High-order difference methods for Cartesian and curvilinear grids

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BOUT++ 2013 Workshop,
Livermore Valley Open Campus, Livermore, CA, USA, September 4, 2013.
LLNL-PRES-643398

Acknowledgments.

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Supported by:

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

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

NSF National Science Foundation.

Topics to be covered

1. Overture : overlapping grids for complex geometry
2. Applications using high-order methods
   1. Maxwell's equations for time domain electromagnetic applications
   2. Incompressible Navier-Stokes equations for turbulence flows
3. High-order difference methods (conservative, non-conservative, compact)
4. Boundary conditions for high-order schemes.

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.

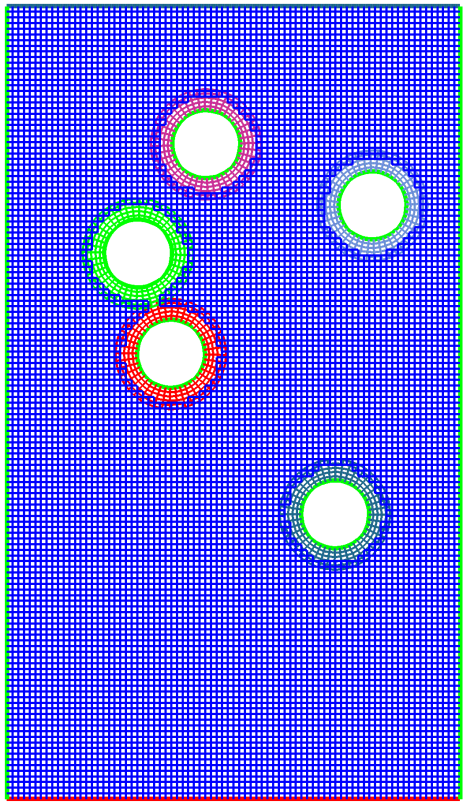
Overture and CG are available from www.llnl.gov/CASC/Overture.

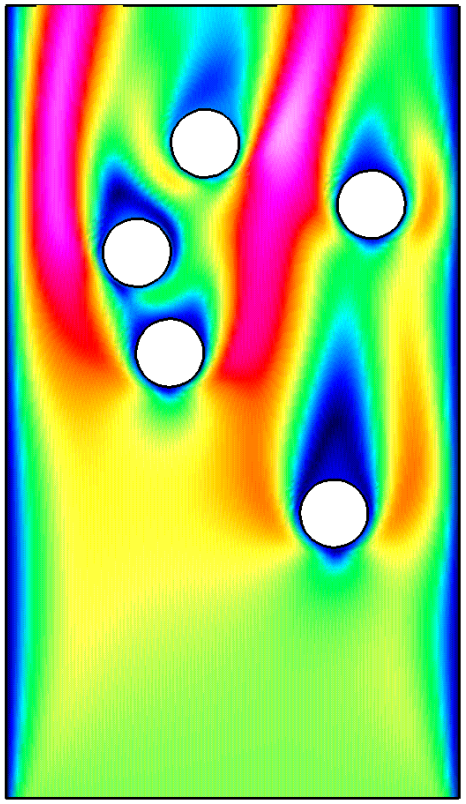
We are looking at a variety of applications:

- 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).

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.
- Smooth grids for accuracy at boundaries.
- Efficient for high-order methods.

Asymptotic Performance Principle for overlapping grids

As grids are refined, total CPU/memory usage can approach that of a Cartesian grid.

The simple case for high-order accurate schemes

Approximate form of errors: (h_p =grid-spacing, T = time)

$$E = C_2\, T\, h_2^2, \qquad \text{Error in a 2nd-order accurate scheme,}$$
$$E = C_4\, T\, h_4^4, \qquad \text{Error in a 4th-order accurate scheme.}$$

To match errors we need $h_2^2 \approx h_4$

To match a 4th-order accurate scheme with N grid points, a second-order accurate scheme needs N^2 grid points.

