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The Role of Theory in Calculation Verification

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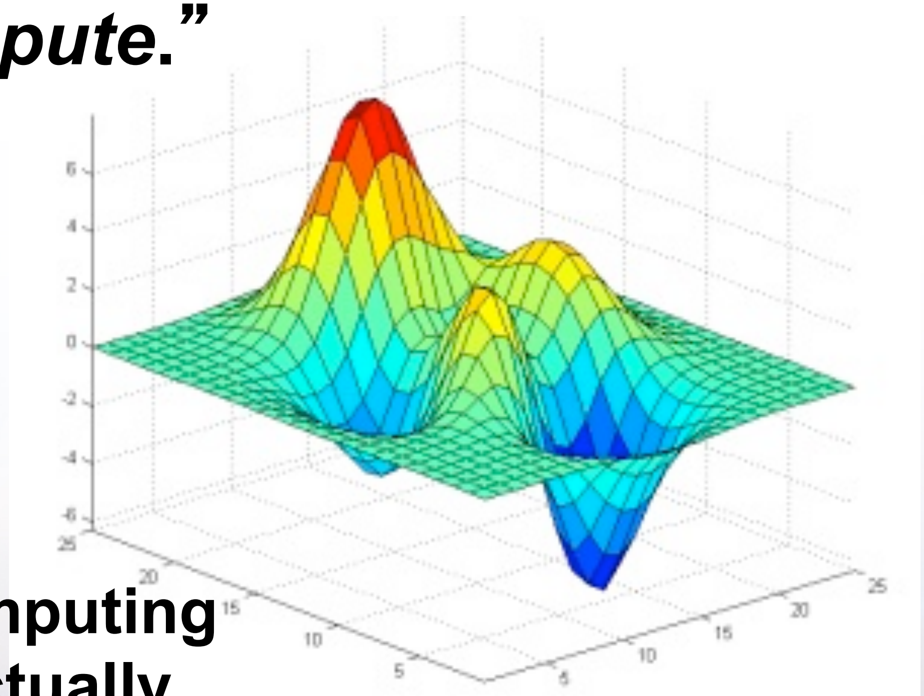
Outline

- Defining Verification (Code vs Calculation)
- What is difficult about verification
- The (less than completely obvious) connections of verification and numerical analysis
- New methods for numerical analysis of under-resolved calculations
- Putting this together with methodology for calculation verification

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!

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 evidence 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.

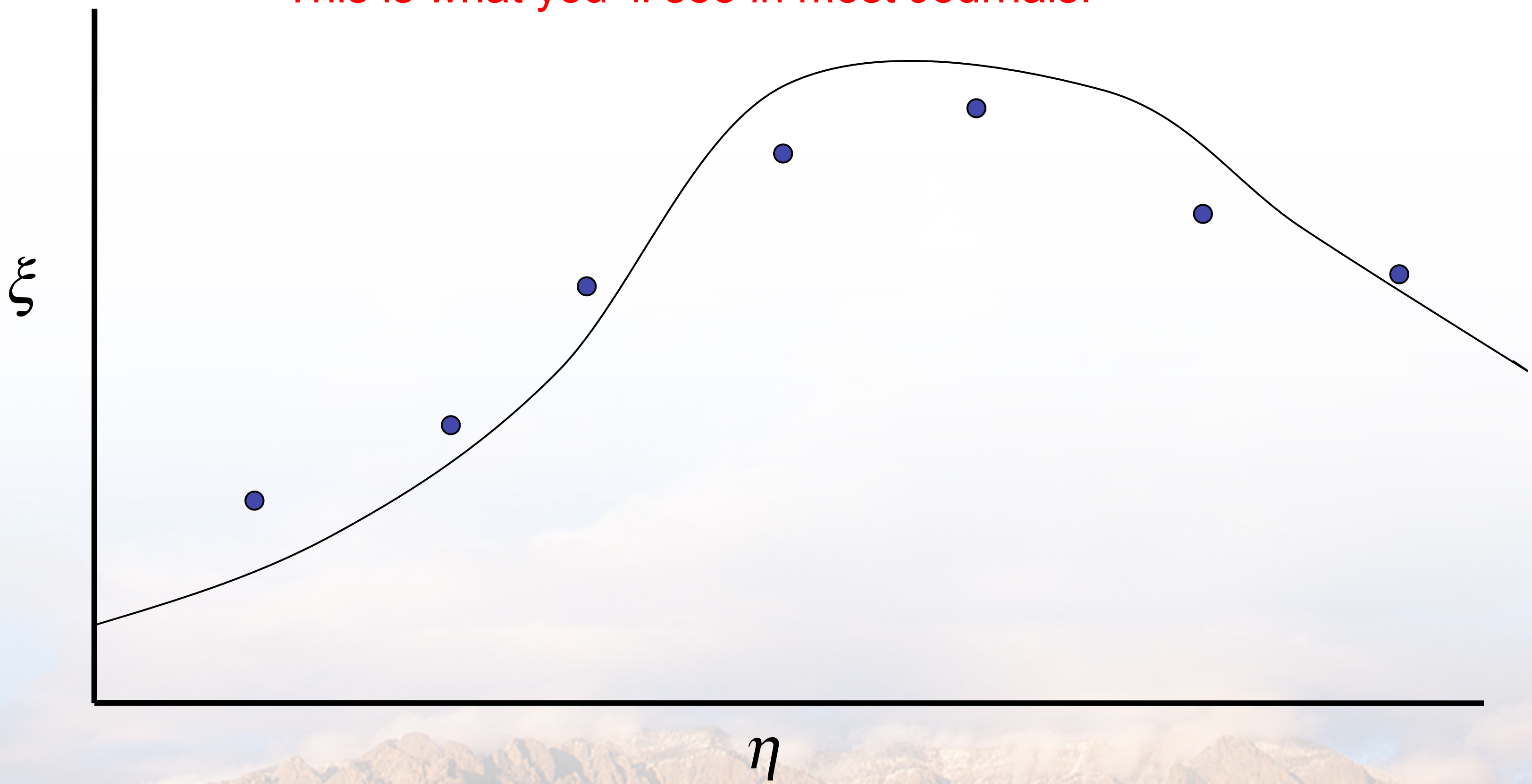
*I am adopting the common separation of verification and validation, i.e., ***Validation*** is comparison with experimental data.

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!**

This is the way validation is typically presented.

This is what you'll see in most Journals.



