An overview of the Kadath library

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Mathematical Aspects of Black Hole Theory, Meudon, December 12-14, 2022

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`KADATH` library

`KADATH` **is a library that implements spectral methods in the context of theoretical physics.**

- It is written in C++, making extensive use of object oriented programming.
- Versions are maintained via git.
- Website : *www.kadath.obspm.fr*
- The library is described in the paper : *JCP* **220**, *3334 (2010).*
- Designed to be very modular in terms of geometry and type of equations.
- LateX-like user-interface.
- More general than its predecessor LORENE.

A test problem

Find the conformal factor Ψ of the Schwarzschild black hole in QI coordinates.

System of equations

- Bulk : $\Delta\Psi = 0$.
- Inner BC : $\Psi_{,r} + \frac{1}{2a}\Psi = 0$
- Outer BC : $\Psi = 1$

a is the radius of the black hole and the solution is

$$\Psi(r) = 1 + \frac{a}{r}.$$

Concept in 1D

Given a set of orthogonal functions Φ_i on an interval Λ, spectral theory gives a recipe to approximate f by

$$f \approx I_N f = \sum_{i=0}^{N} a_i \Phi_i$$

Properties

- the Φ_i are called the basis functions.
- the a_i are the coefficients : it is the quantity stored on the computer.
- Multi-dimensional generalization is done by direct product of basis.
- The computation of the a_i comes from the Gauss quadratures.

Coefficient and configuration spaces

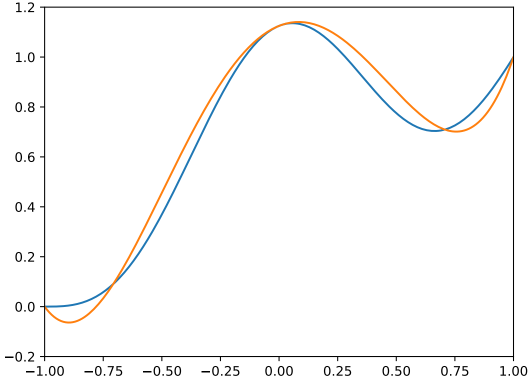
There exist $N+1$ point x_i in Λ such that

$$f(x_i) = I_N f(x_i)$$

Two equivalent descriptions

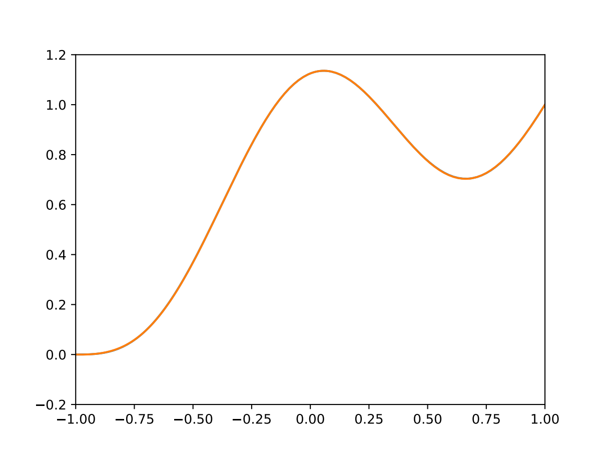
- Formulas relate the coefficients a_i and the values $f(x_i)$.
- Complete duality between the two descriptions.
- One works in the coefficient space when the a_i are used (for instance for the computation of f').
- One works in the configuration space when the $f(x_i)$ are employed (for the computation of $\exp(f)$)

Example of interpolant for $N = 4$



blue curve $f(x) = \cos^3(\pi x/2) + (x+1)^3/8$; *orange* : $I_4 f$.

Example of interpolant for $N = 8$



blue curve $f(x) = \cos^3(\pi x/2) + (x+1)^3/8$; *orange* : $I_8 f$.

Sturm-Liouville problems

Eigenvalue problem of the form :

$$-\left(pu'\right)' + qu = \lambda wu$$

- p strictly positive and continuous (can vanish at the boundaries).
- q continuous, non-negative and bounded.
- w continuous, non-negative and integrable (can diverge at the boundaries for instance).

