FYS-GEO 4500

Lecture Notes #4 Boundary Conditions & Accuracy

FYS-GEO 4500

Where we are today

		date	Торіс	Chapter in LeVeque
	1	1.Sep 2011	introduction to conservation laws, Clawpack	1 & 2
	2	15.Sep 2011	the Riemann problem, characteristics	3 & 5
	3	22.Sep 2011	finite volume methods for linear systems, high resolution	4 & 6
	4	29.Sep 2011	boundary conditions, accuracy, variable coeff.	7,8, part 9
	5	6.Oct 2011	nonlinear conservation laws, finite volume methods	11 & 12
	6	13.Oct 2011	nonlinear equations & systems	13 & 14
	7	20.Oct 2011	finite volume methods for nonlinear systems	14 & 15
	8	27.Oct 2011	source terms and multidimensions	16,17,18,19
	9	3.Nov 2011	multidimensional systems	20 & 21
		10.Nov 2011	no lecture	
	10	17.Nov 2011	waves in elastic media	22
	11	24.Nov 2011	unfinished business: capacity functions, source terms, project plans	
	12	1.Dec 2011	student presentations	
		8.Dec 2011	no lecture	
	*13	15.Dec 2011	FINAL REPORTS DUE	

We improve the first-order upwind method by introducing corrections, and writing:

$$Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} \left(\mathcal{A}^{+} \Delta Q_{i-1/2} + \mathcal{A}^{-} \Delta Q_{i+1/2} \right) - \frac{\Delta t}{\Delta x} \left(\widetilde{F}_{i+1/2} - \widetilde{F}_{i-1/2} \right)$$

We derive the corrections by considering piece-wise linear (instead of piecewise constant) reconstructions.



Taking the basic Lax-Wendroff formula:

$$Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{2\Delta x} A \left(Q_{i+1}^{n} - Q_{i-1}^{n} \right) + \frac{1}{2} \left(\frac{\Delta t}{\Delta x} \right)^{2} A^{2} \left(Q_{i+1}^{n} - 2Q_{i}^{n} + Q_{i-1}^{n} \right)$$

we re-write it in the flux form

$$Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} \left(F_{i+1/2}^{n} - F_{i-1/2}^{n} \right)$$

with

$$F_{i-1/2}^{n} = \frac{1}{2} A \left(Q_{i}^{n} + Q_{i-1}^{n} \right) - \frac{1}{2} \frac{\Delta t}{\Delta x} A^{2} \left(Q_{i}^{n} - Q_{i-1}^{n} \right)$$

Then making use of the divided matrices A^{\pm} we can write this as

$$F_{i-1/2}^{n} = \left(A^{-}Q_{i}^{n} + A^{+}Q_{i-1}^{n}\right) + \frac{1}{2}|A|\left(I - \frac{\Delta t}{\Delta x}|A|\right)\left(Q_{i}^{n} - Q_{i-1}^{n}\right)$$

FYS-GEO 4500

$$F_{i-1/2}^{n} = \left(A^{-}Q_{i}^{n} + A^{+}Q_{i-1}^{n}\right) + \frac{1}{2}|A|\left(I - \frac{\Delta t}{\Delta x}|A|\right)\left(Q_{i}^{n} - Q_{i-1}^{n}\right)$$

This version of the Lax-Wendroff formula has a correction term that can be limited, if we choose, to avoid oscillations around extrema.

For a one-equation system (the advection equation), we can apply a simple functional limiter to the slope:

$$\sigma_i^n = \left(\frac{Q_{i+1}^n - Q_i^n}{\Delta x}\right)\phi_i^n$$

Examples of limiters:

Lax-Wendroff:
$$\phi(\theta) = 1$$

minmod: $\phi(\theta) = \min(1,\theta)$
superbee: $\phi(\theta) = \max(0,\min(1,2\theta),\min(2,\theta))$
MC: $\phi(\theta) = \max(0,\min((1+\theta)/2,2,2\theta))$
vanLeer: $\phi(\theta) = \frac{(\theta + |\theta|)}{(1+|\theta|)}$

