I. WAVE EQUATION

The aim is to solve the three-dimensional homogeneous wave equation $\Box\phi = 0$ in a sphere of radius R, using spherical coordinates:

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} - \frac{\partial^2\phi}{\partial r^2} - \frac{2}{r}\frac{\partial\phi}{\partial r} - \frac{\Delta_{\theta\varphi}\phi}{r^2} = 0. \tag{1}$$

Here, $\Delta_{\theta\varphi}$ is the angular part of the Laplacian. In what follows $c = 1$ is assumed. There shall be possibly three types of boundary conditions (BC) to be implemented:

1. Homogeneous BC : $\phi(r = R) = 0$, which models the reflection on the boundary.
2. Sommerfeld BC : $\partial(r\phi)/\partial t + \partial(r\phi)/\partial r|_{r=R} = 0$, which models a transparent boundary (at least for $\ell = 0$ wave modes).
3. Enhanced outgoing BC : $\partial(r\phi)/\partial t + \partial(r\phi)/\partial r|_{r=R} = \xi(\theta, \varphi)$, which is analogous to the Sommerfeld BC, but is also transparent to $\ell = 1, 2$ wave modes. The function $\xi(\theta, \varphi)$ verifies a wave-like equation on the boundary (see Sec. VI).

II. EXPLICIT SOLVER

The constant time-step is noted dt and $\phi^J = \phi(J \times dt)$, where the spatial coordinates are skipped. The simple forward Euler scheme writes:

$$\phi^{J+1} = 2\phi^J - \phi^{J-1} + dt^2\Delta\phi^J + O(dt^4). \tag{2}$$

This scheme can be safely used for small time-steps and spherical symmetry ($\ell = 0$ only).

Second-order time discretisation of the Sommerfeld BC writes:

$$\left(\frac{3}{2dt} + \frac{1}{R}\right)\phi^{J+1}(R) + \left.\frac{\partial\phi^{J+1}}{\partial r}\right|_{r=R} = \frac{4\phi^J(R) - \phi^{J-1}(R)}{2dt} + O(dt^2). \tag{3}$$

III. SUGGESTED STEPS

- Setup a spherically-symmetric one-domain grid (`Mg3d`, but only nucleus), with a mapping and associated r coordinate.
- Define an initial profile for ϕ^0 and ϕ^1 (*e.g.* the same Gaussian one for both), which should be of type `Scalar`.
- Make a time loop for 2-3 grid-crossing times with a graphical output (with the function `des_meridian`, see Lorene documentation).
- Doing so, the problem is ill-posed and therefore unstable. Add the BC requirement (homogeneous or Sommerfeld BC) by modifying at each time-step the value in physical space of the point situated at $r = R$, with the method `Scalar::set_outer_boundary`. Note that the initial profile must satisfy the BC!
- Make runs with varying the time-step to see the Courant limitation.

IV. IMPLICIT SOLVER

The 3D extension of the previous approach is very uneasy, it is therefore recommended to used implicit schemes, namely the Crank-Nicholson one:

$$\left[1 - \frac{dt^2}{2}\Delta\right]\phi^{J+1} = 2\phi^J - \phi^{J-1}\frac{dt^2}{2}\Delta\phi^{J-1} \tag{4}$$

The angular part of the Laplacian $\Delta_{\theta\varphi}$ admits spherical harmonics as eigen-functions:

$$\Delta_{\theta\varphi}Y_\ell^m = -\ell(\ell+1)Y_\ell^m \tag{5}$$

so that when developing ϕ onto spherical harmonics, the operator in (4) becomes

$$1 - \frac{dt^2}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2}\right) \tag{6}$$

for each harmonic.

V. SUGGESTED STEPS

- Take a symmetric grid (in θ and φ), with x and y coordinate fields, to define an $\ell \leq 2$ initial profile (*e.g.* $xy\times$ a Gaussian).
- At every time-step after transforming to Y_ℓ^m, make a loop on ℓ, m (use `Base_val::give_quant_numbers` to get ℓ and m) and build the matrix associated with the operator (6), acting on coefficient space, using elementary operators `Diff`. Be careful to take into account the mapping!
- Within the same loop on ℓ, m, fill a `Tbl` with the coefficients of the right-hand side of (4).
- Add the BC and a regularity condition (when necessary) using the tau method.
- Invert the system to get ϕ^{J+1}, go back to Fourier coefficients and, eventually, compute the energy stored in the grid:

$$E = \int \left(\frac{\partial \phi}{\partial t}\right)^2 + (\nabla\phi)^2 \tag{7}$$

using the method `Scalar::integrale`.

VI. ENHANCED BOUNDARY CONDITIONS

These are a modification of the Sommerfeld BC (Sec. I), with $\xi(\theta, \varphi)$ verifying:

$$\frac{\partial^2 \xi}{\partial t^2} - \frac{3}{4R^2}\Delta_{\theta\varphi}\xi + \frac{3}{R}\frac{\partial \xi}{\partial t} + \frac{3\xi}{2R^2} = \frac{1}{2R^2}\Delta_{\theta\varphi}\left(\frac{\phi}{R} - \left.\frac{\partial\phi}{\partial r}\right|_{r=R}\right); \tag{8}$$

When developing ξ and ϕ onto Y_ℓ^m and using again Crank-Nicholson time scheme:

$$\frac{\xi_{\ell m}^{J+1} - 2\xi_{\ell m}^{J} + \xi_{\ell m}^{J-1}}{dt^2} + \frac{3}{8}\frac{\ell(\ell+1)}{R^2}\left(\xi_{\ell m}^{J+1} + \xi_{\ell m}^{J-1}\right) + \frac{3}{R}\frac{\xi_{\ell m}^{J+1} - \xi_{\ell m}^{J-1}}{2dt}$$
$$+ \frac{3}{4R^2}\left(\xi_{\ell m}^{J+1} + \xi_{\ell m}^{J-1}\right) = -\frac{\ell(\ell+1)}{2R^2}\left(\frac{\phi_{\ell m}^{J}(R)}{R} - \left.\frac{\partial \phi_{\ell m}^{J}}{\partial r}\right|_{r=R}\right),$$

one gets a simple numeric linear equation in terms of $\xi_{\ell m}^{J+1}$, which is to be solved at every time-step.

Implement this BC and test it against the Sommerfeld one either by doubling the grid, or by looking at the energy left inside the grid.