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MODELING THE LIGHT FIELD IN MACROALGAE AQUACULTURE

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Oliver Graham Evans

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# MODELING THE LIGHT FIELD IN MACROALGAE AQUACULTURE

Oliver Graham Evans

Thesis

Approved:

---

Advisor  
Dr. Kevin Kreider

Accepted:

---

Dean of the College  
Dr. Linda Subich

---

Co-Advisor  
Dr. Curtis Clemons

---

Dean of the Graduate School  
Dr. Chand Midha

---

Faculty Reader  
Dr. Gerald Young

---

Date

---

Department Chair  
Dr. Kevin Kreider

## ABSTRACT

A mathematical model is developed to describe the light field in vertical line seaweed cultivation to determine the degree to which the seaweed shades itself and limits the amount of light available for photosynthesis. A probabilistic description of the spatial distribution of kelp is formulated using simplifying assumptions about frond geometry and orientation. An integro-partial differential equation called the radiative transfer equation is used to describe the light field as a function of position and angle. A finite difference solution is implemented, providing robustness and accuracy at the cost of large CPU and memory requirements, and a less computationally intensive asymptotic approximation is explored for the case of low scattering. Conditions for applicability of the asymptotic approximation are discussed, and depth-dependent light availability is compared to the predictions of simpler light models. The 3D model of this thesis is found to predict significantly lower light levels than the simpler 1D models, especially in regions of high kelp density where a precise description of self-shading is most important.

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# CHAPTER I

## INTRODUCTION

### 1.1 Motivation

Given the consistent global increase in population, efficient and innovative resource utilization is increasingly important. Our generation faces major challenges regarding food, energy, and water and must confront major issues associated with global climate change. Growing concern for the negative environmental impacts of petroleum-based fuel has generated a market for biofuel, especially corn-based ethanol; however, corn-based ethanol has been heavily criticized for diverting land usage away from food production, for increasing use of fertilizers and pesticides that impair water quality, and for the high carbon footprint involved in its development [20]. Meanwhile, a great deal of unutilized coastline is available for both food and fuel production through seaweed cultivation. Specifically, the sugar kelp *Saccharina latissima* has been demonstrated to be a viable source of food, both for direct human consumption and biofuel production, especially in conjunction with other aquatic species in *integrated multi-trophic aquaculture* (IMTA) [9, 12, 16, 17].

Furthermore, seaweed cultivation has been proposed as a nutrient remediation technique for natural waters [21]. Nitrogen leakage into water bodies is a

significant ecological problem, and is especially relevant in close proximity to large conventional agriculture facilities and wastewater treatment plants. Waste water treatment plants (WWTPs) in particular are facing increasingly stringent regulation of nutrients in their effluent discharges from the US Environmental Protection Agency (USEPA) and state regulatory agencies. Nutrient management at WWTPs requires significant infrastructure, operations, and maintenance investments for tertiary treatment processes. Many treatment works are constrained financially or by space limitations in their ability to expand their operations. As an alternative to conventional nutrient remediation techniques, the cultivation of the *Saccharina latissima* within the nutrient plume of WWTP ocean outfalls has been proposed [46]. The purpose of such an undertaking would be twofold: to prevent eutrophication of the surrounding ecosystem by sequestering nutrients, and to provide supplemental nutrients that benefit macroalgae cultivation.

Large scale macroalgae cultivation has long existed in Eastern Asia due to the popularity of seaweed in Asian cuisine, and low labor costs that facilitate its manual seeding and harvest. More recently, less labor-intense and more industrialized kelp aquaculture has been developing in Scandinavia and in the Northeastern United States and Canada. For example, the MACROSEA project is a four year international research collaboration led by SINTEF, an independent research organization in Norway, and funded by the Research Council of Norway. The project's aim is to achieve "successful and predictable production of high quality biomass thereby making significant steps towards industrial macroalgae cultivation in Norway". Figure



Figure 1.1: *Saccharina latissima* being harvested

1.1 shows seaweed being harvested onboard a SINTEF research vessel. The project includes both cultivators and scientists, working to develop a precise understanding of the full life cycle of kelp and its interaction with its environment.

A fundamental aspect of this endeavor is the development of mathematical models to describe the growth of kelp. The development of mathematical models enables insight into a system which would be otherwise difficult or impossible to obtain. For example, imagine that a company is interested in a new IMTA site, and is looking for a suitable location. Running simulations to predict the potential productivity for each site would help determine the best one. Similarly, if a new

cultivation technique is under consideration, simulation can estimate its viability without deploying it on a large scale and risking failure or avoidable inefficiency.

Recently, a growth model [8] for *S. latissima* has been produced and integrated into the SINMOD [45] hydrodynamic and ecosystem model of SINTEF. This kelp model considers factors such as temperature, nutrient concentration, light availability, and water current. The amount of light available is informed by spatially varying attenuation coefficients from SINMOD, which considers optical properties of the water as well as concentrations of various organic and inorganic constituents. However, it does not consider the effect of the kelp itself on the light field. This is an important consideration, as high kelp densities should lead to low light levels which would inhibit further growth. However, without accounting for self-shading, the kelp is not adequately penalized for growing too densely, which is expected to cause overpredictions in the total biomass production. The purpose of this thesis is to develop a first principles light model which adequately predicts the effects of self-shading on seaweed.

## 1.2 Background on Kelp Models

Mathematical modeling of macroalgae growth is not a new topic, although it is a reemerging one. Several authors in the second half of the twentieth century were interested in describing the growth and composition of the macroalgae *Macrocystis pyrifera*, commonly known as “giant kelp,” which grows prolifically off the coast of southern California. The first such mathematical model was developed by W.J. North

for the Kelp Habitat Improvement Project at the California Institute of Technology in 1968 using seven variables. By 1974, Nick Anderson greatly expanded on North's work, and created the first comprehensive model of kelp growth which he programmed using FORTRAN [3]. In his model, he accounts for solar radiation intensity as a function of time of year and time of day, and refraction on the surface of the water. He uses a simple model for shading, specifying a single parameter which determines the percentage of light that is allowed to pass through the kelp canopy floating on the surface of the water. He also accounts for attenuation due to turbidity using Beer's Law. Using this data on the availability of light, he calculates the photosynthesis rates and the growth experienced by the kelp.

Over a decade later in 1987, G.A. Jackson expanded on Anderson's model for *Macrocystis pyrifera* [19], with an emphasis on including more environmental parameters and a more complete description of the growth and decay of the kelp. The author takes into account respiration, frond decay, and sub-canopy light attenuation due to self-shading. Light attenuation is represented with a simple exponential model, and self-shading appears as an added term in the decay coefficient. The author does not consider radial or angular dependence on shading. Jackson also expands Anderson's definition of canopy shading, treating the canopy not as a single layer, but as 0, 1, or 2 discrete layers, each composed of individual fronds. While this is a significant improvement over Anderson's light model, it is still rather simple.

Both Anderson's and Jackson's models were carried out by numerically solving a system of differential equations by integrating over small time steps. In 1990,

M.A. Burgman and V.A. Gerard developed a stochastic population model [10]. This approach functions by dividing kelp plants into groups based on size and age and generating random numbers to determine how the population distribution over these groups changes over time based on measured rates of growth, death, decay, light availability, etc. In the same year, Nyman et. al. [29] published a similar model alongside a Markov chain model, and compared the results with experimental data collected in New Zealand.

In 1996 and 1998 respectively, P. Duarte and J.G. Ferreira used the size-class approach to create a more general model of macroalgae growth, and Yoshimori et. al. created a differential equation model of *Laminaria religiosa* with specific emphasis on temperature dependence of growth rate [14, 47]. These were some of the first models of kelp growth that did not specifically relate to *Macrocystis pyrifera* (“giant kelp”).

The model developed by Broch et. al. at SINTEF [7, 8, 17] uses a super-individual approach, whereby a small number of individual kelp fronds are explicitly simulated at several discrete depth layers. Each super-individual is assumed to represent a certain number of actual individuals in the population. The number of individuals represented by each super-individual may change over the course of the simulation due to population loss. The super-individual approach has the advantage of capturing some of the dynamics at the individual scale, while compromising full detail for the sake of reduced computational cost.

### 1.3 Background on Radiative Transfer

In terms of optical quantities, of primary interest is the radiance, which describes the rate of energy flow through each point in space in *each* direction. Irradiance, on the other hand, describes the total energy flow through a point in space over *every* direction, and is calculated by integrating radiance over all angles. Irradiance, in turn, determines the photosynthetic rate of the kelp, and therefore the total amount of biomass producible in a given area as well as the total nutrient remediation potential. The equation governing the radiance throughout the system is known as the radiative transfer equation (RTE), which has been used extensively in stellar astrophysics [11, 30]; its application to marine biology is fairly recent [26]. In its full form, radiance is a function of 3 spatial dimensions, 2 angular dimensions, and frequency, making for a formidable problem. In this work, frequency is ignored; only the total radiation in the photosynthetic spectrum, known as photosynthetically active radiation (PAR), is considered. The RTE states that along a given path, radiance is decreased by absorption and scattering out of the path, while it is increased by emission and scattering into the path. In the case of macroalgae cultivation, emission is negligible, owing only perhaps to some small luminescent phytoplankton or other anomaly, and can therefore be safely ignored. However, the emission term will be retained in the calculations of this thesis, as it is mathematically useful to verify the correctness of the solution algorithm.

## 1.4 Overview of Thesis

The remainder of this document is organized as follows. In Chapter II, a probabilistic model is developed to describe the spatial distribution of kelp by assuming simple distributions for the lengths and orientations of fronds. Chapter III begins with a survey of fundamental radiometric quantities and optical properties of matter. The spatial kelp distribution from Chapter II is used to determine optical properties of the combined water-kelp medium, and the radiative transfer equation, an integro-partial differential equation which describes the light field as a function of position and angle, is discussed. An asymptotic expansion is explored for the case of low scattering, allowing for analytical, ordered approximations to the true light field. In Chapter IV, details are given for the numerical solution of the equations from Chapters II and III. Both the full finite difference solution and the asymptotic approximation are thoroughly developed.

Chapter V is an in-depth discussion of sources of error in both solution procedures. The concepts of verifying codes in general as well as specific calculations are discussed. Exact discretization errors are calculated via the method of manufactured solutions in order to demonstrate that the methods exhibit their theoretical convergence properties, which builds confidence in the correctness of their implementations. A method for estimating errors for realistic cases is also developed.

Next, Chapter VI surveys practical considerations to keep in mind when applying the algorithms in real situations. Relevant model parameter values from the

literature are collected, and estimates are given for those not readily available. Following that is a set of guidelines for choosing which algorithm and which algorithm parameters to use based on the optical scenario to be simulated. Advantages and disadvantages of both approaches are presented. While the finite difference technique can be applied to any situation, it often requires prohibitively large CPU and memory resources, whereas the numerical asymptotic solution is generally faster and its memory footprint never exceeds the capacity of a standard laptop for reasonable grid sizes. The chapter concludes with a comparison to two simpler light models, and specific qualitative differences are noted. As expected, the presence of self-shading in this model results in the prediction of lower light levels regions of high kelp density. However, the presence of scattering in the model increases light levels elsewhere, especially near the surface of the water.

Finally, Chapter VII concludes the thesis by briefly summarizing the model, discussing its achievements and limitations, and suggesting improvements and avenues for future work. Several appendices follow with further details about the algorithm, as well as the full source code of the Fortran model developed.

## CHAPTER II

### KELP MODEL

In order to properly model the spatial distribution of light around the kelp, it is first necessary to formulate a spatial description of the kelp. Probability distributions are given for the size and orientation of the individual kelp fronds, which are inverted to determine the probability of a point in space being occupied by kelp. Ultimately, the kelp density at any point in space is calculated, which informs the absorption coefficient of the effective kelp-water medium.

#### 2.1 Physical Setup

The life of cultivated macroalgae generally begins in the laboratory, where microscopic kelp spores are inoculated onto a thread in a small laboratory pool. This thread is wrapped around a larger rope as in Figure 2.1, which is hung from buoys in the ocean. The two primary configurations are vertical and horizontal or “long” lines. In the case of vertical lines, the seaweed rope hangs straight down from a single buoy, and is either weighted or anchored. In the case of long lines, the rope is strung from one buoy to another. Long lines allow more light to reach the seaweed since it grows closer to the surface, but more vertical lines can be set up in a given area, which may be advantageous for IMTA.



Figure 2.1: *Saccharina latissima* inoculated onto a thread wrapped around a rope on which it is to be grown.

We consider only the case of a rigid vertical rope which does not sway in the current. The mature *Saccharina latissima* plant consists of a single frond (leaf), a stipe (stem) and a holdfast (root structure). For the sake of this model, only the kelp frond is considered, and its base is attached directly to the rope. The “gentle undulation approximation” is employed, whereby the fronds are modeled as perfectly horizontal. While at any given time they may point up or down due to water current and gravity, we consider the horizontal state to be an average configuration. This simplification allows for the three-dimensionally distributed population of kelp fronds to be considered a collection of independent populations in two-dimensional depth layers. A computer rendering of this scenario is shown in Figure 2.2.



Figure 2.2: Rendering of four nearby vertical kelp ropes as represented in the spatial distribution model. Note the kite-shaped fronds and horizontal orientation.

## 2.2 Coordinate System

Consider the rectangular domain

$$x_{\min} \leq x \leq x_{\max},$$

$$y_{\min} \leq y \leq y_{\max},$$

$$z_{\min} \leq z \leq z_{\max}.$$

For all three dimensional analysis, we use the absolute coordinate system depicted in Figure 2.3. The vectors  $\mathbf{x} = (x, y, z)$  and  $\boldsymbol{\omega} = (\sin \phi \cos \theta, \sin \phi \sin \theta, \cos \phi)$  are also used throughout. Also, the notation  $\hat{x}, \hat{y}, \hat{z}$  is used for the Cartesian unit vectors.

In the following sections, it is necessary to convert between Cartesian and spherical coordinates, which we do using the relations

$$\begin{cases} x = r \sin \phi \cos \theta, \\ y = r \sin \phi \sin \theta, \\ z = r \cos \phi. \end{cases} \quad (2.1)$$

Therefore, for some function  $f(x, y, z)$ , we can write its derivative along a path in spherical coordinates in terms of Cartesian coordinates using the chain rule,

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial r} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial r}.$$

Then, calculating derivatives from (2.1) yields

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x} \sin \phi \cos \theta + \frac{\partial f}{\partial y} \sin \phi \sin \theta + \frac{\partial f}{\partial z} \cos \phi. \quad (2.2)$$

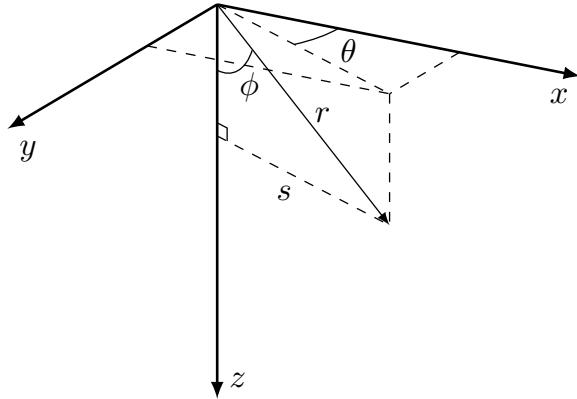


Figure 2.3: Downward-facing right-handed coordinate system with radial distance  $r$  from the origin, distance  $s$  from the  $z$  axis, zenith angle  $\phi$  and azimuthal angle  $\theta$ .

