Multidomain spectral methods based on spherical coordinates for numerical relativity

Éric Gourgoulhon
Laboratoire de l’Univers et de ses Théories (LUTH)
CNRS / Observatoire de Paris
F-92195 Meudon, France

on behalf of LUTH numerical relativity team:
Silvano Bonazzola, Philippe Grandclément, José Luis Jaramillo,
François Limousin & Jérôme Novak

eric.gourgoulhon@obspm.fr

ICOSAHOM 2004 (Brown University, Providence, USA, 21-25 June 2004)
Plan

1. General features of spectral methods developed in Meudon

2. Resolution of elliptic equations: the initial value problem of general relativity

3. Resolution of tensorial wave equations: spacetime dynamics
1

General features of spectral methods developed in Meudon
An overview

• Multidomain three-dimensional **spectral method**

• Spherical-type coordinates \((r, \theta, \varphi)\)

• Expansion functions: \(r\) : Chebyshev; \(\theta\) : cosine/sine or associated Legendre functions; \(\varphi\) : Fourier

• Domains = spherical shells + 1 nucleus (contains \(r = 0\))

• Entire space \((\mathbb{R}^3)\) covered: compactification of the outermost shell

• Adaptative coordinates : domain decomposition with spherical topology

• Multidomain PDEs: patching method (strong formulation)

• Treatment of non-linear terms: pseudospectral method
Domain decomposition

physical coordinates
$(r, \theta, \varphi)$

comput. coordinates
$(\xi, \theta', \varphi')$

$r = \frac{1}{\alpha_3(1-\xi)}$

$0 < \xi < 1$

$-1 < \xi < 1$

$r = \alpha_0 \xi$

$0 < \xi < 1$

$r = \alpha_1 \xi + \beta_1$

$-1 < \xi < 1$

$r = \alpha_2 \xi + \beta_2$

$-1 < \xi < 1$
Starlike domain decomposition

\( N \) nonoverlapping starlike domains:

- \( D_0 : \text{nucleus} \)
- \( D_q \ (1 \leq q \leq N - 2) : \text{shell} \)
- \( D_{N-1} : \text{external domain} \)

\[ D_0 \cup D_1 \cup \cdots \cup D_{N-1} = \mathbb{R}^3 \]
Mapping computational space $\rightarrow$ physical space

Mapping for domain $\mathcal{D}_q$:

$$[-1 + \delta_0, 1] \times [0, \pi] \times [0, 2\pi] \quad \rightarrow \quad \mathcal{D}_q$$

$$(\xi, \theta', \varphi') \quad \mapsto \quad (r, \theta, \varphi)$$

**Radial mapping**: $\theta = \theta'$ and $\varphi = \varphi'$

- **in the nucleus**: $\xi \in [0, 1]$
  $$r = \alpha_0 \left[ \xi + (3\xi^4 - 2\xi^6) F_0(\theta, \varphi) + \frac{1}{2} (5\xi^3 - 3\xi^5) G_0(\theta, \varphi) \right]$$

- **in the shells**: $\xi \in [-1, 1]$
  $$r = \alpha_q \left[ \xi + \frac{1}{4} (\xi^3 - 3\xi + 2) F_q(\theta, \varphi) + \frac{1}{4} (-\xi^3 + 3\xi + 2) G_q(\theta, \varphi) \right] + \frac{\beta_q}{r}$$

- **in the external domain**: $\xi \in [-1, 1]$
  $$\frac{1}{r} = \alpha_{\text{ext}} \left[ \xi + \frac{1}{4} (\xi^3 - 3\xi + 2) F_{\text{ext}}(\theta, \varphi) - 1 \right]$$


ICOSAHOM 2004 (Brown University, Providence, USA, 21-25 June 2004)
Example: binary star with surface fitted coordinates

Double domain decomposition

Surface fitted coordinates:
$F_0(\theta, \varphi)$ and $G_0(\theta, \varphi)$ chosen so that $\xi = 1 \Leftrightarrow$ surface of the star

[Taniguchi, Gourgoulhon & Bonazzola, Phys. Rev. D 64, 064012 (2001)]
Basis functions

Polynomial interpolant of a field $u$ in a given domain $\mathcal{D}_q$:

$$I_N u_q(\xi, \theta, \varphi) = \sum_{m=0}^{N_\varphi/2} \sum_{j=0}^{N_\theta-1} \sum_{i=0}^{N_r-1} \hat{u}_{qmi} X_i(\xi) \Theta_j(\theta) e^{im\varphi}$$

with $N := (N_r, N_\theta, N_\varphi)$

Regularity at the origin and on the axis $\theta = 0 +$ equatorial symmetry:

- $\varphi$ expansion: **Fourier series**

- $\theta$ expansion: **Trigonometric polynomials** or **associated Legendre functions**
  - for $m$ even: $\Theta_j(\theta) = \cos(2j\theta)$ or $\Theta_j(\theta) = P_{2j}^m(\cos \theta)$
  - for $m$ odd: $\Theta_j(\theta) = \sin((2j + 1)\theta)$ or $\Theta_j(\theta) = P_{2j+1}^m(\cos \theta)$

- $\xi$ expansion: **Chebyshev polynomials**
  - in the kernel: $X_i(\xi) = T_{2i}(\xi)$ for $m$ even, $X_i(\xi) = T_{2i+1}(\xi)$ for $m$ odd
  - in the shells and the external compactified domain: $X_i(\xi) = T_i(\xi)$
Numerical implementation: LORENE

A library of C++ classes devoted to multi-domain spectral methods, with adaptive spherical coordinates.

- 1997: start of Lorene project (Jean-Alain Marck, EG)
- 1999: Accurate models of rapidly rotating strange quark stars
- 1999: Neutron star binaries on closed circular orbits
- 2001: Black hole binaries on closed circular orbits
- 2002: 3-D wave equation with non-reflecting boundary conditions
- 2002: Maclaurin-Jacobi bifurcation point in general relativity
- 2004: 3-D time evolution of Einsteins equations

ICOSAHOM 2004 (Brown University, Providence, USA, 21-25 June 2004)
2

Resolution of elliptic equations: the initial value problem of general relativity
Resolution of Poisson equation with noncompact source

Consider the three-dimensional Poisson equation on $\mathbb{R}^3$:

$$\Delta u(r, \theta, \varphi) = s(r, \theta, \varphi)$$  \hfill (1)

with the boundary condition

$$u(r, \theta, \varphi) \to 0 \quad \text{when} \quad r \to +\infty$$  \hfill (2)

The source $s$ has a non-compact support and obeys to the fall-off conditions

$$s(r, \theta, \varphi) \sim \sum_{q=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} \frac{Y_{\ell m}(\theta, \varphi)}{r^{\ell+4}} \quad \text{when} \quad r \to +\infty$$  \hfill (3)
Spherical harmonics expansions

Interpolant of the source in a domain \( D_q \) (notation: \( s_q := s|_{D_q} \)):

\[
I_N s_q(\xi, \theta, \varphi) = \sum_{\ell=0}^{N_\theta-1} \sum_{m=-\ell}^\ell \hat{s}_{q \ell m}(\xi) Y_{\ell m}(\theta, \varphi)
\]

Search for a numerical solution under the form

\[
\bar{u}_q(\xi, \theta, \varphi) = \sum_{\ell=0}^{N_\theta-1} \sum_{m=-\ell}^\ell \hat{u}_{q \ell m}(\xi) Y_{\ell m}(\theta, \varphi)
\]

Shorthand notation: \( u_\bullet(\xi) := \hat{u}_{q \ell m}(\xi) \).
Eq. (1) becomes an ODE system:

- In the nucleus \((r = \alpha \xi)\):

  \[
  \frac{d^2 u}{d\xi^2} + \frac{2}{\xi} \left( \frac{du}{d\xi} - \frac{du}{d\xi}(0) \right) - \frac{\ell(\ell + 1)}{\xi^2} \left( u - u(0) - \xi \frac{du}{d\xi}(0) \right) = \alpha^2 s_{0\ell m}(\xi)
  \]

- In the shells \((r = \alpha \xi + \beta)\):

  \[
  \left( \xi + \frac{\beta}{\alpha} \right)^2 \frac{d^2 u}{d\xi^2} + 2 \left( \xi + \frac{\beta}{\alpha} \right) \frac{du}{d\xi} - \ell(\ell + 1) u = (\alpha \xi + \beta)^2 s_{q\ell m}(\xi)
  \]

- In the external domain \((r^{-1} = \alpha(\xi - 1))\):

  \[
  \frac{d^2 u}{d\xi^2} - \frac{\ell(\ell + 1)}{(\xi - 1)^2} \left( u - u(1) - (\xi - 1) \frac{du}{d\xi}(1) \right) = \frac{s_{q\ell m}(\xi)}{\alpha^4(\xi - 1)^4}
  \]
Resolution by means of a Chebyshev tau method

