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Finding Confidence and Meaning in Verification

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NNSA National Nuclear Security Administration

Outline

- Code verification
- Solution verification
- Foundation of verification
- Importance of theory in guiding verification
- Examples from hyperbolic PDE’s (compressible flow)

Verification and validation are essential to the quality of simulation.

Complementary

- Verification ≈ Solving the equations correctly
  - Mathematics/Computer Science issue
  - Applies to both codes and calculations
- Validation ≈ Solving the correct equations
  - Physics/Engineering (i.e., modeling) issue
  - Applies to both codes and calculations
- Calibration ≈ Adjusting ("tuning") parameters
  - Parameters chosen for a specific class of problems
- Benchmarking ≈ Comparing with other codes
  - "There is no democracy in physics."*

*L.Alvarez, in D. Greenberg, *The Politics of Pure Science*, U. Chicago Press, 1967.

For verification it is important to understand theoretical expectations.

Truncation or approximation error

Stability

Lax (Richtmyer) Equivalence Theorem

FEM: Strang & Fix, Ciarlet, Brezzi, Babuska

In hyperbolic PDEs

The Lax-Wendroff theorem

Godunov's theorem

Entropy conditions

The LeFloch-Hou theorem

Local truncation error is the most basic concept in numerical approximation

This can be estimated with the aid of a Taylor series expansion.

$$\exp(at) \underset{t \to 0}{\approx} 1 + at + \frac{a^2 t^2}{2} + \frac{a^3 t^3}{6} + \frac{a^4 t^4}{24} + \cdots \frac{a^n t^n}{n!}$$

This measures the difference between the discrete and continuous versions of the equations.

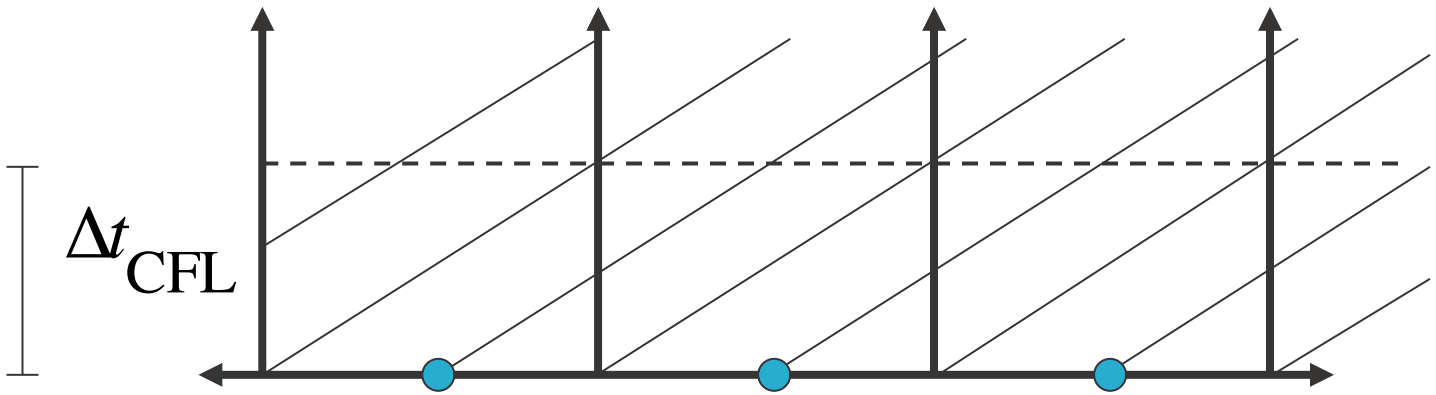
$$\text{truncation error} \underset{h \to 0}{=} \text{exact} - \text{numerical}$$

When combined with stability it forms the foundation of numerical analysis.

Domain of dependence of a solution leads directly to the Courant or CFL number.

This is the region of space that can be physically effected by another space due to the finite speed of propogation.

The idea originated with Courant, Friedrichs and Lewy in 1928 related to the analytic existence of solutions to PDEs (discretization was used as a device in the proofs).