## 2.3 Population Distributions

In order to construct a spatial distribution of kelp fronds, a simple kite-shaped geometry is introduced, and frond lengths and azimuthal orientations are assumed to be distributed predictably. Since it is assumed that fronds extend perfectly horizontally, no angular elevation distribution is required.

### 2.3.1 Frond Shape

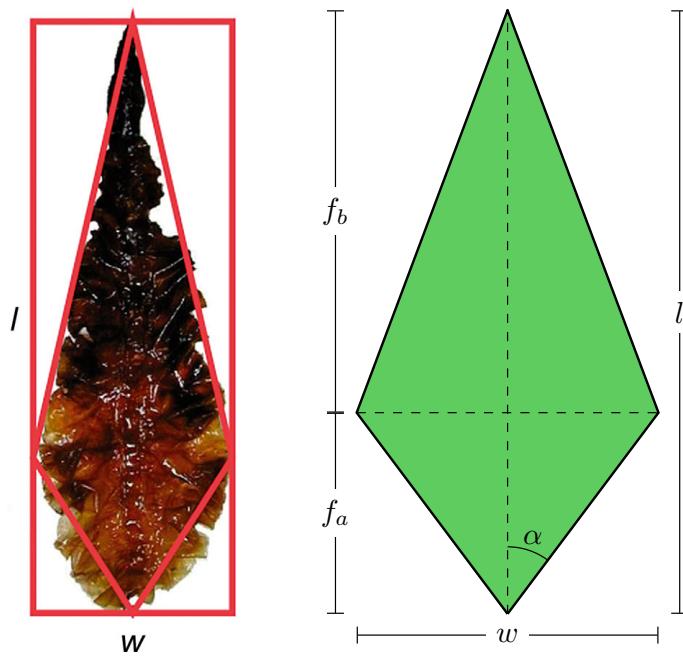


Figure 2.4: Simplified kite-shaped frond. Reproduced with permission from [7].

The frond is assumed to be kite-shaped with length  $l$  from base to tip, and width  $w$  from left to right. In Figure 2.4, the base is shown at the bottom and the tip is shown at the top. The proximal length is the shortest distance from the base to the diagonal connecting the left and right corners, and is notated as  $f_a$ . Likewise,

the distal length, notated  $f_b$ , is the shortest distance from that diagonal to the tip.

It is therefore clear that

$$f_a + f_b = l.$$

When considering a whole population with varying sizes, it is more convenient to specify ratios than absolute lengths. Define the ratios

$$\begin{aligned} f_r &= \frac{l}{w}, \\ f_s &= \frac{f_a}{f_b}. \end{aligned}$$

These ratios are assumed to be constant among the entire population, so that all fronds are geometrically similar. Thus, the shape of the frond can be fully specified by  $l$ ,  $f_r$ , and  $f_s$ ; it is possible to redefine  $w$ ,  $f_a$  and  $f_b$  from the preceding formulas as

$$w = \frac{l}{f_r}, \tag{2.3}$$

$$f_a = \frac{lf_s}{1 + f_s}, \tag{2.4}$$

$$f_b = \frac{l}{1 + f_s}. \tag{2.5}$$

The angle  $\alpha$ , half of the angle at the base corner, is also noteworthy. From the above equations, it follows that

$$\alpha = \tan^{-1} \left( \frac{2f_rf_s}{1 + f_s} \right).$$

It is useful to convert between frond length and surface area, which can be done via the relations

$$A = \frac{lw}{2} = \frac{l^2}{2f_r}, \tag{2.6}$$

$$l = \sqrt{2Af_r}. \tag{2.7}$$

### 2.3.2 Length and Angle Distributions

In any given depth layer, the distribution of frond lengths is assumed to be normal, with mean  $\mu_l$  and standard deviation  $\sigma_l$ . That is, it has the probability density function (PDF)

$$P_l(l) = \frac{1}{\sqrt{2\pi\sigma_l^2}} \exp\left(-\frac{(l - \mu_l)^2}{2\sigma_l^2}\right). \quad (2.8)$$

It is further assumed that frond orientation angle varies according to the von Mises distribution, which is the periodic analogue of the normal distribution, defined on  $[-\pi, \pi]$  rather than  $(-\infty, \infty)$ . The von Mises distribution has two parameters,  $\mu$  and  $\kappa$ , which shift and sharpen its peak respectively, as shown in Figure 2.5.  $\kappa$  is analogous to  $1/\sigma$  in the normal distribution. In the absence of current, the frond angles are distributed uniformly, while as current velocity increases, they become increasingly likely to align parallel to the current, depending on the stiffness of the frond and stipe. Assuming a linear relationship between the current velocity and the steepness of the angular distribution, define the *frond alignment coefficient*  $\eta$ , with units of inverse velocity ( $\text{s m}^{-1}$ ). Then, use  $\mu = \theta_w$  and  $\kappa = \eta v_w$  as the von Mises distribution parameters. Note that  $\theta_w$  and  $v_w$  vary over depth, while  $\eta$  is assumed constant for the population. Then, the PDF for the von Mises frond angle distribution is

$$P_{\theta_f}(\theta_f) = \frac{\exp(\eta v_w \cos(\theta_f - \theta_w))}{2\pi I_0(\eta v_w)}, \quad (2.9)$$

where  $I_0(x)$  is the modified Bessel function of the first kind of order 0. Notice that unlike the normal distribution, the von Mises distribution approaches a *non-zero*

uniform distribution as  $\kappa$  approaches 0, so

$$\lim_{v_w \rightarrow 0} P_{\theta_f}(\theta_f) = \frac{1}{2\pi} \quad \forall \theta_f \in [-\pi, \pi].$$

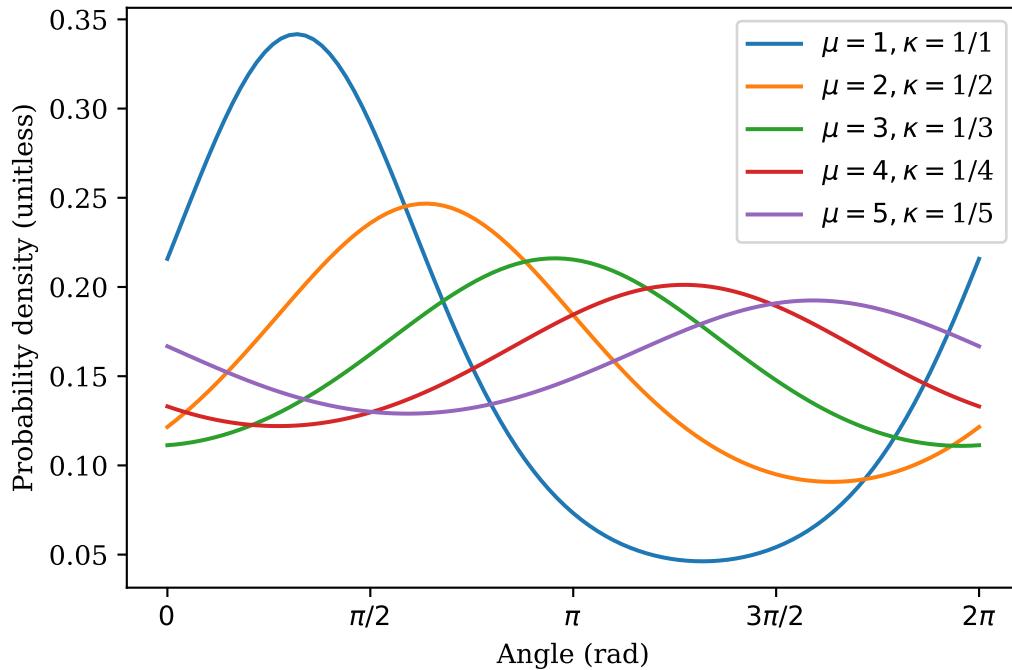


Figure 2.5: The von Mises distribution for a variety of parameters.

### 2.3.3 Joint Length-Orientation Distribution

The previous two distributions can reasonably be assumed to be independent of one another. That is, the angle of the frond does not depend on the length, or vice versa. Therefore, the probability of a frond simultaneously having a given frond length and angle is the product of their individual probabilities. Given independent events  $A$  and  $B$ , the probability of their intersection is the product of their individual

probabilities. That is,

$$P(A \cap B) = P(A)P(B).$$

Therefore, the probability of frond length  $l$  and frond angle  $\theta_f$  coinciding is

$$P_{2D}(\theta_f, l) = P_{\theta_f}(\theta_f) \cdot P_l(l). \quad (2.10)$$

A contour plot of this 2D distribution for a specific set of parameters is shown in Figure 2.6, where probability is represented by color in the 2D plane. Darker green represents higher probability, while lighter beige represents lower probability. In Figure 2.7, 50 samples are drawn from this distribution and plotted.

It is important to note that if  $P_{\theta_f}$  were dependent on  $l$ , the above definition of  $P_{2D}$  would no longer be valid. For example, it might be more realistic to say that larger fronds are less likely to bend towards the direction of the current. In this case, (2.3.3) would no longer hold, and it would be necessary to use the more general Bayes' Theorem,

$$P(A \cap B) = P(A)P(B|A) = P(B)P(B|A),$$

which is currently not taken into consideration in this model.

## 2.4 Spatial Distribution

In this section, the population length and angle distributions from the previous section are used to construct a spatial distribution of kelp. This is made possible by the simple kite-shape fronds, and would be considerably more difficult with more general frond shapes.

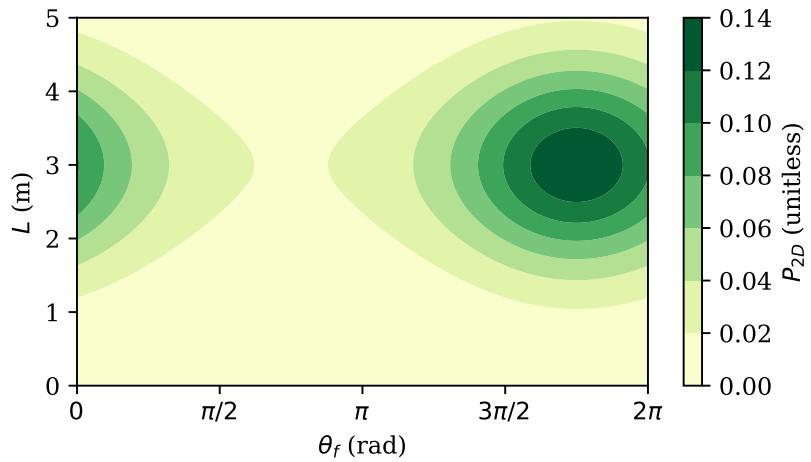


Figure 2.6: 2D length-angle probability distribution with  $\theta_w = 7\pi/4$ ,  $v_w = 1$ ,  $\mu_l = 3$ ,  $\sigma_l = 1$ .

#### 2.4.1 Rotated Coordinate System

To determine under what conditions a frond will occupy a given point, we begin by describing the shape of the frond in Cartesian coordinates and then convert to polar coordinates. Of primary interest are the edges connected to the frond tip. For convenience, we will use a rotated polar coordinate system  $(\theta', s)$  such that the line connecting the base to the tip points in the  $+y$  direction ( $\theta' = \pi/2$ ), with the base at  $(0, 0)$ . Denote the Cartesian analogue of this coordinate system as  $(x', y')$  which

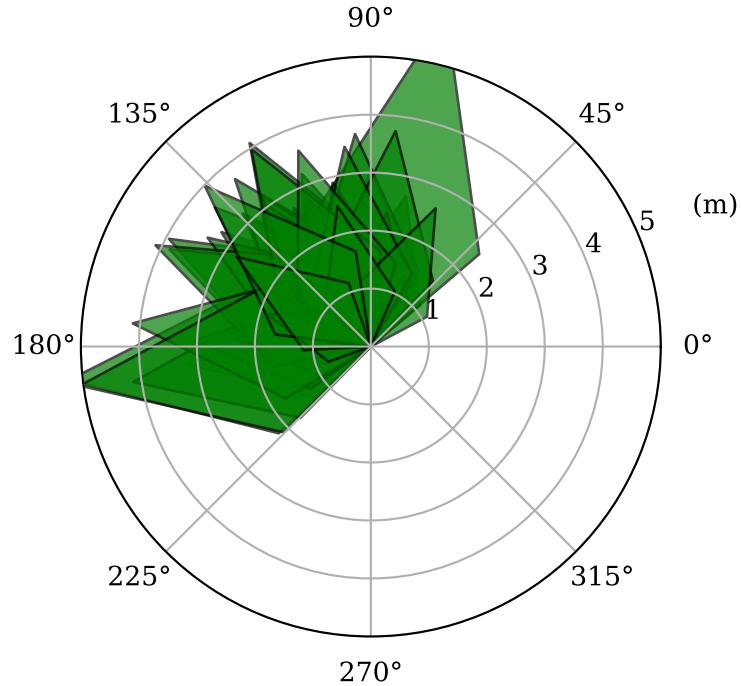


Figure 2.7: A sample of 50 kelp fronds with shape parameters  $f_s = 0.5$  and  $f_r = 2$  whose lengths are picked from a normal distribution and whose angles are picked from a von Mises distribution.

is related to  $(\theta', s)$  by

$$x' = s \cos \theta'$$

$$y' = s \sin \theta'$$

$$s = \sqrt{x'^2 + y'^2},$$

$$\theta' = \text{atan2}(y', x').$$

### 2.4.2 Functional Description of Frond Edge

With this coordinate system established, the outer two edges of the frond can be described in Cartesian coordinates as a piecewise linear function connecting the left corner:  $(-w/2, f_a)$ , the tip:  $(0, l)$ , and the right corner:  $(w/2, f_a)$ . This function has the form

$$y'_f(x') = l - \text{sign}(x') \frac{f_b}{w/2} x'.$$

Using the equations in Section 2.4.1, this can be written in polar coordinates after some rearrangement as

$$s'_f(\theta'; l) = \frac{l}{\sin \theta' + S(\theta') \frac{2f_b}{w} \cos \theta'},$$

where

$$S(\theta') = \text{sign}(\cos \theta').$$

Then, using the relationships in Section 2.3.1, the above equation can be rewritten in terms of the frond ratios  $f_s$  and  $f_r$  as

$$s'_f(\theta'; l) = \frac{l}{\sin \theta' + S(\theta') \frac{2f_r}{1+f_s} \cos \theta'}. \quad (2.11)$$

For convenience, denote the denominator of (2.11) as  $d'_f(\theta')$ . To generalize to a frond pointed at an angle  $\theta_f$ , we introduce the coordinate system  $(\theta, s)$  such that

$$\theta = \theta' + \theta_f - \frac{\pi}{2}.$$

Then, for a frond pointed at the arbitrary angle  $\theta_f$ , the function for the outer edges can be written as

$$s_f(\theta; l) = s'_f \left( \theta - \theta_f + \frac{\pi}{2}; l \right). \quad (2.12)$$

Similarly, define

$$d_f(\theta) = d'_f \left( \theta - \theta_f + \frac{\pi}{2} \right). \quad (2.13)$$

### 2.4.3 Conditions for Occupancy

We now formulate the conditions under which a kite shape frond occupies a point in the sense that the point lies within its interior. Combining these conditions with the size and orientation distributions from 2.3.2 allows a spatial distribution of the kelp fronds to be calculated.

