

Underwater Acoustic Simulation Theory

mv-2

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1 Background & Motivation

This project is intended as a learning exercise for both the physics of sound propagation and the programming aspects required for this project.

The intended theory to be explored is initially to develop ray propagation simulation based on repeated application of Snell's law and then to layer on Gaussian Beam Tracing (GBT) to eventually develop a well rounded sound prediction tool for higher frequency acoustics. If this is successful, a nodal based solver for low frequency noise will be developed although this would be a large undertaking and is a stretch goal at this time.

2 Geometric Ray Tracing

2.1 Physical Theory

The geometric ray trace theory used in this simulation is based on work from **Hovem13**. This methodology discretises the sound speed profile into evenly spaced layers and applies Snell's law (Equation 1) across each layer in order to determine the ray path.

$$\frac{\sin(\theta_1)}{\sin(\theta_2)} = \frac{c_1}{c_2} \quad (1)$$

By assuming that the ray is only refracted between all fluid layers across the entire solution space then this relationship can be reduced to the parameter ξ as shown in Equation 2.

$$\xi = \frac{\cos(\theta(z))}{c(z)} = \frac{\cos(\theta_0)}{c_0} \quad (2)$$

For a full derivation see **Hovem13**. For the purposes of the acoustic simulation, Equations 3 and 4 are required.

$$\Delta r = \int_{z_1}^{z_2} \frac{\xi c(z)}{\sqrt{1 - \xi^2 \cdot c^2(z)}} dz \quad (3)$$

$$\Delta t = \int_{z_1}^{z_2} \frac{1}{c(z) \sqrt{1 - \xi^2 \cdot c^2(z)}} dz \quad (4)$$

To compute these intervals the function for $c(z)$ must be known. Based on the form of the integrals in Equations 3 and 4 not all function forms allow for the integrals to be solved analytically. The most obvious and consequently useful form of $c(z)$ is to assume it is a set of piecewise linear functions along each layer of the fluid medium. Assuming that a general function is known for $c(z)$ either analytically or from curve fitting then the fluid layer i should have the form shown in Equation 5.

$$c_i(z) = c_i + g_i \cdot (z - z_i), \text{ for } z \in [z_i, z_{i+1}) \quad (5)$$

where $g_i = \frac{c_{i+1} - c_i}{\Delta z}$

Solving the integrals with this form of sound speed profile leads to the relationships shown in Equations 6 and 7.

$$\Delta r = \frac{\sqrt{1 - \xi^2 \cdot c^2(z_i)} - \sqrt{1 - \xi^2 \cdot c^2(z_{i+1})}}{\xi \cdot g_i} \quad (6)$$

$$\Delta t = \frac{\ln \left(\frac{c(z_{i+1})}{c(z_i)} \frac{1 + \sqrt{1 - \xi^2 \cdot c^2(z_i)}}{1 + \sqrt{1 - \xi^2 \cdot c^2(z_{i+1})}} \right)}{|g_i|} \quad (7)$$

Note that upon inspection of these equations it is clear that if the term $\xi \cdot c(z_j) \geq 1$ then the equations will both return imaginary quantities. This is non-physical behaviour and must be handled as an edge case. If the increment in range or time is imaginary then it can be concluded that the ray does not reach the next layer of the fluid medium and instead reverses depth direction and $z_{i+1} = z_i$. This lays the groundwork for the ray tracing algorithms although some extra details need to be considered such as how the sound speed profile is to be expressed and other programmatic elements.

Algorithm 1 Ray tracing algorithm

Initialise:

```
 $r_0 \leftarrow \text{sourcerange}$   
 $z_0 \leftarrow \text{sourcedepth}$   
 $\theta_0 \leftarrow \text{sourcerayangle}$   
 $z_{\text{sign}} = \text{sign}(\sin(\theta_0))$   
 $i \leftarrow 0$   
 $t \leftarrow 0$   
 $\text{maximumiterations}$   
 $c_0 \leftarrow c(z_0), c_1 \leftarrow c(z_0 + z_{\text{sign}} \cdot \Delta z)$   
 $\xi \leftarrow \frac{\cos(\theta_0)}{c_0}$   
while  $i < \text{max iterations}$  do  
   $g_i = \frac{c_{i+1} - c_i}{\Delta z}$   
  if  $\xi \cdot g_i < 1$  then  
     $\Delta r = \frac{\sqrt{1 - \xi^2 \cdot c^2(z_i)} - \sqrt{1 - \xi^2 \cdot c^2(z_{i+1})}}{\xi \cdot g_i}$   
     $\Delta t = \frac{\ln\left(\frac{c(z_{i+1})}{c(z_i)} \frac{1 + \sqrt{1 - \xi^2 \cdot c^2(z_i)}}{1 + \sqrt{1 - \xi^2 \cdot c^2(z_{i+1})}}\right)}{|g_i|}$   
     $z_{i+1} \leftarrow z_i + z_{\text{sign}} \cdot \Delta z$   
  else  
     $\Delta r = \frac{2 \cdot \sqrt{1 - \xi^2 \cdot c^2(z_i)}}{\xi \cdot g_i}$   
     $\Delta t = \frac{2 \cdot \ln\left(\frac{1 + \sqrt{1 - \xi^2 \cdot c^2(z_i)}}{\xi \cdot c(z_i)}\right)}{|g_i|}$   
     $z_{\text{sign}} \leftarrow -z_{\text{sign}}$   
   $r_{i+1} \leftarrow r_i + \Delta r$   
   $t_{i+1} \leftarrow t_i + \Delta t$   
   $i \leftarrow i + 1$   
return  $r, z, t$ 
```

2.2 Ray Tracing Algorithm

The generic ray tracing algorithm is included below in Algorithm 1.

2.3 Reflection

In order to accurately model reflection of rays two problems must be handled. Firstly, the point of intersection between a ray and an object must be accurately calculated and then the entry and exit angles of the ray can be calculated as needed.

2.3.1 Body Intersection

Within the **gUAcS** software package, bodies are all defined as polygons. This means intersection between a ray and polygonal body can be calculated by determining the location at which the line defined by a ray and each side of the polygon meet in order to determine a valid intersection.

