Verification in Scientific Computing: from Pristine to Practical to Perimeter-Extending

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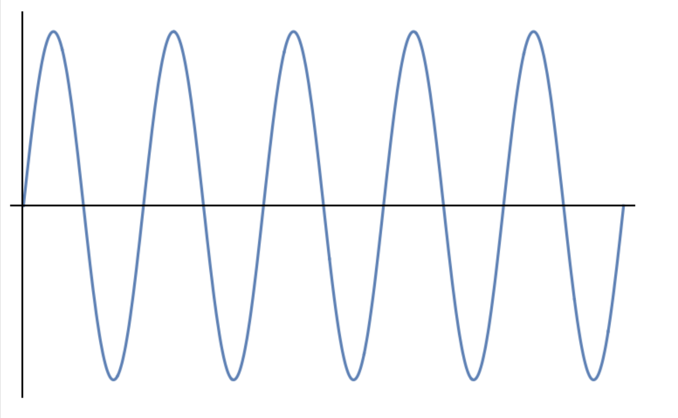
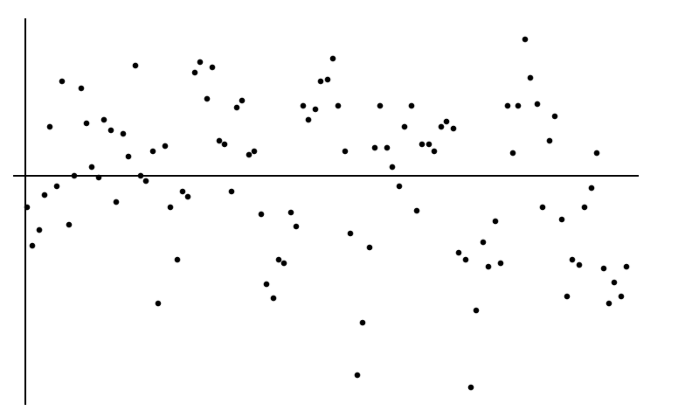
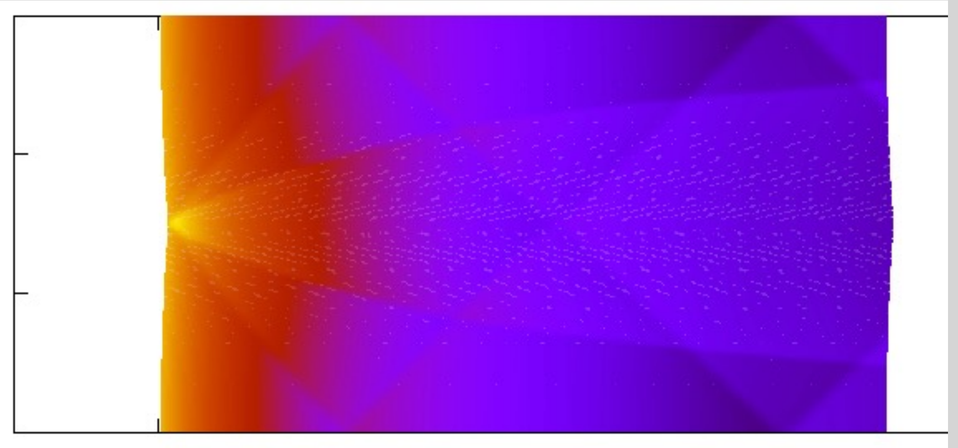
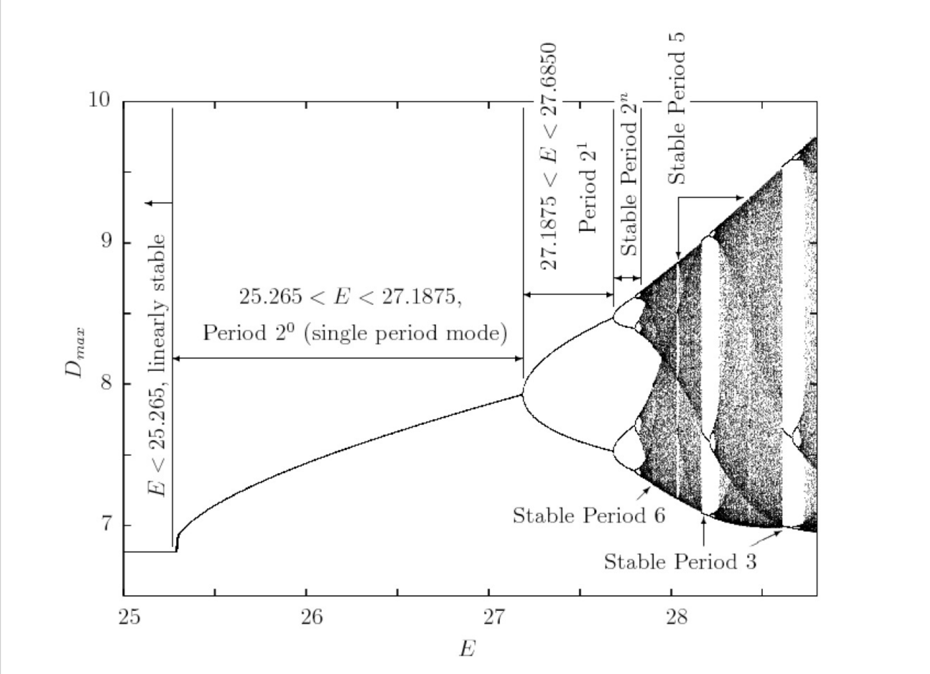
Outline





$$L_2 = ||y_a - y_e||_2 = \sqrt{\int (y_a - y_e)^2 \, dx}$$

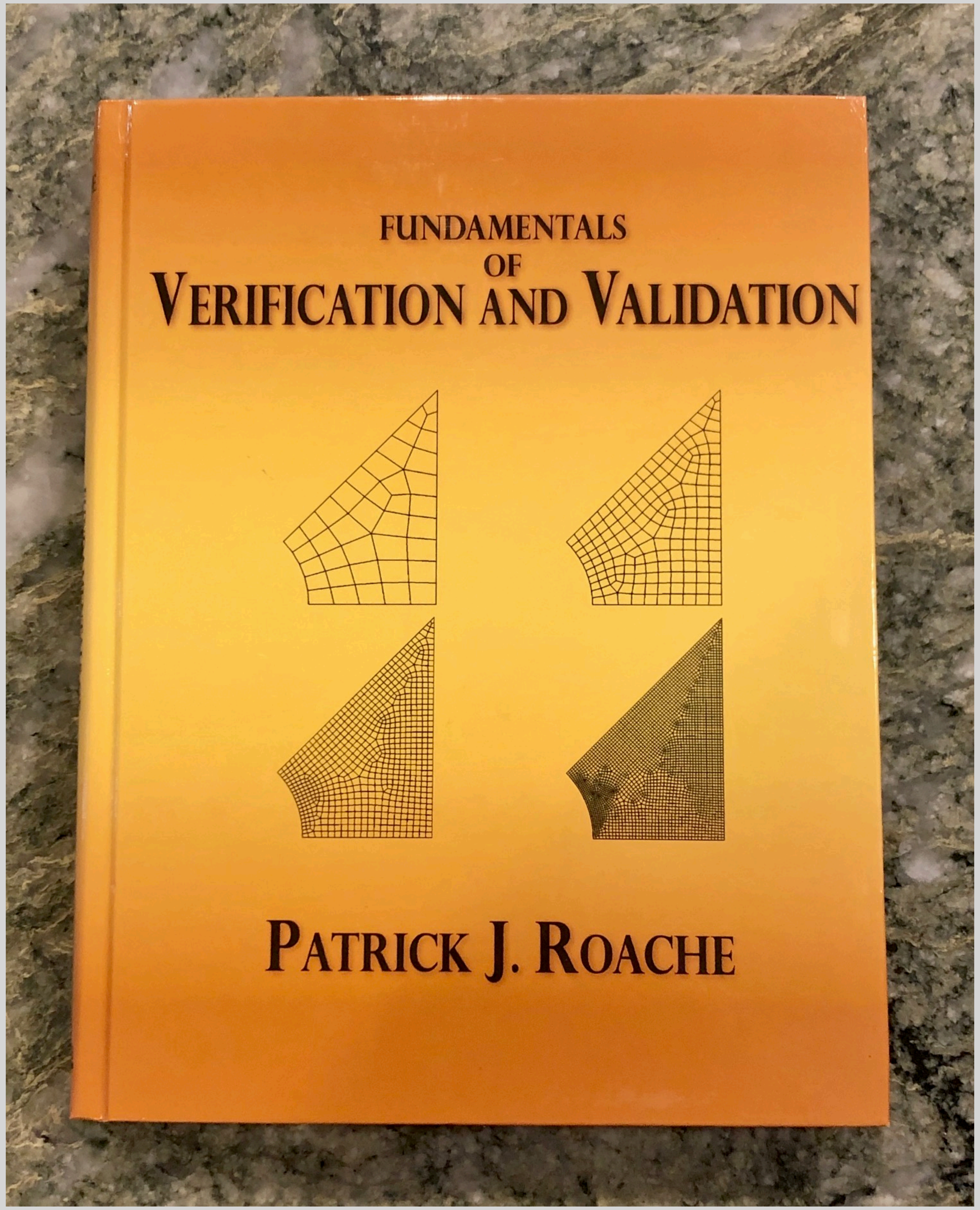




Henrick, 2008

- Signal v. Noise: first resolve the physics, then verify!
- Pristine: convergence, asymptotic convergence rates, multi-scale physics.
- Practical: scarce computational resources, error difficult to define, what should referees expect.
- Perimeter-Extending: nonlinear dynamics, transition to chaos.
- Focus on continuum calculus-based models of reacting fluid dynamics.

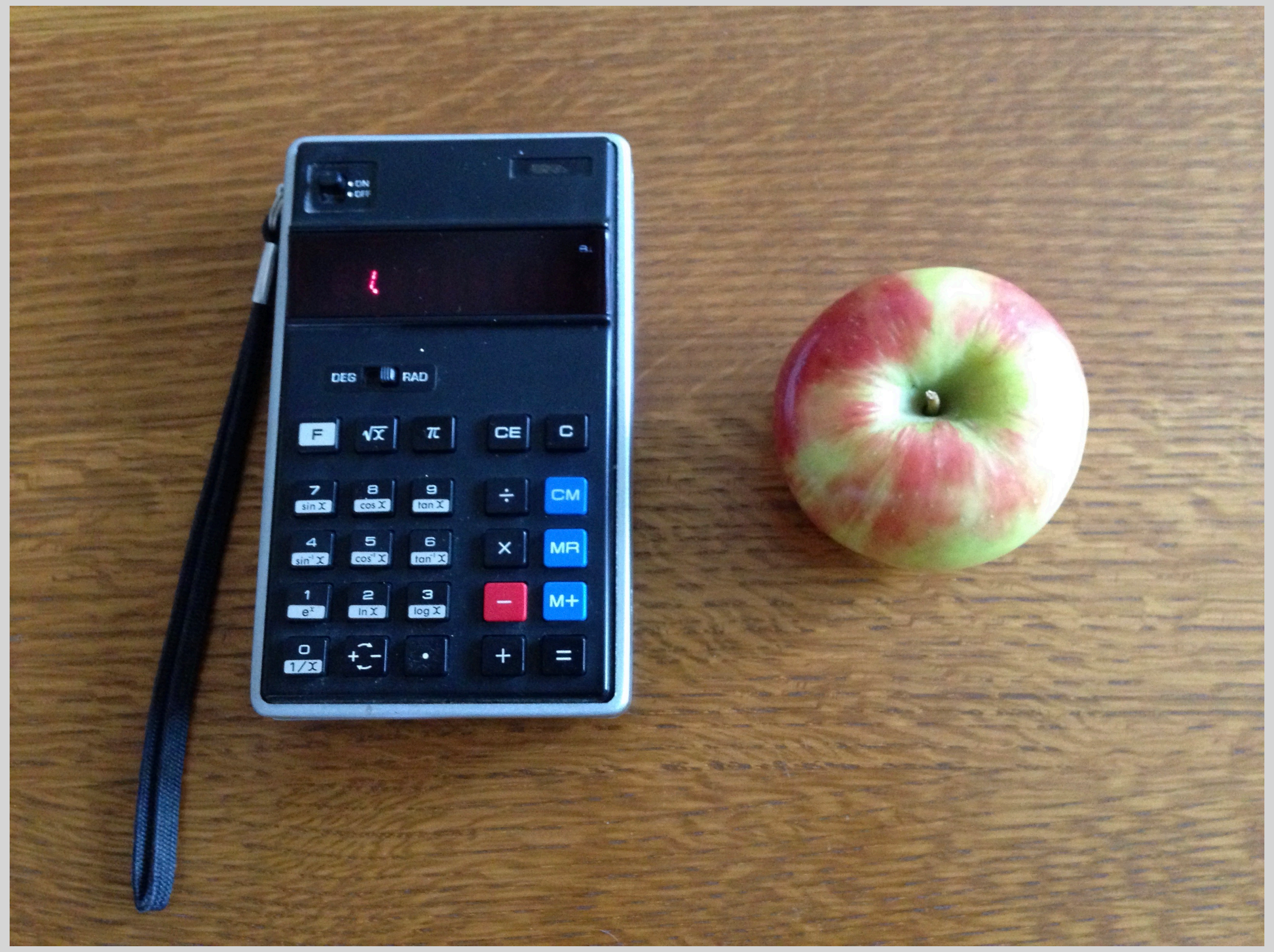
Verification v. Validation



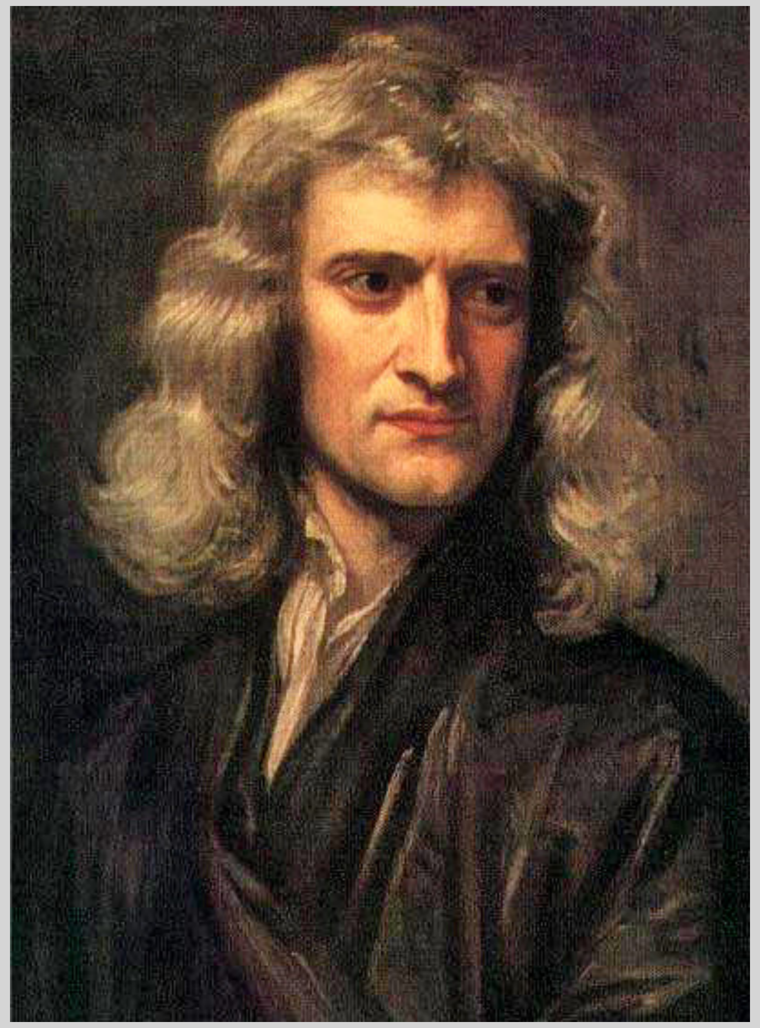
Roache, 2009

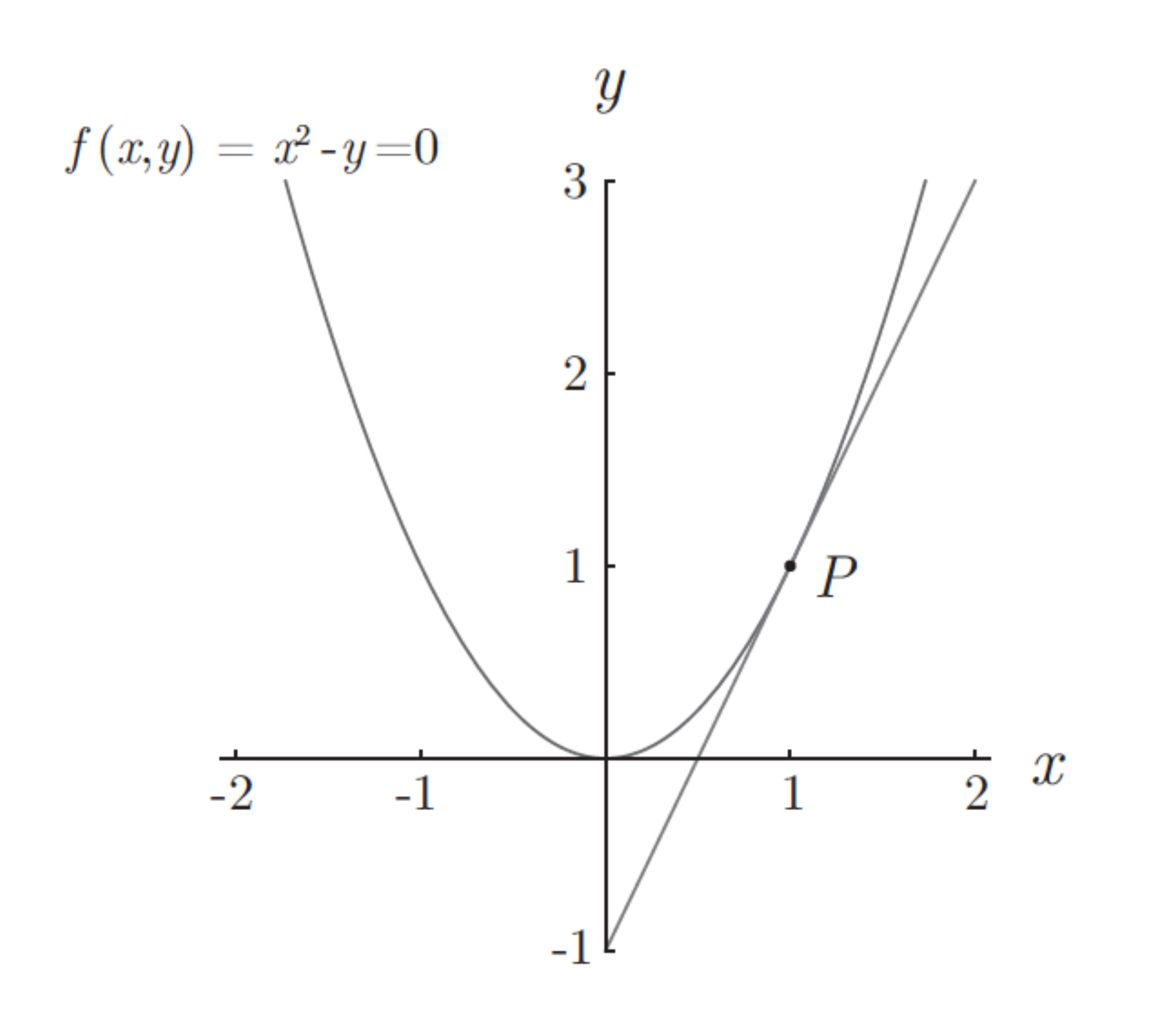
- Verification: solving the equations right.
- Validation: solving the right equations.
- Pat Roache informed me in 1990 I was doing verification. (I was, but didn't know it.)
- Seemed unnecessary.
- I was wrong. The need exists.
- Widespread misunderstanding of V&V.
- Getting it right is important!
- Focus here is solution verification: ASME V&V20: "Estimates the numerical accuracy of a particular calculation."

Verification and Calculus



$$y = x^2$$
$$\frac{dy}{dx} = 2x$$
$$\left.\frac{dy}{dx}\right|_{x=1} = 2$$
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{y(x+\Delta x) - y(x)}{\Delta x}$$





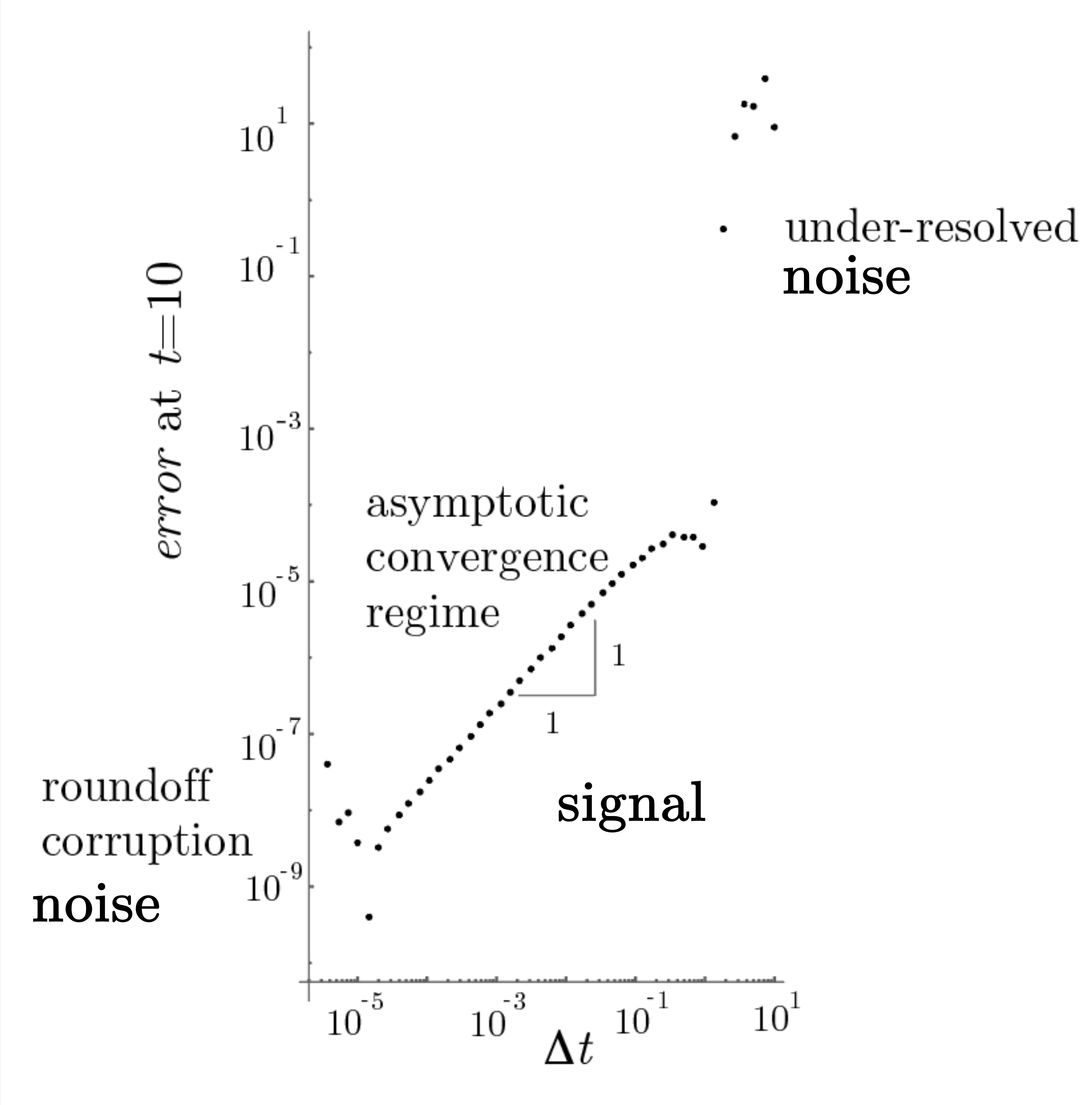
Powers and Sen, 2015

- Cathartic moment in 1978 when I saw a finite difference estimation of the derivative approached the prediction given by Newton's calculus begun in 1665.
- Getting the low order estimate "right" is important!
- We can (and should) do high order corrections later!

Contentions

- Getting a prediction that resolves the modeled physics is ultimately the most important.
- This is often not achieved.
- Low order methods, with appropriate resolution, can get the "signal."
- Once this "signal" has been identified, one can and should *verify* it. ("h-refinement").
- Once this "signal" has been identified, high order methods may be used for enhanced accuracy and efficiency ("p-refinement").

