DETERMINISTIC APPROACH FOR ESTIMATION OF DISCRETIZATION ERROR

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VV&A TWG at COMOPTEVFOR
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On the question of determinism

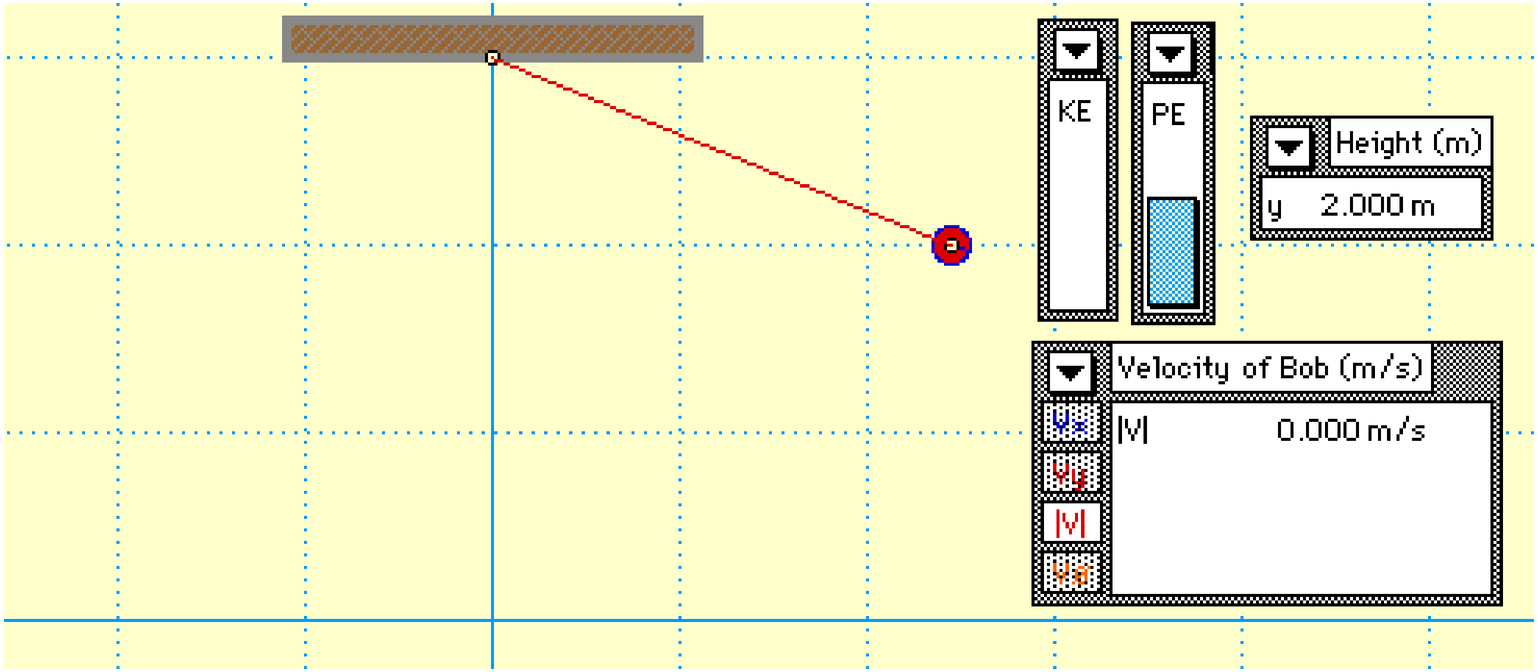
- " … the randomness of quantum mechanics is like a coin toss*. It looks random, but it's not really random."

  Carsten van de Bruck

  – from Musser , G. (2004) 'Was Einstein Right?' Scientific American September issue, pp. 88-91

  – * A*ll coins tossed from a skyscraper with different initial velocities will reach the same terminal velocity due to friction loss (i.e. information loss)*

Introduction



Animation taken from http://www.glenbrook.k12.il.us/gbssci/phys/mmedia/energy/pe.html

Theoretical Model

Displacement:

$$\frac{d\theta}{dt} = \frac{V}{L}$$

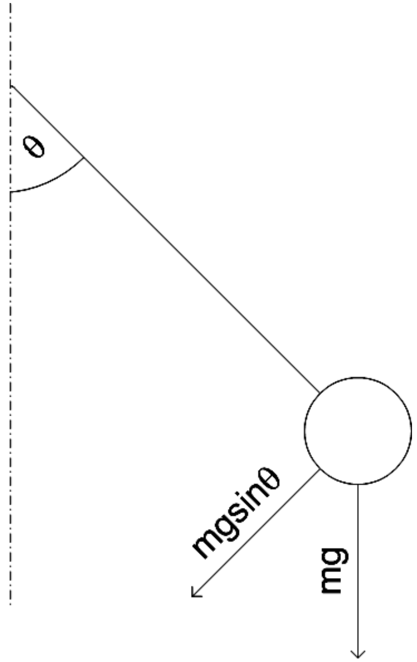
Velocity/Momentum:

$$\frac{dV}{dt} = -g\sin\theta + a_D$$

$$a_D = \tfrac{3}{4} C_D \frac{\rho_a}{\rho}\left(\frac{V - V_a}{D}\right)^2$$

$$C_D = f\left(\mathrm{Re}\right) = \frac{24}{\mathrm{Re}} + \frac{6}{\left(1+\sqrt{\mathrm{Re}}\right)} + 0.4$$

$$\mathrm{Re} = \frac{\rho_a \,|V - V_a|\, D}{\mu_a}$$

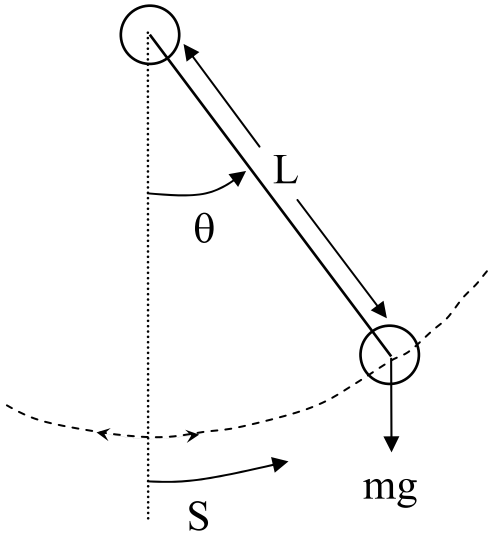


$0<\mathrm{Re}<2\mathrm{x}10^5$ (uncertainity in $C_d \pm 10\%$

V is velocity, θ is angle in radians, L is the length of the rod.

Assumption: Rigid, thin rod so that tangential force exerted on the body by the rod is negligible.

Physical Reality



$$\theta = \frac{S}{L}$$

time t=0, V_0=0.0, θ_0=45°

L = 0.2484 m

g = 9.8066 m/s^2

ρ = 1000 kg/m^3 (bob density)

D = 0.5 m (bob diameter)

Fluid properties etc.

ρ_f=1000 kg/m^3

μ_f=1.5×10^{-3}

Question:

θ = ? after 5 seconds

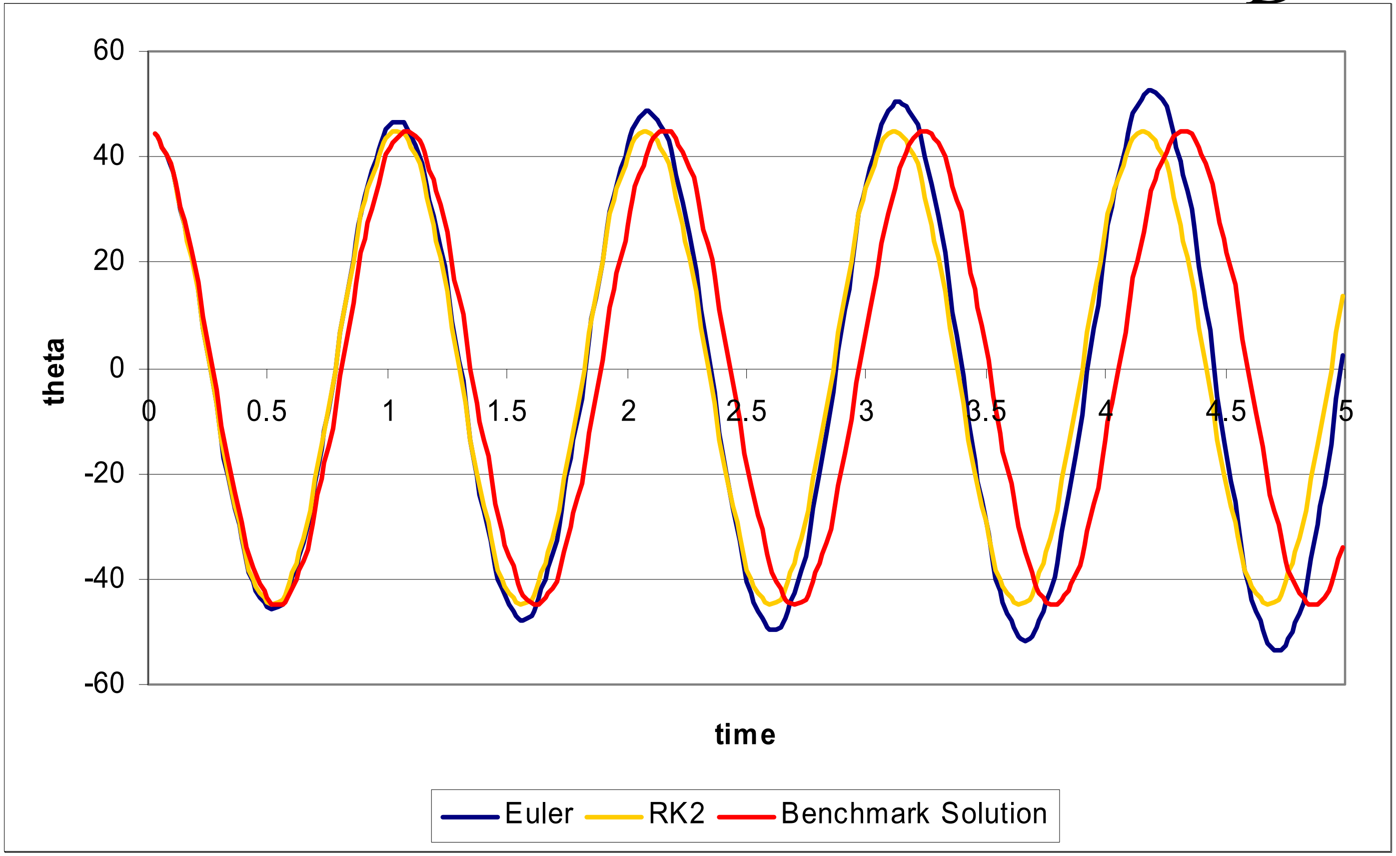
Measured value

$(\theta_E+\delta_E)$ = 20 ± 2 degrees

at 5 ± 0.010 seconds

(*hypothetical*!)

Approximate Solution to Pendulum Problem with C_D=0



dt=2 ms

How accurate are these results?

Experimental Uncertainty

- Uncertainty in input parameters (measured!)
  - Rod length: $L_E \pm\delta_L$
  - Bob diameter: $d_E\pm\delta_d$
  - Bob density: $\rho\pm\delta_\rho$
- Similarly for the surrounding fluid properties:
  - Air speed: $V_a\pm\delta_{Va}$
  - Air density: $\rho\pm\delta_\rho$
  - Air viscosity: $\mu\pm\delta_{\mu a}$
  - Drag coefficient: $C_D\pm\delta_{Cd}$
- Experimental Result
  - $\theta=\theta_E\pm\delta_\theta$ at $t=t_E\pm\delta_t$
- Benchmark Solution: non-linear problem + drag
  - $\Delta t=1.9531$ μs, $e_a=0.002\%$
  - $\theta=20.7379$ deg

Computational Issues

- Numerical Errors / Uncertainty (δ_{num})
  - Uncertainty in input parameters
  - Round off / chop off error
    - Smearing / subtractive cancellation
  - Iterative convergence (incomplete iteration)
  - Truncation / grid error (incomplete grid convergence)
  - Others, i.e. finite domain
- Modeling Errors / Uncertainty (δ_{mod})
  - Approximations and/or assumptions in development of the theoretical mathematical model
  - Example: Pendulum problem
    - Rod is infinitely thin (zero mass)
    - Drag force negligible
    - Small angle (linearization)
- Computational / Prediction Uncertainty (δ_{comp})
  - $\delta_{comp} = \text{func}(\delta_{num}, \delta_{mod})$
  - $\delta^2_{comp} = \delta^2_{num} + \delta^2_{mod}$ (May not be decomposable!)

Verification & Validation (V^2&V)

- Phase I – Code Verification
  - Computer code: Must be debugged and verified for a wide range of problems

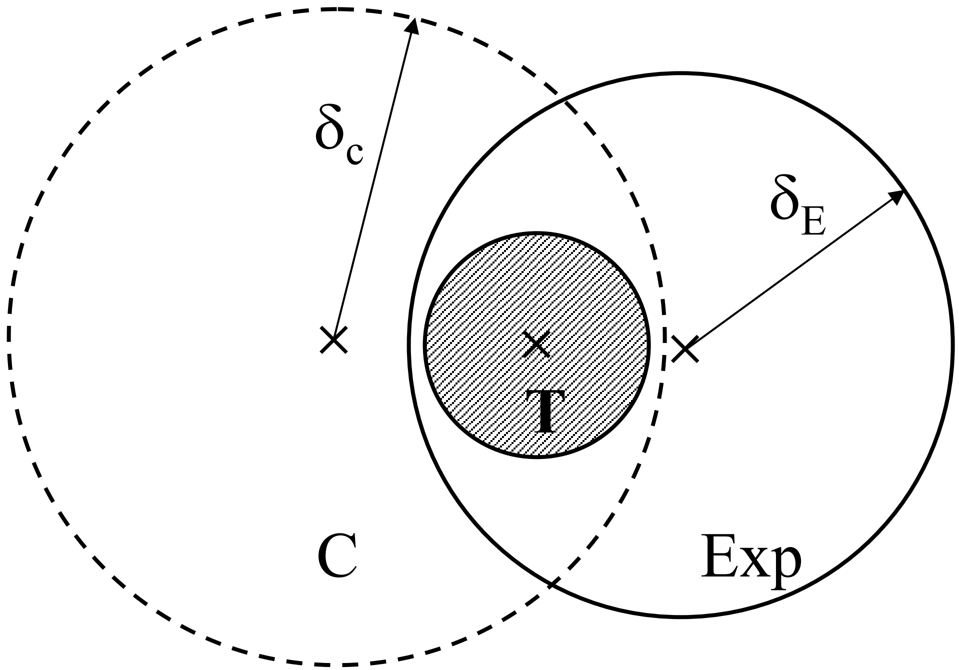
- Phase II – Calculation Verification
  - Show that equations are being solved right
- Phase III – Model Validation
  - Show that the theoretical model produces acceptable results when implemented appropriately

Difficulties:

- Experimental results are not always available (e.g. nuclear explosions)
- Experimental uncertainty may not be available

Challenge

Predict the 'truth' within an acceptable confidence interval without knowing the 'truth'

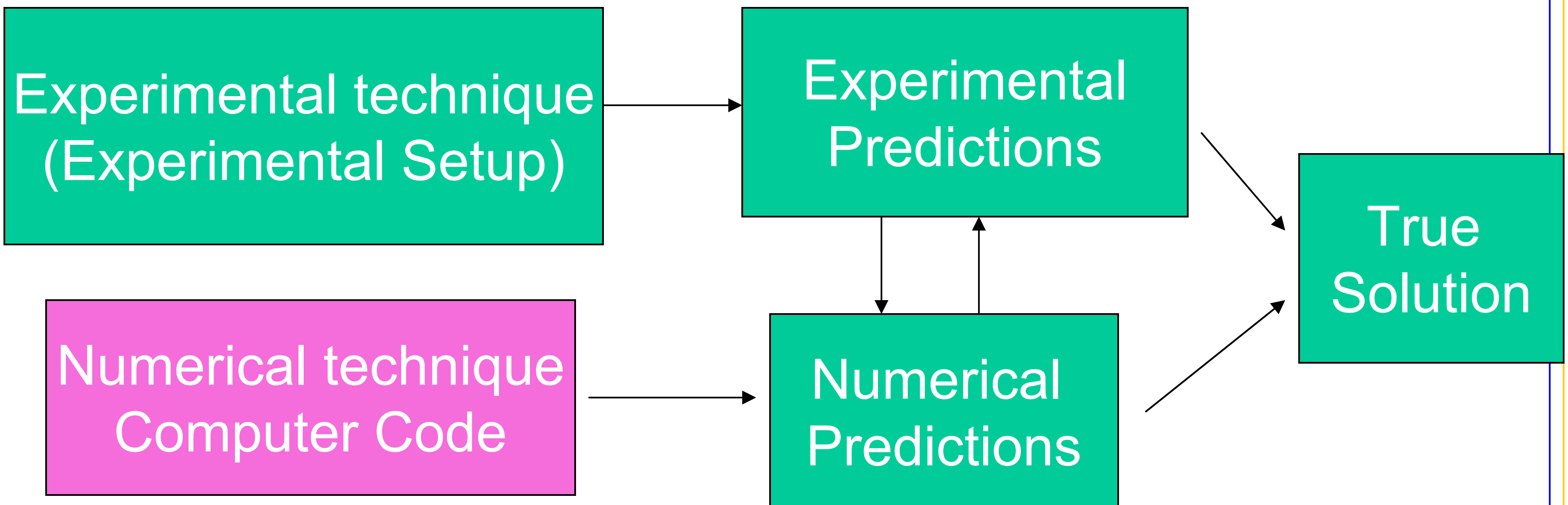


"What can not be computed is meaningless!"