Example: 4th-order: $N = 10^3 \approx$ second-order: $N = 10^6$ grid points!

Maxwell's equations are solved in second-order form

Maxwell's equations:

$$\epsilon\mu\, \partial_t^2 \mathbf{E} = \Delta \mathbf{E} + \nabla\Big(\nabla \ln \epsilon \;\cdot \mathbf{E}\Big) + \nabla \ln \mu \times \Big(\nabla \times \mathbf{E}\Big) - \mu \partial_t \mathbf{j}$$

$$\epsilon\mu\, \partial_t^2 \mathbf{H} = \Delta \mathbf{H} + \nabla\Big(\nabla \ln \mu \;\cdot \mathbf{H}\Big) + \nabla \ln \epsilon \times \Big(\nabla \times \mathbf{H}\Big) + \epsilon \nabla \times (\frac{1}{\epsilon}\mathbf{j})$$

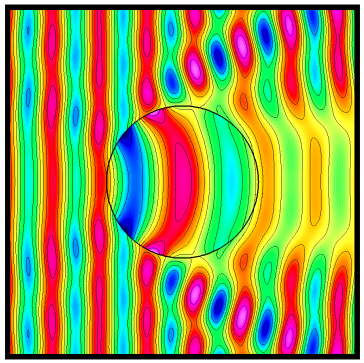
Advantages of the second-order form:

- No need for a staggered grid since the operator Δ is elliptic.
- One can solve for **E** alone.

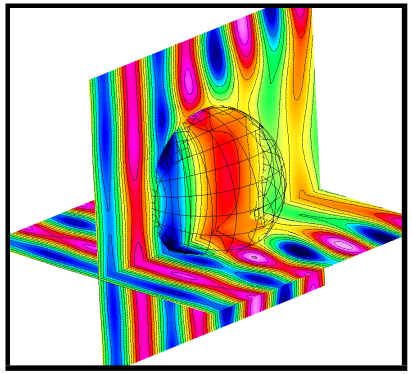
WDH, "A High-Order Accurate Parallel Solver for Maxwell's Equations on Overlapping Grids", SIAM J. Scientific Computing, 2006.

Key ingredients of the Cgmx Maxwell solver.

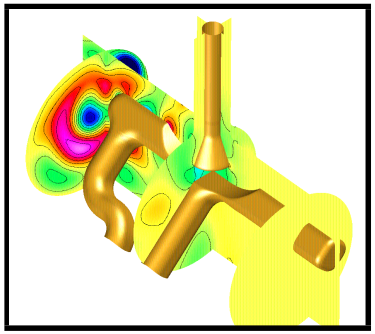
1. Fourth-order accurate space-time scheme with large (CFL=1) time step.
2. Symmetric difference approximations for curvilinear grids are energy conserving.
3. Compatibility based numerical boundary and interface conditions are more stable than one-side approximations.
4. Nearly as efficient as a Cartesian grid method.



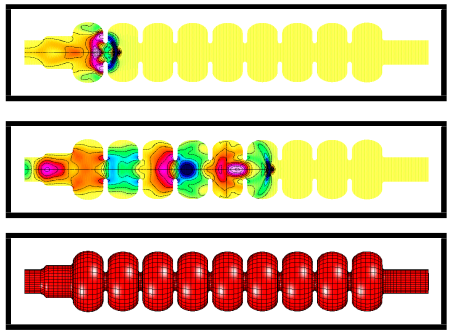
EM scattering from a dielectric cylinder.



Scattering from a dielectric sphere.



Accelerator HOM coupler.



Charge pulse in an accelerator.