Convergence of the Forward Euler Method



$$\frac{dy}{dt} = -y, \qquad y(0) = 1$$

$$y = e^{-t}$$

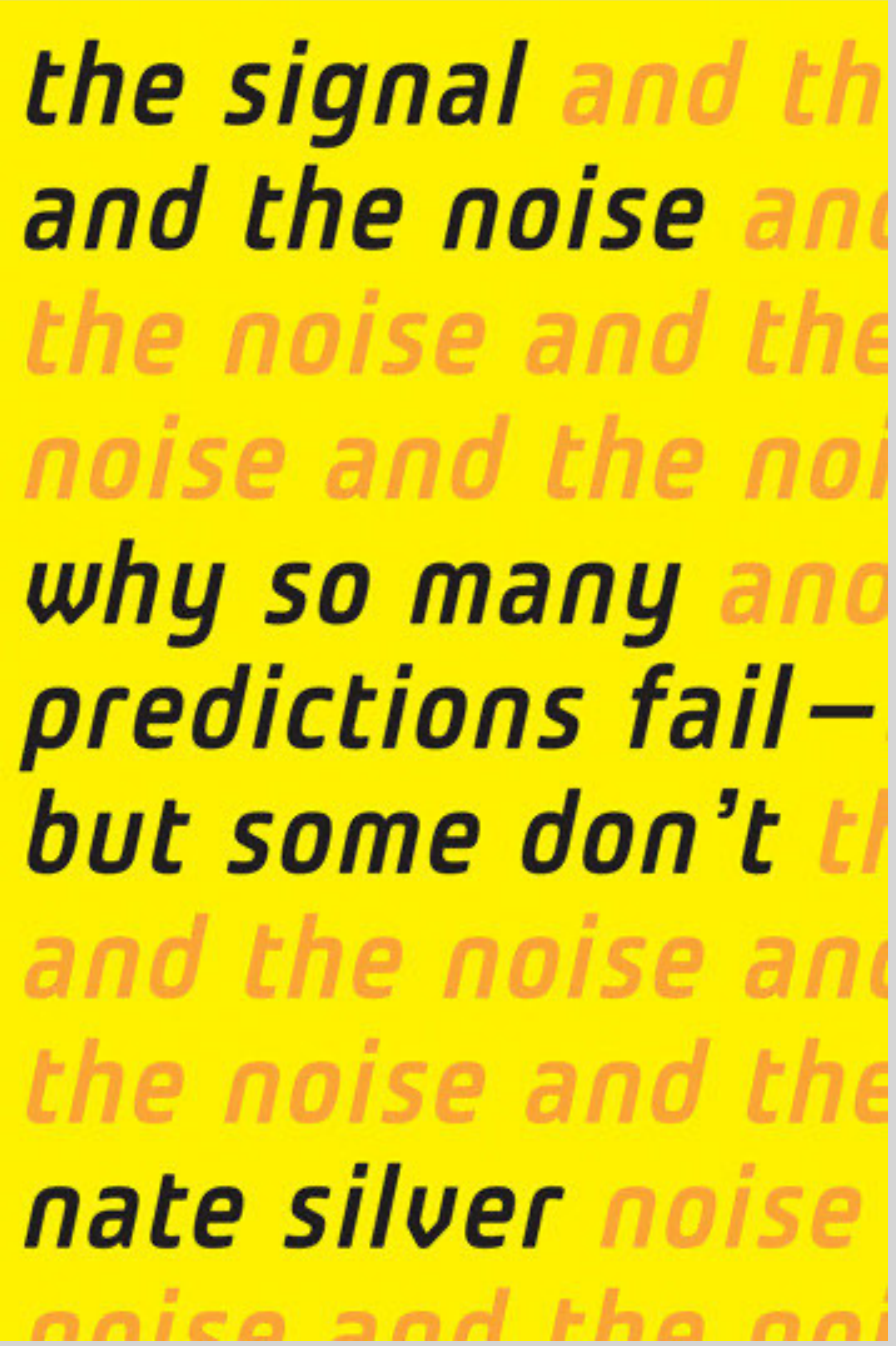
relaxation time constant, $\tau \sim 1$,

$$y_{n+1} = y_n - \Delta t y_n, \qquad n = 1, \ldots, N$$

$$error = ||y_N - e^{-N\Delta t}||.$$

- $\Delta t > \tau$: Solution not captured.
- $\Delta t \sim \tau$: Solution captured.
- $\Delta t < \tau$: Solution expensively captured.

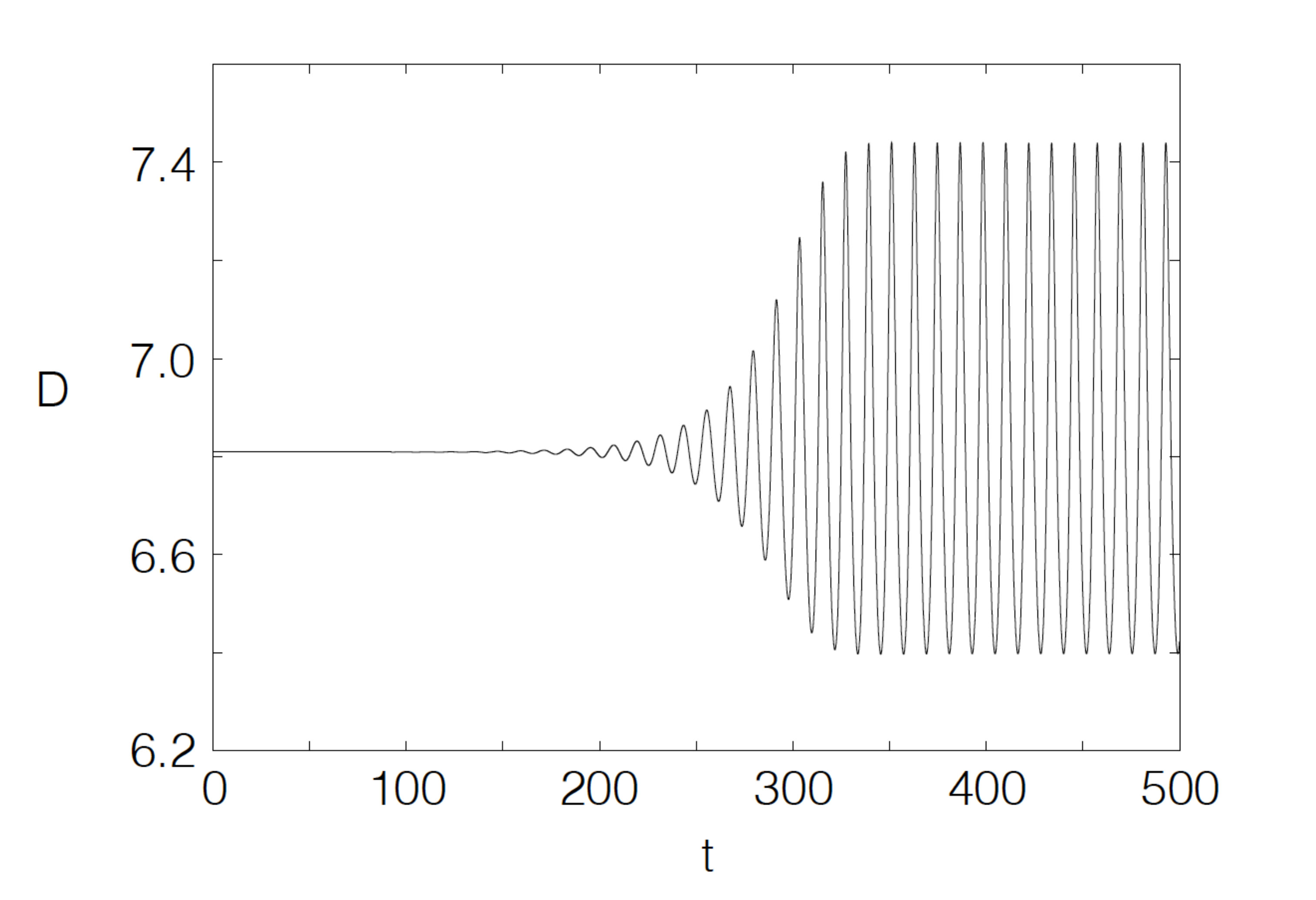
Signal v. Noise



Silver, 2012

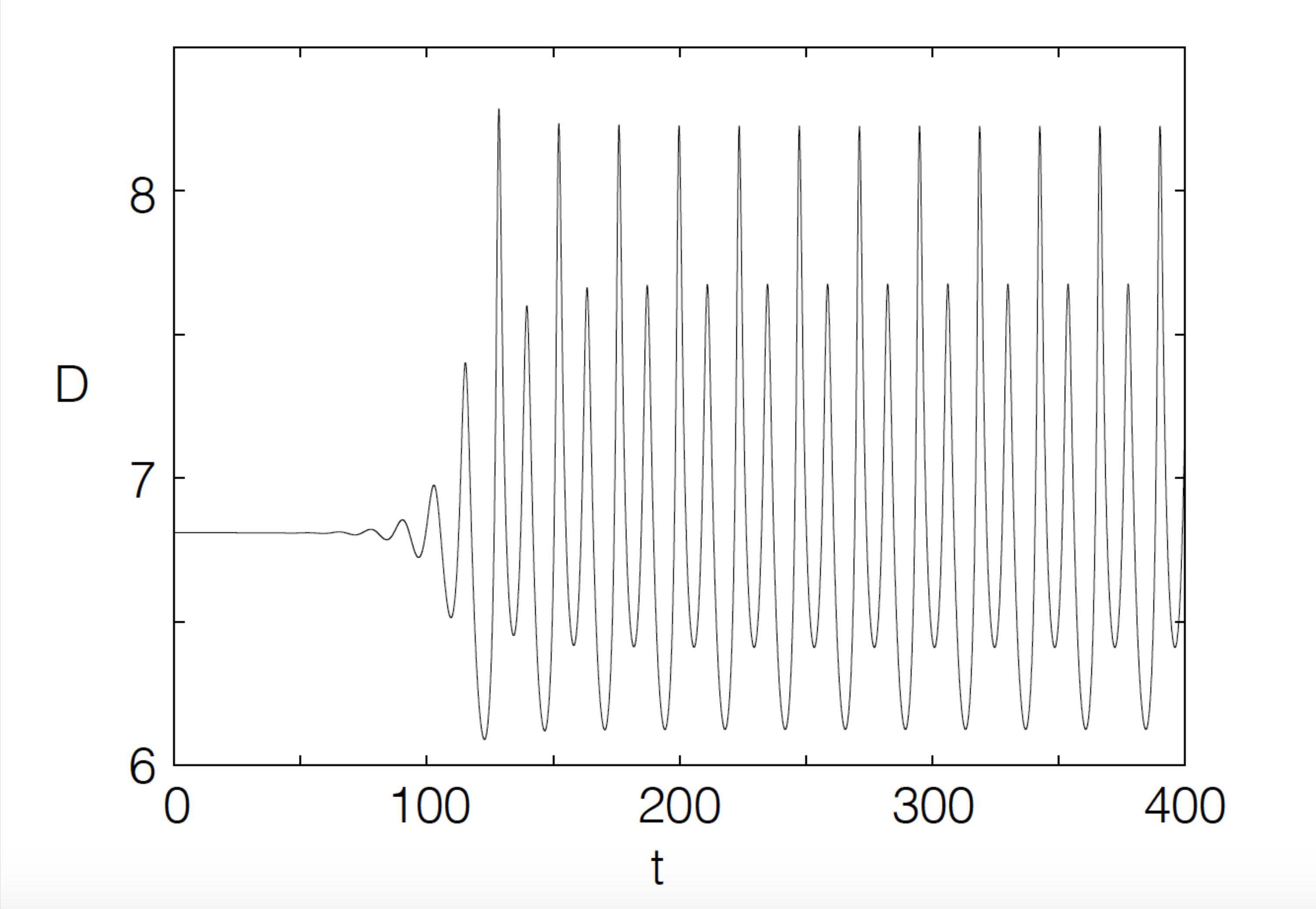
- First order of business: tune to the signal to steer clear of the noise.
- Getting the low order estimate "right" is important!
- A simple AM radio, tuned to the station, conveys the signal with some noise.
- A sophisticated FM radio, still properly tuned, conveys the signal with less noise.

Signal v. Noise in Computational Simulation

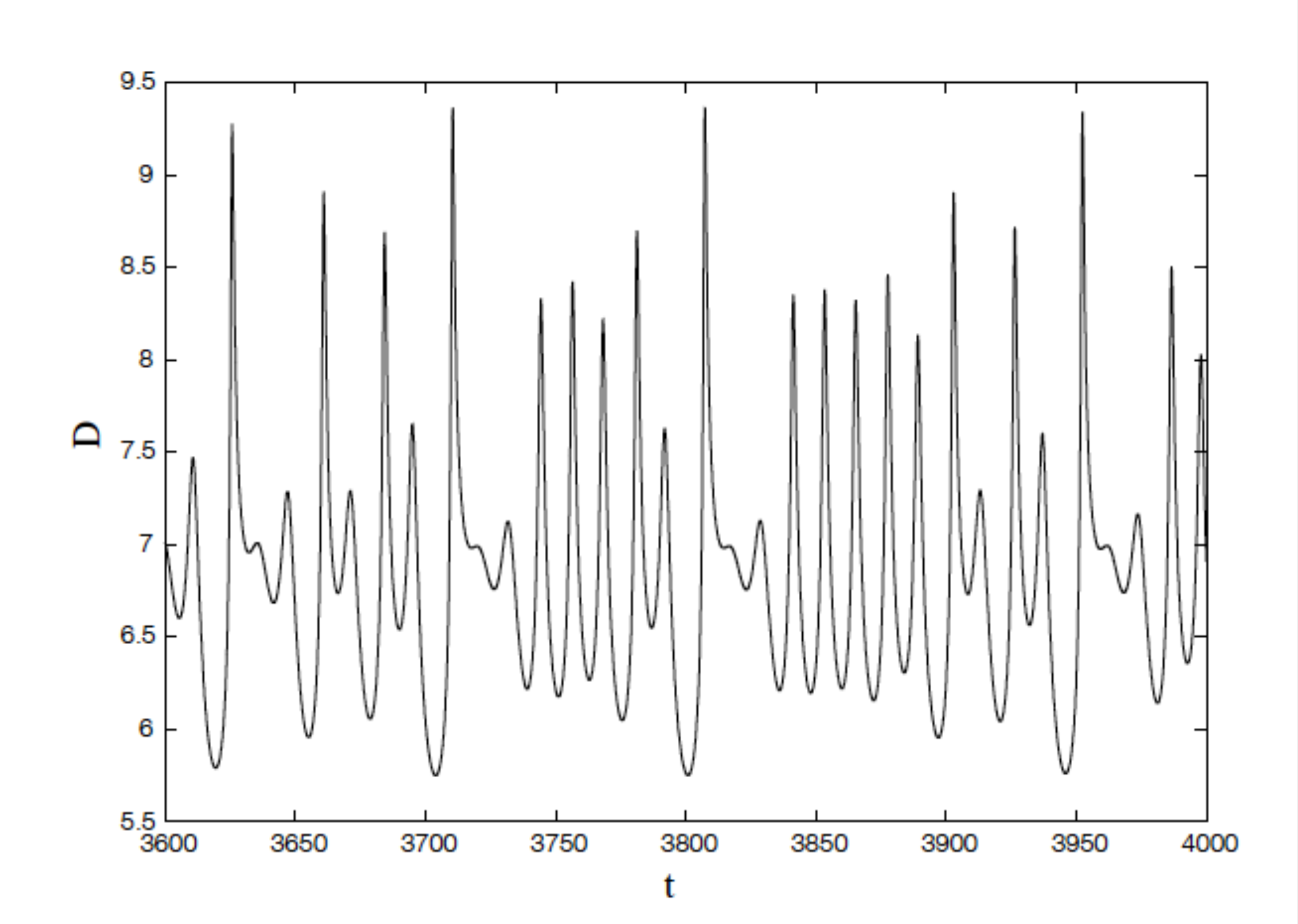


Henrick, 2008

Signal

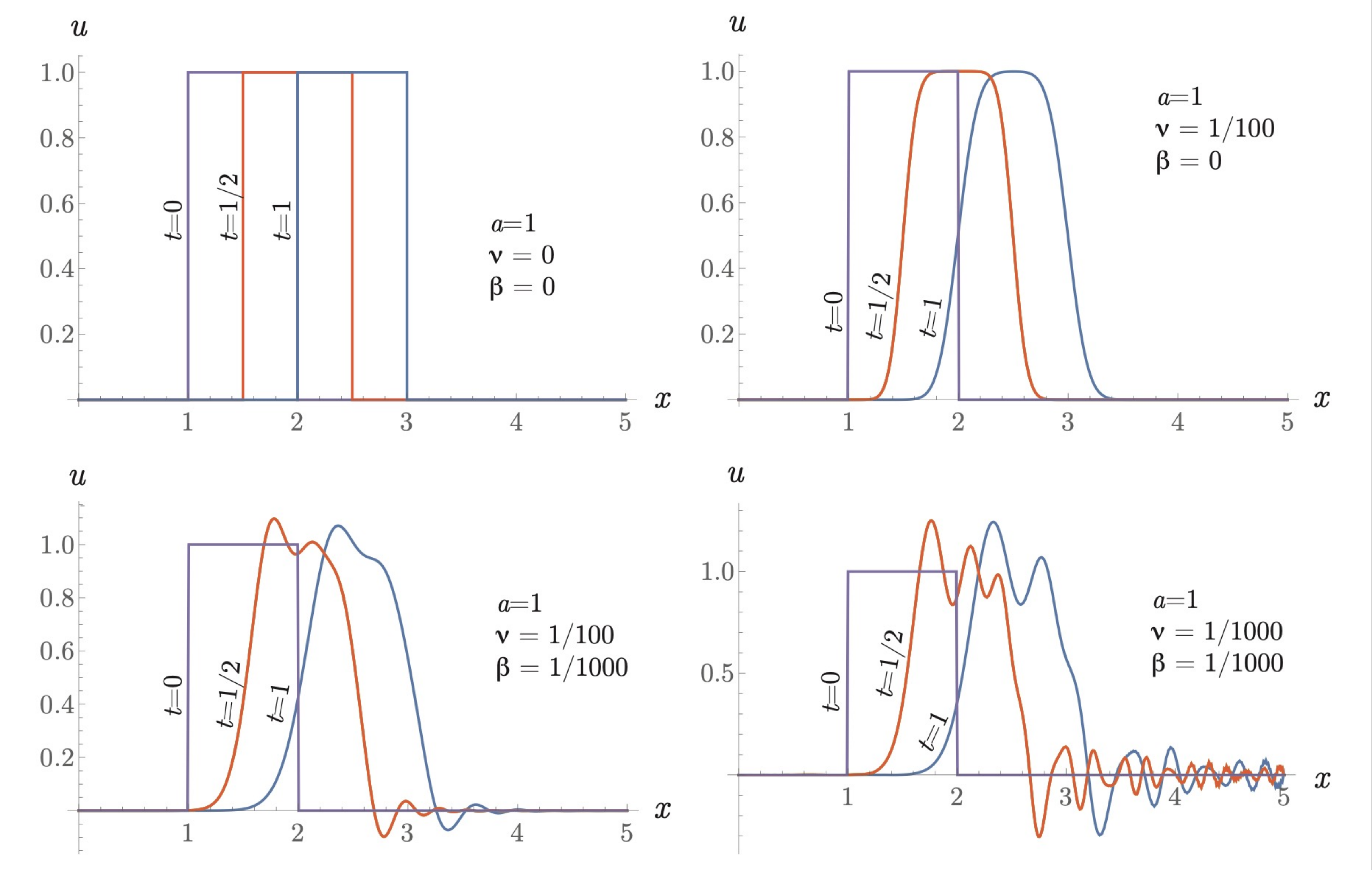


Signal



Signal or Noise?

Signal v. Noise Generated by Discretization

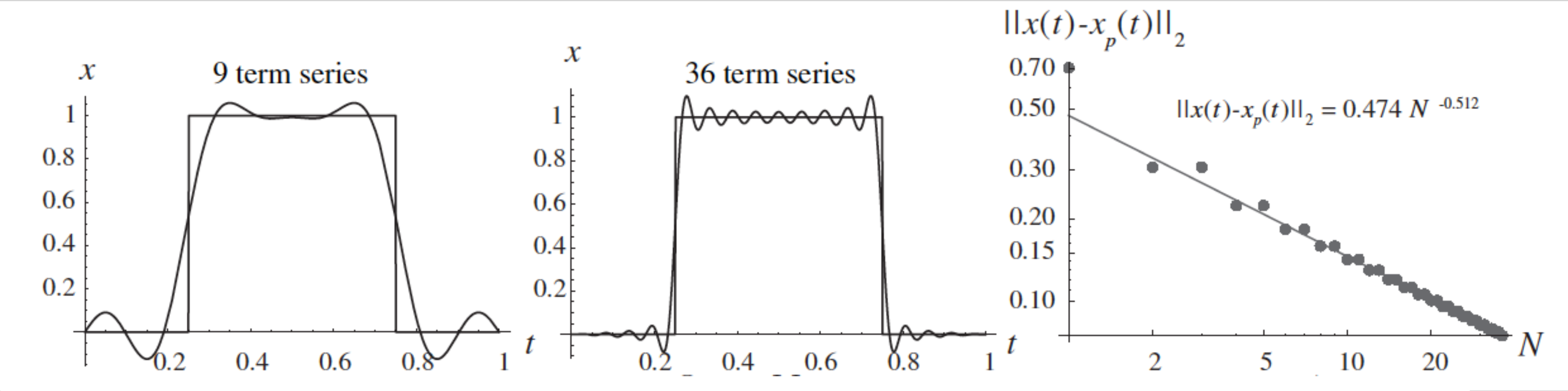


$$\underbrace{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}}_{\text{signal}} = 0 \qquad u = f(x - at)$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1}^n - u_i^n}{\Delta x} = 0.$$

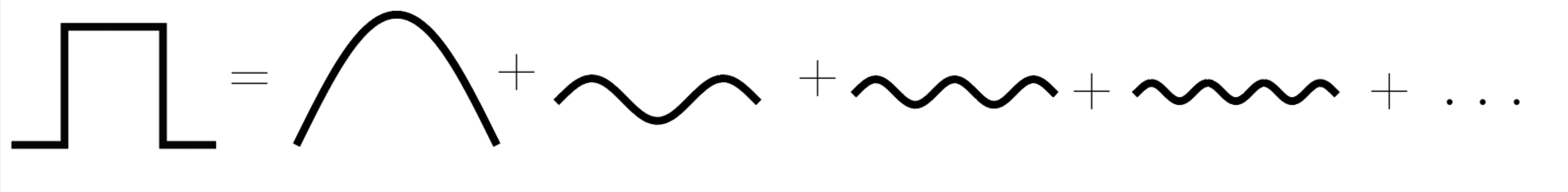
$$\underbrace{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}}_{\text{signal}} = \underbrace{\underbrace{\nu(\Delta x, \Delta t)\frac{\partial^2 u}{\partial x^2}}_{\text{numerical diffusion}} + \underbrace{\beta(\Delta x, \Delta t)\frac{\partial^3 u}{\partial x^3}}_{\text{numerical dispersion}} + \dots}_{\text{noise}}$$

Fourier Series Decomposition Example



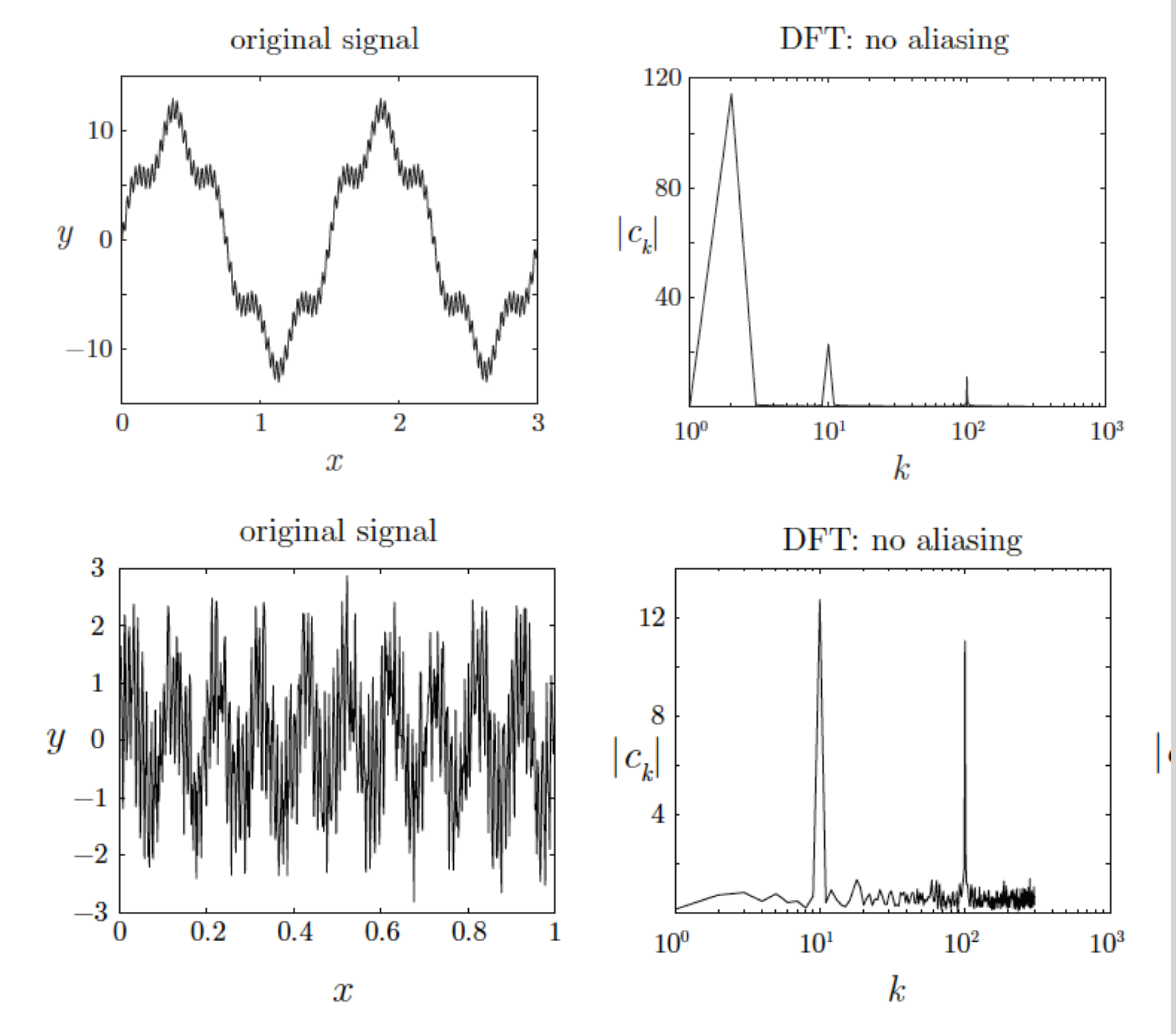
$$H\left(t-\frac{1}{4}\right)-H\left(t-\frac{3}{4}\right)=\frac{2\sqrt{2}}{\pi}\left(\sin(\pi t)-\frac{\sin(3\pi t)}{3}-\frac{\sin(5\pi t)}{5}+\frac{\sin(7\pi t)}{7}+\frac{\sin(9\pi t)}{9}+\ldots\right).$$

Powers and Sen, 2015



- All frequencies represented in an arbitrary signal.
- Typically neglect low amplitude, high frequency modes.
- Such neglect may not be justified, especially for nonlinear problems.

