Analysis and verification of numerical methods outside the *asymptotic* range

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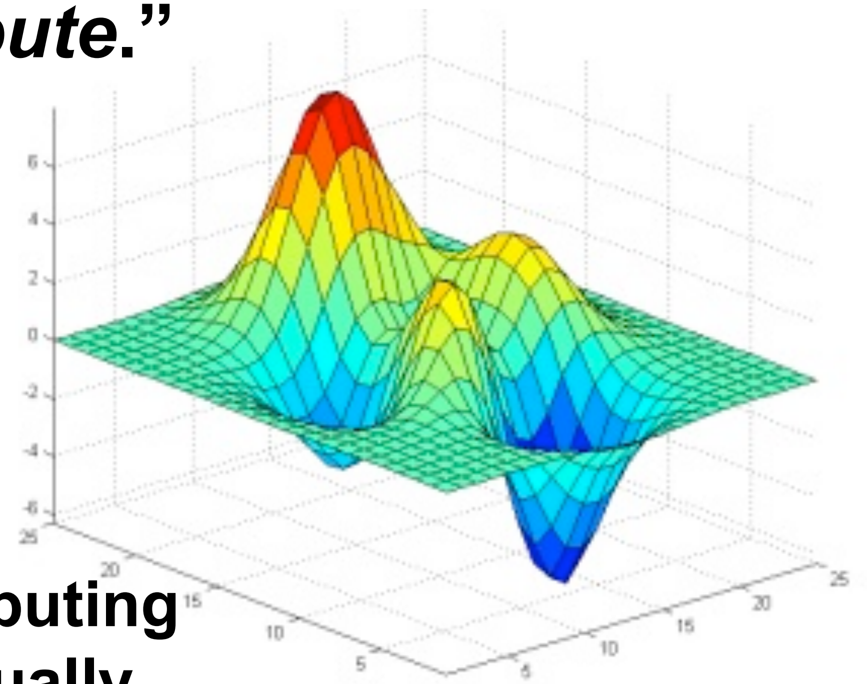
What verification means in numerical analysis!

"For the numerical analyst there are two kinds of truth; the truth you can prove *and the truth you see when you compute*."

– Ami Harten



Corollary: when proof and computing provide the same truth, you actually have something!

Outline

- Defining Verification
- Why do verification and issues associated with conducting it
- The connection of verification and numerical analysis
- Standard verification using standard numerical analysis
- New methods for numerical analysis of under-resolved calculations

Let's define verification first to make sure we are on the same page. *

- **Verification is used to do a couple of things:**
  - Provide evidence that the code is correct and correctly implemented
  - Produce an estimate of numerical error, and proof that the mesh is adequate.
- **Two types of verification are relevant here:**
  - ***Code verification***: the proof that the code is correctly implemented
  - ***Calculation (solution) verification***: the estimate of numerical error and implicitly, discretization adequacy.
  - Software verification is important, but off topic.

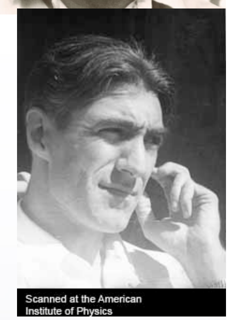
*I am adopting the common separation of verification and validation, i.e., ***Validation*** is comparison with experimental data.

Verification and numerical analysis are intimately and completely linked.

- **The results that verification must produce are defined by the formal analysis of the methods being verified.**
- **The numerical analysis results are typically (always) defined in the asymptotic range of convergence for a method.**
  - This range is reached as the discretization parameter (i.e., mesh, time step, angle, etc.) becomes "small" i.e., asymptotically "*close to zero*".
- **Practically, the asymptotic range is rarely achieved by verification practitioners or simulations.**
- **Hence verification is not generally practiced where it is formally valid!**

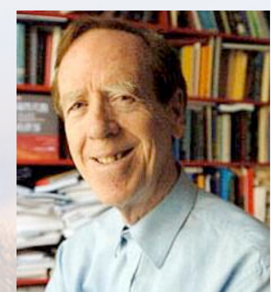
One theorem is absolutely essential to the conduct of verification.

- **The fundamental theorem of numerical analysis defined by Lax and Richtmyer (similar theorem by Dahlquist for ODEs, but it applies to nonlienar equations!),**



A numerical method for a linear differential equation will converge if that method is consistent and stable. Comm. Pure. Appl. Math. 1954

Restated by Strang - *The fundamental theorem of numerical analysis, The combination of consistency and stability is equivalent to convergence.*



Continuing the discussion of this fundamental mathematical concept.

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

Stable - the method produces bounded approximations

In the practice of verification *stability* is generally assumed by the presence of a solution, convergence is sought as evidence of *consistency*.

<u>This means verification is not completely rigorous with regard to the Lax-Richtmyer theorem</u>.

There are a number of typical numerical analysis techniques

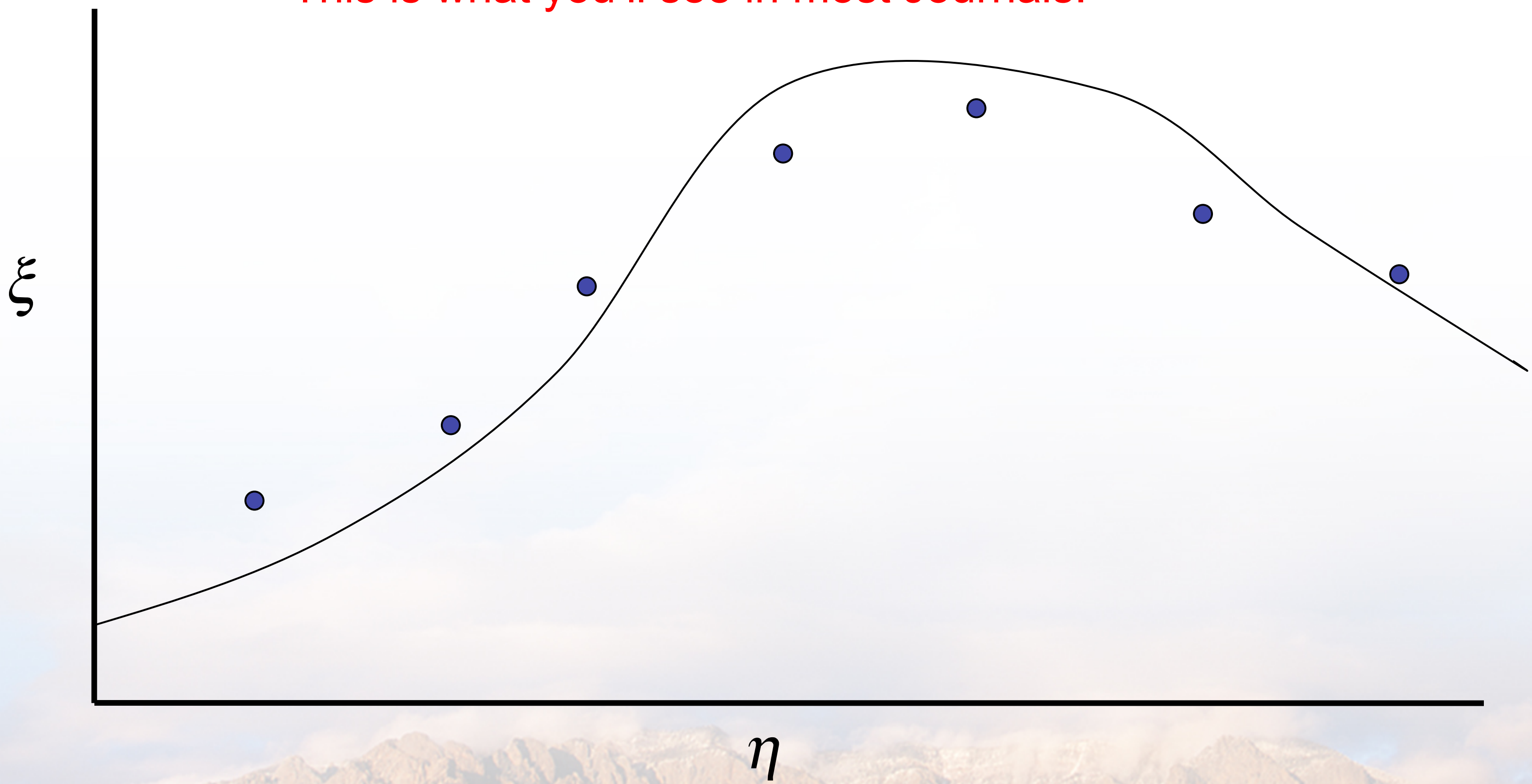
- Method are analyzed through methods providing stability and accuracy information.
- These techniques include Fourier (von Neumann), modified equations, and energy methods.
- These methods provide information about the discrete stability, accuracy, and error structure for methods typically limited to linear problems.
- Order of convergence is discussed in the limit where the discretization parameter becomes small.
- I will demonstrate the basic analysis on a simple method