Consider the line l_i defined by the two points $(r_{i,0}, z_{i,0}), (r_{i,1}, z_{i,1})$. Now determine the intersection between the lines l_{ray} and l_{edge} .

$$\begin{aligned} l_{\text{ray}} : \mathbf{p}_{\text{ray},0} &= (r_{\text{ray},0}, z_{\text{ray},0}), \mathbf{p}_{\text{ray},1} = (r_{\text{ray},1}, z_{\text{ray},1}) \\ l_{\text{edge}} : \mathbf{p}_{\text{edge},0} &= (r_{\text{edge},0}, z_{\text{edge},0}), \mathbf{p}_{\text{edge},1} = (r_{\text{edge},1}, z_{\text{edge},1}) \end{aligned}$$

Parameterise the lines l_{ray} and l_{edge} and consider for our case a ray will only propagate forwards and the side of the polygon must lie between the points used to define it. This means constraints can be imposed on t and τ in order to

determine when valid intersections are made.

$$\begin{aligned} l_{ray} : \mathbf{p}(t) &= \mathbf{p}_{ray,0} + t \cdot (\mathbf{p}_{ray,1} - \mathbf{p}_{ray,0}), \text{ for } t \geq 0 \\ l_{edge} : \mathbf{p}(\tau) &= \mathbf{p}_{edge,0} + \tau \cdot (\mathbf{p}_{edge,1} - \mathbf{p}_{edge,0}), \text{ for } \tau \in [0, 1] \end{aligned}$$

By setting $\mathbf{p}(t) = \mathbf{p}(\tau)$ a point of intersection can be calculated.

$$\begin{aligned} \mathbf{p}_{edge,0} + \tau \cdot (\mathbf{p}_{edge,1} - \mathbf{p}_{edge,0}) &= \mathbf{p}_{ray,0} + t \cdot (\mathbf{p}_{ray,1} - \mathbf{p}_{ray,0}) \\ \begin{bmatrix} r_{edge,0} \\ z_{edge,0} \end{bmatrix} + \tau \cdot \left(\begin{bmatrix} r_{edge,1} \\ z_{edge,1} \end{bmatrix} - \begin{bmatrix} r_{edge,0} \\ z_{edge,0} \end{bmatrix} \right) &= \begin{bmatrix} r_{ray,0} \\ z_{ray,0} \end{bmatrix} + t \cdot \left(\begin{bmatrix} r_{ray,1} \\ z_{ray,1} \end{bmatrix} - \begin{bmatrix} r_{ray,0} \\ z_{ray,0} \end{bmatrix} \right) \\ \begin{bmatrix} r_{edge,0} + \tau \cdot (r_{edge,1} - r_{edge,0}) \\ z_{edge,0} + \tau \cdot (z_{edge,1} - z_{edge,0}) \end{bmatrix} &= \begin{bmatrix} r_{ray,0} + t \cdot (r_{ray,1} - r_{ray,0}) \\ z_{ray,0} + t \cdot (z_{ray,1} - z_{ray,0}) \end{bmatrix} \end{aligned}$$

Now split into equations for x and y .

$$\begin{aligned} r_{edge,0} - r_{ray,0} + \tau \cdot (r_{edge,1} - r_{edge,0}) &= t \cdot (r_{ray,1} - r_{ray,0}) \\ \implies t &= \frac{r_{edge,0} - r_{ray,0} + \tau \cdot (r_{edge,1} - r_{edge,0})}{r_{ray,1} - r_{ray,0}} \\ z_{edge,0} - z_{ray,0} + \tau \cdot (z_{edge,1} - z_{edge,0}) &= t \cdot (z_{ray,1} - z_{ray,0}) \\ \implies t &= \frac{z_{edge,0} - z_{ray,0} + \tau \cdot (z_{edge,1} - z_{edge,0})}{z_{ray,1} - z_{ray,0}} \\ \implies \frac{r_{edge,0} - r_{ray,0} + \tau \cdot (r_{edge,1} - r_{edge,0})}{r_{ray,1} - r_{ray,0}} &= \frac{z_{edge,0} - z_{ray,0} + \tau \cdot (z_{edge,1} - z_{edge,0})}{z_{ray,1} - z_{ray,0}} \\ \frac{r_{edge,0} - r_{ray,0}}{r_{ray,1} - r_{ray,0}} - \frac{z_{edge,0} - z_{ray,0}}{z_{ray,1} - z_{ray,0}} &= \tau \cdot \left(\frac{z_{edge,1} - z_{edge,0}}{z_{ray,1} - z_{ray,0}} - \frac{r_{edge,1} - r_{edge,0}}{r_{ray,1} - r_{ray,0}} \right) \\ &= \frac{(r_{edge,0} - r_{ray,0}) \cdot (z_{ray,1} - z_{ray,0}) - (z_{edge,0} - z_{ray,0}) \cdot (r_{ray,1} - r_{ray,0})}{(r_{ray,1} - r_{ray,0})(z_{ray,1} - z_{ray,0})} \\ \tau \cdot \left(\frac{(z_{edge,1} - z_{edge,0}) \cdot (r_{ray,1} - r_{ray,0}) - (r_{edge,1} - r_{edge,0}) \cdot (z_{ray,1} - z_{ray,0})}{(r_{ray,1} - r_{ray,0})(z_{ray,1} - z_{ray,0})} \right) &= \frac{(r_{edge,0} - r_{ray,0}) \cdot (z_{ray,1} - z_{ray,0}) - (z_{edge,0} - z_{ray,0}) \cdot (r_{ray,1} - r_{ray,0})}{(z_{edge,1} - z_{edge,0}) \cdot (r_{ray,1} - r_{ray,0}) - (r_{edge,1} - r_{edge,0}) \cdot (z_{ray,1} - z_{ray,0})} \end{aligned} \tag{8}$$

$$t = \frac{z_{edge,0} - z_{ray,0} + \tau \cdot (z_{edge,1} - z_{edge,0})}{z_{ray,1} - z_{ray,0}} \tag{9}$$

Equation 8 can be used to directly calculate τ and by extension t can then be calculated from Equation 9. Note that in this form of the equation if both the direction of the edge and the ray is the same such that $\Delta r_{edge} = k \cdot \Delta r_{ray}$ and $\Delta z_{edge} = k \cdot \Delta z_{ray}$ for $k \in \mathbb{R}$ then the denominator of this equations tends to 0 resulting in an undefined result. This makes intuitive sense as there should be no solution for parallel lines having a point of intersection. As stated above the calculated intersection is valid if and only if $t \geq 0$ and $\tau \in [0, 1]$.

2.3.2 Reflection Angle

Reflection angle off an object can be simply calculated by noting that the angle of the outgoing ray relative to the object surface is equivalent to that of the incoming ray to the object surface. Inspecting the phenomena shown in Figure 1 allows the relationship in equation 10 to be derived.

