Recent Developments in Overture

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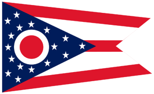

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Primary contributors:
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- **NSF** National Science Foundation .

The Overture project is developing PDE solvers for a wide class of continuum mechanics applications.

Overture is a toolkit for solving PDE's on overlapping grids and includes CAD, grid generation, numerical approximations, AMR and graphics.

The CG (Composite Grid) suite of PDE solvers (cgcns, cgins, cgmx, cgsm, cgad, cgmp) provide algorithms for modeling gases, fluids, solids and E&M.

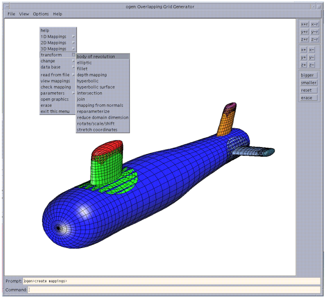
Overture and CG are available from www.llnl.gov/CASC/Overture.

We are looking at a variety of applications:

- wind turbines, building flows (cgins),
- explosives modeling (cgcns),
- fluid-structure interactions (e.g. blast effects) (cgmp+cgcns+cgsm),
- conjugate heat transfer (e.g. NIF holhraum) (cgmp+cgins+cgad),
- damage mitigation in NIF laser optics (cgmx).

Ogen: overlapping grid generator.

Ogen cuts holes and computes interpolation points.

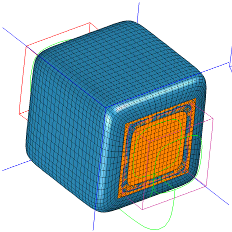


- automatic (implicit) hole cutting algorithm.
- supports arbitrary order of accuracy (stencil width and interpolation width).
- implicit and explicit interpolation.
- backup rules.
- parallel.
- optimized for Cartesian grids.

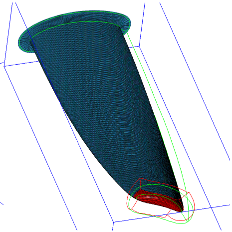
- WDH., *Ogen: An Overlapping Grid Generator for Overture*, UCRL-MA-132237, 1998.

Ogen: recent developments.

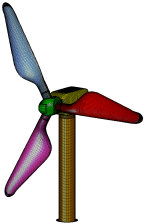
1. lofted mapping (esp. useful for defining *wing tips*).
2. explicit hole cutters (sometimes needed with overlapping refinements).
3. parallel grid generation improvements.
4. improvements to the hyperbolic grid generator and grids on CAD geometry (e.g. for high-order accuracy).

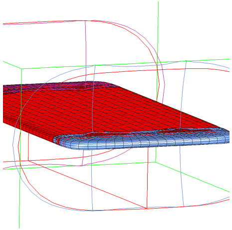


lofted box



lofted Joukowsky, flat tip





lofted mapping and hyperbolic grid generation

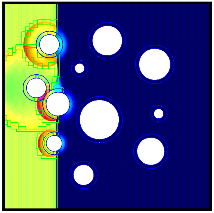
Ogen: recent developments.

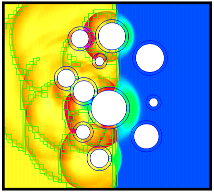
Parallel grid generation results (fourth-order accurate grids).

	Sphere		Turbine		Two-spheres	
	275M pts		185M pts		710M pts	
N_p	CPU	r	CPU	r	CPU	r
2	1060.					
4	606.	1.7	950.			
8	266.	2.3	575.	1.7	2270	
16	162.	1.6	425.	1.4	1370	1.7
32	106.	1.5	271.	1.6	914	1.5
64	67	1.6	235.	1.2	629	1.4

Figure : CPU time in seconds to generate various overlapping grids as a function of the number of processors. All grids are constructed for fourth-order accurate methods.

Cgcns: compressible N-S and reactive-Euler.