In practice, one encounters problems when conducting verification

- **The convergence rates are (almost) never equal to the theoretical values.**
  - If the value is larger than the theoretical value, practitioners are usually comforted.
  - If the values are smaller, the practitioners will become increasingly nervous, e.g. a second order method produces a rate of 1.95 or 1.87, or 1.71, or 1.55, 1.13…
  - Sometimes the rate is too large, 2.14, 2.56, 3.12, 4.67, …
  - Where is it viewed as being incorrect? When should one worry about the result?
- **Sometimes the method will diverge, or oscillate.**
- **The asymptotic range is usually unreasonable to compute especially for applied problems.**

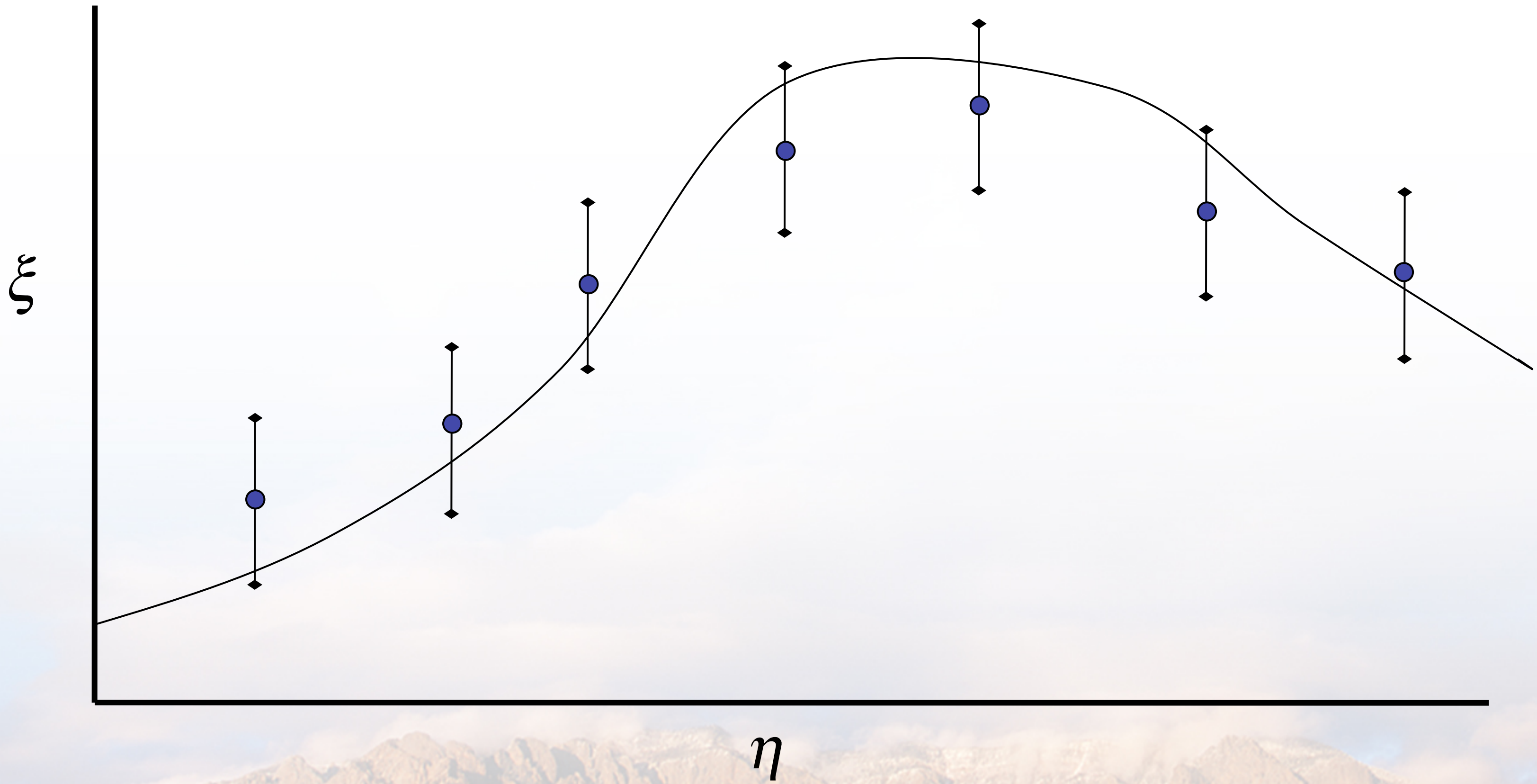
This is the way validation is typically presented.

This is what you'll see in most Journals.



This presentation is an improvement because experimental error is shown.

This is *not* what you'll see in most Journals, but you should.



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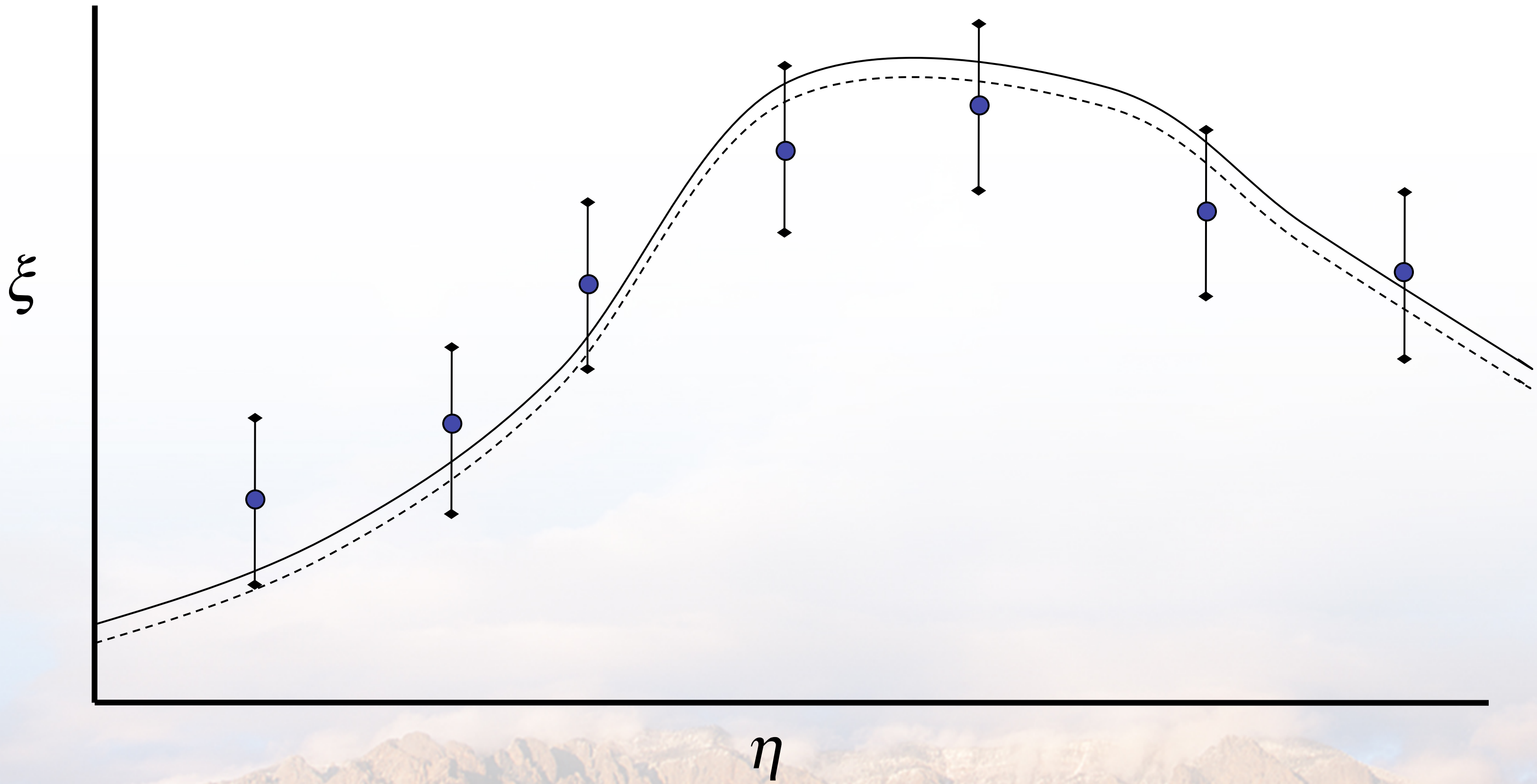
Here is a notion of how a "converged" solution might be described.