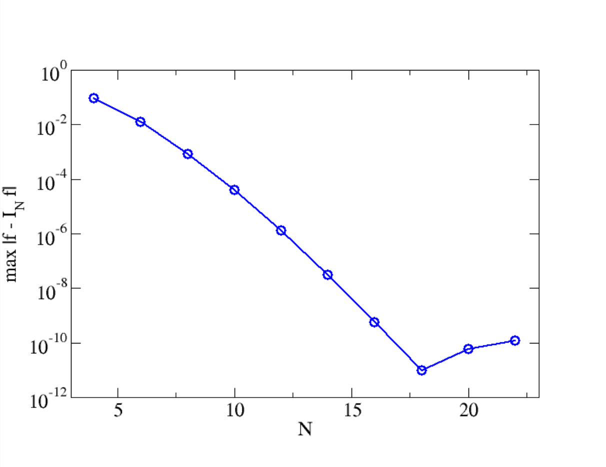
The solutions are :

- the eigenvalues λ_n
- the eigenfunctions u_n.
- orthogonality : $(u_n, u_m)_w = 0$ for $m \neq n$.

Spectral convergence

- Singular problem if and only if p vanishes at the boundaries of Λ.
- If the basis functions are solutions of a singular Sturm-Liouville problem, then $I_N f$ converges to f (when N increases), faster than any power-law of N (typically exponentially) **for smooth functions** (i.e. $\mathcal{C}^\infty$).
- This is called **spectral convergence**.
- this is to be contrasted with finite difference schemes.
- One of the main reason to use spectral methods.
- Legendre or Chebyshev polynomials are solutions of singular SL problems.

Example convergence



Discrete Fourier transform

Discrete version of standard Fourier transform

$$I_N f = \sum_{n=0}^{N/2} \tilde{a}_n \cos(nx) + \sum_{n=1}^{N/2} \tilde{b}_n \sin(nx)$$

$$\tilde{a}_n = \frac{2}{(N+1)(1+\delta_0^n)} \sum_{i=0}^{N} f(x_i) \cos(n x_i)$$

$$\tilde{b}_n = \frac{2}{(N+1)} \sum_{i=0}^{N} f(x_i) \sin(n x_i).$$

A spectral expansion with :

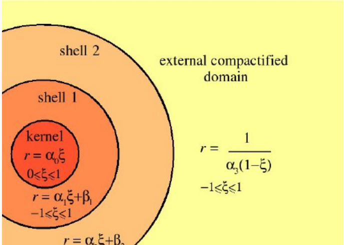
- $\Lambda = [0, 2\pi]$
- $x_i = \frac{2\pi i}{N+1}$.
- $w_i = 1$.

Multi-domain setting

Numerical coordinates

- Space is divided into several numerical domains.
- In each domain there is a link between the physical coordinates X and the numerical ones $X^\star$.
- Spectral expansion is performed with respect to $X^\star$.
- Non-periodic coordinates are expanded wrt to polynomials.
- Periodic coordinates (i.e. angles) are described by trigonometrical functions.

Example spherical space

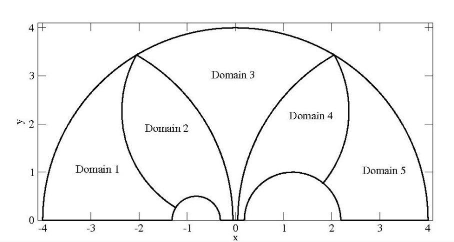


Setting the space in KADATH

```
// 3D :
int dim = 3 ;

// Number of points in each dimension
Dim_array res (dim) ;
res.set(0) = 13 ; res.set(1) = 5 ; res.set(2) = 4 ;

// Center of the coordinates
Point center (dim) ;
for (int i=1 ; i<=dim ; i++)
    center.set(i) = 0 ;

// Number of domains and boundaries :
int ndom = 4 ;
Array<double> bounds (ndom-1) ;
// Radius of the BH
double aa = 1.323 ;
bounds.set(0) = aa ; bounds.set(1) = 1.7557*aa ; bounds.set(2) = 2.9861*aa ;

// Chebyshev or Legendre :
int type_coloc = CHEB_TYPE ;

// Spherical space :
Space_spheric space(type_coloc, center, res, bounds) ;
```

