Spectral methods for core collapse

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Introduction:
Representation of functions

Functions on a computer

Simplified picture

How to deal with functions on a computer?

⇒a computer can manage only integers

In order to represent a function $\phi(x)$ (e.g. interpolate), one can use:

- a finite set of its values $\{\phi_i\}_{i=0\ldots N}$ on a grid $\{x_i\}_{i=0\ldots N}$,
- a finite set of its coefficients in a functional basis $\phi(x) \simeq \sum_{i=0}^{N} c_i \Psi_i(x)$.

In order to manipulate a function (e.g. derive), each approach leads to:

- finite differences schemes

$$\phi'(x_i) \simeq \frac{\phi(x_{i+1}) - \phi(x_i)}{x_{i+1} - x_i}$$

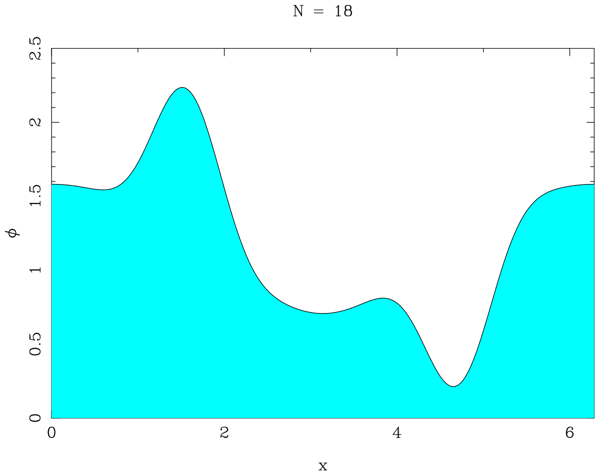
- spectral methods

$$\phi'(x) \simeq \sum_{i=0}^{N} c_i \Psi_i'(x)$$

Convergence of Fourier series

$$\phi(x) = \sqrt{1.5 + \cos(x)} + \sin^7 x$$

$$\phi(x) \simeq \sum_{i=0}^{N} a_i \Psi_i(x) \text{ with } \Psi_{2k} = \cos(kx), \ \Psi_{2k+1} = \sin(kx)$$



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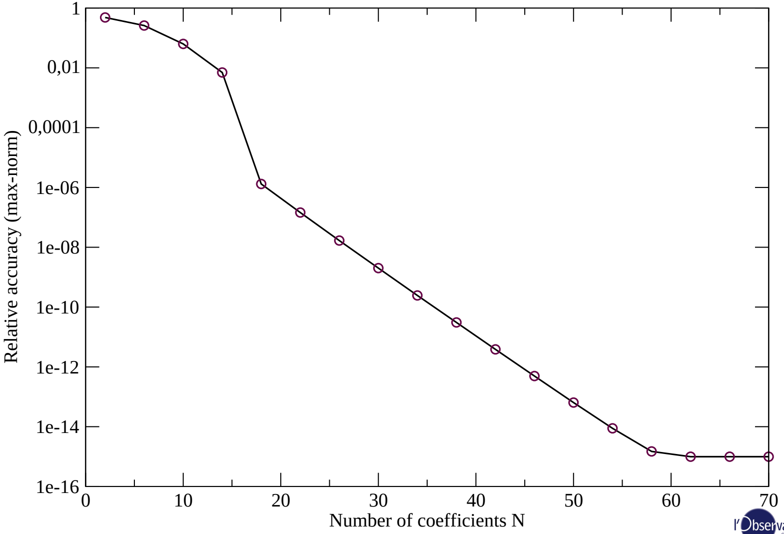
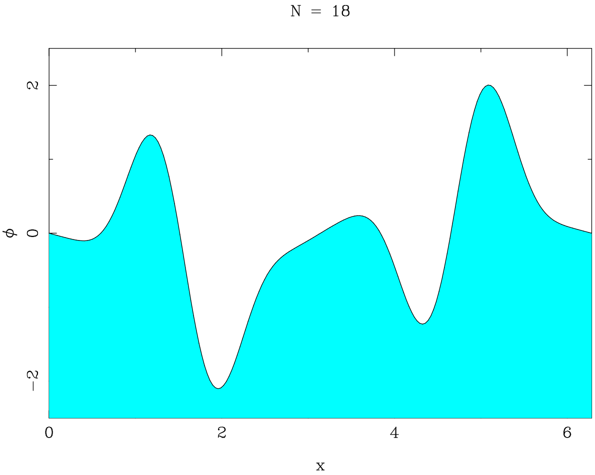