(Davies, 1992)

T = 'truth' ± fuzziness about truth

Climbing to the "true solution"



Parallelism between Experiments and Numerical Methods:

$$\left|T - T_{\exp}\right| < U_{\exp}$$

$$\left|T - T_{num}\right| < U_{num}$$

$$U_{tot} = \sqrt{U^2{}_{\exp} + U^2{}_{num}}$$

Uncertainty v.s. Error

After Roache (2003)

An Error Bar...

...is a U95.

...uses |E1| > 0

...is not an ordered approximation
but an empirical correlation

…based on computational experiments.

...may be accurate (statistically) even outside the asymptotic range.

...could be determined from data for the problem ensemble without error estimator.

...is what we want for calculation Verification prior to Validation.

An Error Estimator...

...is a U50.

...uses signed E1 > 0 or < 0

...is an ordered approximation

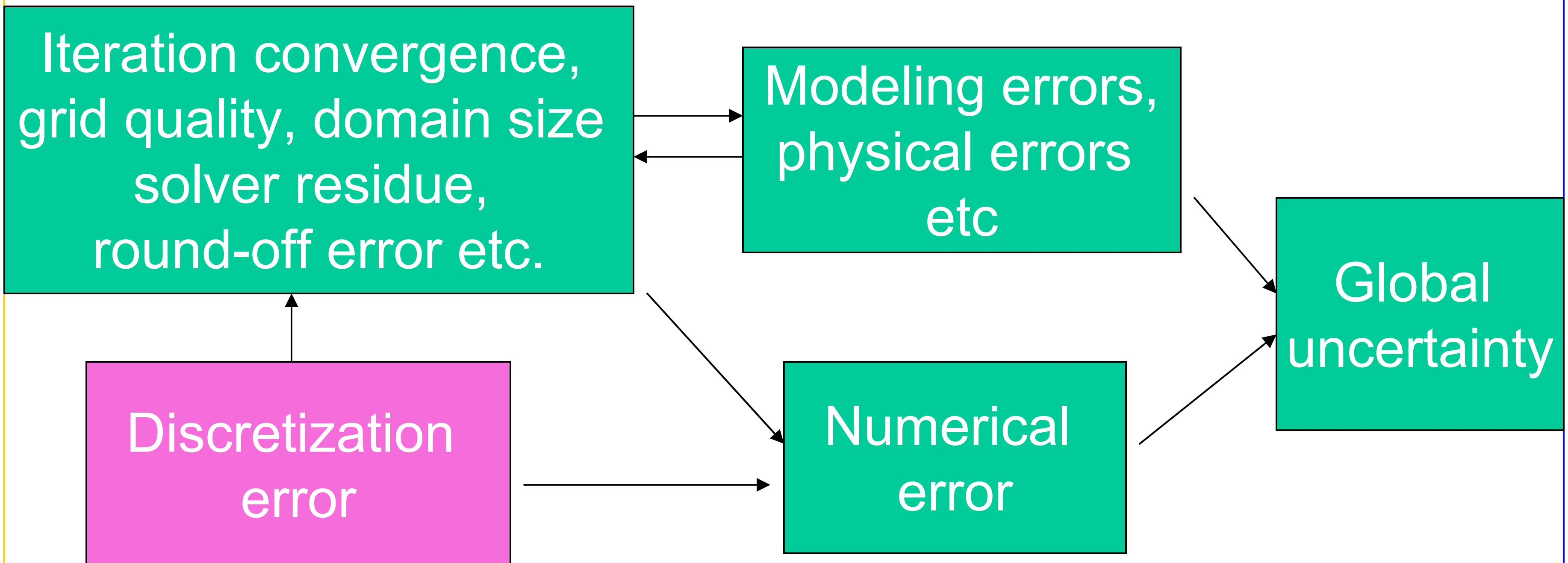
…based only on asymptotic theory

...accuracy depends upon the grid sequence being in the asymptotic range,

…for any problem.

...is what is commonly given (at best) and is what is needed for an RE corrected solution.

Discretization Error



Common methods of quantifying discretization error:

- Richardson extrapolation (RE)
- Zhu-Zienkiewicz (ZZ) and energy norm methods
- Error transport method (ETE)

Literature review of RE

- Richardson (1910, 1927)
- Roache (1993, 1998, 2003)
- Celik et al (1993, 1997)
- Stern et al (2001, 2002)
- Cadafalch et al. (2002)
- Eca & Hockstra (2002)

Richardson Extrapolation

$$E_h = \phi_{ext} - \phi_h = C_1 h + C_2 h^2 + C_3 h^3 + \Lambda$$

$$\phi_{ext} - \phi_1 = C\ (h_1)^p$$

$$\phi_{ext} - \phi_2 = C\ (h_2)^p$$

$$\phi_{ext} - \phi_3 = C\ (h_3)^p$$

Let $h_1 < h_2 < h_3$ and $r_{21} = h_2/h_1$, $r_{32} = h_3/h_2$

$$p = (1/\ln(r_{21}))[\ln|\varepsilon_{32}/\varepsilon_{21}| + q(p)]$$

$$q(p) = \ln\left(\frac{r_{21}^p - s}{r_{32}^p - s}\right) \qquad s = 1 \cdot \mathrm{sign}(\varepsilon_{32}/\varepsilon_{21})$$

where $\varepsilon_{32} = \phi_3 - \phi_2$, $\varepsilon_{21} = \phi_2 - \phi_1$

Original idea: Richardson (1910, 1927)

Procedure for estimation of discretization error

(i) Define a representative cell, mesh or grid size h.
Let

$$h = \sum_{i=1}^{N} (\Delta V_i / N)^{1/3}$$

where ΔV_i is the volume of the i^{th} cell, and N is the total number of cells used for the computations.
For three dimensional, structured, geometrically similar grids, one can use

$$h = \left[(\Delta x_{\max})(\Delta y_{\max})(\Delta z_{\max})\right]^{1/3}$$

(ii) Select three significantly different set of grids and run simulations

- The grid refinement factor, $r=h_{coarse}/h_{fine}$, should be greater than 1.3.
- The grid refinement should be made systematically, that is, the refinement itself should be structured even if the grid is unstructured.
- Geometrically similar cells are preferable.

Procedure for estimation of discretization error-Continued

(iii) Calculate the order "p" according to Richardson Extrapolation

(iv) Calculate the extrapolated values from

$$\phi_{ext}^{21} = (r_{21}^{p}\phi_1 - \phi_2)/(r_{21}^{p} - 1) \qquad \phi_{ext}^{32} = (r_{32}^{p}\phi_2 - \phi_3)/(r_{32}^{p} - 1)$$

(v) Calculate the error estimates along with the apparent order *p*:

Approximate relative error:

$$e_a^{12} = \left| \frac{\phi_1 - \phi_2}{\phi_1} \right| ,$$

extrapolated "true" relative error:

$$e_a^{12} = \left| \frac{\phi_{ext}^{12} - \phi_1}{\phi_{ext}^{12}} \right| ,$$

The fine grid convergence index:

$$\mathrm{GCI}_{\mathrm{fine}}^{12} = \frac{1.25 e_a^{12}}{r_{21}^{p} - 1} ,$$

Note: If calculated order, *p*, is less than 1.0, error estimates should also be given by assuming $p=1$

Example 1: The Pendulum Problem

Simplifications:

1. Drag ~ 0

$$\frac{dv}{dt} = -g \sin\theta \qquad a_D \cong 0$$

2. θ is small

$$\frac{dv}{dt} = -g\theta$$

$$\frac{d\theta}{dt} = V$$

Code Verification: Euler Method

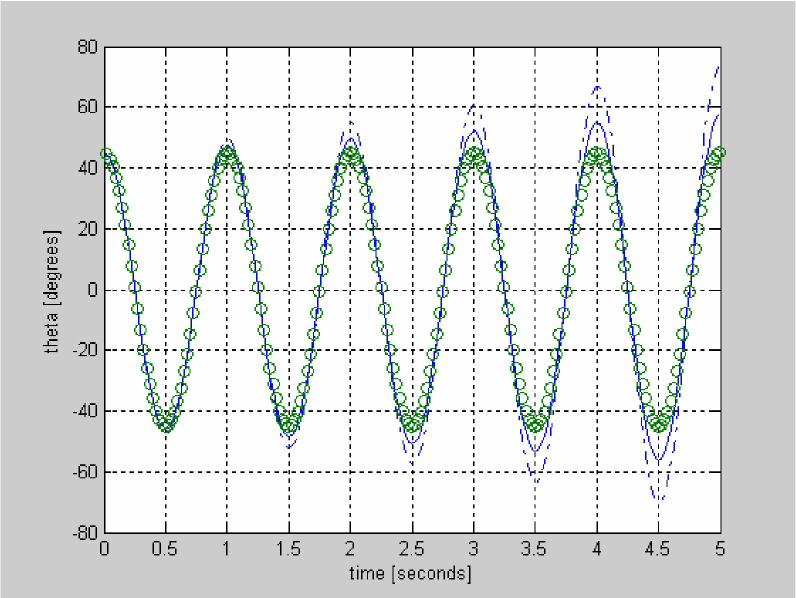


Figure: Verification of Euler Method applied to linearized pendulum problem (Cd=0). Dashed line: dt = 5.0ms, thick line: dt = 2.5 ms, Symbols: exact

h/hmax (hmax= 4ms)	phi (deg)	Apparent Order p
0.0078	45.139	1.0072
0.0156	45.2784	1.0128
0.0313	45.5586	1.0014
0.0625	46.124	1.0902
0.125	47.2559	1.0582
0.25	49.6657	1.2341
0.5	54.6836	
1	66.4872	

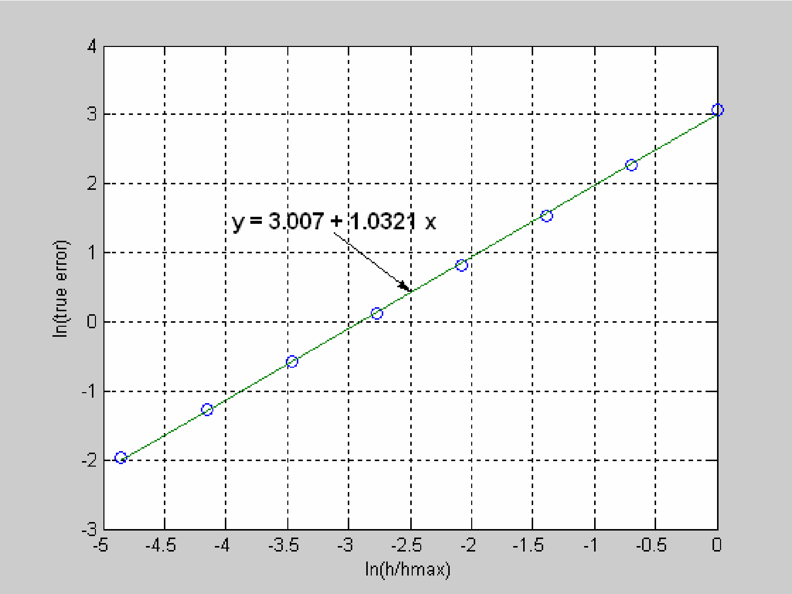


Figure: Error analysis for Euler method applied to the linearized pendulum problem; hmax = 4 ms

Code Verification: Runge-Kutta

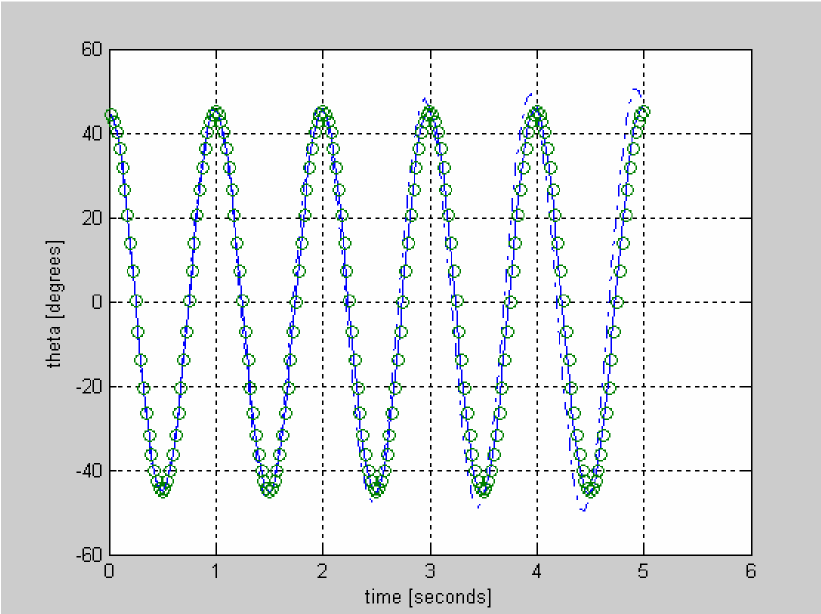


Figure: Verification of RK2 Method applied to linearized pendulum problem (Cd=0), dashed line: dt = 50ms, thick line: dt = 25 ms, Symbols: exact

h/hmax (hmax= 4ms)	phi (deg)	Apparent Order p
0.0078	44.9999	2.1699
0.0156	44.9997	1.6374
0.0313	44.9988	1.0995
0.0625	44.996	2.8843
0.125	44.99	1.891
0.25	45.0343	0.267
0.5	45.1986	
1	45.3963	

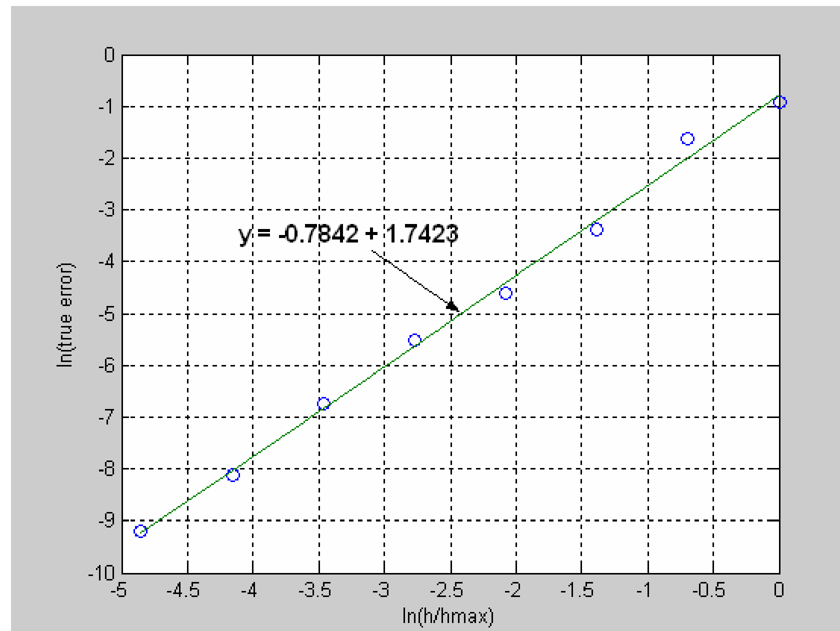
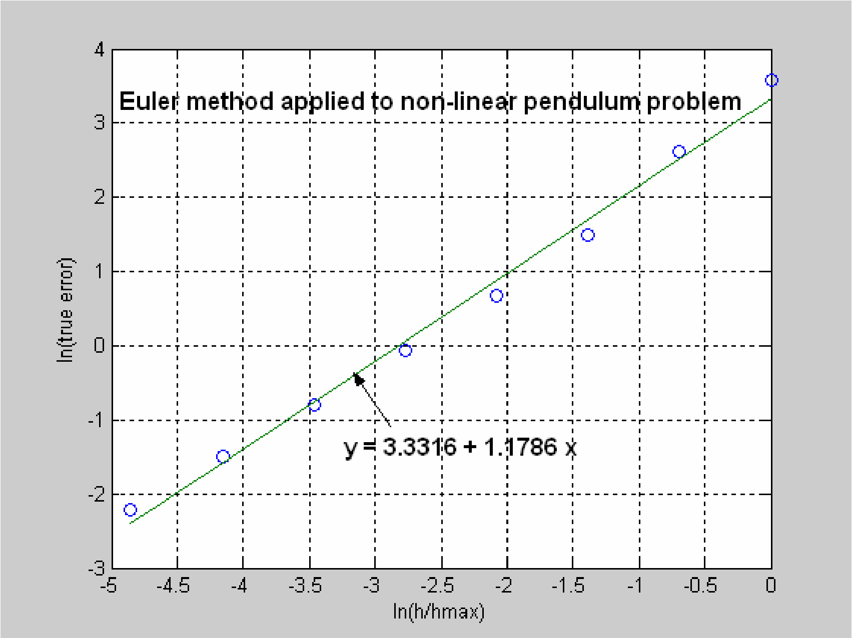
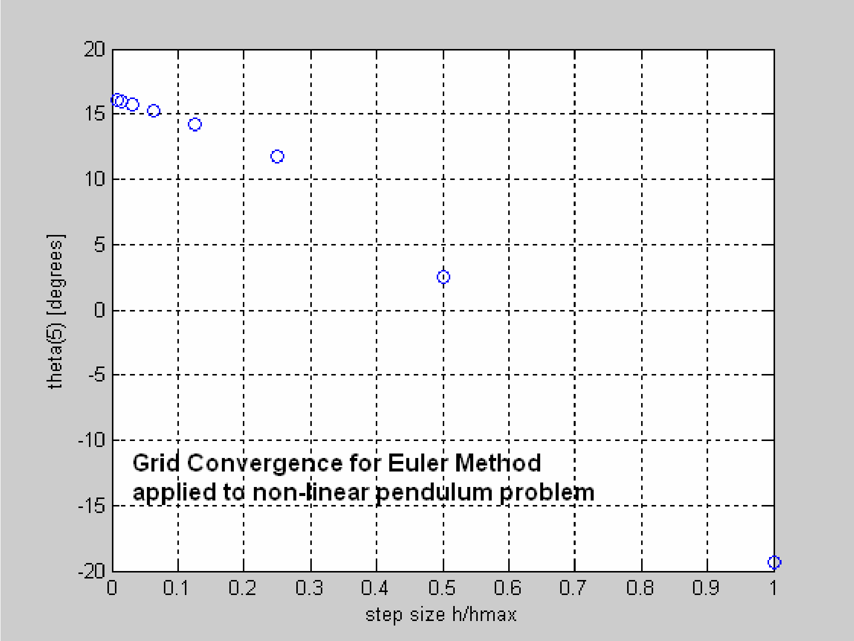