Summary of the fourth-order numerical scheme

♢ Overlapping grids are used to cover the domain. The grids usually consist of narrow boundary fitted curvilinear grids and one or more large Cartesian background grids.
♢ Where grids overlap the solutions are interpolated using a 5th-order interpolation stencil with 5^d points in $d-$dimensions (with a double fringe of interpolation points).
♢ The vector wave equation is discretized in time using a modified-equation approach, giving, for example, the fourth-order accurate scheme

$$U^{n+1} - 2U^n + U^{n-1} = (c\Delta t)^2 \Delta_{4h} U^n + \frac{(c\Delta t)^4}{12} \Delta_{2h}^2 U^n$$

Here Δ_{mh} is a mth-order approximation to the Laplace operator.
This scheme is very efficient and allows a large (cfl=1) time step.

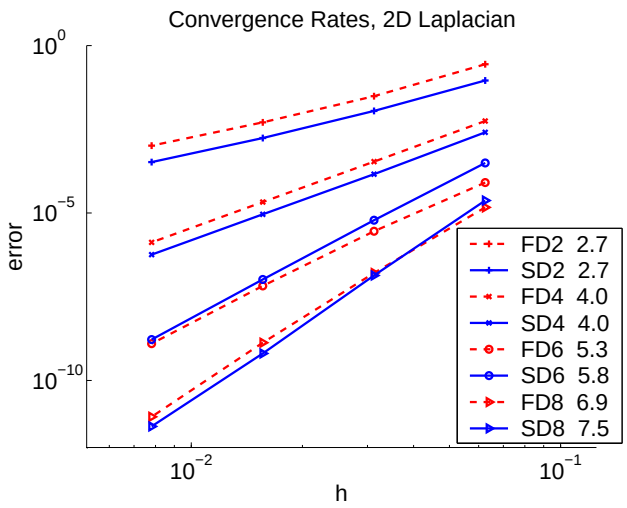
$$Lw = \nabla \cdot (a \nabla w) \; .$$

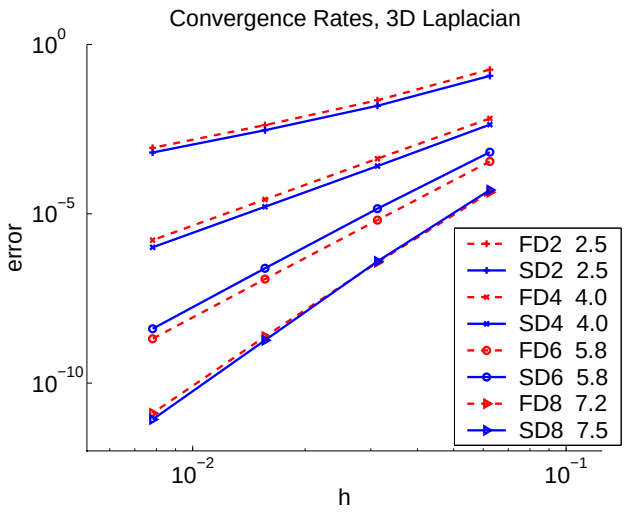
Standard finite difference approximations are based on transforming the equations from physical space **x** to computational space **r**,

$$Lw = a(\mathbf{r}) \frac{\partial r_n}{\partial x_i} \frac{\partial r_m}{\partial x_i} \frac{\partial^2 w}{\partial r_m \partial r_n} + \frac{\partial r_n}{\partial x_i} \left\{ a(\mathbf{r}) \frac{\partial}{\partial r_n} \left(\frac{\partial r_m}{\partial x_i} \right) + \frac{\partial a}{\partial r_n} \frac{\partial r_m}{\partial x_i} \right\} \frac{\partial w}{\partial r_m}. \tag{1}$$

The symmetric approximations are based on the *self-adjoint* form,

$$Lw = \frac{1}{J} \sum_{m=1}^{d} \sum_{n=1}^{d} \frac{\partial}{\partial r_m} \left(A^{mn} \frac{\partial w}{\partial r_n} \right), \quad A^{mn} = kJ \sum_{\mu=1}^{d} \sum_{\nu=1}^{d} \frac{\partial r_m}{\partial x_\mu} \frac{\partial r_n}{\partial x_\nu},$$





