Spectral methods for numerical relativity

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Plan of the lecture

1. Introduction: representation of functions
2. Linear Ordinary Differential Equations
3. Time-dependent problems
4. Multi-domain techniques
5. Fields in 2D and 3D: coordinates and mappings
6. Examples in numerical relativity

Introduction:
Representation of functions

How to deal with functions on a computer?

$\Rightarrow$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

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

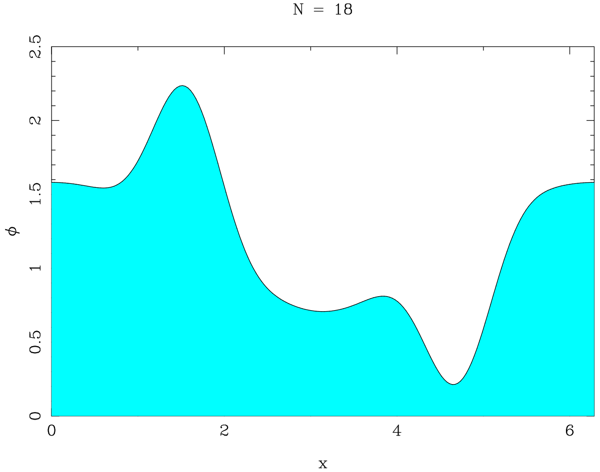
- spectral methods

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

Convergence of Fourier series

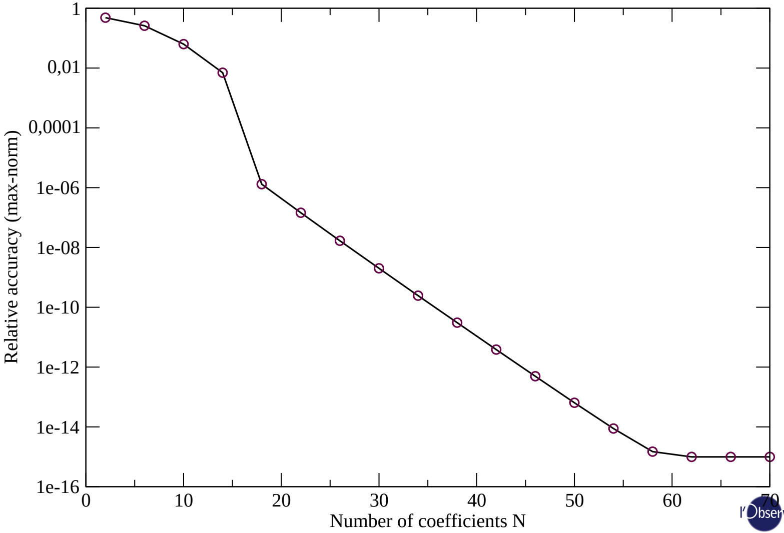
$$\phi(x) = \sqrt{1.5 + \cos(x)} + \sin^7 x$$

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



Convergence of Fourier series

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



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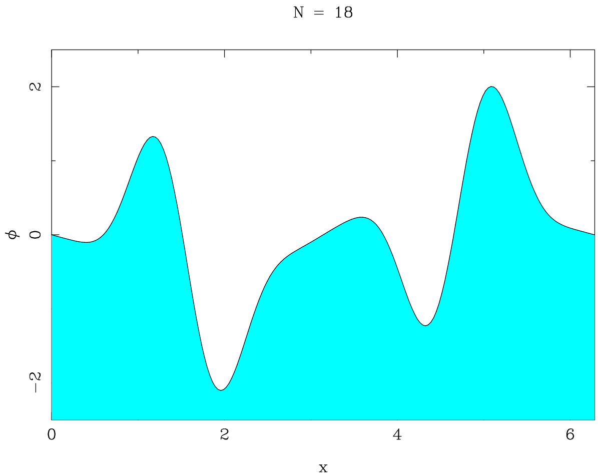
Convergence to the derivative

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

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



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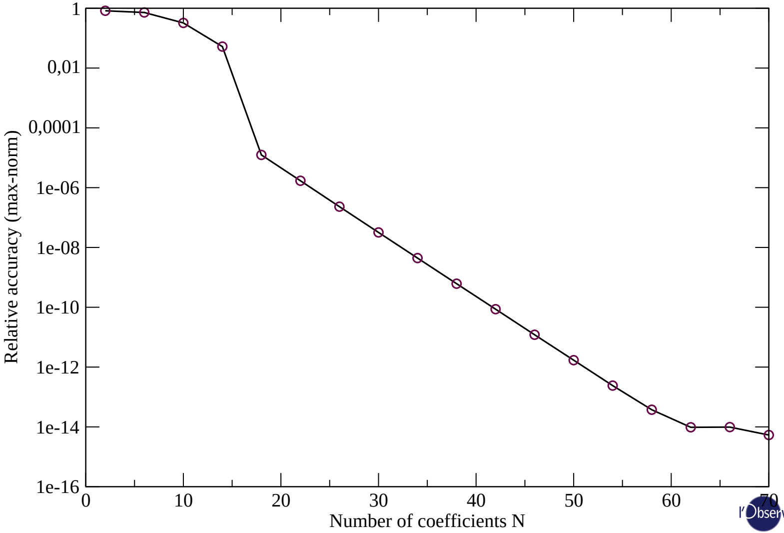
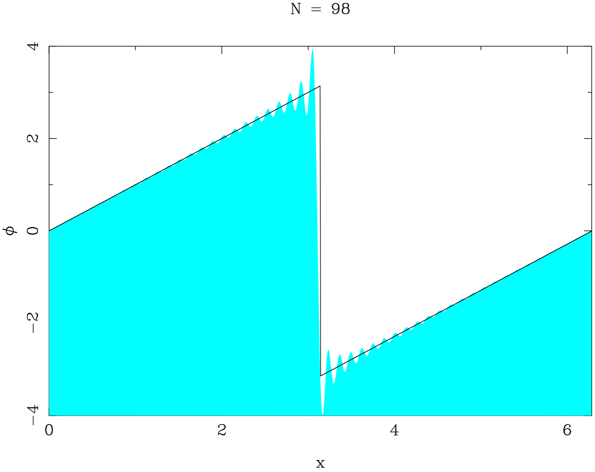


