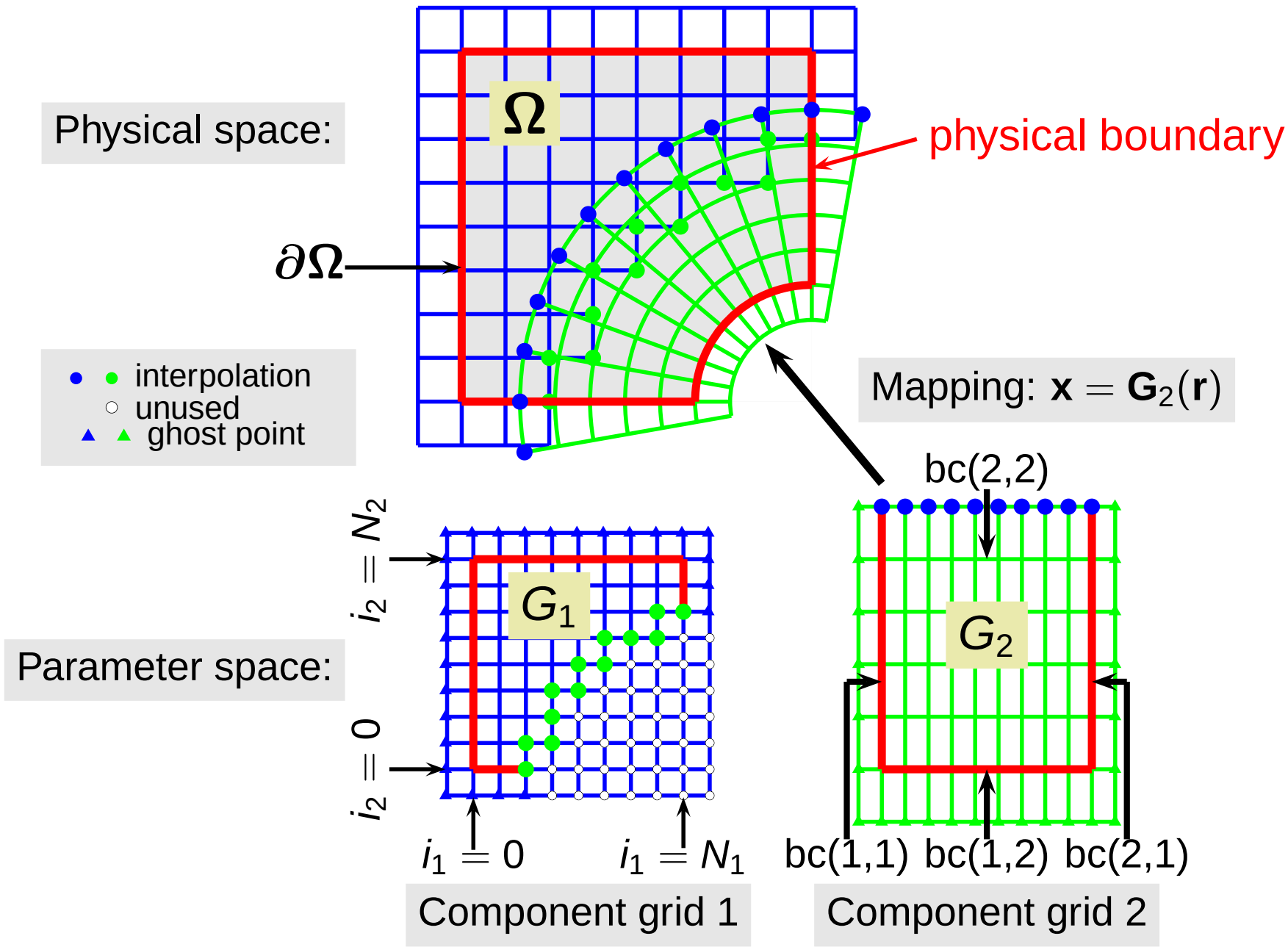
CG: Composite Grid PDE solvers built with Overture

