Hyperbolic Conservation Laws
And
Visualization and Data Analysis
In Chombo

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Overview

• Hyperbolic Conservation Laws
  – Introduction
  – Examples
  – Discretization
  – Algorithm
  – Implementation
  – Additional Notes

• Visualization and Data Analysis
  – Introduction
  – Design/Architecture
  – Capabilities (Demonstration and Movies)
  – Features

• Remarks
  – Software Availability
  – Acknowledgments
Hyperbolic Conservation Laws - Introduction

- Hyperbolic Conservation Laws can be written in the form:

\[
\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = S
\]

- More explicit form:

\[
\frac{\partial U}{\partial t} + \sum_{d=0}^{D-1} \frac{\partial F^d(U)}{\partial x^d} = S
\]

- Changing to primitive variables, \( W = W(U) \):

\[
\frac{\partial W}{\partial t} + \sum_{d=0}^{D-1} A^d(W) \frac{\partial W^d}{\partial x^d} = S'
\]

\[
A^d = \nabla_U W \cdot \nabla_U F^d \cdot \nabla_W U
\]

\[
S' = \nabla_U W \cdot S
\]
Hyperbolic Conservation Laws - Examples

- 2D Gas Dynamics (Compressible Euler Equations):

\[ U = (\rho, \rho u_1, \rho u_2, \rho E) \]
\[ F^1 = (\rho u_1, \rho u_1^2 + p, \rho u_1 u_2, \rho u_1 E + u_1 p) \]
\[ F^2 = (\rho u_2, \rho u_1 u_2, \rho u_2^2 + p, \rho u_2 E + u_2 p) \]
\[ S = 0 \]
\[ W = (\rho, u_1, u_2, E) \]

\[ p = (\gamma - 1)\rho e \]
\[ e = (E - \frac{1}{2}(u_1^2 + u_2^2)) \]
Hyperbolic Conservation Laws - Examples

• Ideal MHD:

\[ U = (\rho, \rho\vec{u}, \vec{B}, \rho E) \]
\[ F = (\rho\vec{u}, \rho\vec{u}\cdot\vec{u} + (P + \frac{1}{8\pi}|\vec{B}|^2)I - \frac{1}{4\pi}\vec{B}\vec{B}, \]
\[ \vec{u}\vec{B} - \vec{B}\vec{u}, \]
\[ (\rho E + P + \frac{1}{8\pi}|\vec{B}|^2)\vec{u} - \frac{1}{4\pi}(\vec{u}\cdot\vec{B})\vec{B}) \]

\[ S = 0 \]

\[ W = (\rho, \vec{u}, \vec{B}, E) \]

\[ \rho E = (\frac{1}{2}\rho|\vec{u}|^2 + \frac{1}{8\pi}|\vec{B}|^2 + \frac{1}{\gamma-1}P) \]

\[ \nabla\cdot\vec{B} = 0 \]
Hyperbolic Conservation Laws - Discretization

- Notation and indexing: $i$ is a spatial index and $n$ is a time index:

- The spatial index and the time index are related to physical coordinates via $h$ and $\Delta t$, respectively
• Cells are grouped into boxes:

• Boxes are grouped into levels:
Hyperbolic Conservation Laws - Discretization

• Levels at different resolutions are nested:

• This nesting allows the coarser level to define the boundary conditions for the finer level:
Hyperbolic Conservation Laws - Discretization

- Consider a single level (collection of boxes) at a fixed resolution
- Approximate the divergence of the flux in each cell of each box:

\[ \nabla \cdot \vec{F} \approx D \vec{F} \equiv \frac{1}{h} \sum_{d=0}^{D-1} \left( F_{i+\frac{1}{2}e_d}^d - F_{i-\frac{1}{2}e_d}^d \right) \]

- This is exact if \( \nabla \cdot \vec{F} \) was a cell average and the \( F_{i\pm\frac{1}{2}e_d}^d \) were face averages (divergence theorem)
• Second-order accurate in space if fluxes are second-order accurate

• Update the solution:

\[ U^{n+1} = U^n - \Delta t(D\vec{F}) , \quad \vec{F} = \vec{F}(U^n) \]

• The critical element is the accurate computation of \( F^d \) in space and time

• Second-order accuracy in time is achieved by using a predictor-corrector method
Hyperbolic Conservation Laws - Algorithm