Convergence to the derivative

$$\phi(x) = \sqrt{1.5 + \cos(x)} + \sin^7 x$$

$$\phi'(x) \simeq \sum_{i=0}^{N} a_i \Psi'_i(x) \text{ with } \Psi'_{2k} = -k\sin(kx),\ \Psi'_{2k+1} = k\cos(kx)$$



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Convergence to the derivative

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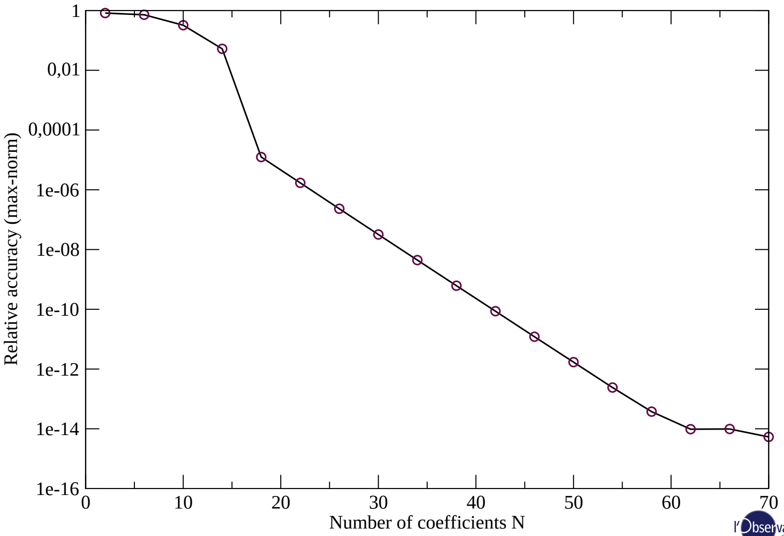
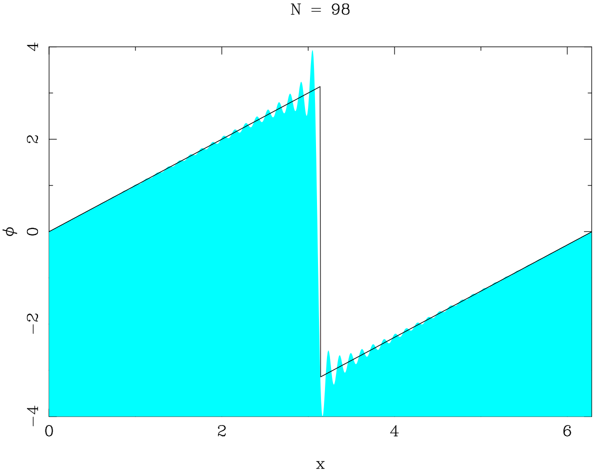


Gibbs phenomenon

no convergence for discontinuous (or non-periodic) functions!

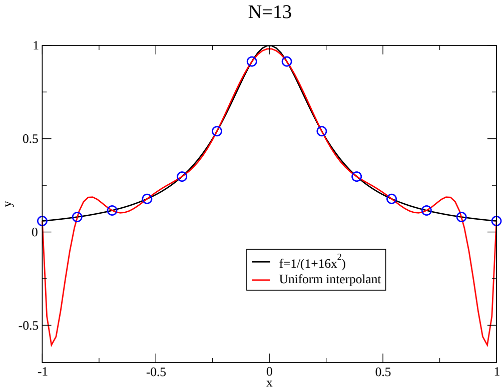
$$\phi(x) = \begin{cases} x & \text{for } x \in [0, \pi] \\ x - 2\pi & \text{for } x \in (\pi, 2\pi) \end{cases}$$



Polynomial interpolation

From the Weierstrass theorem, it is known that any continuous function can be approximated to arbitrary accuracy by a polynomial function.

In practice, with the function known on a grid $\{x_i\}_{i=0\dots N}$, one uses the Lagrange cardinal polynomials:



$$l_i(x) = \prod_{j=0, j\neq i}^{N} \frac{x - x_j}{x_i - x_j}$$

But a uniform grid is not a good choice
⇒Runge phenomenon

Orthogonal polynomials

The solutions $(\lambda_i, u_i)_{i\in\mathbb{N}}$ of a singular Sturm-Liouville problem on the interval $x \in [-1, 1]$:

$$-\left(pu'\right)' + qu = \lambda w u,$$

with $p > 0, \mathcal{C}^1, p(\pm 1) = 0$

- are orthogonal with respect to the measure w:

$$(u_i, u_j) = \int_{-1}^{1} u_i(x) u_j(x) w(x) \mathrm{d}x = 0 \text{ for } m \neq n,$$

- form a spectral basis such that, if $f(x)$ is smooth ($\mathcal{C}^\infty$)

$$f(x) \simeq \sum_{i=0}^{N} c_i u_i(x)$$

converges faster than any power of N.

