

# Agenda

## PDEs with Variable Coefficients

Galerkin Approach

Collocation Approach

Fourier Transforms in Higher Dimensions

## Nonlinear Evolution PDEs

Galerkin approach

Collocation approach & Aliasing Removal

Hybrid Integration Schemes for ODEs

## Chebyshev Polynomials

Review

Numerical Integration Formulae

- ▶ Consider again the problem  $\mathcal{L}u = \nu u'' - au' + bu = f$ , but assume now that the coefficient  $a$  is a function OF SPACE  $a = a(x)$
- ▶ The following Galerkin equations are obtained for  $\hat{u}_k$

$$-\nu k^2 \hat{u}_k - i \sum_{p=-N}^N p \hat{a}_{k-p} \hat{u}_p + b \hat{u}_k = \hat{f}_k, \quad k = -N, \dots, N,$$

where  $a(x) \cong a_N(x) = \sum_{k=-N}^N \hat{a}_k e^{ikx}$  and  $f(x) \cong f_N(x) = \sum_{k=-N}^N \hat{f}_k e^{ikx}$ ; Note that

$$\begin{aligned} \sum_{q=-N}^N \hat{a}_q e^{iqx} \sum_{p=-N}^N \hat{u}_p e^{ipx} &= \sum_{q,p=-N}^N \hat{a}_q \hat{u}_p e^{i(q+p)x} = \sum_{k=-2N}^{2N} \sum_{\substack{q,p=-N \\ q+p=k}}^N \hat{a}_q \hat{u}_p e^{ikx} \\ &= \sum_{k=-2N}^{2N} \sum_{p=-N}^N \hat{a}_{k-p} \hat{u}_p e^{ikx}, \quad \text{where } \hat{a}_q, \hat{u}_q \equiv 0, \text{ for } |q| > N \end{aligned}$$

- ▶ Now the Galerkin equations are **COUPLED** (a system of equations has to be solved)

- ▶ With **FOURIER COEFFICIENTS**  $\hat{u}_k$  as unknowns, the collocation equations are

$$- \sum_{k=-N}^N (\nu k^2 + b) \hat{u}_k e^{ikx_j} - a(x_j) \sum_{k=-N}^N ik \hat{u}_k e^{ikx_j} = f(x_j), \quad j = 1, \dots, M$$

- ▶ Approximations of the Fourier coefficients of  $a(x)$  and  $f(x)$ ,  $\hat{a}_k^c$  and  $\hat{f}_k^c$ , respectively, are calculated using the Discrete Fourier Transform;

$$a(x_j) \sum_{k=-N}^N ik \hat{u}_k e^{ikx_j} = \sum_{p=-N}^N \hat{a}_p^c e^{ipx_j} \sum_{q=-N}^N iq \hat{u}_q e^{iqx_j} =$$

$$i \sum_{k=-N}^N \left( \sum_{\substack{q,p=-N \\ q+p=k}}^N q \hat{a}_p^c \hat{u}_q + \sum_{\substack{q,p=-N \\ q+p=k+N}}^N q \hat{a}_p^c \hat{u}_q + \sum_{\substack{q,p=-N \\ q+p=k-N}}^N q \hat{a}_p^c \hat{u}_q \right) e^{ikx_j}$$

$$\triangleq i \sum_{k=-N}^N \hat{S}_k e^{ikx_j}$$

- ▶ The resulting algebraic system is

$$-\nu k^2 \hat{u}_k - i \hat{S}_k + b \hat{u}_k = \hat{f}_k, \quad k = -N, \dots, N,$$

- ▶ Expressing (hypothetically)  $a(x)$  and  $f(x)$  with **INFINITE** Fourier series we obtain

$$\begin{aligned}
 au' \Big|_{x=x_j} &= i \sum_{k=-N}^N (\hat{S}_k^{(0)} + \hat{S}_k^{(1)} + \hat{S}_k^{(2)} + \hat{S}_k^{(3)}) e^{ikx_j} \\
 &= i \sum_{k=-N}^N \left( \sum_{\substack{q,p=-N \\ q+p=k}}^N q \hat{a}_p^c \hat{u}_q + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \sum_{\substack{q,p=-N \\ q+p=k}}^N q \hat{a}_{p+mM}^c \hat{u}_q \right. \\
 &\quad \left. + \sum_{m=-\infty}^{\infty} \sum_{\substack{q,p=-N \\ q+p=k+N}}^N q \hat{a}_{p+mM}^c \hat{u}_q + \sum_{m=-\infty}^{\infty} \sum_{\substack{q,p=-N \\ q+p=k-N}}^N q \hat{a}_{p+mM}^c \hat{u}_q \right) e^{ikx_j}
 \end{aligned}$$

