Recent Developments in Overture

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Current Overture developers

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Major Contributors

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

Overview of Recent Work

- Solid mechanics on overlapping grids (talk by Jeff Banks).
- Efficient high-order scheme for incompressible flows (talk by Kyle Chand).
- Grid generation: large scale (billions of grid points), parallel, and moving.
- Multigrid solvers for overlapping grids (new high-order accurate and parallel algorithms),
- Maxwell's equations (multi-material electromagnetic problems in 3D),
- Fluid structure interactions (coupling high speed flow with deforming solids).

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

- 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).

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*)

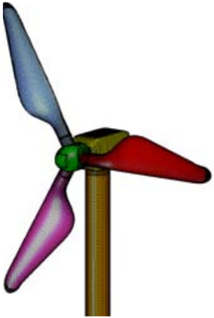
Grid generation.

Two major steps:

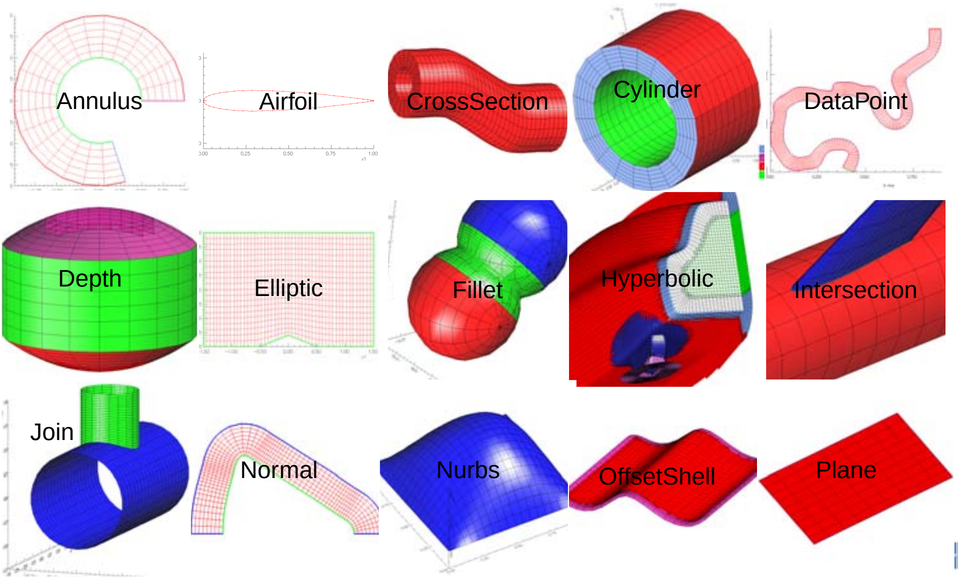
1. construct component grids (Mappings).
2. grid connectivity: cut holes and determine interpolation information (Ogen).

In recent work changes have been made to support

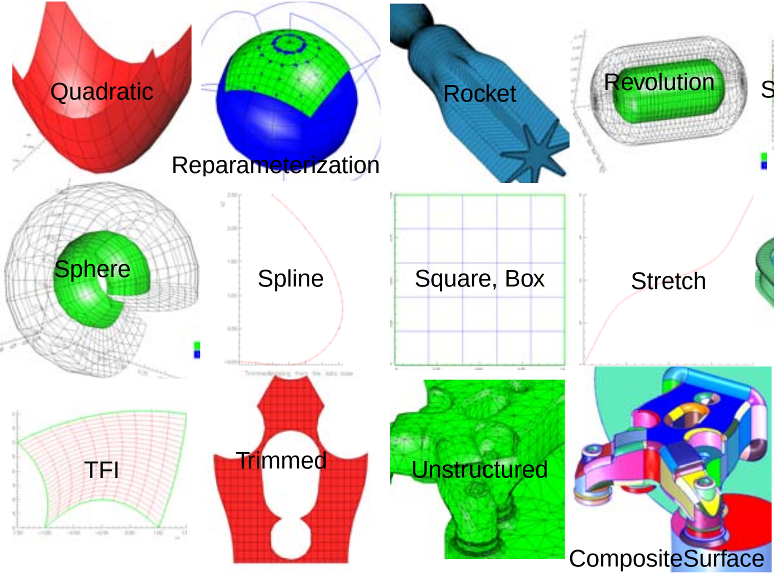
- the generation of large (billion point +) grids.
- parallel moving-grid flow simulations (Ogen is called at each time step).



Overture Mappings (Part I)



Overture Mappings (Part II)



Ogen: overlapping grid generator (grid connectivity)

Brief description of the algorithm:

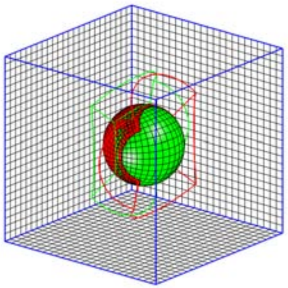
- physical boundaries cut holes (“implicit hole-cutting”).
- grids ordered by priority; interpolation preferred from higher priority grids.
- robust algorithm with backup rules and interactive error diagnostics.