Chebyshev, Legendre and, more generally any type of Jacobi polynomial enters this category.

Gauss quadrature

To get a convergent representation $\{c_i\}_{i=0\dots N}$ of a function $f(x)$, it is sufficient to be able to compute

$$\forall i, \quad c_i = \frac{\int_{-1}^{1} f(x) u_i(x) w(x) \mathrm{d}x}{\int_{-1}^{1} \left(u_i(x)\right)^2 w(x) \mathrm{d}x}.$$

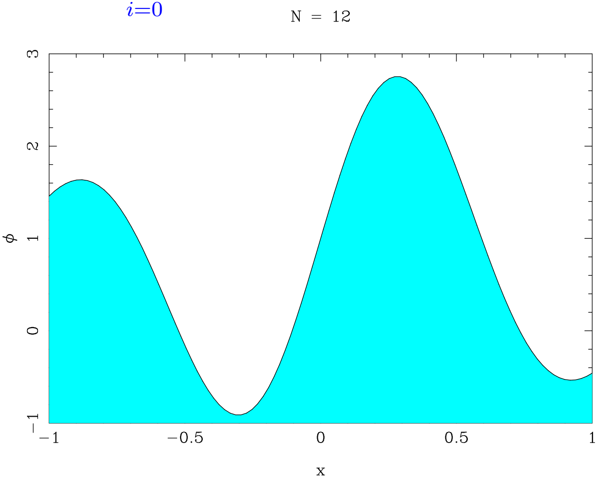
In practice, one can use the Gauss quadrature (here Gauss-Lobatto): for a given $w(x)$ and N, one can find $\{w_i\}_{k=0\dots N}$ and $\{x_i\}_{k=0\dots N} \in [-1, 1]$ such that

$$\forall g \in \mathbb{P}_{2N-1}, \quad \int_{-1}^{1} g(x) w(x) \mathrm{d}x = \sum_{k=0}^{N} g(x_k) w_k.$$

Example with Chebyshev polynomials

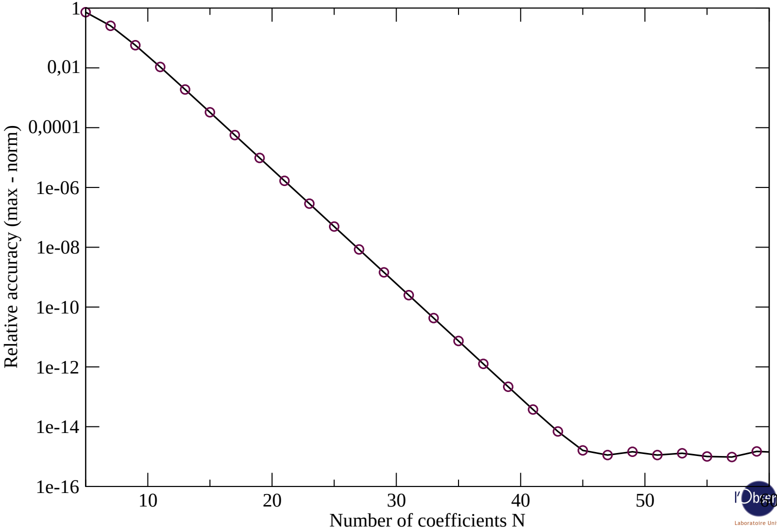
$$\phi(x) = (1 + 2\sin(5x))/(1 + x^2)$$

$$\phi(x) \simeq \sum_{i=0}^{N} a_i \Psi_i(x) \text{ with } \Psi_k = T_k(x) = \cos(k \arccos(x))$$



Example with Chebyshev polynomials

$\phi(x) = (1 + 2\sin(5x))\,/(1 + x^2)$



Linear Ordinary Differential Equations

We consider the general form of an Ordinary Differential Equation (ODE) on an interval, for the unknown function $u(x)$:

$$\begin{aligned} Lu(x) &= s(x), \quad \forall x \in [a,b] \\ Bu(x) &= 0, \quad \text{for } x = a, b, \end{aligned}$$

with L, B being two linear differential operators and $s(x)$ a given source.The approximate solution is sought in the form

$$\bar{u}(x) = \sum_{i=0}^{N} c_i \Psi_i(x).$$

The $\{\Psi_i\}_{i=0\dots N}$ are called trial functions: they belong to a finite-dimension sub-space of some Hilbert space $\mathcal{H}_{[a,b]}$.