5

For a system of equations, we use limiters on the waves. The wavepropagation form for a high-resolution version of Lax-Wendroff is:

$$F_{i-1/2}^{n} = \left(A^{-}Q_{i}^{n} + A^{+}Q_{i-1}^{n}\right) + \frac{1}{2}\sum_{p=1}^{m} \left|s_{i-1/2}^{p}\right| \left(1 - \frac{\Delta t}{\Delta x} \left|s_{i-1/2}^{p}\right|\right) \widetilde{\mathcal{W}}_{i-1/2}^{p}$$

with the limited version of the waves defined as :

$$\widetilde{\mathcal{W}}_{i-1/2}^{p} = \alpha_{i-1/2}^{p} \phi(\theta_{i-1/2}^{p}) r^{p}$$

and a generalised wave speed

$$s_{i-1/2}^p = \lambda^p$$



High-Resolution methods

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Autumn 2011

Boundary Conditions (Chapter 7 in Leveque)

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Real problems have boundaries



In computing the values Q_i^{n+1} for the next time step, we have assumed the availability of data from Q_{i-1}^n and Q_{i+1}^n . But we can never compute on an infinite grid, and in practice we must often deal with physical boundaries such as solid walls or materials with different properties.

Real problems have boundaries



In computing the values Q_i^{n+1} for the next time step, we have assumed the availability of data from Q_{i-1}^n and Q_{i+1}^n . But we can never compute on an infinite grid, and in practice we must often deal with physical boundaries such as solid walls or materials with different properties.

Calculation from the Stanford Center for Turbulence Research of a portion of the main compressor turbine in a modern jet engine. There are inflow and outflow boundaries as well as internal reflective boundaries for the turbine fan blades. The coordinate system rotates with the turbine, which starts slowly and approaches cruising speed.

This calculation couples to a separate calculation for the combustor, which uses the outflow from the compressor, and supplies the energy to rotate the turbine.

FYS-GEO 4500



Calculation from the Stanford Center for Turbulence Research of a portion of the main compressor turbine in a modern jet engine. There are inflow and outflow boundaries as well as internal reflective boundaries for the turbine fan blades. The coordinate system rotates with the turbine, which starts slowly and approaches cruising speed.

This calculation couples to a separate calculation for the combustor, which uses the outflow from the compressor, and supplies the energy to rotate the turbine.

FYS-GEO 4500

Boundary conditions may be of several different types



11

One common approach is to use ghost cells

Physical boundary of problem Ghost cells are cells that participate in the computational scheme, but are reset at the beginning of each time step to values that effectively implement the appropriate boundary condition. If this is done, then no special formulas are needed on the physical boundary during the computational step. A two-dimensional grid with a border Ghost cells of two ghost cells on all boundaries

FYS-GEO 4500

Boundary conditions in one dimension.



The solution in the domain [a,b] is the *interior solution*, and is computed by the wave-propagation procedure, solving Riemann problems at each interface.

To compute the appropriate fluxes to update cells 1 and N, we need values from the neighbouring ghost cells (0,-1) and (N+1, N+2). These are provided by the boundary-condition procedure.

This boundary-condition procedure will depend on the nature of the boundary conditions being used.

FYS-GEO 4500

12

Boundary conditions in one dimension.



The solution in the domain [a,b] is the *interior solution*, and is computed by the wave-propagation procedure, solving Riemann problems at each interface.

To compute the appropriate fluxes to update cells 1 and N, we need values from the neighbouring ghost cells (0,-1) and (N+1, N+2). These are provided by the boundary-condition procedure.

This boundary-condition procedure will depend on the nature of the boundary conditions being used.

Periodic boundary conditions



For periodic boundary conditions, we simply set

$$Q_{-1} = Q_{N-1}, \quad Q_0 = Q_N, \quad Q_{N+1} = Q_1, \quad Q_{N+2} = Q_2.$$

at the beginning of each time step.

In Clawpack, the work is done in the Fortran routine \$CLAW/clawpack/ld/lib/bc1.f

and you invoke it in setrun.py by setting
 clawdata.mthbc_xlower = 2
 clawdata.mthbc_xupper = 2

FYS-GEO 4500

Outflow boundary conditions



For a pure upwind method, we don't need any outflow boundary condition. But we do for higher-order methods, and if waves are travelling in both directions.