You might see this although rarely depicted in this manner.



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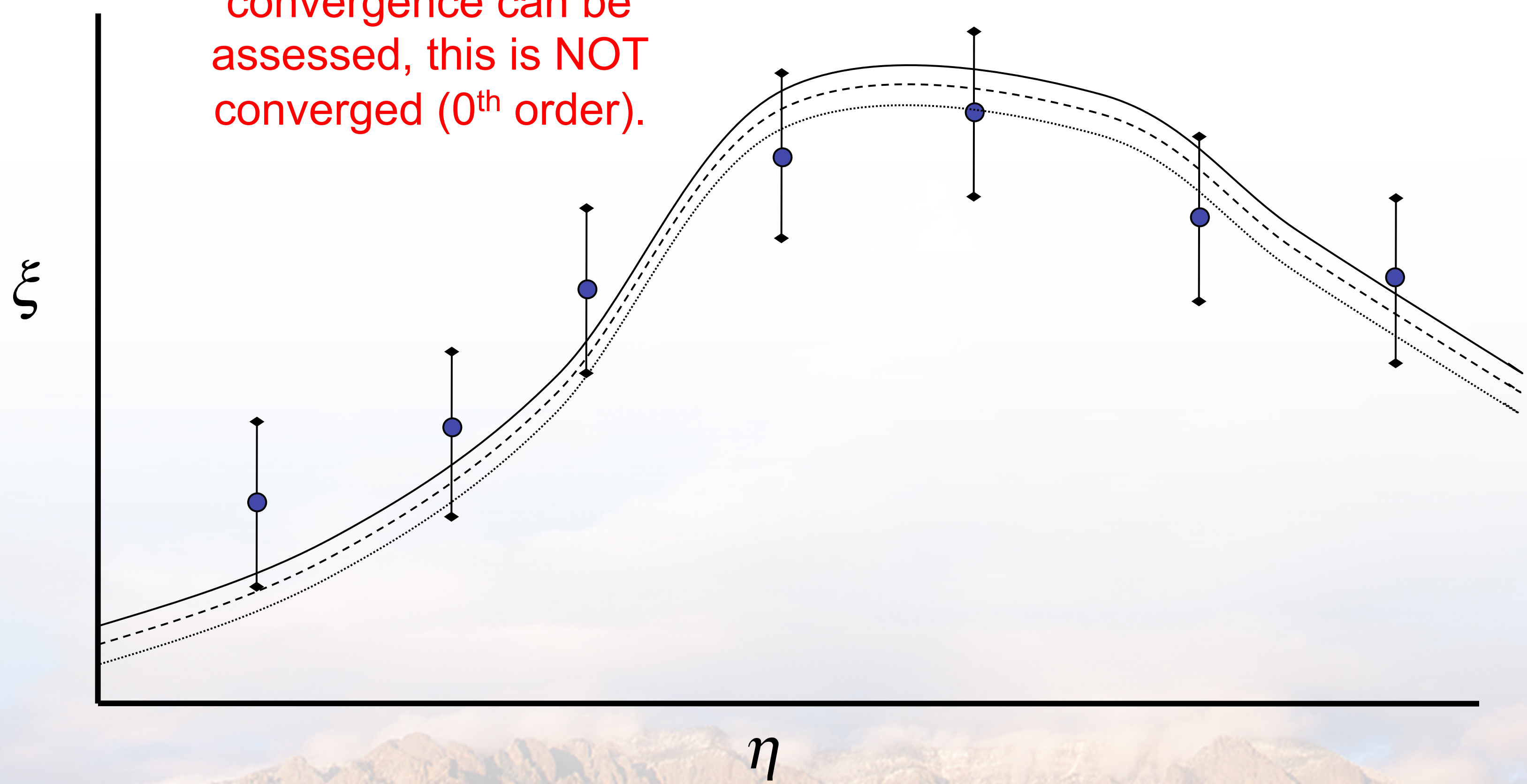
Here is a notion of how a "converged" solution might be described.

With a third resolution convergence can be assessed, this is NOT converged (0th order).