Gibbs phenomenon

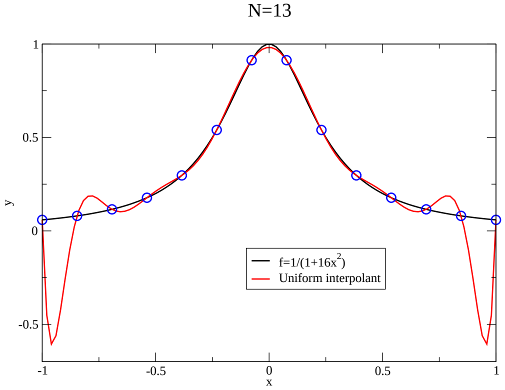
no convergence for discontinuous (or non-periodic) functions!

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



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 $\{x_i\}_{i=0\ldots N}$, 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
$\Rightarrow$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 $\{c_i\}_{i=0\ldots N}$ of a function $f(x)$, it is sufficient to be able to compute

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

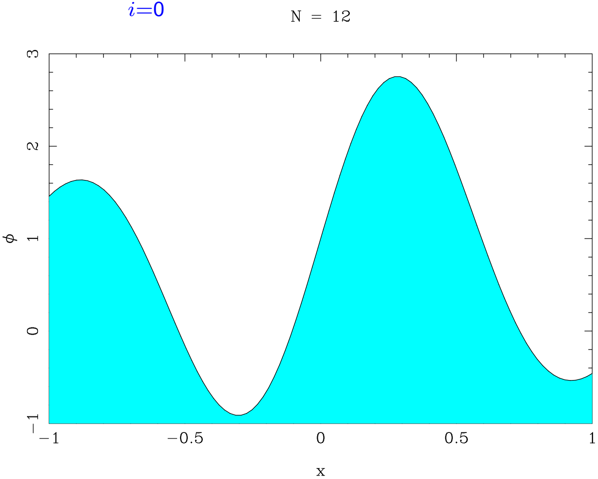
In practice, one can use the Gauss quadrature (here Gauss-Lobatto): for a given $w(x)$ and N, one can find $\{w_i\}_{k=0\ldots N}$ and $\{x_i\}_{k=0\ldots N} \in [-1, 1]$ such that

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

Example with Chebyshev polynomials

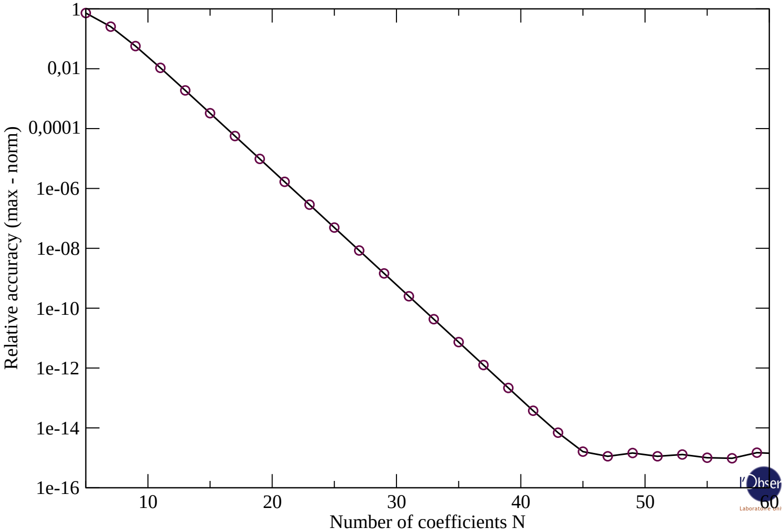
$$\phi(x) = (1 + 2\sin(5x))\,/(1 + x^2)$$

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



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 $\mathcal{H}_{[a,b]}$.

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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 $\{\xi_i\}_{i=0\dots N}$ 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.

Spectral solution of an ODE
Fourier Galerkin method

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

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

with periodic boundary conditions. If one decomposes

$$\bar{u}(x) = \sum_{n=0}^{N} a_n \cos(nx) + b_n \sin(nx) \text{ and } \bar{s}(x) = \sum_{n=0}^{N} \alpha_n \cos(nx) + \beta_n \sin(nx),$$

then, the condition on the residuals translates into

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

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

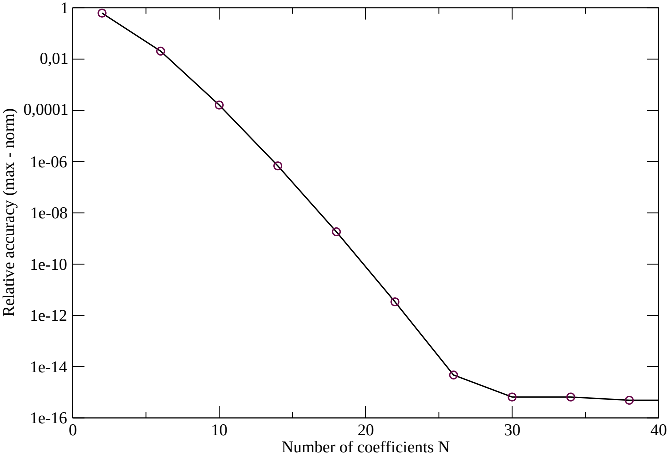
Convergence properties

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 Legendre polynomials $P_n(x), n \in \mathbb{N}$

They are solutions of the singular Sturm-Liouville problem ($p = 1 - x^2, q = 0, w = 1$ and $\lambda_n = -n(n+1)$):

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)\frac{\mathrm{d}P_n}{\mathrm{d}x}\right) = -n(n+1)P_n;$$

they are orthogonal on $[-1, 1]$ with respect to the weight $w = 1$ and, starting from $P_0 = 1$, $P_1 = x$, the recurrence relation is:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

The $\{x_i\}_{i=1\ldots N-1}$ are zeros of $P'_N(x)$, and must be computed numerically. They give the Legendre-Gauss-Lobatto weights

$$w_n = \frac{2}{N(N+1)}\frac{1}{(P_N(x_n))^2}.$$

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

$$Lu(x) = \sum_{i=0}^{N} b_i \left| \begin{array}{l} P_i(x) \\ T_i(x) \end{array} \right., \text{ with } u(x) = \sum_{i=0}^{N} a_i \left| \begin{array}{l} P_i(x) \\ T_i(x) \end{array} \right. .$$

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

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

If $L = x\times$, for Chebyshev polynomials

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

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

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

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 $\{a_i\}_{i=0\dots N}$ 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 (both with Chebyshev and Legendre polynomials).