Consider a fixed frond of length  $l$  at an angle  $\theta_f$ . The point  $(\theta, s)$  lies within the frond if

$$|\theta_f - \theta| < \alpha \text{ and } s < s_f(\theta).$$

Equivalently, the opposite perspective can be taken. Letting the point  $(\theta, s)$  be fixed, a frond occupies the point if

$$\theta - \alpha < \theta_f < \theta + \alpha, \quad (2.14)$$

$$l > l_{\min}(\theta, s), \quad (2.15)$$

where

$$l_{\min}(\theta, s) = s \cdot \frac{l}{s_f(\theta; l)} = s \cdot d_f(\theta). \quad (2.16)$$

Then, considering the point to be fixed, (2.14) and (2.15) define the spacial region  $R_s(\theta, s)$  called the “occupancy region for  $(\theta, s)$ ” with the property that if the tip of a frond lies within this region (i.e.,  $(\theta_f, l) \in R_s(\theta, s)$ ), then it occupies the point.  $R_s(3\pi/4, 1.5)$  is shown in blue in Figure 2.8 and the smallest possible occupying

fronds for several values of  $\theta_f$  are shown in various colors. Any frond longer than these at the same angle will also occupy the point.

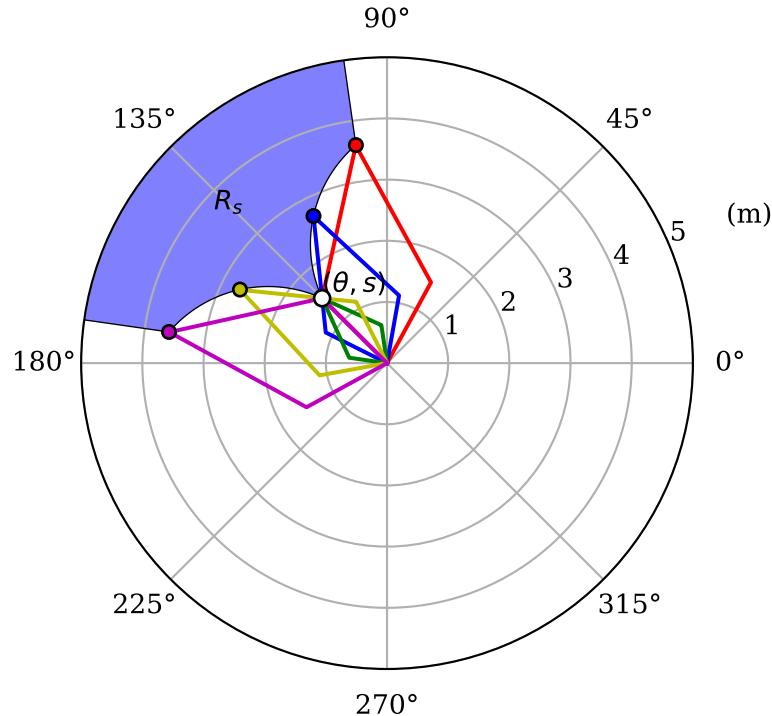


Figure 2.8: Outlines of minimum-length fronds for a variety of angles to occupy the point  $(\theta, s) = (3\pi/4, 3/2)$ .

#### 2.4.4 Probability of Occupancy

We are interested in the probability that, given a fixed point  $(\theta, s)$ , values of  $l$  and  $\theta_f$  chosen from the distributions described in Section 2.3.2 will fall in the occupancy region. This is found by integrating  $P_{2D}(\theta_f, l)$  from (2.10) over  $R_s(\theta, s)$ , the occupancy region for the point of interest.

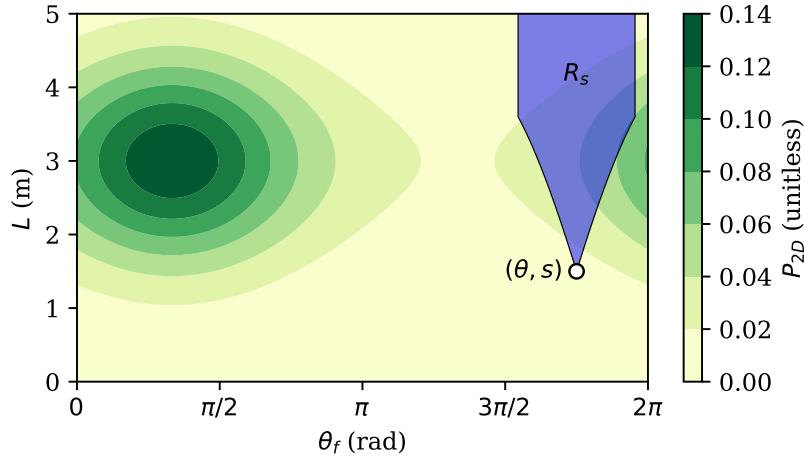


Figure 2.9: Contour plot of  $P_{2D}(\theta_f, l)$  overlayed with the region in the  $\theta_f$ - $l$  plane which results in a frond occupying the point  $(\theta, s) = (3\pi/4, 3/2)$ .

Integrating  $P_{2D}(\theta_f, l)$  over  $R_s(\theta, s)$  as depicted in Figure 2.9 yields the proportion of the population in the depth layer occupying the point  $(\theta, s)$ ,

$$\begin{aligned}\tilde{P}_k(\theta, s, z) &= \iint_{R_s(\theta, s)} P_{2D}(\theta_f, l) dl d\theta_f \\ &= \int_{\theta-\alpha}^{\theta+\alpha} \int_{l_{\min}(\theta_f)}^{\infty} P_{2D}(\theta_f, l) dl d\theta_f.\end{aligned}\quad (2.17)$$

Assuming that the depth layer has thickness  $dz$  and contains  $n_f$  fronds of thickness  $f_t$ , the proportion of the vertical length of the discrete depth layer occupied by kelp at any position  $(x, y, z)$  is given by

$$P_k(x, y) = \frac{n_f f_t}{dz} \tilde{P}_k(x, y). \quad (2.18)$$

In the continuum limit as the number of discrete depth layers approaches infinity,  $P_k(x, y, z)$  can be interpreted as the probability of the point  $(x, y, z)$  being

occupied by kelp. In a three dimensional context, the number of fronds is more likely to be specified by a number density  $\rho_f = n_f/dz$  over the vertical length of the rope with units  $\text{m}^{-1}$ , in which case

$$P_k(x, y, z) = f_t \rho_f(z) \tilde{P}_k(x, y, z). \quad (2.19)$$

Then, since the point  $\mathbf{x}$  has a probability  $P_k(\mathbf{x})$  of being occupied by kelp and a probability  $(1 - P_k(\mathbf{x}))$  of being occupied by the surrounding aquatic medium, the effective absorption coefficient can be calculated as

$$a(\mathbf{x}) = P_k(\mathbf{x})a_k + (1 - P_k(\mathbf{x}))a_w, \quad (2.20)$$

where  $a_k$  is the absorption coefficient of the kelp alone, and  $a_w$  is the absorption coefficient of the water and its dissolved and suspended contents.

## 2.5 Discontinuity at the Rope

While the above model of the kelp distribution is straightforward to evaluate, it does have a noteworthy numerical difficulty in its application. Since the length and orientations are both continuous in the polar coordinates  $s > 0$  and  $\theta$ , the resulting kelp density and effective absorption coefficient are as well. However, they are not necessarily continuous in Cartesian coordinates. In the case of no water current,  $v_w = 0$ , the flat von Mises distribution produces a continuous solution at the origin. In the more general case, though, there is a high kelp density on one side of the origin in the direction of the current, and a low kelp density immediately on the

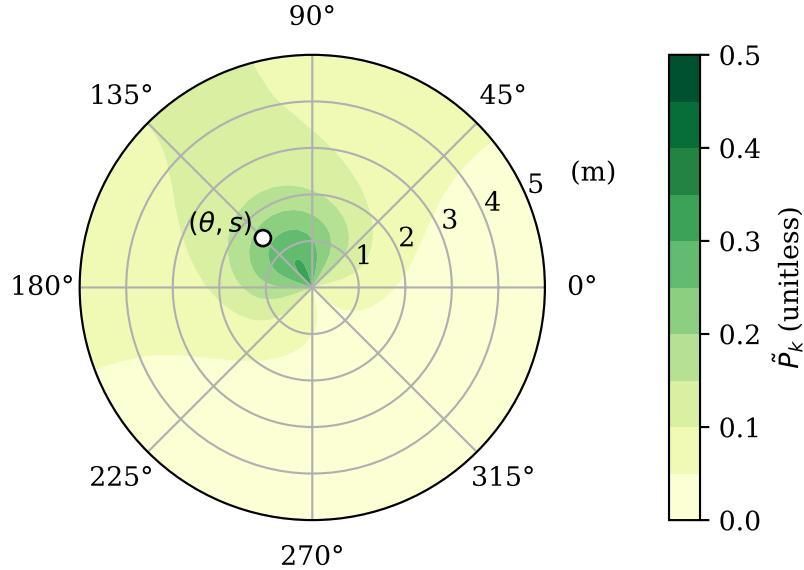


Figure 2.10: Contour plot of the probability of frond occupation sampled at 121 points using  $\theta_f = 2\pi/3$ ,  $\eta v_w = 1$ .

other side. Since the rope is assumed to be infinitely thin and have a fixed position, the sharp corners of the kelp fronds emanate from exactly the same point. Hence, there is in general a discontinuity in the kelp distribution at the origin, and therefore its derivatives are unbounded on the domain.

This is not appealing numerically since the algorithms used in this thesis to solve the differential equation describing the light field are based on interpolation on a discrete Cartesian grid. According to Taylor's theorem, the error incurred by performing such interpolation is bounded by a constant multiple of the appropriate

maximum derivative of the interpolated function over the domain. If the derivatives of the absorption coefficient are unbounded, then so too is the discretization error in the final solution. That is, convergence is not guaranteed in the fine-grid limit.

Luckily, there is a straightforward solution, which is to post-process the spatial kelp distribution with a Gaussian blur in the  $x$  and  $y$  dimensions. This is achieved via convolution of the solution with a 2D Gaussian kernel centered at the origin. Any blur whatsoever is sufficient to bound the derivatives, and the larger the blur radius, the smaller they become. Obviously, as the blur radius is increased, the kelp distribution tends toward a constant and no longer captures any information about the  $x$ - $y$  distribution of the kelp. Therefore, a small blur radius should be used.

### 2.5.1 One dimensional Gaussian Blur

As a one dimensional analogy, consider the Heaviside step function,

$$H(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

Clearly, the function is infinitely steep at the origin. Consider the normalized Gaussian kernel centered at the origin with radius  $\sigma_b$ , given by

$$k(x; \sigma_b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{x^2}{2\sigma_b^2}\right). \quad (2.21)$$

A blur is applied by convolving the function with the kernel according to the formula

$$\begin{aligned} \tilde{H}(x) &= (k * H)(x) = \int_{-\infty}^{\infty} H(\tau)k(x - \tau; \sigma_b) d\tau \\ &= \int_0^{\infty} k(x - \tau; \sigma_b) d\tau. \end{aligned}$$

The substitution  $u = \tau - x$ ,  $du = d\tau$  yields

$$\tilde{H}(x) = \int_{-x}^{\infty} k(u; \sigma_b) du.$$

Note that since the kernel is normalized, the integral from 0 to infinity is  $1/2$ . Further, since the kernel is even, the integral over  $[-x, 0]$  is equal to the integral over  $[0, x]$ .

Hence,

$$\tilde{H}(x) = \frac{1}{2} + \int_0^x k(u; \sigma_b) du.$$

Then, by the fundamental theorem of calculus, the derivative of the convolved function is simply  $k(x; \sigma_b)$ , whose maximum value is  $k(0; \sigma_b) = 1/\sqrt{2\pi\sigma_b^2}$ . Then, since the derivative is a linear operator, this result can be generalized to the following statement: Applying a Gaussian blur of radius  $\sigma_b$  to a function with a maximum discontinuity of size  $J$  produces a function whose first derivative is bounded by

$$\frac{1}{\sqrt{2\pi}} \frac{J}{\sigma_b}.$$

The same logic applies to directional derivatives of multidimensional scalar functions.

### 2.5.2 Multidimensional Gaussian Blur

In light of the above arguments, the derivatives of the absorption coefficient are bounded by applying a Gaussian blur to  $P_k$  before the calculation of  $a(\mathbf{x})$ . This is done by convolving slices of  $P_k$  in the  $x$ - $y$  plane with the two-dimensional normalized Gaussian kernel

$$K(x, y; \sigma_b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(\frac{x^2 + y^2}{2\sigma_b^2}\right). \quad (2.22)$$

Hence, the blurred solution is

$$P_k^b(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K(x', y', z; \sigma_b) P_k(x - x', y - y', z) dx' dy'. \quad (2.23)$$

A physical interpretation of this Gaussian blurring is that  $P_k^b$  is the time-averaged kelp distribution, assuming that the rope is allowed to move horizontally, and  $K(x, y; \sigma)$  is the PDF of the rope's location distribution. This interpretation is a bit incongruous with the rest of the model since there is no other explicit mention of time-averaging; while the frond length and position distributions can be thought of as continuous approximations to the population distribution at a single point in time, this idea does not apply to the rope's position, since there is only one rope.

### 2.5.3 Absorption Coefficient Plots

A variety of numerically calculated absorption coefficient fields are shown here in order to demonstrate some key features of the kelp distribution. In each figure, the absorption coefficient is plotted on the color axis, while the norm of its gradient is shown with contours, with brighter contour lines indicating regions of large derivatives. As mentioned above, large derivatives generate large discretization error, and are therefore undesirable. Of course, the distributions must be sufficiently well-defined to capture the characteristics of the kelp. Note that all of the kelp distributions are periodic in order to easily represent multiple vertical lines grown in close proximity.

Figure 2.11(a) shows a sharp kelp distribution with an unrealistically high current velocity, with all fronds identically equal in length, and with no blurring

applied. Note the kite-shaped distribution, as expected. Also note the regions of high derivatives near the origin and inner edges. This sharp distribution requires excessively large numerical grids to approximate well, and is therefore undesirable.

In Figure 2.11(b), the current velocity has been reduced, and a nonzero standard deviation has been given to the frond distribution. With a variety of frond lengths, the edges are no longer as clearly defined, although the general character of the distribution is sensible—the kelp is most dense near the rope in the direction of the current. However, note that there remains a small neighborhood of sharp derivatives encompassing the origin. Such a distribution may still cause numerical difficulties for the algorithm.

Figure 2.11(c) is similar to Figure 2.11(b), except it has been post-processed with a moderate Gaussian blur of radius 40 cm, not so large that it significantly distorts the shape of the distribution, but sufficient to remove the discontinuity in the origin. Such a kelp distribution is ideal, as it balances accuracy with ease of numerical approximation.

In Figure 2.11(d), too large of a blur has been applied; the character of the Gaussian kernel has overwhelmed that of the kelp distribution. While this may still provide a better spatial description of the kelp than a fully horizontally uniform distribution, an unnecessary amount of information has been sacrificed for marginal gains in smoothness over Figure 2.11(c). Such a large blur is unlikely to reduce the discretization error since other factors discussed later contribute to discretization error as well.