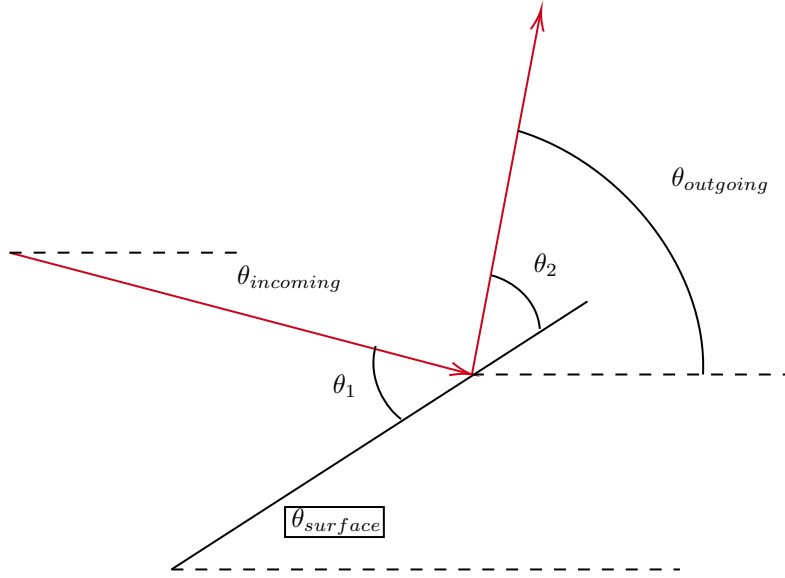


Figure 1: Reflection of ray on solid surface

$$\theta_1 = \theta_2$$

$$\implies \theta_{incoming} + \theta_{surface} = \theta_{outgoing} - \theta_{surface}$$

$$\theta_{outgoing} = \theta_{incoming} + 2 \cdot \theta_{surface} \quad (10)$$

3 Gaussian Beam Tracing

3.1 Arc Step Integration Derivation

$$\begin{aligned} \int_{z_i}^{z_{i+1}} ds &= \int_{z_i}^{z_{i+1}} \frac{dz}{\sqrt{1 - \xi^2 \cdot c^2(z)}} \\ &= \int_{z_i}^{z_{i+1}} \frac{dz}{\sqrt{1 - \xi^2 \cdot (c_i + g_i \cdot (z - z_i))^2}} \\ &= \frac{1}{g_i \cdot \xi} \int_{u_i}^{u_{i+1}} \frac{du}{\sqrt{1 - u^2}} \quad u = \xi(c_i + g_i(z - z_i)) \\ &= \left[\frac{\arcsin(u)}{g_i \cdot \xi} \right]_{u_i}^{u_{i+1}} \\ &= \left[\frac{\arcsin(u)}{g_i \cdot \xi} \right]_{\xi \cdot c_i}^{\xi \cdot c_{i+1}} \\ \therefore \Delta s &= \frac{\arcsin(\xi \cdot c_{i+1}) - \arcsin(\xi \cdot c_i)}{g_i \cdot \xi} \end{aligned}$$

3.2 Derivation of c_{nn}

$$\begin{aligned}
c_{nn} &= \frac{\partial^2 c}{\partial n^2} \\
&= \frac{\partial^2 c}{\partial r^2} \left(\frac{dr}{dn} \right)^2 + 2 \cdot \frac{\partial^2 c}{\partial r \cdot \partial z} \left(\frac{dr}{dn} \right) \left(\frac{dz}{dn} \right) + \frac{\partial^2 c}{\partial z^2} \left(\frac{dz}{dn} \right)^2 \\
&= \frac{\partial^2 c}{\partial z^2} \left(\frac{dz}{dn} \right)^2, \quad c(z, r) = c(z) \\
&= \frac{\partial^2 c}{\partial z^2} \left(-\frac{dr}{ds} \right)^2 \\
&= \frac{\partial^2 c}{\partial z^2} (-\cos(\theta)) \\
\therefore c_{nn} &= \frac{\partial^2 c}{\partial z^2} (-\xi \cdot c)
\end{aligned}$$

With the continuous definition of c_{nn} known, the discretised form can then be derived.

$$\begin{aligned}
\frac{\partial^2 c}{\partial z^2} &= \frac{c_{i+1} - 2 \cdot c_i + c_{i-1}}{\Delta z^2} \\
\therefore c_{nn}|_{z=z_i} &= -\xi \cdot c_i \cdot \left(\frac{c_{i+1} - 2 \cdot c_i + c_{i-1}}{\Delta z^2} \right)
\end{aligned}$$

3.3 Derivation of discretised $p - q$ ODEs

Consider that p and q are linked by equations 11 and 12.

$$\frac{dq}{ds} = c(s) \cdot p(s) \quad (11)$$

$$\frac{dp}{ds} = \frac{-c_{nn}}{c^2(s)} q(s) \quad (12)$$

3.3.1 Explicit Solver

Using the classic Runge-Kutta 4th order solver defined by the following Butcher Tableau.

0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0
1	0	0	1	0
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

Such that:

$$\begin{aligned}
y_{n+1} &= y_n + \frac{h}{6} \cdot (k_{n1} + 2 \cdot k_{n2} + 2 \cdot k_{n3} + k_{n4}) \\
k_{n1} &= f(t_n, y_n) \\
k_{n2} &= f\left(t_n + \frac{h}{2}, y_n + \frac{k_{n1}}{2}\right) \\
k_{n3} &= f\left(t_n + \frac{h}{2}, y_n + \frac{k_{n2}}{2}\right) \\
k_{n4} &= f(t_n + h, y_n + k_{n3})
\end{aligned}$$