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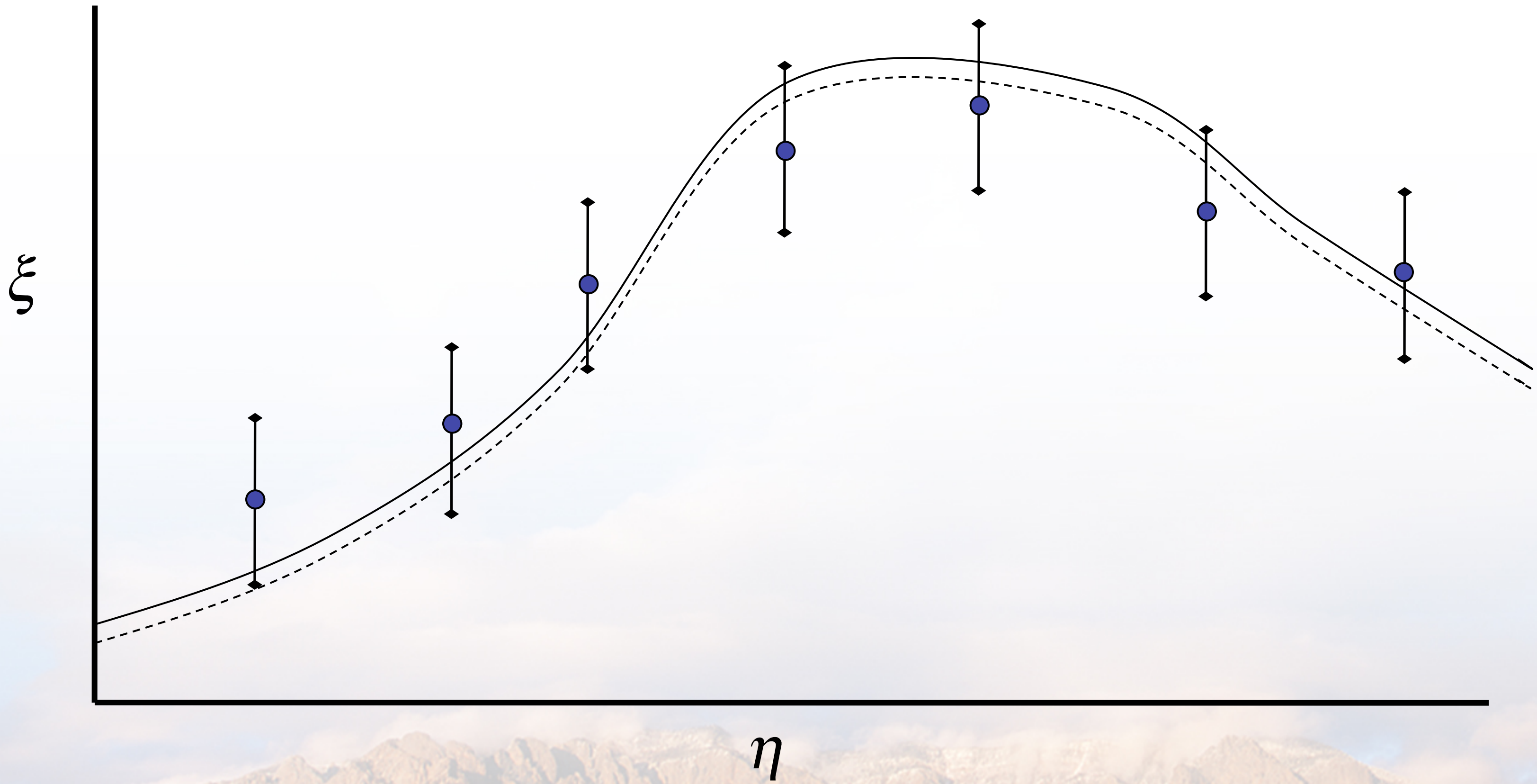
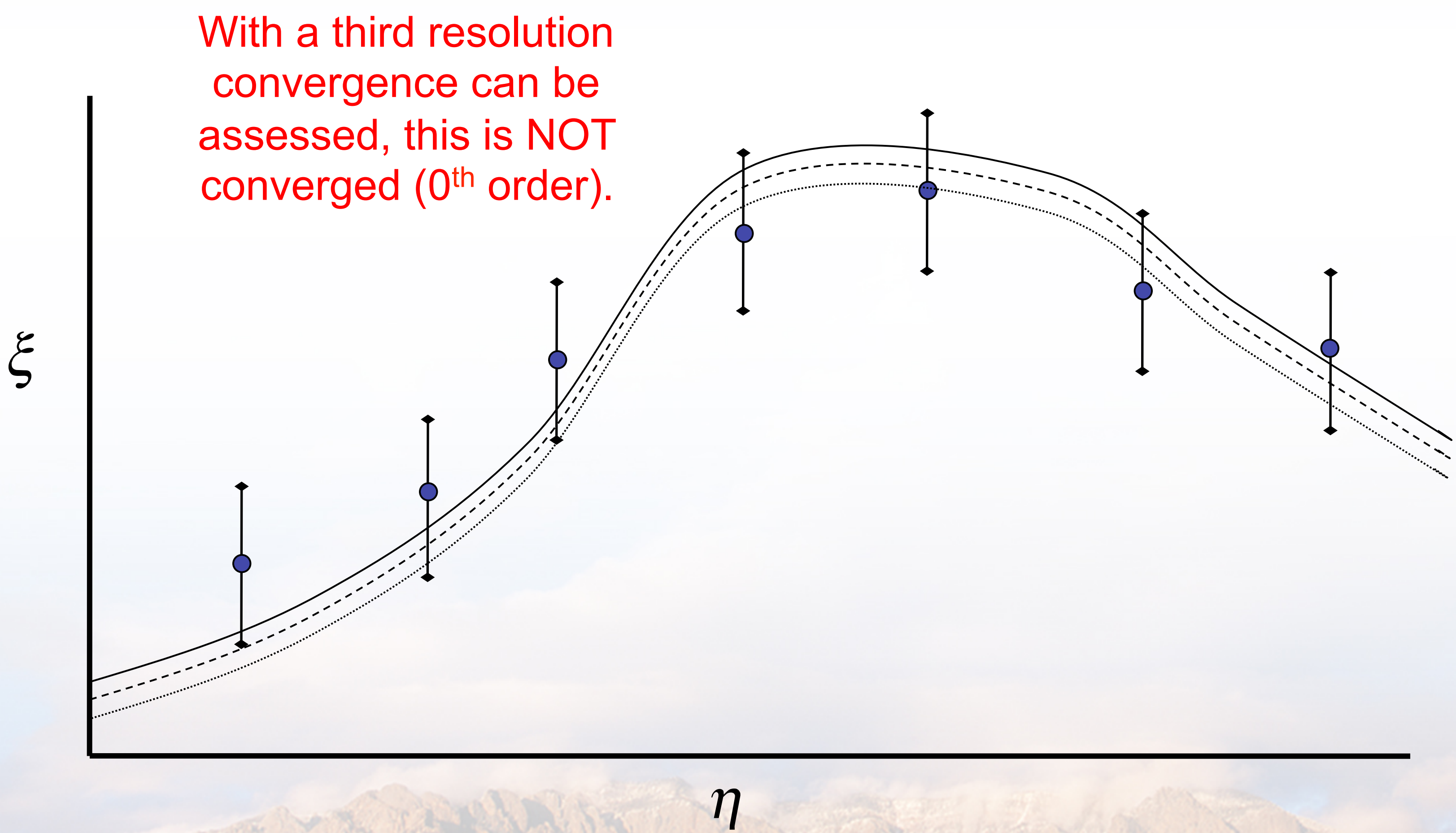
Here is a notion of how a "converged" solution might be described.

