Pseudospectral methods - a finite difference introduction to the non-periodic case

Bengt Fornberg

Department of Applied Mathematics
University of Colorado
Boulder, CO 80309

INTRODUCTION OF SPECTRAL METHODS VIA ORTHOGONAL FUNCTIONS

Approximate $u(x) \approx \sum_{k=0}^{N} a_k \phi_k(x)$; Key questions:

FUNCTION CLASS TO CHOOSE $\phi_k(x)$, $k = 0, 1, 2, \ldots$ FROM	HOW TO DETERMINE THE EXPANSION COEFFICIENTS a_k.

Requirements:

1. $\sum_{k=0}^{N} a_k \phi_k(x)$ must converge fast for smooth functions
2. Given a_k, there must be a fast way to determine b_k such that $\frac{d}{dx}\left(\sum_{k=0}^{N} a_k \phi_k(x) \right) = \sum_{k=0}^{N} b_k \phi_k(x)$
3. It must be fast to convert between coefficients a_k and values of the sum at some set of nodes x_i, $i=0,1,\ldots,N$

Main techniques:

1. Tau
2. Galerkin
3. **Collocation (PS)**

PERIODIC PROBLEMS: TRIGONOMETRIC EXPANSIONS (equivalent to FD limit...)

NON-PERIODIC PROBLEMS: ***ORTHOGONAL POLYNOMIALS***

Next topics to be discussed:

- **What are orthogonal polynomials?**

  Arise in contexts such as
  - Gaussian integration formulas
  - Singular Sturm-Liouville eigen-problems
  - Approximation theory

- **Why are they any good?**

  FD viewpoint that again will offer the best insight, and source for method enhancements.

Different bases for polynomials $P_N(x)$ of degree N:

- **Powers of x:**

  $1, x, x^2, x^3, \ldots, x^N$. Not orthogonal; interpolation terribly ill conditioned.

- **Chebyshev polynomials:**

  $T_n(x) = \cos(n \arccos x)$

  $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1, \ldots$

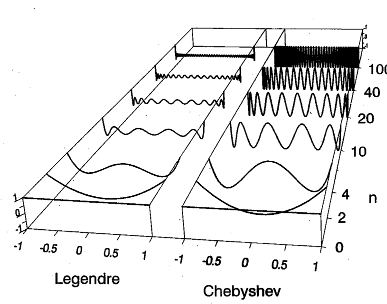
  Orthogonality: $\int_{-1}^{1} \frac{T_m(x)\, T_n(x)}{\sqrt{1-x^2}} dx = 0$ (if $m \neq n$)

- **Legendre polynomials:**

  $L_n(x)$

  $L_0(x) = 1$, $L_1(x) = x$, $L_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, \ldots$

  Orthogonality: $\int_{-1}^{1} L_m(x)\, L_n(x)\, dx = 0$ (if $m \neq n$)