Different PDE solvers in the CG suite:

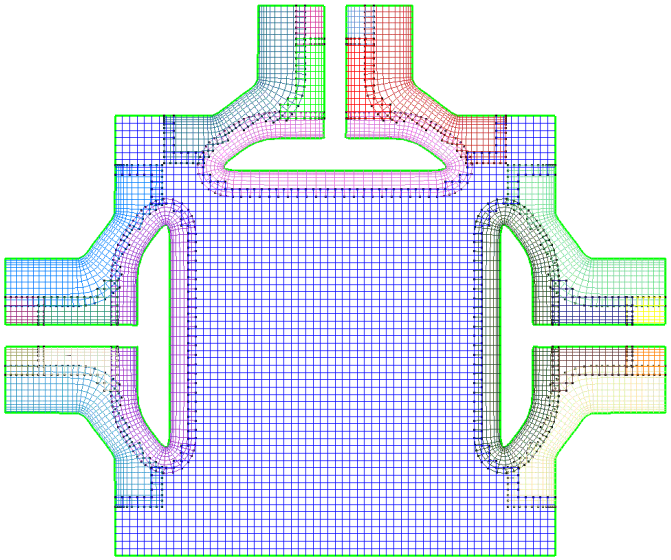
- cgad: advection diffusion equations.
- cgins: incompressible Navier-Stokes with heat transfer.
- cgcns: compressible Navier-Stokes, reactive Euler equations.
- cgmp: multi-physics solver (e.g. conjugate heat transfer).
- cgmx: time domain Maxwell's equations solver.
- cgsm: solid mechanics (*new*)

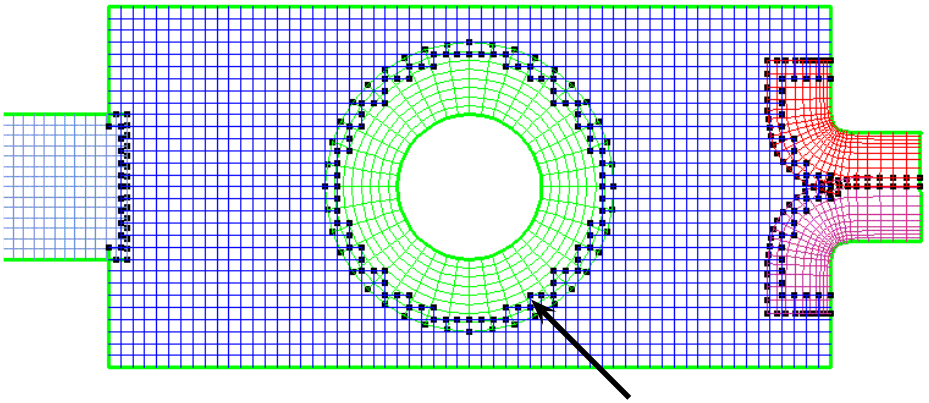
Note: Composite Grid is another name for an overlapping grid.