The simplest and most effective procedure is simply to extrapolate the solution from the last physical cell. If the outflow boundary is at right, we set:

$$Q_{N+1}=Q_N, \quad Q_{N+2}=Q_N$$

for a zero-order or constant extrapolation, or

$$Q_{N+1} = 2Q_N - Q_{N-1}, \ Q_{N+2} = 3Q_N - 2Q_{N-1}$$

for a first-order or linear extrapolation. In most circumstances, constant extrapolation gives better stability.

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

14

Inflow boundary conditions



For inflow conditions it is sufficient to reset the ghost cells on the inflow boundary to the desired source values, which may be time-dependent.

For the advection equation with velocity u, and the inflow boundary at right, set

$$Q_0 = Q_{source}\left(t + \frac{\Delta x}{2u}\right), \quad Q_{-1} = Q_{source}\left(t + \frac{3\Delta x}{2u}\right).$$

Note that we advance the time by the travel time from the centre of each of these cells to the physical boundary.

FYS-GEO 4500

15



For systems with both positive and negative eigenvalues, each boundary may have both incoming and outgoing characteristics.

Then you treat the boundary cells with the normal Riemann solution, for example

$$Q_1 - Q_0 = \sum_{p=1}^m \mathcal{W}_{1/2}^p,$$

but the incoming waves have strength zero. The outgoing waves may have nonzero strength, but it doesn't matter since the ghost cells will be reset at the start of the next cycle.

It should be possible to apply the appropriate boundary conditions for the separate characteristics, with some knowledge of the appropriate physics.

FYS-GEO 4500

16

An example from the acoustics equation

solid reflecting wall



Recall the acoustics equations

$$p_t + Ku_x = 0$$
$$\rho_0 u_t + p_x = 0$$

To implement a solid reflecting wall in this system, we reverse the velocity in the ghost cells and make the pressure the same:

for
$$Q_0$$
: $p_0 = p_1$, $u_0 = -u_1$
for Q_{-1} : $p_{-1} = p_2$, $u_{-1} = -u_2$

FYS-GEO 4500

17

Set the boundary conditions in setrun.py



FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Advection equation: left inflow, right outflow

from \$CLAW/book/chap7/advinflow

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Autumn 2011

19

Advection equation: left inflow, right outflow



FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

19

20

Acoustic equations: left inflow, right reflective

from \$CLAW/book/chap7/acouinflow

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Acoustic equations: left inflow, right reflective



from \$CLAW/book/chap7/acouinflow

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

20

Acoustic equations: left and right reflective

from \$CLAW/book/chap7/standing

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Autumn 2011

21

Acoustic equations: left and right reflective



from \$CLAW/book/chap7/standing

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Accuracy and Convergence (Chapter 8 in Leveque)

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Accuracy, stability, and convergence: how do we ensure confidence in the code?

Numerical computation is still an art; there are many things that can go wrong in a calculation.

It is important to be suspicious of peculiar behaviour, but even if things *look* right, they may not *be* right!

Code systems are subject to a variety of tests to ensure correct behaviour:

Verification: test the code solutions against analytical solutions for simple problems.

Validation: test the code solutions against experimental results.

Convergence: prove that the code solution converges to the correct solution as the grid is refined.

Uncertainty Quantification: develop confidence measures that tell us how much we can rely on the results.

23

One way of putting it:

One way of putting it:

Precision - the number of significant digits in a measurement

24

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

24

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

Precision - is improved by reducing *experimental* or *measurement* error

24

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

Precision - is improved by reducing *experimental* or *measurement* error

Accuracy - is improved by reducing systematic error

24
Do you understand the difference between precision and accuracy?

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

Precision - is improved by reducing *experimental* or *measurement* error

Accuracy - is improved by reducing systematic error

In calculations:

Do you understand the difference between precision and accuracy?

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

Precision - is improved by reducing *experimental* or *measurement* error

Accuracy - is improved by reducing systematic error

In calculations:

Precision - is related to the correct implementation of the numerical algorithm

Do you understand the difference between precision and accuracy?