	LEGENDRE	CHEBYSHEV	JACOBI
Weight function $W(x)$	1	$\frac{1}{\sqrt{1-x^2}}$	$(1-x)^\alpha (1+x)^\beta$, $\alpha > -1$, $\beta > -1$; $\alpha = \beta = 0$ Legendre; $\alpha = \beta = -\frac{1}{2}$ Chebyshev
Customary normalization	$L_n(1) = 1$	$T_n(1) = 1$	$p_n(1) = \binom{n+\alpha}{n}$
First few polynomials	1 x $\frac{3}{2}x^2 - \frac{1}{2}$ $\frac{5}{2}x^3 - \frac{3}{2}x$ $\frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}$ $\frac{63}{8}x^5 - \frac{35}{4}x^3 + \frac{15}{8}x$ ⋮	1 x $2x^2 - 1$ $4x^3 - 3x$ $8x^4 - 8x^2 + 1$ $16x^5 - 20x^3 + 5x$ ⋮	1 $\frac{1}{2}(2+\alpha+\beta)x + \frac{1}{2}(\alpha-\beta)$ $\frac{1}{8}(3+\alpha+\beta)(4+\alpha+\beta)x^2 + \frac{1}{4}(\alpha-\beta)(3+\alpha+\beta)x + \frac{1}{8}[(\alpha-\beta)^2 - (4+\alpha+\beta)]$ General n: $2^{-n} \sum_{k=0}^{n} \binom{n+\alpha}{k} \binom{n+\beta}{n-k} (x-1)^{n-k} (x+1)^k$
Orthogonality $\int_{-1}^{1} \Phi_m \Phi_n W dx$	0 $m \neq n$ $\frac{2}{2n+1}$ $m = n$	0 $m \neq n$ π $m = n = 0$ $\frac{\pi}{2}$ $m = n > 0$	0 $m \neq n$ $\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\, n!\, \Gamma(n+\alpha+\beta+1)}$ $m = n$
Three term recursion	$(n+1)L_{n+1} - (2n+1)xL_n + nL_{n-1} = 0$	$T_{n+1} - 2xT_n + T_{n-1} = 0$	$2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)P_{n+1} - [(2n+\alpha+\beta+1)(\alpha^2-\beta^2) + (2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)x]P_n + 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1} = 0$
Differential equation	$(1-x^2)L_n'' - 2xL_n' + n(n+1)L_n = 0$	$(1-x^2)T_n'' - xT_n' + n^2 T_n = 0$	$(1-x^2)P_n'' + [(\beta-\alpha) - (\alpha+\beta+2)x]P_n' + n(n+\alpha+\beta+1)P_n = 0$
First derivative recursion	$L_{n+1}' = (2n+1)L_n + L_{n-1}'$	$\frac{T_{n+1}'}{n+1} = 2T_n + \frac{T_{n-1}'}{n-1}$	$2(2n+\alpha+\beta)(n+\alpha+\beta)(n+\alpha+\beta+1)P_{n+1}' + 2(\alpha-\beta)(n+\alpha+\beta)(2n+\alpha+\beta+1)P_n' - 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1}' = (n+\alpha+\beta)(2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)P_n$

WHY WOULD WE EXPECT EXPANSIONS IN CHEBYSHEV (OR LEGENDRE) POLYNOMIALS TO BE ESPECIALLY SUITABLE?

- Truncated Chebyshev expansions come very close to the optimal polynomial for approximating a function.
- The error in a fast convergent Chebyshev expansion is dominated by the first omitted term - so nearly uniform across the domain.
- If we put our grid points at the extrema of $T_N(x)$ (i.e. at $x_k = -\cos\frac{\pi k}{N}$, $k = 0, 1, \dots, N$), then the interpolating polynomial becomes a very close approximation to the truncated Chebyshev expansion.
- We can then very quickly convert between node values and Chebyshev expansion coefficients (a FCT - Fast Cosine Transform)..

RECALL FROM PREVIOUS LECTURE:

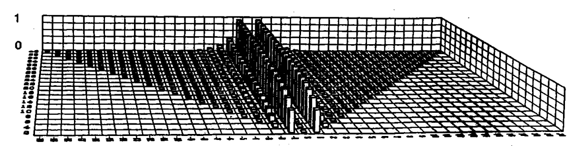
FD approximations to $\frac{\partial}{\partial x}$ (divide weights by h)

Weights:

				$-\frac{1}{2}$	0	$\frac{1}{2}$					2
			$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$				4
		$-\frac{1}{60}$	$\frac{3}{20}$	$-\frac{3}{4}$	0	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$			6
	$\frac{1}{280}$	$-\frac{4}{105}$	$\frac{1}{5}$	$-\frac{4}{5}$	0	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$		8
...	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	...	⋮
... ...	$\frac{1}{4}$	$-\frac{1}{3}$	$\frac{1}{2}$	-1	0	1	$-\frac{1}{2}$	$\frac{1}{3}$	$-\frac{1}{4}$	... ...	∞

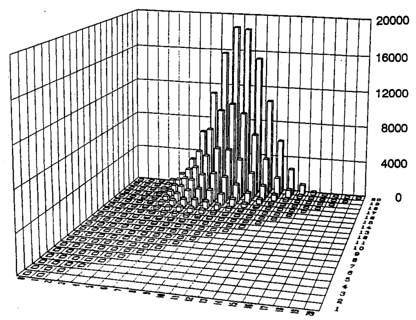
- Weights on equi-spaced grids can be calculated easily by Padé algorithm
- Well-defined limit exists as order tends to infinity
- Limit equivalent to periodic pseudospectral method

Magnitudes of weights for increasing orders:



FIRST DERIVATIVE - ONE-SIDED APPROXIMATIONS

Magnitude of weights shown

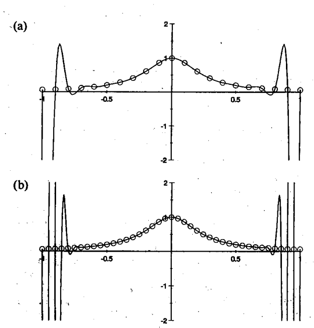


Weights:

$$c^1_{p,j} = \begin{cases} \frac{(-1)^{j+1}}{j}\binom{p}{j} & j = 1, 2, \dots, p \\ -\sum_{k=1}^{p}\frac{1}{k} & j = 0 \end{cases}$$

LIMIT $p \to \infty$ DOES NOT EXIST

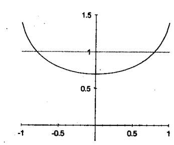
RUNGE PHENOMENON



Results of equi-spaced interpolation on [−1, 1] in the case of (a) $N = 20$ and (b) $N = 40$.

Extensive error analysis available

Errors $|\alpha(x)|^N$ where $\alpha(x)$:



$\alpha(x) = C \cdot e^{-\phi(x)}$,

$\phi(x) = -\frac{1}{2}(1-x)\ln(1-x) - \frac{1}{2}(1+x)\ln(1+x)$

Function that is interpolated affect only the value of the constant C !

ANY REMEDY?

Cluster points towards the ends of the interval !

If we distribute points like $x_k = \cos\frac{\pi k}{N}$, $k = 0, 1, \dots, N$ (or like zeros or extrema of ANY Jacobi polynomial), then

$\phi(x) \equiv 0$ (on [-1,1]) and $\alpha(x) \equiv C$

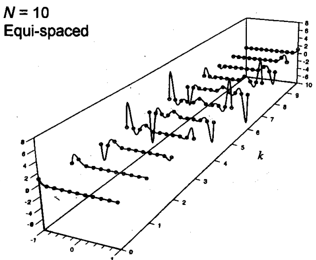
Exactly the same convergence rate everywhere across the interval.

Illustration with Lagrange's interpolation formula:

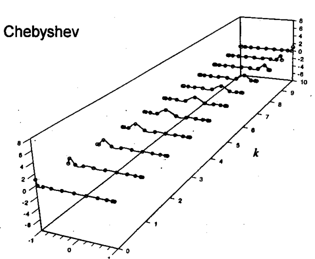
$$p_N(x) = \sum_{k=0}^{N} L_k(x) \cdot \frac{(x-x_0)\cdot\ldots\cdot(x-x_{k-1})(x-x_{k+1})\cdot\ldots\cdot(x-x_N)}{(x_k-x_0)\cdot\ldots\cdot(x_k-x_{k-1})(x_k-x_{k+1})\cdot\ldots\cdot(x_k-x_N)}$$

$N = 10$

Equi-spaced



Chebyshev



Generation of FD formulas on general grids

Examples of FD formulas:

$f'(x) = [\quad -\frac{1}{2}f(x-h) + 0f(x) + \frac{1}{2}f(x+h) \quad]/h + \quad O(h^2)$

$= [\frac{1}{12}f(x-2h) - \frac{2}{3}f(x-h) + 0f(x) + \frac{2}{3}f(x+h) - \frac{1}{12}f(x+2h)]/h + \quad O(h^4)$

etc.

GENERAL CASE:

GIVEN: $x_0, x_1, \dots, x_n$ grid points (non-repeated, otherwise arbitrary)
ξ point $x = \xi$ at which the approximations are wanted
m highest order of derivative of interest

FIND: weights $c^k_{i,j}$ such that the approximations

$$\left.\frac{\partial^k f}{\partial x^k}\right|_{x=\xi} \approx \sum_{j=0}^{i} c^k_{i,j}\, f(x_j) \quad , k=0,1,\dots,m \ , \ i = k, k+1, \dots, n$$

are all optimal.

$$\left.\frac{\partial^k f}{\partial x^k}\right|_{x=\xi} \approx \sum_{j=0}^{i} c_{i,j}^k f(x_j) \qquad , k=0,1,\dots,m \ , \ i=k,k+1,\dots,n$$

ALGORITHM:

$c_{0,0}^0 := 1\ ,\ \alpha := 1$
for $i := 1$ to n
  $\beta := 1$
  for $j := 0$ to $i-1$
    $\beta := \beta(x_i - x_j)$
    for $k := 0$ to $\min(i,m)$
      $c_{i,j}^k := ((x_i-\xi)c_{i-1,j}^k - k c_{i-1,j}^{k-1})/(x_i - x_j)$
  for $k := 0$ to $\min(i,m)$
    $c_{i,i}^k := \alpha(k c_{i-1,i-1}^{k-1} - (x_{i-1}-\xi) c_{i-1,i-1}^k)/\beta$
  $\alpha := \beta$