High-order accurate symmetric approximations for general curvilinear grids

The idea is approximate the derivative at the cell mid-point,

$$\frac{\partial w}{\partial r}(r \pm h/2) = D_{\pm}\left[1 + \sum_{n=1}^{m} \alpha_n h^{2n} (D_+ D_-)^n\right] w(r \pm h/2) + \mathcal{O}(h^{2m+2}),$$

and use this to approximate the second-derivative in conservation form:

$$\frac{\partial}{\partial r}\left(a\frac{\partial}{\partial r}\right) = D_+(a^{(m)}_{i-1/2} D_-) - \frac{h^2}{24}\left[D_+(a^{(m-2)}_{i-1/2} D_+ D_-^2) + D_+^2 D_-(a^{(m-2)}_{i-1/2} D_-)\right]$$
$$+ \frac{h^4}{24^2}\left[D_+^2 D_-(a^{(m-4)}_{i-1/2} D_+ D_-^2)\right] + \frac{3h^4}{640}\left[D_+(a^{(m-4)}_{i-1/2} D_+^2 D_-^3) + D_+^3 D_-^2(a^{(m-4)}_{i-1/2} D_-)\right] \ldots$$

where $D_+ w_i = (w_{i+1} - w_i)/h$, and $D_- w_i = (w_i - w_{i-1})/h$, and

$$a^{(2)}_{i-1/2} = \frac{1}{2}(a_i + a_{i-1}), \quad a^{(4)}_{i-1/2} = \frac{9}{16}(a_i + a_{i-1}) - \frac{1}{16}(a_{i+1} + a_{i-2}),$$

The resulting schemes are compact, symmetric and lead to energy conservation.

CBC: Compatibility boundary conditions

Numerical boundary conditions for high-order approximations

High-order accurate finite difference schemes with wide stencils need NBC's.

CBC's are more stable and accurate than one-side approximations.

$$\mathbf{E}_{tt} = \mathbf{E}_{xx} + \mathbf{E}_{yy} \quad \mathbf{x} \in \Omega = [0,1]^2$$

PEC (perfect electrical conductor) boundary at $x = 0$:

$$\begin{aligned} E^y(0,y,t) &= 0 \qquad (\text{from } \mathbf{n} \times \mathbf{E} = 0), \\ \partial_x E^x(0,y,t) &= 0 \qquad (\text{from } \nabla \cdot \mathbf{E} = 0). \end{aligned}$$

Taking time derivatives of the above and using the equations:

$$\begin{aligned} \partial_x^{2m} E^y(0,y,t) &= 0 \quad m = 0,1,2,3,\ldots \\ \partial_x^{2m+1} E^x(0,y,t) &= 0 \quad m = 0,1,2,3,\ldots \end{aligned}$$

These CBC's are used on the boundary instead of one-sided approximations. The extension to curvilinear geometry is nontrivial.

High-order accurate algorithms for incompressible flow

We have been developing high efficiency algorithms for modeling

1. incompressible flows and moving geometry,
2. fast solution of elliptic boundary value problems in complex geometry,