Components of an Overlapping Grid

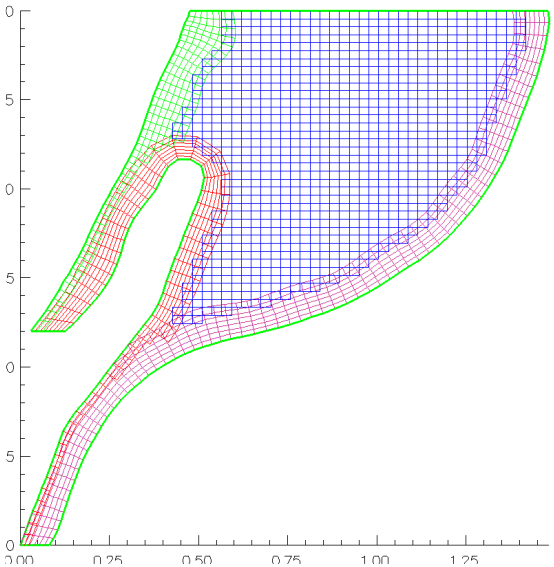


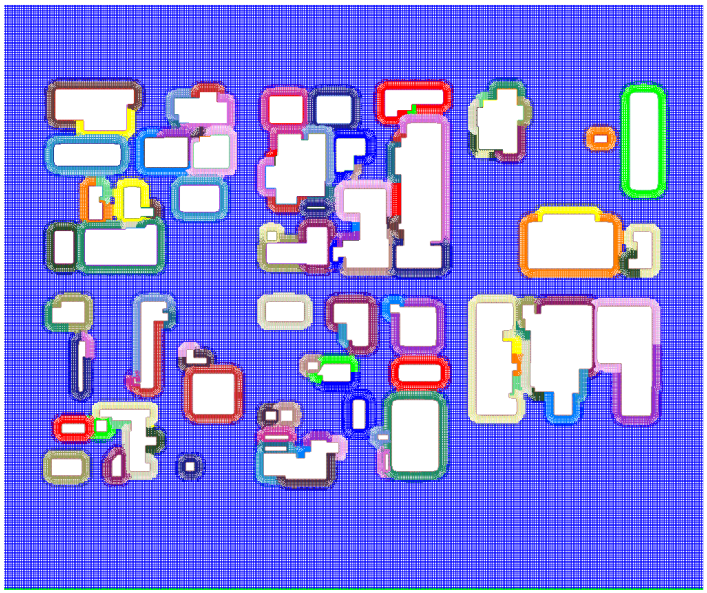
Ogen can be used to build 2D overlapping grids:



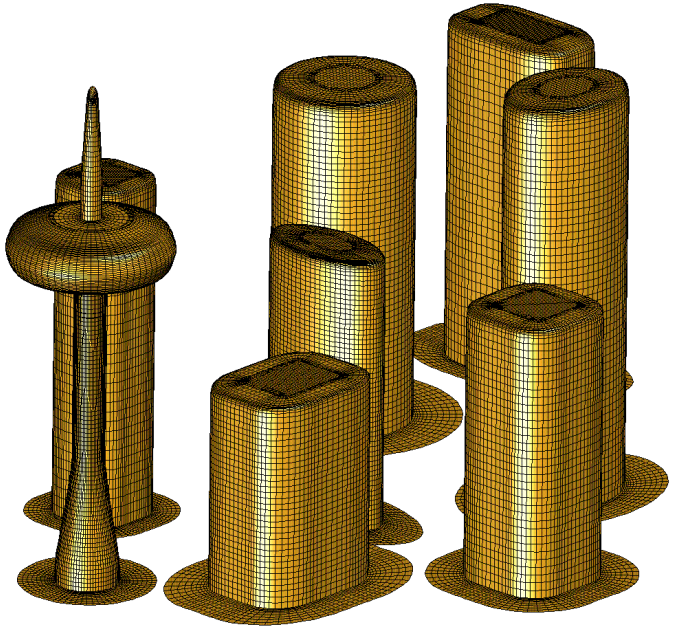


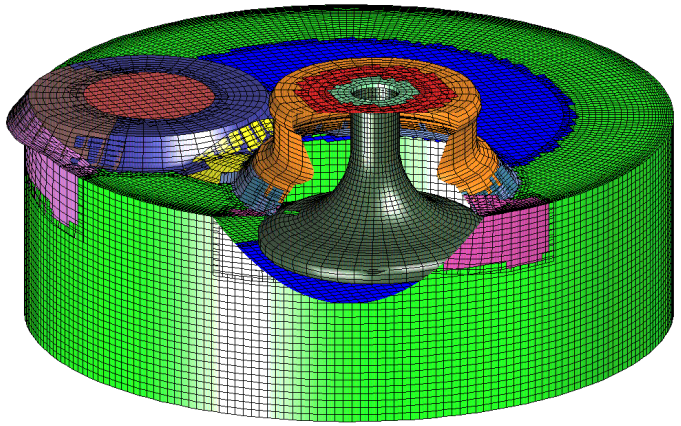
Solutions coupled by interpolation

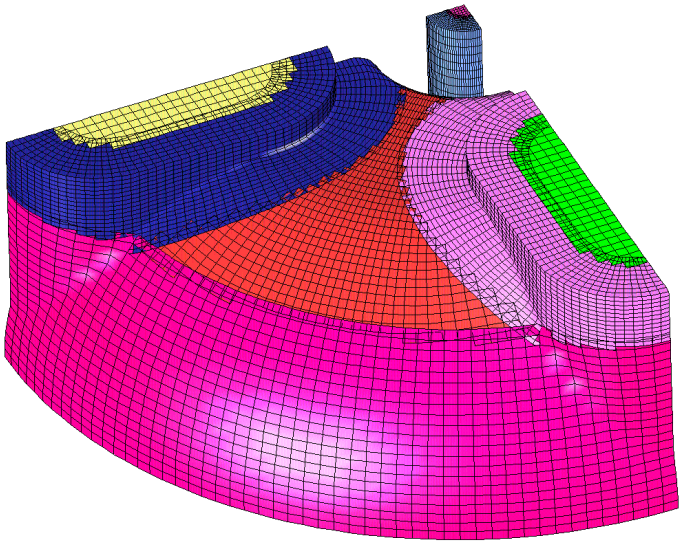


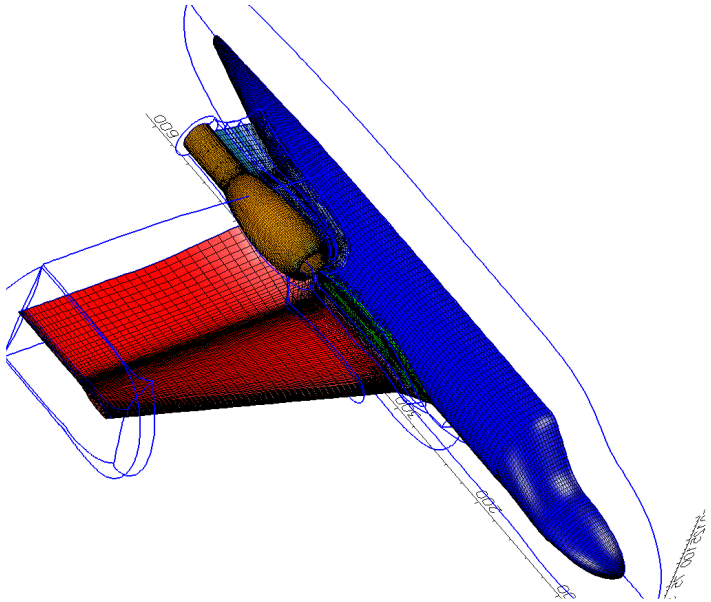


Ogen can be used to build 3D overlapping grids:









Overture supports a high-level C++ interface

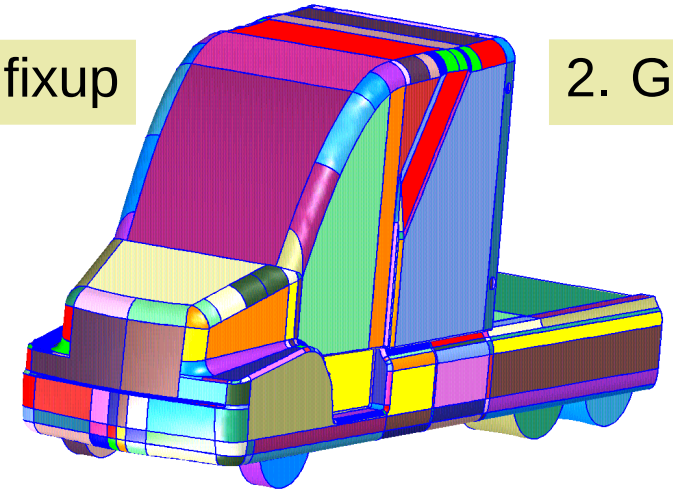
But is built upon mainly Fortran kernels.