- ▶ The collocation equation become

$$-\nu k^2 \hat{u}_k - i \hat{S}_k^{(0)} + i \left( \hat{S}_k^{(1)} + \hat{S}_k^{(2)} + \hat{S}_k^{(3)} \right) + b \hat{u}_k = \hat{f}_k^e + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \hat{f}_{k+mM}^e, \quad k = -N, \dots, N,$$

- ▶ Note that the terms **IN RED** are absent in the corresponding **GALERKIN FORMULATION** ; hence the two approaches are not **NUMERICALLY EQUIVALENT** anymore.

- ▶ With the **NODAL VALUES**  $u(x_j)$ ,  $j = 1, \dots, M$  as unknowns, the collocation equations are

$$(\nu \mathbb{D}_2 - \mathbb{D}' + b\mathbb{I})U_N = F,$$

where the matrix  $\mathbb{D}' = \left[ a(x_j) d_{jk}^{(1)} \right]$ ,  $j, k = 1, \dots, M$

- ▶ Again, solution of an algebraic system is required

- ▶ Consider a function  $u = u(x, y)$   $2\pi$ -periodic in both  $x$  and  $y$ ;  
**DIRECT DISCRETE FOURIER TRANSFORM**

$$\hat{u}_{k_x, k_y} = \frac{1}{2\pi} \int_0^{2\pi} \left[ \frac{1}{2\pi} \int_0^{2\pi} u(x, y) e^{-ik_x x} dx \right] e^{-ik_y y} dy = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} u(x, y) e^{-i\mathbf{k} \cdot \mathbf{r}} dx dy,$$

where  $\mathbf{k} = [k_x, k_y]$  is the **WAVEVECTOR** and  $\mathbf{r} = [x, y]$  is the position vector.

- ▶ Representation of a function  $u = u(x, y)$  as a **DOUBLE FOURIER SERIES**

$$u(x, y) = \sum_{k_x, k_y = -N}^N \hat{u}_{k_x, k_y} e^{i(k_x x + k_y y)} = \sum_{k_x, k_y = -N}^N \hat{u}_{k_x, k_y} e^{i\mathbf{k} \cdot \mathbf{r}}$$

- ▶ Fourier transforms in two (and more) dimensions can be efficiently performed using most standard FFT packages.

- ▶ Replacing the term  $au'$  with the **NONLINEAR** the term  $uu'$  and applying Galerkin or collocation method leads to a **SYSTEM OF NONLINEAR EQUATIONS** that need to be solved using iterative techniques
- ▶ From now on we will focus on **TIME-DEPENDENT** (evolution) PDEs and as a model problem will consider the **BURGERS EQUATION**

$$\begin{cases} \partial_t u + u \partial_x u - \nu \partial_{xx} u = 0 & \text{in } [0, 2\pi] \times [0, T] \\ u(x) = u_0(x) & \text{at } t = 0 \end{cases}$$

Note that steady problems can sometimes be solved as a steady limit of certain time-dependent problems.