- In the nucleus:
  \[ u\bullet(\xi) = \sum_{i=0}^{N_r-1} \hat{u}_{q\ell mi} T_{2i}(\xi) \text{ for } \ell \text{ even} \]
  \[ u\bullet(\xi) = \sum_{i=0}^{N_r-2} \hat{u}_{q\ell mi} T_{2i+1}(\xi) \text{ for } \ell \text{ odd} \]

- In the shells and external domain:
  \[ u\bullet(\xi) = \sum_{i=0}^{N_r-1} \hat{u}_{q\ell mi} T_i(\xi) \]

Linear combinations → banded matrices (5 bands)
Patching method

Number of solutions of the homogeneous equation:

- In the nucleus: 1 \( (r^\ell) \)
- In the shells: 2 \( (r^\ell \text{ and } r^{-(\ell+1)}) \)
- In the external domain: 1 \( (r^{-(\ell+1)}) \)

Total: \( 1 + 2(N - 2) + 1 = 2N - 2 \)

Matching conditions: continuity of \( u \) and its first radial derivative across the \( N - 1 \) boundaries between the domains \( D_q \rightarrow 2N - 2 \) conditions
Behavior of the numerical error

Source with a non-compact support, decaying as $r^{-k}$:

- evanescent error ($\text{error} \propto \exp(-N r)$) if the source does not contain any spherical harmonics of index $\ell \geq k - 3$

- error decreasing as $N^{-2(k-2)}$ otherwise

Extension to vector Poisson-type equations

Minimal distortion equation for the shift vector: \[ \Delta \vec{\beta} + \frac{1}{3} \vec{\nabla} (\vec{\nabla} \cdot \vec{\beta}) = \vec{S} \]

Error on the \( z \) component of the solution of the minimal distortion equation with a non-compact source

Application to the Cauchy data for 3+1 numerical relativity

Quasi-equilibrium sequences of orbiting binary black holes and neutron stars

Initial data within the conformal thin sandwich framework: a set of two scalar and one vectorial elliptic equations (conformal factor $\Psi$, lapse function $N$ and shift vector $\beta$).

← binary neutron star system ($M/R = 0.16$ and $M/R = 0.18$, EOS $\gamma = 2.5$)
[Taniguchi & Gourgoulhon, PRD 68, 124025 (2003)]

← binary black hole system
[Grandclément, Gourgoulhon, Bonazzola, PRD 65, 044021 (2002)]
3

Resolution of tensorial wave equations:
spacetime dynamics
Scalar wave equation with nonreflecting boundary conditions

Consider the wave equation

\[ \Box u(t, r, \theta, \phi) = s(t, r, \theta, \phi) \]  \hspace{1cm} (4)

with the radiating boundary condition

\[ \lim_{r \to \infty} \left( \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial}{\partial t} \right) (ru) = 0. \]  \hspace{1cm} (5)

Solve (4) in a finite ball \( \mathcal{D} \) of radius \( R \) with some boundary conditions which approximate (5) when \( R \to \infty \).

Decompose \( \mathcal{D} \) in \( N \) spherical subdomains \( \mathcal{D}_q \) with \( \mathcal{D}_0 = \) nucleus and the other domains = shells (no external compactified domain).

Finite-differencing in time: second-order implicit Crank-Nicolson scheme.  
Space part: patching with Chebyshev tau
Non reflecting BC up to $\ell = 2$


$$B_1 u := \frac{\partial u}{\partial t} + \frac{\partial u}{\partial r} + \frac{u}{r}$$

$$B_2 u := \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial r} + \frac{3}{r} \right) B_1 u$$

$$B_3 u := \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial r} + \frac{5}{r} \right) B_2 u$$

Boundary condition: $B_3 u|_{r=R} = 0$.