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

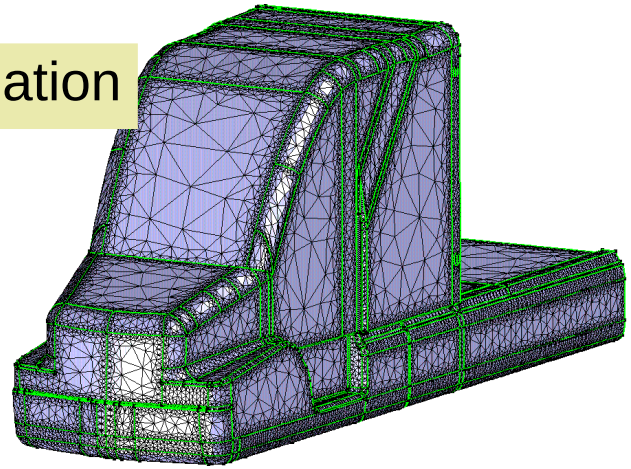
```
CompositeGrid cg; // create a composite grid
getFromADataBaseFile(cg,"myGrid.hdf");
floatCompositeGridFunction u(cg); // create a grid function
u=1.;
CompositeGridOperators op(cg); // operators
u.setOperators(op);
float t=0, dt=.005, a=1., b=1., nu=.1;
for( int step=0; step<100; step++ )
{
   u+=dt*(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

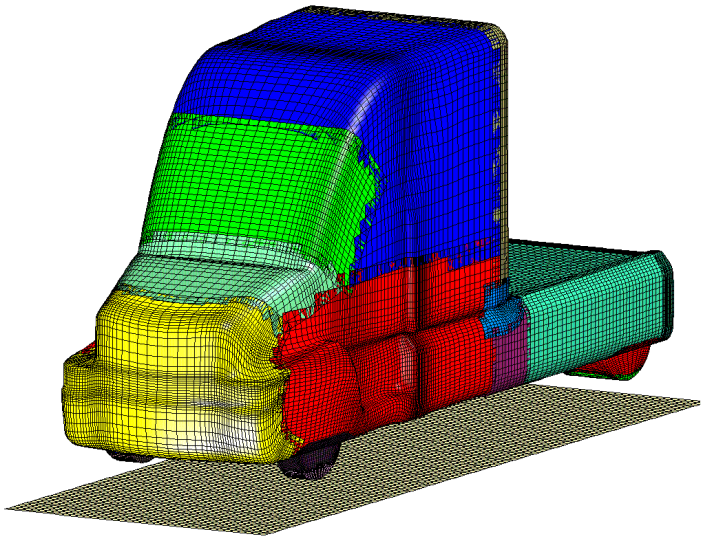
1. Cad fixup



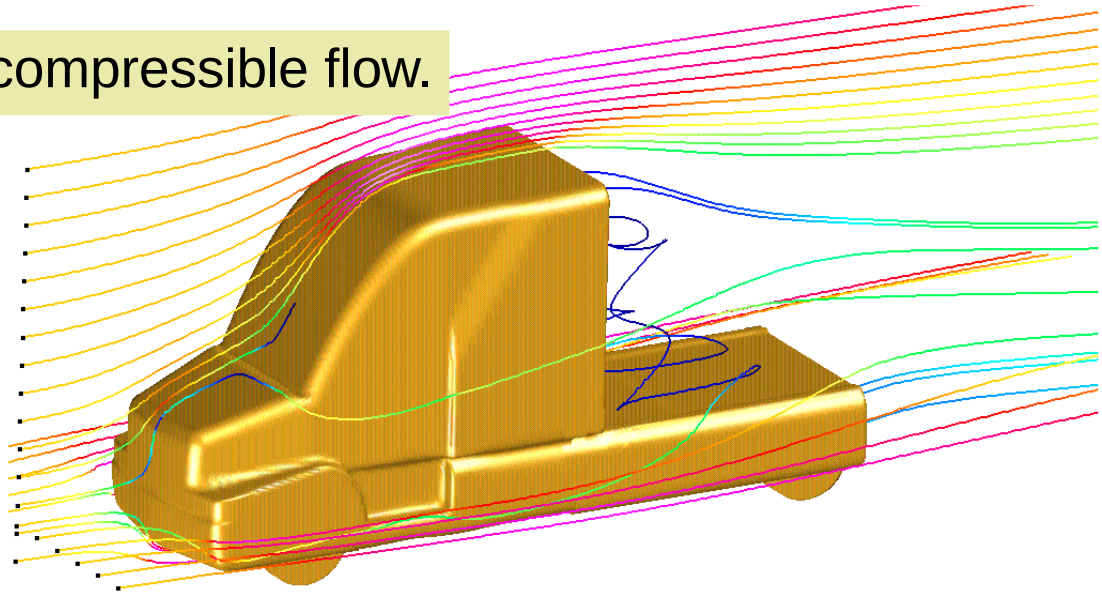
2. Global triangulation



3. Overlapping grid



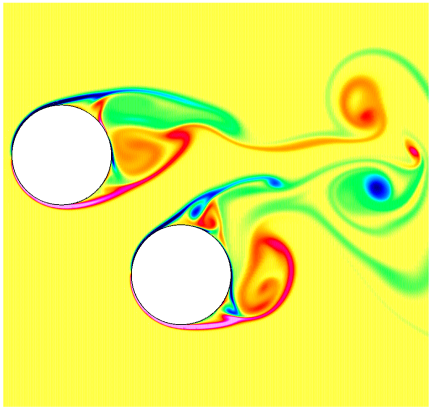
4. Incompressible flow.

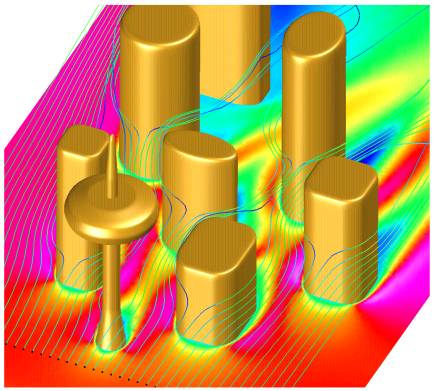


Overture is used by research groups worldwide