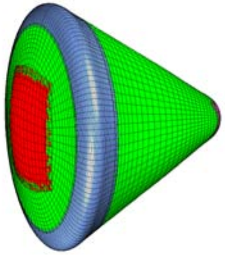
Brief description of capabilities:

- arbitrary stencil widths (1,2,3... fringes),
- arbitrary order of interpolation (linear, quadratic, cubic,...),
- fast searching algorithms and fast “inverse” map.
- inverse optimized for common mappings (spheres, cylinders, ...),
- optimized for Cartesian grids,
- script files with embedded perl commands for "automatic" parameterized grid generation.

Ogen: two examples

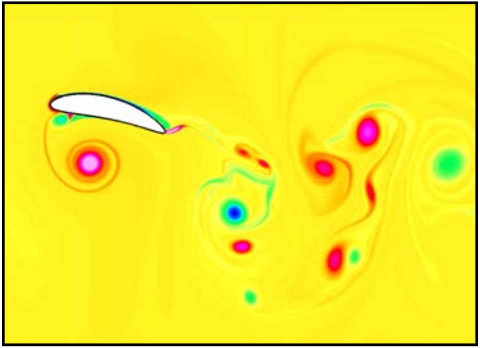
Grid	order of accuracy	grid points	processors (nodes $\times$ p/n)	cpu (s)
Sphere in a box	2	2.1 billion	16 (8 $\times$ 2)	136
Re-entry vehicle	4	215 million	128 (16 $\times$ 8)	1990





Significant performance improvements can still be made.

Parallel Flow Solution on Moving Grids.



- Flow past a pitching and plunging airfoil.
- Demonstrates new parallel moving grid capabilities.

Multigrid: fast in theory and practice (if careful)

- For elliptic problems, multigrid algorithms can have near optimal complexity requiring O(N) work to solve for N unknowns (c.f. conjugate gradient: $O(N^{3/2})$).
- multigrid uses a sequence of coarser and coarser meshes to accelerate the convergence rate on the finest grid.
- For overlapping grids, coarse grid generation is a difficulty.

Ogmg: Overlapping Grid Multigrid Solver

Ogmg: solves scalar elliptic boundary value problems.

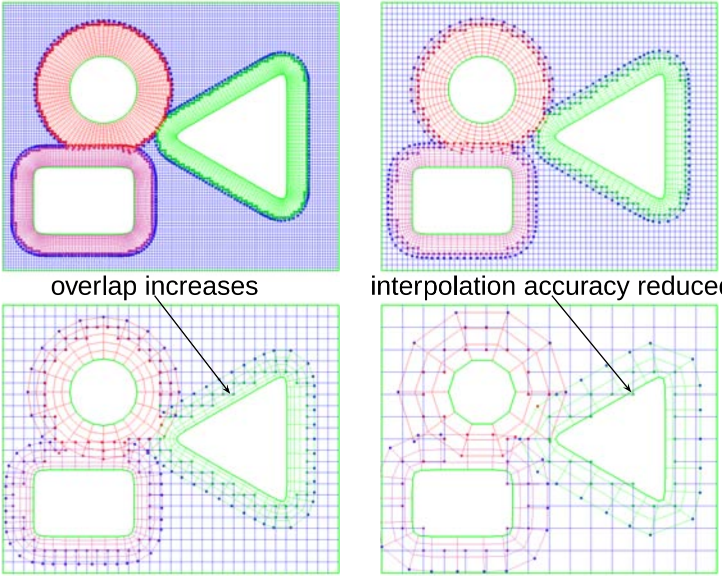
- automatic coarse grid generation of “any” number of levels.
- adaptive smoothing
  - variable sub-smooths per component grid
  - interpolation-boundary smoothing (IBS)
  - over-relaxed Red-Black smoothers
- Galerkin coarse grid operators (operator averaging)
- numerical boundary conditions for Dirichlet and Neumann problems

WDH., *On Multigrid For Overlapping Grids*, SIAM J. Sci. Comput. **26**, no. 5, (2005) 1547–1572.