This is the usually called mesh sensitivity, this is rather flimsy evidence



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



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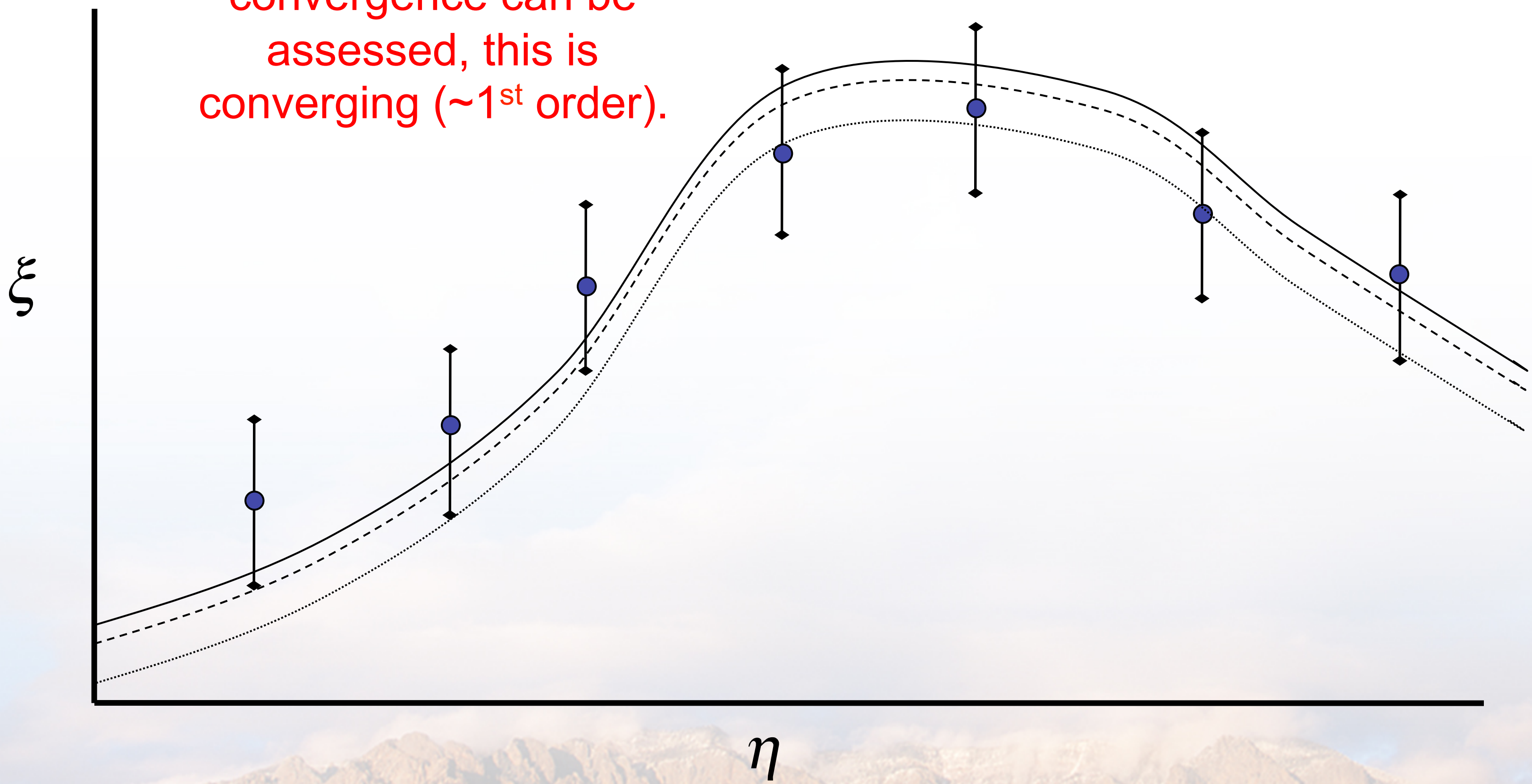
Here is a notion of how a "converged" solution should be described.