Method of weighted residuals

A function $\bar{u}$ is said to be a numerical solution of the ODE if:

- $B\bar{u} = 0$ for $x = a, b$,
- $R\bar{u} = L\bar{u} - s$ is “small”.

Defining a set of test functions $\{\xi_i\}_{i=0...N}$ and a scalar product on $\mathcal{H}_{[a,b]}$, R is small iff:

$$\forall i = 0 \dots N, \quad (\xi_i, R) = 0.$$

It is expected that

$$\lim_{N\to\infty} \bar{u} = u,$$

the “true” solution of the ODE.

Various numerical methods

type of trial functions Ψ

- finite-differences methods for local, overlapping polynomials of low order,
- finite-elements methods for local, smooth functions, which are non-zero only on a sub-domain of $[a, b]$,
- spectral methods for global smooth functions on $[a, b]$.

type of test functions ξ for spectral methods

- tau method: $\xi_i(x) = \Psi_i(x)$, but some of the test conditions are replaced by the boundary conditions.
- collocation method (pseudospectral): $\xi_i(x) = \delta(x - x_i)$, at collocation points. Some of the test conditions are replaced by the boundary conditions.
- Galerkin method: the test and trial functions are chosen to fulfill the boundary conditions.

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Let $u(x)$ be the solution on $[0, 2\pi)$ of

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + 3\frac{\mathrm{d}u}{\mathrm{d}x} + 2u = s(x),$$

with periodic boundary conditions. If one decomposes $\bar{u}(x) = \sum_{n=0}^{N} a_n \cos(nx) + b_n \sin(nx)$ and $\bar{s}(x) = \sum_{n=0}^{N} \alpha_n \cos(nx) + \beta_n \sin(nx)$,

then, the condition on the residuals translates into

$$\begin{cases} -n^2 a_n + 3nb_n + 2a_n &= \alpha_n \\ -n^2 b_n - 3na_n + 2b_n &= \beta_n \end{cases}$$

$$\iff \begin{cases} a_n &= \frac{(2-n^2)\alpha_n + 3n\beta_n}{(n^2+1)(n^2+4)} \\ b_n &= \frac{3n\alpha_n + (2-n^2)\beta_n}{(n^2+1)(n^2+4)} \end{cases}$$

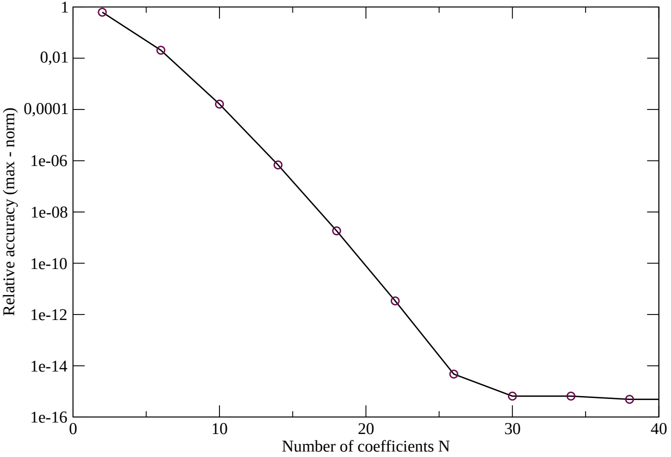
Convergence properties

Fourier Galerkin method

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + 3\frac{\mathrm{d}u}{\mathrm{d}x} + 2u = e^{\cos x}\left(\sin^2 x - \cos x - 3\sin x + 2\right)$$

Convergence of the numerical solution to the analytical one:

$$u(x) = e^{\cos x}$$



Properties of Chebyshev polynomials $T_n(x), n \in \mathbb{N}$

They are solutions of the singular Sturm-Liouville problem ($p = \sqrt{1-x^2}, q = 0, w = 1/\sqrt{1-x^2}$ and $\lambda_n = -n$). They are orthogonal on $[-1, 1]$ with respect to the weight $w = 1/\sqrt{1-x^2}$ and, starting from $T_0 = 1$, $T_1 = x$, the recurrence relation is:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

They have the simple expression which allows for the use of FFT to compute the Chebyshev transform:

$$\forall x \in [-1, 1], \quad T_n(x) = \cos(n \arccos x),$$

also, the Chebyshev-Gauss-Lobatto nodes and weights are known

$$x_n = -\cos\frac{n\pi}{N}, \quad w_0 = w_N = \frac{\pi}{2N}, w_n = \frac{\pi}{N}.$$

