Example 1

Self-interacting Klein-Gordon field on Minkowski metric

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1. Example problem

A relevant use-case of the GridRipper template library is the Klein-Gordon equation with the mass and self-interacting terms taken into account, taken on flat Minkowski metric.

1.1. Analytic formulation

1.1.1. Lagrangian and action

Our differential Lagrangian reads as the following:

$$d\mathcal{L} \coloneqq dV_g \left(g^{ab} \overline{\nabla_a(\phi)} \nabla_b(\phi) - V(\phi) \right)$$

where $dV_g = d^4x\sqrt{|\det(g)|}$ is the general differential 4-volume. Note that the Lagrangian holds the inverse metric, while the 4-volume holds the regular metric.

The action in this case is written as:

$$S \coloneqq \int d\mathcal{L} d^4x = \int \sqrt{|\det(g)|} \left[g^{\mu\nu} \overline{\partial_\mu \phi}\, \partial_\nu \phi - V(\phi) \right] d^3x dt$$

1.1.2. Chosing of coordinates

Now let us use the Boyer-Lindquist (t, r, θ, φ) coordinates, which in turn will render our metric and the inverse of the metric respectively into the form

$$g_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & r^2 & 0 \\ 0 & 0 & 0 & r^2 \sin^2\theta \end{pmatrix}, g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & r^{-2} & 0 \\ 0 & 0 & 0 & r^{-2} \sin^{-2}\theta \end{pmatrix}$$

1.1.3. Euler-Lagrange

The minimal of the action is obtained by the variation of the the Euler-Lagrange, which will take the form of the well known Klein-Gordon equation. This reads as:

$$\begin{gathered} 0 \coloneqq \frac{\partial d\mathcal{L}}{\partial \phi} - \partial_a \frac{\partial d\mathcal{L}}{\partial \nabla_a \phi} = \\ g^{\mu\nu} \partial_\mu \partial_\nu \phi - V'(\phi) = \\ -\partial_t^2 \phi + \Delta\phi - V'(\phi) = \\ -\partial_t^2 \phi + \frac{2}{r} \partial_r \phi + \partial_r^2 \phi + \frac{1}{r^2} \Delta_{S^2} \phi - V'(\phi) = 0 \end{gathered}$$

Where we took a shortcut in our calculations by making use of the knowledge on the Laplace operator in various coordinate systems, in our case in spherical coordinates. The operator Δ_{S^2} is the Laplace-Beltrami operator on the unit 2-sphere and collects the derivates in the angular directions. This will be the most convenient form as later we will see.

1.1.4. Equation of motion

Rearranging the equation will yield our equation of motion to be the following:

$$\partial_t^2 \phi = \frac{2}{r} \partial_r \phi + \partial_r^2 \phi + \frac{1}{r^2} \Delta_{S^2} \phi - V'(\phi)$$

Chosing the potential to be the self-interacting term of a scalar Higgs particle, $V(\phi)$ and $V'(\phi)$ will read as

$$V(\phi) = \frac{1}{2}m^2\phi^2 + \frac{1}{4}\lambda\phi^4$$
$$V'(\phi) = m^2\bar{\phi} + \lambda\phi^2\bar{\phi}$$

which will give us our final equation of motion:

$$\partial_t^2\phi = \frac{2}{r}\partial_r\phi + \partial_r^2\phi + \frac{1}{r^2}\Delta_{S^2}\phi - m^2\bar{\phi} - \lambda\phi^2\bar{\phi}$$

1.1.5. Sommerfeld outgoing radiation boundary condition

In order to increase stability on the borders, but more importantly eliminate the singularity of the origin, we use the widely adopted Sommerfeld reformulation, which substitutes the field variables with a non-physical quantity. Making the

$$\psi \coloneqq r\phi$$

substitution, one arrives at the equation

$$\partial_t^2\psi = 2\partial_r\frac{1}{r}\psi + r\partial_r^2\frac{1}{r}\psi + \frac{1}{r^2}\Delta_{S^2}\psi - m^2\bar{\psi} - \frac{1}{r^2}\lambda\psi^2\bar{\psi}$$