Figure: Error analysis for Runge-Kutta method applied to the linearized pendulum problem; hmax = 40 ms

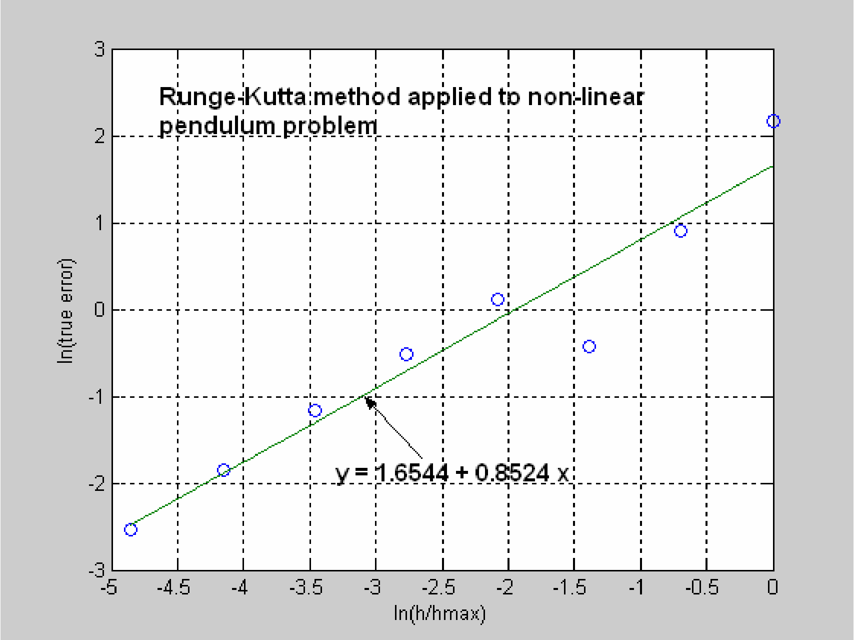
Calculation Verification: Euler method

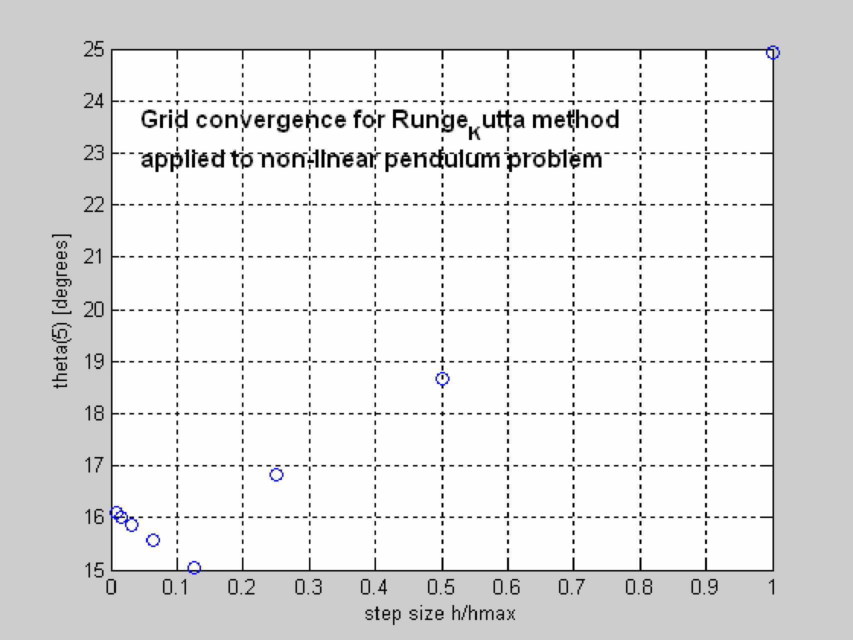




h/hmax (hmax= 4ms)	phi (deg	Apparent Order p
0.0078	16.0665	1.0324
0.0156	15.9543	1.063
0.0313	15.7248	1.1227
0.0625	15.2453	1.2336
0.125	14.2012	1.9085
0.25	11.746	1.2477
0.5	2.5287	
1	-19.3582	

Calculation Verification: Runge Kutta





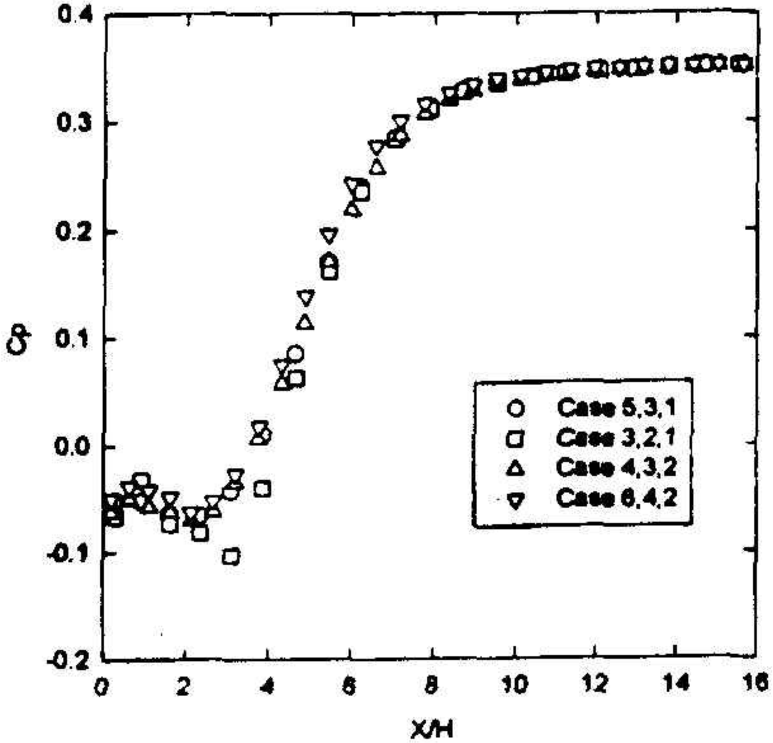
h/hmax (hmax= 40ms)	phi (deg)	Apparent Order p
0.0078	16.0977	0.9626
0.0156	16.0195	0.9272
0.0313	15.8671	0.8415
0.0625	15.5773	1.7729
0.125	15.058	0.041
0.25	16.8327	1.7771
0.5	18.6585	
1	24.9161	

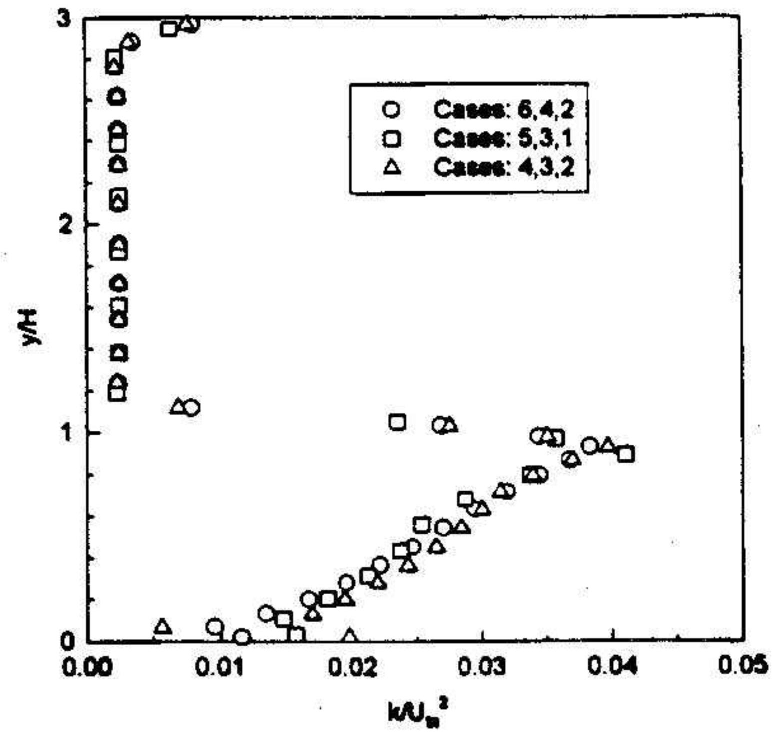
Example Calculations of Discretization Error*

	ϕ = dimensionless reattachment length (*with monotonic convergence*)	ϕ = axial velocity at x/H=8, y=0.0526 ($p < 1$)	ϕ = axial velocity at x/H=8, y=0.0526 (*with oscillatory convergence*)
N_1, N_2, N_3	$1.8*10^4$, $8*10^3$, $4.5*10^3$	$8*10^3$, $4.5*10^3$, $9.8*10^2$	$8*10^3$, $4.5*10^3$, $9.8*10^2$
r_{21}	1.5	2.0	2.0
r_{32}	1.333	2.143	2.143
ϕ_1	6.063	10.7880	6.0042
ϕ_2	5.972	10.7250	5.9624
ϕ_3	5.863	10.6050	6.0909
p	1.53	0.75	1.51
ϕ_{ext}^{21}	6.1685	10.8801 (10.8510)*	6.0269
e_a^{12}	1.50%	0.58% (0.58%)*	0.70%
e_{ext}^{12}	1.71%	0.85% (0.58%)*	0.38%
GCI_{fine}^{12} (error bars)	± 2.18%	± 1.07% (± 0.73%)*	± 0.48%

* calculated with p=1 *(worst case)*; *Data from Celik and Kanatekin(1997)*

Example Calculations of Discretization Error -- Continued



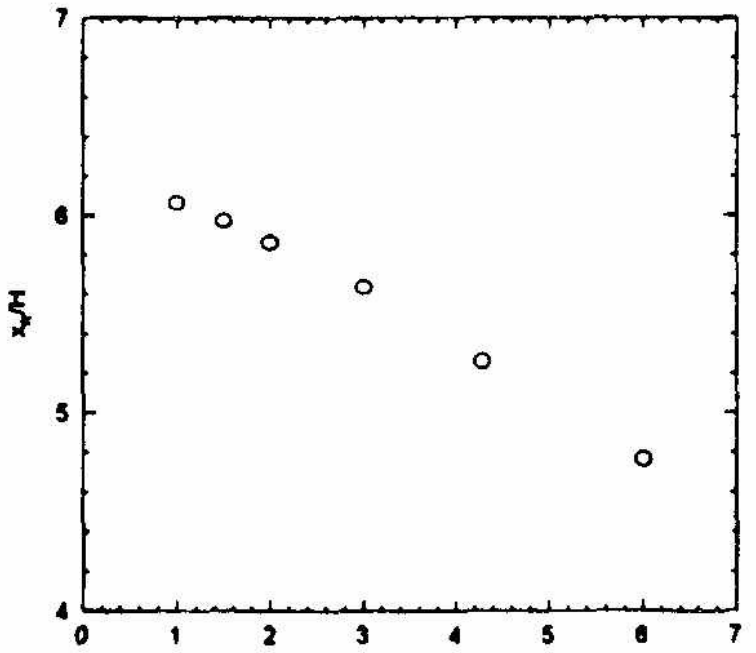


Extrapolated Cp on step side wall

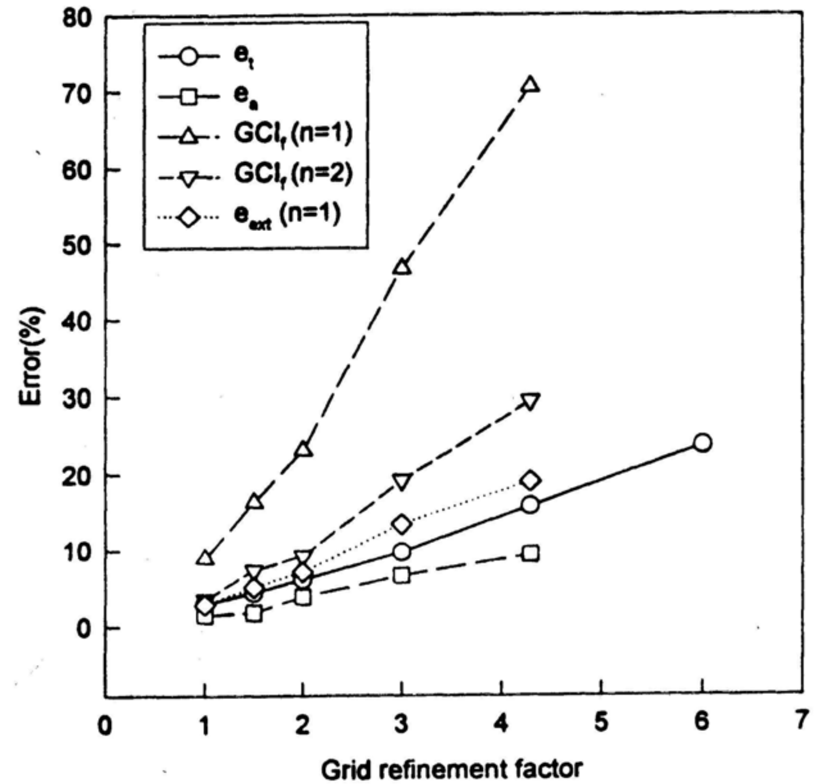
Extrapolated k-profiles at x/H = 2.67

(source: Celik and Karatekin, 1997)

Example Calculations of Discretization Error -- Continued



Grid refinement factor



Variation of reattachment length with grid refinement factor

Variation of various uncertainty estimates with grid refinement factor: Computed reattachment length

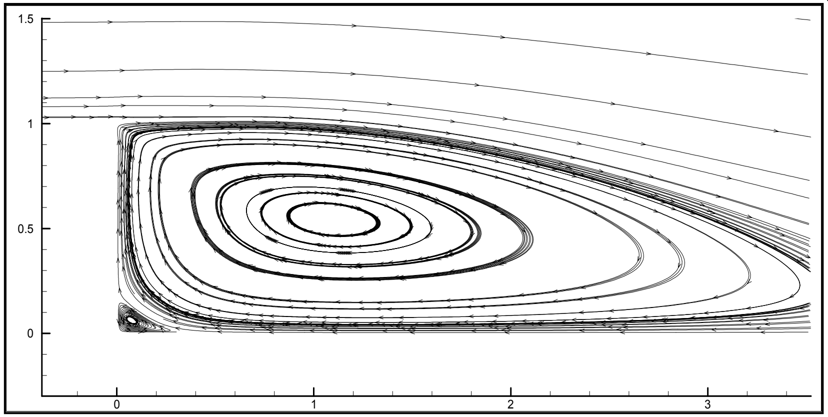
(source: Celik and Karatekin, 1997)

Calculation Verification in Practice

Problem description

• 2D turbulent backward facing step flow
Re_H=50,000

• Expansion ratio 8/9



Calculation issues (Fluent 6.0)

•Grid: similar structured grid, non-cartesian

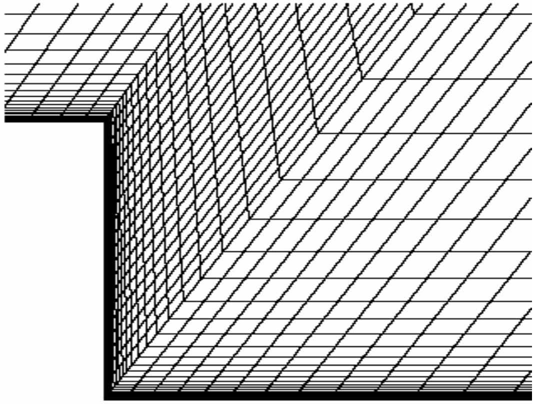
Grid	101*101	121*121	141*141	161*161	181*181	201*201	241*241
Grid refinement ratio	1.00	1.20	1.17	1.14	1.13	1.11	1.20

•Turbulence model: Spalart-Allmaras

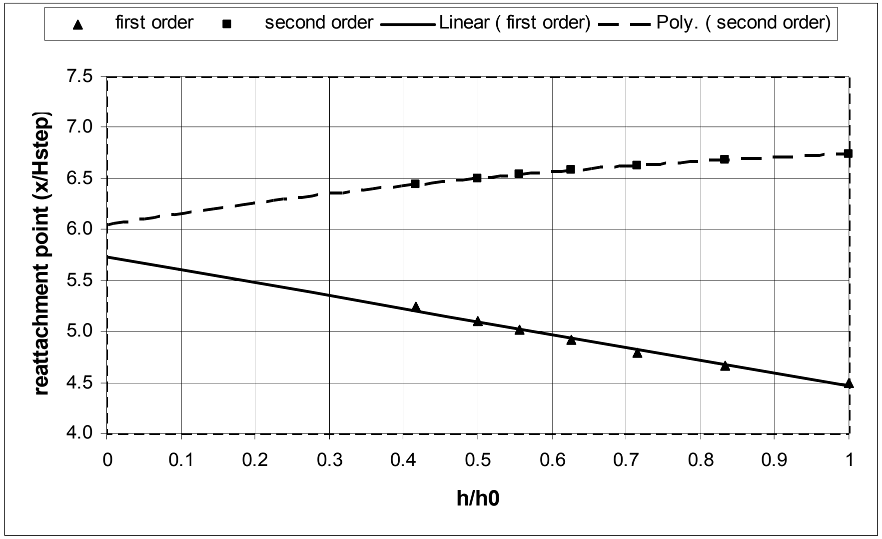
•Numerical scheme: first/second order upwinding for convectior