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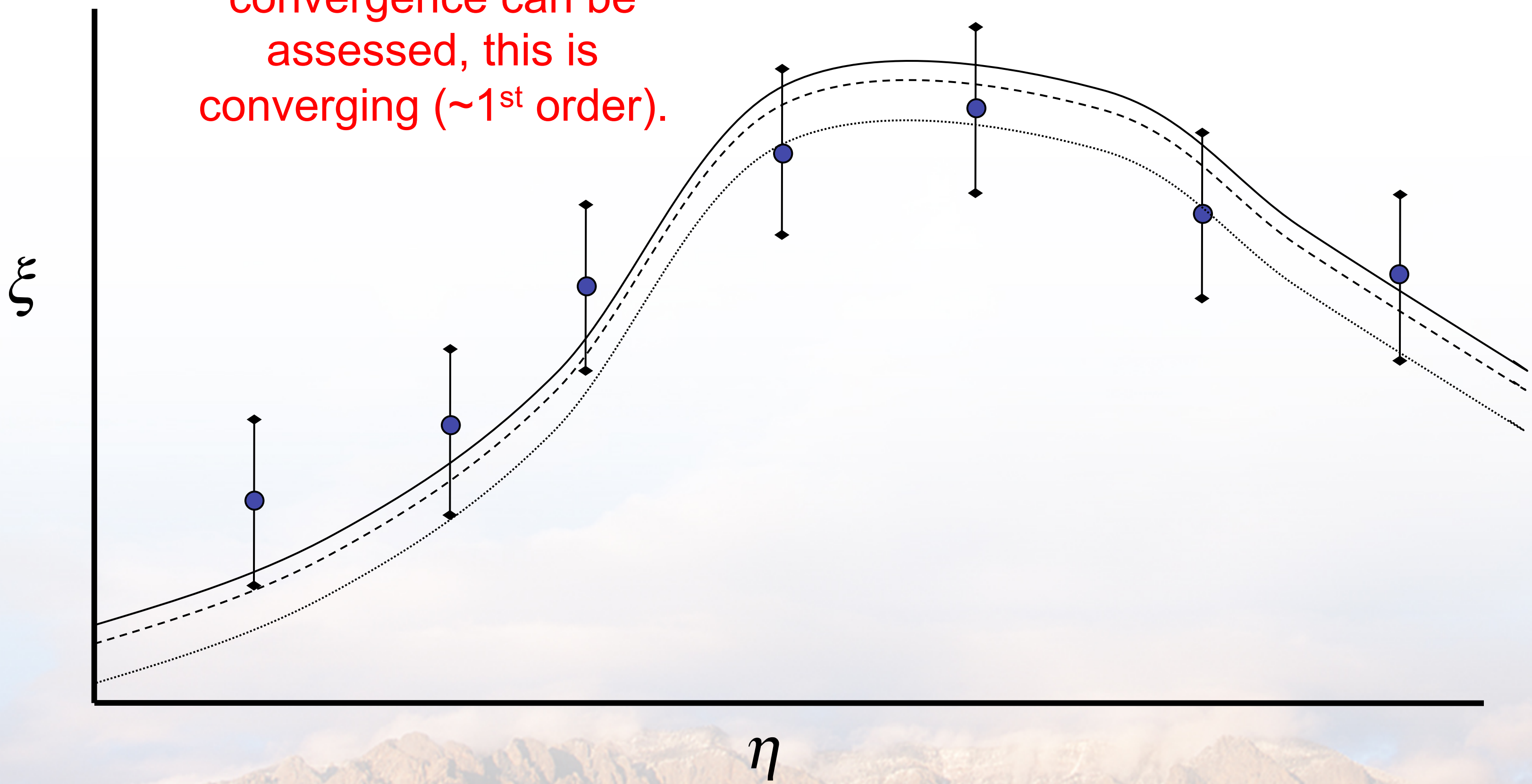
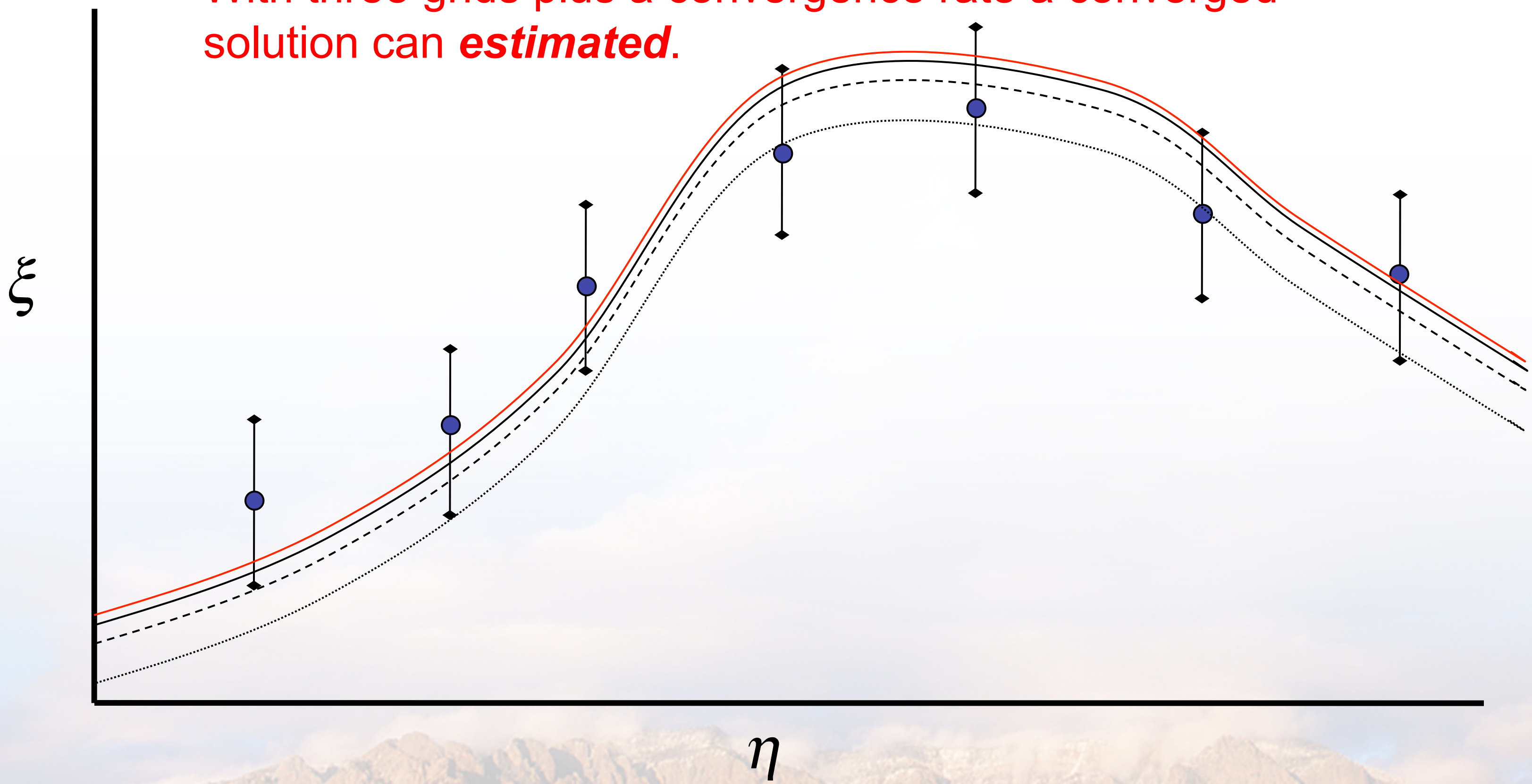
Here is a notion of how a "converged" solution should be described.

With a third resolution convergence can be assessed, this is converging (~1st order).



Even better, a sequence of meshes can be used to extrapolate the solution.

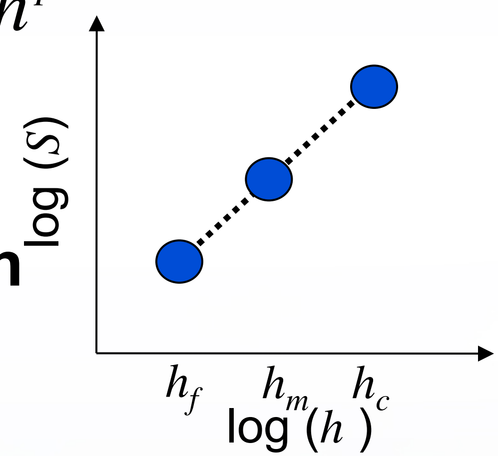
With three grids plus a convergence rate a converged solution can ***estimated***.



Roache's Grid Convergence Index (GCI)* uses a fixed safety factor for numerical uncertainty.

- **The standard power error ansatz,** $S = A + Ch^p$

$$S = A_k + Ch_k^p ;\text{unknowns } S, C, p$$



gives an estimate of numerical error based on extrapolation

$$\delta = \frac{\Delta_{mf}}{r_{mf}^p - 1} ; \Delta_{mf} = S_f - S_m , r_{mf} = \frac{h_m}{h_f}$$

- **A safety factor gives the uncertainty estimate:**

$$U_{num} = F_s \delta ; F_s = 1.25$$

- **This safety factor is described as giving a 95% confidence interval (the consequence of CFD experience).**

*P. Roache, *Verification and Validation in Computational Science and Engineering*, Hermosa(1996).

Another uncertainty Estimate has a variable "safety factor" or asymptotic correction.

- **The estimate developed by Stern uses the same basic framework, but with a key difference…**
- **The safety factor is not constant, but depends on two pieces of information,**
  - The observed order of convergence p_{ob}
  - The theoretical order of convergence p_{th}

$$F_s = \frac{r^{p_{ob}} - 1}{r^{p_{th}} - 1}$$

- ***This potentially makes it attractive when the computation is not in the asymptotic range***
- **I am going to describe a way to extend this approach.**

We can start by showing how convergence rates are usually analyzed (forward Euler method, here).

- **Starting with an ODE we can analyze stability and accuracy using the standard methodology.**
- Analysis of ODE's are primal for anything else, start with the simplest ODE and discretization, $\dot{u} = \lambda u \rightarrow u^{n+1} = u^n + h\lambda u^n$
- The analysis includes the analytical solution and the Taylor series analysis of each