⇒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 $\dfrac{f}{g}$.

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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 (or Legendre) 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)

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

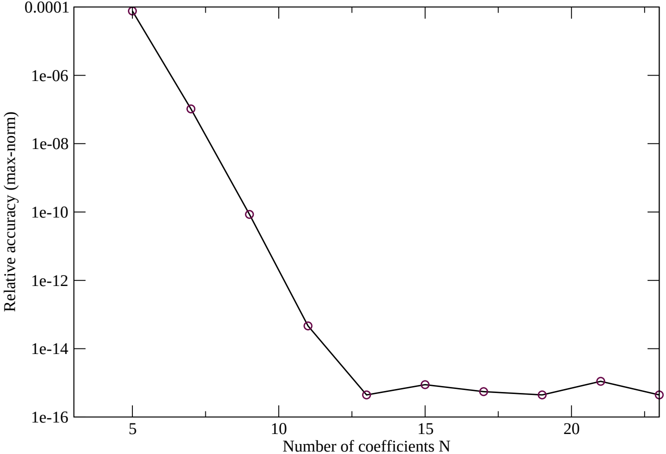
Convergence of the solution

Chebyshev-tau method

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

Convergence of the numerical solution to the analytical one:

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



Time-dependent problems

Time discretization

Formally, the representation (and manipulation) of $f(t)$ is the same as that of $f(x)$.
$\Rightarrow$in principle, one should be able to represent a function $u(x,t)$ and solve time-dependent PDEs only using spectral methods...but this is not the way it is done! Two works:

- Ierley *et al.* (1992): study of the Korteweg de Vries and Burger equations, Fourier in space and Chebyshev in time $\Rightarrow$time-stepping restriction.
- Hennig and Ansorg (2008): study of non-linear (1+1) wave equation, with conformal compactification in Minkowski space-time. $\Rightarrow$nice spectral convergence.

WHY?

- poor *a priori* knowledge of the exact time interval,
- too big matrices for full 3+1 operators ($\sim 30^4 \times 30^4$),
- finite-differences time-stepping errors can be quite small.

Explicit / Implicit schemes

Let us look for the numerical solution of (L acts only on x):

$$\forall t \geq 0, \quad \forall x \in [-1, 1], \quad \frac{\partial u(x,t)}{\partial t} = Lu(x,t),$$

with good boundary conditions. Then, with δt the time-step:

$$\forall J \in \mathbb{N}, \quad u^J(x) = u(x, J \times \delta t),$$

it is possible to discretize the PDE as

- $u^{J+1}(x) = u^J(x) + \delta t\, Lu^J(x)$: explicit time scheme (forward Euler); from the knowledge of $u^J(x)$, it is possible to compute directly u^{J+1}, by applying L ("deriving").
- $u^{J+1}(x) - \delta t\, Lu^{J+1}(x) = u^J(x)$: implicit time scheme (backward Euler); one must solve an equation (ODE) to get u^{J+1}, the matrix approximating it here is $I - \delta t\, L$.

Temporal stability analysis

For each t, the field $u(x,t)$ is approximated by $U_N(t)$, the vector of $N+1$ time-dependent spectral coefficients (Galerkin / tau methods) or values at grid points (collocation method)

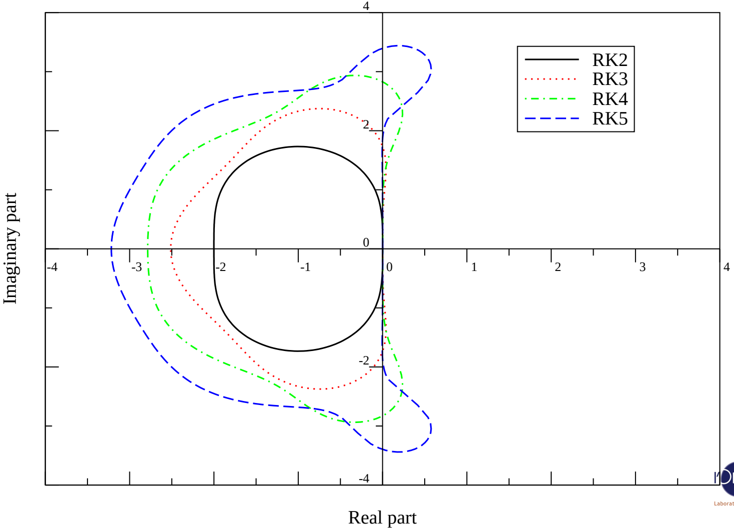
$$\forall t \geq 0, \quad \frac{\partial U_N}{\partial t} = L U_N(t).$$

The matrix L (including the boundary conditions) admits $N+1$ complex eigenvalues $\{\lambda_i\}_{i=0\dots N}$ and the PDE is equivalent to a set of time ODEs

$$\forall t \geq 0, \forall i = 0 \dots N, \quad \frac{\mathrm{d}a_i}{\mathrm{d}t} = \lambda_i a_i(t).$$

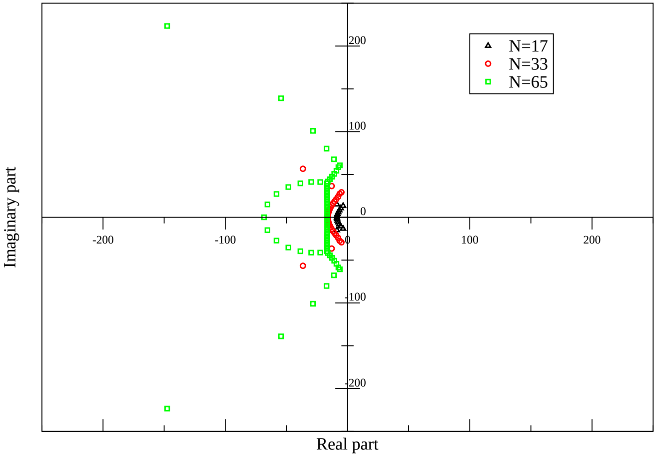
$\Rightarrow$for a given ODE time-integration scheme, the region of absolute stability is the set of the complex plane containing all the $\lambda_i \delta t$, for which all the $\{a_i(t)\}_{i=0\dots N}$ remain bounded in time.