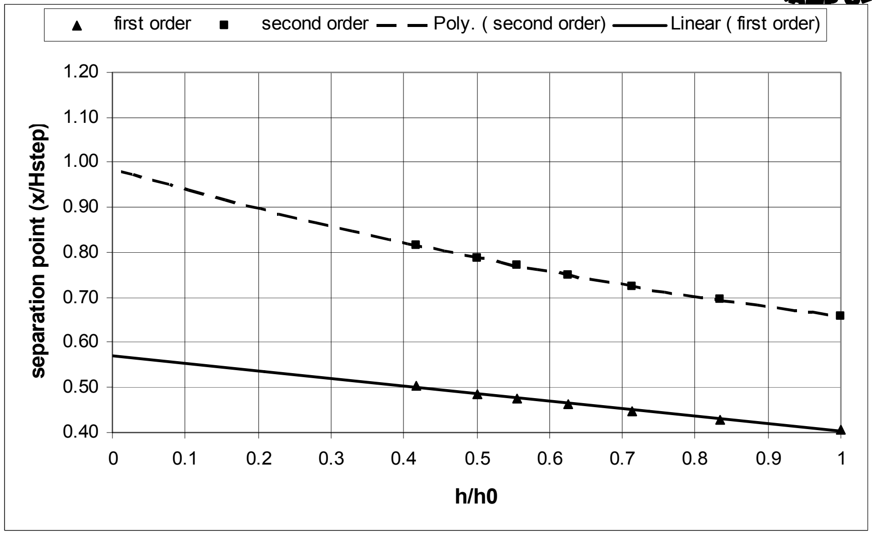
•Interpolation for post process: Bilinear

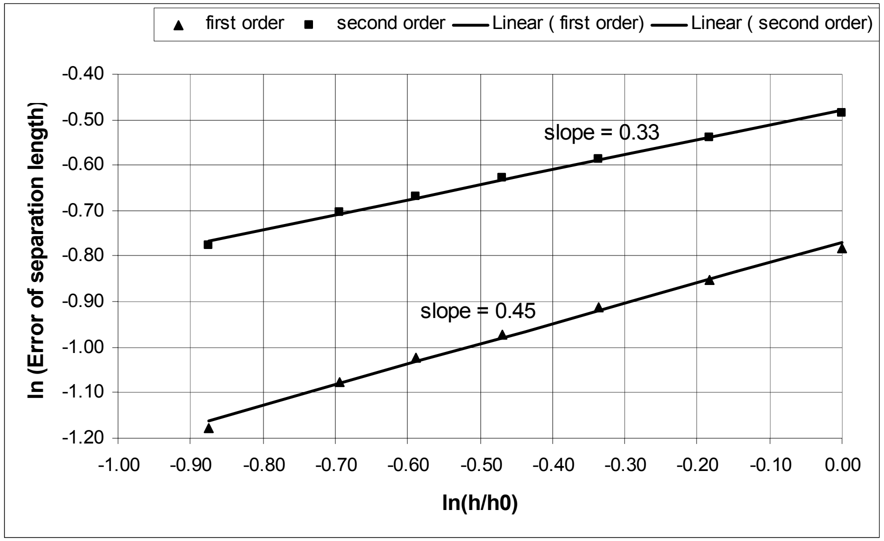
•Extrapolation to limit: ***Power law, Cubic spline, Polynomial, Approximate Spline*** (Celik, et al., 2004)

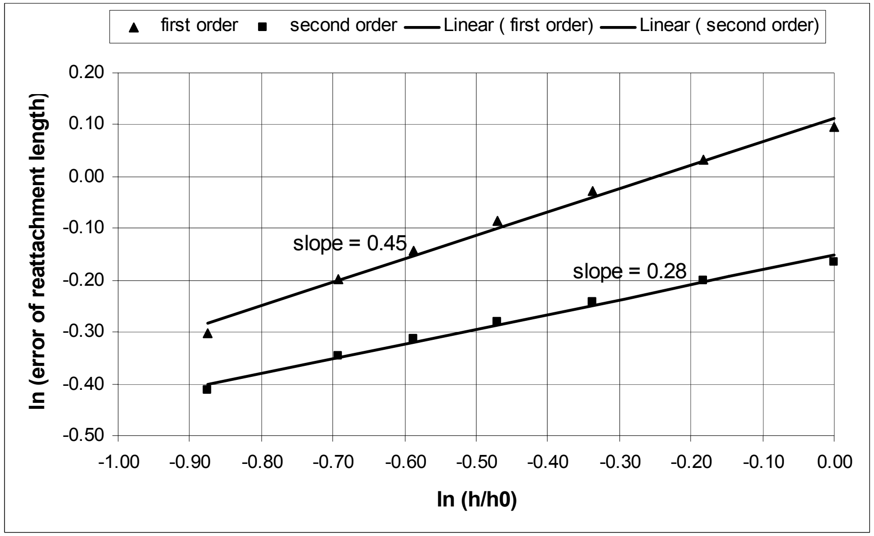


Grid Convergence of Reat. and Sep. Points









Extrapolated reattachment length

first order

Grid - triplets	101-141-181	101-141-201	101-141-241	101-181-241	141-181-241
Power law (p)	11.46 (0.67)	8.77 (1.22)	8.13 (0.26)	7.13 (0.38)	6.54 (0.53)
Approximation Error Spline	5.00	5.07	5.21	5.22	5.22
Polynomial	6.06	6.03	6.05	6.04	6.03
Cubic spline method	5.78	5.80	5.84	5.88	5.88

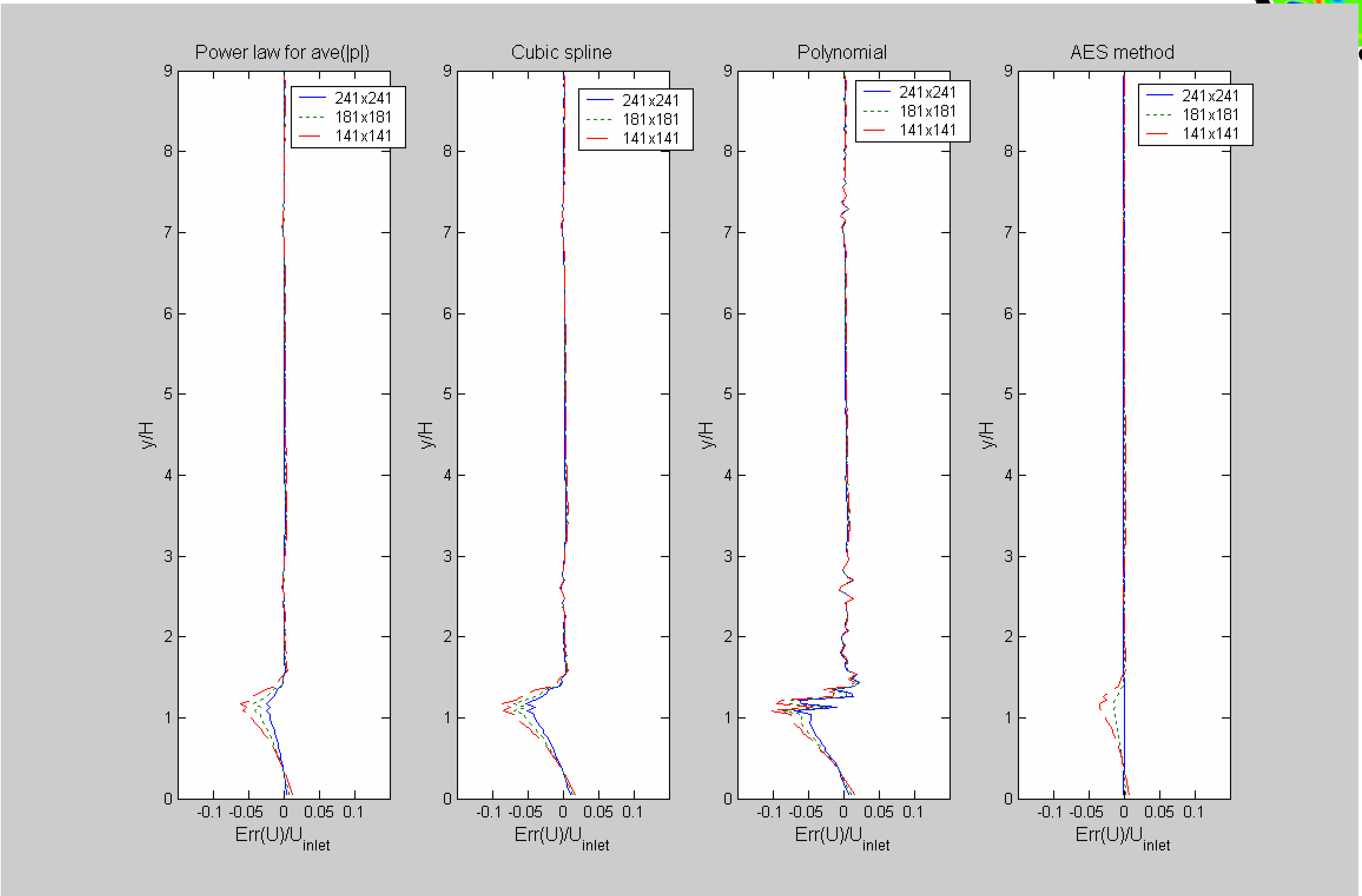
mean = 6.36 $\sigma = 1.50$

Second order

Grid - triplets	101-141-181	101-141-201	101-141-241	101-181-241	141-181-241
Power law (p)	7.38 (-0.48)	7.86 (-0.28)	7.24 (-0.59)	7.15 (-0.69)	7.05 (-0.81)
Approximation Error Spline	6.54	6.50	6.41	6.40	6.40
Polynomial	6.01	6.04	5.87	5.78	5.69
Cubic spline method	6.20	6.19	6.07	5.99	5.99

mean = 6.44 $\sigma = 0.58$

Relative error in velocity profile at x/H=3.0



141-181-241, second order

Introduction to Oscillatory Convergence

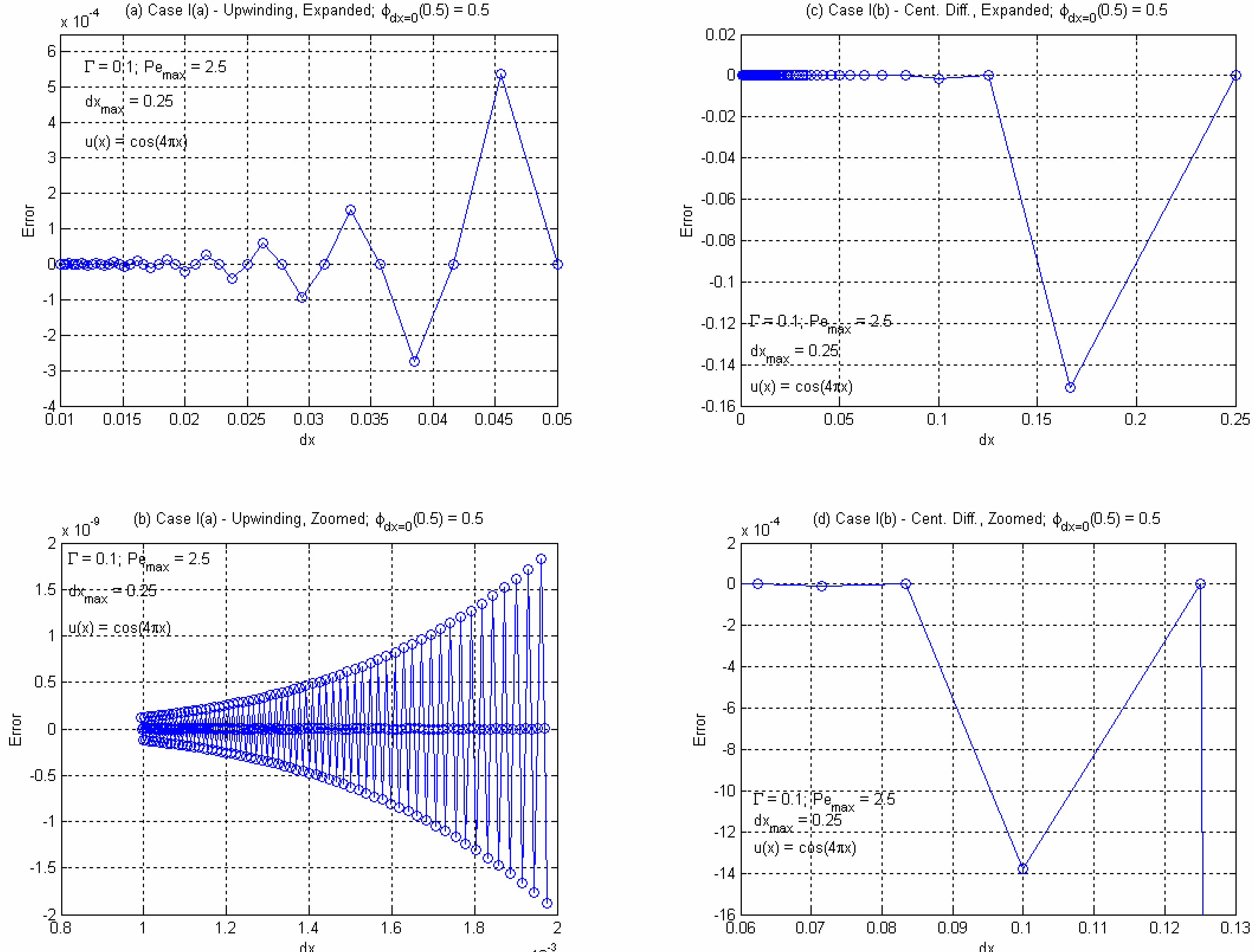
(1) Does oscillatory convergence occur?

(2) What happens in the asymptotic range? Asymptotic range means the leading error term dominates in the Taylor expansion of the error function.

(3) Is Richardson extrapolation applicable to oscillatory converging cases?

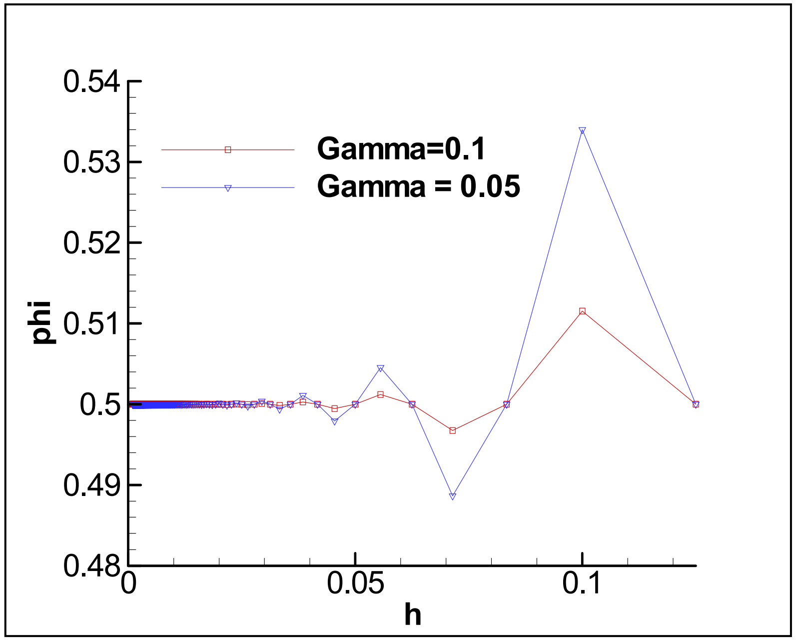
(4) How can one best make use of results from an oscillatory converging computation?