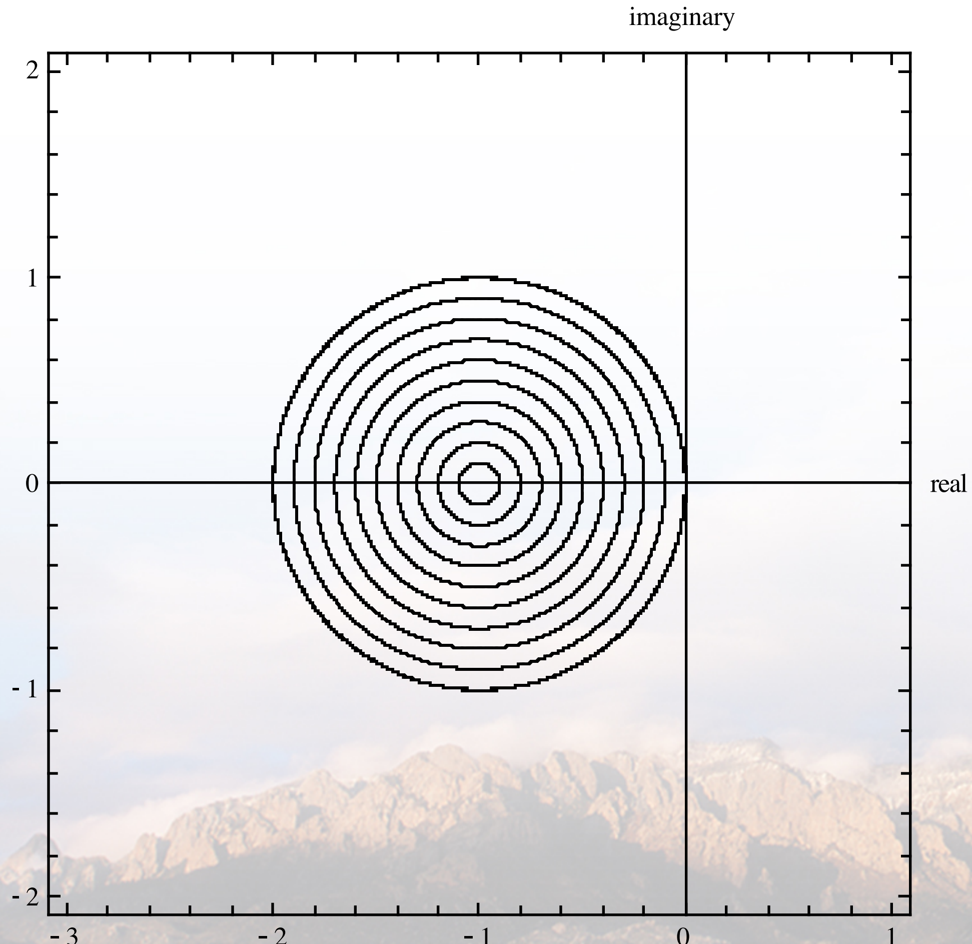
$$\dot{u} = \lambda u \xrightarrow[h \to 0]{} u(0)\left(1 + \lambda h + \tfrac{1}{2}(\lambda h)^2 + \tfrac{1}{6}(\lambda h)^3 + O\left(h^4\right)\right)$$

$$\dot{u} = \lambda u \rightarrow u(0) + h\lambda u(0)$$

- Error is the difference $\text{Error} \approx u(0)\left(\tfrac{1}{2}(\lambda h)^2 + \tfrac{1}{6}(\lambda h)^3 + O\left(h^4\right)\right)$
- The stability can be studied via an energy method by using an expansion of the ODE, $\lambda = a + bi$

Here, we examine the usual stability analysis techniques.

- The magnitude of the amplification factor is plotted to display the stability region where it is less than one,

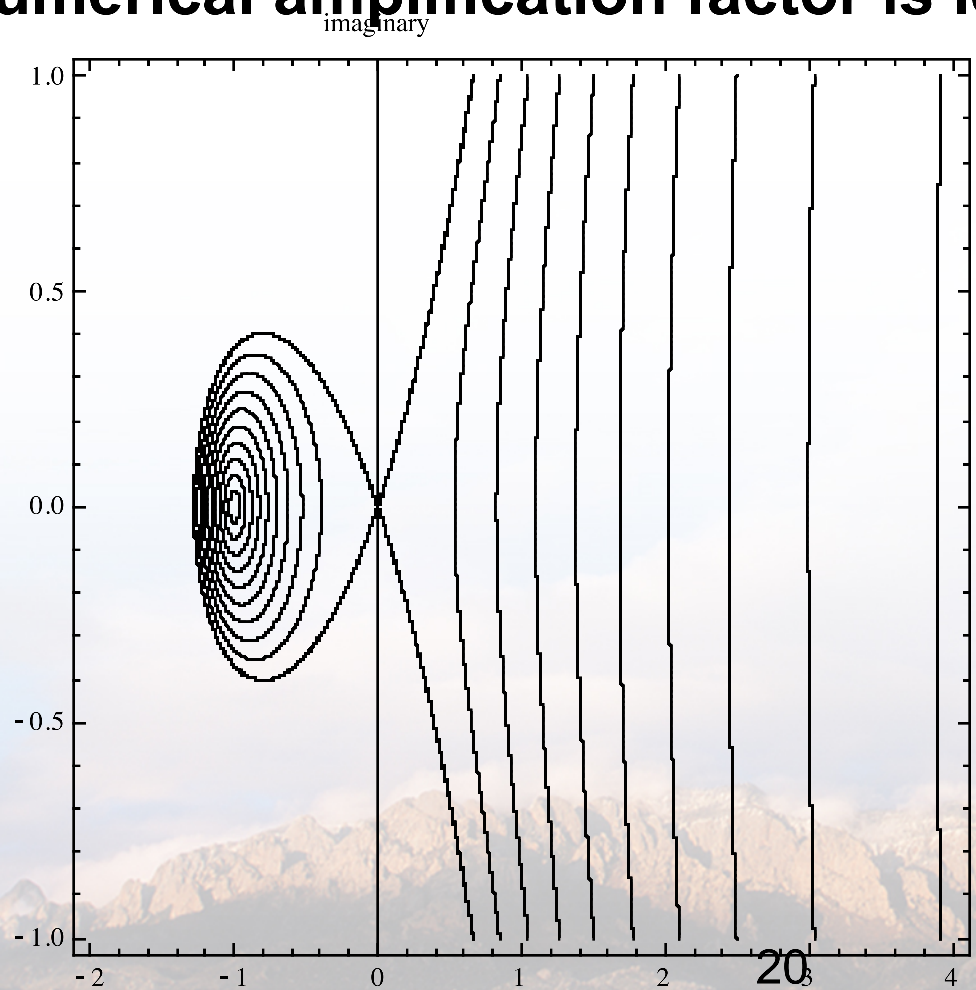


$$A=\sqrt{(1+ha)^2+(hb)^2}$$

The method can be safely used inside the region plotted

Here, we examine the usual stability analysis techniques (continued).

- Another interesting view are the “order stars” where the numerical amplification factor is less than the analytical



$$\frac{\sqrt{(1+ha)^2+(hb)^2}}{Exp[a-b]} \le 1$$

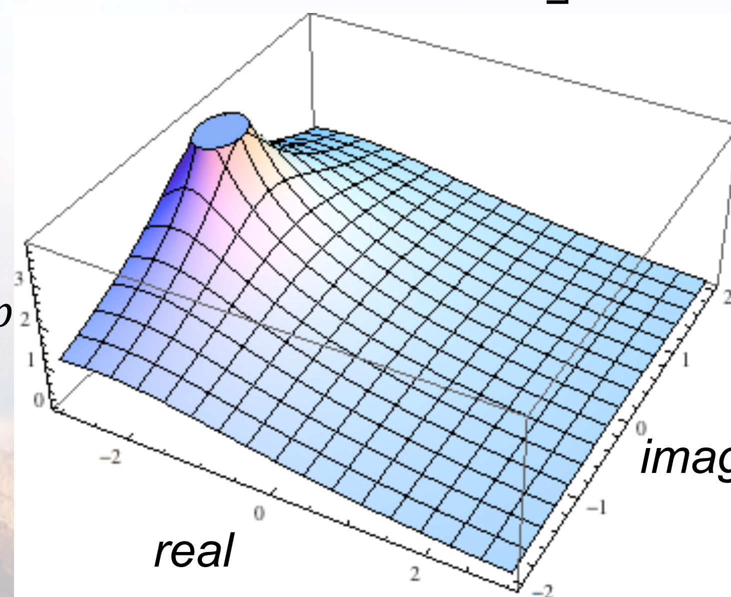
The method can be safely used inside the region plotted because the solution is damped more than the analytical solution

With this foundation, we can augment these techniques to provide extended results.