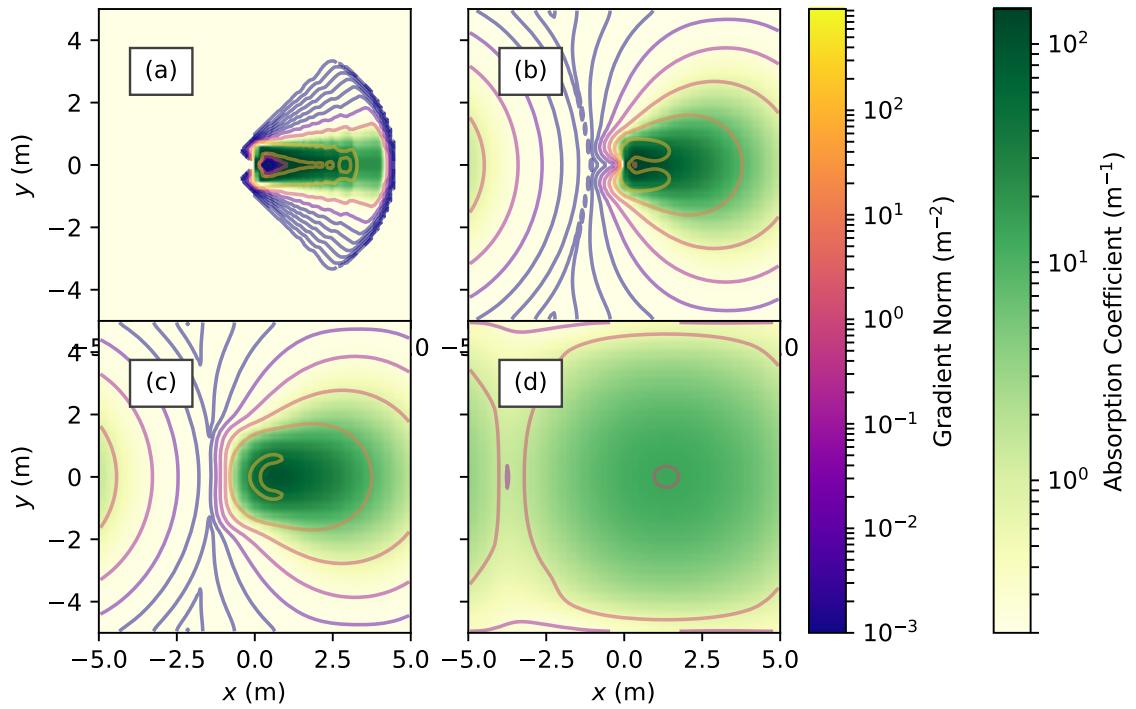


Figure 2.11:  $z$  slices of several absorption coefficient distributions from kelp distributions with varying parameters. The norm of the gradient is depicted with contours.

(a)  $\eta v_w = 90$ ,  $\sigma_l = \sigma_b = 0$ . Unrealistically sharp distribution shows kite-shaped character. (b)  $\eta v_w = 10$ ,  $\sigma_b = 0$ ,  $\sigma_l = 1$  m. More realistic kelp distribution, but still has large derivatives near the origin. (c)  $\eta v_w = 10$ ,  $\sigma_b = 0.4$  m,  $\sigma_l = 1$  m. Moderate Gaussian blur bounds derivatives near the origin. (d)  $\eta v_w = 10$ ,  $\sigma_b = 2$  m,  $\sigma_l = 1$  m. Over-blurred distribution; should be avoided.

## CHAPTER III

### LIGHT MODEL

Now that the spatial kelp distribution has been modeled, the radiative transfer equation is introduced, which is used to calculate the light field. An asymptotic series centered at the case of no scattering is developed, which forms the basis for the faster and less memory-intensive of the two solution algorithms presented in Chapter IV.

#### 3.1 Optical Definitions

Before introducing the radiative transfer equation, it is necessary to discuss some basic radiometric quantities of interest which characterize the light field, as well as inherent optical properties which describe the medium of propagation. It is necessary to begin by saying that the study of light is riddled with different sets of units which vary between disciplines.

From a physics point of view, light is a form of electromagnetic radiation which carries energy determined exclusively by its wavelength. *Radiometric units* thus describe the transfer of energy, measured in Watts, with quantities such as radiance, irradiance, and radiant flux to describe various types of energy transfer. These quantities come in frequency-dependent and frequency-integrated varieties, depending on the context. From the standpoint of human perception, the importance

of light is not in the raw energy that it transfers, but the degree to which it facilitates vision from a physiological perspective.

Therefore, *Photometric units* take all of the quantities from radiometry, rename them, and weight them by a *luminosity function* which describes frequency dependence of the human eye's sensitivity to light. Various luminosity functions exist which describe the eye's response to light in different circumstances. In photometric units, radiance becomes luminance, irradiance illuminance, and so on.

Meanwhile, plant biologists prefer to measure light by counting photons in the photosynthetic frequency band. The most common quantity in plant biology is *photosynthetically active radiation* (PAR), which is generally measured in moles of photons per square meter per second. All photons in the photosynthetic band (400 nm–700 nm) may be counted equally or weighted according to a plant's photosynthetic response. Radiometric quantities are used throughout this thesis.

### 3.1.1 Radiometric Quantities

One of the most fundamental quantities in optics is radiant flux  $\Phi$ , which has units of energy per time (Watts). Considering an element of surface area  $A$ , the energy density moving through the surface is called irradiance, denoted  $I$ , and has units energy per time. Note that the angle  $\vartheta$  of the surface relative to the light source should also be considered for full detail. Assuming the surface to be flat and the light source to be distant (parallel rays), the flux through the surface is  $\Phi = IA \cos \vartheta$ . Further, the angular dependence of the light field must be considered. The radiance,

$L$ , expresses this dependence, and is defined as the radiant flux per steradian per projected surface area perpendicular to the direction of propagation of the beam [11].

That is,

$$L = \frac{d^2\Phi}{dAd\omega},$$

where  $\omega$  is an element of solid angle. Once the radiance  $L$  is calculated everywhere, the irradiance is

$$I(\mathbf{x}) = \int_{4\pi} L(\mathbf{x}, \omega) d\omega,$$

This quantity is also called *scalar irradiance* since it does not consider light through particular surface, but rather weights radiance from all directions equally [22]. For brevity, this quantity is simply called irradiance here.

Irradiance can be approximately converted to PAR units of moles of photons (a mole of photons is also called an Einstein) per second, with the conversion being

$$1 \text{ W} = 4.2 \mu\text{mol photons/m}^2/\text{s}. \quad (3.1)$$

This is not an exact conversion, but has been found to be accurate to roughly  $\pm 10\%$  across a variety of waters [25].

### 3.1.2 Perceived Irradiance

Assuming that the irradiance  $I(\mathbf{x})$  is known, the average irradiance at a depth  $z$  is calculated as

$$\bar{I}(z) = \frac{\iint I(x, y, z) dx dy}{\iint 1 dx dy}. \quad (3.2)$$

More relevant, however, is the average irradiance perceived by the kelp. To calculate this value, the irradiance is weighted by the normalized spatial kelp distribution

before taking the mean. Then, the average perceived irradiance at each depth is

$$I_{\text{perc}}(z) = \frac{\iint P_k(x, y, z) I(x, y, z) dx dy}{\iint P_k(x, y, z) dx dy}. \quad (3.3)$$

The irradiance perceived by the kelp is expected to be lower than the average irradiance, since the kelp is more densely located at the center of the domain where the light field is reduced, whereas the simple average is influenced by regions of higher irradiance at the edges of the domain where kelp is not present.

### 3.1.3 Inherent Optical Properties

We now define a few inherent optical properties (IOPs) which depend only on the medium of propagation. The absorption coefficient  $a(\mathbf{x})$  (units  $\text{m}^{-1}$ ) defines the proportional loss of radiance per unit length due to absorption by the medium. For example, this includes radiant energy which is converted to heat. The scattering coefficient  $b$  (units  $\text{m}^{-1}$ ), defines the proportional loss of radiance per unit length due to scattering, and is assumed to be constant over space. Scattered light is not lost from the light field, it simply changes direction.

The volume scattering function (VSF)  $\beta(\Delta) : [-1, 1] \rightarrow \mathbb{R}^+$  (units  $\text{sr}^{-1}$ ) defines the probability of light scattering at any given angle from its source, where  $\Delta = \cos \vartheta$  is the cosine of the angle between the initial and final directions. Formally, given two directions  $\omega$  and  $\omega'$ ,  $\beta(\omega \cdot \omega')$  is the probability density of light scattering from  $\omega$  into  $\omega'$  (or vice-versa). Now, since a single direction subtends no solid angle, the probability of scattering occurring exactly from  $\omega$  to  $\omega'$  is 0. Rather, we say

that the probability of radiance being scattered from a direction  $\omega$  into an element of solid angle  $\Omega$  is  $\int_{\Omega} \beta(\omega \cdot \omega') d\omega'$ .

The VSF is normalized such that

$$\int_{-1}^1 \beta(\Delta) d\Delta = \frac{1}{2\pi},$$

so that for any  $\omega$ ,

$$\int_{4\pi} \beta(\omega \cdot \omega') d\omega' = 1,$$

i.e., the probability of light being scattered to some direction on the unit sphere is 1.

### 3.2 The Radiative Transfer Equation

We are now prepared to present the full details of radiative transfer equation, whose solution is the radiance in the medium as a function of position  $\mathbf{x}$  and angle  $\omega$ .

#### 3.2.1 Ray Notation

Consider a fixed position  $\mathbf{x}$  and direction  $\omega$  such that  $\omega \cdot \hat{z} \neq 0$  (the ray is not horizontal). Let  $\mathbf{l}(\mathbf{x}, \omega, s)$  denote the linear path from one domain boundary to another containing  $\mathbf{x}$  in the direction  $\omega$ . Since the ray is not horizontal, it originates either at the surface or bottom of the domain, with initial  $z$  coordinate given by

$$z_0 = \begin{cases} 0, & \omega \cdot \hat{z} > 0 \\ z_{\max}, & \omega \cdot \hat{z} < 0. \end{cases}$$

Hence, the ray path is parameterized as

$$\mathbf{l}(\mathbf{x}, \omega, s) = \frac{1}{\tilde{s}}(s\mathbf{x} + (\tilde{s} - s)\mathbf{x}_0(\mathbf{x}, \omega)), \quad (3.4)$$

where

$$\mathbf{x}_0(\mathbf{x}, \boldsymbol{\omega}) = \mathbf{x} - \tilde{s}\boldsymbol{\omega} \quad (3.5)$$

is the origin of the ray, and

$$\tilde{s} = \frac{\mathbf{x} \cdot \hat{\mathbf{z}} - z_0}{\boldsymbol{\omega} \cdot \hat{\mathbf{z}}}$$

is the path length from  $\mathbf{x}_0(\mathbf{x}, \boldsymbol{\omega})$  to  $\mathbf{x}$ .

### 3.2.2 Colloquial Description

Denote the radiance at  $\mathbf{x}$  in the direction  $\boldsymbol{\omega}$  by  $L(\mathbf{x}, \boldsymbol{\omega})$ . As light travels along  $\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s)$ , interaction with the medium produces four phenomena of interest:

1. Radiance is decreased due to absorption.
2. Radiance is decreased due to scattering out of the path to other directions.
3. Radiance is increased due to scattering into the path from other directions.
4. Radiance is increased or decreased due to light sources or sinks.

### 3.2.3 Equation of Transfer

Combining these phenomena yields the radiative transfer equation along  $\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s)$  evaluated at  $(\mathbf{x}, \boldsymbol{\omega})$ ,

$$\begin{aligned} \left. \frac{dL(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega})}{ds} \right|_{s=\tilde{s}} &= -(a(\mathbf{x}) + b)L(\mathbf{x}, \boldsymbol{\omega}) \\ &\quad + b \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L(\mathbf{x}) d\boldsymbol{\omega}' + \sigma(\mathbf{x}, \boldsymbol{\omega}), \end{aligned} \quad (3.6)$$

where  $\int_{4\pi}$  denotes integration over the unit sphere. The derivative of  $L$  over the path can be rewritten as

$$\begin{aligned} \frac{dL(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega})}{ds} \Big|_{s=\tilde{s}} &= \left[ \frac{d\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s)}{ds} \cdot \nabla L(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega}', \boldsymbol{\omega}) \right] \Big|_{s=\tilde{s}} \\ &= \boldsymbol{\omega} \cdot \nabla L(\mathbf{x}, \boldsymbol{\omega}), \end{aligned}$$

which reveals the vector form of the radiative transfer equation,

$$\boldsymbol{\omega} \cdot \nabla L(\mathbf{x}, \boldsymbol{\omega}) = -(a(\mathbf{x}) + b)L(\mathbf{x}, \boldsymbol{\omega}) + b \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' + \sigma(\mathbf{x}, \boldsymbol{\omega}),$$

or equivalently,

$$\boldsymbol{\omega} \cdot \nabla L(\mathbf{x}, \boldsymbol{\omega}) + a(\mathbf{x})L(\mathbf{x}, \boldsymbol{\omega}) = b \left( \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' - L(\mathbf{x}, \boldsymbol{\omega}) \right) + \sigma(\mathbf{x}, \boldsymbol{\omega}). \quad (3.7)$$

### 3.2.4 Boundary Conditions

We use periodic boundary conditions in the  $x$  and  $y$  directions,

$$L((x_{\min}, y, z), \boldsymbol{\omega}) = L((x_{\max}, y, z), \boldsymbol{\omega}),$$

$$L((x, y_{\min}, z), \boldsymbol{\omega}) = L((x, y_{\max}, z), \boldsymbol{\omega}).$$

In the  $z$  direction, we specify a spatially uniform downwelling light just under the surface of the water by a function  $f(\boldsymbol{\omega})$ . Or if  $z_{\min} > 0$ , then the radiance at  $z = z_{\min}$  should be specified instead (as opposed to the radiance at the first grid cell center). Further, we assume that no upwelling light enters the domain from the bottom. Letting  $\mathbf{x}_s$  be a point on the surface of the domain and  $\mathbf{x}_b$  a point on the bottom,

we have

$$L(\mathbf{x}_s, \boldsymbol{\omega}) = f(\boldsymbol{\omega}) \text{ if } \boldsymbol{\omega} \cdot \hat{z} > 0,$$

$$L(\mathbf{x}_b, \boldsymbol{\omega}) = 0 \text{ if } \boldsymbol{\omega} \cdot \hat{z} < 0.$$

### 3.3 Low-Scattering Approximation

In waters where absorption dominates scattering, an asymptotic series in terms of the scattering coefficient  $b$  can be constructed. The physical interpretation of the asymptotic series is that each term represents a discrete scattering event. With the addition of each term, light from the previous term is scattered and attenuated from each point along the ray path. In reality, the scattering cannot be considered to occur in discrete events, but rather all scattering occurs simultaneously (on a macroscopic timescale).

Since this is only an approximation, it is important to note that while the asymptotic series converges as  $b \rightarrow 0$ , it is not necessarily true that the series converges as the number of terms increases, although it may occur in certain cases. Especially in cases of large scattering, the asymptotic series diverges rapidly. The convergence properties of the algorithm are discussed in detail in Chapter V.

