Recent Developments in Overture

Bill Henshaw

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

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Primary contributors:
Jeff Banks (LLNL),
Kyle Chand (LLNL),
Don Schwendeman (RPI).

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**ASCR** Department of Energy, Office of Science, ASCR Applied Math Program.

**LDRD** LLNL: Laboratory Directed Research and Development (LDRD) program.

**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.

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).
Ogen: recent developments.

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

<table>
<thead>
<tr>
<th>Sphere</th>
<th>Turbine</th>
<th>Two-spheres</th>
</tr>
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<tbody>
<tr>
<td>275M pts</td>
<td>185M pts</td>
<td>710M pts</td>
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<table>
<thead>
<tr>
<th>$N_p$</th>
<th>CPU (s)</th>
<th>CPU (s)</th>
<th>CPU (s)</th>
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<tbody>
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<td>1060.</td>
<td>950.</td>
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<tr>
<td>4</td>
<td>606.</td>
<td>266.</td>
<td>575.</td>
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<td>8</td>
<td>266.</td>
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<td>16</td>
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<tr>
<td>64</td>
<td>67</td>
<td>235.</td>
<td>629</td>
</tr>
</tbody>
</table>

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.
Cgcn5: 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.

Cgns: stable FSI algorithms for light rigid-bodies
Overcoming the *added-mass instability*


Shock hitting an ellipse of zero mass.
Cgcns: new multi-fluid algorithms.

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

Cgcn: multiphase modeling of explosives.

Explosive corner turning problem, grid convergence:

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.

Cgmx: scattering of a plane wave by a glass sphere. Compare the Yee, 2nd and 4th order accurate schemes.
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.


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).

Cgmp: a new stable partitioned FSI algorithm
Overcomes the added-mass instability 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.

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.

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.

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).
- \textit{PDE-based} numerical boundary conditions for Dirichlet and Neumann problems.

Automatic coarse grid generation is a key feature.

Overlap increases, interpolation accuracy reduced.

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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 $\omega$.

$\omega$ : relaxation parameter in Red-Black Gauss-Seidel smoother. 
$\rho_{3G}$ : 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.

Sphere in a Box, Errors versus $h$

Sphere in a Box, Order 4, $V[2,1]$

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Recent Developments in Overture

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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.