- **The key is to realize that the error can be computed everywhere,** $\mathrm{Error}(h) = \left|A(h) - \exp(\lambda h)\right|$
  - Compute the error with a refined step size (h/2),

    $$\mathrm{Error}(h/2) = \left|\left(A(h/2)^2 - \exp(\lambda h)\right)\right|$$

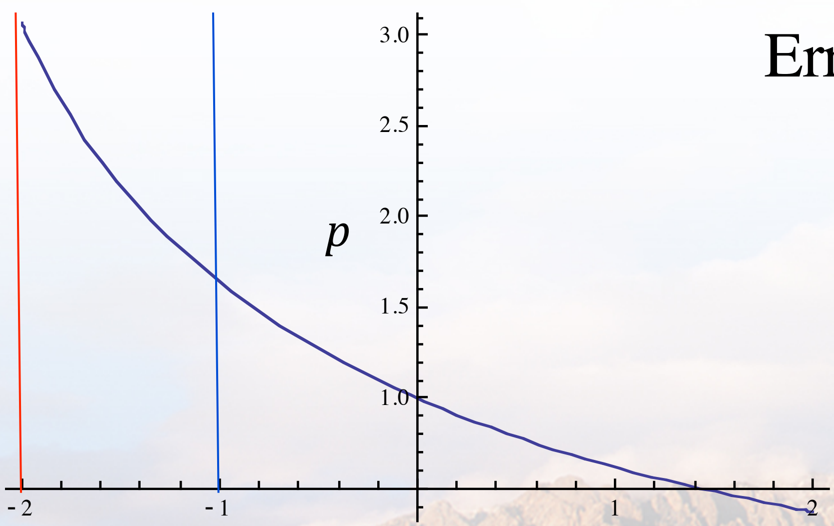
  - The convergence rate can then be easily computed using the standard form, $p = \log\left[\mathrm{Error}(h)/\mathrm{Error}(h/2)\right]/\log(2)$
  - This convergences to the asymptotic limit of 1 as *h* goes to zero.
- **Compute the error as a function of discrete integration steps**



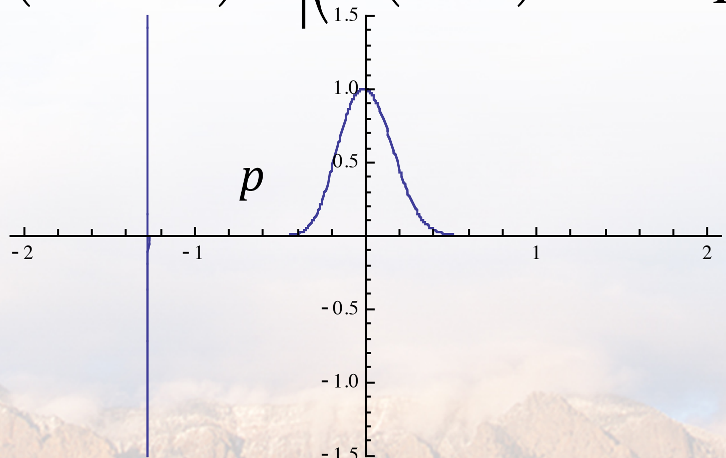
This is the error and convergence for a single step, but multiple steps are used.

- **The results change a bit under two conditions:**
  - The method is applied in the region of strong stability
  - As the step size becomes small, the result becomes less sensitive to the number of steps taken
- **The form can be extended to give**

$$\mathrm{Error}(h/2,m) = \left|\left(A(h/2)^{2m} - \exp(m\lambda h)\right)\right|$$



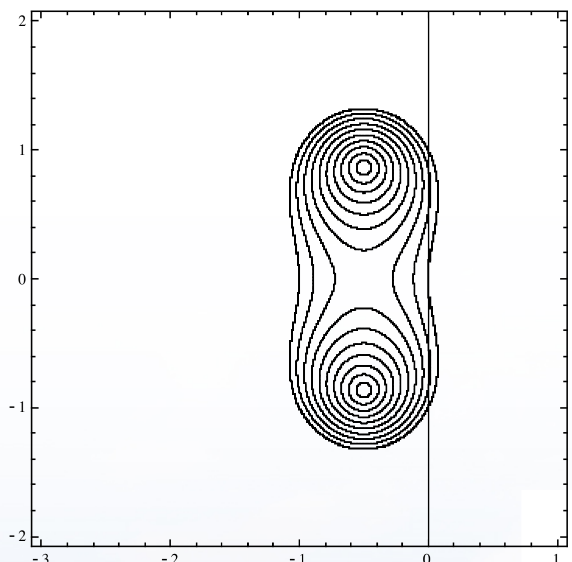
a, b=0, single step



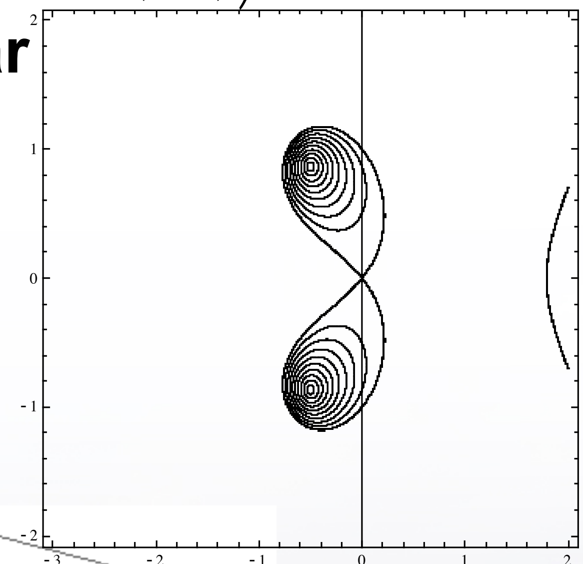
a, b=0, 100 steps

We can analyze the second-order modified Euler method similarly

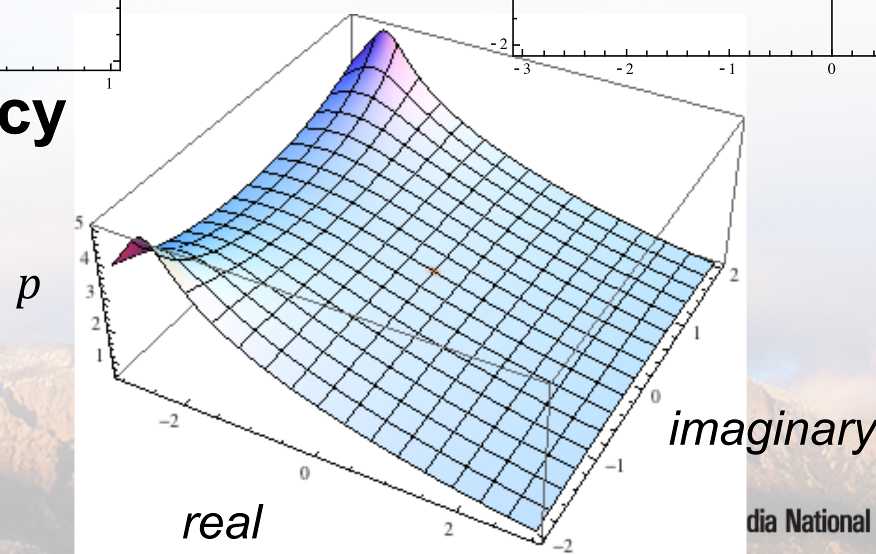
- **Asymptotic accuracy** $\text{Error} \approx u(0)\left(\frac{1}{6}(\lambda h)^3 + O\left(h^4\right)\right)$
- **Stability**



Order star

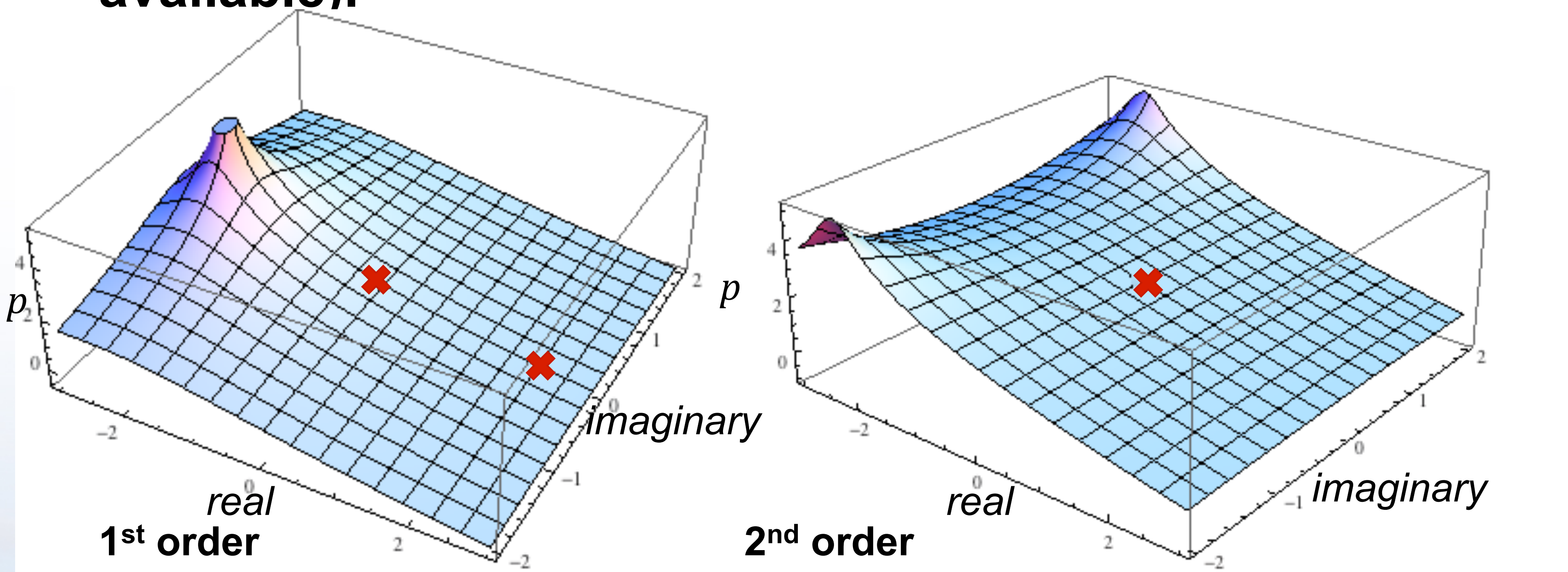


- **Non-asymptotic Accuracy**



We can apply the same methodology to calculation verification (no exact sol'n).