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



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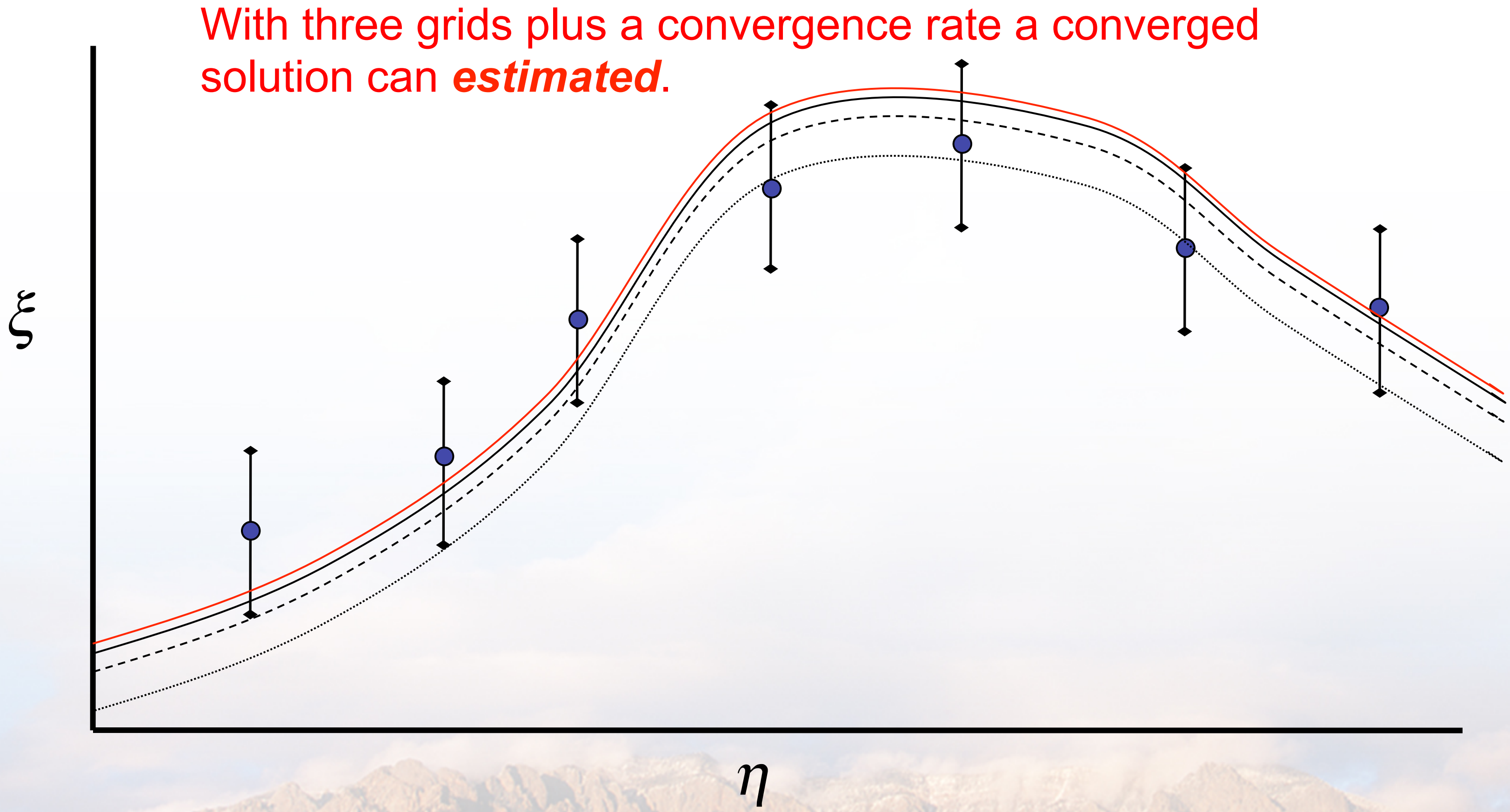
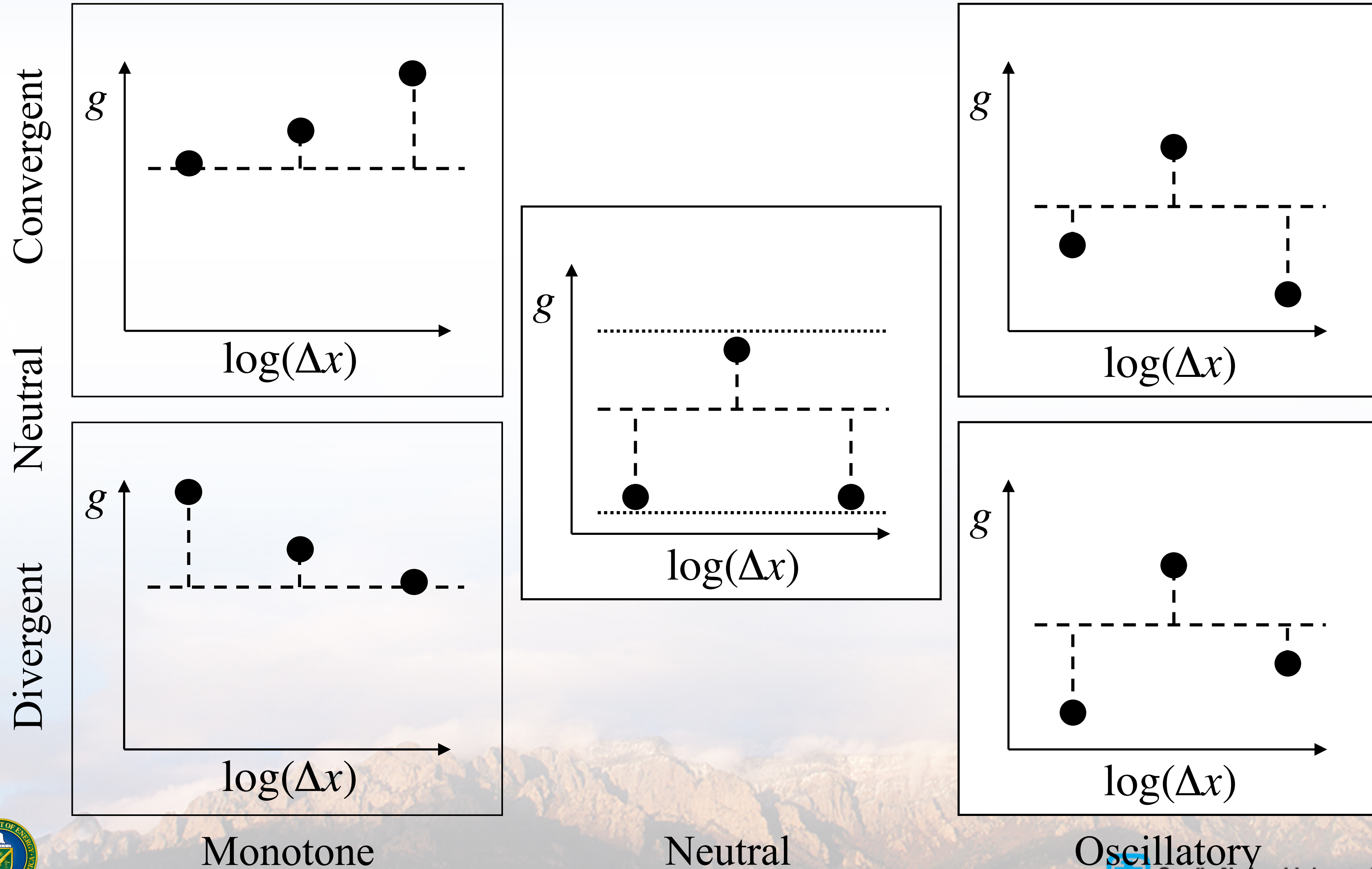
Even better, a sequence of meshes can be used to extrapolate the solution.



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.**

Else if $R > 1$ then monotonic divergence
Else if $R < -1$ then oscillatory divergence
Else ($-1 < R < 0$) oscillatory convergence



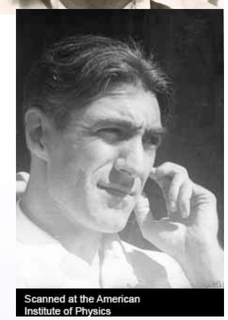
A thought to start us off.

"An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them."

- Werner Heisenberg

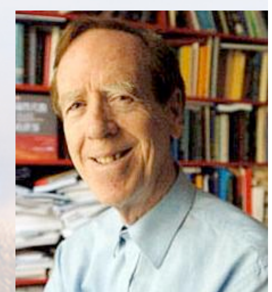
One theorem is absolutely essential to the conduct of verification.

- **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>.

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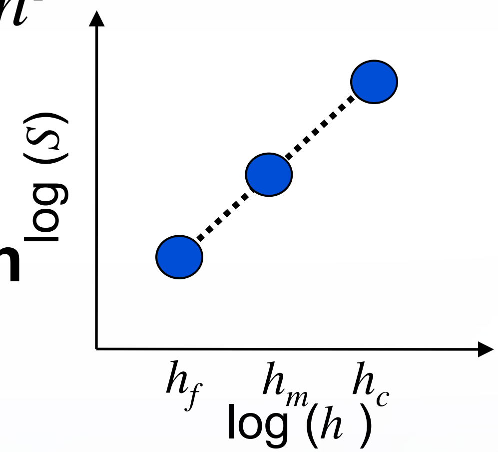
There are a number of typical numerical analysis techniques