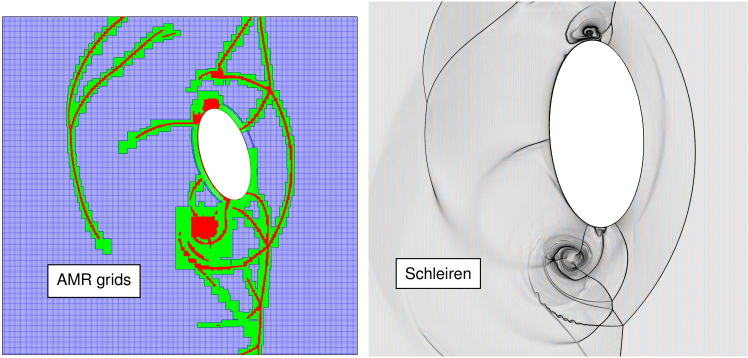


- reactive and non-reactive Euler equations.
  - high-order version of Godunov's method.
  - reactions: one-step, chain-branching, ignition and growth
  - equations of state: ideal, stiffened, JWL
- compressible Navier-Stokes.
- multi-fluid formulations.
- multi-phase formulation.
- adaptive mesh refinement 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).

Cgcns: stable FSI algorithms for light rigid-bodies

Overcoming the *added-mass instability*

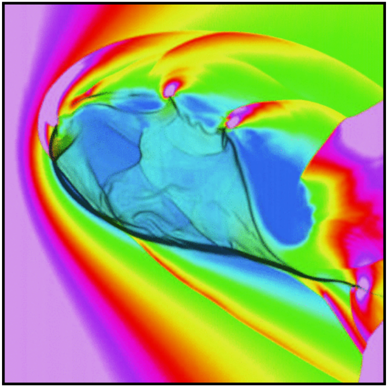


Shock hitting an ellipse of *zero* mass.

- J.W. Banks, WDH, Sjögreen, *A stable FSI algorithm for light rigid bodies in compressible flow*, LLNL-JRNL-558232, submitted, 2012.

Cgcns: new multi-fluid algorithms.

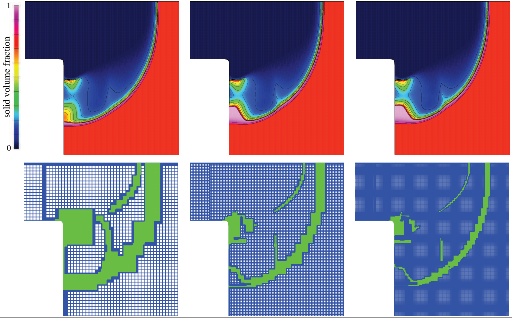
Collapse of a cavity in a solid upon impact by a shock.



- M Ozlem, D.W. Schwendeman, A. Kapila, WDH, *A numerical study of shock-induced cavity collapse*, Shock Waves, 2011.

Cgcns: multiphase modeling of explosives.

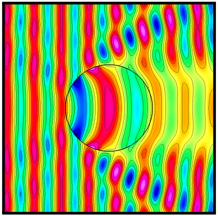
Explosive corner turning problem, grid convergence:

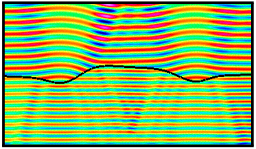


Detonation diffraction around a corner computed with the compressible multiphase model.

- D. W. Schwendeman, A. K. Kapila, WDH, *A Hybrid Two-Phase Mixture Model of Detonation Diffraction with Compliant Confinement*, LLNL-JRNL-57487, submitted, 2012.
- DWS, AKK, WDH, *A Comparative Study of Two Macro-Scale Models of Condensed-Phase Explosives*, IMA Journal of Applied Math, 2012.
- DWS, AKK, WDH, *A study of detonation diffraction and failure for a model of compressible two-phase reactive flow*, Combust. Theory and Modeling, 2010.

Cgmx: an electromagnetics solver.



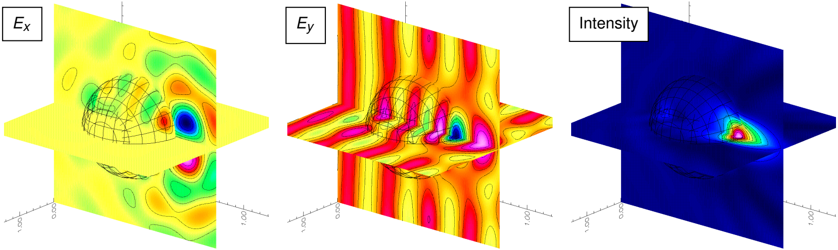


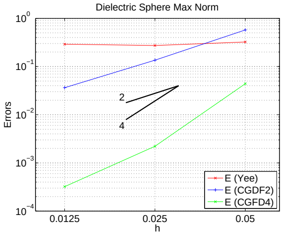
- a time-domain finite difference scheme.
- fourth-order accurate, 2D, 3D.
- Efficient time-stepping with the modified-equation approach.
- High-order accurate symmetric difference approximations.
- High-order-accurate *PDE-based* boundary and interface conditions.
- Computations with over a billion (10^9) grid points have been performed.