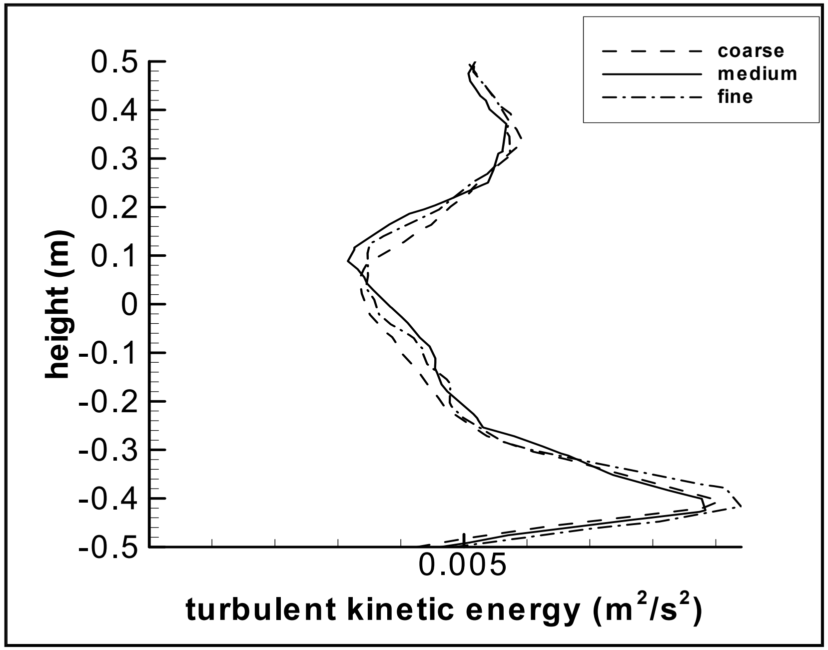
Examples of Oscillatory Convergence



Error plots in both expanded and zoomed form

Examples of Oscillatory Convergence





$$(u\phi)_x = (\Gamma \phi_x)_x + \lambda\phi$$

$\psi(0) = 0$ $\quad u = \cos(4\pi x)$

$\psi(1) = 1$ $\quad$ X=0.5

Convection--First order
Diffusion--2nd order

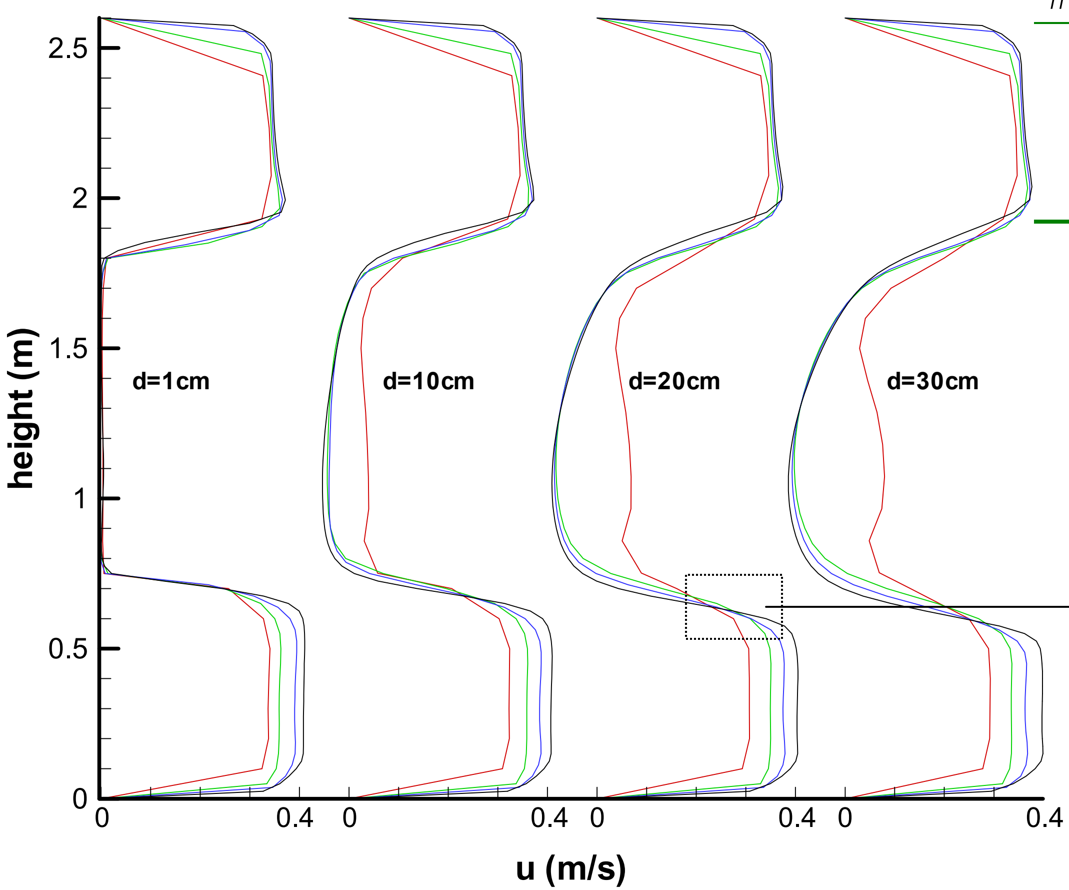
Turbulent kinetic energy along a vertical line 20cm downstream of a human manikin in a wind tunnel (using Fluent and Standard k-ε turbulence model, Li et al., 2003)

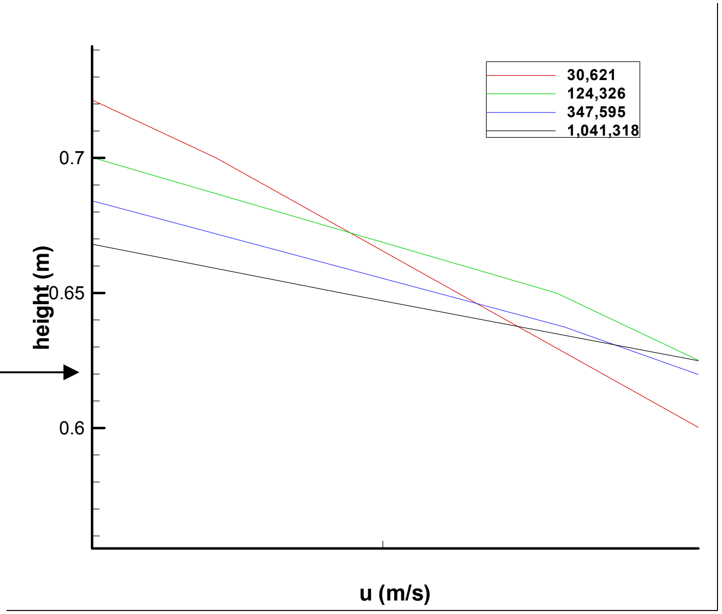
Oscilatory Grid Convergence

Case : Human Exposure (Li et at., 2003)

H= 0.65m

# grid node	u (m/s) (Interpolated)	Δu_{fc}
30,621	0.218	0.023
127,326	0.241	-0.035
347,595	0.206	-0.016
1,041,318	0.190	

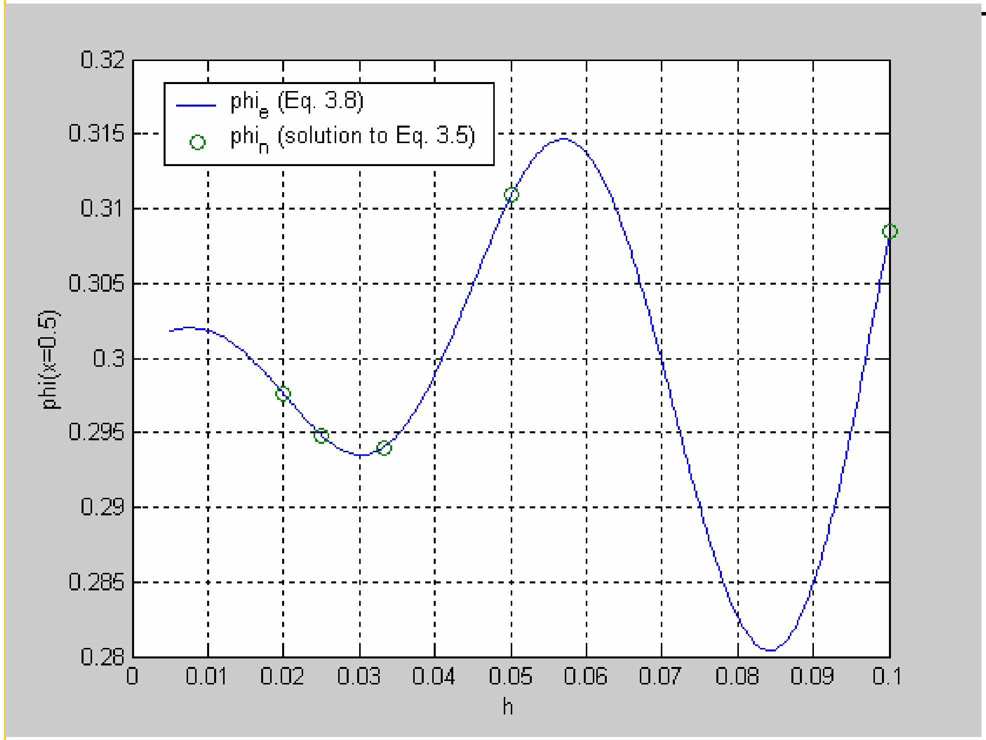




Construction of Oscillatory Convergence

$$u\phi_x = \phi_{xx} - \lambda\phi \qquad \text{with } \phi(0)=0 \quad \phi(1)=1$$

$$-a_i\tilde{\phi}_{i-1} + b_i\tilde{\phi}_i - c_i\tilde{\phi}_{i+1} = 0$$



$$b_i = a_i + c_i + \lambda \qquad (1)$$

Assume $a_i = c_i + \dfrac{u_i}{h}$ (2)

$$E_i \equiv \tilde{\phi}_i - \phi_i = g_i f$$

$$f = h^p \cos(kh)$$

$$g_i = \beta(i-1)(nx-i)$$

$$-a_i(\phi_{i-1} + g_{i-1}f) + b_i(\phi_i + g_i f) - c_i(\phi_{i+1} + g_{i+1}f) = 0 \qquad (3)$$

a_i, b_i and c_i can be solved by combining (1-3)

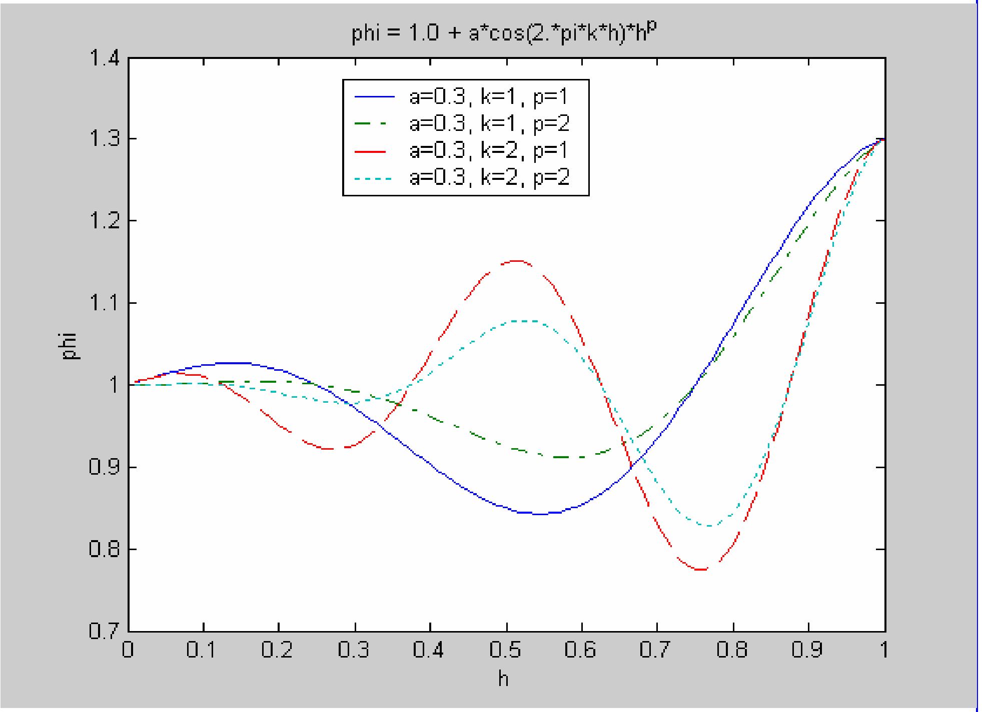
Modeled Equations for Oscillatory Convergence

$$\phi(h) = \phi_0 + a\cos(2\pi kh)h^p$$

$$\phi(h) = \phi_0 + a(1 - e^{-bh})\cos(2\pi kh)h^p$$

$$\phi(h) = \phi_0 \underset{\phi_0}{+} a\log(1+h)\cos(2\pi kh)h^p$$

a	0.2, 0.4, 0.6
k	0.5, 1(for oscillatory); 0.01, 0.02 (for monotonic)
p	1, 2, 3
b	1
	1.0



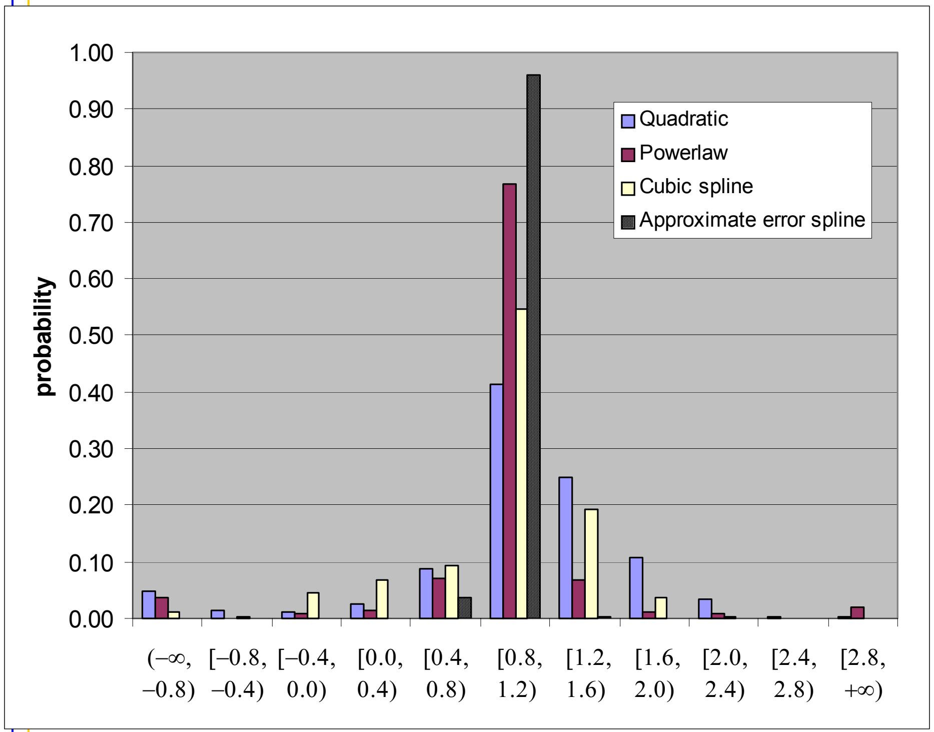
Assessment of above methods

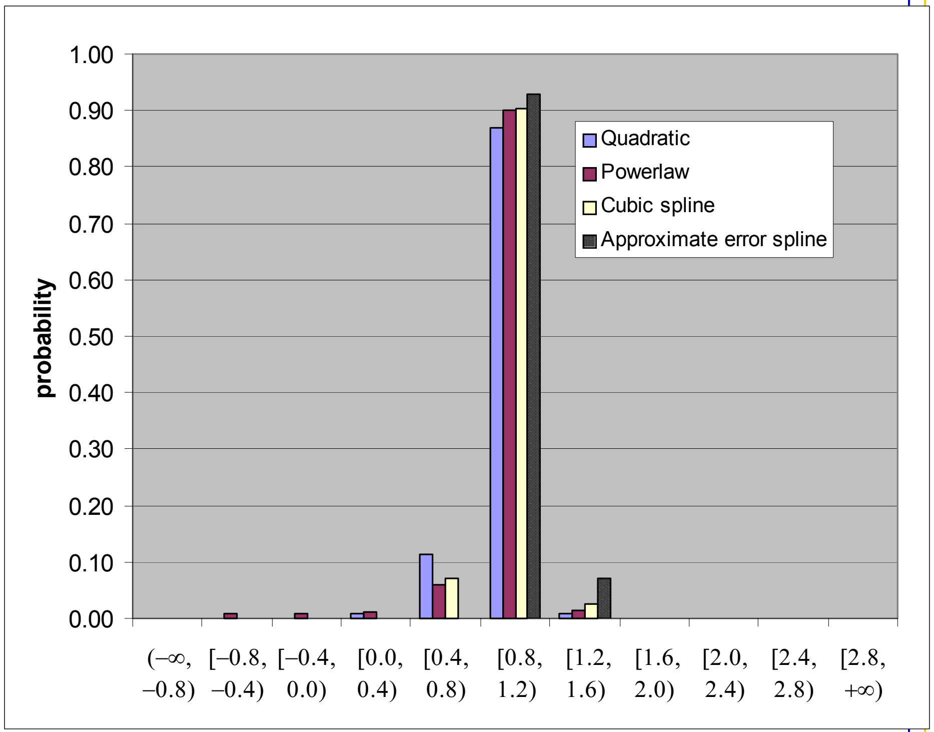
1. Confidence level for the extrapolated value to be in the interval of Phi_exa±20% error.