#### 3.3.1 Asymptotic Expansion

Taking  $b$  to be small, we introduce the asymptotic series

$$L(\mathbf{x}, \boldsymbol{\omega}) = L_0(\mathbf{x}, \boldsymbol{\omega}) + bL_1(\mathbf{x}, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}, \boldsymbol{\omega}) + \dots$$

Since the source  $\sigma$  may also depend on  $b$ , it deserves a similar expansion,

$$\sigma(\mathbf{x}, \boldsymbol{\omega}) = \sigma_0(\mathbf{x}, \boldsymbol{\omega}) + b\sigma_1(\mathbf{x}, \boldsymbol{\omega}) + b^2\sigma_2(\mathbf{x}, \boldsymbol{\omega}) + \dots.$$

Substituting the above into (3.7) yields

$$\begin{aligned} & \boldsymbol{\omega} \cdot \nabla [L_0(\mathbf{x}, \boldsymbol{\omega}) + bL_1(\mathbf{x}, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}, \boldsymbol{\omega}) + \dots] \\ & + a(\mathbf{x}) [L_0(\mathbf{x}, \boldsymbol{\omega}) + bL_1(\mathbf{x}, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}, \boldsymbol{\omega}) + \dots] \\ & = b \left( \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') [L_0(\mathbf{x}, \boldsymbol{\omega}') + bL_1(\mathbf{x}, \boldsymbol{\omega}') + b^2L_2(\mathbf{x}, \boldsymbol{\omega}') + \dots] d\boldsymbol{\omega}' \right. \\ & \quad \left. - [L_0(\mathbf{x}, \boldsymbol{\omega}) + bL_1(\mathbf{x}, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}, \boldsymbol{\omega}) + \dots] \right) \\ & + [\sigma_0(\mathbf{x}, \boldsymbol{\omega}) + b\sigma_1(\mathbf{x}, \boldsymbol{\omega}) + b^2\sigma_2(\mathbf{x}, \boldsymbol{\omega}) + \dots]. \end{aligned}$$

Grouping like powers of  $b$ , we have the decoupled set of equations

$$\boldsymbol{\omega} \cdot \nabla L_0(\mathbf{x}, \boldsymbol{\omega}) + a(\mathbf{x})L_0(\mathbf{x}) = \sigma_0(\mathbf{x}, \boldsymbol{\omega}), \quad (3.8)$$

$$\boldsymbol{\omega} \cdot \nabla L_1(\mathbf{x}, \boldsymbol{\omega}) + a(\mathbf{x})L_1(\mathbf{x}) = \sigma_1(\mathbf{x}, \boldsymbol{\omega}) + \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L_0(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' - L_0(\mathbf{x}, \boldsymbol{\omega}),$$

$$\boldsymbol{\omega} \cdot \nabla L_2(\mathbf{x}, \boldsymbol{\omega}) + a(\mathbf{x})L_2(\mathbf{x}) = \sigma_2(\mathbf{x}, \boldsymbol{\omega}) + \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L_1(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' - L_1(\mathbf{x}, \boldsymbol{\omega}).$$

⋮

In general, for  $n \geq 1$ ,

$$\boldsymbol{\omega} \cdot \nabla L_n(\mathbf{x}, \boldsymbol{\omega}) + a(\mathbf{x})L_n(\mathbf{x}) = \sigma_n(\mathbf{x}, \boldsymbol{\omega}) + \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L_{n-1}(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' - L_{n-1}(\mathbf{x}, \boldsymbol{\omega}). \quad (3.9)$$

For boundary conditions, let  $\mathbf{x}_s$  be a point on the surface of the domain and  $\mathbf{x}_b$  a point on the bottom. Then,

$$\begin{cases} L_0(\mathbf{x}_s, \boldsymbol{\omega}) + bL_1(\mathbf{x}_s, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}_s, \boldsymbol{\omega}) + \dots = f(\boldsymbol{\omega}) & \text{if } \hat{z} \cdot \boldsymbol{\omega} > 0, \\ L_0(\mathbf{x}_b, \boldsymbol{\omega}) + bL_1(\mathbf{x}_b, \boldsymbol{\omega}) + b^2L_2(\mathbf{x}_b, \boldsymbol{\omega}) + \dots = 0 & \text{if } \hat{z} \cdot \boldsymbol{\omega} < 0. \end{cases}$$

Grouping by powers of  $b$ , we have

$$\begin{cases} L_0(\mathbf{x}_s, \boldsymbol{\omega}) = f(\boldsymbol{\omega}) & \text{if } \hat{z} \cdot \boldsymbol{\omega} > 0, \\ L_0(\mathbf{x}_b, \boldsymbol{\omega}) = 0 & \text{if } \hat{z} \cdot \boldsymbol{\omega} < 0, \end{cases} \quad (3.10)$$

for the first term, and

$$\begin{cases} L_n(\mathbf{x}_s, \boldsymbol{\omega}) = 0 & \text{if } \hat{z} \cdot \boldsymbol{\omega} > 0, \\ L_n(\mathbf{x}_b, \boldsymbol{\omega}) = 0 & \text{if } \hat{z} \cdot \boldsymbol{\omega} < 0, \end{cases} \quad (3.11)$$

for  $n > 0$ .

### 3.3.2 Analytical Solution

Given  $\mathbf{x}, \boldsymbol{\omega}$ , consider the path  $\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s)$  from (3.4) for  $s \in [0, \tilde{s}]$ . Denote the leading order radiance, absorption coefficient, and source term along the path by

$$u_0(s) = L_0(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega}),$$

$$\tilde{a}(s) = a(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s)),$$

$$\tilde{\sigma}_0(s) = \sigma_0(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega}).$$

Then, the first equation from the asymptotic expansion, (3.8) and its associated boundary condition, (3.10), can be rewritten as the first order linear ordinary differ-

ential equation and inhomogeneous boundary condition,

$$\begin{cases} \tilde{\sigma}_0(s) = \frac{du_0}{ds}(s) + \tilde{a}(s)u_0(s), \\ u_0(0) = f(\boldsymbol{\omega})H(\boldsymbol{\omega} \cdot \hat{z}), \end{cases} \quad (3.12)$$

where  $H(x)$  is the Heaviside step function. This equation is solved by multiplying by the appropriate integrating factor, as follows.

$$\begin{aligned} \exp\left(\int_0^s \tilde{a}(s') ds'\right) \tilde{\sigma}_0(s) &= \exp\left(\int_0^s \tilde{a}(s') ds'\right) \frac{du_0}{ds}(s) + \exp\left(\int_0^s \tilde{a}(s') ds'\right) \tilde{a}(s)u_0(s) \\ &= \frac{d}{ds} \left[ \exp\left(\int_0^s \tilde{a}(s') ds'\right) u_0(s) \right]. \end{aligned}$$

Then, integrating both sides yields

$$\begin{aligned} \int_0^s \exp\left(\int_0^{s'} \tilde{a}(s'') ds''\right) \tilde{\sigma}_0(s') ds' &= \int_0^s \frac{d}{ds'} \left[ \exp\left(\int_0^{s'} \tilde{a}(s'') ds''\right) u_0(s') \right] ds' \\ &= \exp\left(\int_0^s \tilde{a}(s') ds'\right) u_0(s) - f(\boldsymbol{\omega})H(\boldsymbol{\omega} \cdot \hat{z}). \end{aligned}$$

Hence,

$$\begin{aligned} u_0(s) &= \left[ f(\boldsymbol{\omega})H(\boldsymbol{\omega} \cdot \hat{z}) + \int_0^s \exp\left(\int_0^{s'} \tilde{a}(s'') ds''\right) \tilde{\sigma}_0(s') ds' \right] \exp\left(-\int_0^s \tilde{a}(s') ds'\right) \\ &= \exp\left(-\int_0^s \tilde{a}(s') ds'\right) f(\boldsymbol{\omega})H(\boldsymbol{\omega} \cdot \hat{z}) \\ &\quad + \int_0^s \exp\left(-\int_{s'}^s \tilde{a}(s'') ds''\right) \tilde{\sigma}_0(s') ds'. \end{aligned} \quad (3.13)$$

Then, we convert back from path length  $s$  to the spatial coordinate  $\mathbf{x}$  by evaluating the one-dimensional solution at the end of the ray path. That is,

$$L_0(\mathbf{x}, \boldsymbol{\omega}) = u_0(\tilde{s}).$$

In addition to the explicit source term, the  $n \geq 1$  equations also have a scattering term, which is an integral of the previous term in the series. The sum of these two sources is called the effective source,

$$g_n(\mathbf{x}, \boldsymbol{\omega}) = \sigma(\mathbf{x}, \boldsymbol{\omega}) + \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L_{n-1}(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}' - L_{n-1}(\mathbf{x}, \boldsymbol{\omega}).$$

This can be similarly extracted along a ray path as

$$\tilde{g}_n(s) = \tilde{\sigma}(s) + \int_{4\pi} \beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}') L_{n-1}(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega}') d\boldsymbol{\omega}' - L_{n-1}(\mathbf{l}(\mathbf{x}, \boldsymbol{\omega}, s), \boldsymbol{\omega}).$$

Then, since  $\tilde{g}_n$  depends only on  $L_{n-1}$  and is therefore independent of  $u_n$ , (3.9) and its boundary condition (3.11) can be written as the first order linear ordinary differential equation along the ray path,

$$\begin{cases} \tilde{g}_n(s) = \frac{du_n}{ds}(s) + \tilde{a}(s)u_n(s) \\ u_n(0) = 0 \end{cases} \quad (3.14)$$

This is exactly (3.12) with  $\tilde{\sigma}_0 \rightarrow \tilde{g}_n$  and  $f(\boldsymbol{\omega}) \rightarrow 0$ . Hence,

$$u_n(s) = \int_0^s \tilde{g}_n(s') \exp\left(-\int_{s'}^s \tilde{a}(s'') ds''\right) ds'. \quad (3.15)$$

As before, the conversion back to full spatial and angular coordinates is

$$L_n(\mathbf{x}, \boldsymbol{\omega}) = u_n(\tilde{s}).$$

## CHAPTER IV

### NUMERICAL SOLUTION

In this chapter, the mathematical details involved in the numerical solution of the equations described in Chapters 2 and 3 are presented. Two solution algorithms are used: finite difference and numerical asymptotics. Both algorithms require a discrete spatial-angular grid, described in Section 4.1. In the finite difference algorithm, the continuum differential equation is approximated at every point in the grid. This forms a large sparse system of linear equations which must be solved simultaneously with an iterative method. The computational cost for this approach is high in terms of CPU usage, and especially in its memory requirement. Meanwhile, the numerical asymptotics algorithm is not as robust, but is significantly faster and does not require the allocation of large arrays.

#### 4.1 Discrete Grid

The following is a description of the spatial-angular grid used in the numerical implementation of this model. It is assumed that all simulated quantities are constant over the interior of a grid cell. Other legitimate choices of grids exist; this one was chosen for its relative simplicity.

The domain of the radiative transfer equation is embedded in five dimensions: three spatial ( $x$ ,  $y$ , and  $z$ ) and two angular (azimuthal  $\theta$  and polar  $\phi$ ). The numbers of grid cells in each dimension are denoted  $n_x$ ,  $n_y$ ,  $n_z$ ,  $n_\theta$ , and  $n_\phi$ , with uniform spacings  $dx$ ,  $dy$ ,  $dz$ ,  $d\theta$ , and  $d\phi$  between adjacent grid points. Note that  $n_\phi$  must be even in order to avoid perfectly horizontal rays, as discussed in Section 3.2.1 and Appendix A.

The following indices are assigned to each dimension:  $x \rightarrow i$ ,  $y \rightarrow j$ ,  $z \rightarrow k$ ,  $\theta \rightarrow l$ ,  $\phi \rightarrow m$ . It is convenient, however, to use a single index  $p$  to refer to directions  $\omega$  rather than referring to  $\theta$  and  $\phi$  separately. Then, the center of a generic grid cell will be denoted as  $(x_i, y_j, z_k, \omega_p)$ , and the boundaries between adjacent grid cells will be referred to as *edges*. One-indexing is employed throughout this document (i.e., array elements are counted starting at 1, not 0).

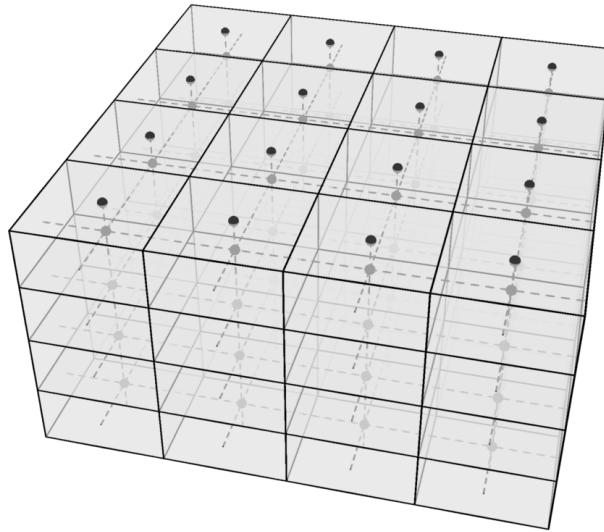


Figure 4.1: Spatial grid. Discrete quantities are calculated at grid cell centers.

Each spatial grid cell is the Cartesian product of  $x$ ,  $y$ , and  $z$  intervals of width  $dx$ ,  $dy$ , and  $dz$  respectively, as shown in Figure 4.1. The three-dimensional interval centered at  $(x_i, y_j, z_k)$  is denoted  $X_{ijk}$ , and has volume  $|X_{ijk}| = dx dy dz$ . Also, note that no grid center is located on the plane  $z = 0$ ; the surface radiance boundary condition is treated separately.

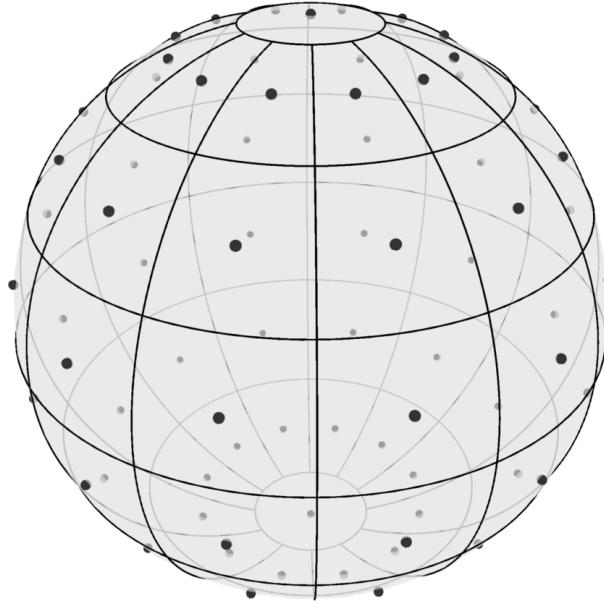


Figure 4.2: Angular grid at each point in space with poles treated separately.