- 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

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

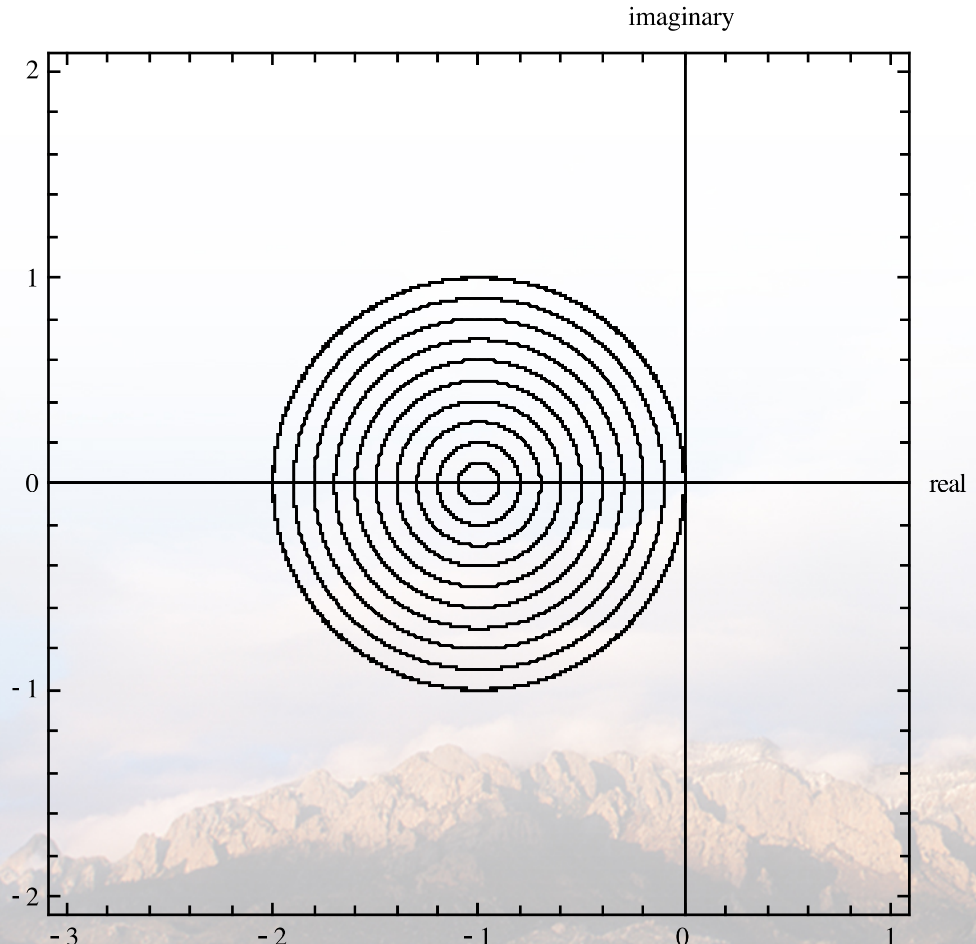
$$\dot{u} = \lambda u \xrightarrow[h \rightarrow 0]{} u(0)\left(1 + \lambda h + \tfrac{1}{2}(\lambda h)^2 + \tfrac{1}{6}(\lambda h)^3 + O\left(h^4\right)\right)$$

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

- 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,**

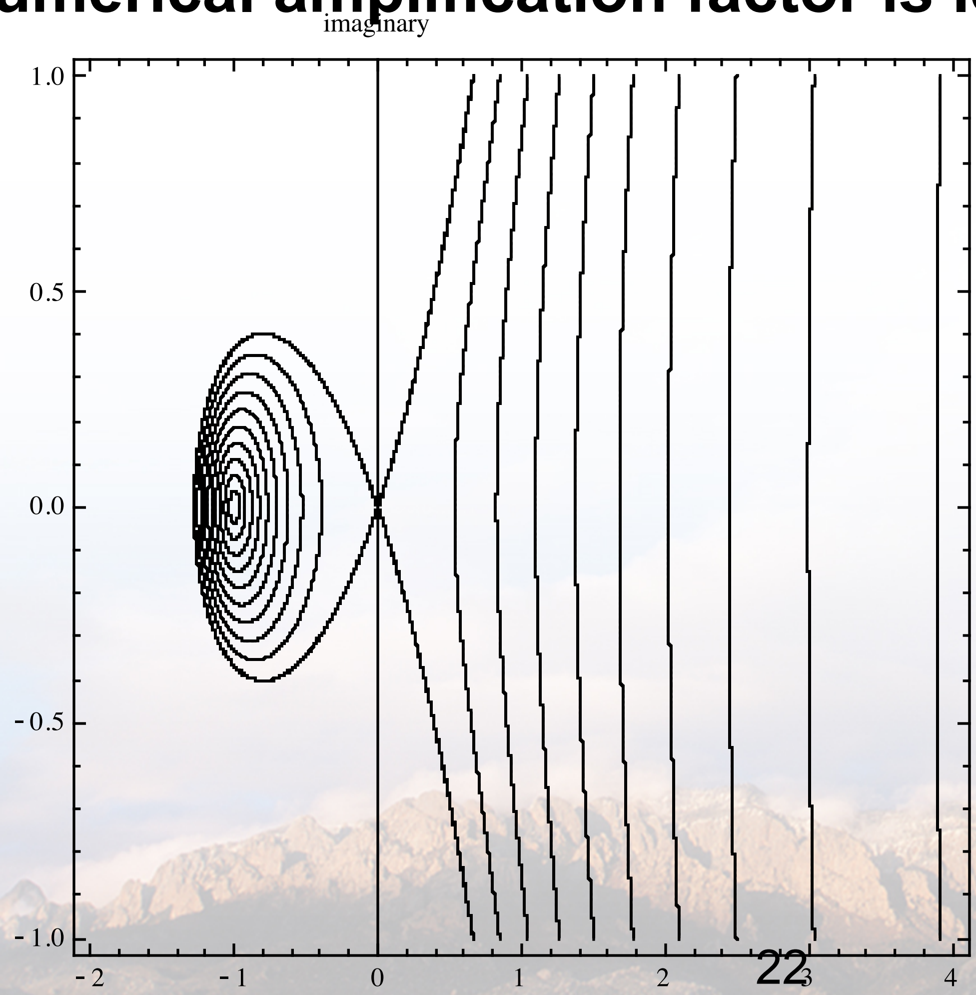


$$A = \sqrt{(1 + ha)^2 + (hb)^2}$$

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



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

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

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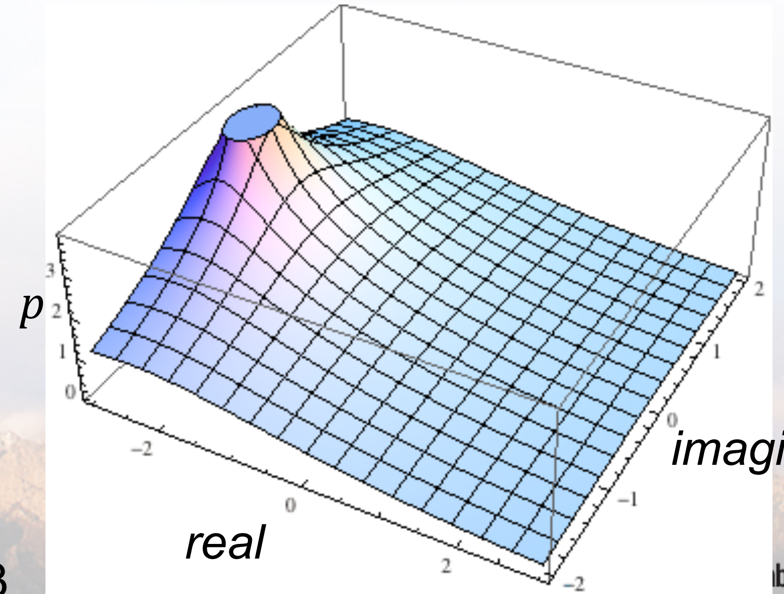
With this foundation, we can augment these techniques to provide extended results.