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

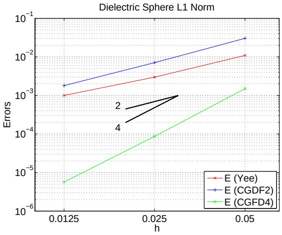
Cgmx: scattering of a plane wave by a glass sphere.

Compare the Yee, 2nd and 4th order accurate schemes





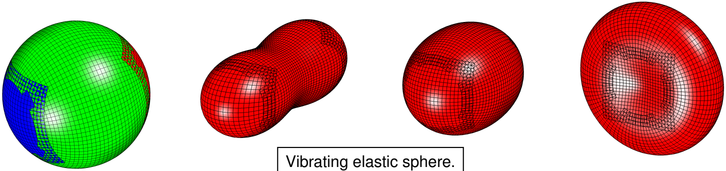
Max-norm errors



L_1-norm errors

Cgsm: a solver for the elastic wave equation.

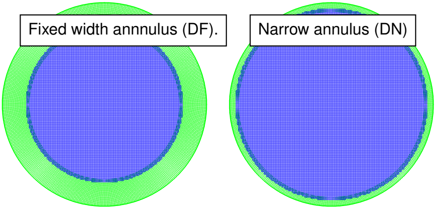
- linear elasticity on overlapping grids, with adaptive mesh refinement,
- conservative finite difference scheme for the second-order system,
- upwind Godunov scheme for the first-order-system.

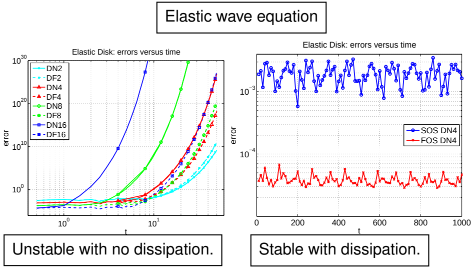


Vibrating elastic sphere.

Diffraction of a p-wave "shock" by a circular cavity.

New stability results for 2nd-order wave equations



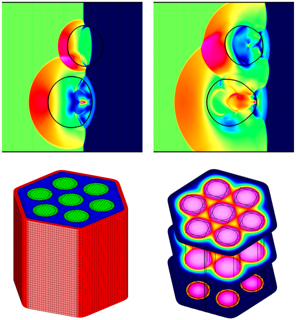


- Non-dissipative schemes for wave equations have an instability.
- Interaction between the interpolation points and boundary.
- The unstable behaviour is more severe for the *narrow* annulus case.
- Theory identifies the required form of the artificial dissipation.
- The Godunov upwind scheme for the first-order-system (FOS) is naturally stable.

- D. Appelö, J.W. Banks , WDH, D.W. Schwendeman, *Numerical Methods for Solid Mechanics on Overlapping Grids: Linear Elasticity*, J. Comput. Phys., 2012.

Cgmp: a multi-domain multi-physics solver.

Cgmp couples different fluids and solid solvers



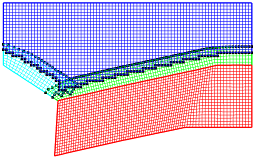
- overlapping grids for each fluid or solid domain,
- a partitioned solution algorithm (separate physics solvers in each sub-domain),
- accurate and stable interface treatments.
- conjugate heat transfer (cgins+cgad, cgcns+cgad).
- fluid-structure interactions (cgcns + cgsm).

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

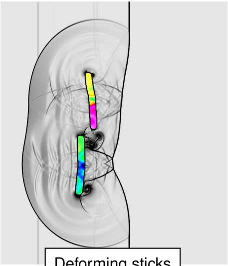
Cgmp: a new stable partitioned FSI algorithm

Overcomes the added-mass instablility for light solids.

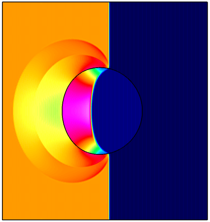
1. embeds the solution of a fluid-solid Riemann problem
2. impedance weighted projection of interface velocity and stress.
3. stable for a wide range of material properties.