Now consider this form based on the form of the $p - q$ equations. Let j define the spatial step for $s = s_j$

$$\begin{aligned}
y_k &\equiv \mathbf{x}_k \\
t_k &\equiv s_k \\
f(t_k, y_k) &\equiv \dot{\mathbf{x}}_k = \begin{bmatrix} 0 & c(s_k) \\ \frac{-c_{nn}|_{s=s_k}}{c^2(s_k)} & 0 \end{bmatrix} \begin{bmatrix} q_k \\ p_k \end{bmatrix} \\
\Rightarrow k_{n1} &= \begin{bmatrix} 0 & c(s_j) \\ \frac{-c_{nn,(j)}}{c^2(s_j)} & 0 \end{bmatrix} \begin{bmatrix} q_j \\ p_j \end{bmatrix} \\
\Rightarrow k_{n2} &= \begin{bmatrix} 0 & c(s_{j+\frac{1}{2}}) \\ \frac{-c_{nn,(j+\frac{1}{2})}}{c^2(s_{j+\frac{1}{2}})} & 0 \end{bmatrix} \left(\begin{bmatrix} q_j \\ p_j \end{bmatrix} + \frac{1}{2} k_{n1} \right) \\
\Rightarrow k_{n3} &= \begin{bmatrix} 0 & c(s_{j+\frac{1}{2}}) \\ \frac{-c_{nn,(j+\frac{1}{2})}}{c^2(s_{j+\frac{1}{2}})} & 0 \end{bmatrix} \left(\begin{bmatrix} q_j \\ p_j \end{bmatrix} + \frac{1}{2} k_{n2} \right) \\
\Rightarrow k_{n4} &= \begin{bmatrix} 0 & c(s_{j+1}) \\ \frac{-c_{nn,(j+1)}}{c^2(s_{j+1})} & 0 \end{bmatrix} \left(\begin{bmatrix} q_j \\ p_j \end{bmatrix} + k_{n3} \right) \\
\Rightarrow \mathbf{x}_{j+1} &= \mathbf{x}_j + \frac{\Delta s}{6} (k_{n1} + 2 \cdot k_{n2} + 2 \cdot k_{n3} + k_{n4})
\end{aligned}$$

Where:

$$\begin{aligned}
c_{nn,(j)} &= -\xi \cdot c_i \cdot \left(\frac{c_{i+1} - 2 \cdot c_i + c_{i-1}}{\Delta z^2} \right) \\
c_{nn,(j+1)} &= -\xi \cdot c_{i+1} \cdot \left(\frac{c_{i+2} - 2 \cdot c_{i+1} + c_i}{\Delta z^2} \right) \\
c_{nn,(j+\frac{1}{2})} &= -\xi \cdot c_{i+\frac{1}{2}} \cdot \left(\frac{c_{i+\frac{3}{2}} - 2 \cdot c_{i+\frac{1}{2}} + c_{i-\frac{1}{2}}}{\Delta z^2} \right) \\
&= -\xi \cdot (c_i + c_{i+1}) \cdot \left(\frac{(c_{i+2} + c_{i+1}) - 2 \cdot (c_i + c_{i+1}) + (c_{i-1} + c_i)}{4 \cdot \Delta z^2} \right) \\
\Rightarrow c_{nn,(j+\frac{1}{2})} &= -\xi \cdot (c_i + c_{i+1}) \cdot \left(\frac{c_{i+2} - c_{i+1} - c_i + c_{i-1}}{4 \cdot \Delta z^2} \right)
\end{aligned}$$

3.3.2 Backward Euler

$$\begin{aligned}
y_{k+1} &= y_k + h \cdot f(t_{k+1}, y_{k+1}) \\
y_k &\equiv \mathbf{x}_k \\
t &\equiv s \\
\Rightarrow \mathbf{x}_{i+1} &= \mathbf{x}_n + \Delta s \dot{\mathbf{x}}_{n+1} \\
\begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} &= \begin{bmatrix} q_i \\ p_i \end{bmatrix} + \Delta s \begin{bmatrix} 0 & c(s_{i+1}) \\ \frac{-c_{nn,i+1}}{c^2(s_{i+1})} & 0 \end{bmatrix} \begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} \\
\begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} &= \begin{bmatrix} q_i \\ p_i \end{bmatrix} + \begin{bmatrix} p_{i+1} \cdot \Delta s \cdot c(s_{i+1}) \\ q_{i+1} \cdot \Delta s \cdot \frac{-c_{nn,i+1}}{c^2(s_{i+1})} \end{bmatrix} \\
\begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} - \begin{bmatrix} p_{i+1} \cdot \Delta s \cdot c(s_{i+1}) \\ q_{i+1} \cdot \Delta s \cdot \frac{-c_{nn,i+1}}{c^2(s_{i+1})} \end{bmatrix} &= \begin{bmatrix} q_i \\ p_i \end{bmatrix} \\
\begin{bmatrix} 1 & -\Delta s \cdot c(s_{i+1}) \\ -\Delta s \cdot \frac{-c_{nn,i+1}}{c^2(s_{i+1})} & 1 \end{bmatrix} \begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} &= \begin{bmatrix} q_i \\ p_i \end{bmatrix}
\end{aligned}$$

To solve this system of equations take the inverse of the matrix to make $\dot{\mathbf{x}}_{i+1}$ the subject of the equation.

$$\begin{aligned}
\text{let } A &= \begin{bmatrix} 1 & -\Delta s \cdot c(s_{i+1}) \\ \Delta s \cdot \frac{c_{nn,i+1}}{c^2(s_{i+1})} & 1 \end{bmatrix} \\
\therefore A^{-1} &= \frac{c(s_{i+1})}{1 - \Delta s^2 \cdot c_{nn,i+1}} \begin{bmatrix} 1 & \Delta s \cdot c(s_{i+1}) \\ -\Delta s \cdot \frac{c_{nn,i+1}}{c^2(s_{i+1})} & 1 \end{bmatrix} \\
\Rightarrow \begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} &= A^{-1} \begin{bmatrix} q_i \\ p_i \end{bmatrix} \\
\therefore \begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} &= \frac{c(s_{i+1})}{1 - \Delta s^2 \cdot c_{nn,i+1}} \begin{bmatrix} q_i + \Delta s \cdot c(s_{i+1}) \cdot p_i \\ p_i - \Delta s \cdot \frac{c_{nn,i+1}}{c^2(s_{i+1})} q_i \end{bmatrix}
\end{aligned}$$