Other spaces available

- Cylindrical space.
- Bispherical space.
- Spaces with periodic time coordinates.
- Spaces with adaptable domains.
- Spaces with various symmetries.
- Additional ones relatively easy to include.



Setting the fields

For a scalar field, in each domain

- one array for the values at the collocation points.
- one array for the values of the coefficients.
- one object describing the spectral basis.
- should be transparent to the user.

The standard spectral base

- A scalar field is regular if it is expressed as a sum of polynomials of Cartesian coordinates $x^m y^n z^p$.
- From that assumption one can deduce some appropriate choice of spectral basis by expressing x, y, z in terms of r, θ, φ, for instance.
- Details depend on the space considered.
- For a spherical space it leads to :
  - for φ : $\cos(m\varphi)$ and $\sin(m\varphi)$.
  - for θ : $\cos(2j\theta)$ for m even and $\sin((2j+1)\theta)$ for m odd.
  - Chebyshev polynomials with respect to $r^\star$
  - In the nucleus : $T_{2i}(r^\star)$ for m even and $T_{2i+1}(r^\star)$ for m odd.

KADATH management of the spectral basis

- For every computation, KADATH tries to assert the basis of the result.
- Straightforward for things like the product, inverse, sum etc...
- For other computations (like $\exp$, $\cos$, $\sqrt{}$) the base cannot be directly obtained and is lost.
- **Important rule** set the base by hand if and only if it is required.
- Be careful when enforcing the standard base. For instance $\rho = \sqrt{x^2 + y^2}$ is not expanded onto the standard base.
- Most of the errors in using KADATH come from inappropriate setting of the basis.

Setting the fields in KADATH

```
// Initial guess for the conformal factor :
Scalar conf (space) ;
conf = 1. ;
conf.std_base() ;

// The analytic solution (except in the nucleus)
Scalar sol (space) ;
sol.set_domain(0) = 0. ;
for (int d=1 ; d<ndom ; d++)
        sol.set_domain(d) = 1 + aa / space.get_domain(d)->get_radius() ;
sol.std_base() ;
```

Higher order tensors

Construction

- Valence
- Types of the various indices (`COV` or `CON`).
- The tensorial basis of decomposition (Cartesian or Orthonormal spherical basis essentially).

Spectral basis of the components

- For a Cartesian tensorial basis : same thing as for scalars (with parity wrt to $z = 0$).
- For a spherical basis : deduced from the Cartesian one by making use of the formulae between the tensorial basis.

Solving equations ; a linear problem

$$Lu\,(x) = S\,(x) \quad x \in U$$

$$Bu\,(y) = 0 \quad y \in \partial U$$

- L is a second order linear differential operator.
- B is a first order linear differential operator on the boundary.

The weighted residual method

Objective : discretize the field equations

- Given a scalar product, one makes the residual $R = Lu - S$ small in the sense
$$(R, \xi_i)_w = 0 \quad ; \quad i \in [0, N] .$$

- The ξ_i are called the test functions.
- There are several different choice for the test functions.
- `KADATH` implements the τ-method where the ξ_i are the basis functions.

Implementation in KADATH

The τ-method

- The ξ_i are the basis functions.
- One solves $R = 0$ by demanding the the coefficients of R vanish.
- The conditions corresponding to the highest order coefficients are relaxed to enforce the boundary conditions.

Galerkin method

- Used to enforced regularity conditions (axis, origin etc).
- Galerkin basis : each term individually fulfills the conditions.
- For instance use $\cos(2j\theta) - 1$ for a function that must vanish on the axis $\theta = 0$.
- The solution is sought as a sum of Galerkin terms.