2. The L^2 norm of the true error defined by

$$L^2 = \left(\sum_{cases} (\phi_0 - \phi(0))^2 \right)^{1/2}$$

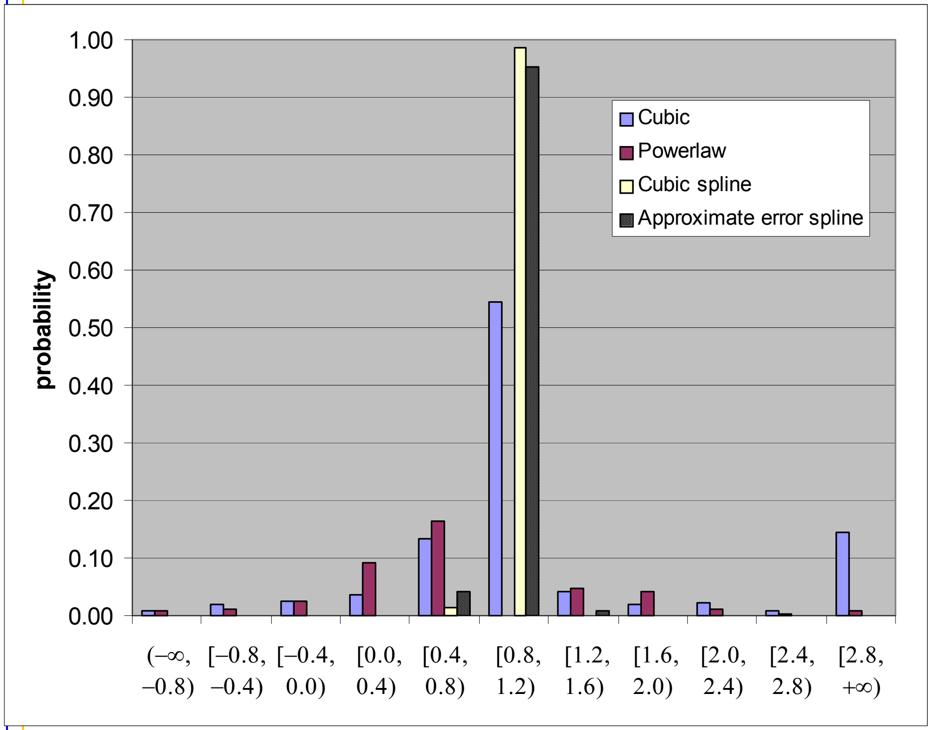
Assessment of above methods --- continued 1



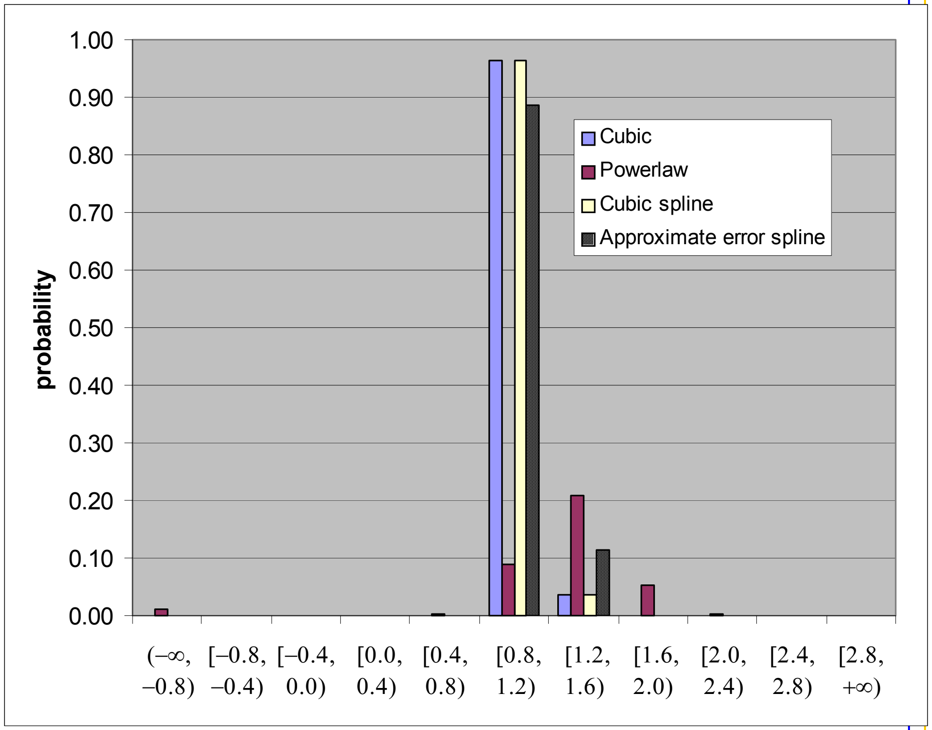


with 3-point oscillatory samples **with 3-point monotonic samples**

Assessment of above methods --- continued 2



with 4-point oscillatory samples



with 4-point monotonic samples

Assessment of above methods --- continued 3

			Polynomial	Powerlaw	Cubic spline	Approximate error spline
3 points	Oscillatory	probability in [0.8, 1.2)	41%	77%	55%	96%
		norm	15.3	25.2	8.10	1.38
	Monotonic	probability in [0.8, 1.2)	87%	90%	90%	93%
		norm	2.62	3.55	2.01	1.69
4 points	Oscillatory	probability in [0.8, 1.2)	54%	0%	99%	95%
		norm	37.2	112	0.85	1.48
	Monotonic	probability in [0.8, 1.2)	96%	9%	96%	89%
		norm	1.43	353	1.27	2.20

Conclusions

- The oscillatory convergence behavior can occur in the asymptotic region

- By way of manufactured solution to FD equations and constructing a corresponding finite difference scheme, it is shown that there exist infinitely many finite difference methods that will exhibit oscillatory convergence even in the asymptotic range.

- Using the data obtained from the model error equations, the newly proposed approximate error spline (AES) method performs superior to the others, the commonly used power-law method ranking the second best.

Proposed Error Transport Equation Method (ETE)

- Richardson extrapolation (RE)
  - Popular, relatively reliable (+)
  - At least three sets of grid, expensive (-)
  - Difficult to identify asymptotic range (-)
  - Does not work for oscillatory grid convergence (-)

- Error transport method (ETE)
  - No extra effort in grid generation (+)
  - Can be solved using the same scheme (+)
  - Can be used as a post-processing tool for steady problems(+)
  - Additional recourses for code development (-)
  - Difficulty in determining source term of ETE (-)
  - Reliability still under investigation (-)

Literature review of ETE

- Roache (1993 & 1998)
- Van Straalen et al. (1995)
- Zhang et al. (1997)
- Wilson & Stern (2001)
- Celik & Hu (2002, 2003)
- Qin & Shih (2003)

Error Transport Equation (ETE)

Non-linear: $L(\phi) = 0$

Linearized: $L_h(\tilde{\phi}) = 0$ (1)

$L_h(\phi) = R = \tau(\phi)$ (2)

L : differential operator (PDE)
L_h : difference operator (FDE)
ϕ : exact solution to PDE
ϕ~ : numerical solution
R : residual

error is defined as: $\varepsilon = \phi - \tilde{\phi}$

ETE: $L_h(\varepsilon) \equiv L_h(\phi) - L_h(\tilde{\phi}) = \tau(\phi)$

τ represents the truncation error of a discretized equation, i.e. the *error source term*

Error Transport Equation Applied to Linearized Pendulum Problem

ETE solves the following two additional equations for errors in the velocity $E^{(V)}$ and the angle $E^{(\theta)}$, respectively:

$$E_{n+1}^{(V)} = E_n^{(V)} + h\left[E_n^{(\theta)} \frac{\partial F}{\partial \theta} + E_n^{(V)} \frac{\partial F}{\partial V} \right] + \frac{h^2}{2} \frac{\partial^2 V}{\partial t^2}$$

$$E_{n+1}^{(\theta)} = E_n^{(\theta)} + h\left[E_n^{(V)} \frac{\partial G}{\partial V} + E_n^{(\theta)} \frac{\partial G}{\partial \theta} \right] + \frac{h^2}{2} \frac{\partial^2 \theta}{\partial t^2}$$

Table: Analysis of the pendulum problem: L=0.2484 m, g=9.8066 m/s^2, $\theta(0) = 45^o$.
After 5 seconds $\theta_{exact}^{linear} = 45^o$, $\theta_{exact}^{non-lin.}$=16.177^o; observed order from RE, p=1.21

$h = \Delta t$ (ms)	θ_{num}(deg.)	E_{num}(deg.)	θ_{ext}(deg.)	E_a^{RE}	E_a^{ETE}
4	66.77	-21.77	42.87	-21.03	-26.26
2	54.82	-9.82	44.52	-9.06	-10.81
1	49.67	-4.67			-4.90

Example: a fully implicit method

$$\mathrm{L}(\phi) = \phi_t + (u\phi)_x - (\Gamma \phi_x)_x - S_P\phi - S_C = 0$$

$$(a_P + a_P^o - \overline{S}_P \Delta x)\widetilde{\phi}_P - a_W \widetilde{\phi}_W - a_E \widetilde{\phi}_E - \overline{S}_C \Delta x - a_P^o \widetilde{\phi}_P^o = 0 \qquad (1)$$

$$(a_P + a_P^o - \overline{S}_P \Delta x)\phi_P - a_W \phi_W - a_E \phi_E - \overline{S}_C \Delta x - a_P^o \phi_P^o = \tau(\phi) \qquad (2)$$

τ can be obtained by Taylor Series expansion about point P

Eq. (2) – Eq. (1) → ETE:

$$(a_P + a_P^o - \overline{S}_P \Delta x)\varepsilon_P - a_W \varepsilon_W - a_E \varepsilon_E - \overline{S}_C \Delta x - a_P^o \varepsilon_P^o = \tau(\phi)$$

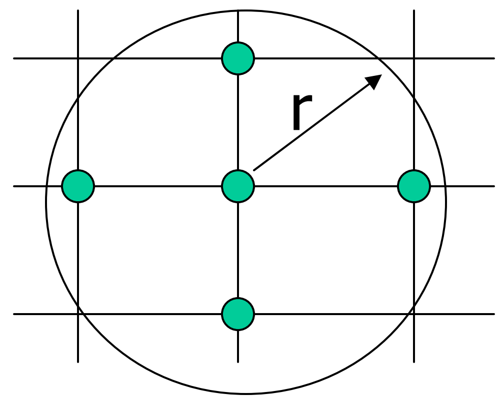
where

$$\tau(\phi) = -\sum_{m=1}^{\infty} \frac{\Delta x^{m-1}}{m!}\left((-1)^m a_W + a_E\right)\phi_{x,(m)} - \sum_{n=1}^{\infty} (-1)^n \frac{\Delta t^n}{n!\,\Delta x} a_P^o \phi_{t,(n)}$$

Generalized Derivation of Error Source

$$\begin{pmatrix}\text{implicit}\\\text{coefficient}\\\text{matrix}\end{pmatrix}\begin{pmatrix}\phi^{new}\end{pmatrix} = \begin{pmatrix}\text{explicit}\\\text{coefficient}\\\text{matrix}\end{pmatrix}\begin{pmatrix}\phi^{old}\end{pmatrix}$$

Influence circle →



Need to know:
1. Access to the coefficient matrix
2. Influence circle (or radius)

Generalized Derivation of Error Source

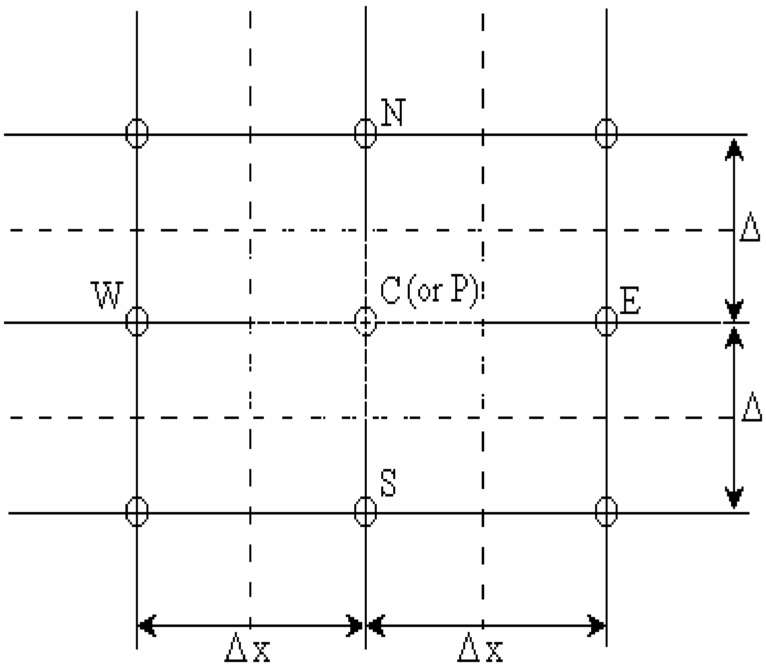
$$L_h(\tilde{\phi}) \equiv a_{C,imp}\tilde{\phi}_P - \sum a_{nb,imp}\tilde{\phi}_{nb} - (a_{C\exp}\tilde{\phi}_P^o + \sum a_{nb,\exp}\tilde{\phi}_{nb}^o) = 0$$

$$L_h(\phi) \equiv a_{C,imp}\phi_P - \sum a_{nb,imp}\phi_{nb} - (a_{C\exp}\phi_P^o + \sum a_{nb,\exp}\phi_{nb}^o) = \tau(\phi)$$

$$a_{C,imp}\varepsilon_P - \sum a_{nb,imp}\varepsilon_{nb} = (a_{C\exp}\varepsilon_P^o + \sum a_{nb,\exp}\varepsilon_{nb}^o) + \tau(\phi)$$

$$\tau(\phi) = -\sum_{m=1}^{\infty}\frac{\Delta x^{m-1}}{m!\,\Delta y}\left((-1)^m a_{W,imp} + a_{E,imp}\right)\phi_{x,(m)}$$
$$-\sum_{m=1}^{\infty}\frac{\Delta y^{m-1}}{m!\,\Delta x}\left((-1)^m a_{S,imp} + a_{N,imp}\right)\phi_{y,(m)}$$
$$-\sum_{m=1}^{\infty}\frac{\Delta x^{m-1}}{m!\,\Delta y}\left((-1)^m a_{W,exp} + a_{E,exp}\right)\phi_{x,(m)}$$
$$-\sum_{m=1}^{\infty}\frac{\Delta y^{m-1}}{m!\,\Delta x}\left((-1)^m a_{S,exp} + a_{N,exp}\right)\phi_{y,(m)}$$
$$-\sum_{n=1}^{\infty}(-1)^n\frac{\Delta t^n}{n!\,\Delta x\Delta y}a_P^o\phi_{t,(n)}$$

Example: 2D, five point stencil



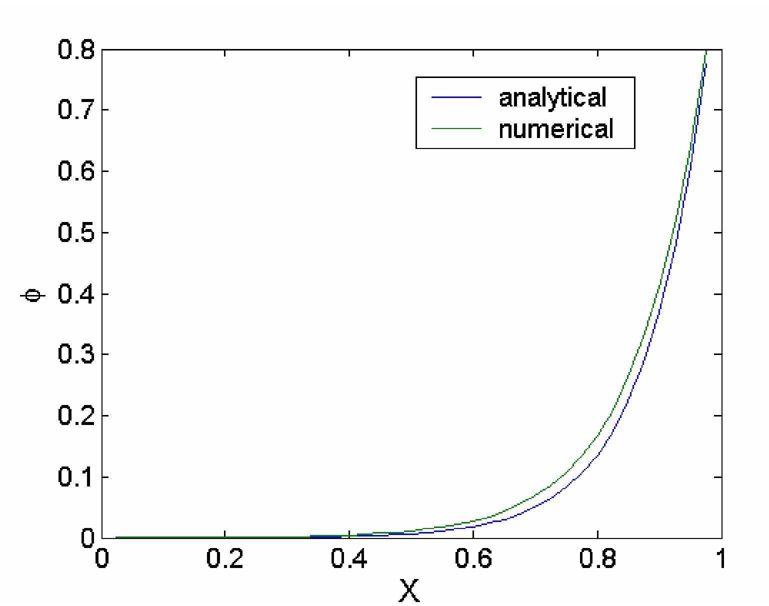
1D Convection Diffusion

$$u\phi_x - \Gamma\phi_{xx} = 0$$

$$0 \le x \le 1$$

B.C. $\quad$ at $x = 0, \ \ \phi = 0$

at $x = 1, \ \ \phi = 1$



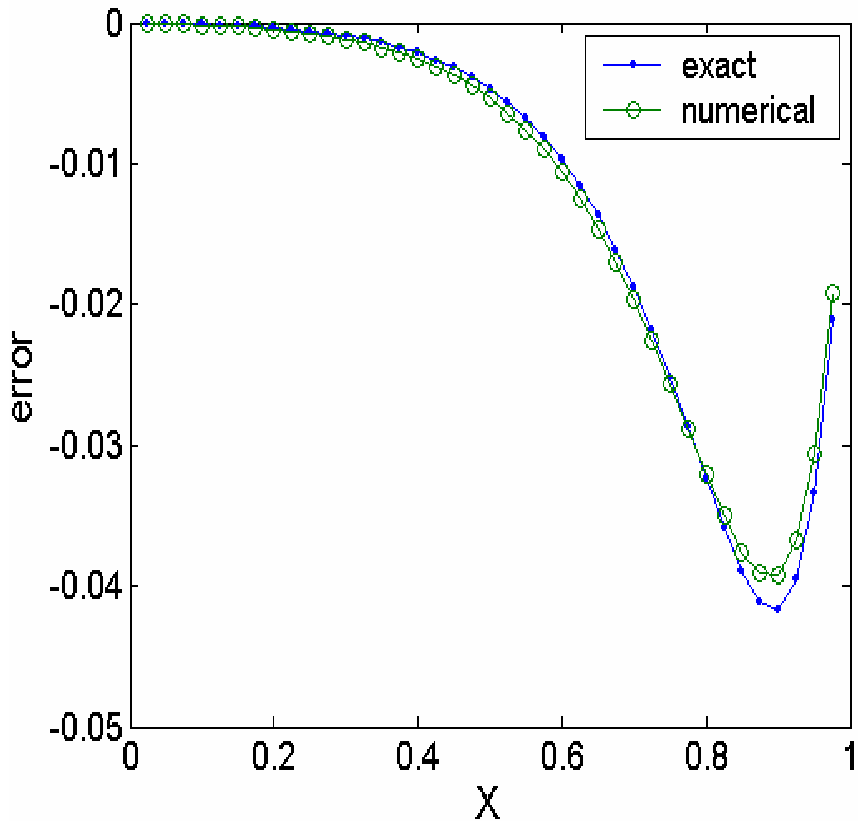
Analytical solution

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp(P_e x / L) - 1}{\exp(P_e) - 1}$$

where $\quad P_e = uL / \Gamma$

1D Convection Diffusion

Predicted error



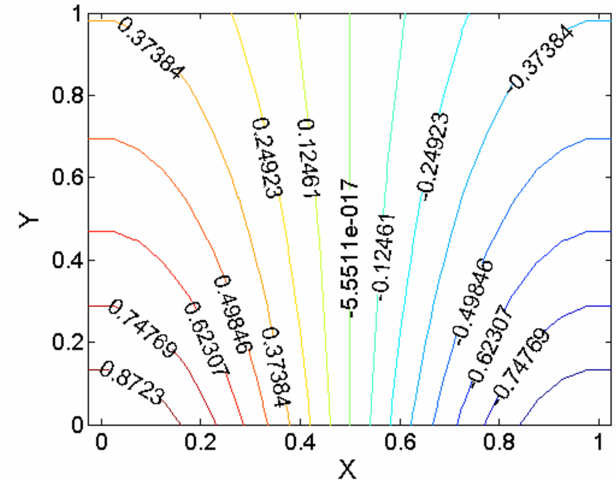
- 1^{st} order Upwind for convection and central differencing for diffusion
- Derived tau used with numerical solution
- Central differencing used to evaluate tau-terms