⇒ ensures that spherical harmonics with $\ell = 0$, $\ell = 1$ and $\ell = 2$ are perfectly outgoing. This is important for gravitational waves.
Comparison with Sommerfeld boundary condition

Test on a 3D case

Square root of the fraction of remaining energy $\varepsilon$

2 domains:
98 points in $r$
17 points in $\theta$
16 points in $\phi$

[Novak & Bonazzola, J. Comp. Phys. 197, 186 (2004)]
Tensorial wave equations $\Box h^{\mu\nu} = \sigma^{\mu\nu}$ occurs in general relativity in various cases:

- in **harmonic coordinates** (4-dimensional tensor)
- in the **TT gauge** of linearized gravity (3-dimensional tensor)
- in the **Dirac gauge** within the 3+1 formalism (3-dimensional tensor) [Bonazzola, Gourgoulhon, Grandclément & Novak, gr-qc/0307082]
3+1 spacetime evolution in Dirac gauge

Conformal decomposition of the metric $\gamma_{ij}$ of the spacelike hypersurfaces $\Sigma_t$ of the 3+1 formalism of general relativity (cf. S.A. Teukolsky's talk):

$$\gamma^{ij} = \Psi^4 (f^{ij} + h^{ij})$$

where $f^{ij}$ is a flat metric on $\Sigma_t$, $h^{ij}$ a symmetric tensor and $\Psi$ a scalar field defined by

$$\Psi = \left( \frac{\det \gamma_{ij}}{\det f_{ij}} \right)^{1/12}$$

The Dirac gauge is expressed as a divergence-free condition on $h^{ij}$:

$$D_j h^{ij} = 0$$

where $D_j$ denotes the covariant derivative with respect to $f_{ij}$.

$\Rightarrow$ Ricci tensor of space metric $\gamma_{ij}$ becomes an elliptic operator for $h^{ij}$

$\Rightarrow$ the dynamical Einstein equations become a wave equation for $h^{ij}$
Resolution of the tensor wave equation

Rewrite the evolution equation for $h^{ij}$ as

$$\frac{\partial^2 h^{ij}}{\partial t^2} - \Delta h^{ij} = \sigma^{ij}$$

Split $h^{ij}$ into its trace $h := f_{ij} h^{ij}$ and its traceless-transverse (TT) part:

$$\bar{h}^{ij} := h^{ij} - \frac{1}{2} (h f^{ij} - D^i D^j \Phi)$$

with $\Delta \Phi = h$.

The TT part of the wave equation is

$$\frac{\partial^2 \bar{h}^{ij}}{\partial t^2} - \Delta \bar{h}^{ij} = \bar{\sigma}^{ij}$$
Taking advantage of spherical components

In spherical components, the TT tensor wave equation is reduced to two scalar wave equations:

\[
\frac{\partial^2 \chi}{\partial t^2} - \Delta \chi = \sigma \chi
\]

\[
\frac{\partial^2 \mu}{\partial t^2} - \Delta \mu = \sigma \mu
\]

Thanks to its TT character, all the components of \( \bar{h}^{ij} \) can be deduced from \( \chi \) and \( \mu \) quasi-algebraically. For instance, in a spherical orthonormal basis,

\[
\bar{h}^{\hat{r}\hat{r}} = \frac{\chi}{r^2}
\]

\[
\bar{h}^{\hat{r}\hat{\theta}} = \frac{1}{r} \left( \frac{\partial \eta}{\partial \theta} - \frac{1}{\sin \theta} \frac{\partial \mu}{\partial \phi} \right)
\]

\[
\bar{h}^{\hat{r}\hat{\phi}} = \frac{1}{r} \left( \frac{1}{\sin \theta} \frac{\partial \eta}{\partial \phi} + \frac{\partial \mu}{\partial \theta} \right)
\]

with \( \Delta_{\theta\phi} \eta = -\frac{\partial \chi}{\partial r} - \frac{\chi}{r} \)
Example: evolution of a vacuum spacetime

Pure gravitational wave spacetime

Initial data: same as [Baumgarte & Shapiro, PRD 59, 024007 (1998)], namely a Teukolsky wave $\ell = 2, m = 2$: $\chi = 10^{-3} x y \exp(-r^2)$ and $\mu = 0$, momentarily static: $K_{ij} = 0$
Constraint equations solved within the conformal thin sandwich framework

Evolution: fully constrained scheme based on Dirac gauge and maximal slicing [Bonazzola, Gourgoulhon, Grandclément & Novak, gr-qc/0307082]

Evolution of $h_{\hat{\phi}\hat{\phi}}$ in the plane $z = 0$

Evolution of the scalar curvature $R$ of the hypersurface $\Sigma_t$ in the plane $z = 0$
Test of the code: conservation of the ADM mass

Number of coefficients in each domain: $N_r = 17$, $N_\theta = 9$, $N_\phi = 8$
Test of the code: conservation of the ADM mass (zoom)

For $dt = 5 \times 10^{-3}$, the ADM is conserved within a relative error lower than $10^{-4}$. 