One way of putting it:

Precision - the number of significant digits in a measurement

Accuracy - how close a measurement is to a true value

Another way:

Precision - is improved by reducing *experimental* or *measurement* error

Accuracy - is improved by reducing systematic error

In calculations:

Precision - is related to the correct implementation of the numerical algorithm

Accuracy - is related to the physical relevance of the algorithm, the validity of the assumptions and the proper use of input data

FYS-GEO 4500

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

 $(v-c)/c = (2.48 \pm 0.28 \text{ (stat.)} \pm 0.30 \text{ (sys.)}) \times 10^{-5}$

25

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

 $(v-c)/c = (2.48 \pm 0.28 \text{ (stat.)} \pm 0.30 \text{ (sys.)}) \times 10^{-5}$

Is this result precise?

FYS-GEO 4500

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

 $(v-c)/c = (2.48 \pm 0.28 \text{ (stat.)} \pm 0.30 \text{ (sys.)}) \times 10^{-5}$

Is this result precise?

Is this result accurate?

FYS-GEO 4500

25

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

 $(v-c)/c = (2.48 \pm 0.28 \text{ (stat.)} \pm 0.30 \text{ (sys.)}) \times 10^{-5}$

Is this result precise?

Is this result accurate?

How about this one: $(v-c)/c = 5.1 \pm 2.9 \times 10^{-5}$?

25

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

 $(v-c)/c = (2.48 \pm 0.28 \text{ (stat.)} \pm 0.30 \text{ (sys.)}) \times 10^{-5}$

Is this result precise?

Is this result accurate?

How about this one: $(v-c)/c = 5.1 \pm 2.9 \times 10^{-5}$? Or this one: $|v-c|/c < 2 \times 10^{-9}$ 25

From a recent experimental result:

$$\Delta t = (60.7 \pm 6.9 \text{ (stat.)} \pm 7.4 \text{ (sys.)}) \text{ ns}$$

(v-c)/c = (2.48 ± 0.28 (stat.) ± 0.30 (sys.)) ×10⁻⁵

Is this result precise?

Is this result accurate?

How about this one:

Or this one:

Do we really know yet?

 $|v-c|/c < 2 \times 10^{-9}$

 $(v-c)/c = 5.1 \pm 2.9 \times 10^{-5}$?

FYS-GEO 4500

OPERA

MINOS

SN 1987A

Truncation error: Your functional representation is incomplete; you can't include all the terms in the Taylor series, for example.

26

- **Truncation error**: Your functional representation is incomplete; you can't include all the terms in the Taylor series, for example.
- **Roundoff error**: The computer's representation of a real number is imprecise; least significant digits are dropped. *Beware subtracting numbers of similar magnitude!*

- **Truncation error**: Your functional representation is incomplete; you can't include all the terms in the Taylor series, for example.
- **Roundoff error**: The computer's representation of a real number is imprecise; least significant digits are dropped. *Beware subtracting numbers of similar magnitude!*
- Numerical diffusion, numerical viscosity: The finite resolution of a gridded calculation fails to resolve fine physical structures, which then diffuse on the scale of the grid resolution.

- **Truncation error**: Your functional representation is incomplete; you can't include all the terms in the Taylor series, for example.
- **Roundoff error**: The computer's representation of a real number is imprecise; least significant digits are dropped. *Beware subtracting numbers of similar magnitude!*
- Numerical diffusion, numerical viscosity: The finite resolution of a gridded calculation fails to resolve fine physical structures, which then diffuse on the scale of the grid resolution.
- **Imperfect boundary conditions**: Outgoing waves may partially reflect back into the grid, causing distortions.

- **Truncation error**: Your functional representation is incomplete; you can't include all the terms in the Taylor series, for example.
- **Roundoff error**: The computer's representation of a real number is imprecise; least significant digits are dropped. *Beware subtracting numbers of similar magnitude!*
- Numerical diffusion, numerical viscosity: The finite resolution of a gridded calculation fails to resolve fine physical structures, which then diffuse on the scale of the grid resolution.
- **Imperfect boundary conditions**: Outgoing waves may partially reflect back into the grid, causing distortions.

The most obvious, and easiest to deal with, are the following:

Errors in setup, incorrect initial conditions, or bogus material properties Coding errors (bugs)

FYS-GEO 4500

26

Measures of error

In a finite volume method, the numerical solution value Q_i^n in grid cell *i* is an approximation to the cell integral of the true solution

$$q_i^n = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x,t_n) dx.$$

If the solution is sufficiently smooth, this is also reasonably close to the value $q(x_i, t_n)$ at the cell centre. We may choose to compare Q_i^n with either of q_i^n or $q(x_i, t_n)$.