As shown in Figure 4.2,  $\phi = 0$  and  $\phi = \pi$ , called the north ( $+z$ ) and south ( $-z$ ) poles respectively, are treated separately from other angular grid cells. A generic interior angular grid cell centered at  $\omega_p$  is the Cartesian product of an azimuthal interval of width  $d\theta$  and a polar interval of width  $d\phi$ . However, the two pole cells are the Cartesian product of a polar interval of width  $d\phi/2$  and the full azimuthal domain,  $[0, 2\pi)$ .

With this configuration, the total number of angles considered is  $n_{\omega} = n_{\theta}(n_{\phi} - 2) + 2$ . Then, cells are indexed by  $p = 1, \dots, n_{\omega}$  and are ordered such that  $p = 1$  and  $p = n_{\omega}$  refer to the north and south poles respectively,  $p \leq n_{\omega}/2$  refers to the northern hemisphere, and  $p > n_{\omega}/2$  refers to the southern hemisphere. Further, the symbol  $\Omega_p$  is used to refer to the two dimension angular interval centered at  $\omega_p$ . The solid angle subtended by  $\Omega_p$  is denoted  $|\Omega_p|$ . The functions  $\hat{p}(l, m)$ ,  $\hat{l}(p)$ , and  $\hat{m}(p)$  are mappings between the two sets of angular indices. Refer to Appendix A for a more rigorous discussion of the discrete spatial-angular grid.

## 4.2 Kelp Distribution

In order to determine the appropriate spatial dependence for the absorption coefficient to use in the radiative transfer equation, the spatial kelp distribution, described by (2.18) and its tributaries, is calculated at every point in space. Several computational details related to the kelp distribution are worth mentioning, from the determination of input parameters to algorithmic instructions for the required numerical integration.

### 4.2.1 Super-Individuals

Rather than model each kelp frond, subsets of the population, called super-individuals, are modeled explicitly, and are considered to represent many identical individuals, as in [41]. Specifically, at each depth  $k$ , there are  $S_k$  super-individuals, indexed by  $q$ . Super-individual  $q$  has a frond area  $A_{kq}$  and represents  $S_{kq}$  individual fronds.

From (2.7), the frond length of the super-individual is  $l_{kq} = \sqrt{2A_{kq}f_r}$ . Given the super-individual data, we calculate the mean  $\mu$  and standard deviation  $\sigma$  frond lengths using the formulas

$$\mu_k = \frac{\sum_{q=1}^{S_k} l_{kq}}{\sum_{q=1}^{S_k} S_{kq}}, \quad (4.1)$$

$$\sigma_k = \frac{\sum_{q=1}^{S_k} (l_{kq} - \mu_k)^2}{\sum_{q=1}^{S_k} S_{kq}}. \quad (4.2)$$

We then assume that frond lengths are normally distributed in each depth layer with mean  $\mu_k$  and standard deviation  $\sigma_k$ .

#### 4.2.2 Integration of Population Distributions

The computational crux of calculating the kelp distribution is to evaluate (2.17) by integrating  $P_{2D}(\theta_f, l)$  from (2.10) over the occupancy region  $R_s(\theta, s)$ , defined by (2.14) and (2.15), for every point  $(\theta, s)$  in the  $xy$ -domain. To recap, the population distribution is

$$\begin{aligned} P_{2D}(\theta_f, l) &= P_{\theta_f}(\theta_f) \cdot P_l(l), \\ P_l(l) &= \frac{1}{\sqrt{2\pi\sigma_l^2}} \exp\left(\frac{-(l - \mu_l)^2}{2\sigma_l^2}\right), \\ P_{\theta_f}(\theta_f) &= \frac{\exp(\eta v_w \cos(\theta_f - \theta_w))}{2\pi I_0(\eta v_w)}, \end{aligned}$$

and the occupancy region for  $(\theta, s)$  is  $R_s(\theta, s) \ni (\theta_f, l)$  such that

$$\theta - \alpha < \theta_f < \theta + \alpha,$$

$$l > l_{\min}(\theta, s).$$

To compute the integral, we symbolically convert the two-dimensional integral to a one-dimensional integral in terms of the error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt, \quad (4.3)$$

which is a built-in function in most programming languages, including Fortran. So, we evaluate

$$\begin{aligned} \tilde{P}_k(\theta, s) &= \int_{R_s(\theta, s)} P_{2D}(\theta_f, l) d\theta_f dl \\ &= \int_{\theta-\alpha}^{\theta+\alpha} \int_{l_{\min}(\theta, s)}^{\infty} P_{\theta_f}(\theta_f) \cdot P_l(l) dl d\theta_f, \\ &= \frac{1}{\sqrt{2\pi\sigma_l^2}} \int_{\theta-\alpha}^{\theta+\alpha} P_{\theta_f}(\theta_f) \int_{l_{\min}(\theta, s)}^{\infty} \exp\left(-\frac{(l - \mu_l)^2}{2\sigma_l^2}\right) dl d\theta_f. \end{aligned}$$

The substitution  $u = (l - \mu_l)/\sqrt{2\sigma_l^2}$ ;  $du = dl/\sqrt{2\sigma_l^2}$  produces

$$\begin{aligned} \tilde{P}_k(\theta, s) &= \frac{1}{\sqrt{\pi}} \int_{\theta-\alpha}^{\theta+\alpha} P_{\theta_f}(\theta_f) \int_{\frac{l_{\min}(\theta, s) - \mu_l}{\sqrt{2\sigma_l^2}}}^{\infty} e^{-u^2} du d\theta_f \\ &= \frac{1}{2} \int_{\theta-\alpha}^{\theta+\alpha} P_{\theta_f}(\theta_f) \left[ 1 - \text{erf}\left(\frac{l_{\min}(\theta, s) - \mu_l}{\sqrt{2\sigma_l^2}}\right) \right] d\theta_f \end{aligned}$$

Note that the above integrand can be explicitly evaluated at any value of  $\theta_f$ , and is not restricted to values on a discrete grid. The integral is then evaluated

numerically using a quadrature rule of any chosen degree. At present, a Gauss-Legendre quadrature with degree 101 is applied. If the quadrature degree is chosen too low (e.g. 5), the resulting distribution is marked by numerical artifacts including discontinuities. Since the kelp calculation is orders of magnitude faster than the light field calculation, there is no issue with choosing a high quadrature degree.

#### 4.2.3 Gaussian Convolution

In order to blur the kelp distribution as described in Section 2.5.2,  $P_k(x, y, z)$  is first calculated without blurring according to Equations (2.17) and (2.18) at every point  $(x_i, y_j)$  in each depth layer, which yields a matrix  $P_{ij}^k = P_k(x_i, y_j, z)$ . Then, the discrete convolution of  $P_{ij}^k$  with the Gaussian kernel  $K(x, y; \sigma_b)$  from Equation (2.22) is numerically computed by the same process used to post-process pixelated image with a Gaussian blur.

Notice first that the integral from Equation (2.23) has infinite extent. For numerical computation, a discrete grid with finite bounds must be chosen. Specifically, an array of uniformly spaced quadrature points  $(x'_{i'}, y'_{j'})$  is chosen for the integration variables  $x'$  and  $y'$  with spacings  $dx$  and  $dy$  to match the existing grid. In order to capture up to two standard deviations of the Gaussian distribution, the number of quadrature points in each dimension is chosen to be

$$n_K = 2r_K + 1, \quad (4.4)$$

where

$$r_K = \text{ceil} \left( \max \left( \frac{2\sigma_b}{dx}, \frac{2\sigma_b}{dy} \right) \right). \quad (4.5)$$

Then, the quadrature points are

$$x'_{i'} = (i' - r_K)dx, \quad i' = 1, \dots, n_k,$$

$$y'_{j'} = (j' - r_K)dy, \quad j' = 1, \dots, n_k.$$

The kernel is then evaluated at the quadrature points to form the matrix

$$K_{i'j'} = K(x'_{i'}, y'_{j'}; \sigma_b).$$

Note that the continuous  $K(x, y; \sigma_b)$  is normalized only on the infinite plane; the discrete  $K_{ij}$  must therefore be re-normalized on the finite grid as

$$K_{i'j'} = \frac{K_{i'j'}}{\sum_{ij} K_{ij}}.$$

Then, letting

$$\delta_x(i, i') = i - r_K + i' \bmod n_x,$$

$$\delta_y(j, j') = j - r_K + j' \bmod n_y,$$

the convolved kelp distribution  $P_{ij}^{kb}$  is evaluated as

$$\begin{aligned} P_{ij}^{kb} &= P_k^b(x_i, y_j, z; \sigma_b) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K(x', y', z; \sigma_b) P_k(x_i - x', y_j - y', z) dx' dy' \\ &= dx dy \sum_{i'=1}^{n_k} \sum_{j'=1}^{n_k} K_{i'j'} P_k(x_i - x'_{i'}, y_j - y'_{j'}, z) \\ &= dx dy \sum_{i'=1}^{n_k} \sum_{j'=1}^{n_k} K_{i'j'} P_k(x_{\delta_x(i, i')}, y_{\delta_y(j, j')}, z) \\ &= dx dy \sum_{i'=1}^{n_k} \sum_{j'=1}^{n_k} K_{i'j'} P_{\delta_x(i, i'), \delta_y(j, j')}^k. \end{aligned}$$

That is, at each grid point  $(x_i, y_j)$ , a weighted sum of periodic-adjacent values is taken according to the Gaussian kernel in order to perform the blur.

### 4.3 Quadrature Rules

As a prerequisite to algorithm development, a few key integrals are calculated here.

Since it is assumed that all quantities are constant within a spatial-angular grid cell, the midpoint rule is employed for both spatial and angular integration. Presented here is a basic derivation of the formulas for integration in the spatial-angular grid. Further details are found in Appendix B.

#### 4.3.1 Spatial Quadrature

Define the *spatial characteristic function* as

$$\mathcal{X}_{ijk}^X(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in X_{ijk}, \\ 0, & \text{otherwise.} \end{cases}$$

The double integral of a function  $f(\mathbf{x})$  over a depth layer  $k$  is approximated as

$$\begin{aligned} \int_{x_{\min}}^{x_{\max}} \int_{y_{\min}}^{y_{\max}} f(x, y, z_k) dy dx &\approx \int_{x_{\min}}^{x_{\max}} \int_{y_{\min}}^{y_{\max}} \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} \mathcal{X}_{ijk}^X(x, y, z_k) f(x_i, y_j, z_k) dy dx \\ &= \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} f(x_i, y_j, z_k) \int_{x_{\min}}^{x_{\max}} \int_{y_{\min}}^{y_{\max}} \mathcal{X}_{ijk}^X(x, y, z_k) dy dx \\ &= \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} |X_{ijk}| f(x_i, y_j, z_k) \\ &= dx dy \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} f(x_i, y_j, z_k). \end{aligned}$$

The path integral of  $f(\mathbf{x})$  over a path  $\mathbf{l}(s)$  from  $s = 0$  to  $s = \tilde{s}$  is

$$\int_0^{\tilde{s}} f(\mathbf{l}(s)) ds \approx \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} \sum_{k=1}^{n_z} f(x_i, y_j, z_k) ds_{ijk},$$

where  $ds_{ijk}$  is the total path distance of  $\mathbf{l}(s)$  through  $X_{ijk}$ . Full details of the path integral algorithm for straight line paths are found in Appendix B.

### 4.3.2 Angular Quadrature

Define the *angular characteristic function* as

$$\mathcal{X}_p^\Omega(\omega) = \begin{cases} 1, & \omega \in \Omega_p, \\ 0, & \text{otherwise.} \end{cases}$$

Then, the integral of a function  $f(\omega)$  over all angles is approximated as

$$\begin{aligned} \int_{4\pi} f(\omega) d\omega &\approx \int_{4\pi} \sum_{p=1}^{n_\omega} f(\omega_p) \mathcal{X}_p^\Omega(\omega) d\omega \\ &= \sum_{p=1}^{n_\omega} f(\omega_p) \int_{4\pi} \mathcal{X}_p^\Omega(\omega) d\omega \\ &= \sum_{p=1}^{n_\omega} f(\omega_p) \int_{\Omega_p} d\omega \\ &= \sum_{p=1}^{n_\omega} f(\omega_p) |\Omega_p|. \end{aligned}$$

Similarly, the amount of light scattered between angular grid cells is found by integrating  $\beta$  over specific regions. Consider two angular grid cells,  $\Omega_p$  and  $\Omega_{p'}$ . Since  $\beta(\omega \cdot \omega')$  is the probability density of scattering between  $\omega$  and  $\omega'$ , the average probability density of scattering from  $\omega \in \Omega_p$  to  $\omega' \in \Omega_{p'}$  (or vice versa) is

$$\beta_{pp'} = \frac{1}{|\Omega_p| |\Omega_{p'}|} \int_{\Omega_p} \int_{\Omega_{p'}} \beta(\omega \cdot \omega') d\omega' d\omega \approx \beta(\omega \cdot \omega'),$$

assuming that  $\beta$  is approximately constant over  $\Omega_p$  and  $\Omega_{p'}$ . Denote the radiance at  $(x_i, y_j, z_k, \omega_p)$  by  $L_{ijkp}$ . Then, the total radiance scattered into  $\Omega_p$  from  $\Omega_{p'}$  is

$$\begin{aligned} \int_{\Omega_p} \int_{\Omega_{p'}} \beta(\omega \cdot \omega') L(x, \omega') d\omega' d\omega &\approx L_{ijkp'} \int_{\Omega_p} \int_{\Omega_{p'}} \beta(\omega \cdot \omega') d\omega' d\omega \\ &= \beta_{pp'} |\Omega_p| |\Omega_{p'}| L_{ijkp'}. \end{aligned}$$

Hence, the average radiance scattered from  $\Omega_{p'}$  into some  $\omega \in \Omega_p$  is  $\beta_{pp'} |\Omega'| L_{ijkp'}$ .