3.3.3 3rd Order Radau IA

The Butcher Tableau of Radau IA is as follows:

$$\begin{array}{c|cc}
0 & \frac{1}{4} & -\frac{1}{4} \\
\frac{2}{3} & \frac{1}{4} & \frac{5}{12} \\
\hline
\frac{2}{3} & \frac{1}{4} & \frac{5}{12}
\end{array}$$

$$\begin{aligned}
\Rightarrow y_{n+1} &= y_n + \frac{\Delta t}{4} \cdot (k_{n1} + 3 \cdot k_{n2}) \\
k_{n1} &= f\left(t_n, y_n + \frac{\Delta t}{4}(k_{n1} - k_{n2})\right) \\
k_{n2} &= f\left(t_n + \frac{2 \cdot \Delta t}{3}, y_n + \frac{\Delta t}{12}(3 \cdot k_{n1} + 5 \cdot k_{n2})\right) \\
y_j &\equiv \begin{bmatrix} q_j \\ s_j \end{bmatrix} \\
t &\equiv s \\
f(t_n, y_n) &\equiv \dot{\mathbf{x}}_j = \begin{bmatrix} 0 & c_j \\ \frac{-c_{nn,j}}{c_j^2} & 0 \end{bmatrix} \begin{bmatrix} q_j \\ p_j \end{bmatrix}
\end{aligned}$$

Now solve:

$$\begin{aligned}
\mathbf{x}_{j+1} &= \mathbf{x}_j + \frac{\Delta s}{4} \cdot (k_{n1} + 3 \cdot k_{n2}) \\
k_{n1} &= \begin{bmatrix} 0 & c_j \\ \frac{-c_{nn,j}}{c_j^2} & 0 \end{bmatrix} \left(\begin{bmatrix} q_j \\ p_j \end{bmatrix} + \frac{\Delta s}{4} \cdot (k_{n1} - k_{n2}) \right) \\
k_{n1} &= A_j \left(\mathbf{x}_j + \frac{\Delta s}{4} \cdot (k_{n1} - k_{n2}) \right) \\
k_{n2} &= \begin{bmatrix} 0 & c_{j+\frac{2}{3}} \\ \frac{-c_{nn,j+\frac{2}{3}}}{c_{j+\frac{2}{3}}^2} & 0 \end{bmatrix} \left(\begin{bmatrix} q_{j+\frac{2}{3}} \\ p_{j+\frac{2}{3}} \end{bmatrix} + \frac{\Delta s}{12} \cdot (3 \cdot k_{n1} + 5 \cdot k_{n2}) \right) \\
k_{n2} &= A_{j+\frac{2}{3}} \left(\mathbf{x}_j + \frac{\Delta s}{12} \cdot (3 \cdot k_{n1} + 5 \cdot k_{n2}) \right)
\end{aligned}$$

Consider solving for k_{n1} and k_{n2} .

$$\begin{aligned}
k_{n1} &= A_j \left(\mathbf{x}_j + \frac{\Delta s}{4} \cdot (k_{n1} - k_{n2}) \right) \\
\Rightarrow A_j^{-1} k_{n1} &= \mathbf{x}_j + \frac{\Delta s}{4} \cdot (k_{n1} - k_{n2}) \\
\therefore k_{n2} &= \frac{4}{\Delta s} \mathbf{x}_j + k_{n1} - \frac{4}{\Delta s} A_j^{-1} k_{n1}
\end{aligned}$$

$$\begin{aligned}
k_{n2} &= A_{j+\frac{2}{3}} \left(\mathbf{x}_j + \frac{\Delta t}{12} \cdot (3 \cdot k_{n1} + 5 \cdot k_{n2}) \right) \\
\implies A_{j+\frac{2}{3}}^{-1} k_{n2} &= \mathbf{x}_j + \frac{\Delta s}{12} \cdot (3 \cdot k_{n1} + 5 \cdot k_{n2}) \\
\left(\frac{12}{\Delta s} A_{j+\frac{2}{3}}^{-1} - 5 \cdot \mathbb{I} \right) k_{n2} &= \frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \\
\text{let } B_{j+\frac{2}{3}} &= A_{j+\frac{2}{3}}^{-1} - 5 \cdot \mathbb{I} \\
\implies B_{j+\frac{2}{3}} k_{n2} &= \frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \\
\therefore k_{n2} &= B_{j+\frac{2}{3}}^{-1} \left(\frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \right)
\end{aligned}$$

Now solve for k_{n1} .

$$\begin{aligned}
\frac{4}{\Delta s} \mathbf{x}_j + k_{n1} - \frac{4}{\Delta s} A_j^{-1} k_{n1} &= B_{j+\frac{2}{3}}^{-1} \left(\frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \right) \\
\frac{4}{\Delta s} \mathbf{x}_j + \left(\mathbb{I} - \frac{4}{\Delta s} A_j^{-1} \right) k_{n1} &= B_{j+\frac{2}{3}}^{-1} \left(\frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \right) \\
\left(\mathbb{I} - \frac{4}{\Delta s} A_j^{-1} - 3 \cdot B_{j+\frac{2}{3}}^{-1} \right) k_{n1} &= \left(\frac{12}{\Delta s} B_{j+\frac{2}{3}}^{-1} - \frac{4}{\Delta s} \mathbb{I} \right) \mathbf{x}_j \\
\text{let } C_j &= \mathbb{I} - \frac{4}{\Delta s} A_j^{-1} - 3 \cdot B_{j+\frac{2}{3}}^{-1} \\
\therefore k_{n1} &= C_j^{-1} \left(3 \cdot B_{j+\frac{2}{3}}^{-1} - \mathbb{I} \right) \frac{4}{\Delta s} \mathbf{x}_j
\end{aligned}$$

Wahoo.

Now figure out the details for the terms A , B and C to allow for these equations to be implemented.