Fourier Signal Analysis Example



Powers and Sen, 2015

- Noisy signals may be sampled.
- Discrete Fourier Transform (DFT) reveals periodicity at various frequencies.
- May be possible to discern a signal in an apparently noisy set of data.

Signal Discernment for a Linear Problem

evolution advection diffusion reaction

$$\frac{\partial}{\partial t}Y(x,t) + u\frac{\partial}{\partial x}Y(x,t) = \mathcal{D}\frac{\partial^2}{\partial x^2}Y(x,t) - a(Y(x,t) - Y_{eq}),$$

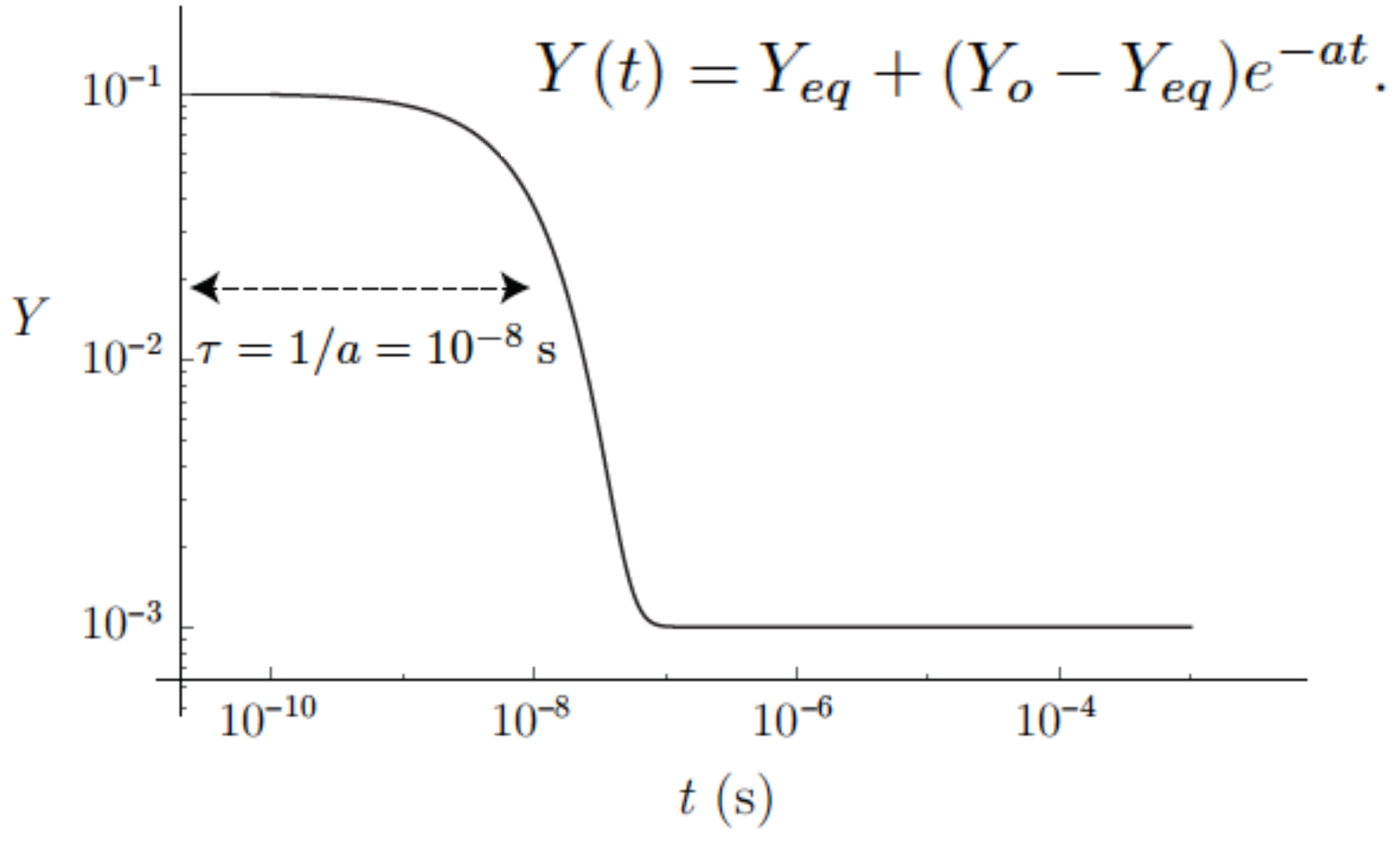
$$Y(x,0) = Y_o, \quad Y(0,t) = Y_o, \quad \frac{\partial Y}{\partial x}(\infty,t) \to 0,$$

Powers, 2016

- Consider a linear advection-reaction-diffusion problem.
- Exact solution exists.
- Gives guidance on fundamental length and time scales that must be resolved for verification.

Time Scale for Spatially Homogeneous Limit

$$\frac{dY(t)}{dt} = -a(Y(t) - Y_{eq}), \qquad Y|_{t=0} = Y_o,$$

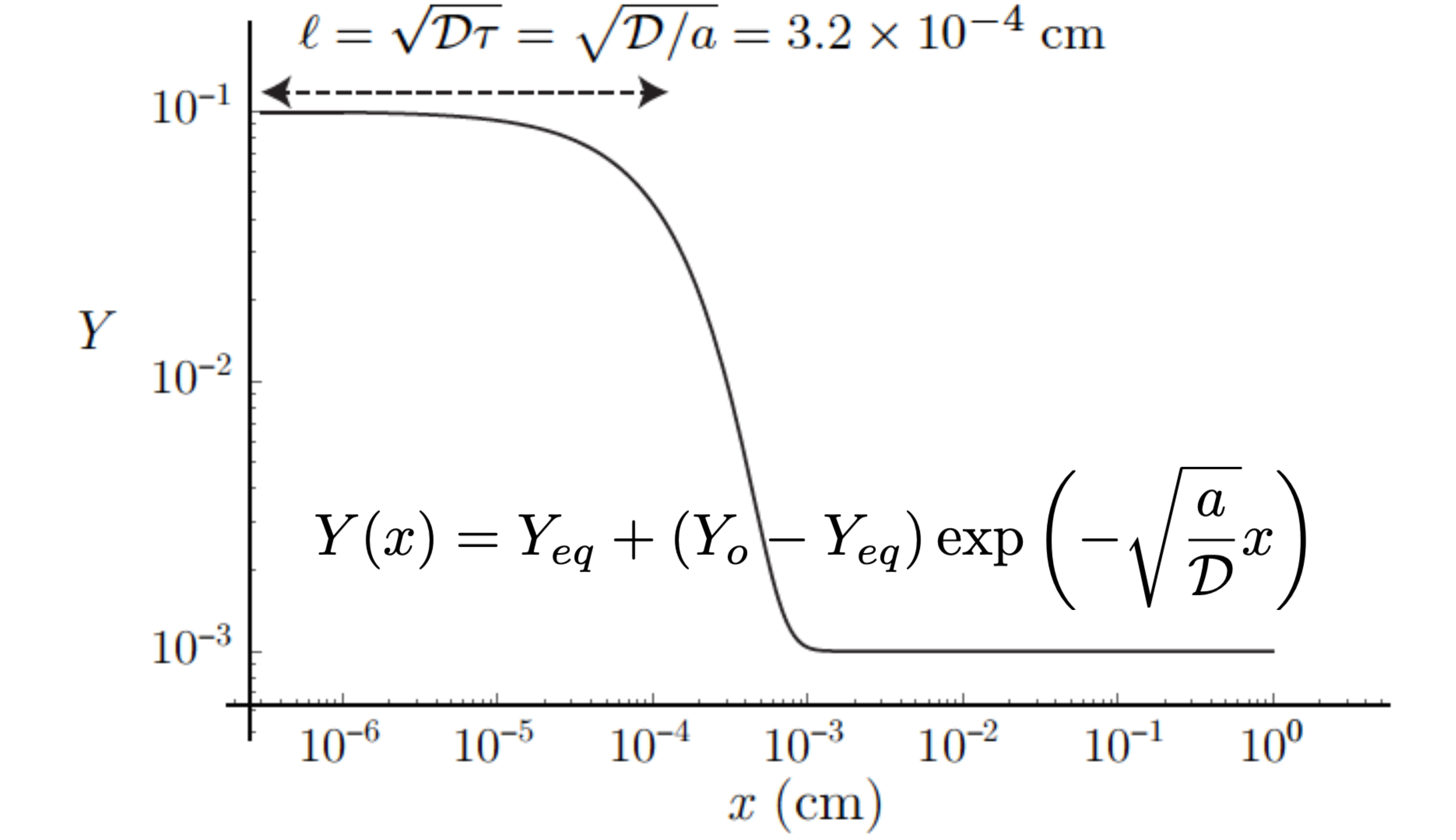


Powers, 2016

- Suppress advection and diffusion.
- Exponential relaxation in time to equilibrium.
- Time scale for reaction identified as $1/a$.

Length Scale for Steady Limit

$$u\frac{dY(x)}{dx} = \mathcal{D}\frac{d^2Y(x)}{dx^2} - a(Y(x) - Y_{eq}),$$



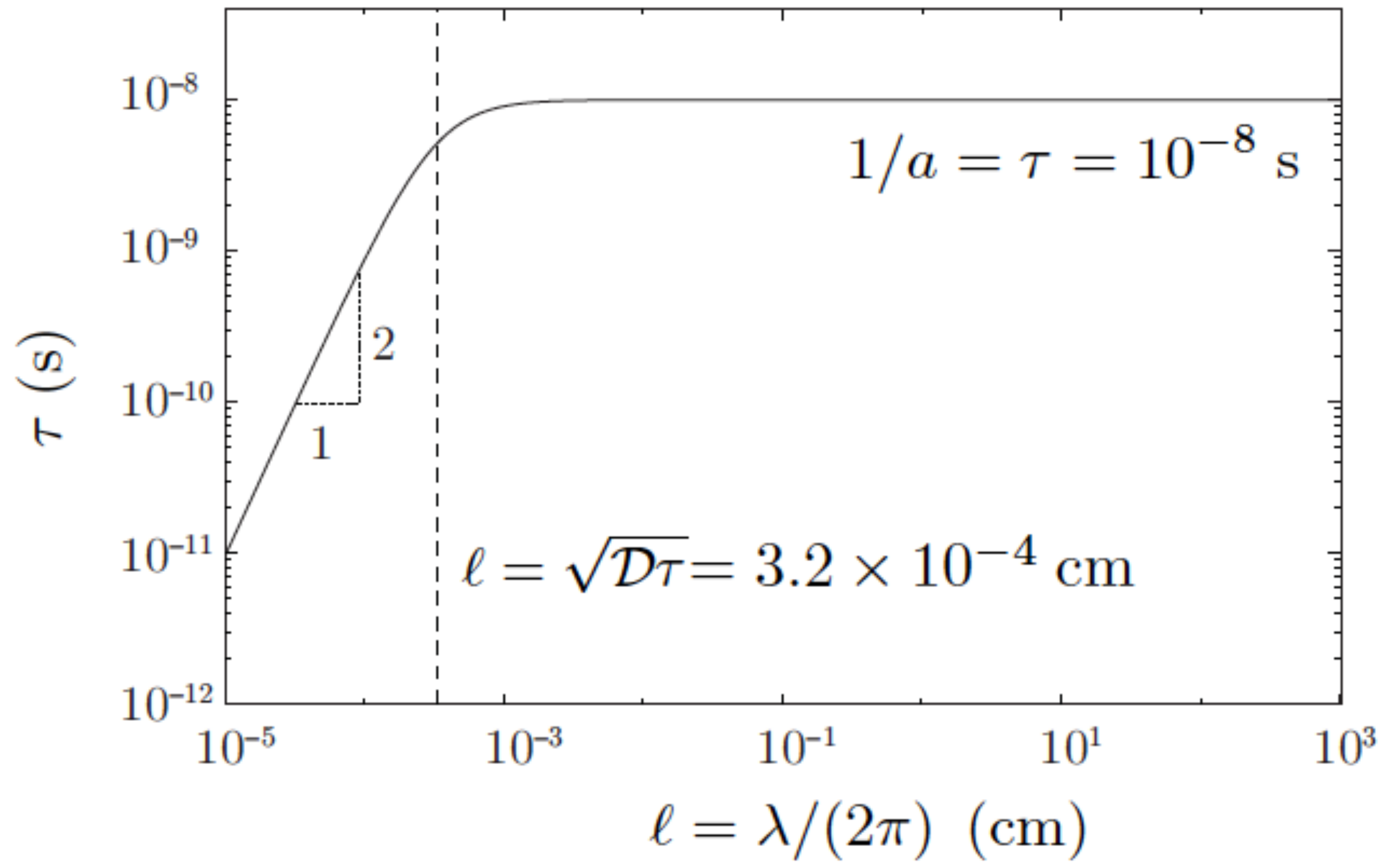
Powers, 2016

- Suppress time-dependency.
- Exponential relaxation in space to equilibrium.
- Length scale for reaction identified as the classical Maxwellian prediction:

$$\ell = \sqrt{\frac{\mathcal{D}}{a}} = \sqrt{\mathcal{D}\tau}$$

Length and Time Scales for a Fourier Mode

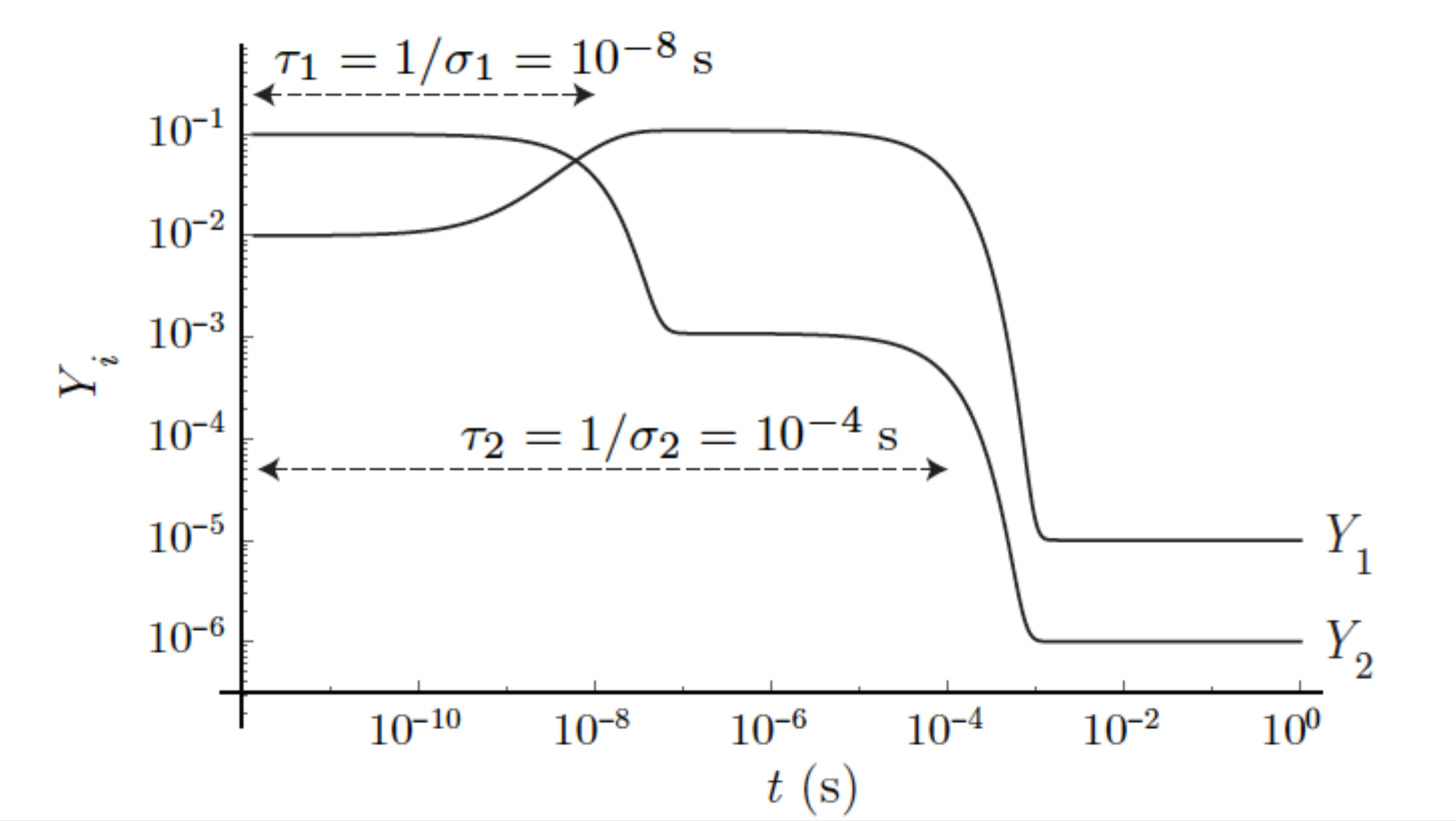
$$Y(x,t) = Y_{eq} + B_o e^{i\hat{k}(x-ut)-\mathcal{D}\hat{k}^2 t - at}.$$



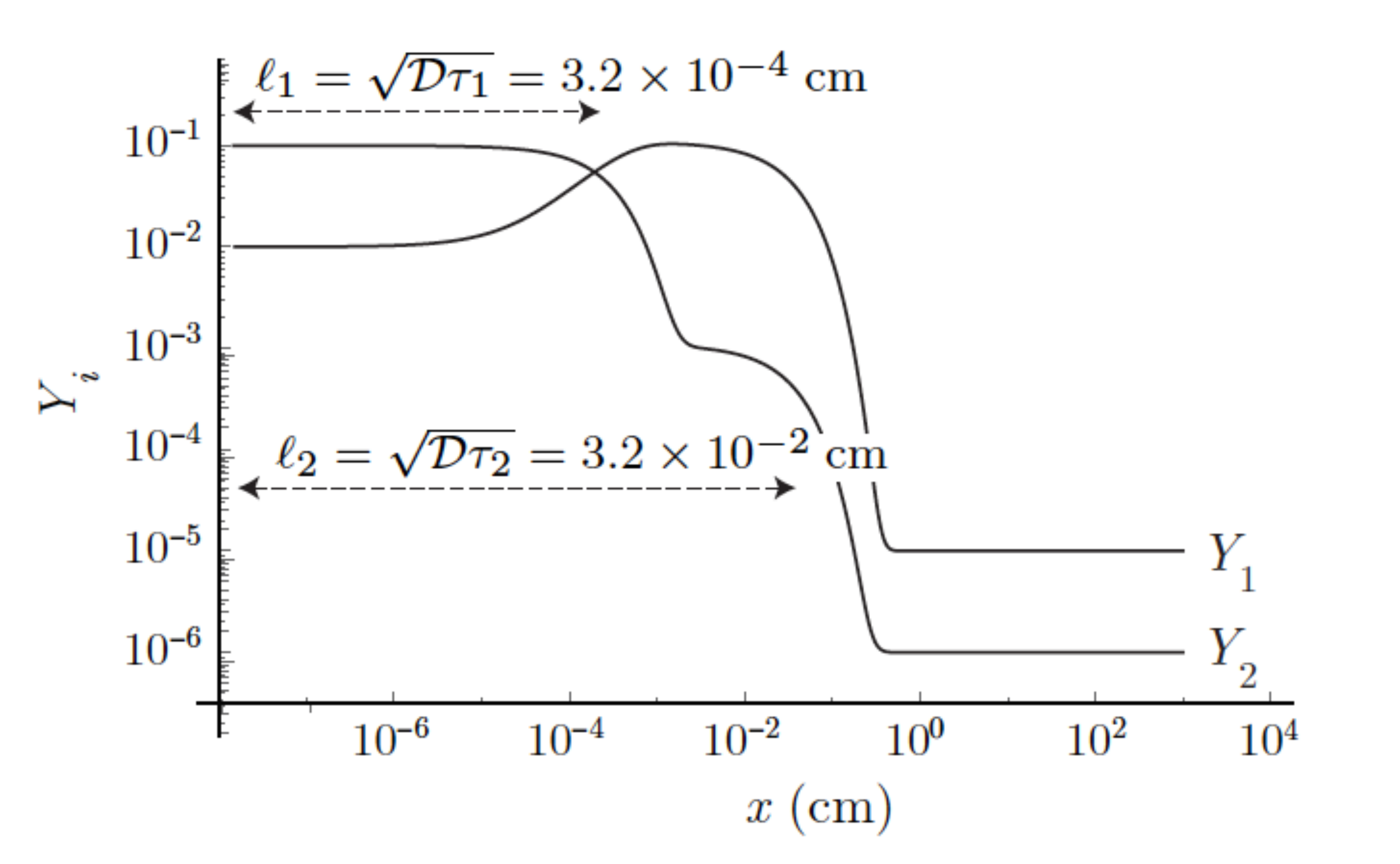
Powers, 2016

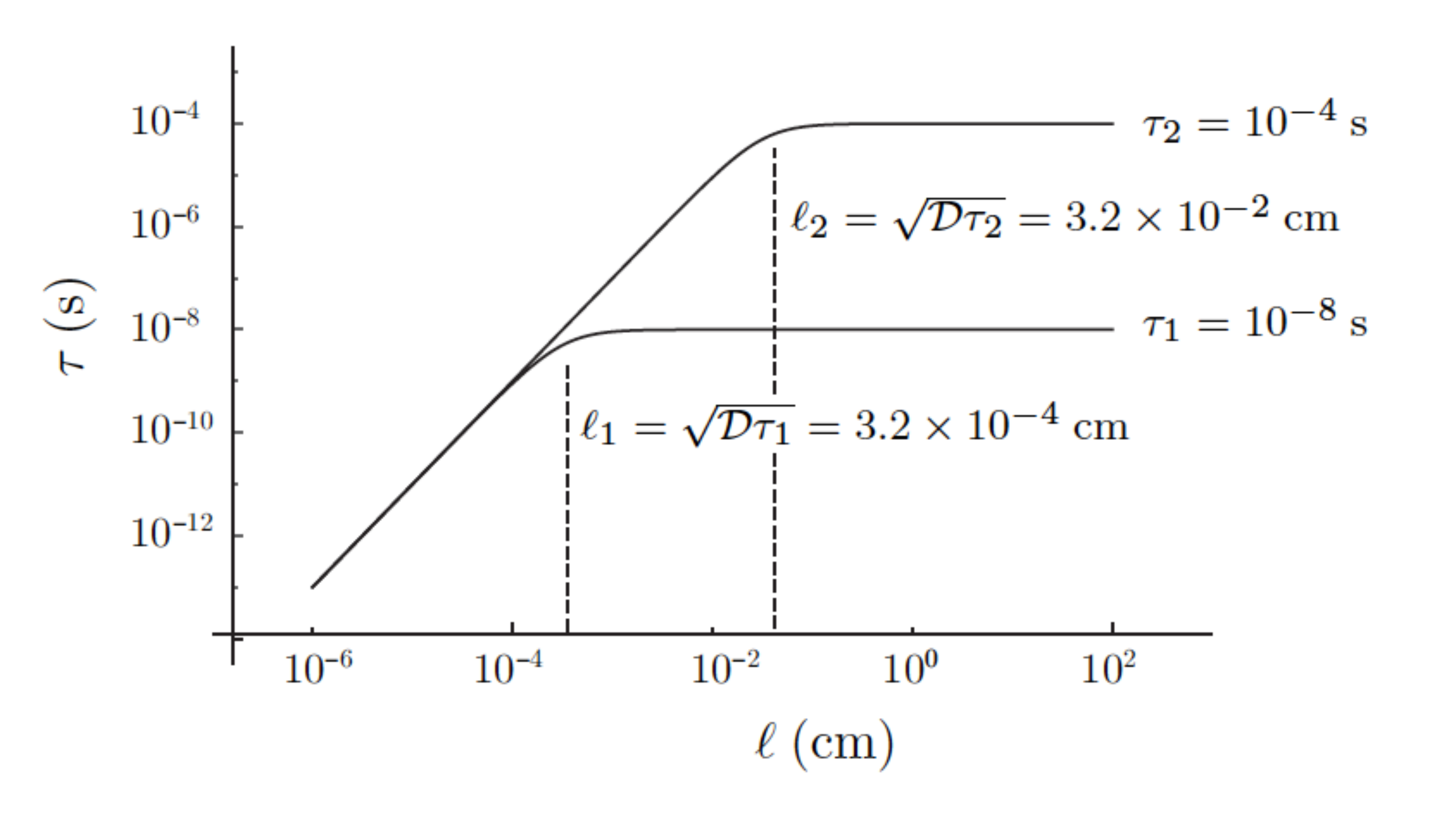
- Long wavelength modes dominated by reaction.
- Short wavelength modes dominated by diffusion.
- For verification, must resolve down to the cutoff length scale where reaction balances diffusion.
- Cutoff scale dictated by physics!