Errors tend to grow with time, so we need to specify the time at which the error comparison of the computed solution against the calculated solution is made. If the comparison is done at time $T = N\Delta t$, we denote the global error as

$$E^N = Q^N - q^N.$$

We will assume that the ratio $\frac{\Delta t}{\Delta x}$ is constant as we refine the grid.

The global error: norms

The global error $E^N = Q^N - q^N$ is computed from the errors at each grid cell by using an appropriate norm. A *p*-norm is defined by:

$$\left\|E\right\|_{p} = \left(\Delta x \sum_{i} \left|E_{i}\right|^{p}\right)^{1/p}$$

The most useful norms are the 1-norm (corresponding to the solution integrals) the 2-norm (the root-mean-square error) and the infinity-norm, or maximum overall error, which measures point-wise convergence:

$$||E||_{\infty} = \max_{i} |E_{i}|.$$

Point-wise convergence is generally impossible when the solutions are not smooth.

28

Convergence and Accuracy

There's some divergence of terminology in this area.

Leveque gives the following definition for *convergence*:

$$\lim_{\Delta t \to 0} \left\| E^N \right\| = 0 \text{ at time } T \text{ where } N\Delta t = T,$$

and he writes that a method is accurate to order s if

$$||E^N|| = \mathcal{O}(\Delta t^s) \text{ as } \Delta t \to 0.$$

Very often you will hear people speak of a method as *convergent to order s* if

$$\frac{\left\|E\right\|_{k\Delta x}}{\left\|E\right\|_{\Delta x}} \sim k^{s},$$

where $||E||_{\Delta x}$ is the error evaluated on a grid with spacing Δx . This latter notion enables convergence (or resolution) studies in the absence of knowledge of the true solution, but invites the danger that a method may be validated while converging to the wrong solution!

FYS-GEO 4500

Variants of the classic shock tube problem are used for code validation



pressure

density

velocity

Above is the exact analytical solution, resolved to a finite grid, for a *spherical* implosion shock. We used this as a validation test for the Sage/Rage code at Los Alamos.

Variants of the classic shock tube problem are used for code validation



Thursday, 6 October 2011

An accuracy and convergence study on an analytical test problem

A calculation of the Noh spherical shock tube problem in two dimensions with the Rage code (Los Alamos, SAIC).

We used the *p*-1 norm, summed in bands instead of over the whole domain, to illustrate differences in convergence in different parts of the solution space.

Outside the shock we saw 2nd order convergence, as expected from the algorithm, but within the shock the convergence was at best linear. The position of the shock was accurately determined, and it was sharp at all resolutions.



An accuracy and convergence study on an analytical test problem

A calculation of the Noh spherical shock tube problem in two dimensions with the Rage code (Los Alamos, SAIC).

We used the *p*-1 norm, summed in bands instead of over the whole domain, to illustrate differences in convergence in different parts of the solution space.

Outside the shock we saw 2nd order convergence, as expected from the algorithm, but within the shock the convergence was at best linear. The position of the shock was accurately determined, and it was sharp at all resolutions.



FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

An accuracy and convergence study on an analytical test problem

A calculation of the Noh spherical shock tube problem in two dimensions with the Rage code (Los Alamos, SAIC).

We used the *p*-1 norm, summed in bands instead of over the whole domain, to illustrate differences in convergence in different parts of the solution space.

Outside the shock we saw 2nd order convergence, as expected from the algorithm, but within the shock the convergence was at best linear. The position of the shock was accurately determined, and it was sharp at all resolutions.



Analytical Solution **RAGE-Analytical** 3 **RAGE Solution** Bands for Analysis 150XI50 300X300

A resolution (not convergence!) study



Thursday, 6 October 2011

A resolution (not convergence!) study



Thursday, 6 October 2011





Near-field wave amplitude is sensitive to resolution, but wave kinematics is not



Consistency, robustness, and numerical stability

Errors occur at each time step as a simulation progresses. These are inevitable because of the approximations involved (*truncation error*) and because of machine accuracy (*round-off error*).

A method is *consistent* if the error introduced at a single time step is small.