The approach is based on

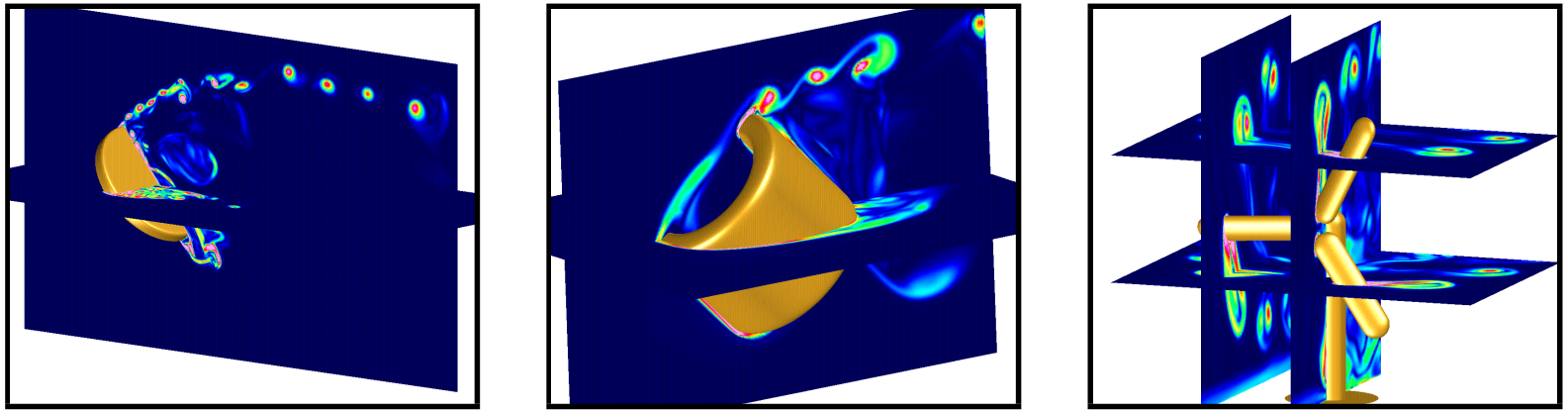
1. overlapping grids for flexible representation of geometry,
2. high-order accurate algorithms,
3. approximate factored operators and compact schemes,
4. matrix free multigrid algorithms,
5. accurate treatment of boundary conditions,
6. fast parallel grid generation.

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.

Compact discretizations to derivatives

Approximation to $\partial u/\partial x$,

$$\alpha\left(\frac{\partial u}{\partial x}\right)_{i+1} + \left(\frac{\partial u}{\partial x}\right)_{i} + \alpha\left(\frac{\partial u}{\partial x}\right)_{i-1} = a\left(\frac{u_{i+1}-u_{i-1}}{2h}\right) + b\left(\frac{u_{i+2}-u_{i-2}}{4h}\right)$$

$\alpha = 0,$	$a = 4/3,$	$b = -1/3$	: explicit 4th-order (5-pt)
$\alpha = 1/4,$	$a = 3/2,$	$b = 0$	: compact 4th-order (3-pt)
$\alpha = 1/3,$	$a = 14/9,$	$b = 1/9$	: compact 6th-order (5-pt)

Advantages: smaller stencil, smaller error constants

Disadvantages: requires solution of a tri-diagonal (penta-diagonal, ...) system, boundary conditions?

Ref. S.K. Lele, *Compact Finite Difference Schemes with Spectral-like Resolution*, JCP, 1992.

Approximate factorization & compact discretizations

A key point is maintaining accuracy at boundaries.

- Approximate factorization (AF) schemes offer larger timesteps with second order accuracy in time:

$$(I + \frac{\Delta t}{2}(A+B))U^{n+1} = (I - \frac{\Delta t}{2}(A+B))U^n$$

becomes

$$(I + \frac{\Delta t}{2}A)(I + \frac{\Delta t}{2}B)U^{n+1} \quad = \quad (I - \frac{\Delta t}{2}A)(I - \frac{\Delta t}{2}B)U^n$$

- *Compact schemes* can be integrated into the AF solves
- Special "combined" compact schemes have been developed:
  $\rightarrow$ reduce the number of factors

$$(a\partial_r + b\partial_{rr}^2)u \rightarrow P^{-1}(D_r a + D_{rr} b)u + \text{corrections}$$

  $\rightarrow$ preserve accuracy at boundaries
  $\rightarrow$ 4th and 6th order accuracy with a 5 point stencil
  $\rightarrow$ special penta-diagonal solvers that handle wider boundary stencils

Summary: High-order accurate approximations (HOA)

1. HOA are effective for wave propagation (e.g. EM) and problems with many scales (e.g. turbulence).
2. HOA work best on **smooth grids**.
3. Compatibility boundary conditions provide stable numerical boundary conditions.
4. Overlapping grids provide smooth grids for complex geometry.