Given \( U^n_i \) and \( S^n_i \), we want to compute a second-order accurate estimate of the fluxes:

\[
F_i^{n+\frac{1}{2}} \approx F^d(x_0 + (i + \frac{1}{2}e^d)h, t^n + \frac{1}{2}\Delta t)
\]

1. Compute the effect of the normal derivative terms and the source term on the extrapolation in space and time from cell centers to faces. For \( 0 \leq d < D \):

\[
W_{i,\pm,d} = W_i^n + \frac{1}{2}(\pm I - \frac{\Delta t}{h}A_i^d)P_\pm(\Delta^dW_i)
\]

\[
A_i^d = A^d(W_i)
\]

\[
P_\pm(W) = \sum_{\pm\lambda_k > 0} (l_k \cdot W)r_k
\]

\[
W_{i,\pm,d} = W_{i,\pm,d} + \frac{\Delta t}{2} \nabla U W \cdot S_i^n
\]
where \( \lambda_k \) are eigenvalues of \( A_i^d \), and \( l_k \) and \( r_k \) are the corresponding left and right eigenvectors.

2. Compute estimates of \( F^d \) suitable for computing 1D flux derivatives \( \frac{\partial F^d}{\partial x^d} \) using a Riemann solver for the interior, \( R \), and for the boundary, \( R_B \). Here, and in what follows, \( \nabla U W \) need only be first-order accurate, e.g., differ from the value at \( U_i^n \) by \( O(h) \):

\[
F_{i+\frac{1}{2}e^d}^{1D} = R(W_{i,+d}, W_{i+e^d,-d}, d) \\
| R_B(W_{i,+d}, (i + \frac{1}{2}e^d)h, d) \\
| R_B(W_{i+e^d,-d}, (i + \frac{1}{2}e^d)h, d)
\]

3. In 3D compute corrections to \( W_{i,\pm,d} \) corresponding to one set of transverse derivatives appropriate to obtain \((1, 1, 1)\)
diagonal coupling. In 2D skip this step:

\[ W_{i,\pm,d_1,d_2} = W_{i,\pm,d_1} - \frac{\Delta t}{3h} \nabla U W \cdot (F_{i+\frac{1}{2}e^{d_2}}^{1D} - F_{i-\frac{1}{2}e^{d_2}}^{1D}) \]

4. In 3D compute fluxes corresponding to corrections made in the previous step. In 2D skip this step:

\[ F_{i+\frac{1}{2}e^{d_1},d_2} = R(W_{i,+,d_1,d_2}, W_{i+e^{d_1},-,d_1,d_2}, d_1) \]

\[ \left| R_B(W_{i,+,d_1,d_2}, (i + \frac{1}{2}e^{d_1})h, d_1) \right| \]

\[ \left| R_B(W_{i+e^{d_1},-,d_1,d_2}, (i + \frac{1}{2}e^{d_1})h, d_1) \right| \]

5. Compute final corrections to \( W_{i,\pm,d} \) due to the final transverse
derivatives:

2D: \( W_{i,\pm,d}^{n+\frac{1}{2}} = W_{i,\pm,d} - \frac{\Delta t}{2h} \nabla U W \cdot (F_{i+\frac{1}{2}e_1}^{1D} - F_{i-\frac{1}{2}e_1}^{1D}) \)

3D: \( W_{i,\pm,d}^{n+\frac{1}{2}} = W_{i,\pm,d} - \frac{\Delta t}{2h} \nabla U W \cdot (F_{i+\frac{1}{2}e_1,d_2}^{1D} - F_{i-\frac{1}{2}e_1,d_2}^{1D}) \)

\[ - \frac{\Delta t}{2h} \nabla U W \cdot (F_{i+\frac{1}{2}e_2,d_1}^{1D} - F_{i-\frac{1}{2}e_2,d_1}^{1D}) \]

6. Compute final estimate of fluxes:

\( F_{i+\frac{1}{2}e_d}^{n+\frac{1}{2}} = R(W_{i,+d}^{n+\frac{1}{2}}, W_{i+e_d,-d}^{n+\frac{1}{2}}, d) \)

\[ \left| R_B(W_{i,+d}^{n+\frac{1}{2}}, (i + \frac{1}{2}e_d)h, d) \right| \]

\[ \left| R_B(W_{i+e_d,-d}^{n+\frac{1}{2}}, (i + \frac{1}{2}e_d)h, d) \right| \]
7. Update the solution using the divergence of the fluxes:

\[ U_{i}^{n+1} = U_{i}^{n} - \frac{\Delta t}{h} \sum_{d=0}^{D-1} (F_{i+\frac{1}{2}e_{d}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}e_{d}}^{n+\frac{1}{2}}) \]