Two Reaction Extension: Stiff Linear Kinetics



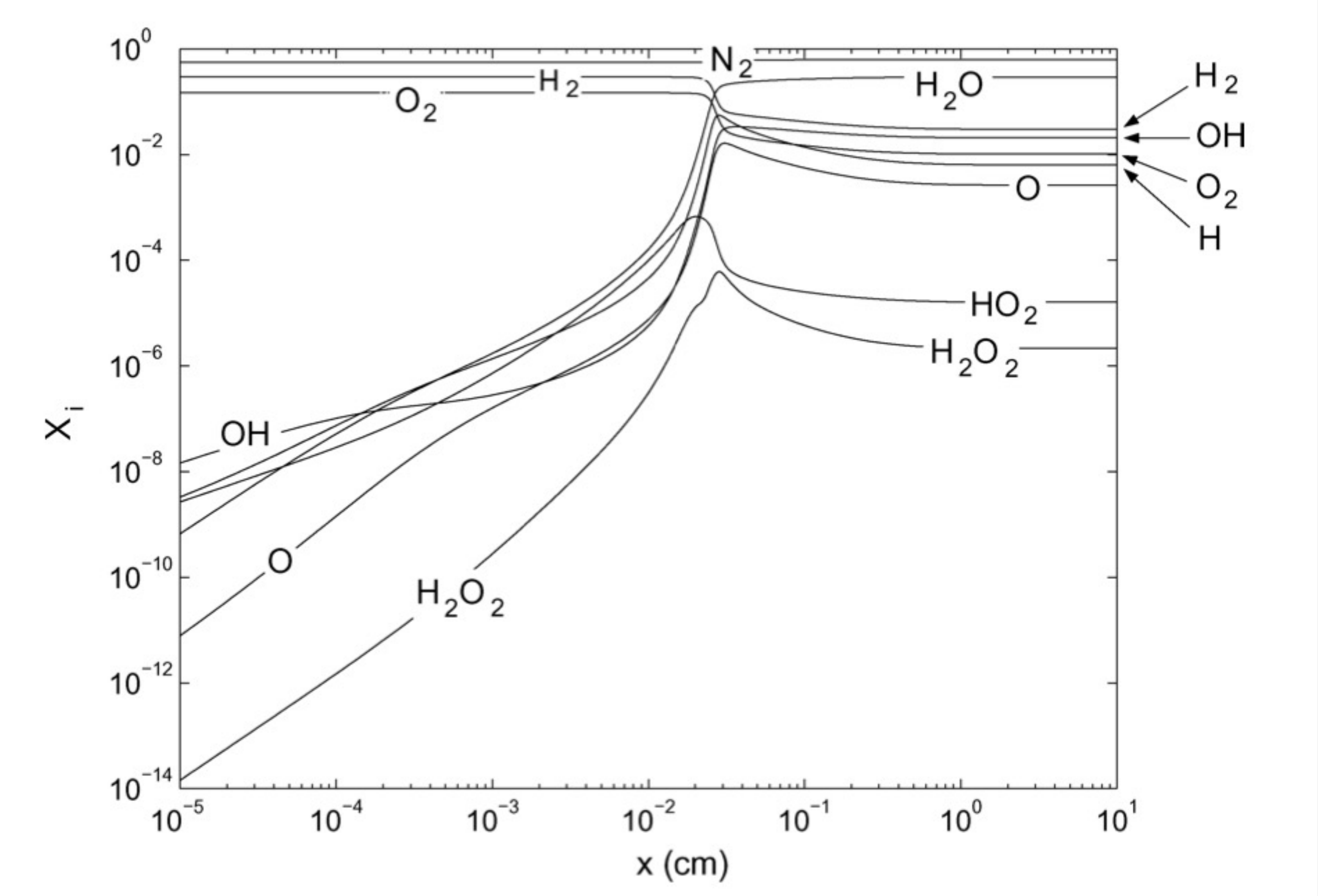
$$\frac{\partial}{\partial t}\mathbf{Y}(x,t) + u\frac{\partial}{\partial x}\mathbf{Y}(x,t) = \mathcal{D}\frac{\partial^2}{\partial x^2}\mathbf{Y}(x,t) - \mathbf{A}\cdot(\mathbf{Y}(x,t) - \mathbf{Y}_{eq}),$$





Powers, 2016

Nonlinear: Stiff Realistic Hydrogen Chemistry



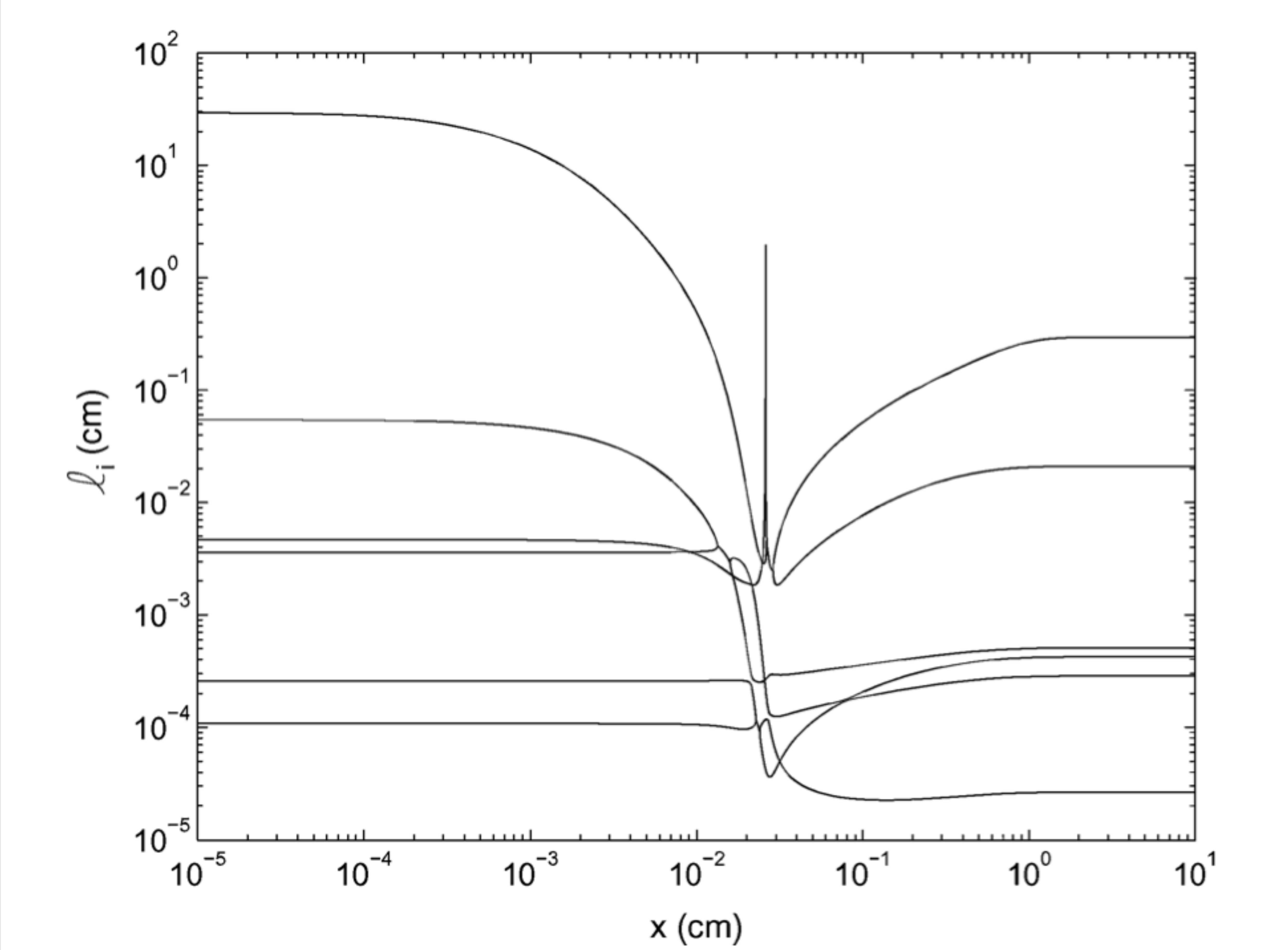
Powers and Paolucci, 2005

- Fully nonlinear steady advection-reaction model of hydrogen-air, of the form

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(\mathbf{y})$$

- Evolution from unreacted to equilibrium on the scale of microns to meters.
- Spatial eigenvalues of the local Jacobian matrix reveal the local length scales.

Nonlinear: Stiff Realistic Hydrogen Chemistry



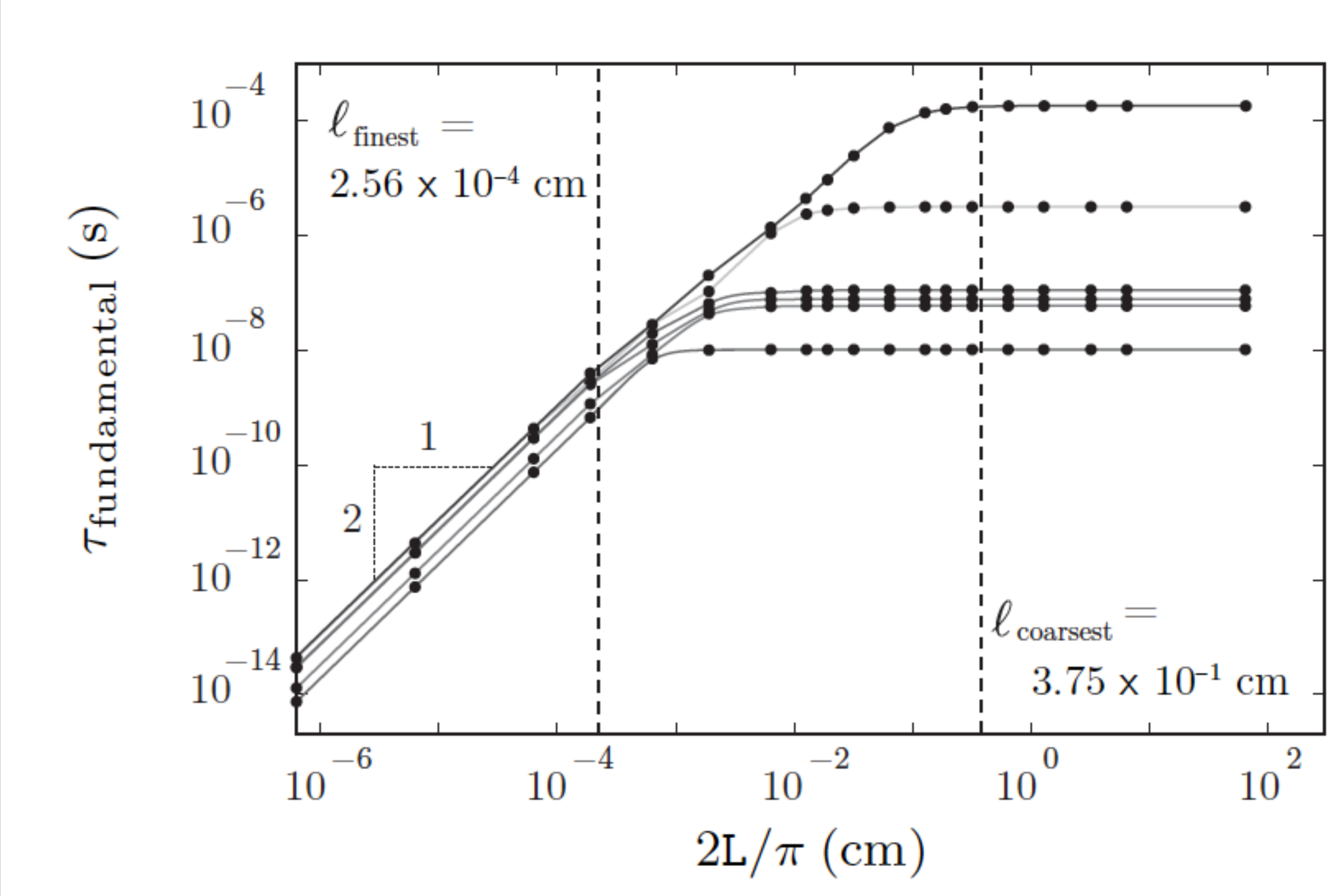
Powers and Paolucci, 2005

- Reciprocals of spatial eigenvalues of Jacobian

$$\frac{\partial \mathbf{f}}{\partial \mathbf{y}}$$

- Yields physical length scales that span microns to meters.
- Gives length scale necessary for verification.

Nonlinear: Stiff Realistic Hydrogen Chemistry: Advection-Reaction-Diffusion



$\tau_{slowest}$ = 1.85×10^{-4} s

$\tau_{fastest}$ = 1.03×10^{-8} s

Powers, 2016

Signal v. Noise: Summary

- Just like the simple Fourier series, for nonlinear and multiscale problems, we find more structure if we include more terms.
- Sometimes the physics demands we retain many terms because high frequency modes can carry a lot of energy.
- We induce error by neglecting some of the structure, and hope we retain enough structure to distinguish signal from noise.
- This is not verification, it is signal identification.
- Once we have a signal, we can try to verify it with pristine studies.

Pristine Verification

- Define a normed error.
- Get a discrete solution that captures the "signal."
- Examine how the error improves as the discretization is refined.
- Compare rate of convergence rate with the rate of the method

$$error = ||\mathbf{y}_{discrete} - \mathbf{y}_{exact}||_p \quad \text{or}$$

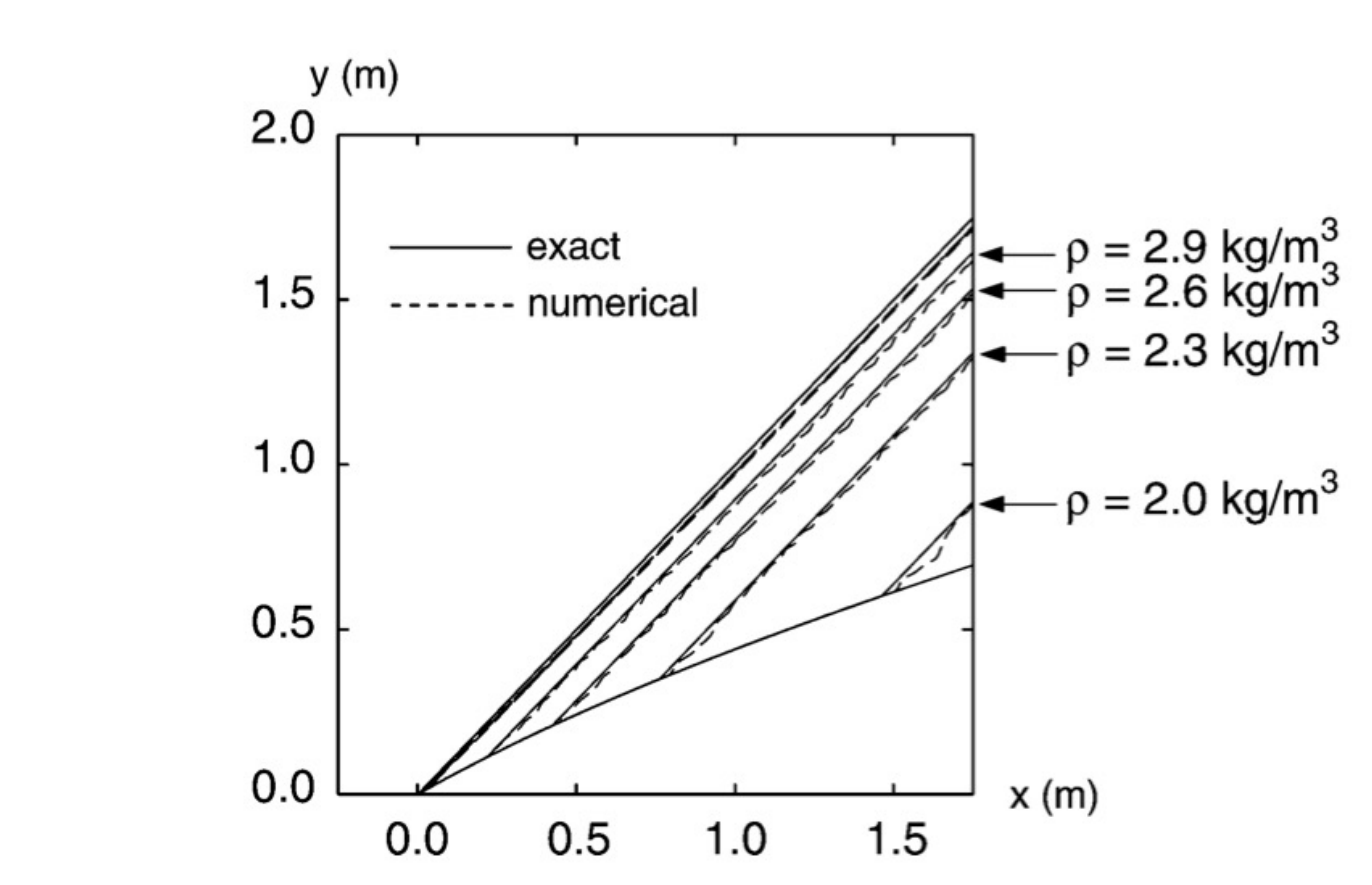
$$error = ||\mathbf{y}_{discrete} - \mathbf{y}_{highly\ refined}||_p$$

Caution: If you use the second method, you might be converging to the wrong exact solution, as nonlinear problems have non-unique solutions!

Either point or entire domain can be considered.

p=1, Manhattan norm; p=2, Euclidean norm; p=∞, Chessboard norm.

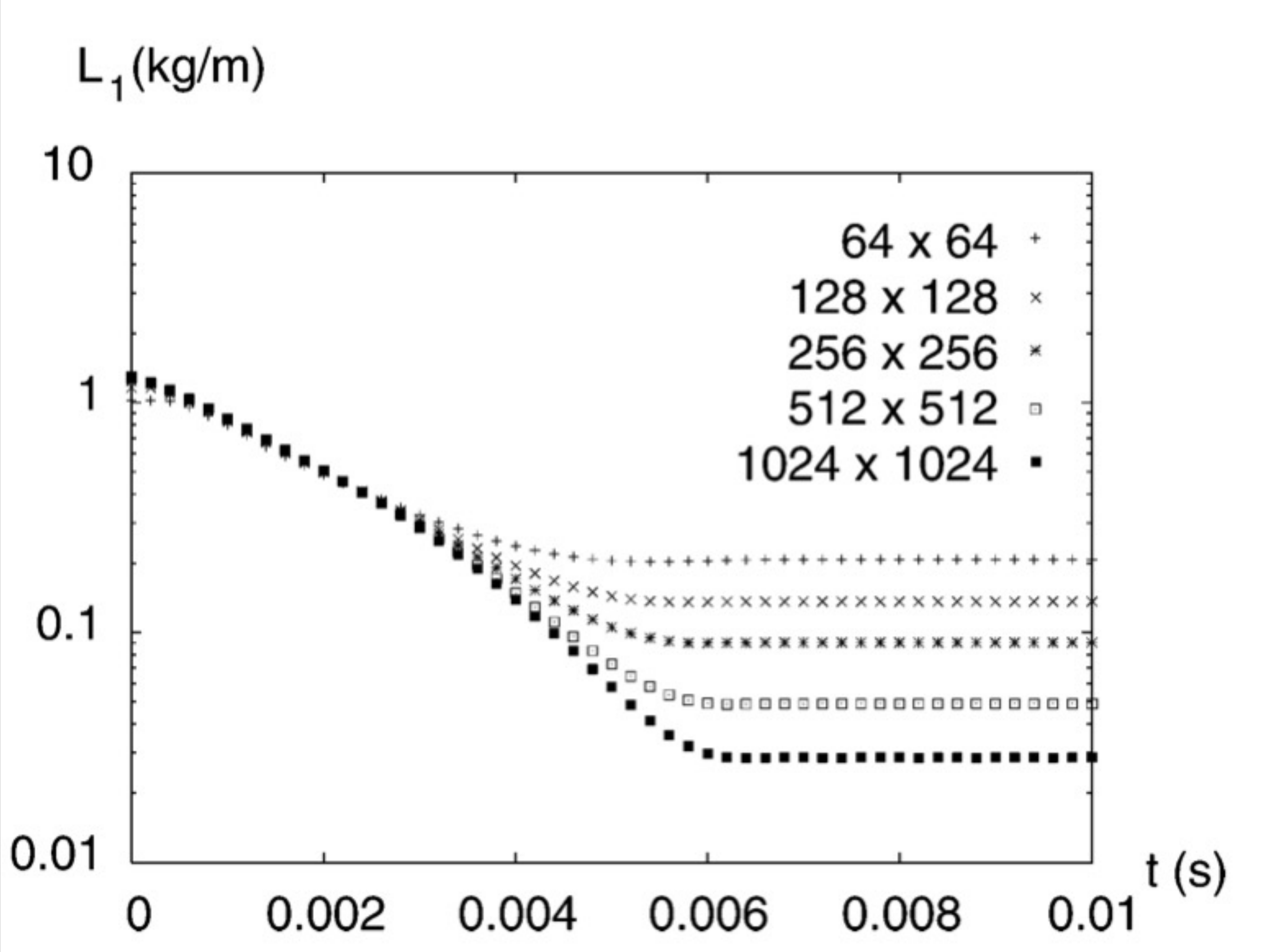
Example: Verification of Oblique Detonation



Powers and Aslam, 2006

- 2D, inviscid reactive flow.
- Straight shock.
- Curved wall.
- Simple one-step kinetics.
- Exact solution exists.
- "Picture norm" reveals the signal is captured by a standard shock-capturing scheme.
- About 10 cells in the reaction zone.