- High-order accurate, compact Hermite-Taylor schemes (Tom Hagstrom, SMU, Dallas).
- Blood flow in veins with blood clot filters. (Mike Singer, LLNL).
- Compressible flow/ice-formation (Graeme Leese, U. Cambridge).
- Relativistic hydrodynamics and Einstein field equations (Philip Blakely, U. Cambridge).
- Visco-plastic flows and friction-stir welding (Graeme Thorn, U. of Liverpool).
- Flow on the surface of the eye (Kara Maki, U. Delaware).
- High-order accurate subsonic/transonic aero-acoustics (Phillipe Lafon, CNRS, EDF, France).
- Low Reynolds flow for pitching airfoils (D. Chandar, M. Damodaran, NTU, Singapore).
- Incompressible flow in pumps (J.P. Potanza, Shell Oil, Houston).

Cgins: incompressible Navier-Stokes solver.

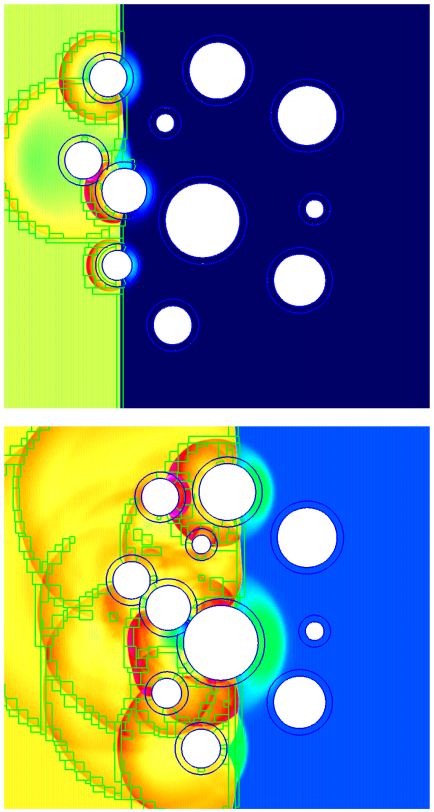




- 2nd-order and 4th-order accurate (DNS).