- Fourth order slope calculations with limiting and flattening
- Extensions to piecewise parabolic methods (PPM)
- Second-order accurate in space and time
- “Accurate” shock capture - robust and stable
- This is an “unsplit” algorithm for the updating of the conservative quantities, \( U \)
- Everything has been reduced to computations that can be computed box by box (if ghost cells are used) and all reduced to 1D
Hyperbolic Conservation Laws - Implementation

• All physics independent code has been implemented and requires no modification by the user:
  – The framework for time dependent, adaptive mesh refinement (AMR) computations, including: AMR mesh generation, time step control, interaction between levels
  – All the computations for hyperbolic conservation laws with the exception of a handful of physics dependent routines
  – Parallel computation without modifications to code - only recompilation
Hyperbolic Conservation Laws - Implementation

• Recall Step 1 of the algorithm:

\[ W_{i,\pm,d} = W_i^n + \frac{1}{2} \left( \pm I - \frac{\Delta t}{h} A_i^d \right) P_\pm (\Delta^d W_i) \]

\[ A_i^d = (\nabla_U W)_i \cdot \nabla_U F_i^d \cdot (\nabla_W U)_i \]

• The following physics dependent routines must be provided by the user:
  
  – Eigen-analysis of the linearization of \( A^d(W) \):
    transformations between characteristic variables (eigenvectors) and primitive variables, computation of eigenvalues
  
  – The solution to 1D Riemann problems given the primitive variable values on each side of a face
  
  – Quasilinear update - computation of: \( A^d(W) P_\pm (\Delta^d W) / h \)
  
  – Maximum wave speed (in a box) given the conserved
variable values (in the box)

- The transformation of conserved variables to primitive variables
- The computation of fluxes on a face given the value of the primitive variables on the face
- Physical boundary conditions - if the boundaries of the domain are periodic then this is trivial to provide
- Various bookkeeping functions - number of conserved variables, number of primitive variables, etc.
Hyperbolic Conservation Laws - Additional Notes

- Some current work using Chombo’s framework:
  - Gas Dynamics - Current example in Chombo library (PLM and PPM)
  - Ideal MHD - Ravi Samtaney (PPPL/ANAG), Rob Crockett (UCB Physics)
  - Self Gravitating Gas Dynamics with MHD and coupling to collisionless particles - Francesco Miniati (ETH)

- Current development:
  - Particle computations
  - Multifluid computations
Visualization and Data Analysis - Introduction

• ChomboVis - visualization and data analysis tool for AMR data

• Some capabilities:
  – Grid display
  – Data slices
  – Contours / Isosurfaces
  – Streamlines
  – Clipping
  – Data selection and spreadsheets
  – State saving and restoring
  – Creation of derived quantities

• Driven by user’s needs and funding

• One fulltime developer
Visualization and Data Analysis - Design/Architecture

- Built modularly using existing software packages: Python, VTK, Tk, HDF5
- Scripting language with all functionality available
- Data viewing and analysis a core requirement
- Use of OpenGL graphics acceleration including advanced graphics capabilities (e.g., texture mapping)
- Reads and writes data using HDF5 which is machine independent/portable
- Customization via startup file using scripting language
- Data read and stored only on demand
- Non-graphical versions of ChomboVis provided
- Core visualization and data analysis tool of developers
Visualization and Data Analysis - Capabilities

Demonstration and Movies
Visualization and Data Analysis - Features

- Different data centerings
- Multiple tools synchronized (master/slave)
- Offscreen rendering
- Rendering directly to encapsulated PostScript (vector output)
- Particles
- Embedded Boundaries
- Multifluids
Remarks - Software Availability

- Software and documentation is available locally on “joshuatreep” under “/usr/local/chombo”

- Also available on the ANAG WWW site: http://seesar.lbl.gov/anag under “Software”

- E-mail to the developers:
  - chombo@hpcrd.lbl.gov (Chombo)
  - chombovis@hpcrd.lbl.gov (ChomboVis)

- This talk is available at:
  - “joshuatreep” under “/usr/local/chombo” as “talk-March28.pdf”
  - http://seesar.lbl.gov/anag/staff/ligocki/index.html under the IPAM link
Remarks - Acknowledgments

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