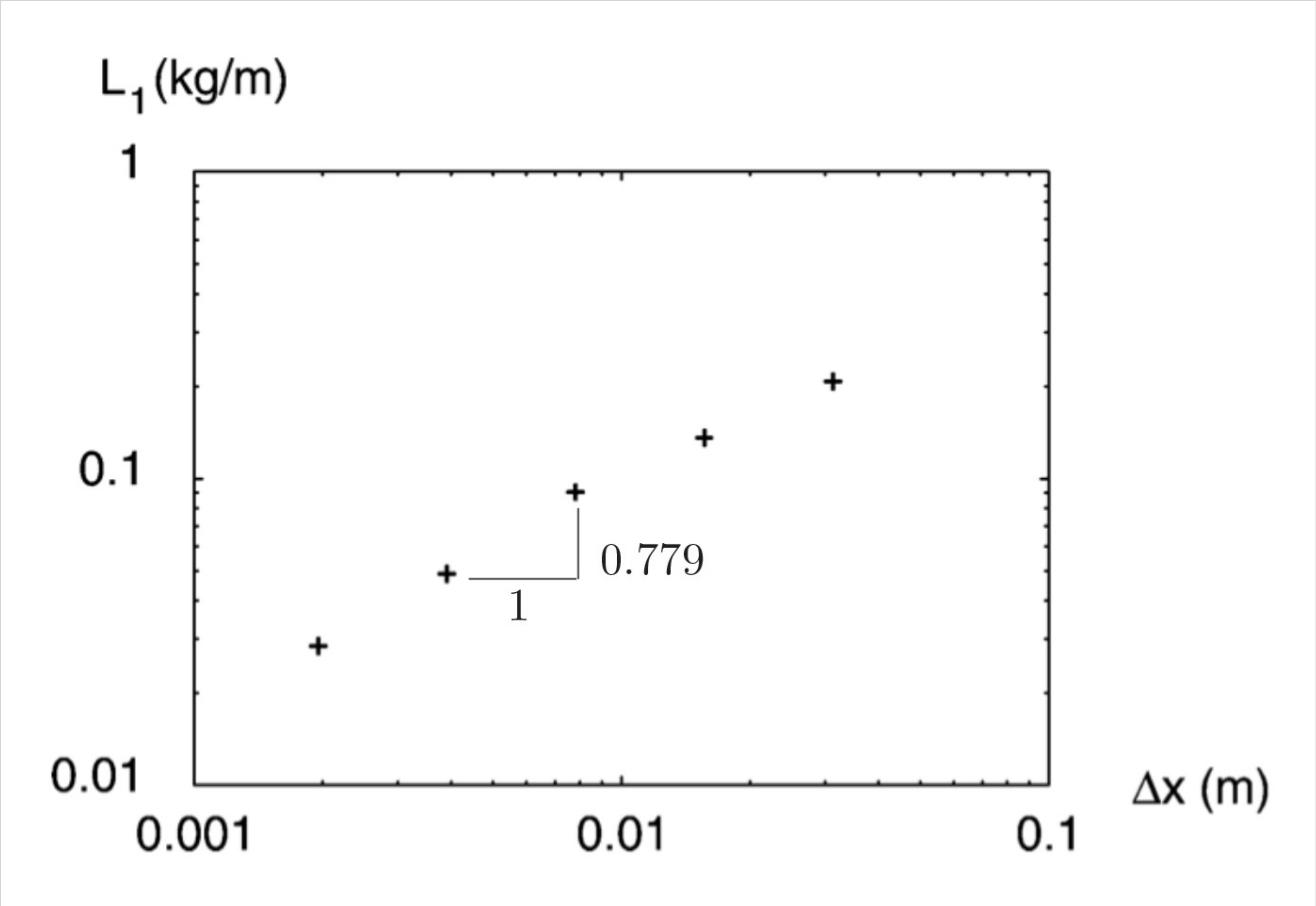
Example: Verification of Oblique Detonation



Powers and Aslam, 2006

- Unsteady algorithm must allow time to relax to steady state.
- Similar to “iterative convergence.”
- Finer grids take longer to relax to steady state.
- Once relaxed, the steady state error is seen to decrease as grid size is increased.

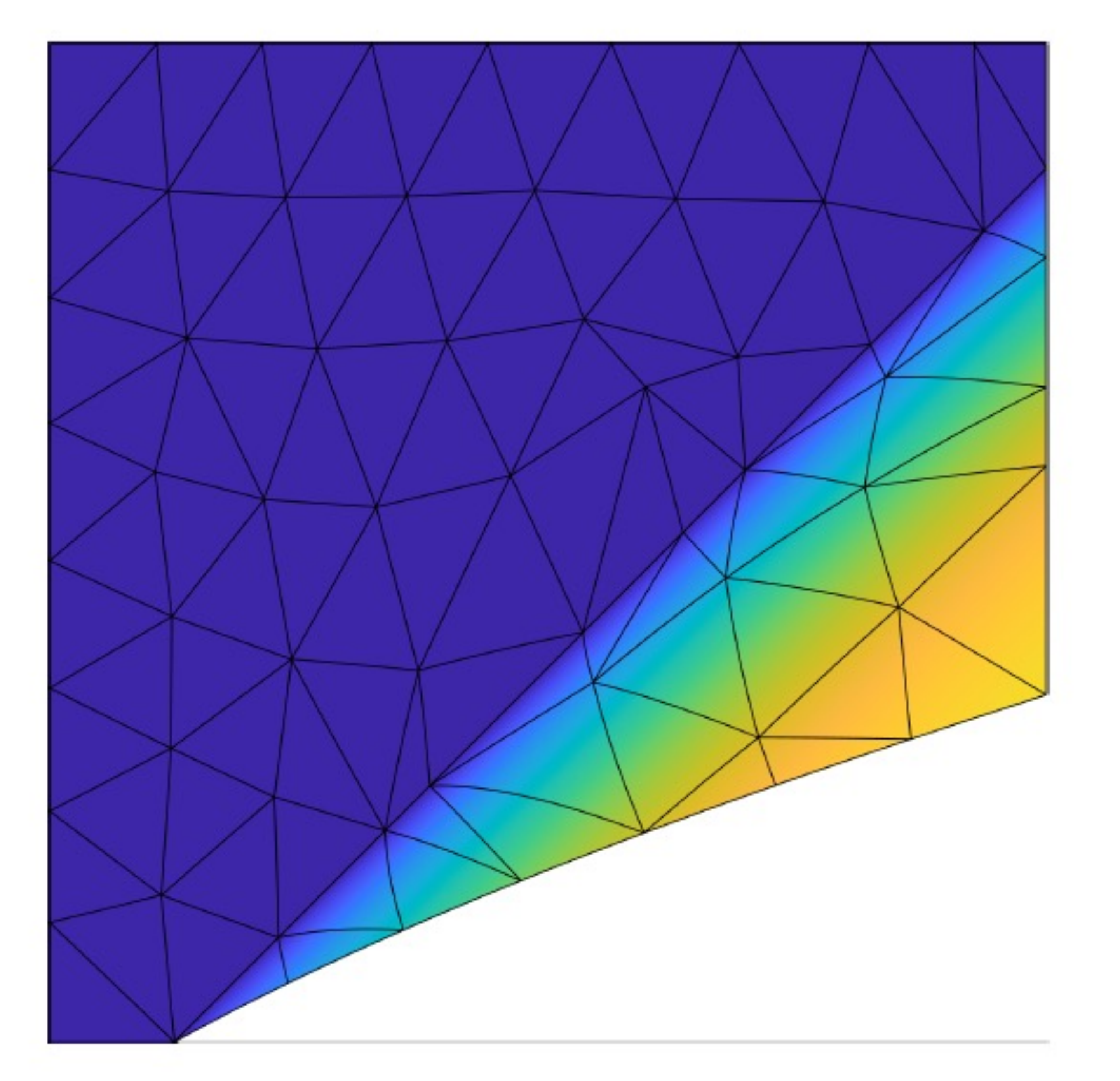
Low Order Verification: Shock-Capturing



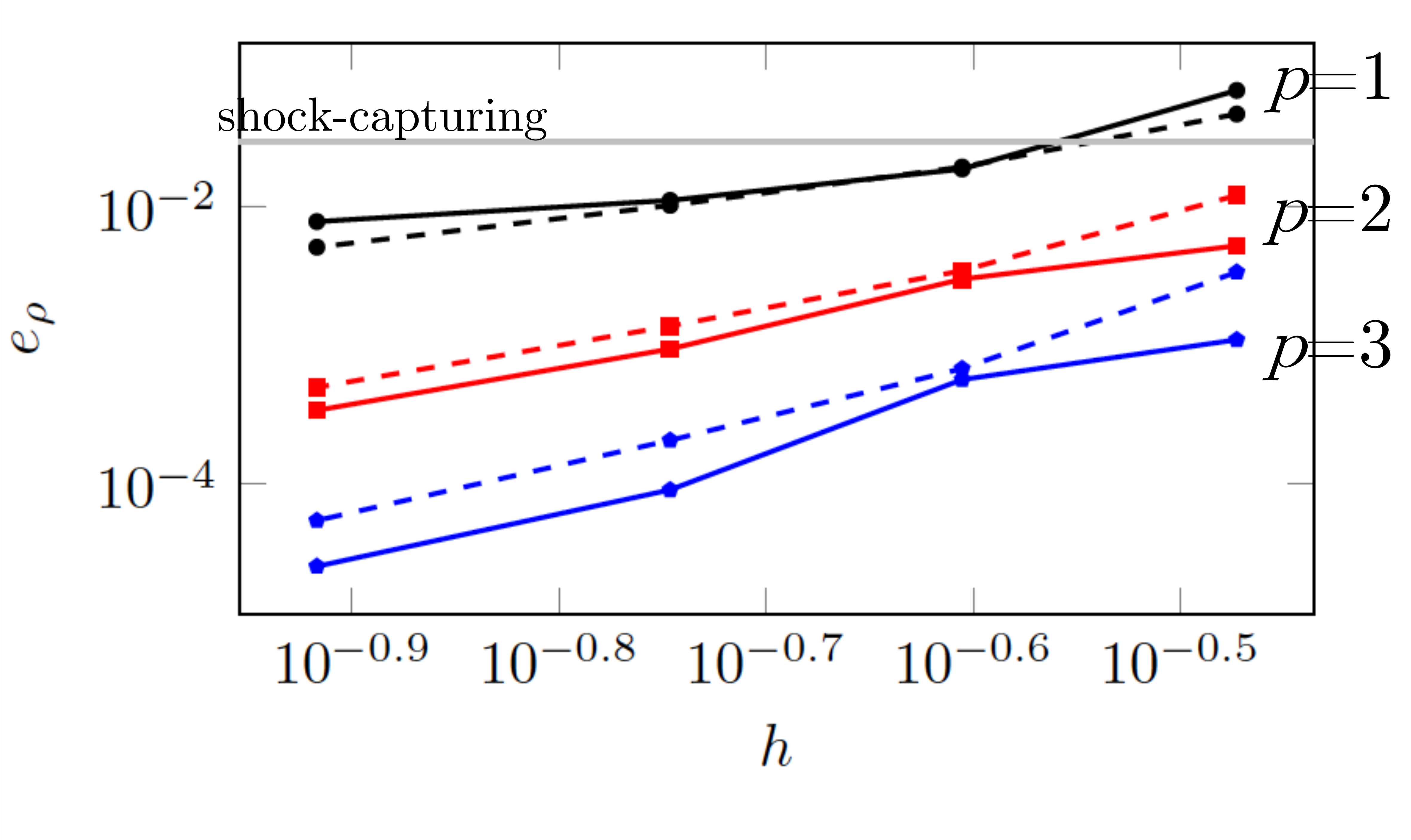
Powers and Aslam, 2006

- Error calculated over the entire domain using the p=1, Manhattan norm.
- Error determined after time relaxation.
- The error is converging!
- The error is converging at 0.779, *much less* than the nominal fifth order method.
- Typical of most shock-capturing.

High Order Verification: Shock-Tracking

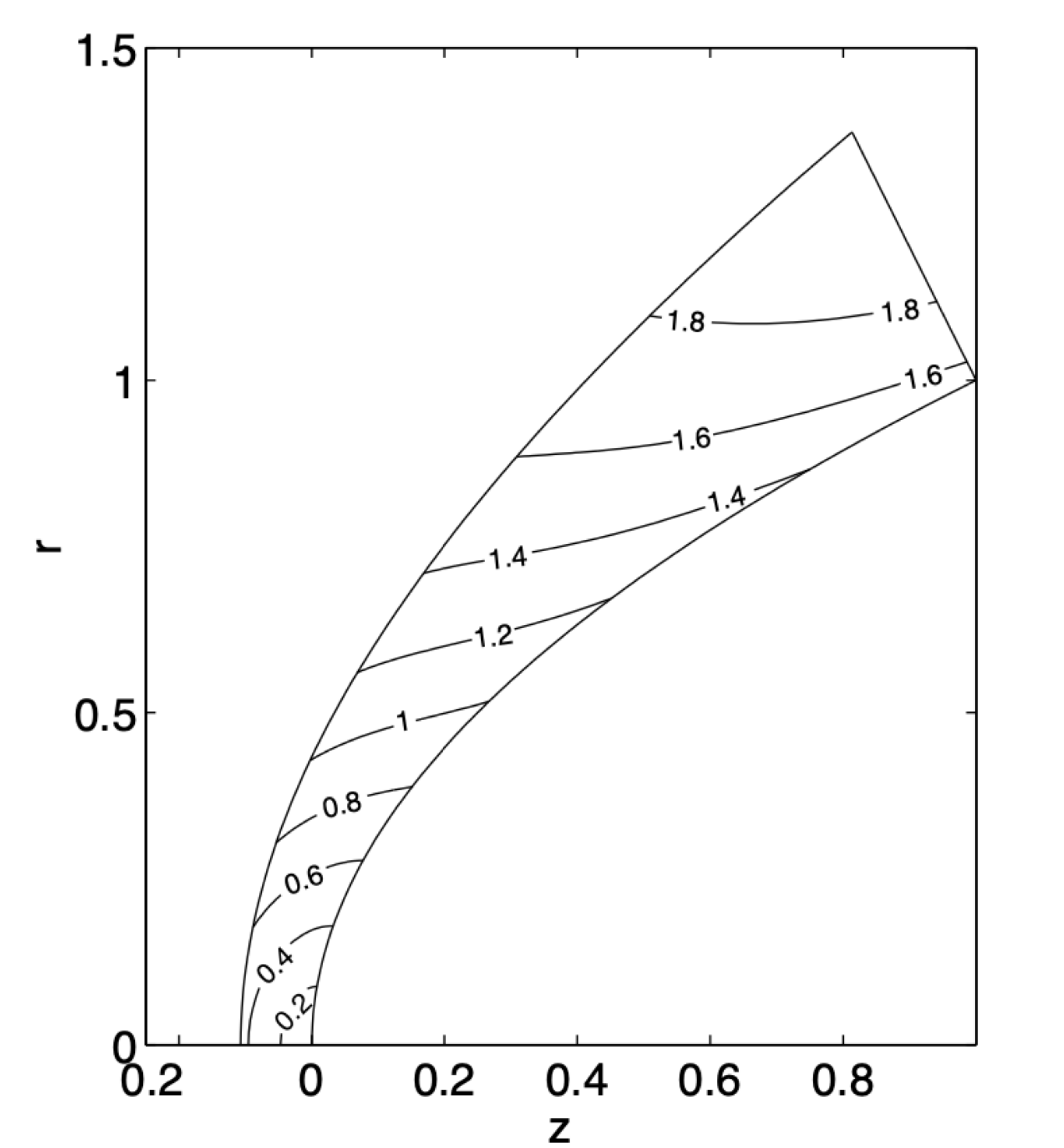


Zahr and Powers, 2021

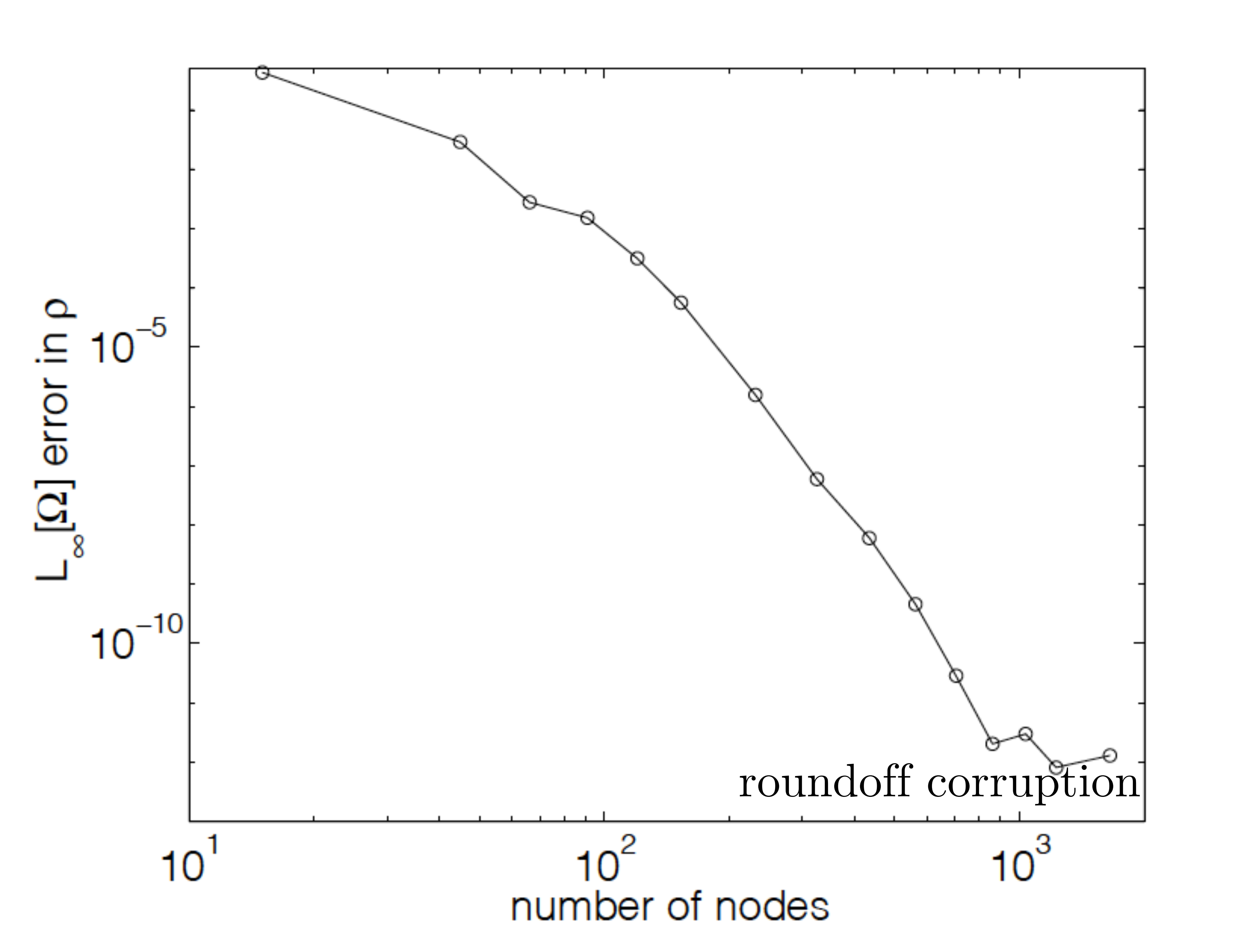


- Implicit shock-tracking and an optimization-based, *r*-adaptive discontinuous Galerkin method lead to *remarkably accurate* solutions, under *h*-*p* refinement.
- Orders of magnitude better than shock-capturing!
- Verified at p=1,2,3.

Highest Order Verification: Spectral Shock-Fitting



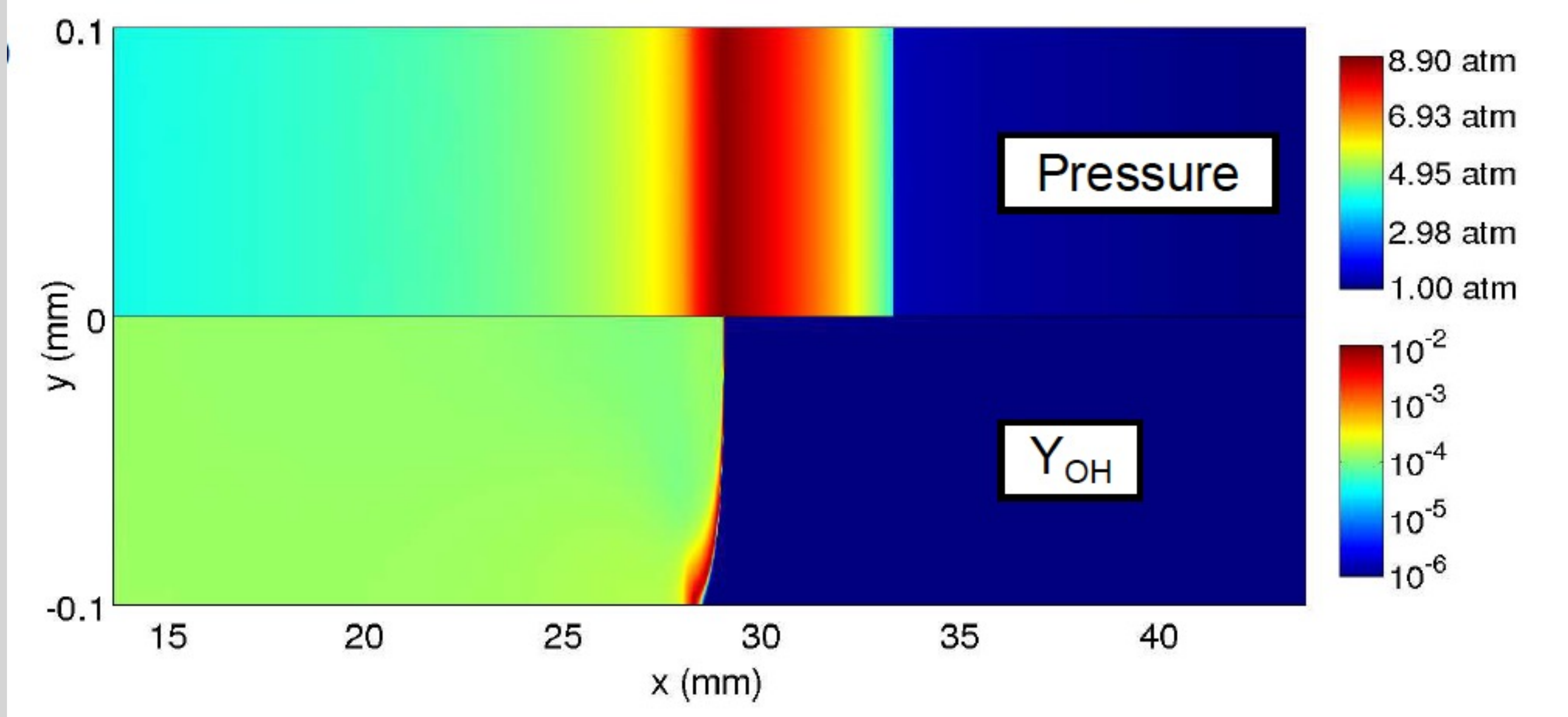
Brooks and Powers, 2004



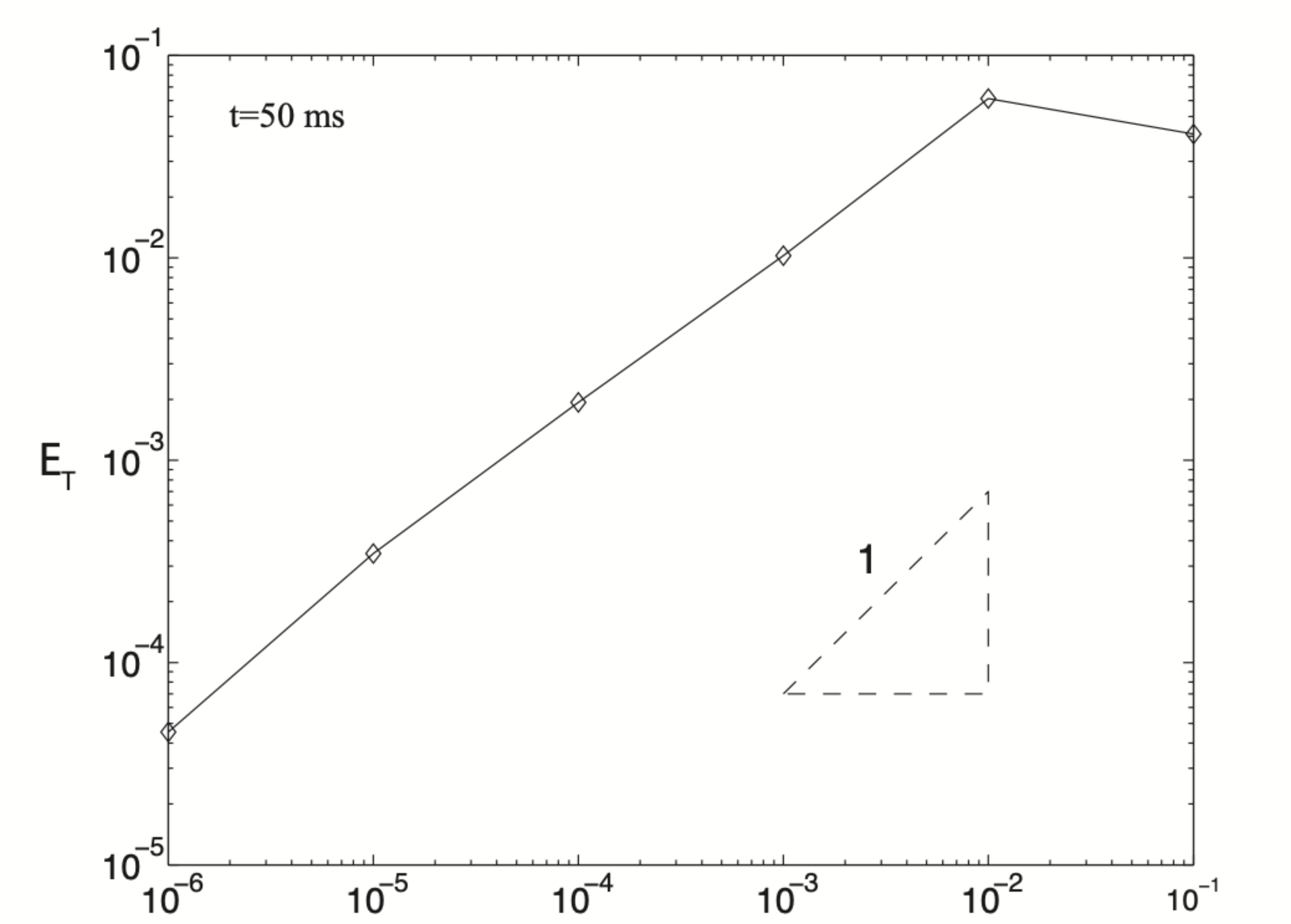
- Blunt body re-entry; 2D Euler equations.
- No exact solution; error small.
- Spectral convergence: verified!