2D Poison Equation

$$\phi_{xx} + \phi_{yy} = \phi + g(x, y)$$

where $g(x, y) = -\pi^2 \exp(-y)\cos(\pi x)$

domain: $-1 \le x \le 1,\ -1 \le y \le 1$



B.C.

$$\text{at } x = 0,\ \ \phi_x = 0$$

$$\text{at } x = 1,\ \ \phi_x = 0$$

$$\text{at } y = 0,\ \ \phi = \cos(\pi x)$$

$$\text{at } y = 1,\ \ \phi = \exp(-1)\cos(\pi x)$$

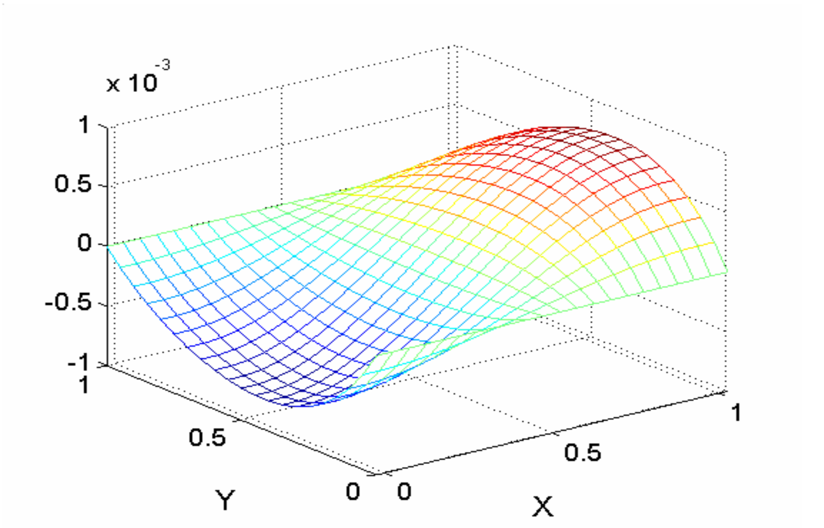
Analytical solution

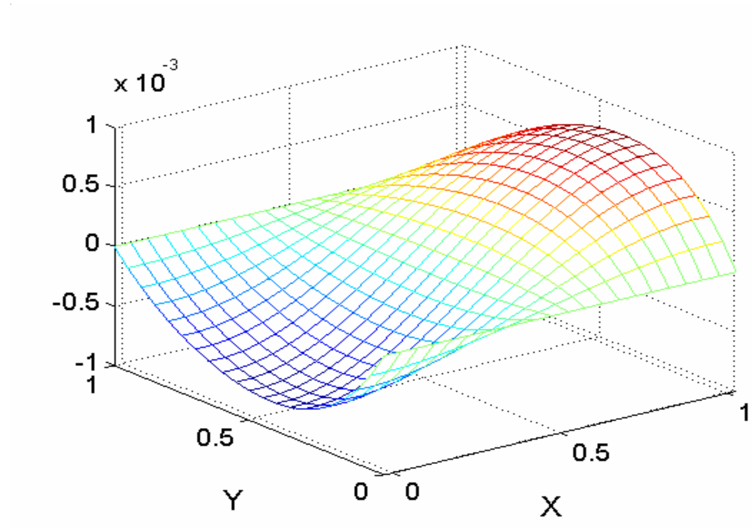
$$\phi(x, y) = \exp(-y)\cos(\pi x)$$

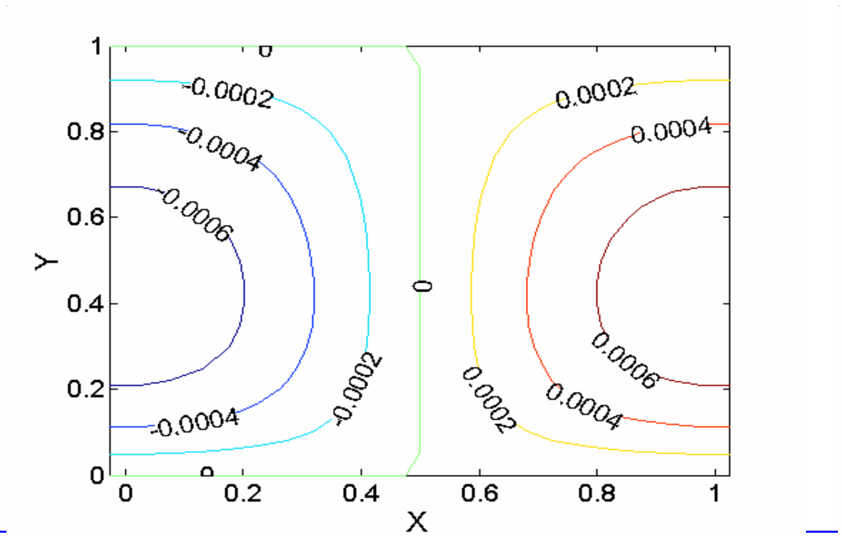
2D Poison Equation: Central difference Scheme

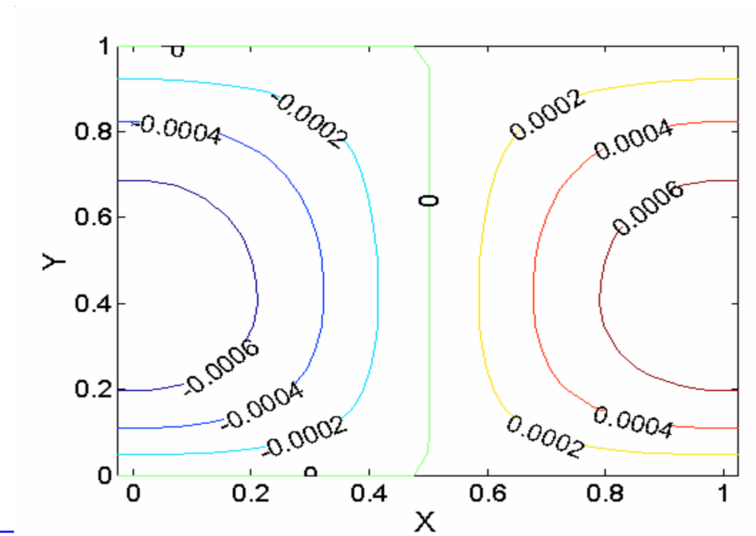
Exact error

ETE error









2D Steady Convection Diffusion

$$u\phi_x + v\phi_y - \Gamma(\phi_{xx} + \phi_{yy}) = 0$$

$$\text{domain: } 0 \le x \le 1, \quad 0 \le y \le 1$$

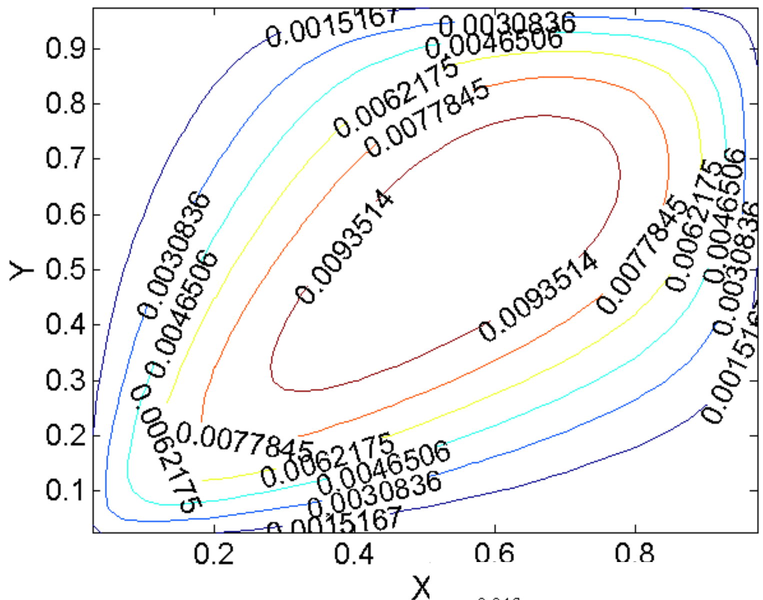
Analytical solution

$$\phi(x,y) = \frac{\dot{m}}{2\pi\Gamma} \exp\left(\frac{Vx'}{2\Gamma}\right) \mathrm{K}_0\left(\frac{r}{2\Gamma}\right)$$

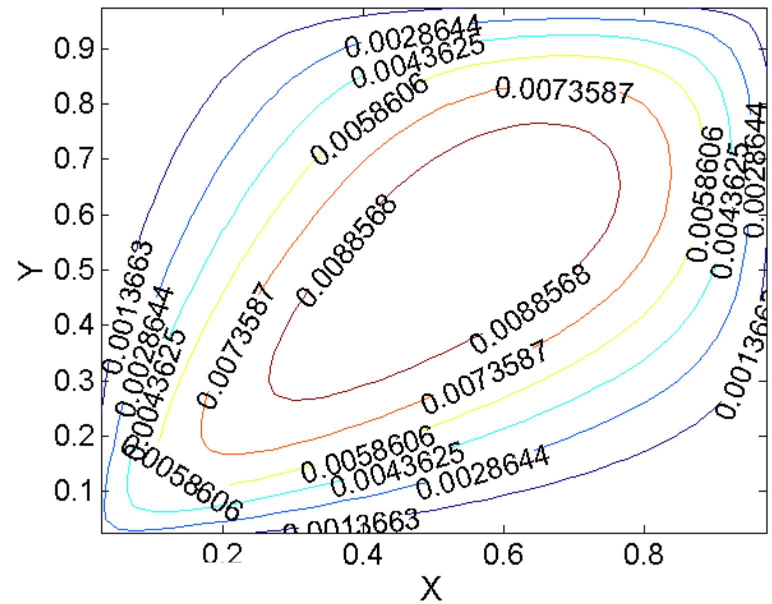
Dirichlet B.C. is imposed using the analytical solution

2D Steady Convection Diffusion

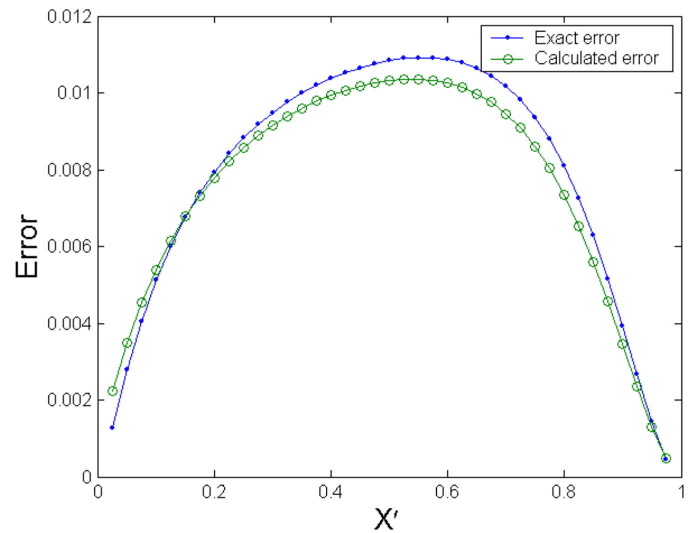
1st order Upwind scheme



Exact error



Calculated error



Line plot along diagonal

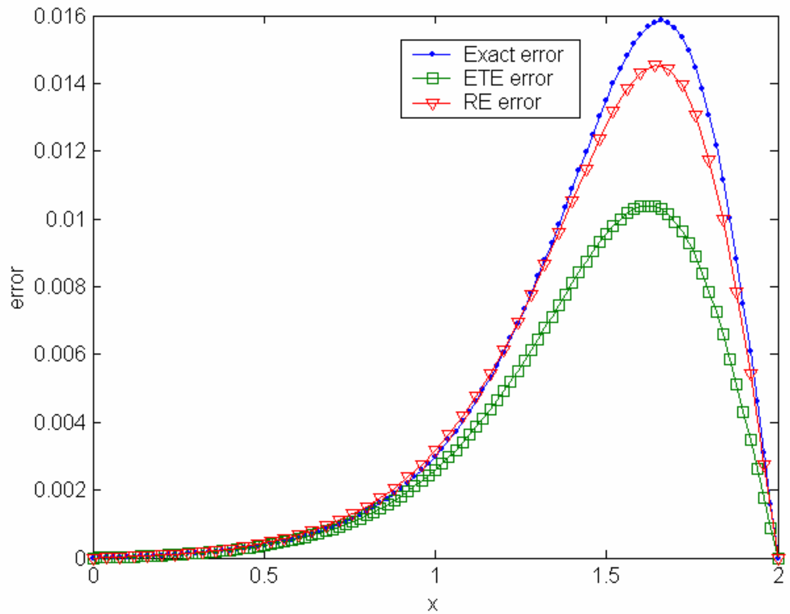
Nonlinear Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2}$$

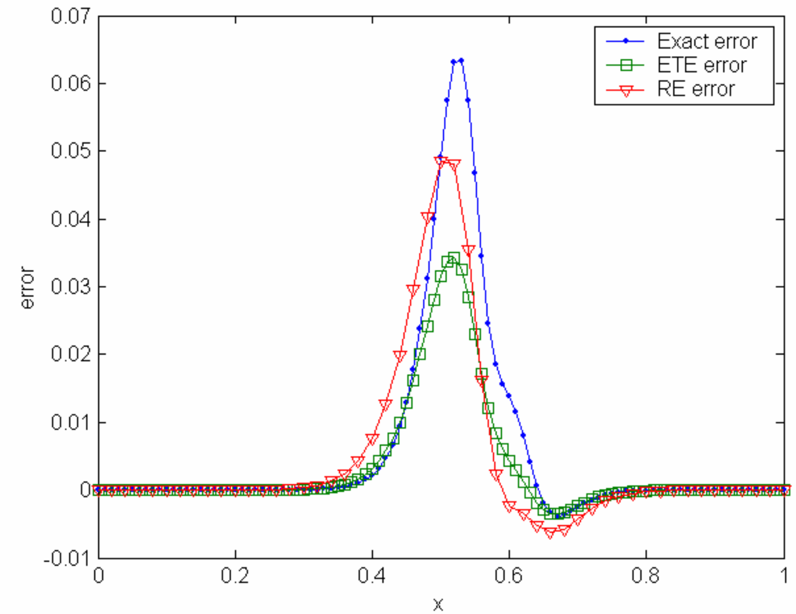
1st order upwind

Steady case b.c.: u(0,t)=1, u(L,t)=0, fully implicit, upwind, Pe=10

Transient case b.c. u(t,0)=f(t,0), u(t,1)=f(t,1),
i.c. u(0,x)=f(0,x), Fully explicit, upwind, t=0.5



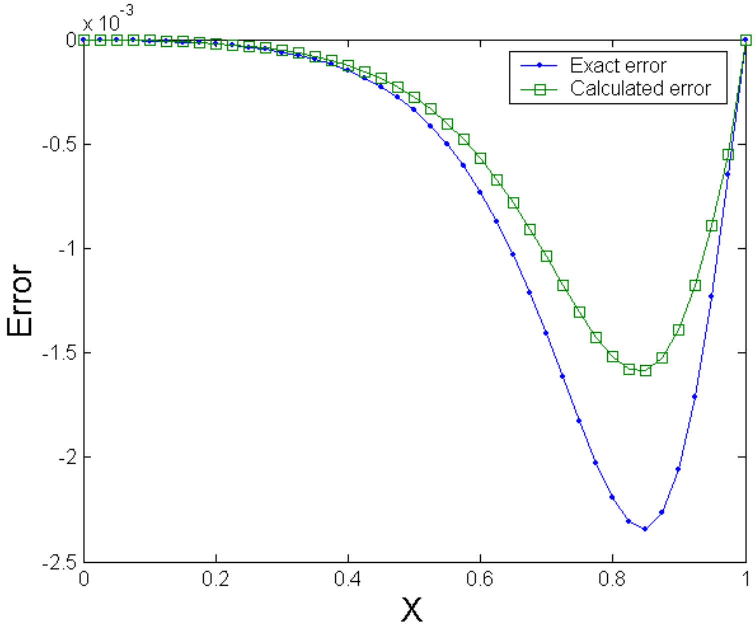
Steady case



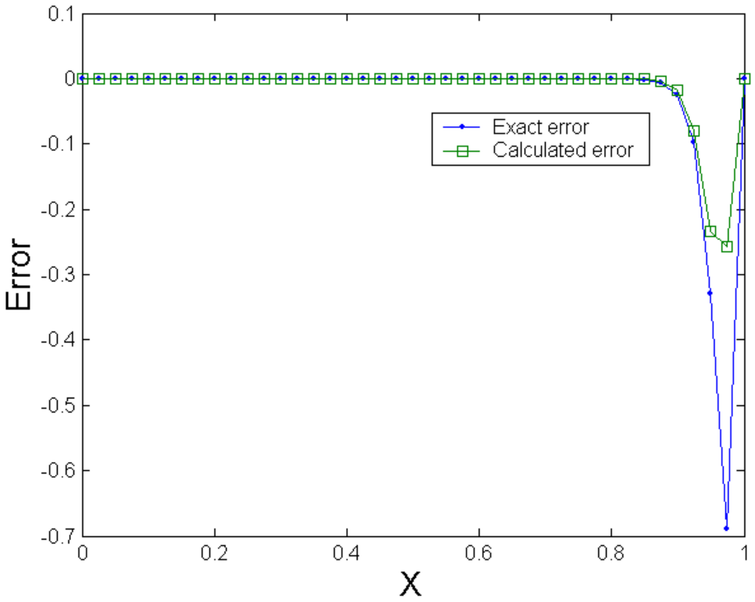
Transient case

Nonlinear Burger's equation (Cont'd)