- ▶ Looking for solution in the form  $u_N(x, t) = \sum_{k=-N}^N \hat{u}_k(t) e^{ikx}$ . Note that the expansion coefficients  $\hat{u}_k(t)$  are now **FUNCTIONS OF TIME**
- ▶ Denote by  $u_N^n$  the approximation of  $u_N$  at time  $t_n = n\Delta t$ ,  $n = 0, 1, \dots$

- ▶ Time-discretization of the residual  $R_N(x, t)$

$$R_N^n = \frac{u_N^{n+1} - u_N^n}{\Delta t} + u_N^n \partial_x u_N^n - \nu \partial_{xx} u_N^{n+1}$$

Points to note:

- ▶ **EXPLICIT** treatment of the nonlinear term avoids costly iterations
  - ▶ **IMPLICIT** treatment of the linear viscous term allows one to mitigate the stability restrictions on the time step  $\Delta t$
  - ▶ here using for simplicity first-order accurate explicit/implicit Euler — can do much better than that
- ▶ System of equations obtained by applying the **GALERKIN FORMALISM**

$$\left( \frac{1}{\Delta t} + \nu k^2 \right) \hat{u}_k^{n+1} = \frac{1}{\Delta t} \hat{u}_k^n - i \sum_{\substack{p, q = -N \\ p+q=k}}^N q \hat{u}_p^n \hat{u}_q^n, \quad k = -N, \dots, N$$

Note truncation of higher modes in the nonlinear term.



- ▶ Evaluation of the nonlinear  $i \sum_{\substack{p,q=-N \\ p+q=k}}^N q \hat{u}_p^n \hat{u}_q^n$  term in Fourier space results in a **CONVOLUTION SUM** which requires  $\mathcal{O}(N^2)$  operations – can we do better than that?

- ▶ **PSEUDOSPECTRAL APPROACH** — perform differentiation in **FOURIER SPACE** and evaluate products in **REAL SPACE** ; transition between the two representations is made using FFTs which cost "only"  $\mathcal{O}(N \log(N))$

Outline of the algorithm:

1. calculate (using inverse FFT)  $u_N^n(x_j)$ ,  $j = 1, \dots, M$  from  $\hat{u}_k^n$ ,  $k = -N \dots, N$ ,
  2. calculate (using inverse FFT)  $\partial_x u_N^n(x_j)$ ,  $j = 1, \dots, M$  from  $ik \hat{u}_k^n$ ,  $k = -N \dots, N$ ,
  3. calculate the product  $w_N^n(x_j) = u_N^n(x_j) \partial_x u_N^n(x_j)$ ,  $j = 1, \dots, M$
  4. Calculate (using FFT)  $\tilde{w}_k^n$ ,  $k = -N \dots, N$  from  $w_N^n(x_j)$ ,  $j = 1, \dots, M$
- ▶ Note that, because of the **ALIASING PHENOMENON** , the quantity  $\tilde{w}_k^n$  is different from  $\hat{w}_k^n = i \sum_{\substack{p,q=-N \\ p+q=k}}^N q \hat{u}_p^n \hat{u}_q^n$

- ▶ Analysis of aliasing in the **PSEUDOSPECTRAL** calculation of the nonlinear term

$$w_N^n(x_j) = \sum_{k=-N}^N \tilde{w}_k^n e^{ikx_j}, \quad \text{where } w_N^n(x_j) = u_N^n(x_j) \partial_x u_N^n(x_j)$$

- ▶ The Discrete Fourier Transform

$$\begin{aligned} \tilde{w}_k^n &= \frac{1}{M} \sum_{j=1}^M w_N^n(x_j) e^{-ikx_j} = \frac{1}{M} \sum_{j=1}^M \left( \sum_{p=-N}^N \hat{u}_p^n e^{ipx_j} \right) \left( \sum_{q=-N}^N iq \hat{u}_q^n e^{iqx_j} \right) e^{-ikx_j} \\ &= \frac{1}{M} \sum_{j=1}^M \sum_{p, q=-N}^N iq \hat{u}_p^n \hat{u}_q^n e^{i(p+q-k)x_j} = \frac{1}{M} \sum_{p, q=-N}^N iq \hat{u}_p^n \hat{u}_q^n \sum_{j=1}^M e^{i(p+q-k)x_j} \\ &= \hat{w}_k^n + i \sum_{\substack{p, q=-N \\ p+q=k+M}}^N q \hat{u}_p^n \hat{u}_q^n + i \sum_{\substack{p, q=-N \\ p+q=k-M}}^N q \hat{u}_p^n \hat{u}_q^n \quad k = -N, \dots, N \end{aligned}$$

The term  $\hat{w}_k^n$  is the convolution sum obtained by **TRUNCATING** the fully spectral Galerkin approach. The terms **IN RED** are the **ALIASING ERRORS**.