Automatic Verification: Wavelet Adaptive Method

$$u^J(\mathbf{x}) = \underbrace{\sum_{\mathbf{k}} u_{0,\mathbf{k}}\Phi_{0,\mathbf{k}}(\mathbf{x}) + \sum_{j=0}^{J-1}\sum_{\{\boldsymbol{\lambda}\,:\,|d_{j,\boldsymbol{\lambda}}|\geq\varepsilon\}} d_{j,\boldsymbol{\lambda}}\Psi_{j,\boldsymbol{\lambda}}(\mathbf{x})}_{u^J_\varepsilon} + \underbrace{\sum_{j=0}^{J-1}\sum_{\{\boldsymbol{\lambda}\,:\,|d_{j,\boldsymbol{\lambda}}|<\varepsilon\}} d_{j,\boldsymbol{\lambda}}\Psi_{j,\boldsymbol{\lambda}}(\mathbf{x})}_{R^J_\varepsilon},$$



Romick, 2015



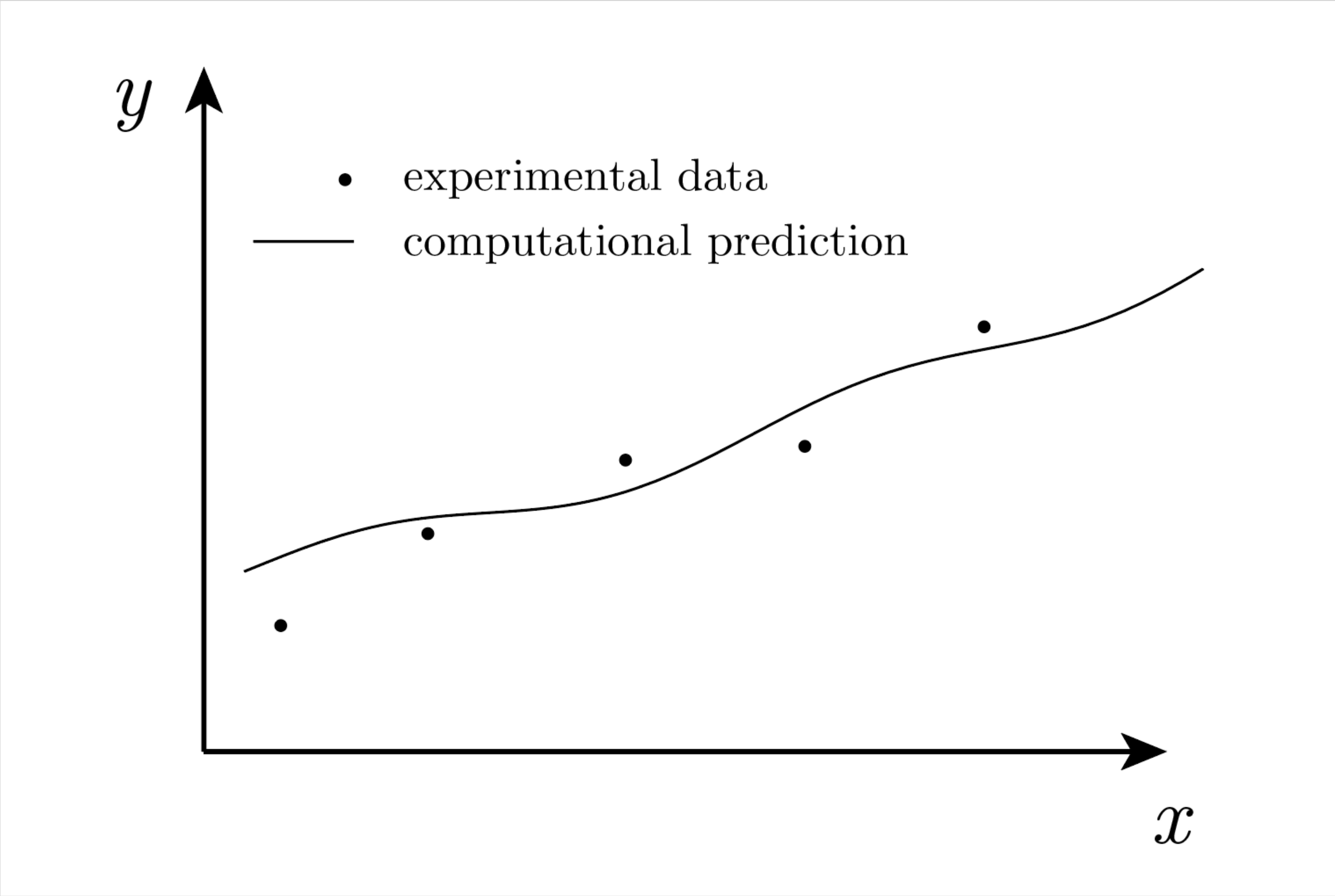
Brill, Grenga, Powers, Paolucci, 2015

- Complicated, highly accurate method.
- Like a Fourier series, *a priori* error estimate allows user to select the automatically verified error.

Practical Verification: What Should One Do?

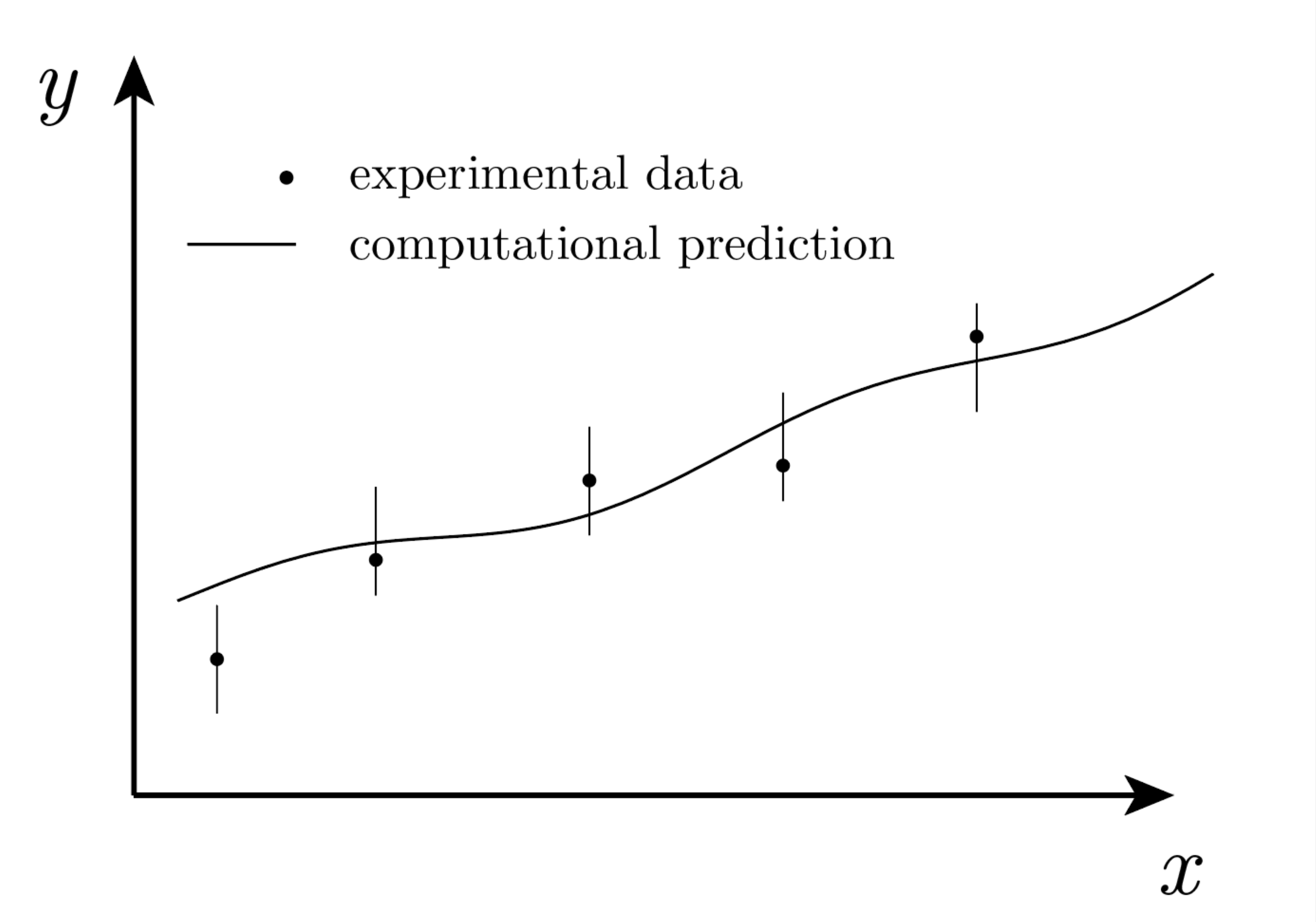
- Most problems do not have exact solutions.
- Many problems are solved with software not developed by the user.
- Many problems have complex geometries and inherent instabilities and/or turbulence.
- Many journals and institutions have strict (and useful) requirements for verification.
- As a referee and journal editor, I see significant confusion, summarized in the next slides, based on a 2011 presentation of Rider.

Typical Plot in the Literature



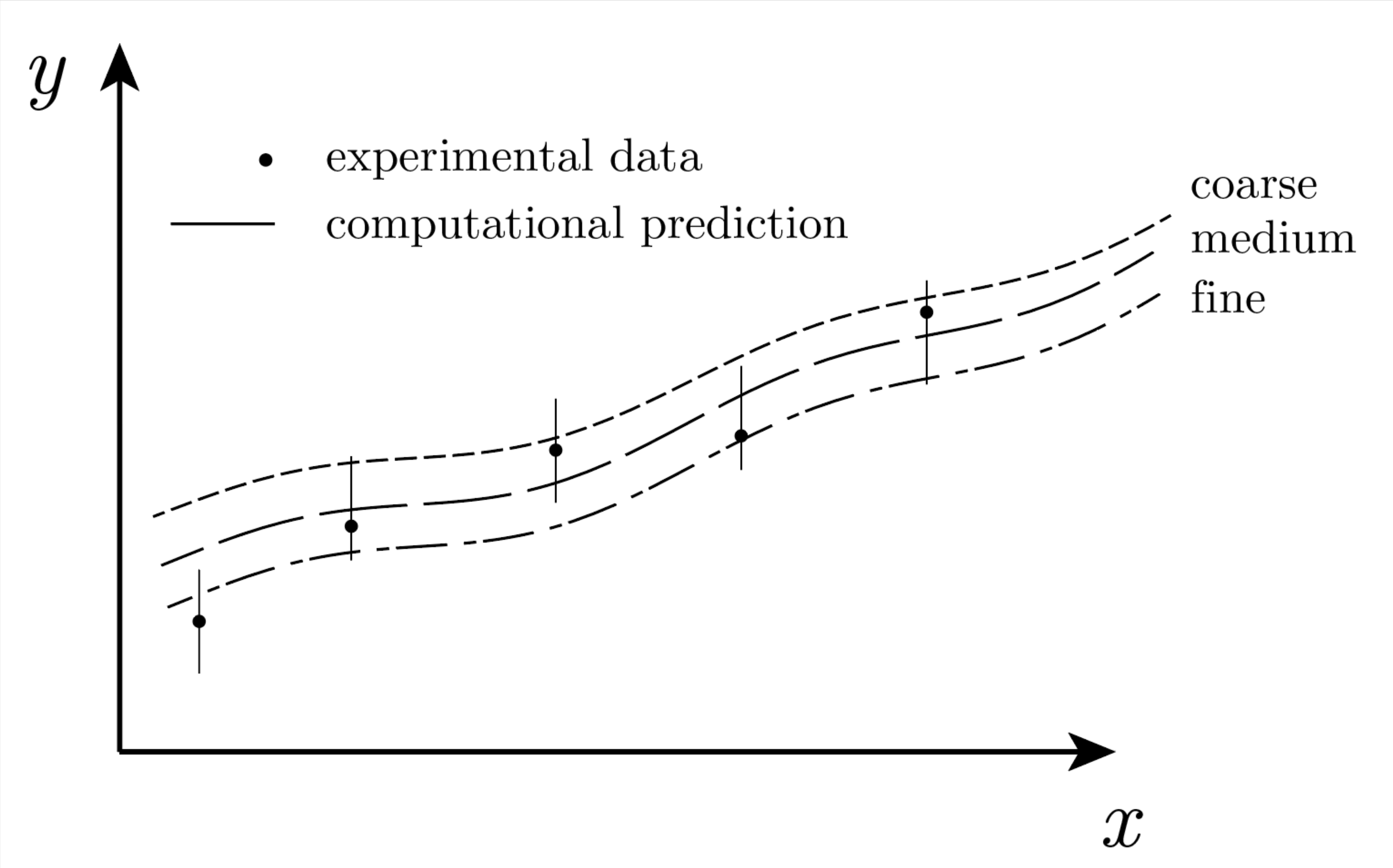
- This is very common.
- It is not verified.
- It is not validated.

A Somewhat Better Plot, Occasionally Seen



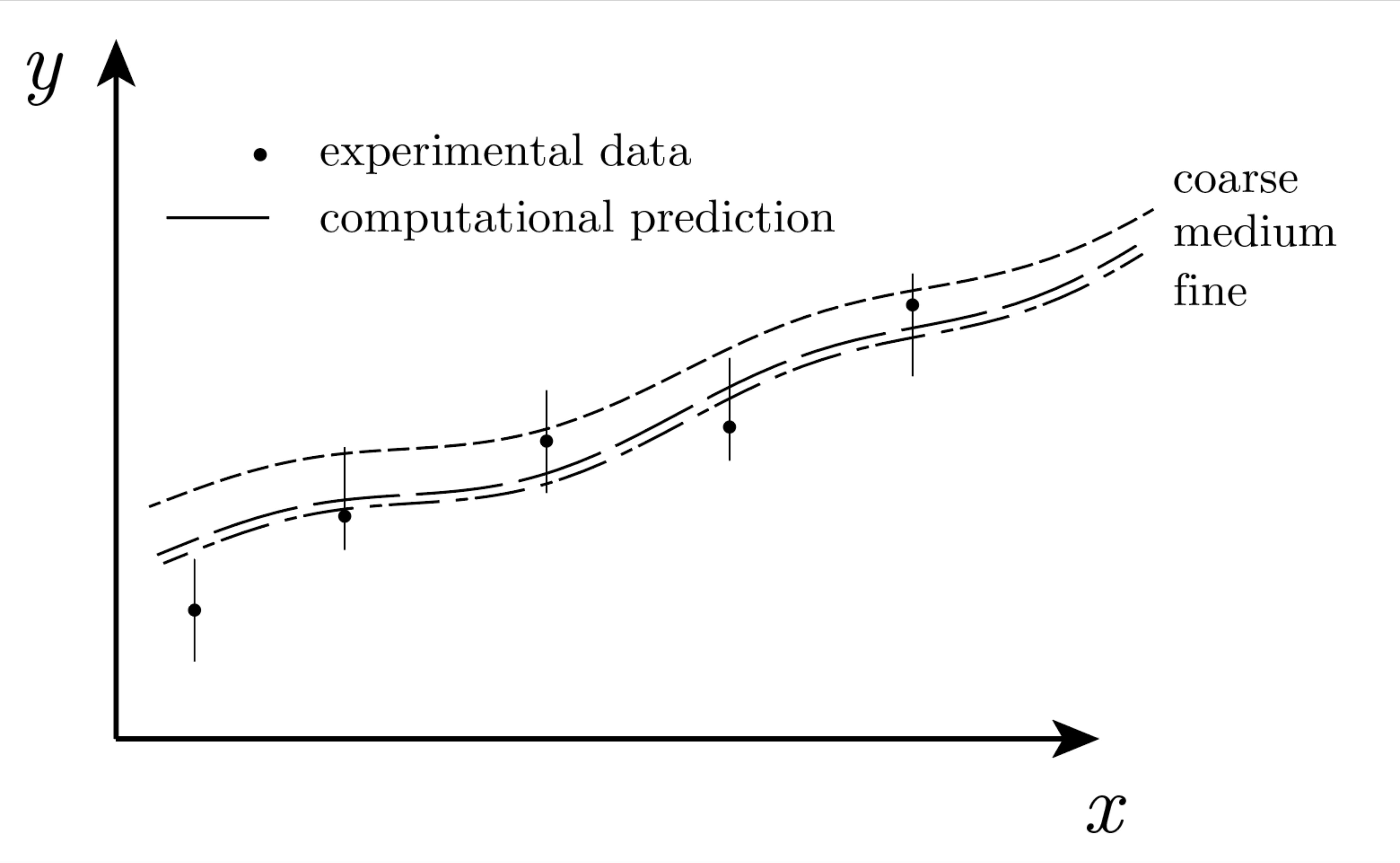
- Better, because an indication of the experimental error is given.
- The prediction calculation remains unverified.
- So the prediction is unvalidated.

An Attempt at Verification, Often Seen



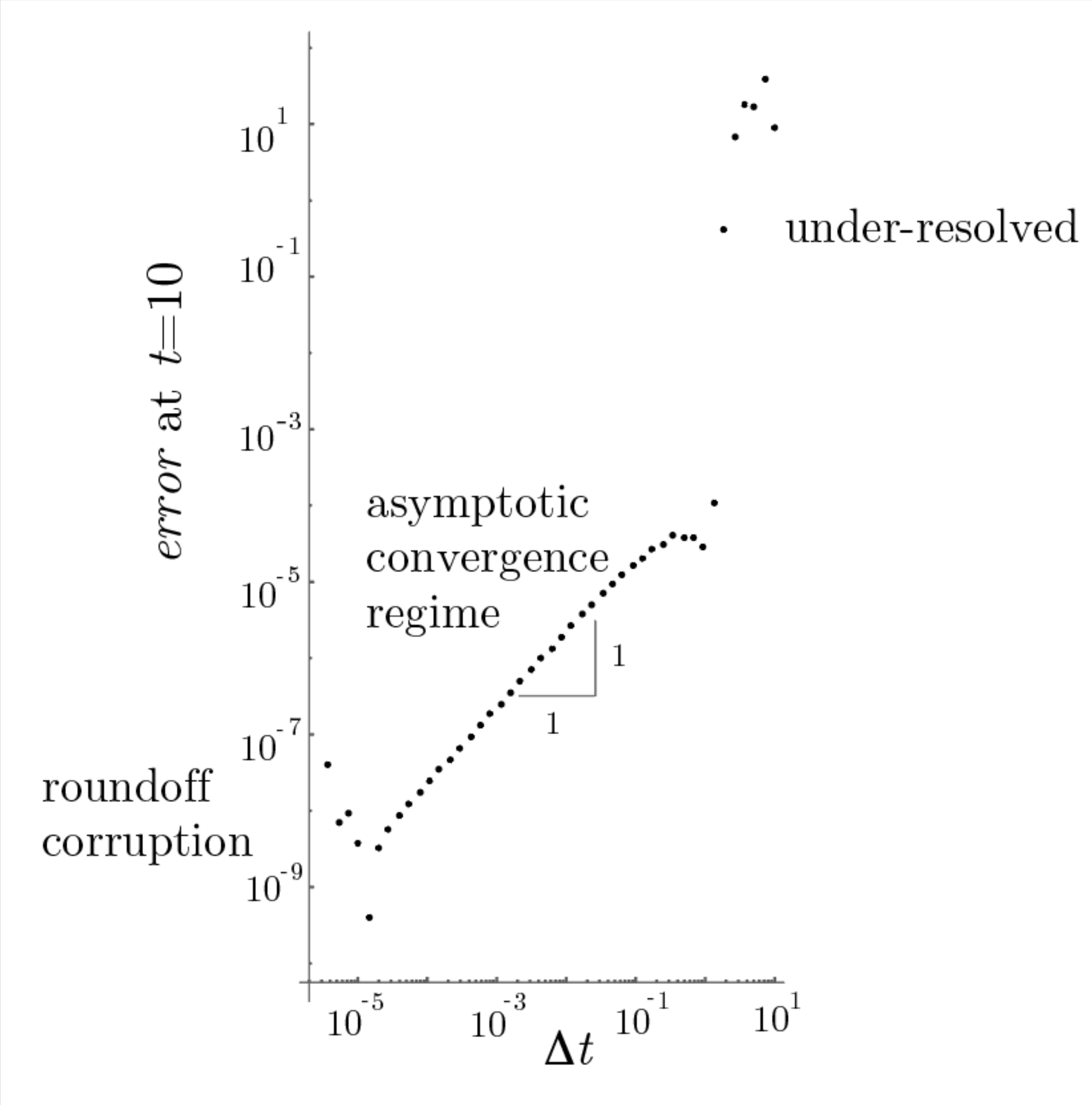
- Showing predictions on several grids is an improvement.
- This does not demonstrate verification, as the solution is not converging.

A Somewhat Better Verification



- Because the solution is approaching something as the grid is refined, it is showing convergence, and perhaps verification.
- The error is not quantified.
- The order of convergence is not quantified.
- We can do better in 2021!

A Much Better Verification



- Give a log-log plot of error as function of grid size.
- Compare to the asymptotic convergence rate.
- Often insist as referee and editor.
- You will get pushback.
- It is usually unwarranted.
- Most authors will comply.
- Some will find real errors and fix them.

A Useful Tool: Journal Policies

Journal of Fluids Engineering

Editorial

Editorial Policy Statement on the Control of Numerical Accuracy

A professional problem exists in the computational fluid dynamics community and also in the broader area of computational physics. Namely, there is a need for higher standards on the control of numerical accuracy.

The numerical fluid dynamics community is aware of this problem but, although individual researchers strive to control accuracy, the issue has not to our knowledge been addressed collectively and formally by any professional society of journal editorial board. The problem is certainly not unique to the JFE and came into even sharper focus at the 1980-81 AFOSRHTTM-Stanford Conference on Complex Turbulent Flows. It was a conclusion of that conference's Evaluation Committee[1] that, in most of the submissions to that conference, it was impossible to evaluate and compare the accuracy of different turbulence models, since one could not distinguish physical modeling errors from numerical errors related to the algorithm and grid. This is especially the case for first-order accurate methods and hybrid methods.

The practice of publishing comparisons based on coarse grid solutions, without systematic truncation error testing, may have been acceptable in the past. Certainly ten to fifteen years ago any calculation was of interest, and much of the exploratory work deserved publication, as many researchers lacked the computational power or funds to do a thorough and systematic error estimation. We are of the opinion that this practice, however understandable in the past, is outmoded and that, with powerful computers becoming more common, standards should be raised. Consequently, this journal hereby announces the following policy:

The Journal of Fluids Engineering will not accept for publication any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation.

Although the formal announcement of this journal policy is new, it has been the practice of many of our conscientious reviewers. Thus the present announcement is not a change in policy so much as a clarification and standardization.

Methods are available to accomplish this task, such as Richardson extrapolation (when applicable), calculations with a high- and low-order method on the same grid, and straightforward repeat calculations with finer or coarser grids. As in the case of experimental uncertainty analysis, "… any appropriate analysis is far better than none as long as the procedure is explained."[2] Whatever the authors use will be considered in the review process, but we must make it clear that *a single calculation in a fixed grid will not be acceptable,* since it is impossible to infer an accuracy estimate from such a calculation. Also, the editors will not consider a reasonable agreement with experimental data to be sufficient proof of accuracy, especially if any adjustable parameters are involved, as in turbulence modeling.

We recognize that it can be costly to do a thorough study, and that many practical engineering calculations will continue to be performed on a single fixed grid. However, this practice is insufficient for publication in an archival journal.

Patrick J. Roache
Kirti N. Ghia
Frank M. White
JFE Editorial Board

"The *Journal of Fluids Engineering* will not accept for publication any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation."

Roache, Ghia, White, 1986, *Journal of Fluids Engineering-Transactions of the ASME*

35 year-old policy!

My Boilerplate Language—Usually Works

An analysis of numerical errors, including grid dependence, etc., must be conducted in accordance with AIAA editorial policy. For more details regarding the latter, see

https://www.aiaa.org/publications/books/Publication-Policies/Editorial-Policy-Statement-on-Numerical-and-Experimental-Accuracy

Please provide a log-log plot of how some error measure decreases as the grid is refined (or equivalently, coarsened) and a comparison of the achieved order of convergence with the nominal convergence rate of your chosen numerical method.