- **The key is to realize that the error can be computed everywhere,** $\text{Error}(h) = \left|A(h) - \exp(\lambda h)\right|$
  - Compute the error with a refined step size (h/2),
    $$\text{Error}(h/2) = \left|\left(A(h/2)^2 - \exp(\lambda h)\right)\right|$$
  - The convergence rate can then be easily computed using the standard form, $p = \log\left[\text{Error}(h)/\text{Error}(h/2)\right]/\log(2)$
  - This convergences to the asymptotic limit of 1 as *h* goes to zero.
- **Compute the error as a function of discrete integration steps**



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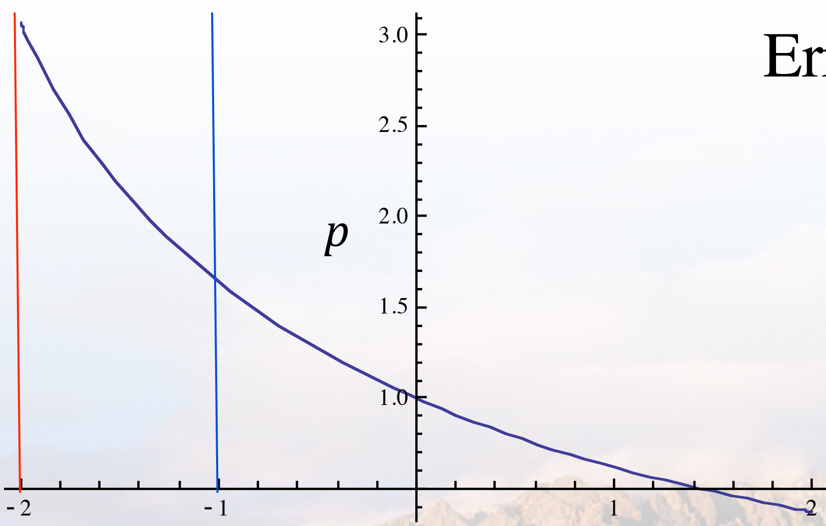
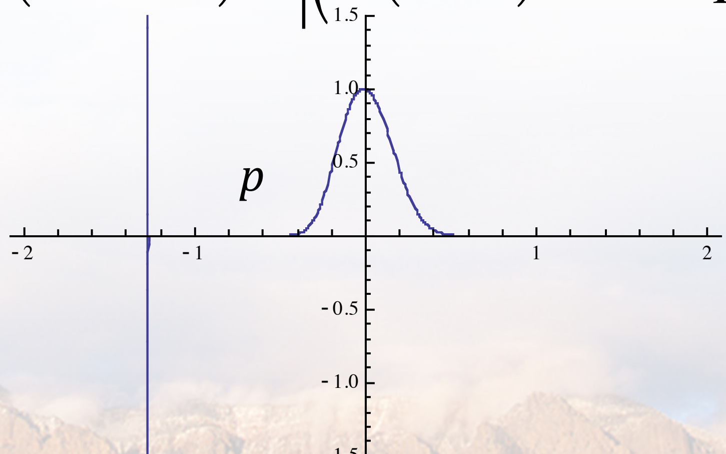
This is the error and convergence for a single step, but multiple steps are used.

- **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**

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



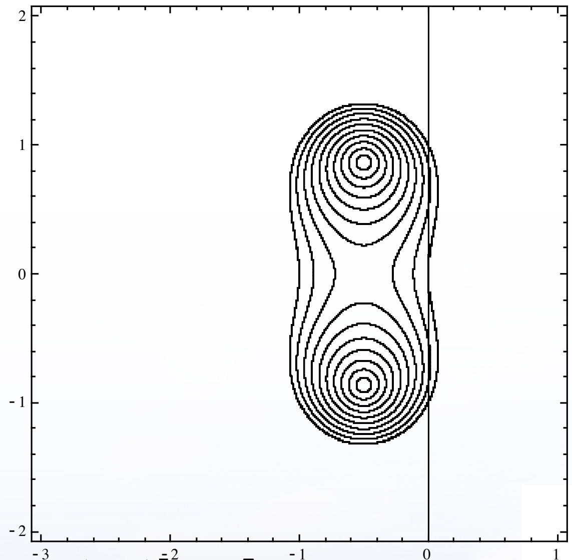
a, *b*=0, single step



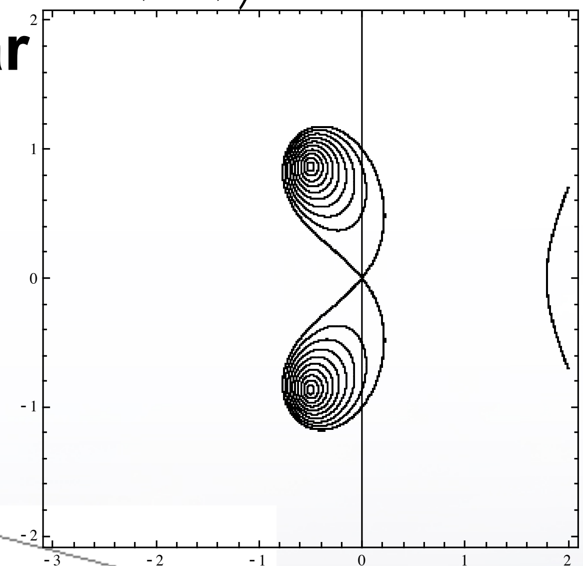
a, *b*=0, 100 steps

We can analyze the second-order modified Euler method similarly

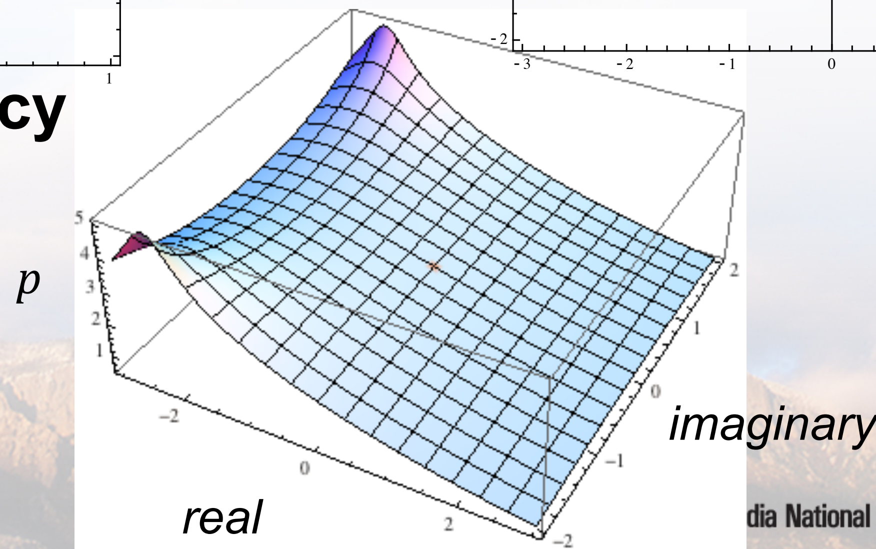
- **Asymptotic accuracy** $\text{Error} \approx u(0)\left(\frac{1}{6}(\lambda h)^3 + O\left(h^4\right)\right)$
- **Stability**