Therefore, the radiance gain due to scattering into  $\omega_p$  from all other angles is

$$\int_{4\pi} \beta(\omega_p \cdot \omega_{p'}) L(x, \omega') d\omega \approx \sum_{p=1}^{n_\omega} \beta_{pp'} |\Omega'| L_{ijkp}. \quad (4.6)$$

#### 4.4 Numerical Asymptotics

The asymptotic approximations (3.13) and (3.15) to the radiative transfer equation (3.7) are evaluated numerically as follows. Given a position  $x$  and direction  $\omega$ , a path through the discrete grid can be constructed using the ray tracing algorithm described in Appendix B. Let  $\nu = 1, \dots, N - 1$  index the spatial grid cells traversed (wholly or partially) by the ray, and define the *path-length characteristic function*

$$\mathcal{X}_\nu^l(s) = \begin{cases} 1, & s_\nu \leq s < s_{\nu+1}, \\ 0, & \text{otherwise,} \end{cases}$$

where  $s \in [s_\nu, s_{\nu+1}]$  parameterizes the path segment traversing cell  $\nu$  and  $ds_\nu = s_{\nu+1} - s_\nu$  is the length of the segment. Then, the piecewise constant representations of the path absorption coefficient  $\tilde{a}(s)$  and the effective source  $\tilde{g}_n(s)$  from Section 3.3.2 are

$$\begin{aligned} \tilde{g}_n(s) &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \mathcal{X}_\nu^l(s), \\ \tilde{a}(s) &= \sum_{\nu=1}^{N-1} \tilde{a}_\nu \mathcal{X}_\nu^l(s). \end{aligned}$$

Given  $s$ , the index of the next edge crossing is

$$\hat{\nu}(s) = \min \{ \nu \in \{1, \dots, N\} : s_\nu > s \},$$

and the path length between  $s$  and the next edge crossing is

$$\tilde{d}(s) = s_{\hat{\nu}(s)} - s.$$

Then, evaluating (3.15) at  $s = \tilde{s}$  is calculated as

$$\begin{aligned} u_n(\tilde{s}) &= \int_0^{\tilde{s}} \tilde{g}_n(s') \exp \left( - \int_{s'}^{\tilde{s}} \tilde{a}(s'') ds'' \right) ds' \\ &= \int_0^{\tilde{s}} \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \mathcal{X}_\nu^l(s') \exp \left( - \int_{s'}^{\tilde{s}} \sum_{j=1}^{N-1} \tilde{a}_j \mathcal{X}_j^l(s'') ds'' \right) ds' \\ &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \int_0^{\tilde{s}} \mathcal{X}_\nu^l(s') \exp \left( - \sum_{j=1}^{N-1} \tilde{a}_j \int_{s'}^{\tilde{s}} \mathcal{X}_j^l(s'') ds'' \right) ds' \\ &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \int_{s_\nu}^{s_{\nu+1}} \exp \left( - \tilde{a}_{\hat{\nu}(s')-1} \tilde{d}(s') - \sum_{j=\hat{\nu}(s')}^{N-1} \tilde{a}_j ds_j \right) ds' \\ &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \int_{s_\nu}^{s_{\nu+1}} \exp \left( - \tilde{a}_\nu (s_{\nu+1} - s') - \sum_{j=\nu+1}^{N-1} \tilde{a}_j ds_j \right) ds'. \end{aligned}$$

This integral is made straightforward by setting

$$b_\nu = -\tilde{a}_\nu s_{\nu+1} - \sum_{j=\nu+1}^{N-1} \tilde{a}_j ds_j,$$

which yields

$$\begin{aligned} u_n(\tilde{s}) &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} \int_{s_\nu}^{s_{\nu+1}} \exp (\tilde{a}_\nu s' + b_\nu) ds' \\ &= \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} e^{b_\nu} \int_{s_\nu}^{s_{\nu+1}} \exp (\tilde{a}_\nu s') ds'. \end{aligned}$$

Define the intermediate variable

$$\begin{aligned} d_\nu &= \int_{s_\nu}^{s_{\nu+1}} \exp (\tilde{a}_\nu s') ds' \\ &= \begin{cases} ds_\nu, & \tilde{a} = 0 \\ (\exp(\tilde{a}_\nu s_{\nu+1}) - \exp(\tilde{a}_\nu s_\nu)) / \tilde{a}_\nu, & \text{otherwise,} \end{cases} \end{aligned}$$

which permits the simple formula

$$u_n(\tilde{s}) = \sum_{\nu=1}^{N-1} \tilde{g}_{n\nu} d_\nu e^{b_\nu}. \quad (4.7)$$

When  $n = 0$ , the boundary condition must be included for downwelling light, and the effective source  $\tilde{g}_{n\nu}$  is reduced to the explicit source  $\tilde{\sigma}_{0\nu}$  for lack of a scattering term. Thus, the numerical solution to (3.13) is given by

$$u_0(\tilde{s}) = f(\boldsymbol{\omega}) H(\boldsymbol{\omega} \cdot \hat{z}) \exp \left( - \sum_{j=1}^{N-1} \tilde{a}_j ds_j \right) + \sum_{\nu=1}^{N-1} \tilde{\sigma}_{0\nu} d_\nu e^{b_\nu}. \quad (4.8)$$

## 4.5 Finite Difference

While the asymptotic solution is valid in the case of low scattering, a more general solution is obtained via finite difference, whereby the derivatives and integrals in the integro-partial differential equation are discretized to differences and sums and evaluated at each grid cell to construct a linear system of equations whose solution approximates that of the analytical equation. The price of a general solution, is greatly increased computational cost, both in terms of memory and CPU usage.

### 4.5.1 Discretization

For the spatial interior of the domain, we use the second order central difference formula (CD2) to approximate the derivatives, which is

$$f'(x) = \frac{f(x + dx) - f(x - dx)}{2dx} + \mathcal{O}(dx^2).$$

When applying the PDE on the upper or lower boundary, we use the forward and backward difference (FD2 and BD2) formulas respectively. The forward

difference is given by

$$f'(x) = \frac{-3f(x) + 4f(x+dx) - f(x+2dx)}{2dx} + \mathcal{O}(dx^2),$$

and the backward difference by

$$f'(x) = \frac{3f(x) - 4f(x-dx) + f(x-2dx)}{2dx} + \mathcal{O}(dx^2).$$

For the upper and lower boundaries, an asymmetric finite difference formula is required since the distance between grid centers in the  $z$  direction is  $dz$ , whereas the distance to the surface is  $dz/2$ . In general, the Taylor Series of a function  $f$  about  $x$  is written as

$$f(x+\varepsilon) = \sum_{n=1}^{\infty} \frac{f^{(n)}(x)}{n!} \varepsilon^n.$$

Truncating after the first few terms, we have

$$f(x+\varepsilon) = f(x) + f'(x)\varepsilon + \frac{f''(x)}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3). \quad (4.9)$$

Similarly, replacing  $\varepsilon$  with  $-\varepsilon/2$  we have

$$f(x - \frac{\varepsilon}{2}) = f(x) - \frac{f'(x)\varepsilon}{2} + \frac{f''(x)\varepsilon^2}{8} + \mathcal{O}(\varepsilon^3). \quad (4.10)$$

Rearranging (4.9) produces

$$f''(x)\varepsilon^2 = 2f(x+\varepsilon) - 2f(x) - 2f'(x)\varepsilon + \mathcal{O}(\varepsilon^3). \quad (4.11)$$

Combining (4.10) with (4.11) gives

$$\begin{aligned} \varepsilon f'(x) &= 2f(x) - 2f(x - \frac{\varepsilon}{2}) + \frac{f''(x)\varepsilon^2}{4} + \mathcal{O}(\varepsilon^3) \\ &= 2f(x) - 2f(x - \frac{\varepsilon}{2}) + \left[ \frac{f(x+\varepsilon)}{2} - \frac{f(x)}{2} - \frac{f'(x)\varepsilon}{2} \right] + \mathcal{O}(\varepsilon^3) \\ &= \frac{3}{2}f(x) - 2f(x - \frac{\varepsilon}{2}) + \frac{f(x+\varepsilon)}{2} - \frac{f'(x)}{2} + \mathcal{O}(\varepsilon^3). \end{aligned}$$

Hence,

$$\frac{3}{2}\varepsilon f'(x) = \frac{3}{2}f(x) - 2f\left(x - \frac{\varepsilon}{2}\right) + \frac{f(x + \varepsilon)}{2} + \mathcal{O}(\varepsilon^3).$$

Then, dividing by  $3\varepsilon/2$  gives

$$f'(x) = \frac{-4f\left(x - \frac{\varepsilon}{2}\right) + 3f(x) + f(x + \varepsilon)}{3\varepsilon} + \mathcal{O}(\varepsilon^2). \quad (4.12)$$

Similarly, substituting  $\varepsilon \rightarrow -\varepsilon$ , we have

$$f'(x) = \frac{-f(x - \varepsilon) - 3f(x) + 4f\left(x + \frac{\varepsilon}{2}\right)}{3\varepsilon} + \mathcal{O}(\varepsilon^2). \quad (4.13)$$

#### 4.5.2 Difference Equations

For every spatial grid cell, the scattering integral is discretized as in Section 4.4 by

$$\boldsymbol{\omega} \cdot \nabla L_p = -(a_{ijk} + b)L_p + \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{p'} + \sigma_{ijkp},$$

or equivalently,

$$\boldsymbol{\omega} \cdot \nabla L_p + (a_{ijk} + b)L_p - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{p'} = \sigma_{ijkp}.$$

On the interior of the spatial domain, we apply the central difference formula in each

dimension, which yields

$$\begin{aligned} \sigma_{ijkp} &= \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\ &\quad + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\ &\quad + \frac{L_{ij,k+1,p} - L_{ij,k-1,p}}{2dz} \cos \hat{\phi}_p \\ &\quad + (a_{ijk} + b)L_{ijkp} - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'}. \end{aligned}$$

Note that since periodic boundary conditions are used in  $x$  and  $y$ , the subscript  $i+1$  should actually read  $(i+1) \bmod 1 n_x$ , where  $\bmod 1$  is the one-indexed modulus. The

same idea applies for  $i - 1$ ,  $j + 1$ , and  $j - 1$ . For the sake of readability, this is omitted from the equations in this section.

For downwelling light at the surface, we apply the asymmetric second order difference approximation (4.10) using the surface radiance value, which gives

$$\begin{aligned}\sigma_{ijkp} = & \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\ & + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\ & + \frac{-4f_p + 3L_{ijkp} + L_{ij,k+1,p}}{3dz} \cos \hat{\phi}_p \\ & + (a_{ijk} + b)L_{ijkp} \\ & - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'}.\end{aligned}$$

Combining  $L_{ijkp}$  terms and moving the boundary condition to the other side gives

$$\begin{aligned}& \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\ & + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\ & + \frac{L_{ij,k+1,p}}{3dz} \cos \hat{\phi}_p \\ & + \left( a_{ijk} + b + \frac{\cos \hat{\phi}_p}{dz} \right) L_{ijkp} \\ & - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'} = \frac{4f_p}{3dz} \cos \hat{\phi}_p + \sigma_{ijkp}.\end{aligned}$$

Likewise, for the bottom boundary condition, we have

$$\begin{aligned}
& \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\
& + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\
& - \frac{L_{ij,k-1,p}}{3dz} \cos \hat{\phi}_p \\
& + \left( a_{ijk} + b - \frac{\cos \hat{\phi}_p}{dz} \right) L_{ijkp} \\
& - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'} = \sigma_{ijkp}
\end{aligned}$$

Now, for upwelling light at the first depth layer (non-BC), we apply FD2.

$$\begin{aligned}
\sigma_{ijkp} &= \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\
& + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\
& + \frac{-3L_{ijkp} + 4L_{ij,k+1,p} - L_{ij,k+2,p}}{2dz} \cos \hat{\phi}_p \\
& + (a_{ijk} + b) L_{ijkp} \\
& - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'}.
\end{aligned}$$

Grouping  $L_{ijkp}$  terms gives

$$\begin{aligned}
\sigma_{ijkp} &= \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\
& + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\
& + \frac{4L_{ij,k+1,p} - L_{ij,k+2,p}}{2dz} \cos \hat{\phi}_p \\
& + \left( a_{ijk} + b - 3 \frac{\cos \hat{\phi}_p}{2dz} \right) L_{ijkp} \\
& - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'}.
\end{aligned}$$

Similarly, for downwelling light at the lowest depth layer, we have

$$\begin{aligned}\sigma_{ijkp} = & \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p \\ & + \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p \\ & + \frac{-4L_{ij,k-1,p} + L_{ij,k-2,p}}{2dz} \cos \hat{\phi}_p \\ & + \left( a_{ijk} + b + 3 \frac{\cos \hat{\phi}_p}{2dz} \right) L_{ijkp} \\ & - \sum_{p'=1}^{n_\omega} \beta_{pp'} L_{ijkp'}.\end{aligned}$$

#### 4.5.3 Structure of Linear System

For each spatial-angular grid cell, one of the above equations is applied. The equation applied at each grid cell involves adjacent radiance values due to the discretized derivatives. Thus, a coupled system of linear equations is produced, which can be written as a sparse matrix equation,  $\mathbb{A}\mathbb{X} = \mathbb{B}$ . In the coefficient matrix  $\mathbb{A}$ , each row is associated with the grid cell at which the discretized equation was evaluated. Each column is the coefficient of the radiance at a particular spatial-angular grid cell.

In principle, the order of the equations, i.e., the order of the rows and columns of the coefficient matrix, is not important so long as consistency is maintained with the solution vector and right-hand side. In practice, some procedure is necessary for constructing an ordered list of the multidimensional grid cells. One option, employed here, is to use a block structure where dimensions are nested within one another. An ordering for the dimensions is chosen, from outermost to innermost. Adjacent rows and columns in the matrix are associated with adjacent grid cells in the innermost

dimension, adjacent blocks of the innermost dimension are adjacent in the second innermost dimension, etc.

In the numerical implementation of this model, we choose the order of dimensions to be  $\omega, z, y, x$ , with  $\omega$  being the outermost and  $x$  being the innermost. Recall that  $\theta$  and  $\phi$  are already combined, both indexed by  $p$ , as discussed in Section 4.1 and Appendix A. This particular ordering is chosen for ease of programming in terms of deciding which of the equations from Section 4.5.2 to apply. Since the choice of equation does not depend on  $x$  or  $y$ , they are the outermost. Then, the surface and bottom  $z$  values have to be considered separately from the rest. And within the surface and bottom depth layers, there are further cases depending on whether the light is upwelling or downwelling. Hence, the chosen ordering follows somewhat naturally from the boundary conditions.

With this storage scheme in mind, the coefficients of the discretized equation applied to  $(x_i, y_j, z_k, \omega_p)$  is stored in row

$$r_{ijkp} = p + n_\omega(k - 1) + n_\omega n_z(j - 1) + n_\omega n_z n_y(i - 1)$$

of the matrix  $\mathbb{A}$ . Since the same ordering is used for rows and columns of the coefficient matrix  $\mathbb{A}$ ,  $L_{ijkp}$  is located at position  $r_{ijkp}$  of the solution vector  $\mathbb{X}$ , and the right-hand side associated with that grid cell, if any, is also stored at position  $r_{ijkp}$  of the right-hand side vector  $\mathbb{B}$ .

Also relevant is the total size of the system and of the sparse matrices necessary to store. The sizes of  $\mathbb{A}$ ,  $\mathbb{X}$ , and  $\mathbb{B}$  are the number of grid cells, which is just

$n_x n_y n_z n_{\omega}$ . Most of these elements, though, are zero, since spatial derivatives only involve adjacent spatial grid cells and the scattering integral only involves angles within a single spatial grid cell. Therefore, by saving only the locations and values of nonzero elements in the coefficient matrix, a considerable amount of storage space is saved. Table 4.1 shows a breakdown of the number of distinct radiance values involved in each application of the discretized equations from Section 4.5.2, as well as the number of times that each of the equations appears in the matrix.

By multiplying the first column of Table 4.1 by the second and summing over the rows, the total number of nonzero matrix elements is calculated to be

$$\begin{aligned}
 N_{\mathbb{A}} &= (n_{\omega} + 6) \cdot n_x n_y (n_z - 2) n_{\omega} \\
 &\quad + (n_{\omega} + 5) \cdot n_x n_y n_{\omega} + (n_{\omega} + 6) \cdot n_x n_y n_{\omega} \\
 &= n_x n_y n_{\omega} [n_{\omega} n_z - n_{\omega} + 6n_z - 6 + n_{\omega} + 5] \\
 &= n_x n_y n_{\omega} [n_z (n_{\omega} + 6) - 1]. \tag{4.14}
 \end{aligned}$$

For example, a  $10 \times 10 \times 10 \times 10 \times 10$  grid involves 7,207,800 matrix elements, while a  $20 \times 20 \times 20 \times 20 \times 20$  grid requires 1,065,583,200 elements to be stored! Clearly, the grid must be kept reasonably small in order to be solved by modern computers. Also, note that in the absence of an explicit source term  $\sigma(\mathbf{x}, \omega)$ ,  $\mathbb{B}$  only has nonzero entries for the downwelling surface grid cells, of which there are  $n_x n_y n_{\omega}/2$ .