Common Responses

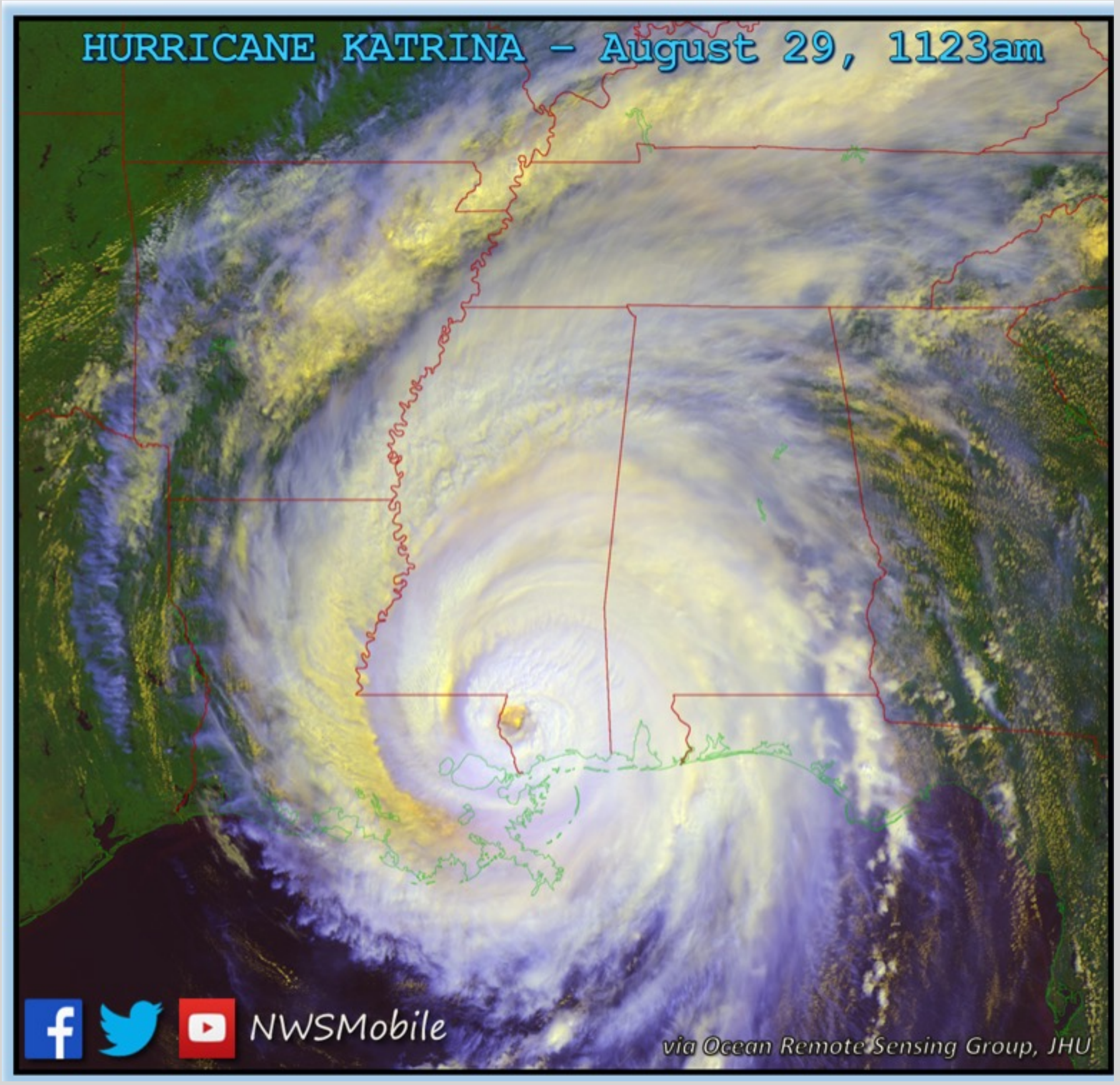
- *I don't have enough computing resources.* Then do grid coarsening.
- *My software package won't let me verify.* Do a point convergence study.
- *My problem is unsteady/turbulent.* Seek an error norm for an integrated quantity like drag coefficient or net thrust.
- *I'm not going to do it.* Decline the manuscript.

Perimeter-Expanding Verification: Challenge Areas

- Non-continuum regime where calculus-methods are difficult.
  - Solutions with embedded surfaces of discontinuity (shocks, material interfaces).
  - Problems with embedded "switches."
- Problems with parameters (geometry, material properties, forcing functions) with a stochastic nature.
- Problems that do not relax to steady-state.
- Nonlinear deterministic problems that may have chaotic nature.

considered here

Nonlinear Dynamics and Verification



https://www.weather.gov/mob/katrina

"Big whorls have little whorls,
Which feed on their velocity;
And little whorls have lesser whorls,
And so on to viscosity."

Lewis Fry Richardson, 1922,
Weather Prediction by Numerical Processes.

- Big can affect small.
- Small can affect big.
- Predictions of "big" and "small" should not be machine-dependent.
- Difficult to guarantee!

Nonlinear Dynamics and Verification

- Nonlinear models reflect that nature can be
  - well-behaved and mainly stable,
  - ill-behaved with intermittent catastrophic events.
- Predictive science needs to predict repeatable phenomena repeatably.
- We can learn about nature by careful charting of unknown territory.
- Careful charting takes time and cannot address all important problems!
- I will show verified results for a nonlinear problem that undergoes a transition to chaos.
- The “verification” lies in taking care that the persistent modes are resolved: the “signal” has been captured.

Local Linear Behavior May be Stable or Unstable

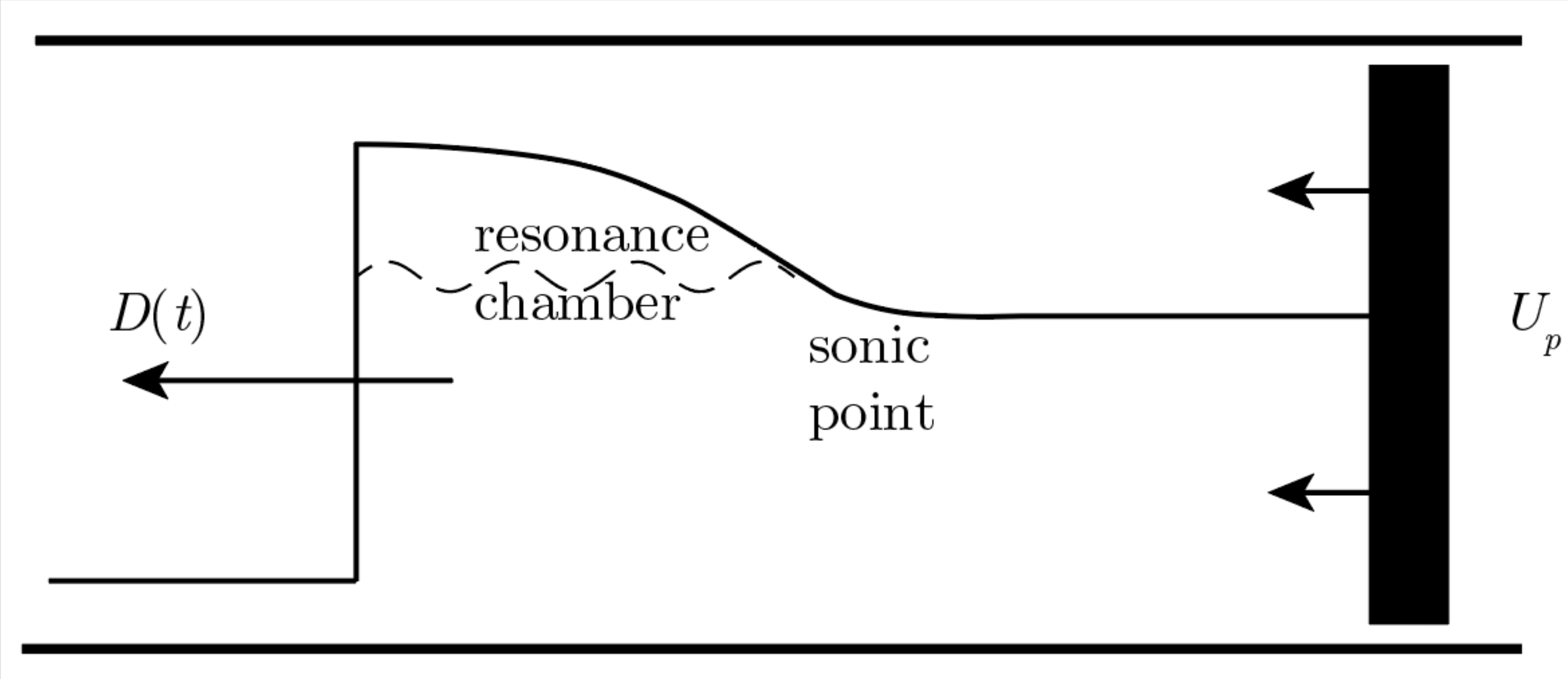
$$f(x,t) = a_1 e^{-t} \sin x + a_2 e^{-4t} \sin 2x + a_3 e^{-9t} \sin 3x + a_4 e^{-16t} \sin 4x + \ldots$$

- All modes stable.
- High frequency modes decay rapidly and can be neglected.

$$f(x,t) = a_1 e^{-t} \sin x + a_2 e^{-4t} \sin 2x + a_3 e^{9t} \sin 3x + a_4 e^{-16t} \sin 4x + \ldots$$

- Push the same system into a different regime.
- Nonlinearity can induce growth of some modes.
- Must be resolved for verified solution.

Viscous 1D Detonation



- Piston at speed U_p drives a detonation at speed $D(t)$.
- Large U_p yields stability, though with some thin zones.
- As U_p is lessened, chemical energy plays a larger role and destablizes.
- Acoustic resonances induce high frequency stable limit cycles.
- "Signal" scales: viscous shock zone, reaction zone, small wavelength resonances.

Continuum Model Equations

Conservation and Evolution Laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + P - \tau\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2}\right) + j^q + \left(P - \tau\right)u\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho Y_B\right) + \frac{\partial}{\partial x}\left(\rho u Y_B + j_B^m\right) = \rho r.$$

Constitutive Models

$$P = \rho R T,$$

$$e = \frac{p}{\rho\left(\gamma - 1\right)} - q Y_B,$$

$$r = H(P - P_s) a \left(1 - Y_B\right) e^{-\frac{\tilde{E}}{p/\rho}},$$

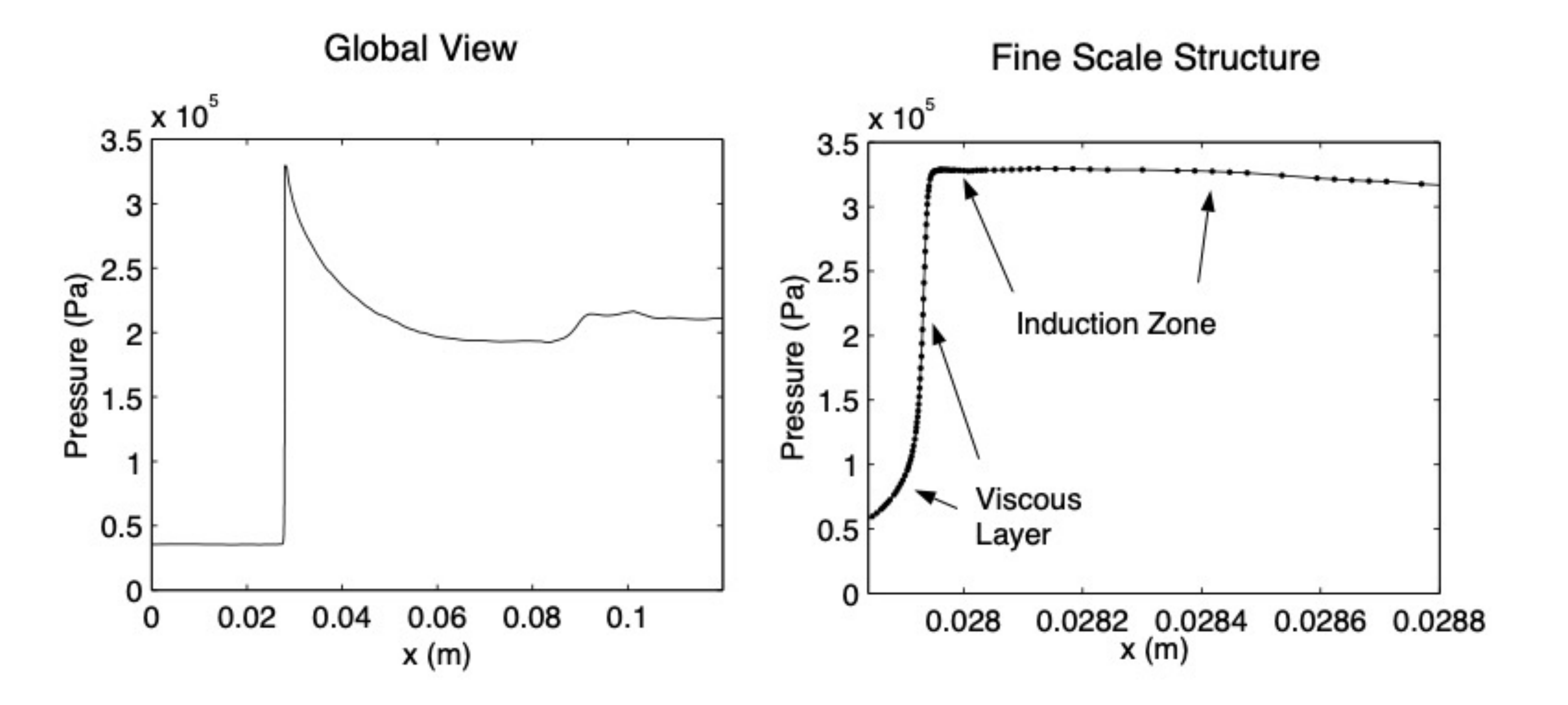
$$j_B^m = -\rho \mathcal{D} \frac{\partial Y_B}{\partial x},$$

$$\tau = \frac{4}{3}\mu\frac{\partial u}{\partial x},$$

$$j^q = -k\frac{\partial T}{\partial x} + \rho \mathcal{D} q \frac{\partial Y_B}{\partial x}.$$

- 1D, compressible, reactive Navier-Stokes.
- 1 step, irreversible Arrhenius kinetics.
- Ideal gas, Newtonian fluid, Fourier's Law, Fick's Law.
- Solved with adaptive wavelet algorithm for full verification.
- Activation energy varied to study stability behavior.

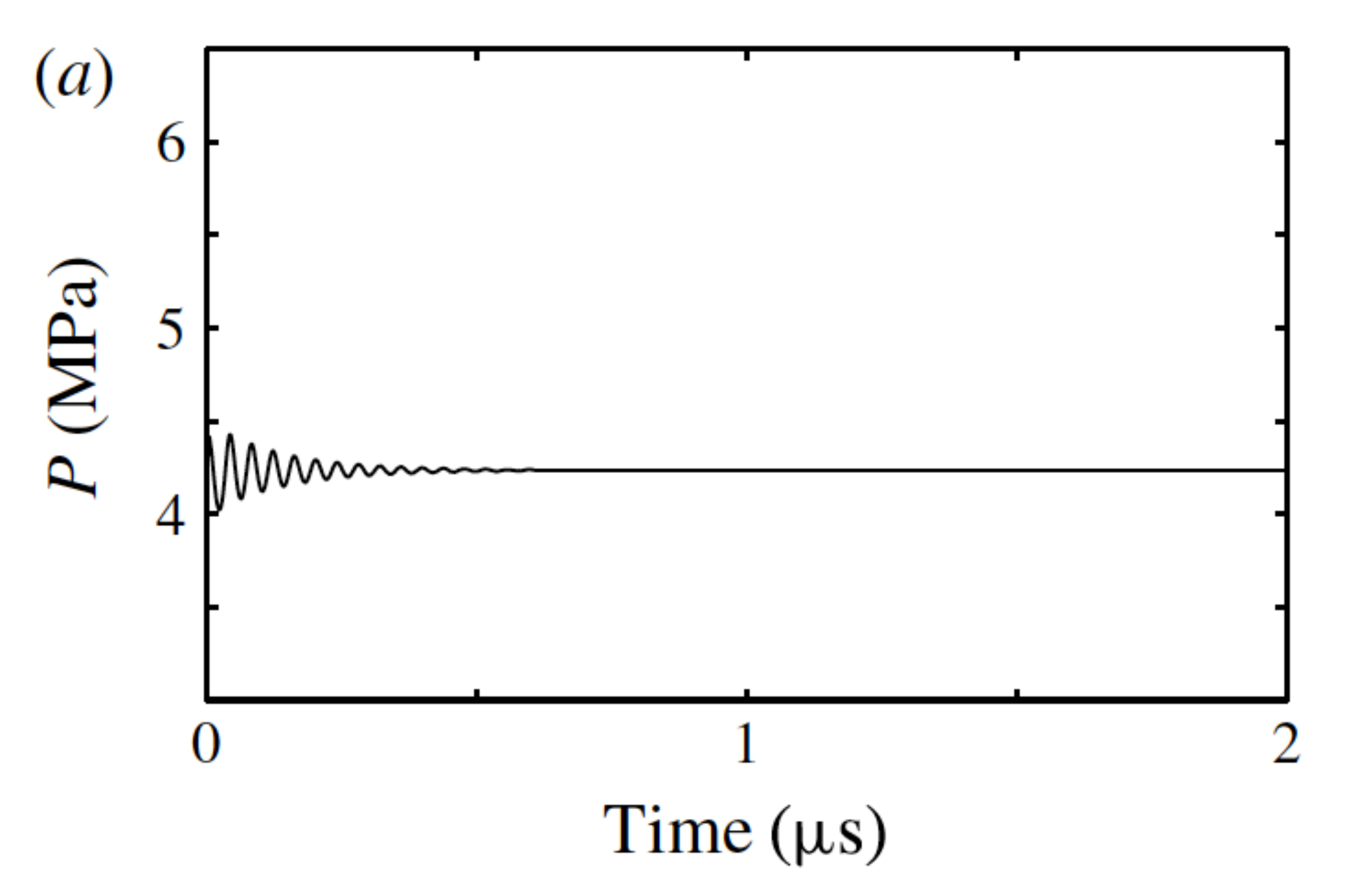
Stable, Viscous, 1D Detonation



Singh, Rastigejev, Paolucci, Powers, 2001

- The wavelet method resolves the viscous shock, induction, and reaction zone. Signal verification!

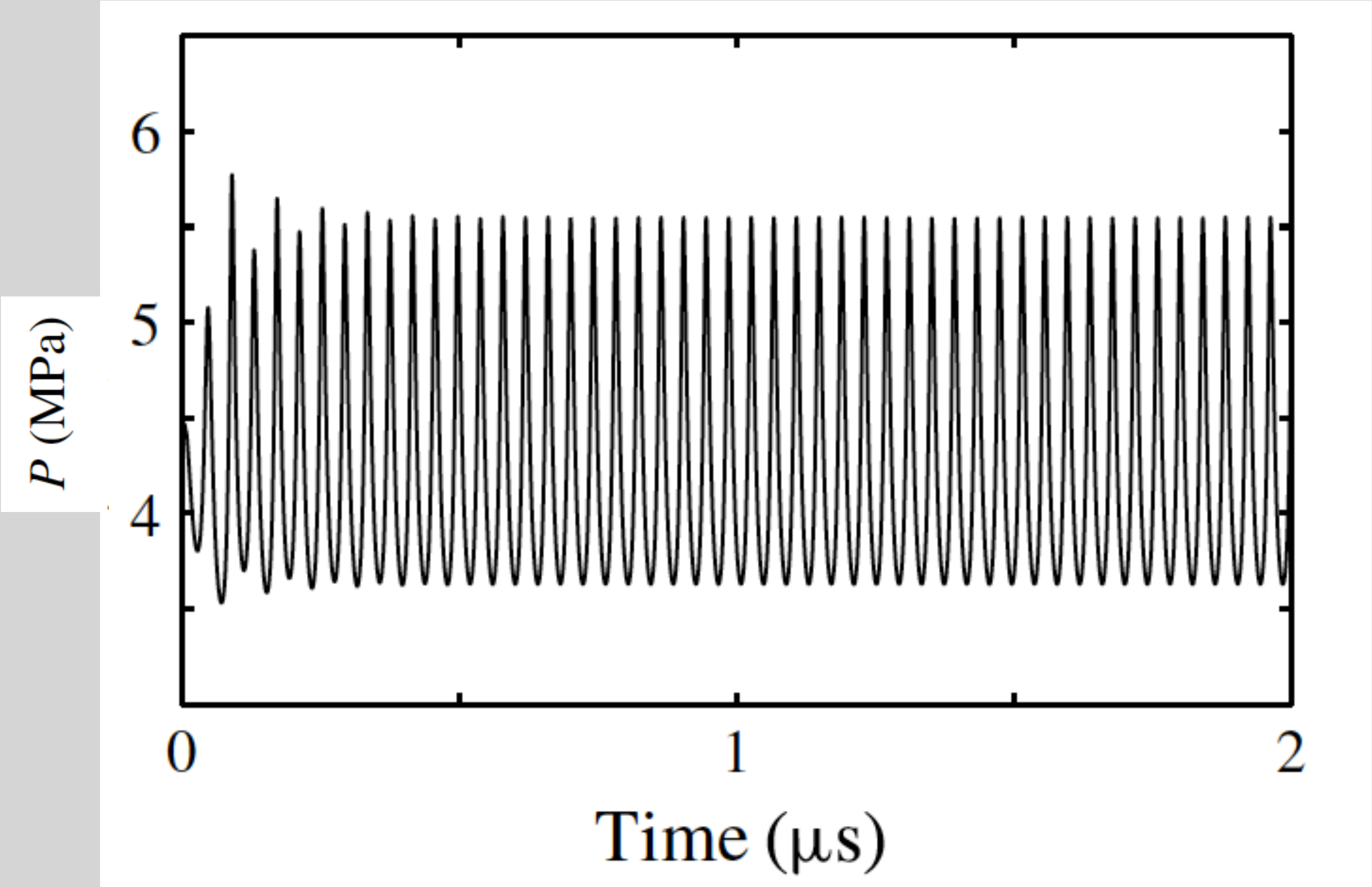
Stable, Viscous, 1D Detonation



Romick, Aslam, and Powers 2012

- Low activation energy results induce stability.
- Peak pressure at viscous shock front evolves with time.
- Relaxes to a steady state value.
- In the inviscid limit, grid refinement is sufficient to capture the linear stability boundary.

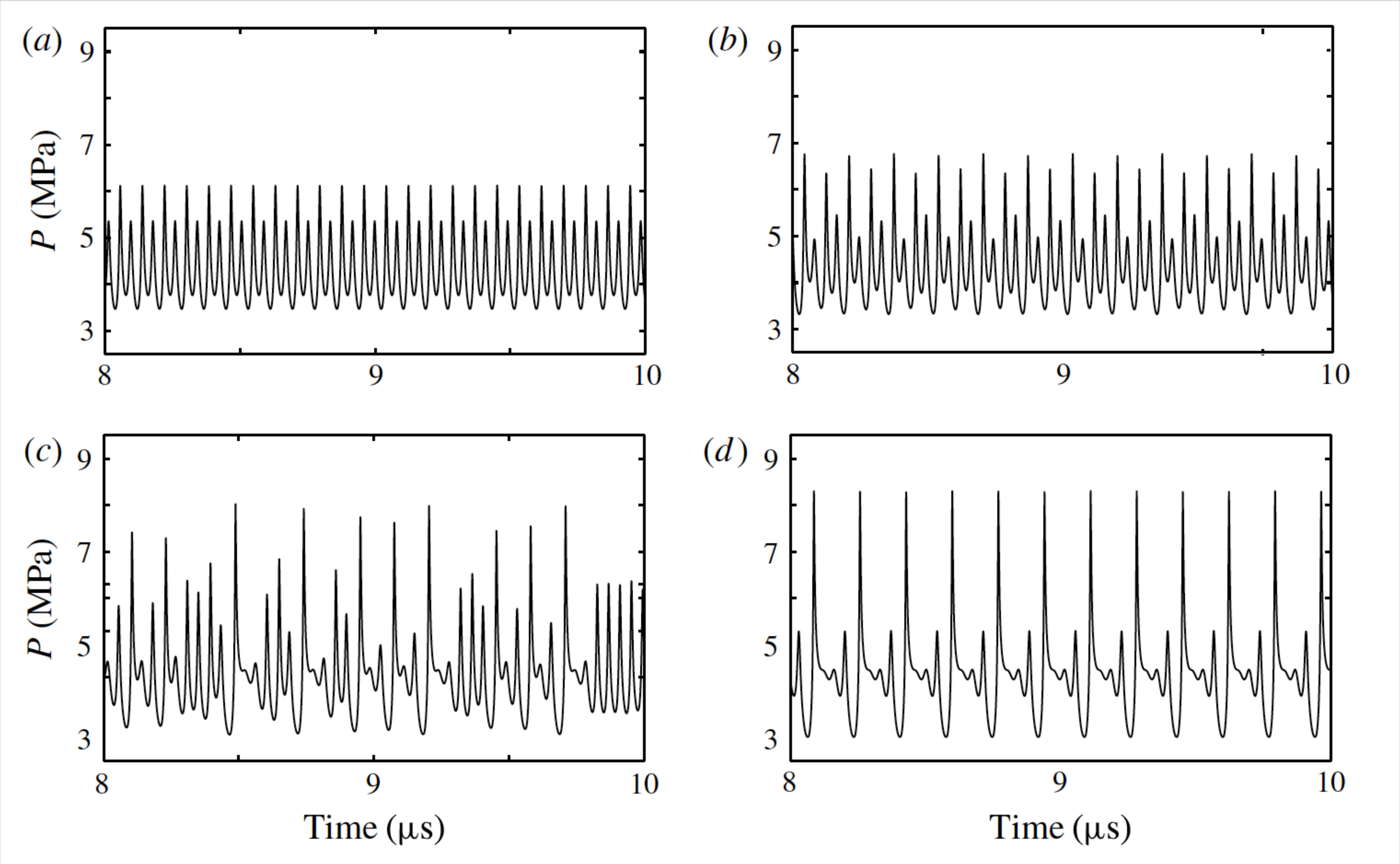
Viscous, 1D Detonation: Period 1 Instability



Romick, Aslam, Powers, 2012

- Raising activation energy induces an unstable mode.
- Peak pressure at viscous shock front evolves with time.
- Relaxes to a long-time limit cycle.