Linear "differential" operators

Thanks to the recurrence relations of Chebyshev polynomials, it is possible to express the coefficients $\{b_i\}_{i=0\ldots N}$ of

$$Lu(x) = \sum_{i=0}^{N} b_i T_i(x), \text{ with } u(x) = \sum_{i=0}^{N} a_i T_i(x).$$

If $L = \mathrm{d}/\mathrm{d}x$,

$$b_n = 2 \sum_{i=n+1, n+i \text{ odd}}^{N} i a_i.$$

If $L = x\times$,

$$b_n = \frac{1}{2}\left((1+\delta_{0\,n-1})a_{n-1} + a_{n+1}\right) \quad (n \geq 1).$$

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The numerical solution $\bar{u}(x)$ of

$$x^2 u''(x) - 6xu'(x) + 10u(x) = s(x),$$

can be seen as a solution of the system $L\bar{u} = \bar{s}$, where

$$\bar{u} = \sum_{i=0}^{N} a_i T_i(x) \text{ and } \bar{s} = \sum_{i=0}^{N} \alpha_i T_i(x)$$

are represented as vectors and, if $N = 5$

$$L = \begin{pmatrix} 10 & 0 & -10 & 0 & 4 \\ 0 & 4 & 0 & -18 & 0 \\ 0 & 0 & 0 & 0 & -8 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

$$L = \begin{pmatrix} 10 & 0 & -10 & 0 & 4 \\ 0 & 4 & 0 & -18 & 0 \\ 0 & 0 & 0 & 0 & -8 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

is not an invertible matrix. In order to get the solution of the ODE, one must specify exactly two boundary conditions. e.g.

1. $u(x=-1)=0$, and
2. $u(x=1)=0$.

Since

$$\forall i, \quad T_i(-1) = (-1)^i, \text{ and } T_i(1) = 1,$$

in the tau method, the last two lines of the matrix representing L are replaced by the two boundary conditions.

$$L = \begin{pmatrix} 10 & 0 & -10 & 0 & 4 \\ 0 & 4 & 0 & -18 & 0 \\ 0 & 0 & 0 & 0 & -8 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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Singular operators

- The operator $u(x) \mapsto \dfrac{u(x)}{x}$ is a linear operator, inverse of $u(x) \mapsto xu(x)$.
- Its action on the coefficients $\{a_i\}_{i=0\ldots N}$ representing the N-order approximation to a function $u(x)$ can be computed as the product by a regular matrix.

⇒The computation in the coefficient space of $u(x)/x$, on the interval $[-1, 1]$ always gives a finite result.

⇒The actual operator which is thus computed is

$$u(x) \mapsto \frac{u(x) - u(0)}{x}.$$

⇒The same holds for $u(x) \mapsto \dfrac{u(x)}{x-1}$ and $u(x) \mapsto \dfrac{u(x)}{x+1}$.

⇒possibility of computing a singular ratio $\dfrac{f}{g}$.

Spectral solution of an ODE

Chebyshev-tau method

The Poisson equation in spherical symmetry and spherical coordinates writes

$$\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}u}{\mathrm{d}r} = s(r).$$

To be regular, $u(r)$ and $s(r)$ must be even functions of r.

- it is sufficient to use only even Chebyshev polynomials for $x \in [0, 1]$,
- it is necessary to specify one boundary condition at $x = 1$.
- the matrix of the spectral Chebyshev-tau method of approximating the solution is (with $u(x = 1) =$const)

$$L = \begin{pmatrix} 0 & 12 & 32 & 132 & 256 \\ 0 & 0 & 80 & 192 & 544 \\ 0 & 0 & 0 & 168 & 384 \\ 0 & 0 & 0 & 0 & 288 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

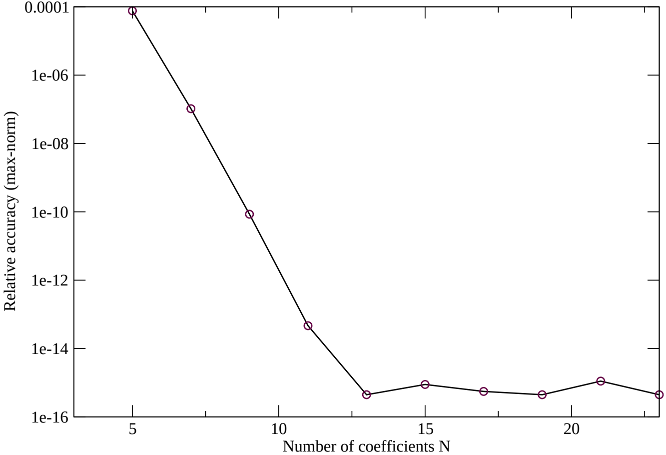
Convergence of the solution

Chebyshev-tau method

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + \frac{2}{x}\frac{\mathrm{d}u}{\mathrm{d}x} = (4x^2 - 6)e^{-x^2} \text{ and } u(x=1) = 1/e.$$