NOTES:

1. Non-initiated quantities assumed equal to zero
2. Only 4 operations / weight
3. Numerically stable
4. Case $m = 0$ fast method for polynomial interpolation

References:

B. Fornberg, Generation of finite difference formulas on arbitrarily spaced grids, *Math. Comput.*, 51 (1988), 699-706.

B. Fornberg, Calculation of weights in finite difference formulas, *SIAM Review*, 40 (1988), 685-691.

EQUIVALENCE BETWEEN SPECTRAL COLLOCATION (PS METHODS) AND FINITE DIFFERENCES

NOTE: Finite difference formulas can be designed also for non-uniform grids.

- If we place our grid points at the Chebyshev extrema and calculate, at each grid point, our derivatives with FD formulas that extend over all the grid points, we have exactly recovered the Chebyshev PS method.

  If we place our grid points at the Legendre extrema and calculate, at each grid point, our derivatives with FD formulas that extend over all the grid points, we have exactly recovered the Legendre PS method.

  Same for any Jacobi polynomial...

- **However we place our nodes, we get a PS method. There is no need to start with any orthogonal polynomial class at all! The FD approach very much generalizes the traditional approach of expanding in some class of classical orthogonal polynomials.**

- **Quadratic clustering of nodes towards the end of an interval is purely a means of defeating the Runge Phenomenon - and a quite desperate action to take. It should be used ONLY if the boundary truly represents the end of the world - and absolutely no extra information is available beyond it.**

Two alternatives for calculating derivatives on a Chebyshev-type grid

1. Using FFT

Turn point data into expansion coefficients $\Sigma_0^n a_k T_k(x)$,

Express $\frac{\partial}{\partial x}(\Sigma_0^n a_k T_k(x))$ as $\Sigma_0^n b_k T_k(x)$

Return from coefficients to node values

Total cost $O(n \log n)$ operations

2. Using Differentiation Matrix

At each grid point, approximate $\frac{\partial}{\partial x}$ by FD stencil that covers rest of interval

$$\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_n \end{bmatrix}' = \begin{bmatrix} & & \\ & D & \\ & & \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_n \end{bmatrix}$$

Total cost $O(n^2)$ operations.

Still usually faster for moderate sizes of n.

POLAR AND SPHERICAL COORDINATE SYSTEMS

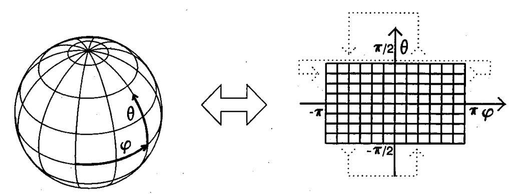
On a unit circle:

Traditionally: $0 \le r \le 1,\ 0 \le \theta \le 2\pi$
Much better: $-1 \le r \le 1,\ 0 \le \theta \le \pi$

No longer any reason to cluster at the center.

Can use periodicity in either case

On a unit sphere:



Would be VERY BAD to consider $-\pi \le \theta \le \pi$ together with end conditions.

Utilize that data is periodic in both φ and θ–directions, and use periodic, equi-spaced Fourier-PS.

EXAMPLE : Axi-symmetric eigenvalue problem in unit circle

Bessel's equation:

$$u'' + \frac{1}{r}u' - \frac{n^2}{r^2}u = -\lambda u$$

$n = 0,1,\dots$
$u(0)$ bounded, $u(1) = 0$

(From separation of variables, Laplace's equation)

Exact eigenvalues $\lambda_{n,k}$, $k = 1,2,\dots$
satisfy $J_n(\sqrt{\lambda_{n,k}}) = 0$