- ▶ Thus, the **PSEUDOSPECTRAL GALERKIN** equations are

$$\left( \frac{1}{\Delta t} + \nu k^2 \right) \hat{u}_k^{n+1} = \frac{1}{\Delta t} \hat{u}_k^n - \tilde{w}_k^n, \quad k = -N, \dots, N$$

- ▶ Looking for the solution in the form  $u_N(x, t) = \sum_{k=-N}^N \hat{u}_k(t) e^{ikx}$ , i.e., with the Fourier coefficients  $\hat{u}_k$  as unknowns
- ▶ Time-discretization of the residual  $R_N(x, t)$

$$R_N^n = \frac{u_N^{n+1} - u_N^n}{\Delta t} + u_N^n \partial_x u_N^n - \nu \partial_{xx} u_N^{n+1}$$

- ▶ Canceling the residual at the collocation points  $x_j$

$$\frac{1}{\Delta t} [u_N^{n+1}(x_j) - u_N^n(x_j)] + u_N^n(x_j) \partial_x u_N^n(x_j) - \nu \partial_{xx} u_N^{n+1}(x_j) = 0, \quad j = 1, \dots, M$$

- ▶ Straightforward calculation shows that the equation for the Fourier coefficients  $\hat{u}_k$  is the same as in the **PSEUDOSPECTRAL GALERKIN APPROACH**. Thus the two methods are numerically equivalent.
- ▶ **QUESTION** — Show equivalence of pseudospectral Galerkin and collocation approaches to a nonlinear PDE

- ▶ “3/2 RULE” — extend the wavenumber range (the “spectrum”), and therefore also the number of collocation points, of the quantities involved in the products, so that the aliasing errors arising in pseudospectral calculations are not present.
- ▶ ALGORITHM — consider two  $2\pi$ -periodic functions

$$a_N(x) = \sum_{k=-N}^N \hat{a}_k e^{ikx}, \quad b_N(x) = \sum_{k=-N}^N \hat{b}_k e^{ikx}$$

Calculated in a naive way, the Fourier coefficients of the product  $w(x) = a(x)b(x)$  are

$$\tilde{w}_k = \hat{w}_k + \sum_{\substack{p,q=-N \\ p+q=k+M}}^N \hat{a}_p \hat{b}_q + \sum_{\substack{p,q=-N \\ p+q=k-M}}^N \hat{a}_p \hat{b}_q, \quad k = -N, \dots, N$$

where  $\hat{w}_k$  are the coefficients of the truncated convolution sum that we want to keep (only)

1. Extend the spectra  $\hat{a}_k$  and  $\hat{b}_k$  to  $\hat{a}'_k$  and  $\hat{b}'_k$  according to

$$\hat{a}'_k = \begin{cases} \hat{a}_k & \text{if } |k| \leq N \\ 0 & \text{if } N < |k| \leq N' \end{cases}, \quad \hat{b}'_k = \begin{cases} \hat{b}_k & \text{if } |k| \leq N \\ 0 & \text{if } N < |k| \leq N' \end{cases}$$

The number  $N'$  will be determined later.

2. Calculate (via FFT)  $a_{N'}$  and  $b_{N'}$  in real space on the extended grid  $x'_j = \frac{2\pi j}{M'}$ ,  $j = 1, \dots, M'$ , where  $M' = 2N' + 1$

$$a_{N'}(x'_j) = \sum_{k=-N'}^{N'} \hat{a}'_k e^{ikx'_j}, \quad b_{N'}(x'_j) = \sum_{k=-N'}^{N'} \hat{b}'_k e^{ikx'_j}$$

3. Multiply  $a_{N'}(x'_j)$  and  $b_{N'}(x'_j)$ :  $w'(x'_j) = a_{N'}(x'_j) b_{N'}(x'_j)$ ,  $j = 1, \dots, M'$
4. Calculate (via FFT) the Fourier coefficients of  $w'(x'_j)$

$$\tilde{w}'_k = \frac{1}{M'} \sum_{j=1}^{M'} w(x'_j) e^{-ikx'_j}, \quad k = -N', \dots, N', \quad M' = 2N' + 1$$