Convergence of the numerical solution to the analytical one:

$$u(x) = e^{-x^2}$$



Multi-domain and multi-dimensional settings

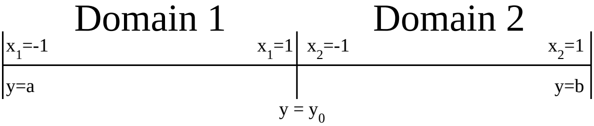
with spherical coordinates

Multi-domains techniques

Motivations and settings

Multi-domain technique consists in having several touching, or overlapping, domains (intervals), each one mapped on $[-1, 1]$.

- the boundary between two domains can be the place of a discontinuity of the function, or its derivatives $\Rightarrow$recover spectral convergence,
- one can set a domain with more coefficients (collocation points) in a region where much resolution is needed $\Rightarrow$fixed mesh refinement,
- 2D or 3D, allows to build a complex domain from several simpler ones,
- it is possible to treat a function in each domain on a different CPU $\Rightarrow$parallelization.



Consider the ODE:

$\forall y \in [a,b], \quad Lu(y) = s(y)$, with boundary conditions on $u(y=a,\, b)$.

The numerical solution is sought in the form

$$\begin{cases} \forall y \leq y_0, & \bar{u}(y) = \sum_{i=0}^{N_1} c_i^1 T_i\left(x_1(y)\right), \\ \forall y \geq y_0, & \bar{u}(y) = \sum_{i=0}^{N_2} c_i^2 T_i\left(x_2(y)\right), \end{cases}$$

To determine the $N_1 + N_2 + 2$ coefficients, one takes:

- $N_1 - 1$ residual equations for domain 1,
- $N_2 - 1$ residual equations for domain 2,
- 2 boundary conditions at $x_1 = -1$ and $x_2 = 1$,
- 2 matching conditions at $y = y_0$:
  $\bar{u}(x_1 = 1) = \bar{u}(x_2 = -1)$ and $\bar{u}'(x_1 = 1) = \bar{u}'(x_2 = -1)$.

$\Rightarrow$considering a big vector of size $N_1 + N_2 + 2$, one has in principle an invertible system and thus a uniquely defined numerical solution.

Domain matching

collocation method / homogeneous solutions

The collocation multi-domain method is like the tau one:

- write the residual equations on the interior collocation points $\{x_{i1}, x_{j2}\}_{i=1\ldots(N_1-1), j=1\ldots(N_2-1)}$,
- write the two boundary conditions at x_{11} and x_{2N_2}, and the matching condition at $y = y_0$ (x_{1N_1} and x_{20}).

If one knows explicitely the homogeneous solutions $u_\lambda(y)$ and $u_\mu(y)$ of

$$\forall y \in [a, b], \quad Lu(y) = 0,$$

then after getting a particular solution in each domain, solving

$$d = 1, 2 \; Lu_p^d(x_d) = \bar{s}(x_d), \text{ with e.g. } u(x_p^d = \pm 1) = 0,$$

one is left with the determination of the linear combination in each domain $$u^d(x_d) = u_p^d(x_d) + \lambda_d u_\lambda(x_d) + \mu_d u_\mu(x_d)$$

such that it verifies the boundary and the matching conditions (system in $\{\lambda_d, \mu_d\}_{d=1,2}$).

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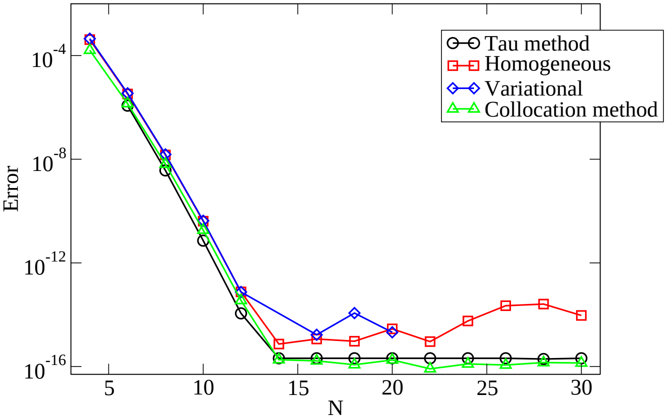
Comparison

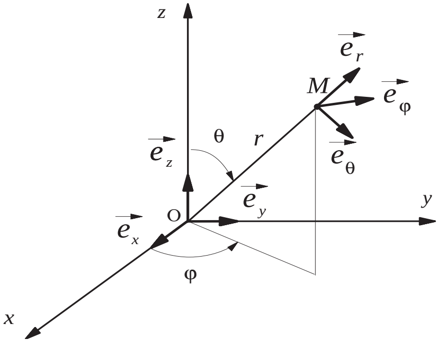
Accuracy on the solution of $\frac{d^2u}{dy^2} + 4u = S$, with $S(y \leq 0) = 1$ and $S(y \geq 0) = 0$. $N_1 = N_2 = N$.