New capabilities under development:

- fourth-order accuracy
- parallel

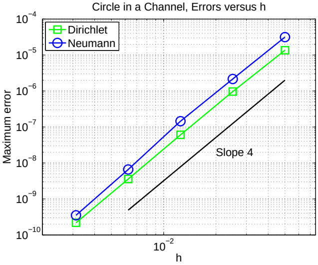
Ogmg: Automatic Coarse Grid Generation

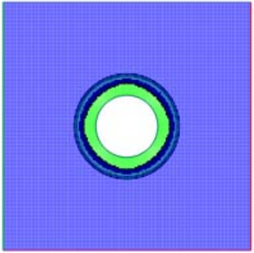


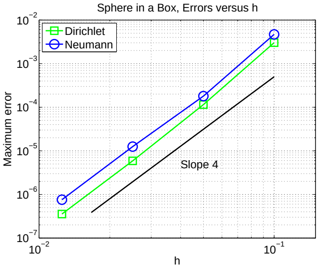
Ogmg: Fourth order accuracy.

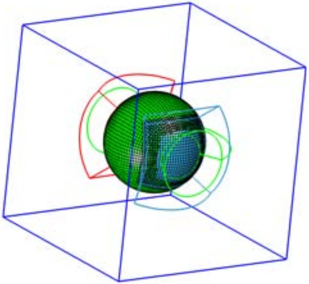
- The equations are solved to fourth-order accuracy on the finest level but only second-order accuracy on lower levels.
- Boundary conditions must be carefully formulated to avoid degradation in convergence rates.
- Neumann boundary conditions require particular care.

Ogmg: Results: fourth order accuracy.









Ogmg: Convergence rates - Cartesian grids.

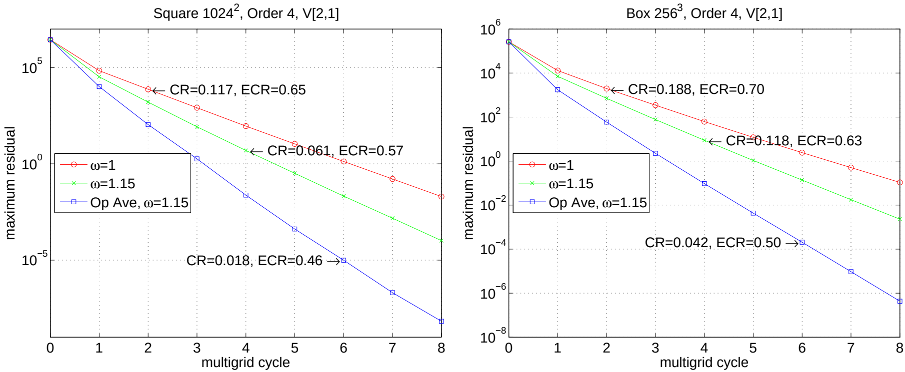
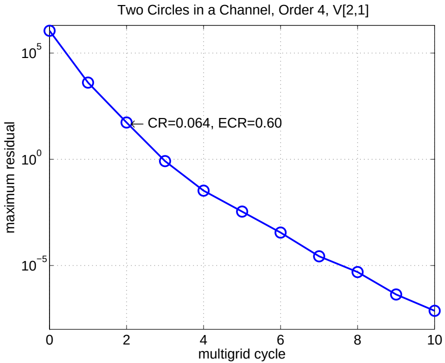


Figure: Multigrid convergence rates for Poisson's equation with Dirichlet boundary conditions on a 1024^2 square and a 256^3 box with a V[2,1] cycle. The rates are significantly improved using operator averaging and over-relaxed Red-Black smoothers with a relaxation parameter ω.

Ogmg: Convergence rates - Overlapping grids.



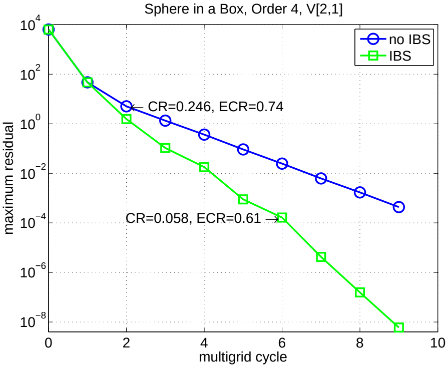
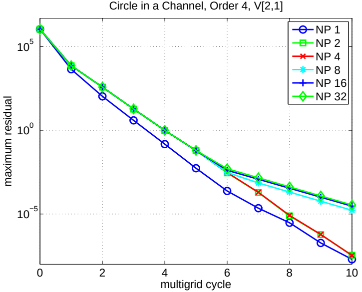


Figure: Left: two-cylinders-in-a-channel. Right: sphere-in-a-box

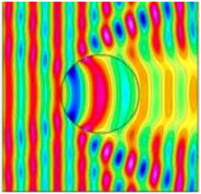
Ogmg: Parallel issues.

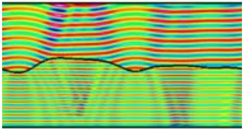
- Each grid is distributed across a set of processors.
- Coarse grids may be distributed over different processors than fine.
- Load balancing - there is less work on coarse grids.
- Coarse grid generation, smoothers, and fine-coarse transfers must account for the parallel distribution.