Regions of absolute stability for various Runge-Kutta schemes.



Eigenvalues of $L = \frac{\partial}{\partial x}$

Chebyshev-tau method



An eigenvalue on the negative part of the real axis, which is too negative, is not displayed $\mathcal{O}(-N^2)$.

Pros and cons

Drawback of explicit schemes:

- CFL time-step limitation $\delta t \lesssim \dfrac{1}{\max(|\lambda_i|)}$,$\Rightarrow$for advection equation with Chebyshev or Legendre

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial u(x,t)}{\partial x}, \text{ the time-step } \delta t \lesssim \frac{1}{N^2}.$$

Drawbacks of implicit schemes:

- more complicated to implement: boundary-value problem at each time-step,
- also limited by CFL-like condition for linear multi-step methods of order higher than 2 (Dahlquist barrier).

Example of time-integration
Fourier Galerkin

Let us solve the PDE:

$$\begin{array}{rcl} \forall x \in [0, 2\pi], \forall t \geq 0, \quad \dfrac{\partial u(x,t)}{\partial t} & = & \dfrac{\partial u(x,t)}{\partial x}, \\ \forall t \geq 0, \quad u(2\pi, t) & = & u(0,t), \\ \forall x \in [0, 2\pi], \quad u(x, 0) & = & e^{\cos x}. \end{array}$$

If one decomposes: $\bar{u}(x,t) = \sum_{n=0}^{N} a_n(t) \cos(nx) + b_n(t) \sin(nx)$
then, the forward Euler scheme writes:

$$\left\{ \begin{array}{rcl} a_n^{J+1} & = & a_n^J + n\,\delta t\, b_n^J \\ b_n^{J+1} & = & b_n^J - n\,\delta t\, a_n^J \end{array} \right.$$

and the backward Euler:

$$\left\{ \begin{array}{rcl} a_n^{J+1} - n\,\delta t\, b_n^{J+1} & = & a_n^J \\ n\,\delta t\, a_n^{J+1} + b_n^{J+1} & = & b_n^J \end{array} \right.$$

Two examples with $\delta t = 0.01$ and $\delta t = 0.1$.

Boundary conditions

Implicit schemes

An ODE is solved to advance from one time-step to the next, e.g.:
$$(I - \delta t\, L)\, U_N^{J+1} = U_N^J,$$
the boundary conditions are imposed as for ODEs.

Explicit schemes

One can directly compute the coefficients at the new time-step, e.g.:
$$U_N^{J+1} = U_N^J + L\, U_N^J.$$
With b boundary conditions, the tau method requires the change of the last b coefficients of U_N^{J+1} so that $\bar{u}^{J+1}(x)$ fulfills the boundary conditions.

For example, if $\bar{u}^{J+1}(x) = \sum_{i=0}^{N} c_i T_i(x)$ and one requires $\bar{u}^{J+1}(x=1) = 0$, the $\{c_i\}_{i=0\dots N-1}$ are advanced and
$$c_N = -\sum_{i=0}^{N-1} c_i.$$

Collocation explicit schemes

- Let $\{x_i\}_{i=0\dots N}$ be (e.g.) the Legendre-Gauss-Lobatto collocation points: $x_0 = -1, x_N = 1$ and $\forall i = 1 \dots N-1, \quad P'_N(x_i) = 0$.
- Using the Lagrange cardinal polynomials, or the Legendre polynomials properties, it is possible to compute the differentiation matrix D_{ij}:

$$\forall i = 0 \dots N, \forall Q \in \mathbb{P}_N[X], \quad Q'(x_i) = \sum_{j=0}^{N} D_{ij} Q(x_j).$$

- The time integration of the advection PDE (with $u(1,t) = 0$ condition) writes:

$$\forall i = 0 \dots N-1, \quad \frac{\partial \bar{u}(x_i,t)}{\partial t} = \sum_{j=0}^{N} D_{ij} \bar{u}(x_j,t)$$
$$\bar{u}(x_N,t) = 0$$

Boundary conditions
Penalty method for collocation schemes

- In all previous examples, the boundary conditions were enforced strongly: the numerical solution $\bar{u}(x,t)$ satisfies the BCs up to machine precision.
- In particular, in collocation methods, the PDE is not satisfied at the (neighborhood of the) boundary point.

In the penalty method, the boundary condition is enforced through a penalty term at the boundary collocation point

$$\forall i = 0 \dots N, \quad \frac{\partial \bar{u}(x_i,t)}{\partial t} = \sum_{j=0}^{N} D_{ij}\bar{u}(x_j,t) - \tau \frac{(1+x_i)P'_N(x_i)}{2P'_N(x_N)} \left(\bar{u}(x_N,t) - 0\right),$$

where τ is an adjustable constant such that the problem be well-posed and stable.⇒The boundary condition is enforced up to the precision of the scheme.

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Chebyshev collocation example
Advection equation

Initial data $\forall x \in [-1, 1], \quad u(x, 0) = e^{-4x^2} - e^{-4}$
at Chebyshev-Gauss-Lobatto collocation points
$\{x_k = -\cos(k\pi/N)\}_{k=0\dots N}$.