- The calculation verification has some subtle differences from code verification (where an exact solution is available).



- There is no reason we have to use a factor of two step size change (not enough time to go into this!).

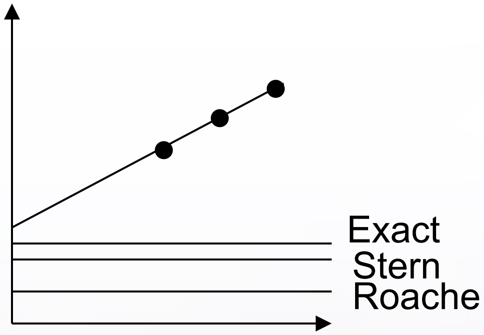
Results for linear ODE can be used to produce "verification" of the analysis

- **We'll start with the simplest thing possible,**

$$\dot{u} = \lambda u \rightarrow u(t) = u(0)\exp(-\lambda t)$$

  - Use a first-order forward Euler method

$$\begin{array}{ccc} p_T = 1 & \Delta_{cm} = 0.027 & F_{\mathrm{Roache}} = 1.25 \\ p = 1.13 & \Delta_{mf} = 0.012 & F_{\mathrm{Stern}} = 1.18 \\ & \delta = 0.015 & F_{\mathrm{Exact}} = 1.12 \end{array}$$



New analysis gives the right rate ***p_T* = 1.13**

  - Compare with a second-order modified Euler

$$\begin{array}{ccc} p_T = 2 & \Delta_{cm} = 0.0036 & F_{\mathrm{Roache}} = 1.25 \\ p = 2.16 & \Delta_{mf} = 0.0008 & F_{\mathrm{Stern}} = 1.16 \\ & \delta = 0.0002 & F_{\mathrm{Exact}} = 1.09 \end{array}$$

Actually, the answers are correct to four digits!

New analysis gives the right rate ***p_T* = 2.16**

Results for linear ODE with a bad choice for time step size further test the methodology.

- We'll continue with the simplest thing possible and forward Euler, $\dot{u} = \lambda u \rightarrow u(t) = u(0)\exp(-\lambda t)$
- Study a "growing" case

$$
\begin{array}{lll}
p_T = 1 & \Delta_{cm} = -29.07 & F_{Roache} = 1.25 \\
p = 0.167 & \Delta_{cm} = -24.46 & F_{Stern} = 5.31 \\
\lambda = -1 & \delta = -129.9 & F_{Exact} = 3.49
\end{array}
$$

New analysis gives $\boldsymbol{p_T = 0.167}$

- In each of these three cases, the new analysis gives quite precise estimates of the observed convergence rate.

Applying the same methodology to other PDEs

- Exact solutions in Fourier space are available for a broad class of PDEs, 1st, 2nd order operators, etc…
- For example 1st order hyperbolic operators analyzed with Von Neumann analysis can be accomplished here for donor differencing of , $u_j^n = \exp\left(ij\theta\right) \Rightarrow u_j^{n+1} = u_j^n - c\left(u_j^n - u_{j-1}^n\right) \Rightarrow$

$$A\exp\left(ij\theta\right) = \exp\left(ij\theta\right) - C\left(\exp\left(ij\theta\right) - \exp\left(i\left(j-1\right)\theta\right)\right)$$

$$A = 1 - C\left(1 - \cos\left(\theta\right) + i\sin\left(\theta\right)\right)$$

$$\mathbf{amp} = \sqrt{\left[1 - C\left(1 + \cos\left(\theta\right)\right)\right]^2 + \left(-C\sin\left(\theta\right)\right)^2} \quad \mathbf{phase} = \arctan\left(\frac{-C\sin\left(\theta\right)}{\left[1 - C\left(1 + \cos\left(\theta\right)\right)\right]}\right) \Big/ \left(-c\theta\right)$$

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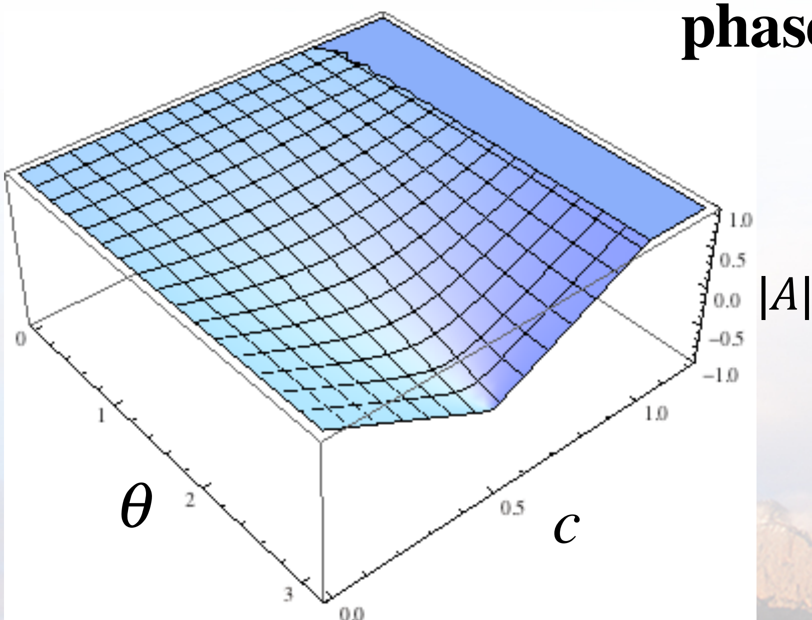
Standard Fourier analysis for PDEs (continued)

- **Take an expansion to find the asymptotic error relations,**
  - Amplitude error even order errors

$$\mathbf{amp} \approx 1 + \left(-\frac{c}{2} + \frac{c^2}{2}\right)\theta^2 + O\left(\theta^4\right)$$

  - Phase error odd order (divide by the angle!)

$$\mathbf{phase} \approx 1 + \left(-\frac{1}{6} + \frac{c}{2} - \frac{c^2}{3}\right)\theta^2 + O\left(\theta^4\right)$$



What does the convergence analysis look like? First, some preliminaries…

- **We can converge in either space, time or both.**
- **For some hyperbolic integrators, space & time are linked, and time only refinement is not convergent, but calculation verification is.**
  - These methods are based on the “Lax-Wendroff” procedure where time accuracy is achieved with spatial derivatives.
$$u_j^{n+1} = u_j^n - \nu\left(u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}\right); u_{j+1/2}^{n+1/2} = u_j^n + \tfrac{1}{2}(1-\nu)\left(u_j^n - u_{j-1}^n\right)$$
  - Other methods are based on the “method of lines” and do converge independently in space and time
  - This is because time and space are discretized independently. $u_j^{n+1/2} = u_j^n - \tfrac{\nu}{2}\left(u_{j+1/2}^n - u_{j-1/2}^n\right); u_{j+1/2}^n = u_j^n + \tfrac{1}{2}\left(u_j^n - u_{j-1}^n\right)$
$$u_j^{n+1} = u_j^n - \nu\left(u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}\right); u_{j+1/2}^{n+1/2} = u_j^{n+1/2} + \tfrac{1}{2}\left(u_j^{n+1/2} - u_{j-1}^{n+1/2}\right)$$

We worked on a verification exercise that resulted in some seemingly mysterious results.