1.1.6. First order reduction

To be able to handle the equation of motion numerically, we have to use the usual first-order reduction of the partial derivate. Introducing

$$\partial_t\psi \coloneqq \psi_t$$
$$\partial_r\psi \coloneqq \psi_r$$

the equation decomposes into a partial differential equation system governing the evolution of $(\psi_t, \psi_r, \psi)^T$

$$\partial_t\psi_t = \partial_r\psi_r + \frac{1}{r^2}\Delta_{S^2}\psi - m^2\bar{\psi} - \frac{1}{r^2}\lambda\psi^2\bar{\psi}$$
$$\partial_t\psi_r = \partial_r\psi_t$$
$$\partial_t\psi = \psi_t$$

The constraint of the initial condition $\psi_r = \partial_r\psi$ is conserved throughout the evolution.

1.1.7. Decomposition into spherical harmonics

The choice of Boyer-Lindquist coordinates to express our metric is not by chance. The field ψ can be decomposed on the base of spherical harmonics in the following way:

$$\psi(t, r, \theta, \varphi) \equiv \sum_{l,m} A_l^m(t, r)Y_l^m(\theta, \varphi)$$

where $A_l^m(t, r)$ are the coefficients of the various spherical harmonic functions. This can be interpreted as a dimension reduction, as we have expressed our field using solely the $A_l^m(t, r)$ coefficients - henceforth referred to as multipole coefficients – as opposed to using $\psi(t, r, \theta, \varphi)$.

Substituting back this formula into our equation system, we get the following:

$$\partial_t \sum_{l,m} A_{t,l}^m Y_l^m = \partial_r \sum_{l,m} A_{r,l}^m Y_l^m + \frac{1}{r^2} l(l+1) \sum_{l,m} A_l^m Y_l^m - m^2 \sum_{l,m} \overline{A_l^m} Y_l^m + \frac{1}{r^2} \lambda \left(\sum_{l,m} A_l^m Y_l^m \right)^3$$
$$\partial_t \sum_{l,m} A_{r,l}^m Y_l^m = \partial_r \sum_{l,m} A_{t,l}^m Y_l^m$$
$$\partial_t \sum_{l,m} A_l^m Y_l^m = \sum_{l,m} A_{t,l}^m Y_l^m$$

where A, A_r, A_t correspond to the multipole coefficients of ψ, ψ_r, ψ_t respectively. Plus we have made use of the Eigen values of the spherical Laplace-Beltrami operator in spherical coordinates.

The time evolution equation can be obtained by scalar multiplying the equations by Y_l^m which will result in

$$\partial_t A_{t,l}^m = \partial_r A_{r,l}^m + \frac{1}{r^2} l(l+1) A_l^m - m^2 A_l^m + \frac{1}{r^2} \lambda (A_l^m)^3$$
$$\partial_t A_{r,l}^m = \partial_r A_{t,l}^m$$
$$\partial_t A_l^m = A_{t,l}^m$$

So it would seem that the equations fully decouple along the distinct multipole directions, however coupling of the various multipole coefficients arise in the multiplication operator of the field coefficients. The multiplication of fields are defined by

$$A \cdot B = C_l^m = \sum_{l_1,m_1} \sum_{l_2,m_2} A_{l_1}^{m_1} B_{l_2}^{m_2} \int_0^\pi d\theta \int_0^{2\pi} d\varphi Y_{l_1}^{m_1} Y_{l_2}^{m_2} Y_l^m$$

The double integral on the right side can be pre-computed. It's values are the Gaunt-coefficients and they can be written in matrix form:

$$G_{l_1,l_2,l}^{m_1,m_2,m} \equiv \int_0^\pi d\theta \int_0^{2\pi} d\varphi Y_{l_1}^{m_1} Y_{l_2}^{m_2} Y_l^m$$

The matrix of Gaunt-coefficients is a sparse matrix, thus each multipole direction is only connected to a handful of other multipole directions. However, taking high-order coefficients into account, this multiplication will tend to dominate our numerical calculations.