Order star

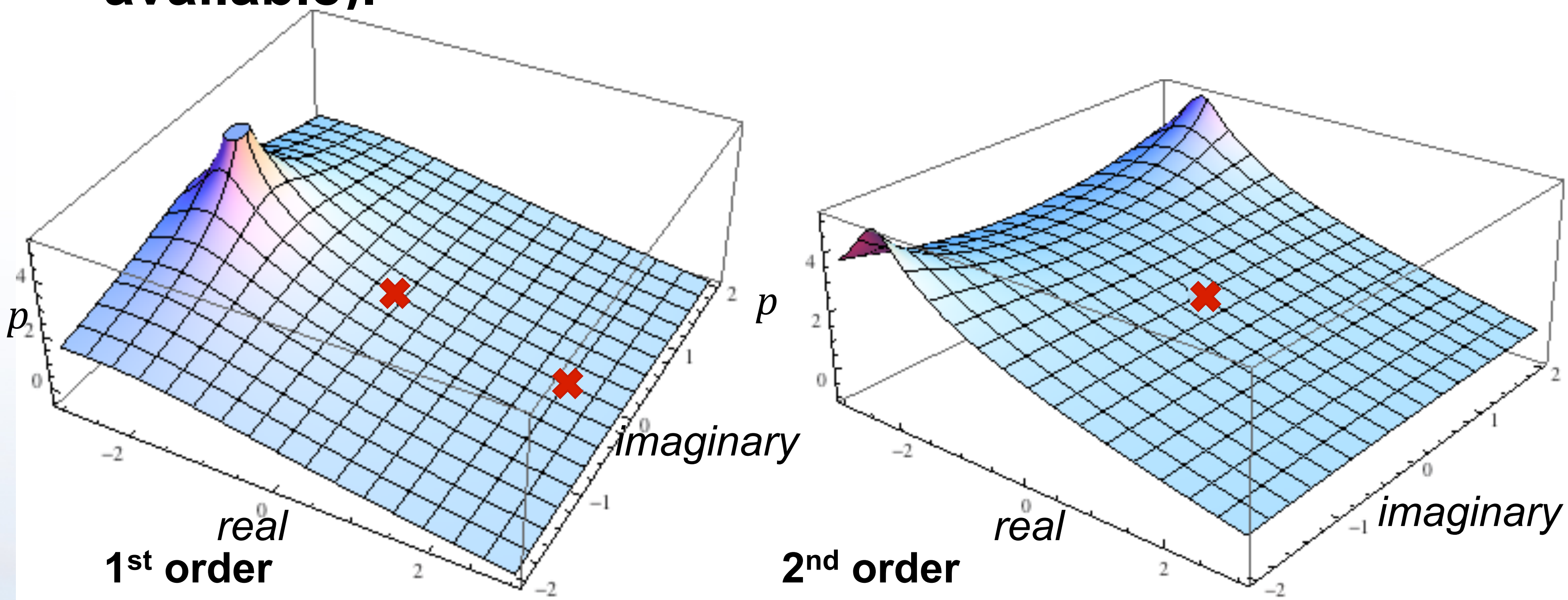


- **Non-asymptotic Accuracy**



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!).

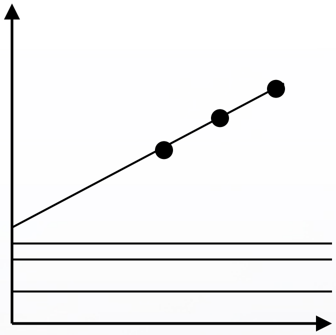
Results for linear ODE can be used to produce "verification" of the analysis

- **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

$$p_T = 1 \quad \Delta_{cm} = 0.027 \quad F_{\text{Roache}} = 1.25$$
$$p = 1.13 \quad \Delta_{mf} = 0.012 \quad F_{\text{Stern}} = 1.18$$
$$\delta = 0.015 \quad F_{\text{Exact}} = 1.12$$



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

  - Compare with a second-order modified Euler

$$p_T = 2 \quad \Delta_{cm} = 0.0036 \quad F_{\text{Roache}} = 1.25$$
$$p = 2.16 \quad \Delta_{mf} = 0.0008 \quad F_{\text{Stern}} = 1.16$$
$$\delta = 0.0002 \quad F_{\text{Exact}} = 1.09$$

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 , $u_j^n = \exp(ij\theta) \Rightarrow u_j^{n+1} = u_j^n - c(u_j^n - u_{j-1}^n) \Rightarrow$

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

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

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

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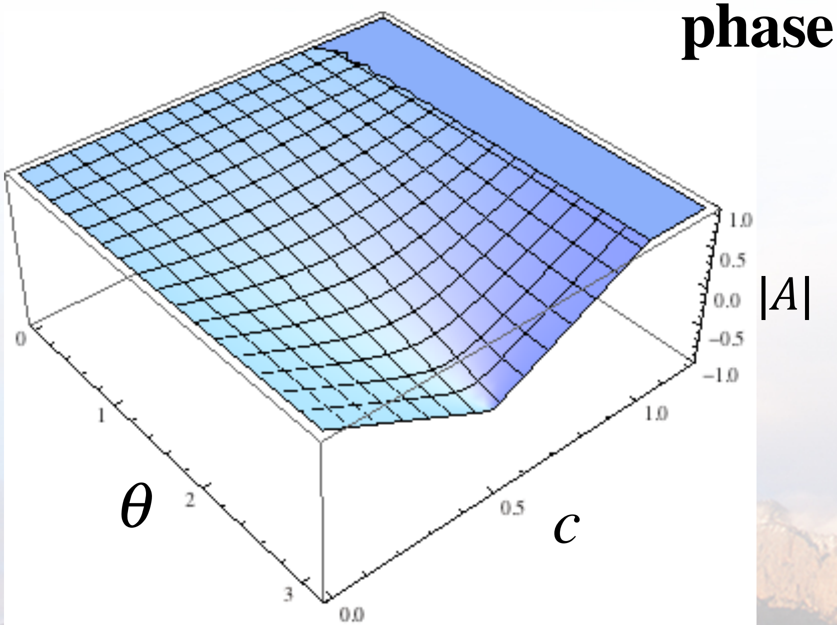
Standard Fourier analysis for PDEs (continued)