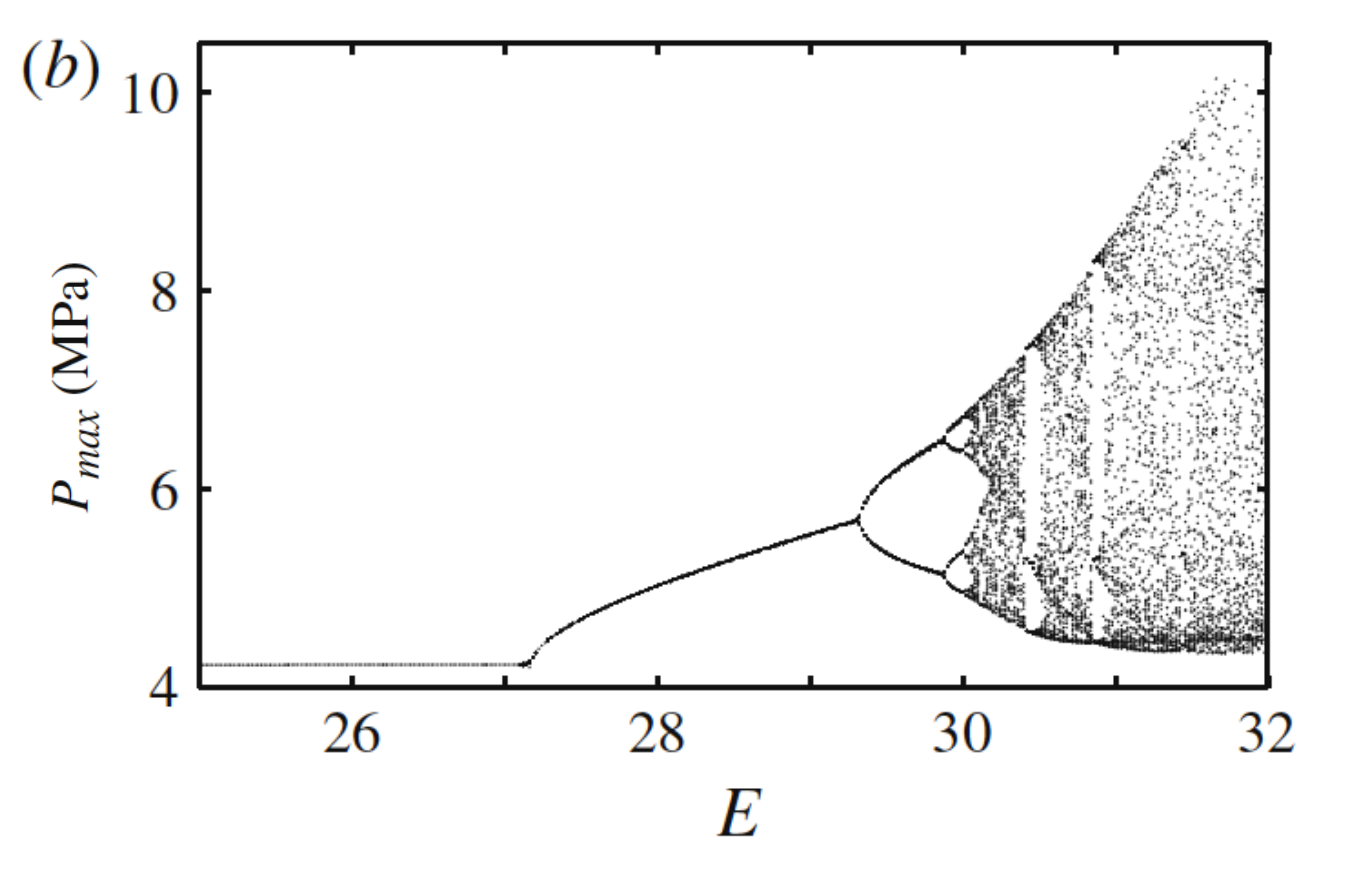
Viscous, 1D Detonation: Various Instabilities



Romick, Aslam, Powers, 2012

- Raising activation energy induces more and more instabilities.
- Can induce chaos c).
- Raising activation energy further can induce low frequency limit cycles, d).

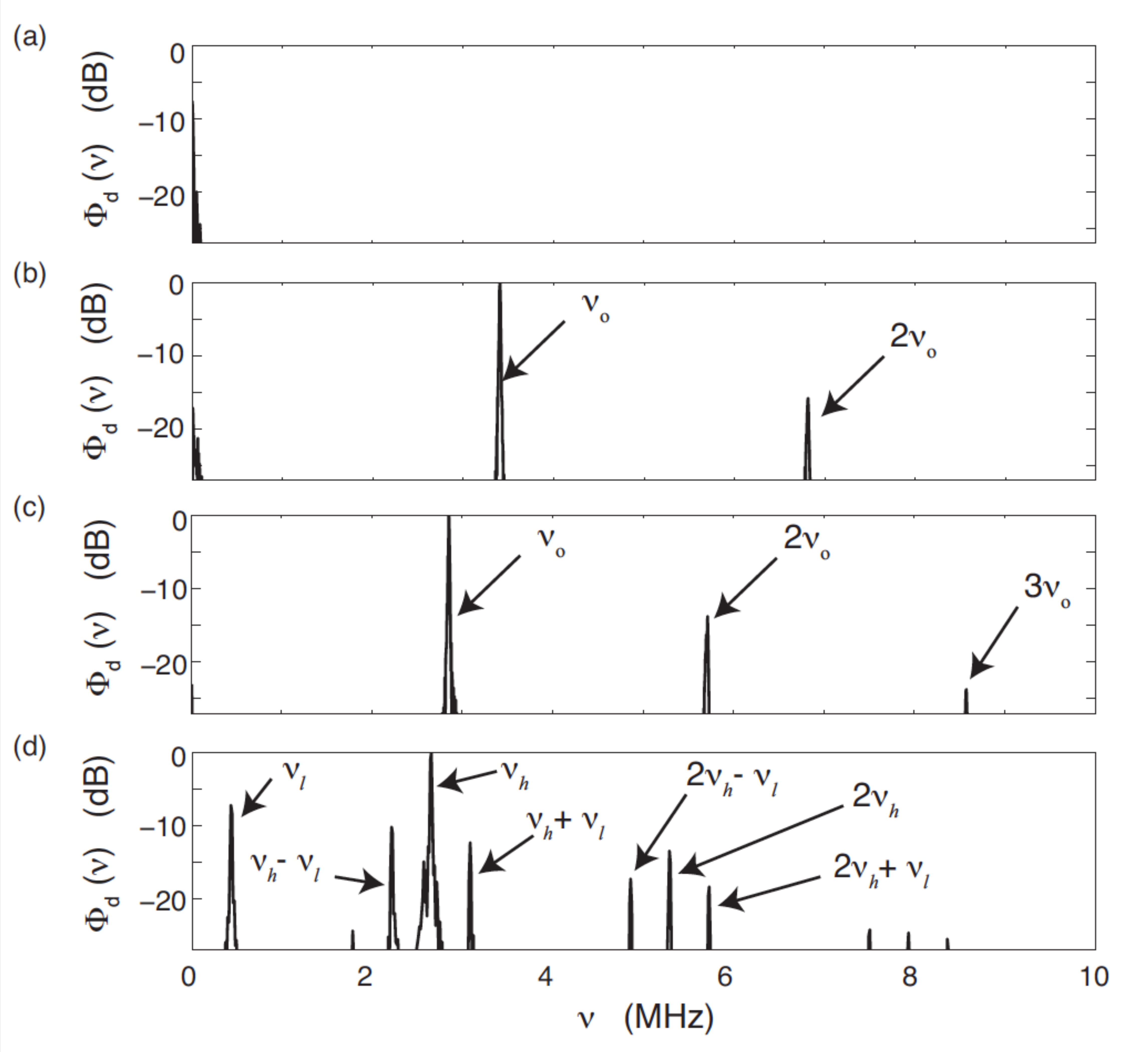
Viscous, 1D Detonation: Transition to Chaos



Romick, Aslam, Powers, 2012

- With activation energy as a bifurcation parameter, a transition to chaos is predicted.
- Feigenbaum constant predicted as 4.67.

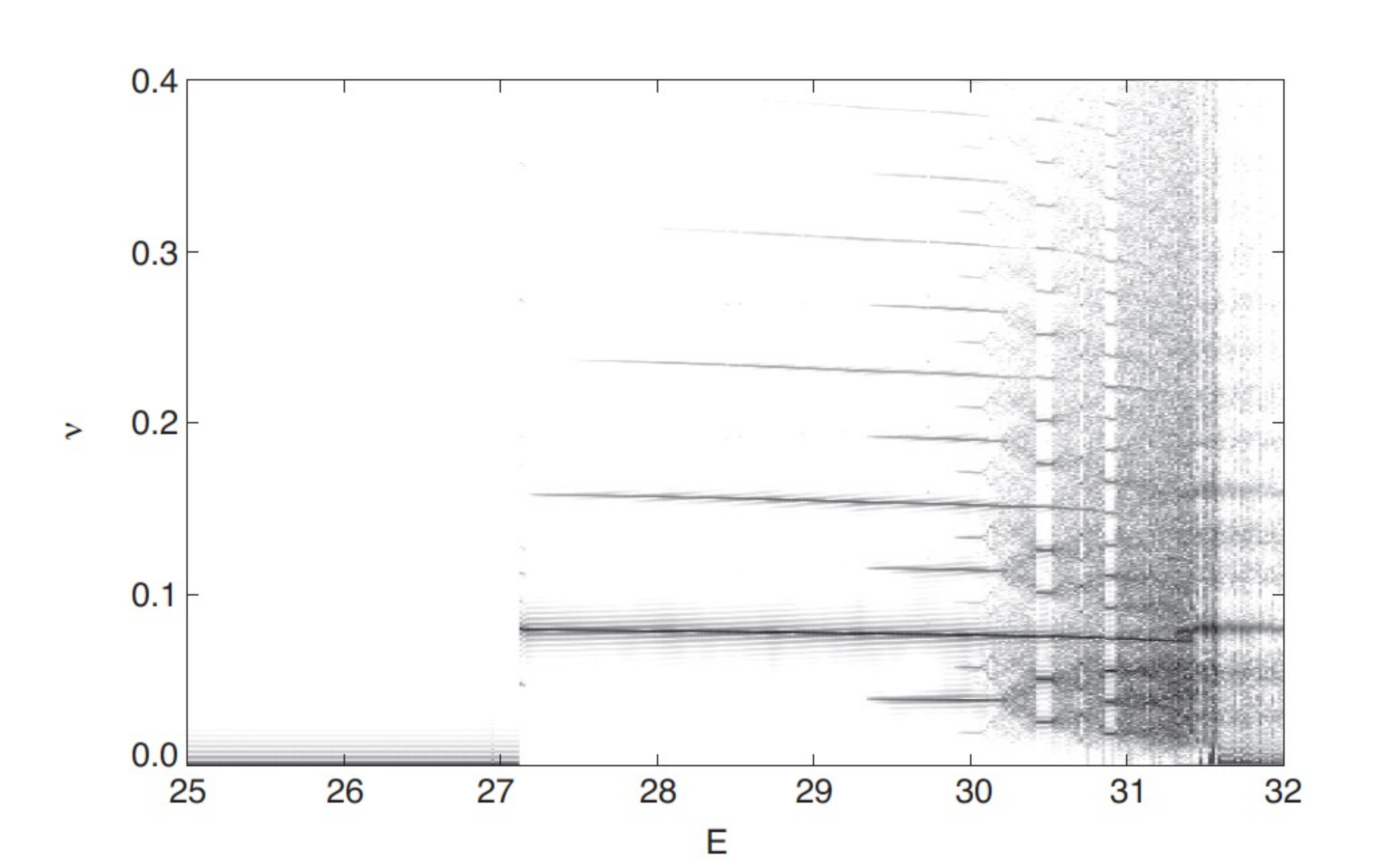
Spectral Analysis of the Signal for Verification



Romick, Aslam, Powers, 2015; results for detailed H_2-air kinetics.

- *a posteriori* spectral analysis of the signal via Discrete Fourier Transform (DFT).
- Fundamental modes and harmonic overtones revealed.
- Sideband instabilities revealed.
- They persist under grid resolution: verification!
- Refine until stability results do not change (Reed, et al., 2015).

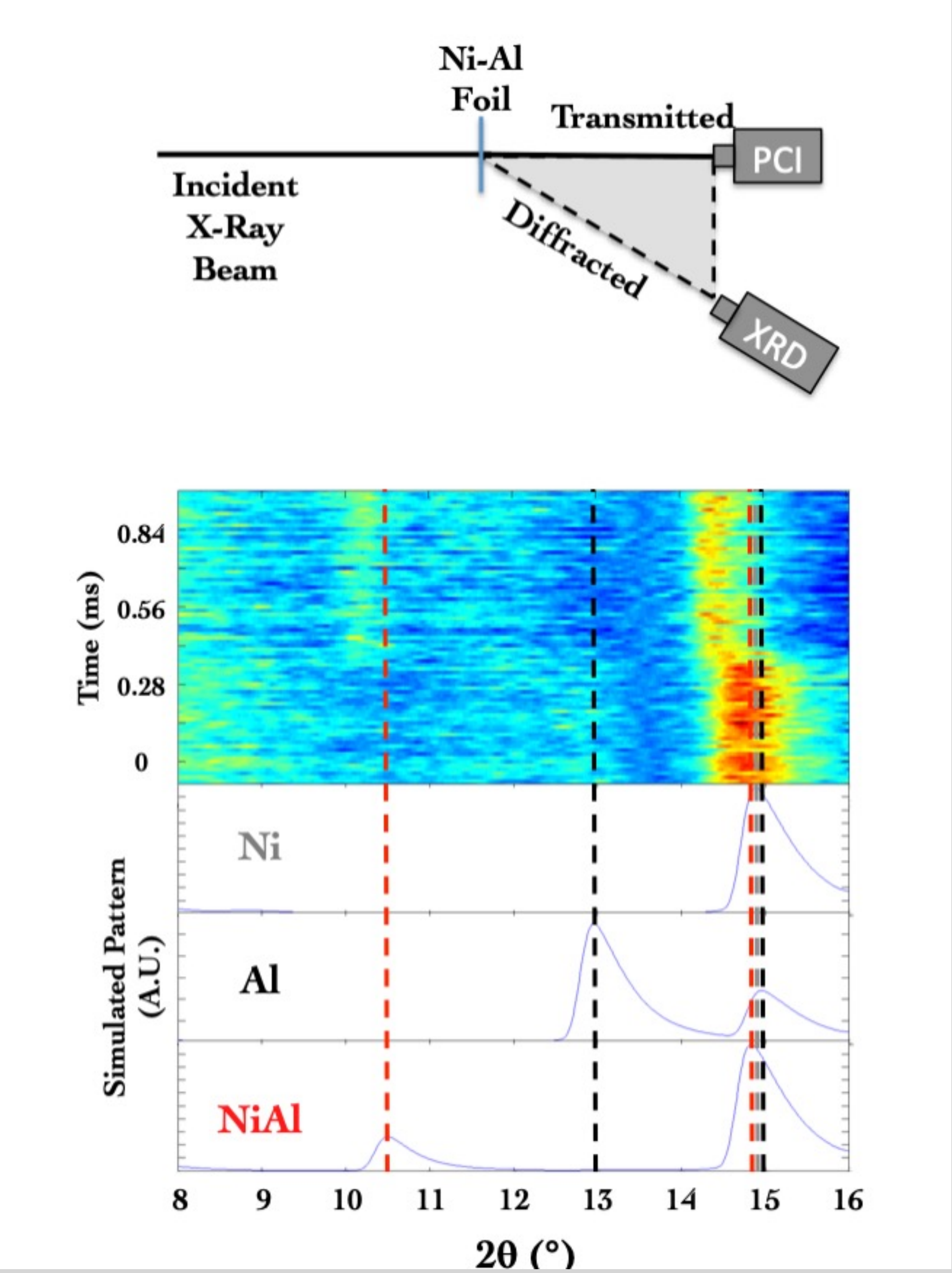
Spectral Analysis of the Signal for Verification



Romick, 2015

- DFT at various activation energies.
- Reveals the discrete, ordered, verified set of active Fourier modes.

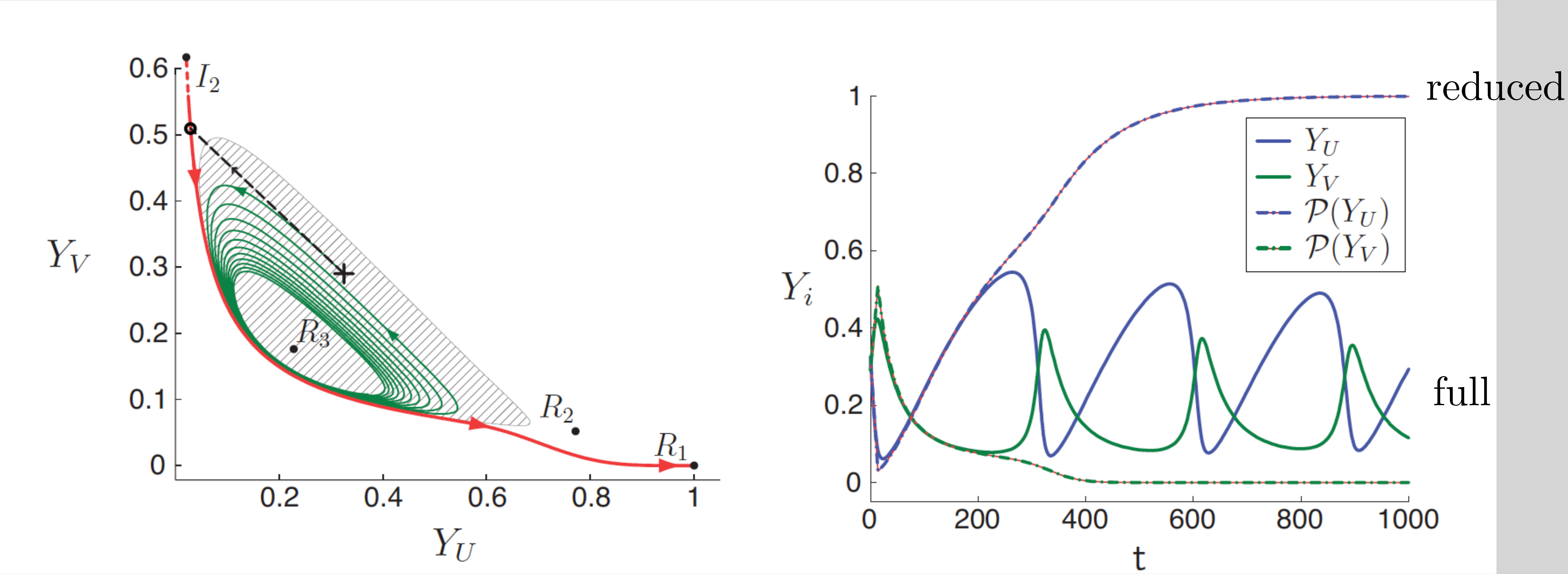
Computational Science can Learn from Material Science



Mukasyan, et al., 2018; data obtained from ANL with time-resolved XRD, 13 μs/frame, 10×50 μm.

- Experimental colleagues in material science use spectral analysis in X-Ray Diffraction (XRD) as a precision tool for material characterization.
- Here, spectral peaks associated with Ni, Al, and NiAl shown.
- Effective tool for segregating signal from noise.
- This tool should be used more in verification of computational predictions of unsteady phenomena.

Model Reduction: The Signal May Be Lost!



Mengers, 2012

- Gray-Scott reaction-diffusion model.
- Reduction to analytically filter fast kinetics falsely suppresses limit cycle.

Conclusions

- Computational science requires the *essence* of prediction of deterministic continuum systems to be machine- and algorithm-independent.
- What constitutes "essence" always requires user-choices; hopefully the neglected terms are not influential!
- Capturing the "essence" must be informed by the underlying physics.
- Pristine verification is a useful exercise to give the user confidence that the results are scientific, but unrealistic for many problems.
- Practical verification is important for the integrity of science.
- Perimeter-extending verification, e.g. *verifying spectral amplitudes*, is ongoing and highly challenging!
- Segregating "signal" and "noise" will never be easy!

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References

- Al-Khateeb, 2010, *Fine Scale Phenomena in Reacting Systems: Identification and Analysis for Their Reduction*, Ph.D. Dissertation, U. Notre Dame.
- ASME, 2009, *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*, ASME V&V 20, ISBN 9780791832097.
- Brill, Grenga, Powers, and Paolucci, 2014, "Automatic Error Estimation and Verification Using an Adaptive Wavelet Method," WCCM XI, Barcelona.
- Brooks, G. P., and Powers, J. M., 2004, "Standardized Pseudospectral Formulation of the Inviscid Supersonic Blunt Body Problem," *Journal of Computational Physics*, 197(1): 58-85.
- Henrick, 2008, *Shock-Fitted Numerical Solution of One- and Two-Dimensional Detonation*, Ph.D. Dissertation, U. Notre Dame.
- Kadanoff, 2003, "Excellence in Computer Simulation," *Computing in Science and Engineering* 6(2): 57-67.
- Mengers, 2012, *Slow Invariant Manifolds for Reaction-Diffusion Systems*, Ph.D. Dissertation, U. Notre Dame.
- Oberkampf and Roy, 2010, *Verification and Validation in Scientific Computing*, Cambridge U. Press.
- Powers and Paolucci, 2005, "Accurate Spatial Resolution Estimates for Reactive Supersonic Flow with Detailed Chemistry," *AIAA Journal*, 43(5):1088-1099.
- Powers and Sen, 2015, *Mathematical Methods in Engineering*, Cambridge U. Press.
- Powers, 2016, *Combustion Thermodynamics and Dynamics*, Cambridge U. Press.
- Singh, Rastigejev, Paolucci, and Powers, 2001, "Viscous detonation in H_2–O_2–Ar using intrinsic low-dimensional manifolds and wavelet adaptive multilevel representation," *Combustion Theory and Modeling*, 5(2): 163-184.

References

- Reed, Perez, Kuehl, Kocian, and Oliviero, 2015, “Verification and Validation Issues in Hypersonic Stability and Transition Prediction,” *Journal of Spacecraft and Rockets*, 52(1): 29-37.
- Richardson, 1922, *Weather Prediction by Numerical Process*, Cambridge U. Press.
- Rider, 2011, “What Makes a Calculation Good? or Bad?,” Workshop on Verification and Validation in Computational Science, University of Notre Dame.
- Roache, Ghia, and White, 1986, “Editorial Policy Statement on the Control of Numerical Accuracy,” Journal of Fluids Engineering, 108(1): 2.
- Roache, 2009, *Fundamentals of Verification and Validation*, Hermosa.
- Romick, Aslam, and Powers, 2012, “The Effect of Diffusion on the Dynamics of Unsteady Detonations,” *Journal of Fluid Mechanics*, 699: 453-464.
- Romick, C. M., Aslam, T. D., and Powers, J. M., 2015, “Verified and Validated Calculation of Unsteady Dynamics of Viscous Hydrogen-Air Detonations,” *Journal of Fluid Mechanics*, 769: 154-181.
- Romick, 2015, *On the Effect of Diffusion on Gaseous Detonation*, Ph.D. Dissertation, U. Notre Dame.
- Roy, McWherter-Payne, and Oberkampf, 2003, “Verification and Validation for Laminar Hypersonic Flowfields, Part 1: Verification, *AIAA Journal*, 41(10): 1934-1943.
- Silver, 2012, *The Signal and the Noise: Why Most Predictions Fail—but Some Don’t*, Penguin.
- Zahr and Powers, 2021, “High-Order Resolution of Multidimensional Compressible Reactive Flow Using Implicit Shock Tracking,” *AIAA Journal*, 59(1): 150-164.