Taking the latter quantity for  $k = -N, \dots, N$  gives an expression for the convolution sum **FREE OF ALIASING ERRORS**

- ▶ Making a suitable choice for  $N'$

$$\begin{aligned}\tilde{w}'_k &= \hat{w}_k + \sum_{\substack{p,q=-N' \\ p+q=k+M'}}^{N'} \hat{a}'_p \hat{b}'_q + \sum_{\substack{p,q=-N' \\ p+q=k-M'}}^{N'} \hat{a}'_p \hat{b}'_q \\ &= \hat{w}_k + \sum_{\substack{p,q=-N \\ p+q=k+M'}}^N \hat{a}_p \hat{b}_q + \sum_{\substack{p,q=-N \\ p+q=k-M'}}^N \hat{a}_p \hat{b}_q\end{aligned}$$

because  $\hat{a}'_p, \hat{b}'_q = 0$  for  $|p|, |q| > N$

- ▶ The alias terms will vanish, when one of the frequencies  $p$  or  $q$  appearing in each term of the sum is larger than  $N$ . Observe that in the first alias term  $q = M' + k - p = 2N' + 1 + k - p$ , therefore

$$\min_{|k|, |p| \leq N} (q) = \min_{|k|, |p| \leq N} (2N' + 1 + k - p) = 2N' + 1 - 2N > N$$

Hence  $2N' > 3N - 1$ . One may take  $N' \geq 3N/2$  (the “**3/2 RULE**”) [see the diagram on page 212 in Boyd (2001)]

- ▶ Analogous argument for the second aliasing error sum.

- ▶ Consider a model ODE problem

$$\mathbf{y}' = \mathbf{r}(\mathbf{y}) + \mathbf{A}\mathbf{y}$$

- ▶ One would like to use a higher-order ODE integrator with
  - ▶ **EXPLICIT** treatment of nonlinear terms
  - ▶ **IMPLICIT** treatment of linear terms (with high-order derivatives)
- ▶ Combining a **three-step Runge-Kutta method** with the **CRANK-NICOLSON METHOD** results in the following approach:

$$\left(I - \frac{h_{rk}}{2}A\right) \mathbf{y}^{rk+1} = \mathbf{y}^{rk} + \frac{h_{rk}}{2}A\mathbf{y}^{rk} + h_{rk}\beta_{rk}\mathbf{r}(\mathbf{y}^{rk}) + h_{rk}\zeta_{rk}\mathbf{r}(\mathbf{y}^{rk-1}), \quad rk = 1, 2, 3$$

where

$$h_1 = \frac{8}{15}\Delta t$$

$$h_2 = \frac{2}{15}\Delta t$$

$$h_3 = \frac{1}{3}\Delta t$$

$$\beta_1 = 1$$

$$\beta_2 = \frac{25}{8}$$

$$\beta_3 = \frac{9}{4}$$

$$\zeta_1 = 0$$

$$\zeta_2 = -\frac{17}{8}$$

$$\zeta_3 = -\frac{5}{4}$$

▶ General properties of **ORTHOGONAL POLYNOMIALS**

- ▶ Suppose  $I = [a, b]$  is a given interval. Let  $\omega : I \rightarrow \mathbb{R}^+$  be a weight function which is positive and continuous on  $I$
- ▶ Let  $L^2_\omega(I)$  denote the space of measurable functions  $v$  such that

$$\|v\|_\omega = \left( \int_I |v(x)|^2 \omega(x) dx \right)^{\frac{1}{2}} < \infty$$

- ▶  $L^2_\omega(I)$  is a Hilbert space with the scalar products

$$(u, v)_\omega = \int_I u(x) \overline{v(x)} \omega(x) dx$$

▶ **CHEBYSHEV POLYNOMIALS** are obtained by setting:

- ▶ the weight:  $\omega(x) = (1 - x^2)^{-\frac{1}{2}}$
- ▶ the interval:  $I = [-1, 1]$
- ▶ Chebyshev polynomials of degree  $k$  are expressed as

$$T_k(x) = \cos(k \cos^{-1} x), \quad k = 0, 1, 2, \dots$$



- ▶ By setting  $x = \cos(z)$  we obtain  $T_k = \cos(kz)$ , therefore we can derive expressions for the first Chebyshev polynomials

$$T_0 = 1, \quad T_1 = \cos(z) = x, \quad T_2 = \cos(2z) = 2\cos^2(z) - 1 = 2x^2 - 1, \quad \dots$$

- ▶ More generally, using the de Moivre formula, we obtain

$$\cos(kz) = \Re \left[ (\cos(z) + i \sin(z))^k \right],$$

from which, invoking the binomial formula, we get

$$T_k(x) = \frac{k}{2} \sum_{m=0}^{\lfloor k/2 \rfloor} (-1)^m \frac{(k-m-1)!}{m!(k-2m)!} (2x)^{k-2m},$$

where  $\lfloor \alpha \rfloor$  represents the integer part of  $\alpha$

- ▶ Note that the above expression is **COMPUTATIONALLY USELESS** — one should use the formula  $T_k(x) = \cos(k \cos^{-1} x)$  instead!

- ▶ The trigonometric identity  $\cos(k+1)z + \cos(k-1)z = 2\cos(z)\cos(kz)$  results in the following **RECURRENCE RELATION**

$$2xT_k = T_{k+1} + T_{k-1}, \quad k \geq 1,$$

which can be used to deduce  $T_k$ ,  $k \geq 2$  based on  $T_0$  and  $T_1$  only

- ▶ Similarly, for the derivatives we get

$$T'_k = \frac{d}{dz}(\cos(kz)) \frac{dz}{dx} = \frac{d}{dz}(\cos(kz)) \left(\frac{dx}{dz}\right)^{-1} = k \frac{\sin(kz)}{\sin(z)},$$

which, upon using trigonometric identities, yields a **RECURRENCE RELATION** for derivatives

$$2T_k = \frac{T'_{k+1}}{k+1} - \frac{T'_{k-1}}{k-1}, \quad k > 1,$$

- ▶ Note that simply changing the integration variable we obtain

$$\int_{-1}^1 f(x)\omega(x) dx = \int_0^\pi f(\cos \theta) d\theta$$

This also provides an **isometric (i.e., norm-preserving)** transformation  $u \in L^2_\omega(I) \longrightarrow \tilde{u} \in L^2(0, \pi)$ , where  $\tilde{u}(\theta) = u(\cos \theta)$

- ▶ Consequently, we obtain

$$(T_k, T_l)_\omega = \int_{-1}^1 T_k T_l \omega dx = \int_0^\pi \cos(k\theta) \cos(l\theta) d\theta = \frac{\pi}{2} c_k \delta_{kl},$$

where

$$c_k = \begin{cases} 2 & \text{if } k = 0, \\ 1 & \text{if } k \geq 1 \end{cases}$$

- ▶ Note that Chebyshev polynomials are **ORTHOGONAL**, but not **ORTHONORMAL**

- ▶ The Chebyshev polynomials  $T_k(x)$  vanish at the **GAUSS POINTS**  $x_j$  defined as

$$x_j = \cos\left(\frac{(2j+1)\pi}{2k}\right), \quad j = 0, \dots, k-1$$

There are exactly  $k$  distinct zeros in the interval  $[-1, 1]$

- ▶ Note that  $-1 \leq T_k \leq 1$ ; furthermore the Chebyshev polynomials  $T_k(x)$  attain their extremal values at the the **GAUSS-LOBATTO POINTS**  $x_j$  defined as

$$x_j = \cos\left(\frac{j\pi}{k}\right), \quad j = 0, \dots, k$$

There are exactly  $k+1$  real extrema in the interval  $[-1, 1]$ .