- **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. $u_j^{n+1/2} = u_j^n - \frac{\nu}{2}\left(u_{j+1/2}^n - u_{j-1/2}^n\right); u_{j+1/2}^n = u_j^n + \frac{1}{2}\left(u_j^n - u_{j-}^n\right.$
    $$u_j^{n+1} = u_j^n - \nu\left(u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}\right); u_{j+1/2}^{n+1/2} = u_j^{n+1/2} + \tfrac{1}{2}\left(u_j^{n+1/2} - u_{j-1}^{n+1/2}\right)$$

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**

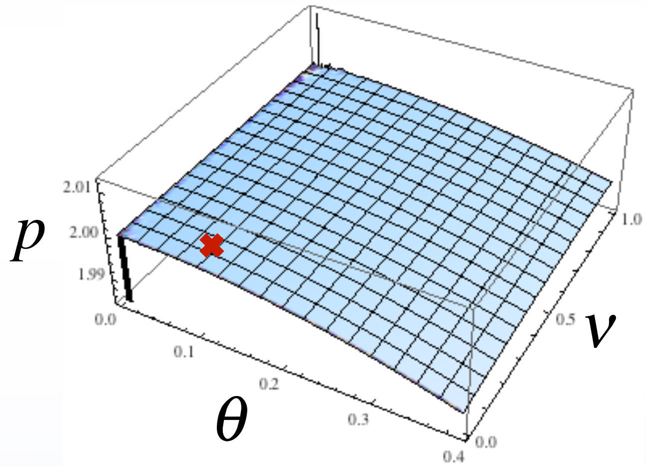
CFL	L^1 error	L^1 rate	L^2 error	L^2 rate
0.10	2.01×10^{-2}	—	2.62×10^{-2}	—
0.05	1.08×10^{-2}	0.96	1.35×10^{-2}	0.96

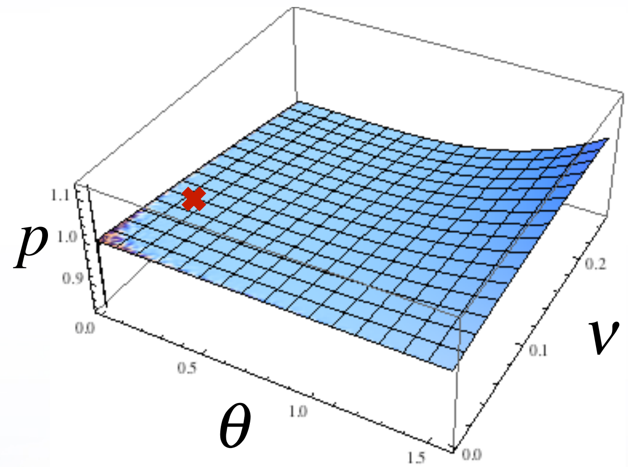
- **MOL time only**

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

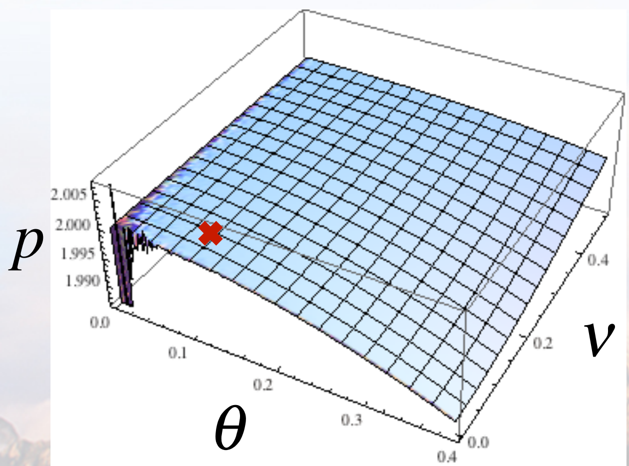
What does the convergence analysis tell us for each case?

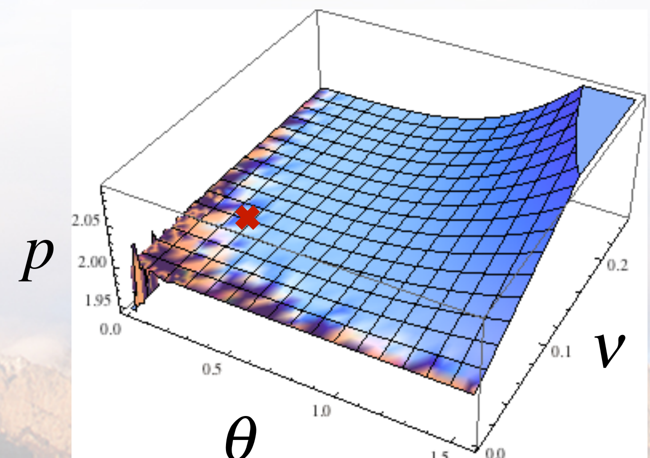
- **L-W scheme** **time-space** **time only**





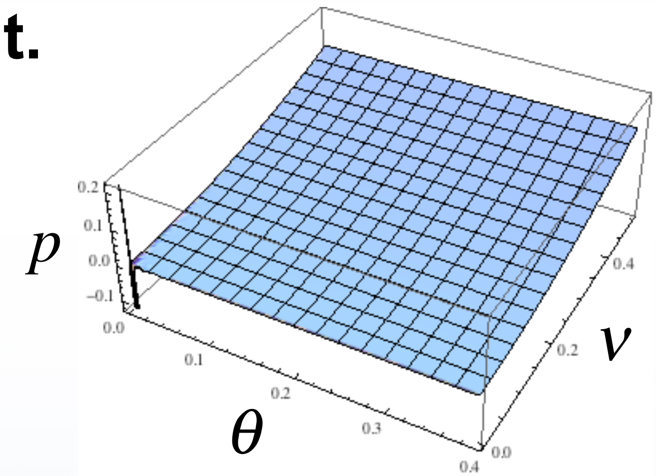
- **MOL scheme**



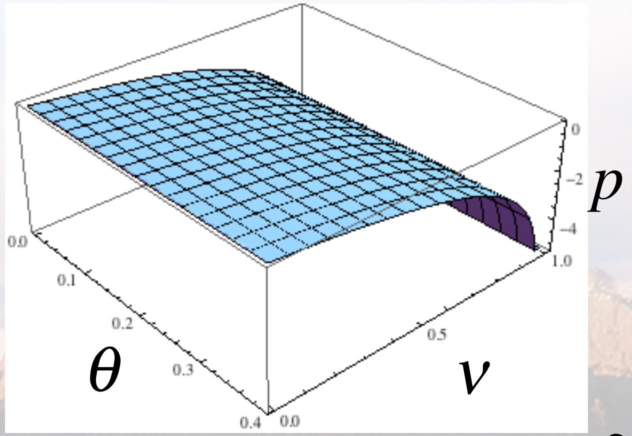


The schemes show distinct difference in convergence toward the exact solution.

- **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)***

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.

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