First a bit of history…

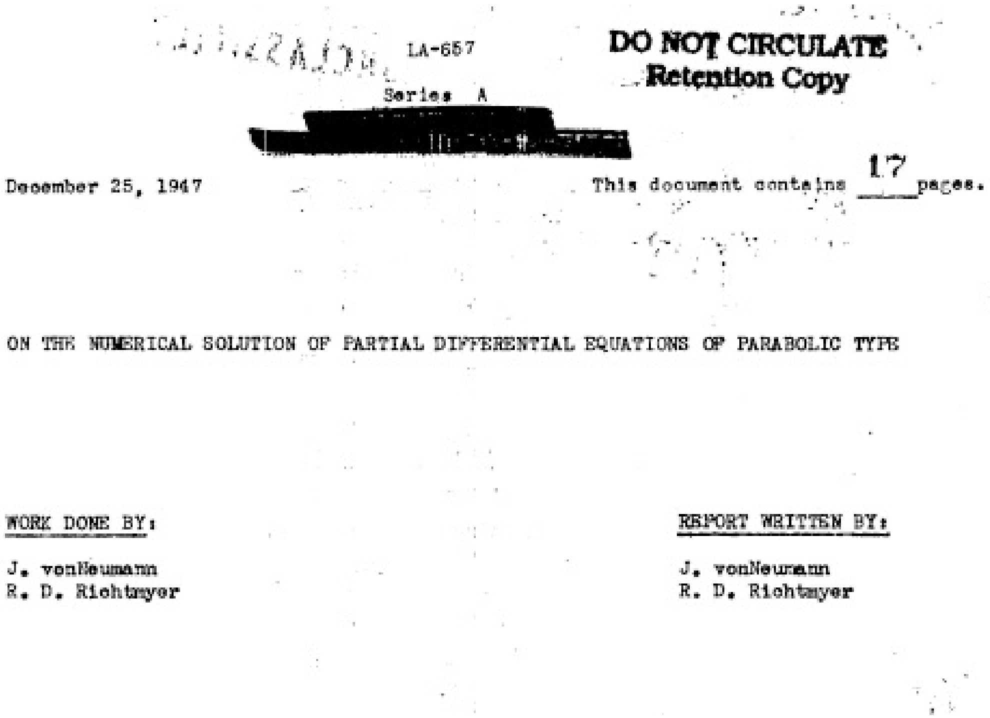
Von Neumann introduced the Fourier technique at Los Alamos in 1946 in a lecture.

It was originally classified.

Used to analyze parabolic PDE integrators in 1947 LA Report (LA-657)

Related to L_2 norm,…

- …Energy norm
- We'll do other norms, L_1



LA-657

Series A

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December 25, 1947

This document contains 17 pages.

ON THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS OF PARABOLIC TYPE

WORK DONE BY:

J. vonNeumann
R. D. Richtmyer

REPORT WRITTEN BY:

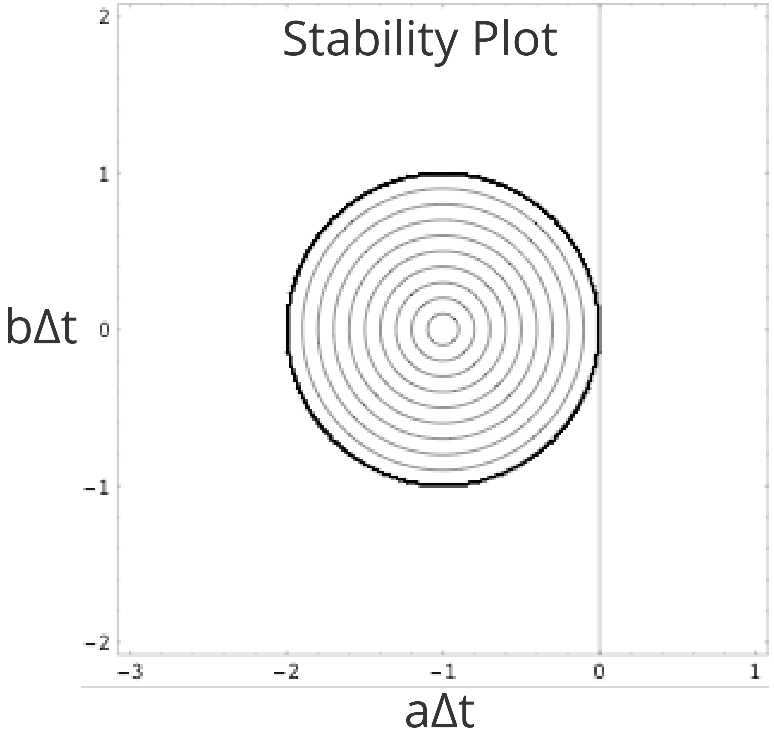
J. vonNeumann
R. D. Richtmyer

We can examine the basic stability concepts with ODEs.

The forward Euler example.

$$\frac{U^{n+1}-U^n}{\Delta t} = L\left(U^n\right) \rightarrow U^{n+1} = U^n + \Delta t L\left(U^n\right)$$

$$L = a + bi$$



Truncation error

$$\frac{\Delta t^2}{2}\frac{\partial^2 L(U)}{\partial t^2} + \frac{\Delta t^3}{6}\frac{\partial^3 L(U)}{\partial t^3} + \text{H.O.T.}$$

Quote by Peter Lax: The American Mathematical Monthly, February 1965:

"...who may regard using finite differences as the last resort of a scoundrel that the theory of difference equations is a rather sophisticated affair, more sophisticated than the corresponding theory of partial differential equations."

He goes on to make two points:

1. The proofs that an approximation converges is analogous to the estimates of the soln's to the PDEs, and

2. These proofs are harder to construct than for the PDEs themselves.

Lax's contributions have recently received a great honor - the 2005 Abel Prize

The Abel prize was created to make up for the lack of a Nobel prize for mathematicians.

Some of the work he was honored for started at Los Alamos and continued while at NYU's Courant Institute.

- It forms much of the theoretical foundation for CFD.
- Basic theory for the analytical and numerical solution of hyperbolic conservation laws.

The Lax-Richtmyer equivalence theorem provides the barest requirements on methods.

Putting numerical stability and truncation error together gets us to the basic requirement for linear methods for differential equations.

<u>Theorem (Lax Equivalence):</u> A numerical method for a linear differential equation will converge if that method is consistent and stable.

Lax, Peter D., and Robert D. Richtmyer. "Survey of the stability of linear finite difference equations." *Communications on pure and applied mathematics* 9, no. 2 (1956): 267-293.

Consistency - means that the method is at least 1st order accurate – means it approximates the correct PDE.

Stable - the method produces bounded approximations

Important to recognize for its relation to verification.

Let's state this differently (Gil Strang, Introduction to Applied Mathematics)

The fundamental theorem of numerical analysis, the combination of consistency and stability is equivalent to convergence.

Godunov’s Theorem relating high-order and montonicity

Godunov’s theorem says that a high-order linear methods (2nd order or higher) cannot be monotone for advection.

Restated: only 1st order linear methods are monotone

A linear method uses the same differencing stencil for all zones.

Godunov also developed a method that has been used extensively (mostly outside the hydrocode community)

He developed the method because of other methods available to him were inadequate, and he did not has access to the US literature (he commented that LxF would have been adequate).

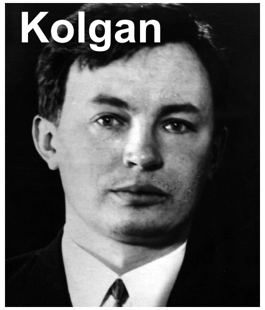
Godunov, Sergei Konstantinovich. "A difference scheme for numerical solution of discontinuous solution of hydrodynamic equations." *Math. Sbornik* 47 (1959): 271-306.

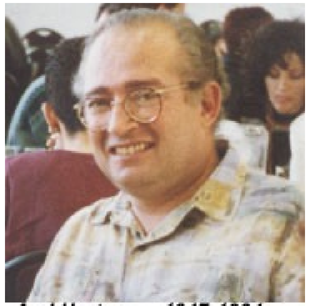
Overcoming Godunov's Theorem with nonlinear methods for advection

The key to overcoming Godunov's theorem is using nonlinear methods – using different stencils dependent on the local solution.