$$\begin{aligned}
A_j &= \begin{bmatrix} 0 & c_j \\ -\frac{c_{nn,j}}{c_j^2} & 0 \end{bmatrix} \\
A_j^{-1} &= \frac{c_j}{c_{nn,j}} \begin{bmatrix} 0 & -c_j \\ \frac{c_{nn,j}}{c_j^2} & 0 \end{bmatrix} \\
\therefore A_j^{-1} &= \begin{bmatrix} 0 & -\frac{c_j^2}{c_{nn,j}} \\ \frac{1}{c_j} & 0 \end{bmatrix} \\
B_j &= A_j^{-1} - 5 \cdot \mathbb{I} \\
B_j &= \begin{bmatrix} -5 & -\frac{c_j^2}{c_{nn,j}} \\ \frac{1}{c_j} & -5 \end{bmatrix} \\
B_j^{-1} &= \frac{1}{25 + \frac{c_j}{c_{nn,j}}} \begin{bmatrix} -5 & \frac{c_j^2}{c_{nn,j}} \\ -\frac{1}{c_j} & -5 \end{bmatrix} \\
&= \frac{c_{nn,j}}{25 \cdot c_{nn,j} + c_j} \begin{bmatrix} -5 & \frac{c_j^2}{c_{nn,j}} \\ -\frac{1}{c_j} & -5 \end{bmatrix} \\
\therefore B_j^{-1} &= \begin{bmatrix} -\frac{5 \cdot c_{nn,j}}{25 \cdot c_{nn,j} + c_j} & \frac{c_j^2}{25 \cdot c_{nn,j} + c_j} \\ -\frac{c_{nn,j}}{25 \cdot c_j \cdot c_{nn,j} + c_j^2} & -\frac{5 \cdot c_{nn,j}}{25 \cdot c_{nn,j} + c_j} \end{bmatrix} \\
C_j &= \mathbb{I} - \frac{4}{\Delta s} A_j^{-1} - 3 \cdot B_{j+\frac{2}{3}}^{-1} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & -\frac{4 \cdot c_j^2}{\Delta s \cdot c_{nn,j}} \\ \frac{4}{\Delta s \cdot c_j} & 0 \end{bmatrix} - \begin{bmatrix} -\frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} & \frac{3 \cdot c_{j+\frac{2}{3}}^2}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \\ -\frac{3 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{j+\frac{2}{3}} \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}^2} & -\frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \end{bmatrix} \\
\therefore C_j &= \begin{bmatrix} 1 + \frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} & \frac{4 \cdot c_j^2}{\Delta s \cdot c_{nn,j}} - \frac{3 \cdot c_{j+\frac{2}{3}}^2}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \\ \frac{4}{\Delta s \cdot c_j} + \frac{3 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{j+\frac{2}{3}} \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}^2} & 1 + \frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \end{bmatrix} \\
\text{let } C_j &= \begin{bmatrix} C_j^{(1,1)} & C_j^{(1,2)} \\ C_j^{(2,1)} & C_j^{(2,2)} \end{bmatrix} \\
C_j^{-1} &= \frac{1}{C_j^{(1,1)} \cdot C_j^{(2,2)} - C_j^{(1,2)} \cdot C_j^{(2,1)}} \begin{bmatrix} C_j^{(2,2)} & -C_j^{(1,2)} \\ -C_j^{(2,1)} & C_j^{(1,1)} \end{bmatrix}
\end{aligned}$$

Now calculate k_{n1} .

$$k_{n1} = C_j^{-1} \left(3 \cdot B_{j+\frac{2}{3}}^{-1} - \mathbb{I} \right) \frac{4}{\Delta s} \mathbf{x}_j$$

$$\text{let } D_j = 3 \cdot B_{j+\frac{2}{3}}^{-1} - \mathbb{I}$$

$$\begin{aligned} \therefore D_j &= \begin{bmatrix} -\frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} - 1 & \frac{3 \cdot c_{j+\frac{2}{3}}^2}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \\ -\frac{3 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{j+\frac{2}{3}} + c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}^2} & -\frac{15 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} - 1 \end{bmatrix} \\ k_{n1} &= \frac{1}{C_j^{(1,1)} \cdot C_j^{(2,2)} - C_j^{(1,2)} \cdot C_j^{(2,1)}} \begin{bmatrix} C_j^{(2,2)} & -C_j^{(1,2)} \\ -C_j^{(2,1)} & C_j^{(1,1)} \end{bmatrix} \begin{bmatrix} D_j^{(1,1)} & D_j^{(1,2)} \\ D_j^{(2,1)} & D_j^{(2,2)} \end{bmatrix} \begin{bmatrix} \frac{4 \cdot q_j}{\Delta s} \\ \frac{4 \cdot p_j}{\Delta s} \end{bmatrix} \\ &= \frac{1}{c_j^{(1,1)} \cdot c_j^{(2,2)} - c_j^{(1,2)} \cdot c_j^{(2,1)}} \begin{bmatrix} C_j^{(2,2)} \cdot D_j^{(1,1)} - C_j^{(1,2)} \cdot D_j^{(2,1)} & C_j^{(2,2)} \cdot D_j^{(1,2)} - C_j^{(1,2)} \cdot D_j^{(2,2)} \\ -C_j^{(2,1)} \cdot D_j^{(1,1)} + C_j^{(1,1)} \cdot D_j^{(2,1)} & -C_j^{(2,1)} \cdot D_j^{(1,2)} + C_j^{(1,1)} \cdot D_j^{(2,2)} \end{bmatrix} \begin{bmatrix} \frac{4 \cdot q_j}{\Delta s} \\ \frac{4 \cdot p_j}{\Delta s} \end{bmatrix} \\ \therefore k_{n1} &= \frac{4}{\Delta s \cdot (C_j^{(1,1)} \cdot C_j^{(2,2)} - C_j^{(1,2)} \cdot C_j^{(2,1)})} \begin{bmatrix} q_j \cdot (C_j^{(2,2)} \cdot D_j^{(1,1)} - C_j^{(1,2)} \cdot D_j^{(2,1)}) + p_j \cdot (C_j^{(2,2)} \cdot D_j^{(1,2)} - C_j^{(1,2)} \cdot D_j^{(2,2)}) \\ q_j \cdot (-C_j^{(2,1)} \cdot D_j^{(1,1)} + C_j^{(1,1)} \cdot D_j^{(2,1)}) + p_j \cdot (-C_j^{(2,1)} \cdot D_j^{(1,2)} + C_j^{(1,1)} \cdot D_j^{(2,2)}) \end{bmatrix} \end{aligned}$$

Now calculate k_{n2} .

$$\begin{aligned} k_{n2} &= B_{j+\frac{2}{3}}^{-1} \left(\frac{12}{\Delta s} \mathbf{x}_j + 3 \cdot k_{n1} \right) \\ &= \begin{bmatrix} -\frac{5 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} & \frac{c_{j+\frac{2}{3}}^2}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \\ -\frac{c_{nn,j+\frac{2}{3}}}{25 \cdot c_{j+\frac{2}{3}} + c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}^2} & -\frac{5 \cdot c_{nn,j+\frac{2}{3}}}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \end{bmatrix} \begin{bmatrix} \frac{12}{\Delta s} \cdot q_j + 3 \cdot k_{n1}^{(1)} \\ \frac{12}{\Delta s} \cdot p_j + 3 \cdot k_{n1}^{(2)} \end{bmatrix} \\ \therefore k_{n2} &= \begin{bmatrix} -\frac{5 \cdot c_{nn,j+\frac{2}{3}} \cdot (\frac{12}{\Delta s} \cdot q_j + 3 \cdot k_{n1}^{(1)})}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} + \frac{c_{j+\frac{2}{3}}^2 \cdot (\frac{12}{\Delta s} \cdot p_j + 3 \cdot k_{n1}^{(2)})}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \\ -\frac{c_{nn,j+\frac{2}{3}} \cdot (\frac{12}{\Delta s} \cdot q_j + 3 \cdot k_{n1}^{(1)})}{25 \cdot c_{j+\frac{2}{3}} + c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}^2} - \frac{5 \cdot c_{nn,j+\frac{2}{3}} \cdot (\frac{12}{\Delta s} \cdot p_j + 3 \cdot k_{n1}^{(2)})}{25 \cdot c_{nn,j+\frac{2}{3}} + c_{j+\frac{2}{3}}} \end{bmatrix} \end{aligned}$$