- ▶ Interpolation on **CLUSTERED GRIDS** has very special properties — **CHEBYSHEV MINIMAL AMPLITUDE THEOREM** : Of all polynomials of degree  $N$  with the leading coefficient (i.e., the coefficient of  $x^N$ ) equal to 1, the unique polynomial which has the smallest maximum on  $[-1, 1]$  is  $T_N(x)/2^{N-1}$ , the  $N$ -th Chebyshev polynomials divided by  $2^{N-1}$ . In other words, all polynomials of the same degree and leading coefficient satisfy the inequality

$$\max_{x \in [-1, 1]} |P_N(x)| \geq \max_{x \in [-1, 1]} \left| \frac{T_N(x)}{2^{N-1}} \right| = \frac{1}{2^{N-1}}$$

- ▶ Hence, the **TRUNCATION ERROR** when given in terms of  $\frac{1}{2^N} T_{N+1}(x)$  will be best behaved
- ▶ Thus, in contrast to interpolation on **UNIFORM** grids, interpolation on **CLUSTERED** grid is less likely to exhibit the **RUNGE PHENOMENON** ; this concerns clustered grids with asymptotic density of points proportional to  $\frac{N}{\pi\sqrt{1-x^2}}$  (e.g., various Chebyshev grids)

- ▶ **FUNDAMENTAL THEOREM OF GAUSSIAN QUADRATURE** — The abscissas of the  $N$ -point Gaussian quadrature formula are precisely the roots of the orthogonal polynomial of order  $N$  for the same interval and weighting function.
- ▶ **THE GAUSS-Chebyshev FORMULA** (exact for  $u \in \mathbb{P}_{2N-1}$ )

$$\int_{-1}^1 u(x)\omega(x) dx = \frac{\pi}{N} \sum_{j=1}^N u(x_j),$$

with  $x_j = \cos\left(\frac{(2j-1)\pi}{2N}\right)$  (the Gauss points located in the interior of the domain only)

Proof via straightforward application of the theorem quoted above.

- THE GAUSS-RADAU-CHEBYSHEV FORMULA (exact for  $u \in \mathbb{P}_{2N}$ )

$$\int_{-1}^1 u(x)\omega(x) dx = \frac{\pi}{2N+1} \left[ u(\xi_0) + 2 \sum_{j=1}^N u(\xi_j) \right],$$

with  $\xi_j = \cos\left(\frac{2j\pi}{2N+1}\right)$  (the Gauss-Radau points located in the interior of the domain and on one boundary, useful e.g., in annular geometry)

- Proof via application of the above theorem and using the roots of the polynomial  $Q_{N+1}(x) = T_N(a)T_{N+1}(x) - T_{N+1}(a)T_N(x)$  which vanishes at  $x = a = \pm 1$

- ▶ **THE GAUSS-LOBATTO-CHEBYSHEV FORMULA** (exact for  $u \in \mathbb{P}_{2N}$ )

$$\int_{-1}^1 u(x)\omega(x) dx = \frac{\pi}{2N+1} \left[ u(\tilde{\xi}_0) + u(\tilde{\xi}_N) + 2 \sum_{j=1}^{N-1} u(\tilde{\xi}_j) \right],$$

with  $\tilde{\xi}_j = \cos\left(\frac{j\pi}{N}\right)$  (the Gauss-Lobatto points located in the interior of the domain and on both boundaries)

- ▶ Proof via application of the theorem quoted above.



- ▶ The **GAUSS-LOBATTO-Chebyshev COLLOCATION POINTS** are most commonly used in Chebyshev spectral methods, because this set of points also includes the boundary points (which makes it possible to easily incorporate the **BOUNDARY CONDITIONS** in the collocation approach)
- ▶ Using the Gauss-Lobatto-Chebyshev points, the orthogonality relation for the Chebyshev polynomials  $T_k$  and  $T_l$  with  $0 \leq k, l \leq N$  can be written as

$$(T_k, T_l)_\omega = \int_{-1}^1 T_k T_l \omega \, dx = \frac{\pi}{N} \sum_{j=0}^N \frac{1}{\bar{c}_j} T_k(\tilde{\xi}_j) T_l(\tilde{\xi}_j) = \frac{\pi \bar{c}_k}{2} \delta_{kl},$$

where

$$\bar{c}_k = \begin{cases} 2 & \text{if } k = 0, \\ 1 & \text{if } 1 \leq k \leq N-1, \\ 2 & \text{if } k = N \end{cases}$$

- ▶ Note similarity to the corresponding **DISCRETE ORTHOGONALITY RELATION** obtained for the trigonometric polynomials