The discrete system

Original system

- Unknowns : tensorial fields.
- Equations : partial derivative equations.

Discretized system

- Unknowns : coefficients $\vec{u}$.
- Equations : algebraic system $\vec{F}(\vec{u}) = 0$.

Properties

- For a linear system $\vec{F}(\vec{u}) = 0 \Longleftrightarrow A^i_j u^j = S^i$
- In general $\vec{F}(\vec{u})$ is even not known analytically.
- $\vec{u}$ is sought numerically.

Newton-Raphson iteration

Given a set of field equations with boundary and matching equations, `KADATH` translates it into a set of algebraic equations $\vec{F}\left(\vec{u}\right)=0$, where $\vec{u}$ are the unknown coefficients of the fields.

The non-linear system is solved by Newton-Raphson iteration

- Initial guess $\vec{u}_0$.
- Iteration :
  - Compute $\vec{s}_i=\vec{F}\left(\vec{u}_i\right)$
  - If $\vec{s}_i$ if small enough $\Longrightarrow$ solution.
  - Otherwise, one computes the Jacobian : $\mathbf{J}_i=\frac{\partial\vec{F}}{\partial\vec{u}}\left(\vec{u}_i\right)$
  - One solves : $\mathbf{J}_i\vec{x}_i=\vec{s}_i$.
  - $\vec{u}_{i+1}=\vec{u}_i-\vec{x}_i$.

Convergence is very fast for good initial guesses.

Computation of the Jacobian

Explicit derivation of the Jacobian can be difficult for complicated sets of equations.

Automatic differentiation

- Each quantity x is supplemented by its infinitesimal variation δx.
- The dual number is defined as $\langle x, \delta x \rangle$.
- All the arithmetic is redefined on dual numbers. For instance $\langle x, \delta x \rangle \times \langle y, \delta y \rangle = \langle x \times y, x \times \delta y + \delta x \times y \rangle$.
- Consider a set of unknown $\vec{u}$, and a its variations $\delta \vec{u}$. When $\vec{F}$ is applied to $\langle \vec{u}, \delta \vec{u} \rangle$, one then gets : $\left\langle \vec{F}\left(\vec{u}\right), \delta \vec{F}\left(\vec{u}\right) \right\rangle$.
- One can show that

$$\delta \vec{F}\left(\vec{u}\right) = \mathbf{J}\left(\vec{u}\right) \times \delta \vec{u}$$

The full Jacobian is generated *column by column*, by taking all the possible values for $\delta \vec{u}$, at the price of a computation roughly twice as long.

Numerical resources

Consider N_u unknown fields, in N_d domains, with d dimensions. If the resolution is N in each dimension, the Jacobian is an $m \times m$ matrix with :

$$m \approx N_d \times N_u \times N^d$$

For $N_d = 5$, $N_u = 5$, $N = 20$ and $d = 3$, one reaches $m = 200\,000$

Solution

- The matrix is distributed on several processors.
- Easy because the Jacobian is computed column by column.
- The library `SCALAPACK` is used to invert the distributed matrix.

- $d = 1$ problems : sequential.
- $d = 2$ problems : 100 processors (mesocenters).
- $d = 3$ problems : 1000 processors (national supercomputers).

Solving the system with KADATH

```
// Solve the equation in space outside the nucleus
System_of_eqs syst (space, 1, ndom-1) ;
// Only one unknown
syst.add_var ("P", conf) ;
// One user defined constant
syst.add_cst ("a", aa) ;

// Inner BC
syst.eq_eq_bc (1, INNER_BC, "dn(P)+0.5/a*P=0") ;

for (int d=1 ; d<ndom ; d++) {
	// Bulk equation (2nd order)
	syst.add_eq_inside (d, "Lap(P)=0") ;
	if (d!=ndom-1) {
		// Matching of the solution
		syst.add_eq_matching (d, OUTER_BC, "P") ;
		// Matching of the radial derivative
		syst.add_eq_matching (d, OUTER_BC, "dn(P)") ;
}
// Outer BC
syst.add_eq_bc (ndom-1, OUTER_BC, "P=1") ;

// Newton-Raphson
double conv ;
bool endloop = false ;
int ite = 1 ;
while (!endloop) {
	endloop = syst.do_newton(1e-8, conv) ;
	cout << "Newton iteration " << ite << " " << conv << endl ;
	ite++ ;
}
```