3.3.4 Radau IIA (3)

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{4}{3} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

$$\begin{aligned} \mathbf{x}_{n+1} &= \mathbf{x}_n + \frac{1}{4} \cdot (3 \cdot F_1 + F_2) \\ F_1 &= \Delta s \cdot \mathbf{f} \left(s_n + \frac{\Delta s}{3}, \mathbf{x}_n + \frac{5}{12} F_1 - \frac{1}{12} F_2 \right) \\ F_2 &= \Delta s \cdot \mathbf{f} \left(s_n + \Delta s, \mathbf{x}_n + \frac{3}{4} F_1 + \frac{1}{4} F_2 \right) \\ &= \Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \end{aligned}$$

Rearrange for a solvable form.

$$\begin{aligned}
\mathbf{x}_{n+1} &= \mathbf{x}_n + \frac{1}{4} \cdot (3 \cdot F_1 + F_2) \\
&= \mathbf{x}_n + \frac{3}{4}F_1 + \frac{\Delta s}{4}\mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}), \quad \mathbf{x}_n + \frac{3}{4}F_1 + \frac{1}{3}F_2 = \mathbf{x}_{n+1} \\
\Rightarrow F_1 &= \frac{4}{3}\mathbf{x}_{n+1} - \frac{4}{3}\mathbf{x}_n - 3 \cdot \Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \\
\Rightarrow \frac{5}{12}F_1 &= \frac{5}{9}\mathbf{x}_{n+1} - \frac{5}{9}\mathbf{x}_n - \frac{5}{36}\Delta s \cdot \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \\
\mathbf{x}_n + \frac{5}{12}F_1 - \frac{1}{12}F_2 &= \mathbf{x}_n \left[\frac{5}{9}\mathbf{x}_{n+1} - \frac{5}{9}\mathbf{x}_n - \frac{5}{36}\Delta s \cdot \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \right] - \frac{1}{12}\Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \\
&= \frac{4}{9}\mathbf{x}_n + \frac{5}{9}\mathbf{x}_{n+1} - \frac{2}{9}\Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \\
\therefore F_1 &= \Delta s \mathbf{f} \left(s_n + \frac{\Delta s}{3}, \frac{4}{9}\mathbf{x}_n + \frac{5}{9}\mathbf{x}_{n+1} - \frac{2}{9}\Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \right) \\
\therefore \mathbf{x}_{n+1} &= \mathbf{x}_n + \frac{3 \cdot \Delta s}{4} \mathbf{f} \left(s_n + \frac{\Delta s}{3}, \frac{4}{9}\mathbf{x}_n + \frac{5}{9}\mathbf{x}_{n+1} - \frac{2}{9}\Delta s \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1}) \right) + \frac{1}{4} \mathbf{f}(s_{n+1}, \mathbf{x}_{n+1})
\end{aligned}$$

Now translate the $p - q$ equations into the above form.

$$\begin{aligned}
\mathbf{x}_j &= \begin{bmatrix} q_j \\ p_j \end{bmatrix} \\
f(s_j, \mathbf{x}_j) &= \begin{bmatrix} 0 & c_j \\ -\frac{c_{nn,j}}{c_j^2} & 0 \end{bmatrix} \begin{bmatrix} q_j \\ p_j \end{bmatrix} = A_j \mathbf{x}_j \quad A_j = A(s_j) \\
\mathbf{x}_{j+1} &= \mathbf{x}_j + \frac{3 \cdot \Delta s}{4} f \left(s_j + \frac{\Delta s}{3}, \frac{4}{9}\mathbf{x}_j + \frac{5}{9}\mathbf{x}_{j+1} - \frac{2}{9}\Delta s \mathbf{f}(s_{j+1}, \mathbf{x}_{j+1}) \right) + \frac{1}{4} \mathbf{f}(s_{j+1}, \mathbf{x}_{j+1}) \\
&= \mathbf{x}_j + \frac{3 \cdot \Delta s}{4} A_{j+\frac{1}{3}} \left(\frac{4}{9}\mathbf{x}_j + \frac{5}{9}\mathbf{x}_{j+1} - \frac{2}{9}\Delta s A_{j+1} \mathbf{x}_{j+1} \right) + \frac{\Delta s}{4} A_{j+1} \mathbf{x}_{j+1} \\
&= \mathbf{x}_j + \frac{3 \cdot \Delta s}{4} A_{j+\frac{1}{3}} \left(\frac{4}{9}\mathbf{x}_j + \left(\frac{5}{9}\mathbb{I} - \frac{2 \cdot \Delta s}{9} A_{j+1} \right) \mathbf{x}_{j+1} \right) + \frac{\Delta s}{4} A_{j+1} \mathbf{x}_{j+1} \\
&= \left(\mathbb{I} + \frac{\Delta s}{3} A_{j+\frac{1}{3}} \right) \mathbf{x}_j + \left(\frac{3 \cdot \Delta s}{4} A_{j+\frac{1}{3}} \left(\frac{5}{9}\mathbb{I} - \frac{2 \cdot \Delta s}{9} A_{j+1} \right) + \frac{\Delta s}{4} A_{j+1} \right) \mathbf{x}_{j+1} \\
\Rightarrow \left(\mathbb{I} + \frac{\Delta s}{3} A_{j+\frac{1}{3}} \right) \mathbf{x}_j &= \left(\mathbb{I} - \frac{3 \cdot \Delta s}{4} A_{j+\frac{1}{3}} \left(\frac{5}{9}\mathbb{I} - \frac{2 \cdot \Delta s}{9} A_{j+1} \right) - \frac{\Delta s}{4} A_{j+1} \right) \mathbf{x}_{j+1} \\
\therefore \mathbf{x}_{j+1} &= \left[\mathbb{I} - \frac{3 \cdot \Delta s}{4} A_{j+\frac{1}{3}} \left(\frac{5}{9}\mathbb{I} - \frac{2 \cdot \Delta s}{9} A_{j+1} \right) - \frac{\Delta s}{4} A_{j+1} \right]^{-1} \left(\mathbb{I} + \frac{\Delta s}{3} A_{j+\frac{1}{3}} \right) \mathbf{x}_j
\end{aligned}$$