Developed *<u>independently</u>* by four men in 1971-1972

- Jay Boris (NRL)
- Bram Van Leer (U. Leiden)
- Vladimir Kolgan (USSR)
- Ami Harten (Israel)





Ami Harten 1947-1994
The developer of TVD & ENO schemes. We'll always miss your originality in science and in life.
SO, (2003)

Lax-Wendroff's method was a major development in computations.

The method was a landmark and dominated the numerical methods for hyperbolic PDE's in the 1960's.

The paper that introduces the method is important theoretically (discussed later) for a theorem introduced.

The method is second-order accurate, stable to a CFL number of one.

The method is derived by expanding the solution in a Taylor series and substituting second-order approximations.

P.D Lax; B. Wendroff (1960). "Systems of conservation laws". *Communications in Pure and Applied Mathematics*. 13 (2): 217–237. doi:10.1002/cpa.3160130205

Lax-Wendroff Theorem is an essential motivator for many numerical methods for hyperbolic equations.

Most methods for hyperbolic PDEs are based on the discrete conservation form following the continuous conservation form because of this theorem.

Theorem (Lax and Wendroff): *If a numerical method is in discrete conservation form, if a solution converges, it will converge to a weak solution of the PDE. A weak solution is not the weak solution. There are infinitely many weak solutions.*

Conservation form: the flux out of one cell is into another (telescoping)

$$\frac{\partial u}{\partial t}+\frac{\partial f\left(u\right)}{\partial x}=0\Rightarrow u_j^{n+1}=u_j^n-\frac{\Delta t}{\Delta x}\left(f_{j+1/2}-f_{j-1/2}\right)$$

Here is an example of what happens without conservation form. Burgers' equation.

Nonconservation form

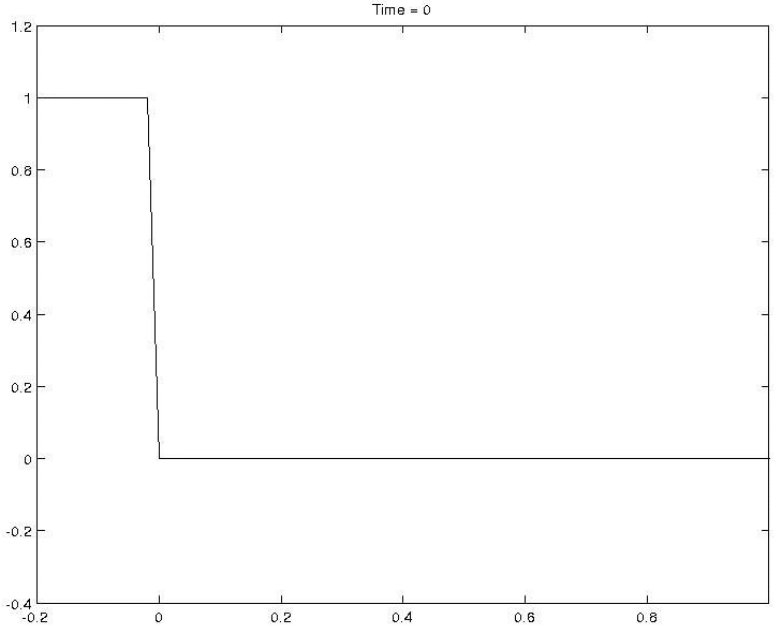
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