Advanced topics : definitions

- When an expression of the unknowns appears often.
- That expression can be made into a definition.
- Simplifies the writing of the equations.
- Makes the code faster as the definitions are computed only when needed.

```
// Extrinsic curvature tensor
syst.add_def ("K_ij=(D_i_B_j+D_j_B_i)2/N") ;

// Can be used in other expressions
// Hamiltonian constraint
syst.add_def ("H=R-K_ij*K^ij") ;
// Momentum constraints
syst.add_def ("M^i=D_j_K^ij") ;
```

Advanced topics : metrics

- Special type of second order tensor.
- Enables the index manipulation.
- Enables the use of covariant derivative.
- Enables the use of Riemann and Ricci tensors

```
// Definition of a metric (from a second order tensor)
// Here met is an unknown also (use Metric_const otherwise)
Metric_general met (gmet) ;

// Associates the metric to the system
met.set_system (syst, "g") ;

// Now you can compute things like
syst.add_def ("derN=D_i_N") ;
// The Ricci is known
syst.add_def ("Ricci_ij=R_ij") ;
```

Advanced topics : global unknowns

- Some unknowns are numbers, not fields.
- Associated with integral equations.

```
double omega = 0. ;

// Omega is an unknown
syst.add_var ("ome", omega) ;

// Equality of the ADM and Komar masses forces the right value of omega
// Can be expressed as
space.add_eq_int_inf (syst, "integ(dn(N)+2*dn(P))=0") ;
```

Example of a complex problem

Kerr black hole in 3+1 formalism

- Based of the paper : P. Grandclément, J. Nicoules, Phys. Rev. D, 105, 104011 (2022).
- Unknowns : N the lapse, B^i the shift and γ_{ij} the spatial metric.
- Maximal slicing $K = 0$.
- Spatial harmonic gauge $g^{kl}\Gamma^i_{kl} = 0$.

Bulk equations

$$
\begin{aligned}
H &: \quad R - D_k V^k - K_{ij} K^{ij} = 0 \\
M_i &: \quad D^j K_{ij} = 0 \\
E_{ij} &: \quad \mathcal{L}_{\boldsymbol{B}} K_{ij} - D_i D_j N + N \left(R_{ij} - \frac{1}{2} \left(D_i V_j + D_j V_i \right) - 2 K_{ik} K^k_j \right) = 0
\end{aligned}
$$

where $V^i = g^{kl} \Gamma^i_{kl}$ and $K_{ij} = \frac{1}{2N} \left(D_i B_j + D_j B_i \right)$.

Outer boundary equations

- $N = 1$
- $B^i = 0$
- $\gamma_{ij} = f_{ij}$.

Inner boundary equations

- $N = N_{\text{const}}$ (time coordinate freedom).
- $B^i = N\tilde{s}^i + \Omega\,(\partial_\varphi)^i$ (horizon at fixed location, with no shear).
- $\gamma_{r\theta} = 0$ and $\gamma_{r\varphi} = 0$ (spatial gauge freedom).
- $E_{\theta\theta} = 0$, $E_{\theta\varphi} = 0$ and $E_{\varphi\varphi} = 0$ (degenerate equations).
- $\gamma_{rr} = g_{\text{const}}$ for $l = m = 0$ and $\Theta = 0$ otherwise.

Last words

- Additional specialized features (adapted domains).
- Many successful applications (boson stars, hairy black holes, initial data for general relativity).
- Additional functionalities are included regularly.
- The number of users increases, at last...

Try it...

Kadath website (https ://kadath.obspm.fr) has some tutorials... Have fun...