Spatial compactification

- A mapping not specific to spectral methods.
- Consider the simple case of $\zeta = \frac{1}{r} = \alpha(x-1),\ x \in [-1,1]$,
- the spherically symmetric Laplace operator writes
$$\Delta u = \frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}u}{\mathrm{d}r} = \zeta^4 \frac{\mathrm{d}^2 u}{\mathrm{d}\zeta^2},$$
- and it is possible to impose boundary conditions at $r \to \infty \iff \zeta = 0$.
- Other types of compactification are possible ($\tan, \dots$), even combining (t, r) coordinates in conformal compactification.
- Keep in mind that properties of some PDEs may change with the mapping: the $\zeta = \frac{1}{r}$ is not compatible with the characteristics of the wave equation $\Box u = \frac{\partial^2 u}{\partial t^2} - \Delta u = s$.

Spherical coordinates



- are well-adapted to describe isolated astrophysical systems: single star or black hole, where the surface is spheroidal,
- compactification needs only to be done for r,
- the boundary surface $r = \text{const}$ is a smooth one.
- allow the use of spherical harmonics,
- the coordinate singularities can be nicely handled with spectral methods,
- spherical and axial symmetries nicely handled.

Regularity conditions

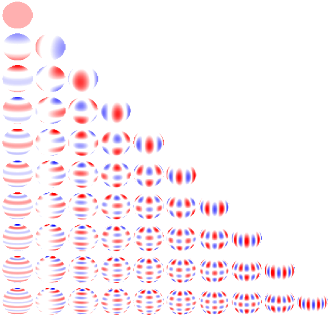
Considering (e.g.) the Laplace operator, which is regular:

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right),$$

division by r or $\sin\theta$ look singular. ⇒a regular field $u(r,\theta,\varphi)$ must have a particular behavior.

- if u is expandable in series of powers of x, y and z, near $r = 0$: $u(x,y,z) = \sum_{i,j,k} a_{ijk} x^i y^j z^k$.
- changing to spherical coordinates $u(r,\theta,\varphi) = \sum_{n,p,q} a_{npq} r^{n+p+q} \cos^q\theta \sin^{n+p}\theta \cos^n\varphi \sin^p\varphi$;
- and rearranging the terms $u(r,\theta,\varphi) = \sum_{m,p,q} b_{mpq} r^{|m|+2p+q} \sin^{|m|+2p}\theta \cos^q\theta e^{im\varphi}$
- introducing $\ell = |m| + 2p + q$ and the spherical harmonics $Y_\ell^m(\theta,\varphi)$, one gets the following consequences for u:
- near $\theta = 0$, $u(\theta) \sim \sin^{|m|}\theta$,
- near $r = 0$, $u(r) \sim r^\ell$ and has the same parity as ℓ.

Spherical harmonics



- are pure angular functions $Y_\ell^m(\theta,\varphi)$, forming an orthonormal basis for the space of regular functions on a sphere:
  $\ell \geq 0,\ |m| \leq \ell,$
  $Y_\ell^m(\theta,\varphi) \propto P_\ell^m(\cos\theta)e^{im\varphi}.$
- are eigenfunctions of the angular part of the Laplace operator:

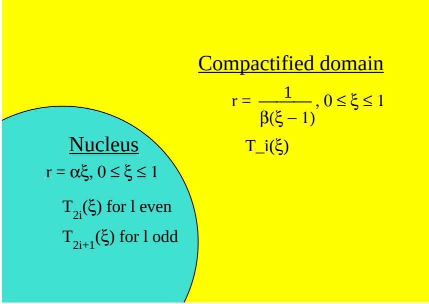
$$\Delta_{\theta\varphi} Y_\ell^m(\theta,\varphi) := \frac{\partial^2 Y_\ell^m}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial Y_\ell^m}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_\ell^m}{\partial\varphi^2} = -\ell(\ell+1)Y_\ell^m(\theta,\varphi).$$

$\Rightarrow$they can form a spectral decomposition basis for functions defined on a spheroid (e.g. apparent horizon)
$\Rightarrow$they can simplify the solution of a Poisson equation

Example:

3D Poisson equation, with non-compact support

To solve $\Delta\phi(r,\theta,\varphi) = s(r,\theta,\varphi)$, with s extending to infinity.