- support for moving rigid-bodies (not parallel yet).
- heat transfer (Boussinesq approximation).
- semi-implicit (time accurate), pseudo steady-state (efficient line solver), full implicit.

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

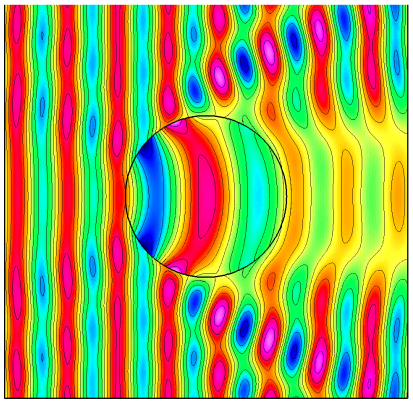
Cgcns: compressible N-S and reactive-Euler.

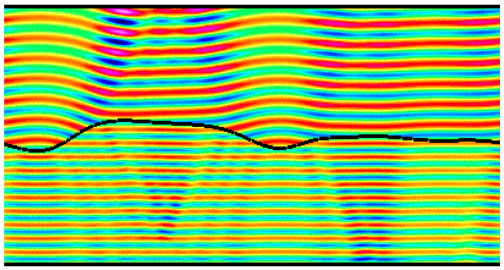


- reactive and non-reactive Euler equations, Don Schwendeman (RPI).
- compressible Navier-Stokes.
- multi-fluid formulation, Jeff Banks (LLNL).
- adaptive mesh refinement and moving grids.

- 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.



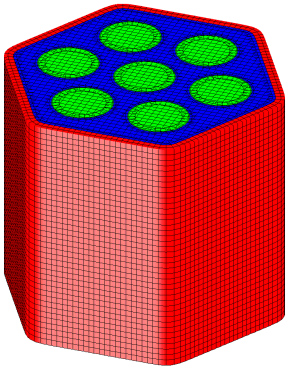


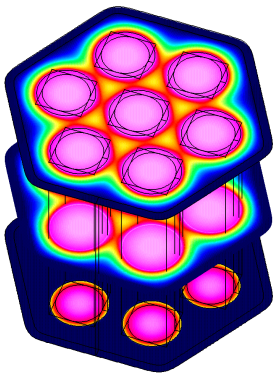
- fourth-order accurate, 2D, 3D.
- Efficient time-stepping with the modified-equation approach