Small single-step errors affect the calculation subsequently. After hundreds or thousands of time steps, these errors accumulate and the numerical solution diverges from the true solution.

The divergence will be *bounded* if the method is *stable*. If the method is unstable, the errors grow exponentially.

The method is *robust* if small changes in the input parameters produce reasonably small changes in the solution after many time steps.

Robustness is tested by running many simulations with different inputs; consistency and stability can be checked analytically.

The Lax-Richtmeyer equivalence theorem states that:

A numerical method for a linear differential equation will converge if that method is *consistent* and *stable*.

Consistency means the single-step error is small.

Stability means that single-step errors do not grow catastrophically with time.

Single-step errors

A single step of a numerical method can be written as

$$Q^{n+1}=\mathcal{N}(Q^n),$$

where the operator \mathcal{N} maps the approximate solution at one time step to the next time step. We define the local truncation error by applying the same operator to the *true* solution at time step n and comparing it to the true solution (resolved to the grid) at time step n+1:

truncation error
$$= \tau^n = \frac{1}{\Delta t} \mathcal{N}(q^n) - q^{n+1}.$$

If $\lim_{\Delta t \to 0} \tau^n = 0$ then the method is consistent with the differential equation.

The truncation error is calculated by doing a Taylor series expansion and estimating the size of all the terms that are omitted from the numerical approximation.

FYS-GEO 4500

38

Assessing stability for linear methods

If at time step *n* we have an error $E^n = Q^n - q^n$, then at time step n+1 our error will be

$$E^{n+1} = \mathcal{N}(q^n + E^n) - q^{n+1}$$

= $\underbrace{\mathcal{N}(q^n + E^n) - \mathcal{N}(q^n)}_{\text{propagation of previous errors}} + \underbrace{\Delta t \tau^n}_{\text{single-step error}}$

If the numerical solution operator \mathcal{N} is *contractive,* that is if

$$\left\|\mathcal{N}(P) - \mathcal{N}(Q)\right\| \leq \left\|P - Q\right\|$$

in an appropriate norm, then the operator is stable in that norm, and we get a bound on the global error:

$$\left\|E^{N}\right\| \leq \left\|E^{0}\right\| + \sum_{n=1}^{N} \Delta t \left\|\tau^{n}\right\|.$$

Unfortunately, it may be difficult to prove contractivity for nonlinear systems. In that case, we insist on Total Variation Diminishing methods, which accomplishes the same thing.

FYS-GEO 4500

The formal order of accuracy isn't a guarantee of true accuracy!



Comparing the 2nd-order accurate Lax-Wendroff with a high-resolution method of lower *formal* order: the high-resolution method is more accurate for all but the finest grids in the max norm.

FYS-GEO 4500

Variable Coefficients (Chapter 9 in Leveque)

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

A brief-look at variable-coefficient problems

Before we get into nonlinear equations and systems, it's useful to consider systems of the form:

$$q_t + A(x)q_x = 0$$

or the similar conservation law:

$$q_t + (A(x)q)_x = 0$$

or the capacity-function form:

$$\kappa(x)q_t + (A(x)q)_x = 0$$

Real examples include: advection of a tracer in a pipe with variable crosssection, two conveyor belts with different speeds, traffic flow on a highway with a sudden change in the speed limit, or linear acoustics in a layered medium.

FYS-GEO 4500
We'll look at the acoustics equations with variable coefficients

The equation is
$$q_t + A(x)q_x = 0$$

with
$$q(x,t) = \begin{bmatrix} p(x,t) \\ u(x,t) \end{bmatrix} A(x) = \begin{bmatrix} 0 & K(x) \\ 1/\rho(x) & 0 \end{bmatrix}$$

and the eigensystem is

$$R(x) = \begin{bmatrix} -Z(x) & Z(x) \\ 1 & 1 \end{bmatrix} \quad \Lambda(x) = \begin{bmatrix} -c(x) & 0 \\ 0 & c(x) \end{bmatrix}$$

where

$$c(x) = \sqrt{\frac{K(x)}{\rho(x)}} \qquad Z(x) = \rho(x)c(x) = \sqrt{K(x)\rho(x)}$$

43

The coefficients are *piece-wise* constant ...