Method 1: 'PS on [0,1]'

$$\begin{cases} n = 0 & u'(0) = 0 \\ n \ne 0 & u(0) = 0 \end{cases}$$

Grid:
$r_k = (1-\cos\frac{k\pi}{N})/2\ ,\ k = 0,1,\dots,N$

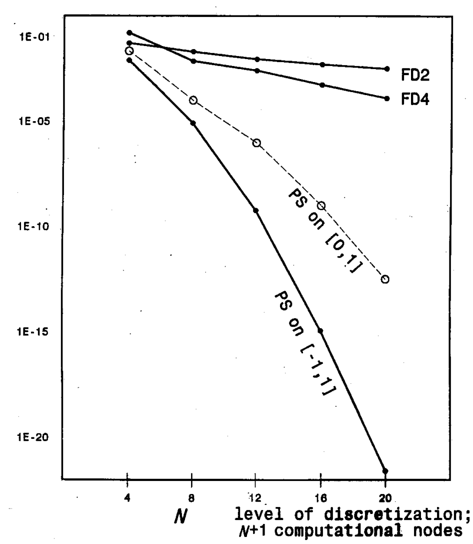
Method 2: 'PS on [-1,1]'

$$\begin{cases} n \text{ even} & u(r) \text{ even} \\ n \text{ odd} & u(r) \text{ odd} \end{cases}$$

Grid:
$r_k = \sin\frac{k\pi}{2N}\ ,\ k = 0,1,\dots,N$

Test problem: $n = 7,\ k = 1,\ \lambda_{7,1} \approx 122.9$.

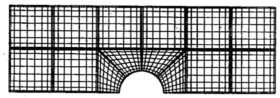
Relative error in eigenvalue
$\lambda_{7,1} \approx 122.9$



Spectral Elements

1-D:

2-D:



Typically:

- Chebyshev- or Legendre grids (stretched if in 2-D),
- Grid points at ends of interval,
- Domains coupled via characteristics

Concerns:

- Grid clustering appears excessive and unnecessary,
- Equations may not have characteristics,
- Complexity in 2-D and 3-D corners

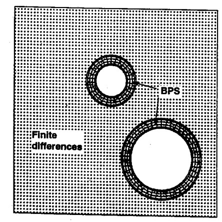
2-D TE Maxwell

$$\begin{cases} \varepsilon(x,y)\dfrac{\partial E_x}{\partial t} = \dfrac{\partial H_z}{\partial y} - \sigma(x,y)\,E_x \\ \varepsilon(x,y)\dfrac{\partial E_y}{\partial t} = -\dfrac{\partial H_z}{\partial x} - \sigma(x,y)\,E_y \\ \mu(x,y)\dfrac{\partial H_z}{\partial t} = \dfrac{\partial E_x}{\partial y} - \dfrac{\partial E_y}{\partial x} - \sigma^*(x,y)\,H_z \end{cases}$$

E_x, E_y Electric field
H_z Magnetic field

ε, μ Permettivity, Permeability
σ, σ^* Electric and magnetic resistivity

Grid structure:



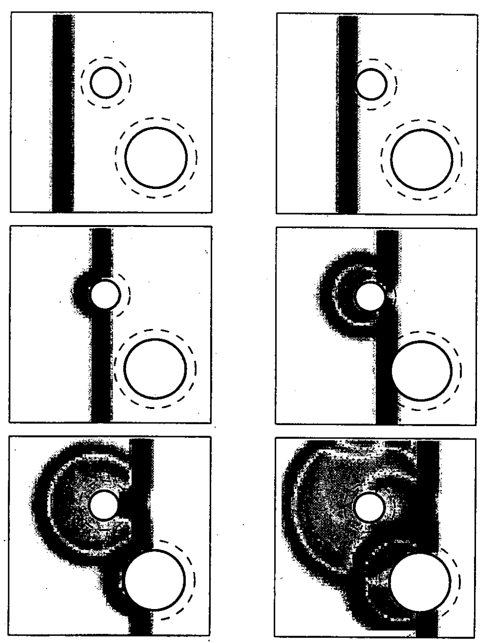
In strips BPS

In background, space-time-steggered 6th order implicit (compact) FD:

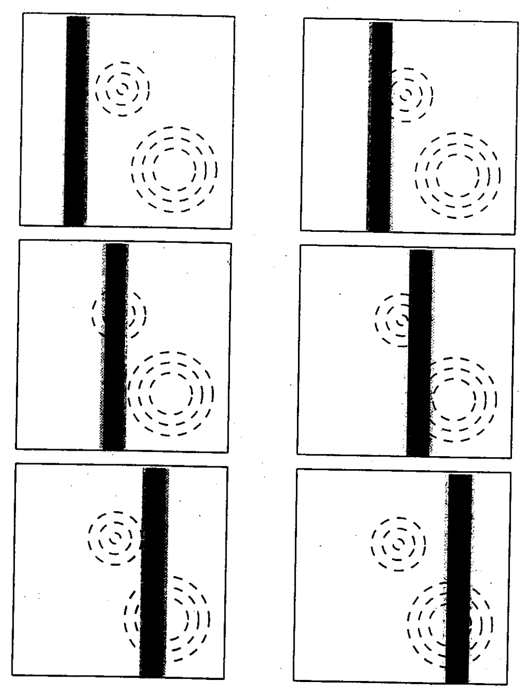
○ ○ ○
■ ■ ■ ■

Test case with two perfectly electrically conducting cylinders

The dotted contours show the zero level



Propagation of plane wave in free space, using same composit grid method



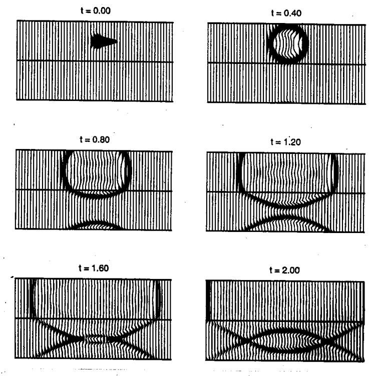
Test case with two dielectric media

Two dielectric materials,

$\varepsilon^+ = 1,\ \varepsilon^- = 4$;

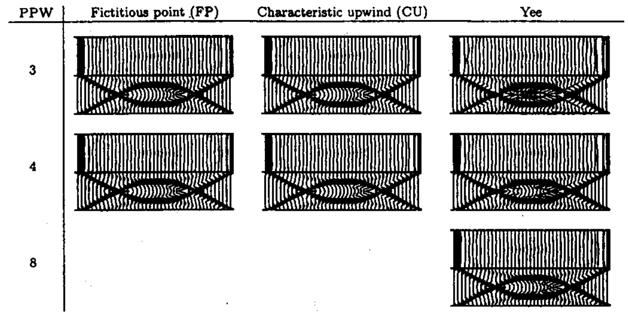
no wave absorption

Snapshots in time for BPS with 3 PPW

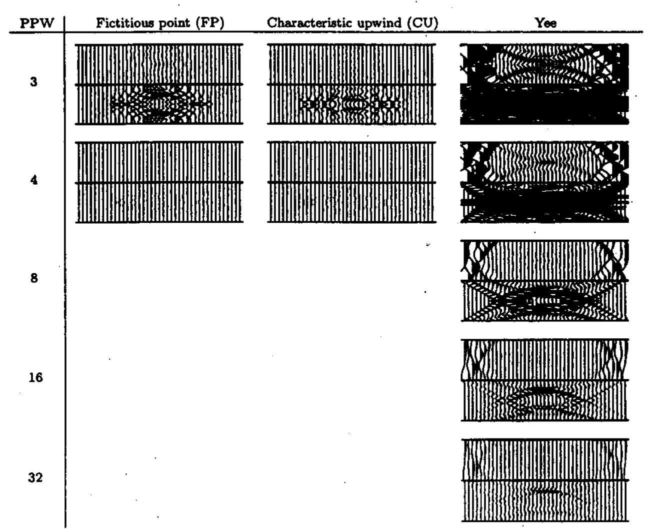


To achieve 3 PPW, we use a 144×36 grid in S^- and a 144×27 grid in S^+

Accuracy comparison between different methods and different resolutions



Solutions at $t = 2$ for the dielectric problem. Errors are seen more clearly in Figure 7.3.



Errors at $t = 2$ for the dielectric problem. As an indication of the scale, the maximum error in the case of CU-4 is about 0.001; *the maximum of the solution is about* 0.23.

Yee needs about 56 PPW to match the BPS methods with 4 PPW

CONCLUSIONS

Periodic PS:

Alternative approaches:
- Collocate with trigonometric functions - take the derivative of the interpolant
- Limit of equi-spaced FD formulas of orders / stencil width tending to infinity

Performance:
- Superior computational efficiency for both linear and mildly nonlinear cases (e.g. nonlinear waves, turbulence etc.)

Non-Periodic PS:

Alternative approaches:
- Collocate with orthogonal polynomials
- Global FD approximation based on end-clustered grid

Performance:
- Accuracy superior to FEM and low order FD approximations, but severely degraded compared to the periodic case
- Time stepping stability in general hurt by grid clustering

Both cases:

- Combine with MOL (Methods of Lines) for time stepping - most ODE solvers effective.