Cylinder-in-a-channel, 6.6M pts, Convergence for different numbers of processors (preliminary).

Cgmx: electromagnetics solver.

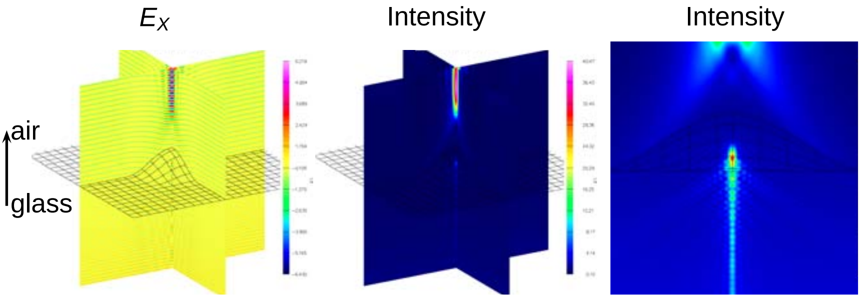




- a time-domain finite difference scheme.
- fourth-order accurate, 2D, 3D.
- Efficient time-stepping with the modified-equation approach
- High-order accurate symmetric difference approximations.
- High-order-accurate *centered* boundary and interface conditions.

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

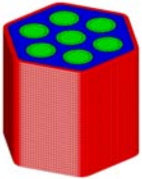
Scattering by a 3d material interface

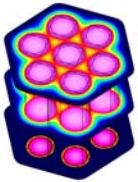


- Uses newly developed 4th-order accurate 3D material interface approximations.
- Scattering of a plane wave by an interface with a bump, glass-to-air.
- 1 billion grid points, 32 nodes (8 processors per node) of a Linux cluster.

Cgmp: a multi-domain multi-physics solver.

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

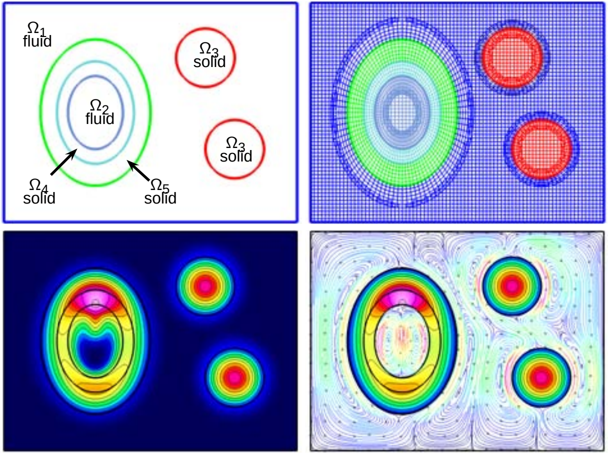




- overlapping grids for each fluid or solid domain,
- a partitioned solution algorithm (separate physics solvers in each sub-domain),
- (cgins) incompressible Navier-Stokes equations (with Boussinesq approximation) for fluid domains,
- (cgad) heat equation for solid domains,
- a key issue is interface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



Each fluid or solid sub-domain is covered by an overlapping grid.
Fluid sub-domains : cgins. Solid sub-domains: cgad.
Coupled problem: cgmp.

Deforming composite grids for Fluid-Structure Interactions (FSI)

Goal: Couple overlapping grid techniques for modeling fluids and gases (using moving grids and AMR) with linear and non-linear solid mechanics codes.

A mixed Eulerian-Lagrangian approach:

- Fluids: Overlapping grid fluid solver.
- Solids : overlapping-grid (or unstructured) solid solver.
- Boundary fitted deforming grids for fluid-solid interfaces.

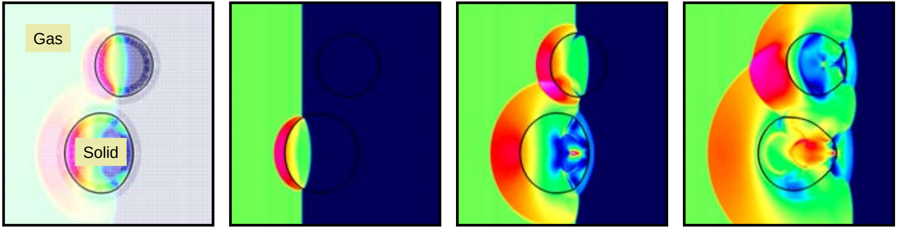
Strengths of the approach:

- Maintains high quality grids for large deformations/displacements.
- efficient structured grid methods optimized for Cartesian grids.

Cgmp: deforming composite grids for FSI

Current status:

- 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.
- Adaptive mesh refinement (in progress).



Mach 2 shock in a gas hitting two elastic cylinders.