- Does the analysis of the methods explain the convergence rates? Its all calculation verification

- Combined space-time

Cells	L^1 error	L^1 rate	L^2 error	L^2 rate
100	2.80×10^{-1}	—	3.75×10^{-1}	—
200	7.06×10^{-2}	1.99	9.53×10^{-2}	1.98

- LW time only

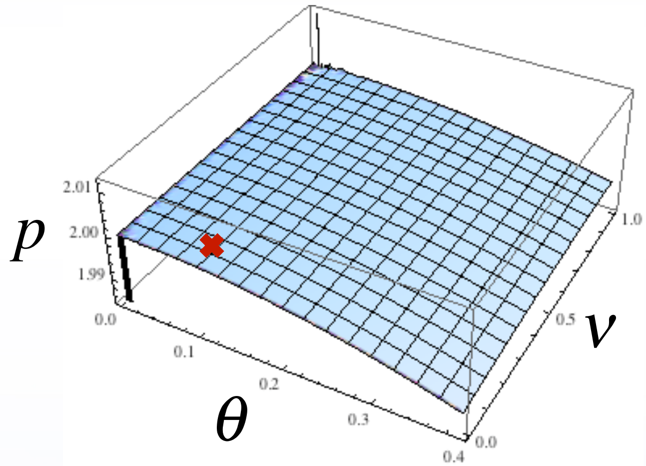
CFL	L^1 error	L^1 rate	L^2 error	L^2 rate
0.10	2.01×10^{-2}	—	2.62×10^{-2}	—
0.05	1.08×10^{-2}	0.96	1.35×10^{-2}	0.96

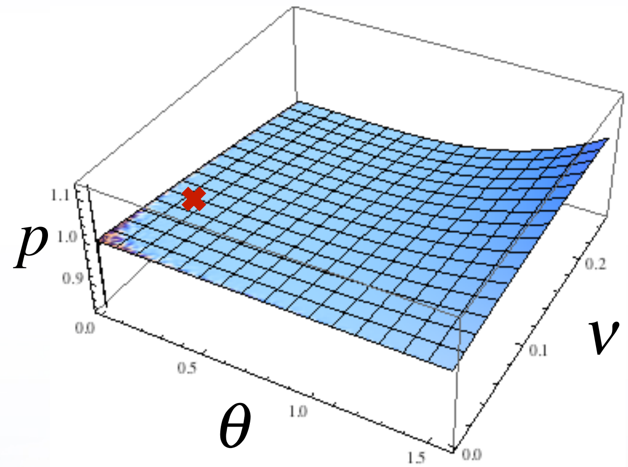
- MOL time only

CFL	L^1 error	L^1 rate	L^2 error	L^2 rate
0.10	1.40×10^{-3}	—	1.87×10^{-3}	—
0.05	3.51×10^{-4}	1.99	4.70×10^{-4}	1.99

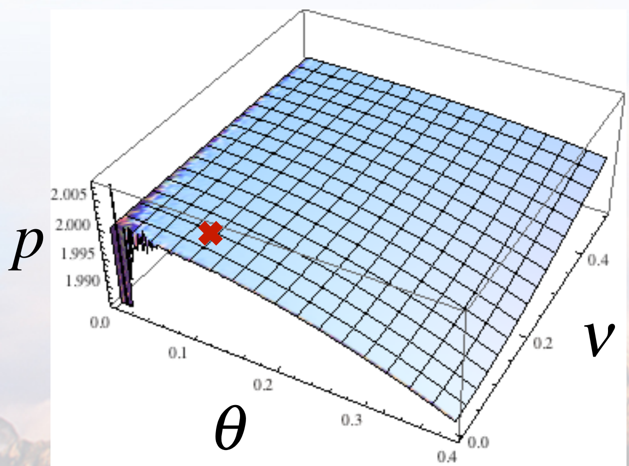
What does the convergence analysis tell us for each case?

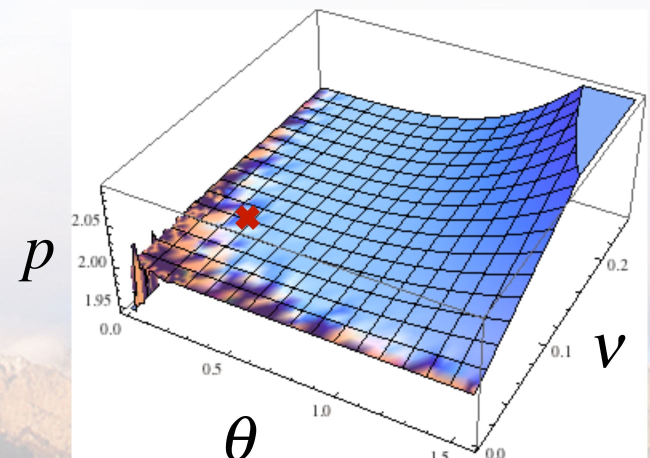
- **L-W scheme** — **time-space** — **time only**





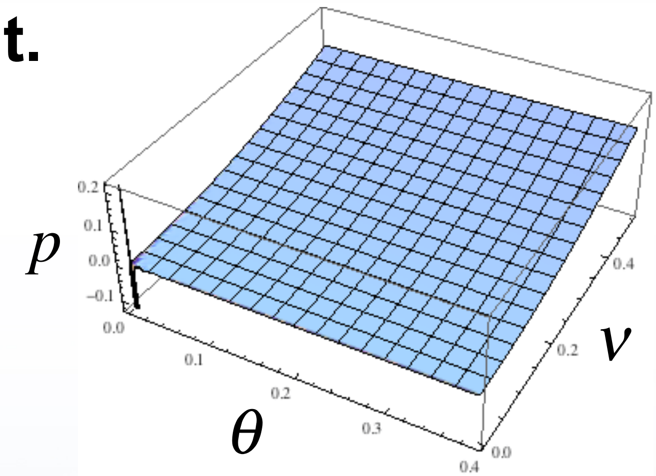
- **MOL scheme**



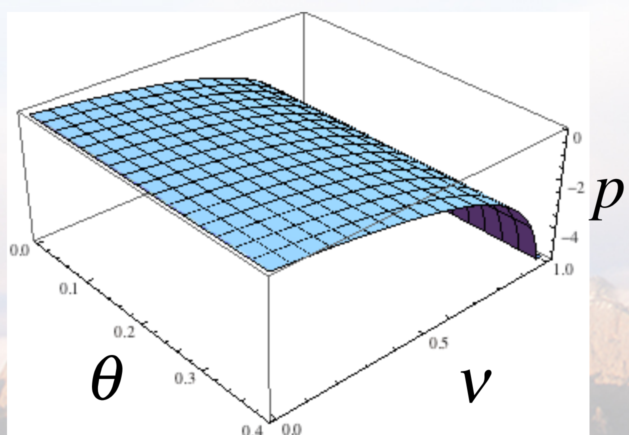


The schemes show distinct difference in convergence toward the exact solution.

- **MOL: very poorly convergent under time only refinement.**



- **L-W: divergent under time only refinement!**



Since we are advecting a Gaussian, we need to find the effective wave number.

- **The function is the following:**

$$u(x) = \tfrac{1}{4} + \tfrac{1}{4}\exp\left[-30\left(x - \tfrac{1}{2}\right)^2\right]$$

  - Solved on a grid of 100 cells.
- **Convert this to an effective wave number for the function through an integration of the second derivative of the Gaussian over the domain [0,1] and finding the effective trigonometric function.**
  - This leads to an effective wave number of $\theta \approx 0.0911$
  - **Estimated L_2 convergence rates**
    - ***L-W space time:1.98 (observed 1.98)***
    - ***L-W time only: 0.96 (observed 0.96)***
    - ***MOL time only:2.00 (observed 1.99)***

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Summary of results

- Verification is usually applied where it is formally invalid, i.e., outside the asymptotic range of convergence, so the theoretical convergence rate is not observed.
- This problem can be addressed by developing analysis methods that can analyze methods without taking the limit of vanishing discretization parameters.
- Several examples have been shown to demonstrate this technique, and the potential accuracy of the predicted convergence rates.
- The work is rather preliminary and further extensions and demonstrations are needed.

“Dilbert isn’t a comic strip, it’s a documentary” – Paul Dubois