- High-order accurate symmetric difference approximations.
- High-order-accurate *centered* boundary and interface conditions.

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

Cgmp: a multi-domain multi-physics solver.

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

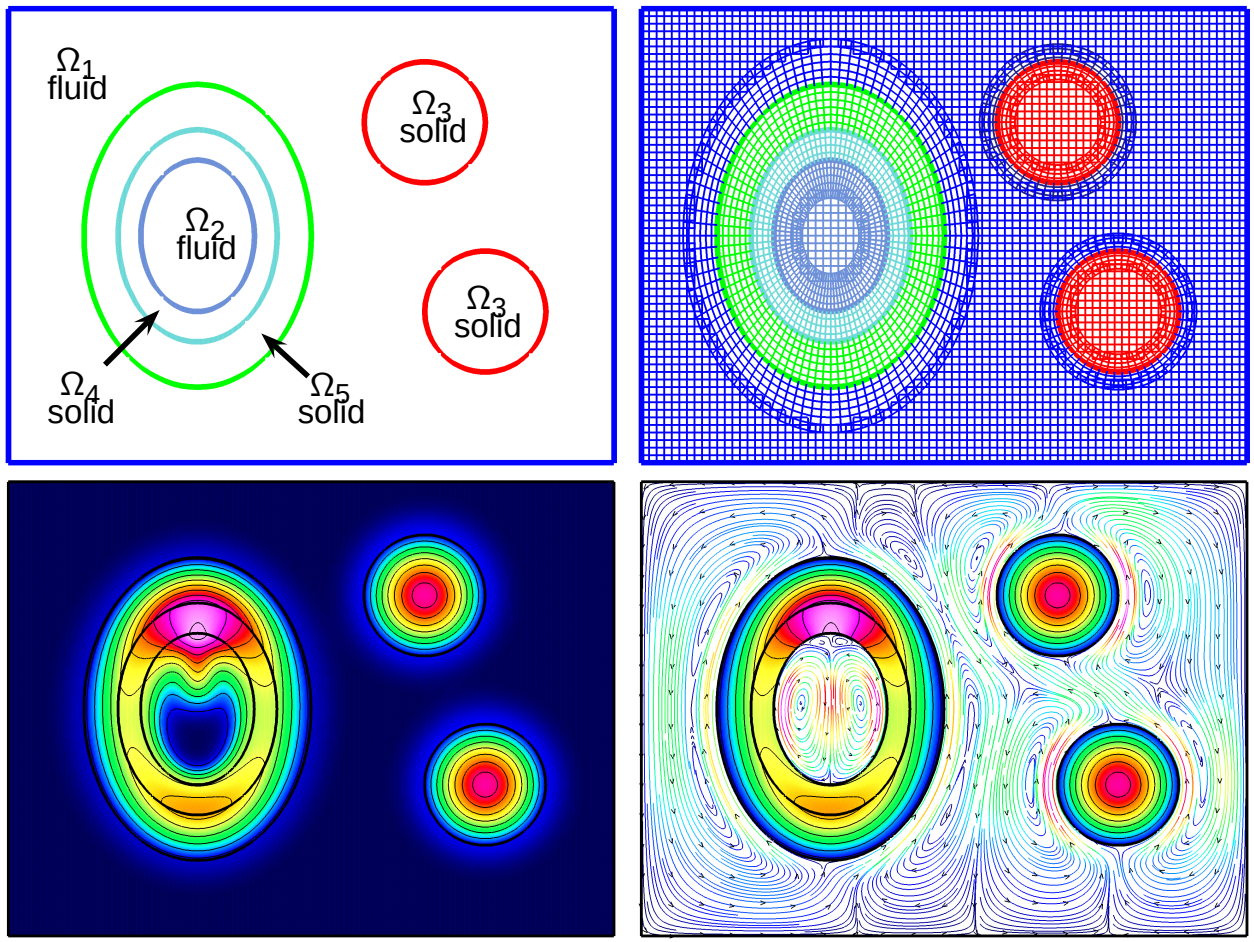




- overlapping grids for each fluid or solid domain,
- a partitioned solution algorithm (separate physics solvers in each sub-domain),
- (cgins) incompressible Navier-Stokes equations (with Boussinesq approximation) for fluid domains,
- (cgad) heat equation for solid domains,
- a key issue is interface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

Summary.

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

www.llnl.gov/CASC/Overture