We consider a medium with a discontinuity in the coefficients:

$$\rho(x) = \begin{cases} \rho_l & \text{if } x < 0, \\ \rho_r & \text{if } x > 0, \end{cases} \quad K(x) = \begin{cases} K_l & \text{if } x < 0, \\ K_r & \text{if } x > 0. \end{cases}$$

and consider it with the piecewise constant initial data

$$q(x,0) = \begin{cases} q_l & \text{if } x < 0, \\ q_r & \text{if } x > 0. \end{cases}$$

Much as before, we have the Riemann problem illustrated here:



... so we apply a mixed matrix, using the appropriate coefficients ...

For each wave the jump is:

$$q_m - q_l = \alpha^1 \begin{bmatrix} -Z_l \\ 1 \end{bmatrix}$$
 and $q_r - q_m = \alpha^2 \begin{bmatrix} Z_r \\ 1 \end{bmatrix}$,

 $q_r - q_l = \alpha^1 \begin{vmatrix} -Z_l \\ 1 \end{vmatrix} + \alpha^2 \begin{vmatrix} Z_r \\ 1 \end{vmatrix}.$

and the total discontinuity is therefore

We can define the special mixed eigenvector matrix $R_{lr} = \begin{bmatrix} -Z_l & Z_r \\ 1 & 1 \end{bmatrix}$,

then
$$R_{lr}\alpha = q_r - q_l$$
.



FYS-GEO 4500

45

Galen Gisler, Physics of Geological Processes, University of Oslo

... and solve the Riemann problem

From
$$R_{lr} = \begin{bmatrix} -Z_l & Z_r \\ 1 & 1 \end{bmatrix}$$
,
We have $R_{lr}^{-1} = \frac{1}{Z_l + Z_r} \begin{bmatrix} -1 & Z_r \\ 1 & Z_l \end{bmatrix}$.
 $\alpha^1 = \frac{-(p_r - p_l) + Z_r(u_r - u_l)}{Z_l + Z_r}$.
Then $\alpha^2 = \frac{(p_r - p_l) + Z_l(u_r - u_l)}{Z_l + Z_r}$



and the intermediate state is simply

$$p_m = p_l - \alpha^1 Z_l$$
$$u_m = u_l + \alpha^1$$

from which transmission and reflection coefficients can be computed.

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

46

Acoustics equations with a partially reflecting interface

from \$CLAW/book/chap9/acoustics/interface

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

Autumn 2011

47

Acoustics equations with a partially reflecting interface



from \$CLAW/book/chap9/acoustics/interface

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

47

Doing the Godunov problem is then relatively easy...

Just assign each cell appropriate values of density and bulk modulus, and then work directly with the waves and speeds.

A Riemann solver that does this is:

\$CLAW/book/chap9/acoustics/interface/rp1.f

The reference in the book (p181) says rplacv.f, but this does not exist. If you examine this Riemann solver, you will see that the limiters are applied within the solver, in contrast to the usual method; section 9.13 explains why this is so.

Studying this file will help in developing any Riemann solver for heterogeneous media.

FYS-GEO 4500

Galen Gisler, Physics of Geological Processes, University of Oslo

48



Implement boundary conditions by using ghost cells and setting them appropriately.

Then treat the boundary cells with the normal Riemann solution:

$$Q_1 - Q_0 = \sum_{p=1}^m \mathcal{W}_{1/2}^p,$$

with incoming waves having strength zero. The outgoing waves may have nonzero strength.

The ghost cells are reset at the start of the next cycle.

FYS-GEO 4500

49

Review: Accuracy and Convergence

A method is *consistent* if the single-step error is small.

Single-step errors include *truncation error* and (*round-off error*).

Small single-step errors accumulate and the numerical solution diverges from the true solution after many time steps.

If the method is *stable,* the divergence will be *bounded.* If the method is unstable, the errors grow exponentially.

The Lax-Richtmeyer equivalence theorem states that:

A numerical method for a linear differential equation will converge if that method is *consistent* and *stable*.

Assignment for next time

Finite Volume

Methods for Hyperbolic Problems

CAMBRIDGE TEXTS

IN APPLIED MATHEMATICS



Read Chapter 7, 8 (through 8.5), and 9 (through 9.9).

Work problems 7.2a, 7.3, 8.2, and 9.5.

Next: Nonlinear Conservation Laws (Ch 11)

52