$\Downarrow$

LOOP

- computation of $\frac{\partial u^J}{\partial x}$ (derivation matrix or coefficients),
- advance to next time-step

$$\forall k = 0 \dots N, \quad u^{J+1}(x_k) = u^J(x_k) + \delta t \, \frac{\partial u^J(x_k)}{\partial x}$$

- and don't forget the boundary condition:

$$u^{J+1}(x_N) = 0.$$

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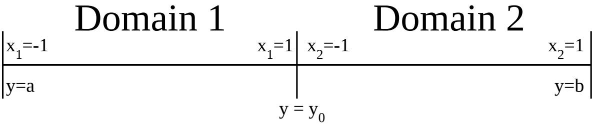
Multi-domain (or patching) techniques

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 ⇒recover spectral convergence,
- one can set a domain with more coefficients (collocation points) in a region where much resolution is needed ⇒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 ⇒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.

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 $\{\lambda_d, \mu_d\}_{d=1,2}$).

Variational matching method
(Legendre, numerically integrated)

Only with Legendre collocation method (i.e. polynomials orthogonal with $w(x) = 1$). Considering only $Lu(y) = u''(y)$ the residual equation gives, in each domain:

$$\int_{-1}^{1} \xi_n u'' \,\mathrm{d}x_d = \int_{-1}^{1} \xi_n S \,\mathrm{d}x_d \Rightarrow \left[\xi_n u'\right]_{-1}^{1} - \int_{-1}^{1} \xi_n' u' \,\mathrm{d}y = \int_{-1}^{1} \xi_n S \,\mathrm{d}y.$$

With Legendre-Gauss-Lobatto quadrature and $\xi_n(x_{di}) = \delta_{nj}$:

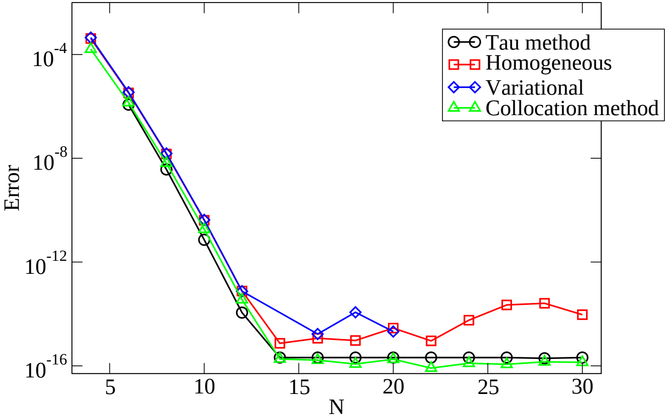
$$\forall n = 1 \dots N_d - 1,\ -\sum_{i=0}^{N_d} \sum_{j=0}^{N_d} D_{ij} D_{in} w_i u\left(x_{dj}\right) = S\left(x_{dn}\right) w_n.$$

2 more equations are obtained from the boundary conditions, and 1 from the continuity requirement at $y = y_0$. The derivative at this point is obtained from the integrated part

$$u'\left(x_1 = 1\right) = \sum_{i=0}^{N_1} \sum_{j=0}^{N_1} D_{ij} D_{iN_1} w_i u\left(x_{1j}\right) + S\left(x_{1N_1}\right) w_{N_1}.$$

Comparison

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



Fields in 2D and 3D: coordinates and mappings

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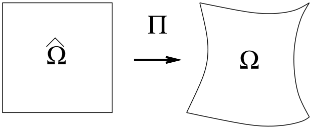
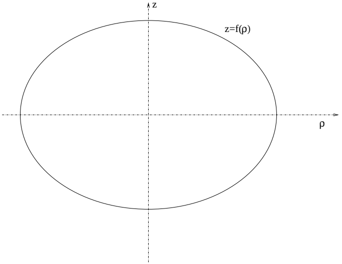
Tensor product and mappings

In two spatial dimensions, the usual technique is to write a function as:

$$f \quad : \quad \hat{\Omega} = [-1,1] \times [-1,1] \rightarrow \mathbb{R}$$

$$f(x,y) \quad = \quad \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} c_{ij} P_i(x) P_j(y)$$





- The domain $\hat{\Omega}$ is then mapped to the real physical domain, trough some mapping $\Pi : (x,y) \mapsto (X,Y) \in \Omega$.
- When computing derivatives, the Jacobian of Π is used.
- For example, the interior of an axisymmetric star can be described

$$(s,t) \in [0,1]^2 \xrightarrow{\Pi} (\rho, z) \in [0, \rho_{\max}] \times [0, z(\rho)].$$

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Example:
Fourier method for 3D Poisson equation

In (e.g.) simulations of cosmic structure formation, one has to solve a Poisson equation to get the gravitational potential:

$$\Delta\phi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\phi = 4\pi G\rho(x, y, z),$$

with periodic boundary conditions.Writing:

$$\begin{aligned}
\phi(x, y, z) &= \sum_{k_x=0}^{N_x}\sum_{k_y=0}^{N_y}\sum_{k_z=0}^{N_z} a_{k_x k_y k_z} e^{i(k_x x + k_y y + k_z z)},\\
\rho(x, y, z) &= \sum_{k_x=0}^{N_x}\sum_{k_y=0}^{N_y}\sum_{k_z=0}^{N_z} c_{k_x k_y k_z} e^{i(k_x x + k_y y + k_z z)},
\end{aligned}$$

one gets the set of simple equations:

$$\forall (k_x, k_y, k_z) \neq (0, 0, 0), \quad a_{k_x k_y k_z} = -\frac{c_{k_x k_y k_z}}{k_x^2 + k_y^2 + k_z^2}.$$

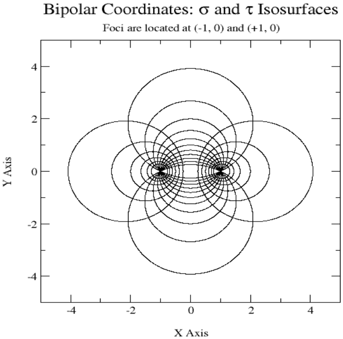
Spatial compactification

- 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 $\Box u = \frac{\partial^2 u}{\partial t^2} - \Delta u = s$.