- setup two domains in the radial direction: one to deal with the singularity at $r = 0$, the other with a compactified mapping.
- In each domain decompose the angular part of both fields onto spherical harmonics:

$$\phi(\xi,\theta,\varphi) \simeq \sum_{\ell=0}^{\ell_{\max}} \sum_{m=-\ell}^{m=\ell} \phi_{\ell m}(\xi) Y_\ell^m(\theta,\varphi),$$

- $\forall(\ell, m)$ solve the ODE: $\dfrac{\mathrm{d}^2\phi_{\ell m}}{\mathrm{d}\xi^2} + \dfrac{2}{\xi}\dfrac{\mathrm{d}\phi_{\ell m}}{\mathrm{d}\xi} - \dfrac{\ell(\ell+1)\phi_{\ell m}}{\xi^2} = s_{\ell m}(\xi),$
- match between domains, with regularity conditions at $r = 0$, and boundary conditions at $r \to \infty$.

Non-linear problems

Solution of a boundary value problem

$$Lu = Nu$$

Newton-Raphson method

- for $F(\bar{u}) = (L - N)\,(c_0, \dots, c_N) = 0$:
- compute $J_{ij} = \dfrac{\partial F_i}{\partial c_j}$,
- start from an initial guess $\bar{u}_0$, and solve $J(\bar{u}_1 - \bar{u}_0) = -F\bar{u}_0 \dots$

$\Rightarrow J$ may be complicated to compute!

iterative method

- if the inversion of L is easy,
- start from initial guess $\bar{u}_0$, compute $N\bar{u}_0$ and
- solve the linear operator to get $\bar{u}_1 = L^{-1}\,N\bar{u}_0 \dots$

$\Rightarrow$no reason to converge!

“Mariage des Maillages” (MdM):

Interpolation and filtering

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Combination of two numerical techniques

- hydrodynamics $\Rightarrow$High-Resolution Shock-Capturing schemes (HRSC), presented by Pablo tomorrow;
- gravity $\Rightarrow$multi-domain spectral solver using spherical harmonics and Chebyshev polynomials, with a compactification of type $u = 1/r$.

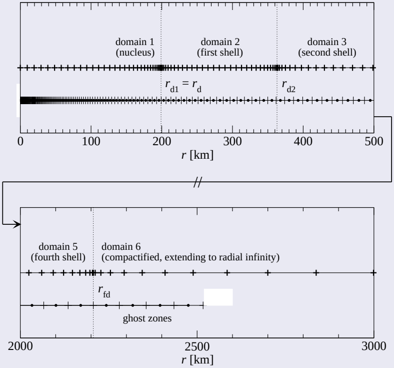
Use of two numerical grids with interpolation:

- matter sources: Godunov (HRSC) grid $\longrightarrow$ spectral grid;
- gravitational fields: spectral grid $\longrightarrow$ Godunov grid.

First achieved in the case of spherical symmetry, in tensor-scalar theory of gravity (Novak & Ibáñez 2000).
Spares a lot of CPU time in the gravitational sector, that can be used for other physical ingredients.

- Godunov grid stops at a finite distance ⇒no matter outside;

Grid setting

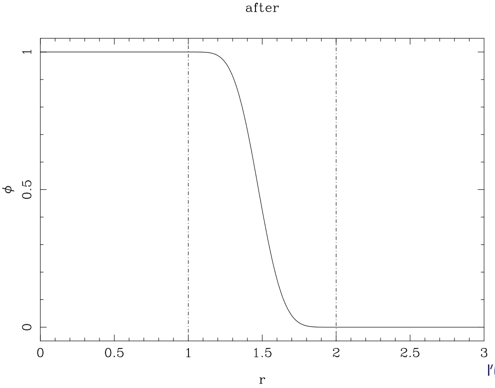


- interpolation to spectral grid using piecewise parabolic formula (many tested);
- fewest possible manipulations of these fields on spectral grid;
- partial summation technique (Orszag 1980) to gain CPU in the spectral summation.

One the main limitations for the use of spectral methods is the Gibbs phenomenon.⇒possibility to use filters: e.g.

$$c_n \mapsto c_n \times e^{-\alpha\left(\frac{n}{N}\right)^{2p}}$$

⇒spectral series converging with order p
⇒quite useful for discontinuous sources in core-collapse simulations.



On spectral methods. . .

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