1.2. Numerical formulation

1.2.1. Treating the boundaries

As with all lattice calculations, the treating of the origin requires extra care.

1.2.1.1. The origin

The C^2 continuity requirement of the field quantities ensure that spatial derivates in the origin are finite. The spatial part of the Laplacian

$$\frac{2}{r} \partial_r \phi + \partial_r^2 \phi + \frac{1}{r^2} \Delta_{S^2} \phi$$

and applying l'Hôspital's rule we obtain the equalities

$$l = 0: \partial_r \phi_l^m = 0$$
$$l = 1: \phi_l^m = 0$$
$$l \geq 2: \phi_l^m = 0, \partial_r \phi_l^m = 0$$

which in turn mean

$$l = 0: \psi_l^m = 0, \partial_r^2 \psi_l^m = 0$$
$$l = 1: \psi_l^m = 0, \partial_r \psi_l^m = 0$$
$$l \geq 2: \psi_l^m = 0, \partial_r \psi_l^m = 0, \partial_r^2 \psi_l^m = 0$$

for our substituted field variables. Given that all multipole directions vanish in both value and first derivate, the time derivate of these will vanish too. Only $l = 0$ will differ in this regard, where only the second derivate vanishes, but not the first. Summarizing, our field equations in the origin will look as following:

$$\partial_t \psi_{t,l}^m(r = 0, t) = 0$$
$$\partial_t \psi_{r,l}^m(r = 0, t) = \begin{cases} l = 0 \to \partial_r \psi_{t,l}^m(r = 0, t) \\ l \neq 0 \to 0 \end{cases}$$
$$\partial_t \psi_l^m(r = 0, t) = 0$$

1.2.1.2. Next to the origin

While the field equations hold true as normal next to the origin, calculating the radial derivates requires obtaining field values from the far side of the origin. These values can be obtained by

$$\psi_{t,l}^m(-r, t) = (-1)^{l+1} \cdot (-1) \cdot \psi_{t,l}^m(r, t)$$
$$\psi_{r,l}^m(-r, t) = (-1)^{l+1} \cdot (+1) \cdot \psi_{r,l}^m(r, t)$$
$$\psi_l^m(-r, t) = (-1)^{l+1} \cdot (+1) \cdot \psi_l^m(r, t)$$

The first parity is that of the multipole direction's, while the second is the parity of the variable, and the resulting parity is the combination of the two.

These however although are analytically correct, the multipole coefficients next to the origin are ill conditioned. Sufficiently large radial resolution will yield high noise close to the origin due to the inverse powers of r in the field equations, as well as the Eigen values of the spherical Laplace operator further magnify numeric inaccuracies.

To eliminate this noise, we make use of the constraints on the field variables at the origin. Taking the symmetric fourth order finite difference stencil

$$\partial_r \psi(r) = \frac{8\big(\psi(r + dr) - \psi(r - dr)\big) + \psi(r - 2dr) - \psi(r + 2dr)}{12dr}$$

and substituting in $r = 1$ plus our knowledge that the field variables are exactly 0 in the origin, we obtain the relations

$$\partial_t \psi_{t,l}^m(r = 1, t) = \begin{cases} l_{\text{even}} \to \psi_{t,l}^m(r = 2, t)/16 \\ l_{\text{odd}} \to \psi_{t,l}^m(r = 2, t)/8 \end{cases}$$
$$\partial_t \psi_{r,l}^m(r = 1, t) = \begin{cases} l = 0 \to \partial_r \psi_{t,l}^m(r = 1, t) \\ l \neq 0 \to \begin{cases} l_{\text{even}} \to \psi_{r,l}^m(r = 2, t)/16 \\ l_{\text{odd}} \to \psi_{r,l}^m(r = 2, t)/8 \end{cases} \end{cases}$$
$$\partial_t \psi_l^m(r = 1, t) = \begin{cases} l_{\text{even}} \to \psi_l^m(r = 2, t)/16 \\ l_{\text{odd}} \to \psi_l^m(r = 2, t)/8 \end{cases}$$