Types of coordinates

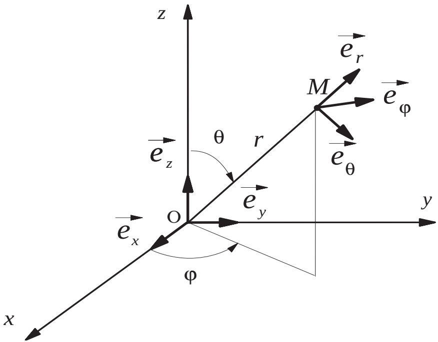
List of coordinates used in numerical relativity, with spectral methods (flat line element):

- Cartesian (rectangular) coordinates: $ds^2 = dx^2 + dy^2 + dz^2$.
- Circular cylindrical coordinates: $ds^2 = d\rho^2 + \rho^2\, d\phi^2 + dz^2$, singular on the z-axis ($\rho = 0$).
- Spherical (polar) coordinates: $ds^2 = dr^2 + r^2\, d\theta^2 + r^2 \sin^2\theta\, d\varphi^2$, singular at the origin ($r = 0$) and on the $z-$axis.



- Prolate spheroidal coordinates: $ds^2 = a^2 \left(\sinh^2\mu + \sin^2\nu\right)\left(d\mu^2 + d\nu^2\right) + a^2 \sinh^2\mu \sin^2\nu\, d\varphi^2$, singular for $\mu = 0$ and $\nu = 0, \pi$ (the foci are at $x = \pm a$).
- Bispherical coordinates: $ds^2 = a^2 \left(\cosh\sigma - \cos\tau\right)^{-2}\left(d\sigma^2 + d\tau^2 + \sin^2\tau\, d\right.$ The foci situated at $x = \pm a$ on the focal axis exhibit coordinate singularities.

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

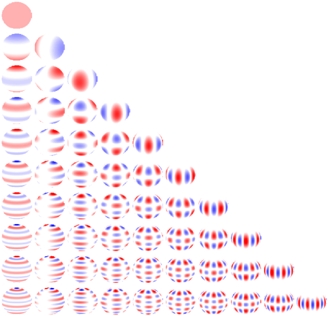
Considering (e.g.) the Laplace operator, which is regular:

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

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:

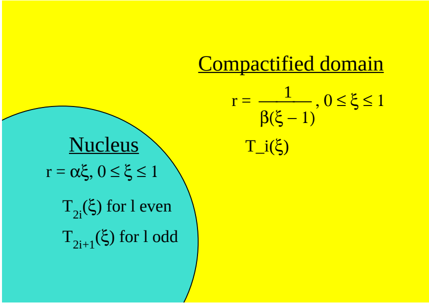
$$\Delta_{\theta\varphi} Y_\ell^m(\theta,\varphi) := \frac{\partial^2 Y_\ell^m}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial Y_\ell^m}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_\ell^m}{\partial\varphi^2} = -\ell(\ell+1)Y_\ell^m(\theta,\varphi).$$

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

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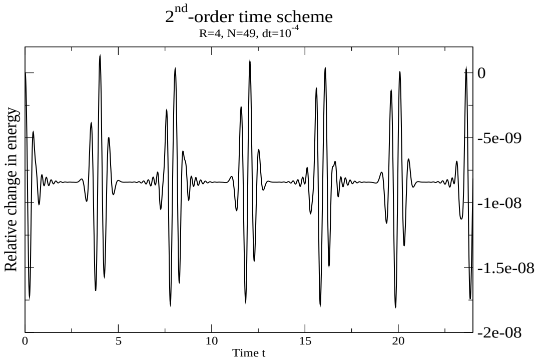
Scalar wave equation

Time-dependent 3D problems can be treated similarly, e.g. the case of the wave equation $\frac{\partial^2 \phi(r,\theta,\varphi)}{\partial t^2} = \Delta\phi(r,\theta,\varphi)$, inside a sphere of radius R, with homogeneous boundary conditions $\phi(r=R)=0$ (reflection), for $\ell = m = 0, 2$ modes.

$\Rightarrow$use of Chebyshev-tau method and explicit second-order time-scheme:

$$\phi^{J+1} = 2\phi^J - \phi^{J-1} + \delta t^2 \Delta\phi^J.$$



$\Rightarrow$Check the conservation of energy in the grid:

$$\mathcal{E} = \sqrt{\sum_{x^i=t,r,\theta,\varphi} \left(\frac{\partial\phi}{\partial x^i}\right)^2},$$

for $\delta t = 0.0001$

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Vector and tensor components

Vector components expressed in the spherical triad do not behave like scalars: they cannot be expanded onto a basis of $Y_\ell^m(\theta, \varphi)$.⇒two solutions:

- use Cartesian triad, where $\beta^{x,y,z}(r, \theta, \varphi)$ can be expanded onto Y_ℓ^m, and use scalar solvers (drawback: needs more points in (θ, φ))
- decompose the spherical components onto pure-spin vector spherical harmonics $(\boldsymbol{Y}_{\ell m}^R, \boldsymbol{Y}_{\ell m}^E, \boldsymbol{Y}_{\ell m}^B)$ and solve for the scalar potentials (drawback: more complicated to implement)

$$
\begin{aligned}
V^r &= \sum_{\ell,m} R_{\ell m}(r) Y_{\ell m}(\theta, \varphi) \\
\eta &= \sum_{\ell,m} E_{\ell m}(r) Y_{\ell m}, \\
\mu &= \sum_{\ell,m} B_{\ell m}(r) Y_{\ell m}
\end{aligned}
$$

Same questions appear in the case of rank-2 tensor (e.g. the 3-metric γ_{ij} in 3+1 formalism).