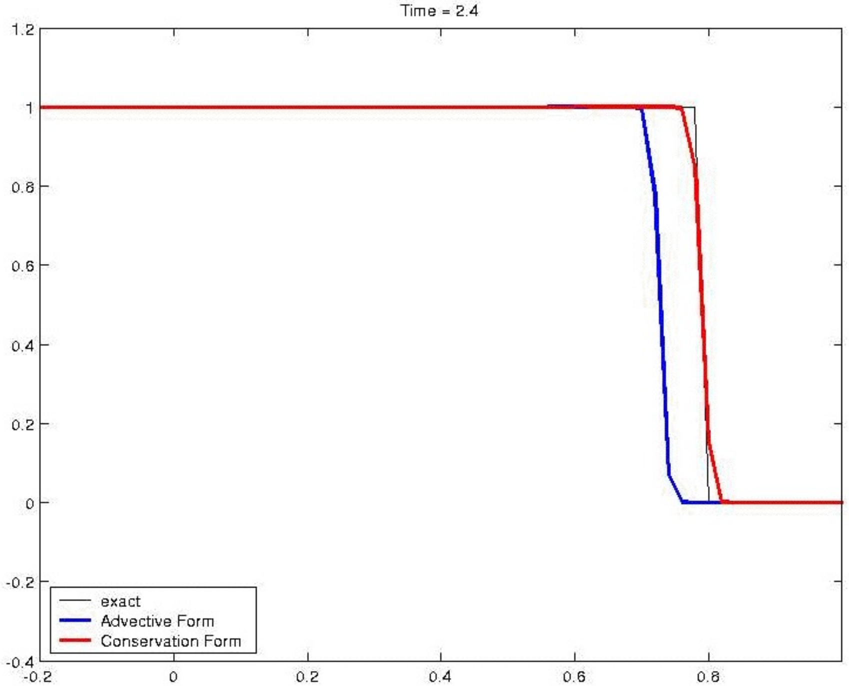
$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} u_j^n \left(u_j^n - u_{j-1}^n \right)$$

Conservation form

$$\frac{\partial u}{\partial t} + \frac{\partial \left(\tfrac{1}{2} u^2 \right)}{\partial x} = 0$$

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} \left(\frac{1}{2}\left(u_j^n\right)^2 - \frac{1}{2}\left(u_{j-1}^n\right)^2 \right)$$





Example from Randy Leveque

The Majda-Osher theorem establishes accuracy expectations for discontinuous flows.

Majda and Osher establish that the approximation of shocked or discontinuous flows will converge at be 1st order at best.

<u>Theorem (Majda and Osher):</u> A numerical solution will converge at 1st order at best for the region between any characteristics emanating from a discontinuity. Comm. Pure Appl. Math. 1977

Nonlinear discontinuties (self-steepening like shocks) converge at 1st order.

Majda, Andrew, and Stanley Osher. "Propagation of error into regions of smoothness for accurate difference approximations to hyperbolic equations." *Communications on Pure and Applied Mathematics* 30, no. 6 (1977): 671-705.

Linear discontinuties converge at less than 1st order (order

m/(m+1) where *m* is the order of the method

Banks, Jeffrey W., T. Aslam, and William J. Rider. "On sub-linear convergence for linearly degenerate waves in capturing schemes." *Journal of Computational Physics* 227, no. 14 (2008): 6985-7002.

Entropy conditions are critical in determining physically meaningful results.

The problem with L-W is that there are an infinity of weak solutions, we need a mechanism to pick out the correct physical one.

The mechanism to do this entropy. The entropy created through dissipation, numerical viscosity.

This is the connection to vanishing viscosity, more generally,

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=\lambda\frac{\partial^2 u}{\partial x^2}$$
$$\lambda \to 0^+$$

via Harten, Hyman and Lax, 1976

Harten, Amiram, James M. Hyman, Peter D. Lax, and Barbara Keyfitz. "On finite-difference approximations and entropy conditions for shocks." *Communications on pure and applied mathematics* 29, no. 3 (1976): 297-322.

The Hou-LeFloch theorem has potentially profound consequences .

What happens when the method is not in conservation form?

The solution does not converge to a weak solution much less a correct one regardless of the dissipation.

Theorem (Hou-LeFloch): For a non-conservative method the solution differs from a weak solution by an amount proportional to the entropy produced in the solution.

Hou, Thomas Y., and Philippe G. LeFloch. "Why nonconservative schemes converge to wrong solutions: error analysis." *Mathematics of computation* 62, no. 206 (1994): 497-530.

Summary

- It is essential to understand the theory related to both the method you are verifying and the problem being solved.
- The method's analysis establishes the upper bound on expected convergence and error
- The problem being solved can lower the rate of convergence and increase error substantially
- For hyperbolic PDE's many theorems exist defining expectations including when convergence should not be expected.