The above formulation trivially holds true for the multipole coefficients as well.

1.2.1.3. *The outer sphere*

There is no compactification involved, therefore the outer end of the lattice is a free boundary. As such, calculating radial derivates becomes problematic. Investigations (CITATION) showed that somewhat counter-intuitively using less precise derivates provides greater stability than using the more and more asymmetric finite difference stencils. Former papers referred to this method as the $\mathcal{O}(4-2-1)$ method, referring to the order of correctness decreasing towards the boundary of the lattice.

1.2.2. Numerical viscosity

In order to suppress high-order oscillations to wreck the stability of the evolution, one needs to introduce a higher order dissipative factor into the evolution, than that of the driving finite difference method.

Since the application uses finite differencing precise to the 4th order in the separation of coordinates, we introduce a 6th order derivate

$$\mathfrak{D} = \sigma \Delta_r^5 \partial_r^6 \phi$$

1.3. Energy conservation

As the first and most important test of the simulation one needs to check whether energy is conserved throughout the evolution. The energy-impulse tensor generally is defined as

$$T^{ab} \coloneqq \frac{\partial d\mathcal{L}/\partial g_{ab}}{dV_g}$$

where we can make use of the analogies

$$\frac{\partial dV_g}{\partial g_{ab}} = \frac{1}{2} g^{ab} dV_g$$
$$\frac{\partial g^{cd}}{\partial g_{ab}} = -\frac{1}{2}\left(g^{ca} g^{bd} + g^{cb} g^{ad}\right)$$

Substituting the differential Lagrangian into the equation and using the formulas above we get

$$T^{ab} = \frac{1}{dV_g}\left\{\frac{1}{2} g^{ab} dV_g \left[g^{cd}\overline{\nabla_c(\phi)}\nabla_d(\phi) - V(\phi)\right] + dV_g\left[-\frac{1}{2}\left(g^{ia}g^{bj} + g^{ib}g^{aj}\right)\overline{\nabla_i(\phi)}\nabla_j(\phi)\right]\right\}$$

The energy inside the evolution is conserved if

$$\Delta E = 0$$

between any two time points holds true. Having one free boundary on the lattice, the total energy of the system will be the sum of the energy that is still inside the lattice and of the energy that has been radiated out through the free boundary up until the given time point. This can be interpreted as a relativistic continuity equation. The energy thus at any given t can be written as

$$E(t) = \int_0^{r_{\max}} \varepsilon(t,r)dr + \int_0^t j_r(t, r_{\max})dt$$

where

$$\varepsilon(t,r) = T^{ab}t_a t_b = T^{tt} =$$
$$= \frac{1}{2}\left[-\overline{\partial_t\phi}\partial_t\phi + \overline{\partial_r\phi}\partial_r\phi + \frac{1}{r^2}\overline{\Delta_{S^2}\phi}\Delta_{S^2}\phi - \left(\frac{1}{2}m^2\phi^2 + \frac{1}{4}\lambda\phi^4\right)\right] - \overline{\partial_t\phi}\partial_t\phi$$
$$j_r = T_{ab}t^a r^b = T_{tr} =$$
$$= 2\left(\overline{\partial_r\phi}\partial_t\phi + \overline{\partial_t\phi}\partial_r\phi\right)$$

given that t^b, r^b are the time-like and radial Killing-vectors of the metric.

2. Results