Non-linear problems

Explicit method for time-dependent problems

$$\frac{\partial u}{\partial t} = N u$$

- knowing the field $\bar{u}^J$ at a given time-step, one can compute the non-linear source $N\bar{u}^J$, and advance in time…

Solution of a boundary value problem

$$L u = N u$$

- Newton-Raphson method for $F(\bar{u}) = (L + N)\,(c_0, \dots, c_N) = 0$: compute $J_{ij} = \frac{\partial F_i}{\partial c_j}$, start from an initial guess $\bar{u}_0$,and solve $J(\bar{u}_1 - \bar{u}_0) = -F\bar{u}_0$… 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 $\bar{u}_1 = L^{-1}\,N\bar{u}_0$…no reason to converge!

Examples in numerical relativity

We consider space-times which are

- stationary: there exists a Killing vector field, timelike at infinity,
- axisymmetric : there exists a Killing vector field, vanishing on a timelike 2-surface (the axis), spacelike elsewhere and whose orbits are closed curves,
- asymptotically flat
- circular: there is no meridional convective current.

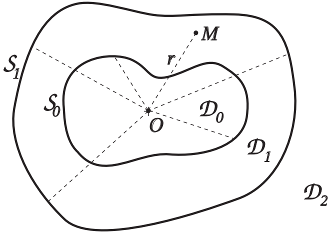
$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + B^2 r^2 \sin^2\theta \, (\mathrm{d}\varphi - \beta^\varphi \mathrm{d}t)^2 + A^2 \left(\mathrm{d}r^2 + r^2\mathrm{d}\theta^2\right).$$

$\Rightarrow$set of 4 coupled non-linear Poisson-like equations for the metric potentials + first integral of motion (hydrostatic equilibrium) + equation of state (EOS).

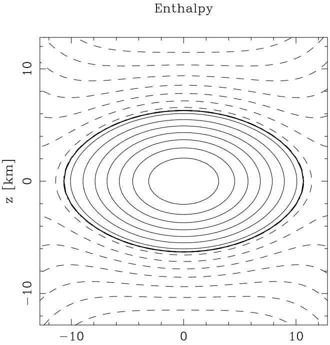
Rotating relativistic stars

Adapted mapping

- The density profile is not smooth at the surface ⇒loss in the convergence rate.
- The multi-domain approach requires that the domain boundary be situated exactly at the (coordinate) surface of the star,



From Bonazzola *et al.* (1998).



For a rotating star, this surface is not a sphere ⇒need of a starred mapping $(\xi, \theta', \varphi') \mapsto (r, \theta, \varphi)$:

$$
\begin{aligned}
r &= \alpha_0 \left[\xi + (3\xi^4 - 2\xi^6) F_{\mathrm{even}}(\theta', \varphi') \right.\\
&\quad \left. + (5\xi^3 - 3\xi^5) G_{\mathrm{odd}}(\theta', \varphi')\right] \\
\theta &= \theta' \text{ and } \varphi = \varphi'
\end{aligned}
$$

to take care of regularity conditions at $r = 0$.

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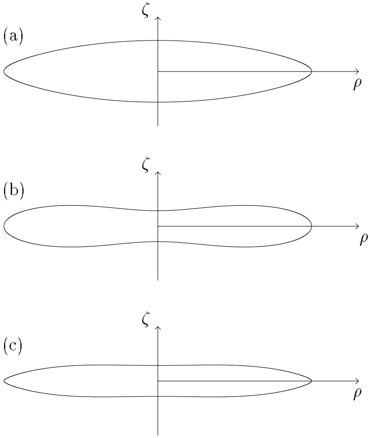
All very fast and differentially rotating stars do no fit into this picture:
$\Rightarrow$use of cylindrical coordinates with the mapping $(s, t) \mapsto (\rho, z)$:

$$\begin{aligned} \rho^2 &= r_e^2 st, \; r_e\text{: equatorial radius} \\ z^2 &= r_p^2 s y_B(t), \; r_p\text{: polar radius} \end{aligned}$$

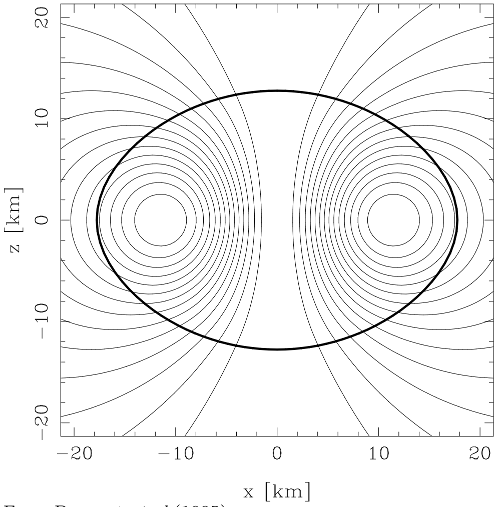
where $y_B(t)$ describes the star surface.
$\Rightarrow y_B(t)$, with other fields, is decomposed on a basis of Chebyshev polynomials and enters the system of equations.



From Ansorg *et al.*(2002)

Rotating relativistic stars
Einstein-Maxwell system

Magnetic field



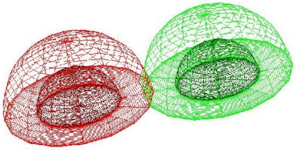
From Bocquet *et al.*(1995)

- One can solve for the electro-magnetic field in addition to the gravitational one,
- Assumption of perfect conductor and self-consistent model (electric currents in hydro equilibrium),
- Matching of the tangential part of electric field at the surface.

Want to model initial data of inspiralling binary systems of compact objects ⇒must be in some quasi-equilibrium state:

- standing waves, or
- no gravitational radiation

use of conformally flat condition (see lectures by Font and Campanelli): the 3-metric is conformally flat (spatial gauge is then fixed) ⇒set of five coupled elliptic (Poisson-like) non-linear equations (two scalar ones and a vector one)

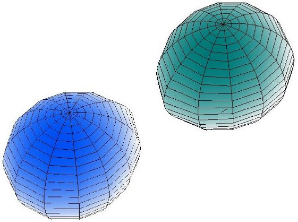


From Gourgoulhon *et al.* (2001)

Several choices for the coordinates:

- Cartesian (compactification?),
- two spherical grids, centered on each object (cost of interpolation?),
- bispherical coordinates (implementation?).