Central difference scheme, exact error vs. calculated error

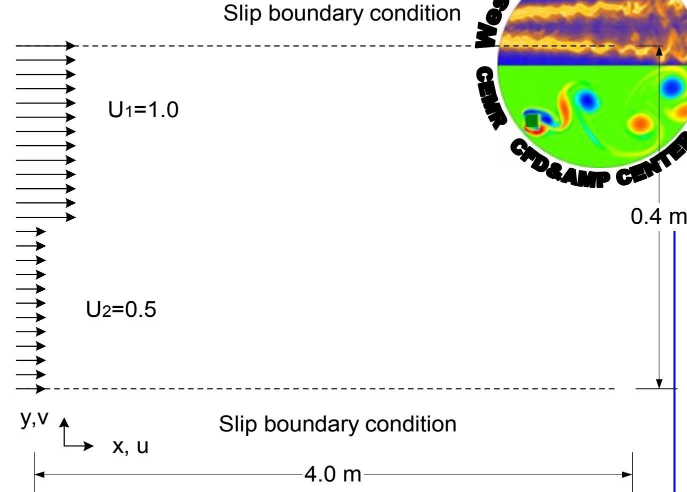


Re=10

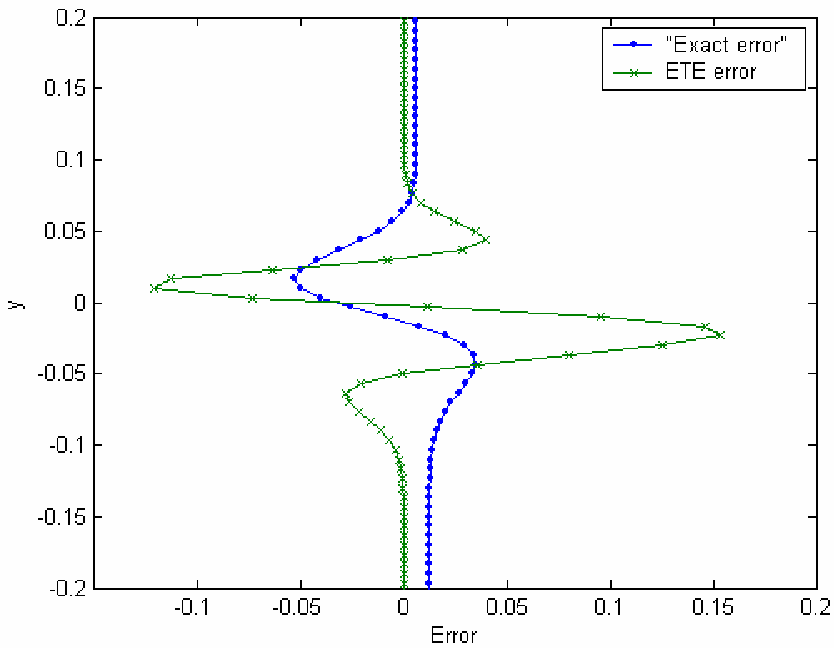


Re=60

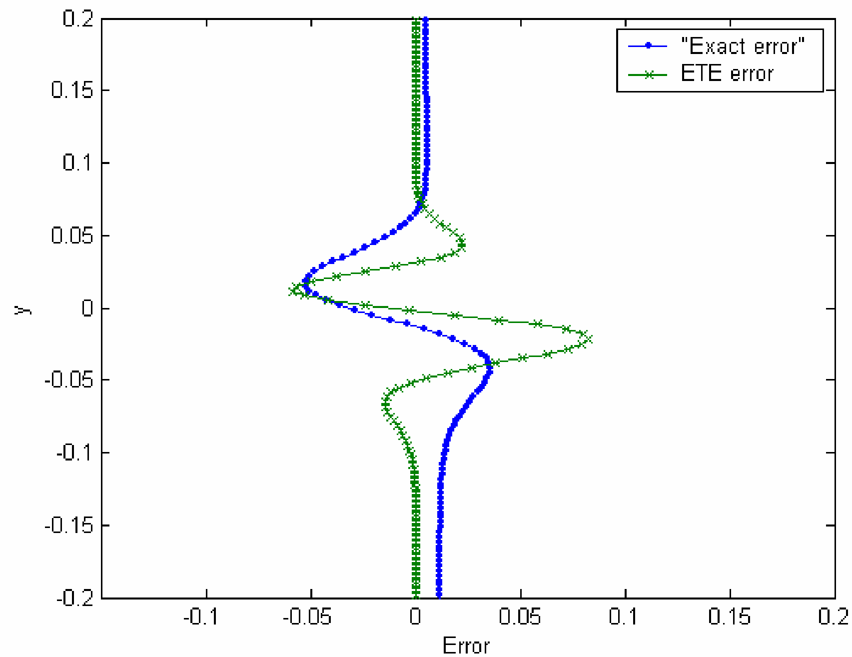
Application on a N-S Solver



2D mixing layer



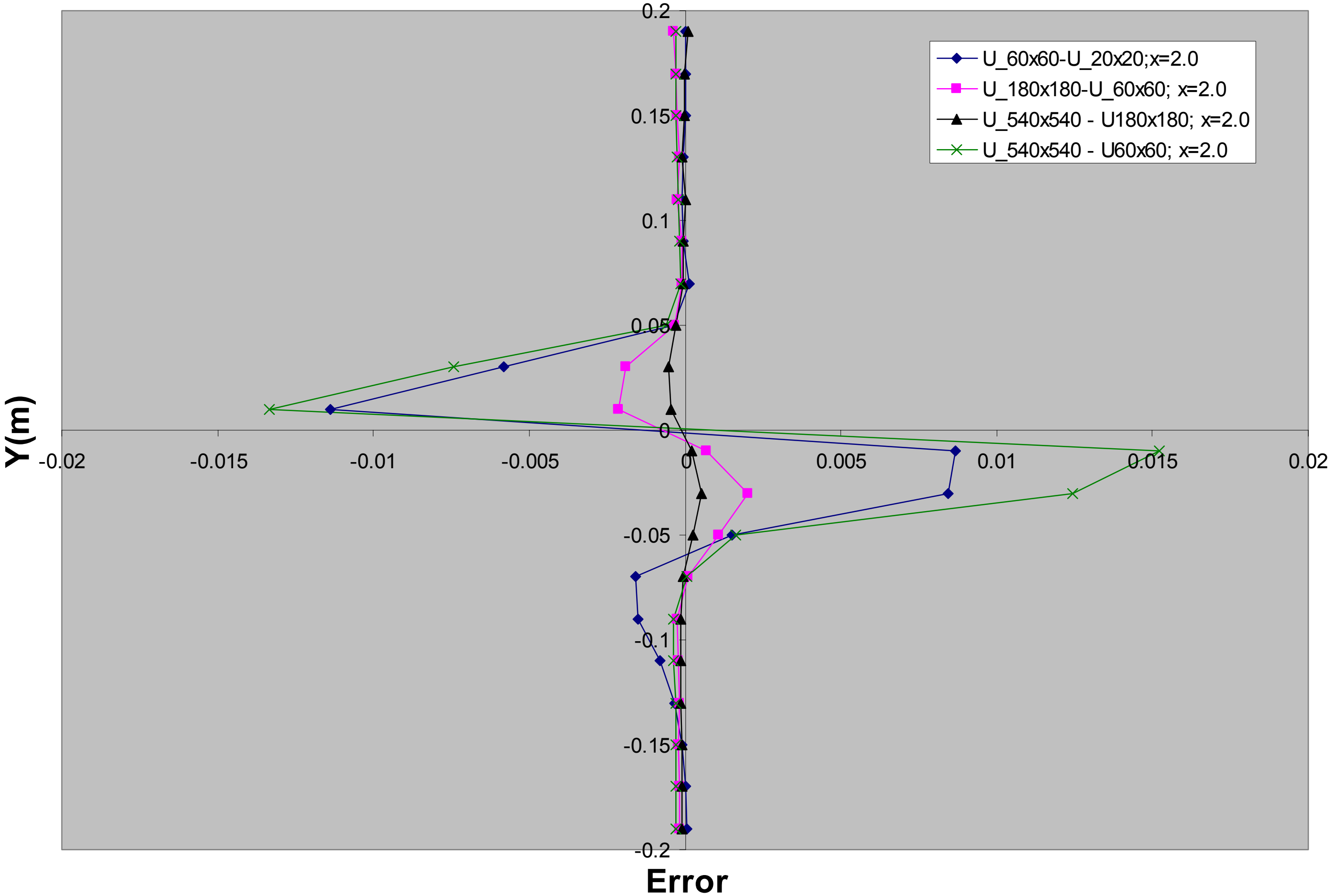
60x60



12x120

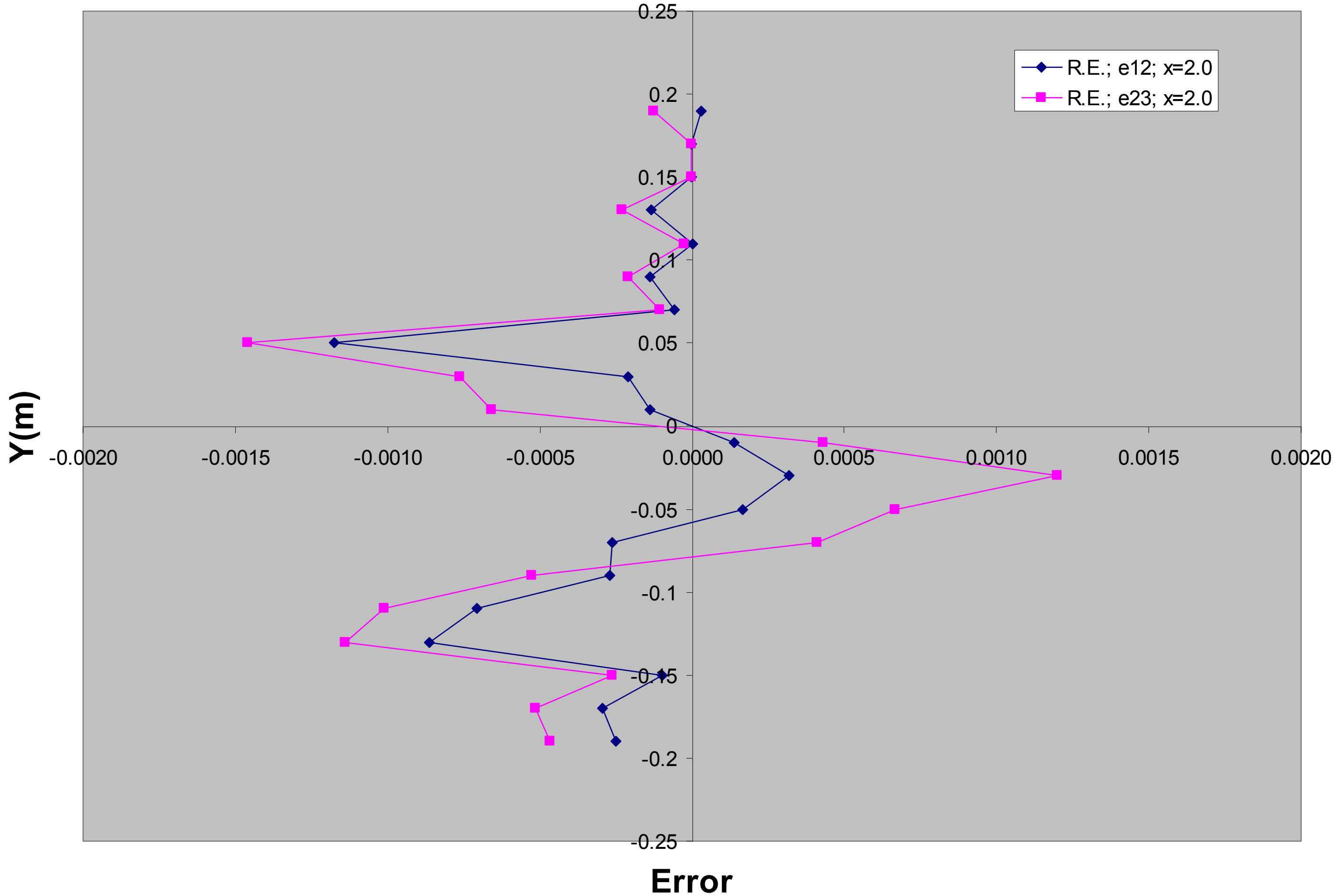
Application on a N-S solver: calculated error

Use grid independent solution as "exact" solution



Application on a N-S solver:

RE results: predicted error is too small and oscillating



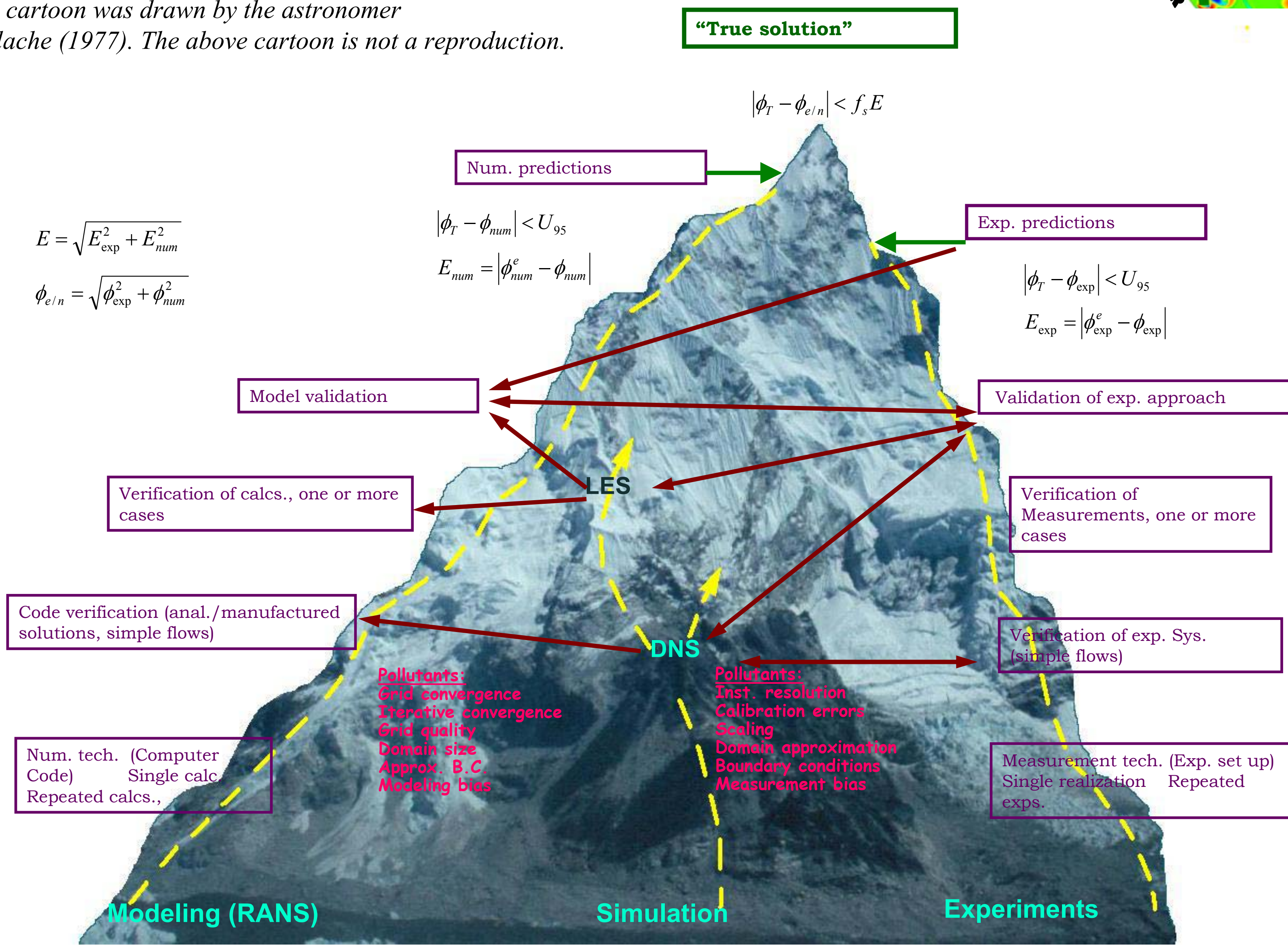
Conclusion for RE & ETE

- ETE works as good as and sometimes better than the RE for simple steady flow problems. Further, for steady calculation ETE can be used as a post-processor tool to save computational expense

- For transient problems, the quality of ETE results are dependent on the primary field variables; a dissipative schemes will lead to large errors in the ETE calculation

- Coefficient-based ETE is a fairly general formulation and can be adopted in the computer codes without much effort; The same solver can be used to calculate the error as that for the primitive variables.

***Acknowledgement**: This cartoon was created after seeing a similar cartoon in the book <u>Turbulence</u> by U. Frisch (1997). The original cartoon was drawn by the astronomer Philippe Delache (1977). The above cartoon is not a reproduction.*



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