Evaluate the terms individually.

$$\begin{aligned}
\text{let } B_j &= \mathbb{I} - \frac{\Delta s}{12} A_{j+\frac{1}{3}} (5\mathbb{I} - 2 \cdot \Delta s A_{j+1}) - \frac{\Delta s}{4} A_{j+1} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{\Delta s}{12} \begin{bmatrix} 0 & c_{j+\frac{1}{3}} \\ -\frac{c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} & 0 \end{bmatrix} \left(\begin{bmatrix} 5 & 0 \\ 0 & 5 \end{bmatrix} - 2 \cdot \Delta s \begin{bmatrix} 0 & c_{j+1} \\ -\frac{c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \right) - \frac{\Delta s}{4} \begin{bmatrix} 0 & c_{j+1} \\ -\frac{c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{\Delta s}{12} \left(\begin{bmatrix} 0 & c_{j+\frac{1}{3}} \\ -\frac{c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} & 0 \end{bmatrix} \left(\begin{bmatrix} 5 & 0 \\ 0 & 5 \end{bmatrix} - 2 \cdot \Delta s \begin{bmatrix} 0 & c_{j+1} \\ -\frac{c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \right) + 3 \begin{bmatrix} 0 & c_{j+1} \\ -\frac{c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \right) \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{\Delta s}{12} \left(\begin{bmatrix} 0 & c_{j+\frac{1}{3}} \\ -\frac{c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} & 0 \end{bmatrix} \begin{bmatrix} 5 & -2 \cdot \Delta s \cdot c_{j+1} \\ \frac{2 \cdot \Delta s \cdot c_{nn,j+1}}{c_{j+1}^2} & 5 \end{bmatrix} + \begin{bmatrix} 0 & 3 \cdot c_{j+1} \\ -\frac{3 \cdot c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \right) \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{\Delta s}{12} \left(\begin{bmatrix} \frac{2 \cdot \Delta s \cdot c_{nn,j+1} \cdot c_{j+\frac{1}{3}}}{c_{j+1}^2} & 5 \cdot c_{j+\frac{1}{3}} \\ -\frac{5 \cdot c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} & \frac{2 \cdot \Delta s \cdot c_{j+1} \cdot c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} \end{bmatrix} + \begin{bmatrix} 0 & 3 \cdot c_{j+1} \\ -\frac{3 \cdot c_{nn,j+1}}{c_{j+1}^2} & 0 \end{bmatrix} \right) \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{\Delta s}{12} \begin{bmatrix} \frac{2 \cdot \Delta s \cdot c_{nn,j+1} \cdot c_{j+\frac{1}{3}}}{c_{j+1}^2} & 5 \cdot c_{j+\frac{1}{3}} + 3 \cdot c_{j+1} \\ -\frac{5 \cdot c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} - \frac{3 \cdot c_{nn,j+1}}{c_{j+1}^2} & \frac{2 \cdot \Delta s \cdot c_{j+1} \cdot c_{nn,j+\frac{1}{3}}}{c_{j+\frac{1}{3}}^2} \end{bmatrix} \\
\therefore B_j &= \begin{bmatrix} 1 - \frac{\Delta s^2 \cdot c_{nn,j+1} \cdot c_{j+\frac{1}{3}}}{6 \cdot c_{j+1}^2} & -\frac{5 \cdot \Delta s}{12} \cdot c_{j+\frac{1}{3}} - \frac{\Delta s}{4} \cdot c_{j+1} \\ \frac{5 \cdot \Delta s \cdot c_{nn,j+\frac{1}{3}}}{12 \cdot c_{j+\frac{1}{3}}^2} + \frac{3 \cdot \Delta s \cdot c_{nn,j+1}}{12 \cdot c_{j+1}^2} & 1 - \frac{\Delta s^2 \cdot c_{j+1} \cdot c_{nn,j+\frac{1}{3}}}{6 \cdot c_{j+\frac{1}{3}}^2} \end{bmatrix} \\
\mathbb{I} + \frac{\Delta s}{3} A_{j+\frac{1}{3}} &= \begin{bmatrix} 1 & \frac{\Delta s \cdot c_{j+\frac{1}{3}}}{3} \\ -\frac{\Delta s \cdot c_{nn,j+\frac{1}{3}}}{3 \cdot c_{j+\frac{1}{3}}^2} & 1 \end{bmatrix} \\
\therefore \mathbf{x}_{j+1} &= B_j^{-1} \left(\mathbb{I} + \frac{\Delta s}{3} A_{j+\frac{1}{3}} \right) \mathbf{x}_j
\end{aligned}$$

3.4 Rederive ODEs

$$\begin{aligned}
\frac{dq}{ds} &= c(s) \cdot p(s) \\
\frac{dp}{ds} &= -\frac{\partial^2 c}{\partial n^2} \cdot \frac{q(s)}{c^2(s)}
\end{aligned}$$

4 General Functions

4.1 Sound Speed Profile Representation

The sound speed profile is treated as range invariant in the current **gUAcS** package. The profile is expressed as the knots, coefficients and degree of a B-spline within the configuration files for the program. This requires the B-spline to be evaluated at each depth point for the program. To do so De Boor's Algorithm is implemented where; $\{c_i\}$ is the set of spline coefficients, $\{t_i\}$ is the set of spline knots and p is the order of the spline. The algorithm is shown below in Algorithm 4.1.

Algorithm 2 De Boor's Algorithm

Initialise:

x

$k \leftarrow i$ for which i satisfies $t_i > x$ and $t_{i-1} \leq x$

$d_i \leftarrow c_{j+k-order}$ for $j \in 0, 1, \dots, p$

for $r \leftarrow 1$ to p **do**

for $j \leftarrow p$ to r **do**

$i \leftarrow j + k - p$

$\alpha_j = \frac{x-t_i}{t_{j+1+k-r}-t_i}$

$d_j = (1 - \alpha_j) \cdot d_{j-1} + \alpha_j \cdot d_i$

return d_p