- For neutron stars, one often considers that the viscosity is too small to synchronize the binary,
- the hydro flow can be considered as irrotational$\Rightarrow$solution of an additional Poisson-like equation for the potential.

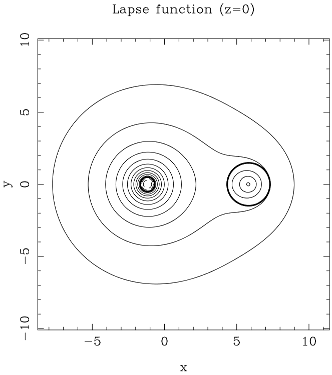


- use of two spherical grids, adapted to the surface of each star,
- most of time spent in the interpolation between grids
- able to treat incompressible fluids, as well as strange quark matter (pressure jump at the surface).

Binary systems

Mixed initial data

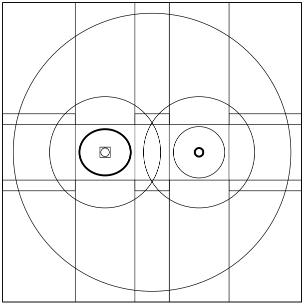
- Irrotational hydro flow and a grid adapted to the surface of the star,
- the black hole is modeled through the presence of an isolated horizon, which is set to be a sphere



From Granclément (2006)

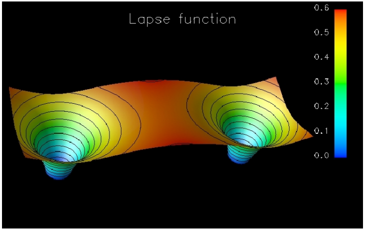
Other grid setting:

- only Cartesian grids and shells (no $r = 0$ coordinate singularity),
- overlapping domain matching.



From Foucart *et al.* (2008)

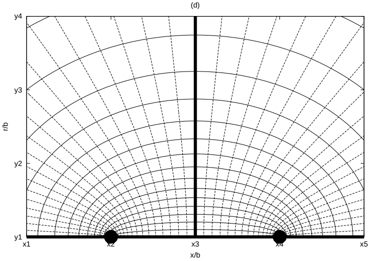
Binary systems
Black hole initial data



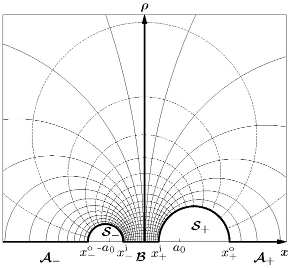
Several “groups” have performed computations of binary-black-hole initial data, using spectral methods:

- the Meudon group (e.g. Gourgoulhon *et al.* 2002),
- the Caltech / Cornell group (e.g. Lovelace *et al.* 2008),
- M. Ansorg (e.g. Ansorg 2005).

punctures



excision



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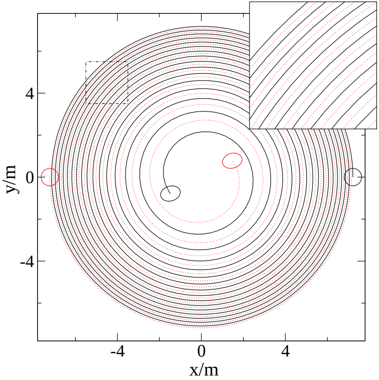
Binary black hole evolution

Only the Caltech/Cornell group is able to perform binary black hole evolution with spectral methods (see lectures by Campanelli and Laguna).



From Boyle *et al.* (2007)

- use free evolution, generalized harmonic gauge and excision,
- multi-domain spectral method, with penalty technique to match the domains,
- dual-frame approach and horizon-tracking grid,
- explicit, high-order Runge-Kutta scheme, spherical harmonics and Chebyshev representation.

$\Rightarrow$15 orbits and merger, up to $\gtrsim 4000M$.

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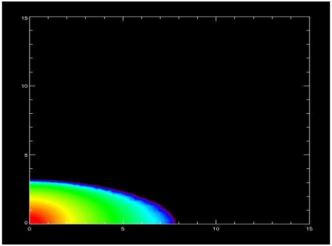
Core-collapse

Combined code spectral/Godunov

Spectral methods may not be used for the hydrodynamics of core-collapse simulations ... High-Resolution Shock-Capturing methods are very efficient (see lecture by J.A. Font).

- Nevertheless, the gravitational field is never discontinuous (no coordinate shocks),
- Although not spectrally convergent, the spectral representation of gravitational field is convergent.
- Define a domain containing the shock, with more points.



⇒ "Mariage des Maillages"/CoCoNuT project (also lecture by Font):

- use high-resolution shock-capturing methods for the hydro system,
- use spectral methods for the Einstein equations.

Cordero-Carrión *et al.* (2008), in preparation

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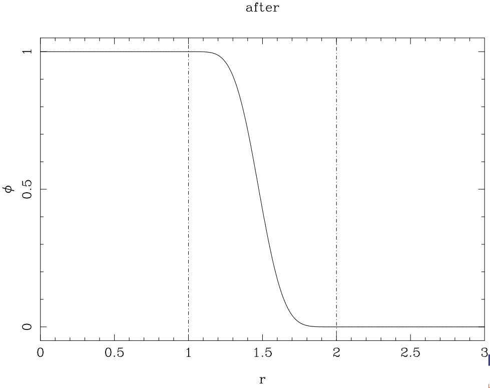
One the main limitations for the use of spectral methods is the Gibbs phenomenon.⇒possibility to use filters: e.g.

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

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



Summary

Summary

- Spectral method can yield rapid convergence in the representation of smooth functions, the computation of their derivatives and for the solution of PDEs/ODEs.
- They can nicely handle coordinate singularities and "$\frac{0}{0}$-like" terms.
- They are limited by the Gibbs phenomenon, which makes them not well-suited for some simulations (shocks,…).
- They can however be combined with other techniques (Godunov, SPH, …) to solve for the gravitational field equations.
- Possible future developments: spectral methods for time representation, spectral elements, …

Some of the techniques/codes described here are available as parts of the publicly available numerical library LORENE:

www.lorene.obspm.fr

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