Superseismic shock



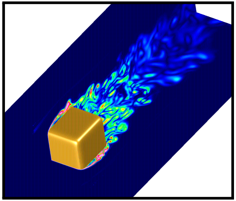
Deforming sticks

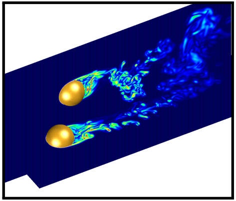


Elastic shock and fluid cavity.

- J. W. Banks, WDH, D.W. Schwendeman, *Deforming Composite Grids for Solving Fluid Structure Problems*, J. Comput. Phys, 2012.
- J. W. Banks and B. Sjögreen, *A Normal Mode Stability Analysis of Numerical Interface Conditions for Fluid/Structure Interaction*, Commun. Comput. Phys., 2011.

Cgins: incompressible Navier-Stokes solver.





- 2nd-order and 4th-order accurate (DNS and LES).
- accurate and stable treatment of boundaries.
- support for moving rigid-bodies.
- heat transfer and buoyancy (Boussinesq approx.).
- semi-implicit (time accurate), pseudo steady-state (efficient line solver), full implicit.
- SSLES nonlinear LES turbulence model.

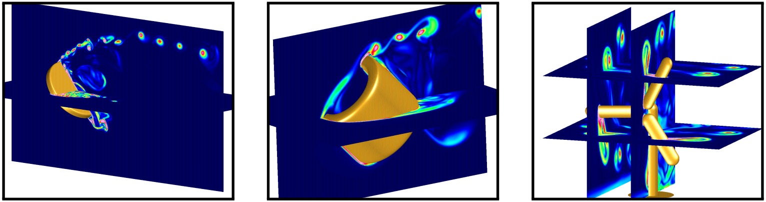
- WDH., *A Fourth-Order Accurate Method for the Incompressible Navier-Stokes Equations on Overlapping Grids*, J. Comput. Phys, **113**, no. 1, (1994) 13–25.
- WDH, N.A. Petersson, *A Split-Step Scheme for the Incompressible Navier-Stokes Equations*, 2003.

Cgins: New 4th-order AFS-MG parallel solver.

Approximate-factored/compact scheme and multigrid pressure solver

A parallel split-step solver is being developed based on:

1. Fourth-order accurate approximate-factored/compact time-stepping scheme for the momentum equations.
2. Fourth-order accurate multigrid solver for the pressure equation.
3. Fast overlapping grid generation for moving geometry.



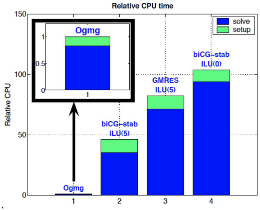
Parallel moving grid computations.

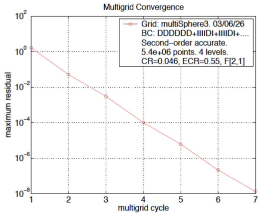
• K.K. Chand and M.A. Singer, *Verification and validation of CgWind: a high-order accurate simulation tool for wind engineering*, 13th International Conference on Wind Engineering (ICWE13), 2011.
• K.K. Chand, WDH, K.A. Lundquist and M.A. Singer, *CgWind: A high-order accurate simulation tool for wind turbines and wind farms*, The Fifth International Symposium on Computational Wind Engineering (CWE2010), 2010.

The Ogmg overlapping grid multigrid solver has been extended to 4th-order accuracy and parallel.

Ogmg is many times faster than Krylov methods.

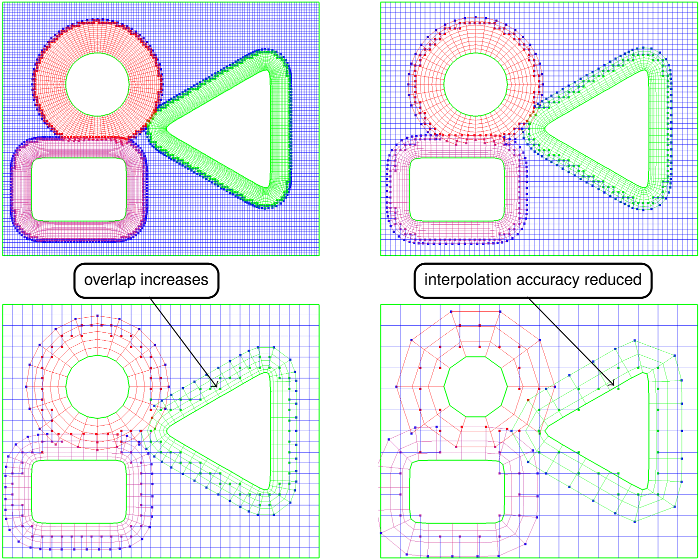
- matrix-free; optimized for Cartesian grids.
- automatic coarse grid generation.
- adaptive smoothing
  - variable sub-smooths per component grid.
  - interpolation-boundary smoothing (IBS).
- Galerkin coarse grid operators (operator averaging).
- *PDE-based* numerical boundary conditions for Dirichlet and Neumann problems.





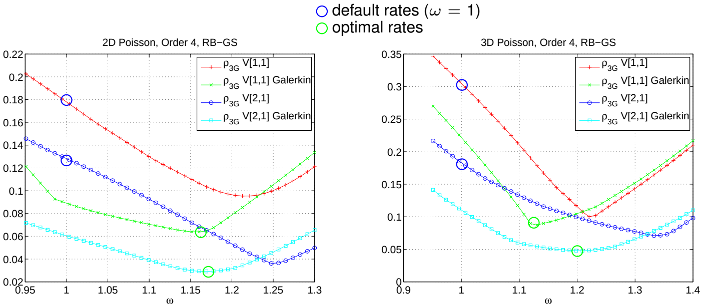
WDH., *On Multigrid For Overlapping Grids*, SIAM J. Sci. Comput. **26**, no. 5, (2005) 1547–1572.

Automatic coarse grid generation is a key feature.



Local Fourier analysis significantly improves convergence rates.

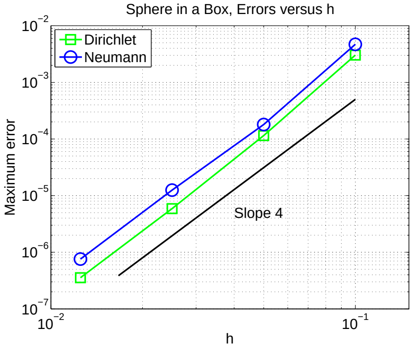
Over-relaxed Red-Black smoothers and Galerkin coarse grid operators.

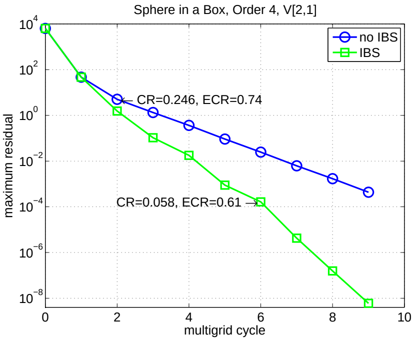


Three-grid multigrid convergence rates as a function ω.

ω : relaxation parameter in Red-Black Gauss-Seidel smoother.
ρ_{3G} : convergence rate per cycle for a 3 grid (i.e. 3 level) MG.
$V[m,n]$: MG V-cycle, m pre-smooths and n-post smooths.
Galerkin : Galerkin coarse grid operators.

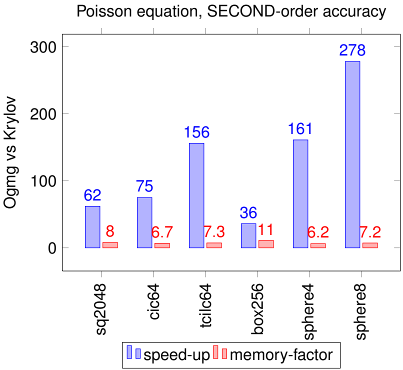
Accuracy and convergence of the new fourth-order accurate parallel version of Ogmg.

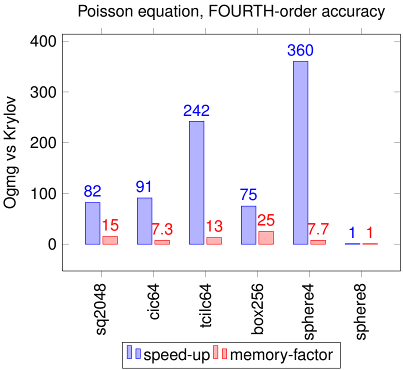




Multigrid is much faster than Krylov based methods.

And uses much less memory.





Performance of Ogmg for solving Poisson's equation to on various grids. Ogmg is compared to a Krylov solver (bi-CG stab, ILU(1)) from PETSc.

Movies