#### 4.5.4 Iterative Solution

Because of the large number of dimensions (three spatial, two angular), the matrix can easily have upwards of millions of nonzero elements, even for modest grid sizes.

Table 4.1: Breakdown of nonzero matrix elements by derivative case.

Derivative case	# nonzero/row	# of rows
interior	$n_\omega + 6$	$n_x n_y (n_z - 2) n_\omega$
surface downwelling	$n_\omega + 5$	$n_x n_y n_\omega / 2$
bottom upwelling	$n_\omega + 5$	$n_x n_y n_\omega / 2$
surface upwelling	$n_\omega + 6$	$n_x n_y n_\omega / 2$
bottom downwelling	$n_\omega + 6$	$n_x n_y n_\omega / 2$

Direct methods such as Gaussian elimination, QR factorization, and singular value decomposition are therefore infeasible due to memory requirements. We therefore turn to iterative solvers. Many such solvers are available, including GMRES [39], LGMRES [4], IDR [43], and BI-CGSTAB [44].

For the code in this thesis, a parallel implementation of GMRES provided by a Fortran package called LIS (Library of Iterative Solvers) [27] is employed. LIS provides several execution environments: multithreading, multiprocessing, and MPI (Message Passing Interface) [23]. At present, the multithreading environment is used. While this is the simplest to set up since threads within a process share memory and all communication between workers is hidden from the user, it requires that a single process on a single machine be able to allocate enough space for the entire coefficient matrix, which can easily reach tens or hundreds of gigabytes for large grids.

## CHAPTER V

### CODE VERIFICATION

The purpose of a numerical simulation is generally to accurately predict the behavior of a real system. All mathematical modeling and numerical calculation, however, deals only with approximations. It is therefore crucial to understand the degree to which these approximations reflect the actual scenario of interest, and to what extent their predictions can be trusted. In this chapter, the validity of the numerical approximations to the continuum model is discussed. Concepts relating to determining the correctness of a whole code and the accuracy of specific results are surveyed. The Fortran implementations of the finite difference and numerical asymptotics solutions of the radiative transfer equation are verified with reasonable confidence to be free of detectable coding mistakes.

#### 5.1 Sources of Error in Numerical Simulations

While simulations attempt to realistically reproduce real-life observations, many factors conspire to distort the numerical results they produce. The following is an overview of the errors incurred throughout the process of creating and evaluating numerical models. Some of these errors are *ordered*, meaning that they can be decreased predictably by performing additional computations, while others are not.

First, any mathematical model is based on simplifying assumptions compared to the real system. Any assumptions which do not hold precisely for the real system contribute to differences between solutions to the model equations and the behavior of the real system. Such differences can be termed *modeling errors*, and are a present in the exact solutions to the mathematical equations comprising the model. Once a model is formulated, it contains free parameters which can be varied to emulate different physical scenarios. To evaluate the model, specific parameters must be used which reflect the scenario of interest. The values of these parameters often are obtained experimentally, and may not be known with exact precision. Error resulting from inaccurate physical parameter values can be called *parameter uncertainty error*.

Mathematical models accurate enough to be useful are usually difficult or impossible to solve analytically. Therefore, either mathematical simplifications or numerical approximations, or both, may be employed in order to obtain a solution. For example, in the low-scattering solution presented in Section 3.3, the exact solution is expanded in a Taylor Series, from which only the first few terms are used, with the rest discarded. The error resulting from using a finite number of terms from an infinite series is referred to as *truncation error*. Truncation error is ordered for a convergent series, as an arbitrary number of terms can be used to better approximate the true solution. When a continuous equation is solved numerically, it is necessary to compute the solution on a finite number of discrete points rather than on the complete domain. The error incurred by doing so is called *discretization error*.

Discretization error is also ordered, as arbitrarily fine grids can be chosen in order to better approximate the continuum solution.

Finally, once the model, solution algorithm, and discretization scheme are chosen, a computer is used to perform the actual calculations. Computers do not operate on the full set of real numbers, but rather on a finite subset of the real numbers with a predetermined floating point precision, depending on the hardware and software environment. The loss of accuracy in computations due to the use of floating point numbers is termed *round-off error* [35].

## 5.2 Verification and Validation

There are two aspects to building confidence in numerical codes, specifically those which solve PDEs: verification and validation. Verification deals with *solving the equations right*, while validation deals with *solving the right equations* [35]. Validation involves comparison with experimental evidence in order to determine that governing equations accurately describe physical phenomenon, and that their solutions match observation. In other words, it is the process of checking that modeling errors are sufficiently small to model the system as accurately as necessary. Validation is an ongoing process; as new experimental data become available, the equations can be solved under appropriate conditions in an attempt to replicate the new observations [37]. Verification, however, is a purely mathematical exercise, and has nothing to do with the physical system being modeled [36]. It deals only with the agreement between an equation and its numerical solution produced by a partic-

ular implementation of an algorithm. It involves checking that ordered sources of numerical error (truncation and discretization errors) decrease as expected when additional computations are performed. Unlike validation, verification is something to be started and finished. If a set of parameters to the model can be chosen to exercise all terms in the equation, comparison between the numerical and exact solution is sufficient to demonstrate the correctness of a computational code, and the process need not be repeated unless the code is modified.

Due to lack of sufficient experimental data, rigorous validation of the present radiative transfer code is left as future work. However, verification of both the finite difference and numerical asymptotics algorithms is demonstrated here. There are two phases of verification. The first is *code verification*, where the overall implementation of an algorithm is tested, and the difference between the numerical and analytical solutions is *explicitly measured* at every point in the numerical solution. The same calculation is repeated for several grid sizes, and it is checked that the convergence order as the grid spacing approaches zero matches the theoretical convergence order of the algorithm. The explicit measurement of errors requires that the analytical solution be known, which is generally only possible for some unrealistic or uninteresting set of parameters. If the analytical solution were available for the real, interesting case, then it would probably not have been necessary to implement a numerical solution in the first place. Nevertheless, analyzing a well-chosen unrealistic situation is sufficient to check that the order of the code's discretization error matches the theoretical order of the algorithm.

For realistic conditions, however, a second stage of verification is employed: *verification of calculations*. In this phase, a specific calculation of interest is performed, and the error is *estimated* since it cannot be measured explicitly when the exact solution is not available. This is generally done by repeating the calculation for several grid sizes, as above, then using a technique called Richardson Extrapolation to estimate the limiting solution as the grid spacing approaches zero. This estimated limiting solution is then compared to the actual numerical solutions.

Since the solutions are known on different grids, they cannot be compared pointwise without interpolation. Rather, a single scalar calculated from some integral of the solution is often used as a simple measure of the global order of accuracy [1]. However, the procedure may also be used to estimate discretization for a variable over the entire domain (e.g. for error bars on a plot) by interpolating the variable from each grid at a predetermined set of points, and applying Richardson extrapolation independently at each interpolated point. Of course, the order of the interpolation should be greater than the order of the algorithm under consideration to avoid reducing the observed order of convergence.

### 5.3 Method of Manufactured Solutions

The most obvious way to obtain an analytical solution to compare to a numerical solution is by choosing a simple case where the PDE can be solved explicitly, perhaps through separation of variables or by reducing it to an ODE. This is referred to as the method of exact solutions (MES). However, such simple cases usually result in such

a loss of generality that they become useless in testing the complicated aspects of the solution algorithm. In order to verify that a code will work in an interesting case, every term in the equation must be exercised during the verification process. An alternative process, the method of manufactured solutions (MMS), retains arbitrary generality in the equations while making analytical solutions readily available [40]. Of course, there is a trade-off: the solutions are not physically realistic. However, this is not an issue; as stated previously, *verification is a purely mathematical endeavor* [36]. Whether a code solves an equation correctly is unrelated to physical realism.

The method of manufactured solutions is performed as follows. Consider a differential equation

$$Du(\mathbf{x}) = \sigma(\mathbf{x}), \quad (5.1)$$

$$u(\mathbf{x}) = f(\mathbf{x}) \text{ for } \mathbf{x} \in \Sigma, \quad (5.2)$$

where  $D$  is a differential operator,  $u$  is the solution,  $\sigma$  is a source term,  $f$  is the boundary condition function, and  $\Sigma$  is the set of boundary points at which the boundary condition is applied. Normally,  $D$ ,  $\sigma$ , and  $f$  are known, and solving for  $u$  involves determining  $D^{-1}$  and calculating  $u = D^{-1}\sigma$  subject to (5.2).

The Method of Manufactured Solutions reverses the normal procedure. Here,  $u$  is hand-picked at the outset to be easy to calculate, all parameters and coefficient functions in  $D$  are chosen to be nonzero, and the source term  $\sigma$  which produces the desired solution is calculated. Similarly, the boundary condition is determined from the chosen solution. In essence, rather than solving  $u = D^{-1}\sigma$  subject to  $u(\Sigma) = f$ ,

it suffices to compute  $\sigma = Du$  and evaluate  $f = u$  at the boundary. Whereas *inverting* a differential operator analytically is impossible for many equations and often requires ingenuity when it is, *applying* one is a plug-and-chug application of algebra and calculus. Of course, it is necessary to construct  $u$  and any coefficient functions in  $D$  from simple, differentiable and integrable functions.

Also,  $u$  must satisfy any constraints imposed by the algorithm such as hard-coded boundary conditions or acceptable coefficient ranges. Finally, the chosen functions should have small derivatives so that convergence can be achieved for reasonable grid sizes. Since these functions may need to be fairly complicated in order to achieve full generality while meeting the necessary constraints, it is advisable to use a *Computer Algebra System* (CAS) such as the Python package Sympy [24] to symbolically compute the source term.

### 5.3.1 Discretization Error Analysis

Once an exact solution is known, code verification is performed by demonstrating that the discretization error of the code matches the theoretical order of accuracy of the algorithm. Numerical calculations are computed on a sequence of discrete grids from coarse to fine, and errors are calculated by evaluating the exact solution pointwise. Then, the norm of the discretization error is calculated for each grid. To verify an algorithm of order  $p$  with grid resolution  $h$ , it should be shown that the norm of the pointwise error is approximately proportional to  $h^p$ .

This behavior is observed only when the grid spacing is within a neighborhood of zero called the *asymptotic range* [33] (a.k.a. “the sweet spot”). Outside of this neighborhood, order  $p$  convergence may not be observed even in a correct implementation since higher order error terms will overpower the order  $p$  term. If the observed convergence order does not match the theoretical order, it is either because a coding mistake is present or the asymptotic range has not been achieved [34].

### 5.3.2 Synthetic Data

In order to perform code verification for the radiative transfer equation, a manufactured solution  $L(\mathbf{x}, \boldsymbol{\omega})$  for radiance, as well as coefficient functions for the absorption coefficient  $a(\mathbf{x})$  and volume scattering function  $\beta(\boldsymbol{\omega} \cdot \boldsymbol{\omega}')$ , must be chosen *a priori*. Together, the chosen solution and coefficient functions are referred to as *synthetic data*. The code developed for this thesis imposes the following conditions on the manufactured solution:

1. Periodic solution and absorption coefficient in  $x$  and  $y$
2. Positive solution and absorption coefficient
3. Position-independent surface downwelling boundary condition
4. Zero upwelling radiance at the bottom boundary
5. Properly normalized VSF  $\beta(\Delta)$ , as described in Section 3.1.3

The actual expressions chosen for the synthetic data are quite unwieldy, and are listed in full in Appendix C.

### 5.3.3 Finite Difference Verification

Since second order finite difference formulas are used, once the asymptotic range for grid spacing has been achieved, decreasing it further should result in the discretization error approaching zero quadratically. The radiative transfer equation involves five discretized variables:  $(x, y, x, \theta, \phi)$ . A five dimensional resolution space is nontrivial to characterize, so we define the generic spatial and angular grid sizes  $n_s = n_x = n_y = n_z$  and  $n_a = n_\theta = n_\phi$  for the sake of reducing dimensionality. Then, we use the geometric mean to describe the spatial and angular resolution, as

$$ds = (dx dy dz)^{1/3}, \quad (5.3)$$

$$da = (d\theta d\phi)^{1/2}. \quad (5.4)$$

This reduces the dimensionality of the resolution space to two, but it would be preferable to deal only with a single variable. Therefore, the finite difference verification is performed by holding  $n_a = 8$ , and varying  $n_s$  between 4 and 64. As shown in Figure 5.1, second order convergence is observed, demonstrating that the code is free of coding mistakes affecting the convergence properties of the algorithm.

### 5.3.4 Numerical Asymptotics Verification

For the numerical asymptotics algorithm, both discretization error and truncation error are present. Therefore, the solutions are not expected to converge to the true solution by increasing the grid size. Neither is it guaranteed that increasing the number of terms will lead to convergence to the true solution. However, since the  $n$  term asymptotic solution is a numerical approximation to the  $n$  term Taylor series,

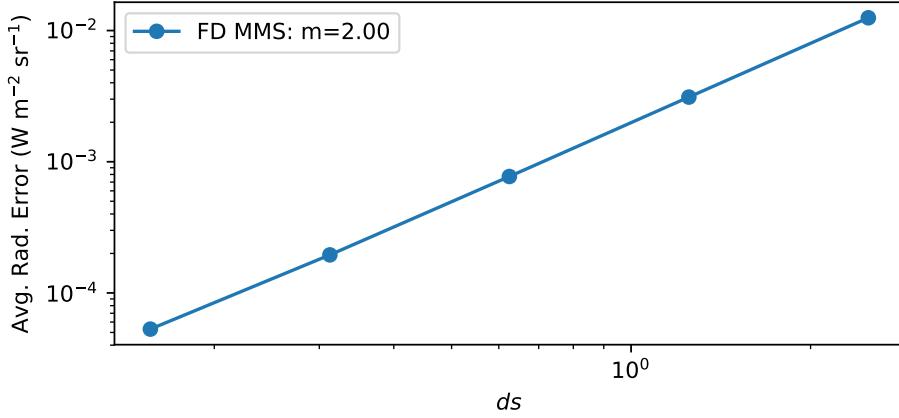


Figure 5.1: Code verification for the finite difference solution. Each point represents the same simulation run with a different spatial grid sizes, with the angular grid held constant at  $n_a = 8$ . A slope of  $m = 2$  on a log-log scale demonstrates second order convergence, as expected, demonstrating the correctness of the code.

the norm of the pointwise error should decrease with order  $n + 1$  as  $b \rightarrow 0$ . As with discretization error, this can only be observed within some asymptotic range of small  $b$  values since higher order error terms dominate the truncation error for large values of  $b$ . However, once  $b$  is sufficiently small, the truncation error is smaller than the discretization error, and no further improvement results from decreasing  $b$  further.

Figure 5.2 demonstrates the convergence of the asymptotic solution as  $b \rightarrow 0$ . The first three approximations are reasonably close, demonstrating order  $n + 1$  convergence, but the  $n = 3$  approximation converges slower than expected. It is unclear whether this is due to a coding mistake, the effect of discretization error, or if there is another cause for the sub-optimal convergence.

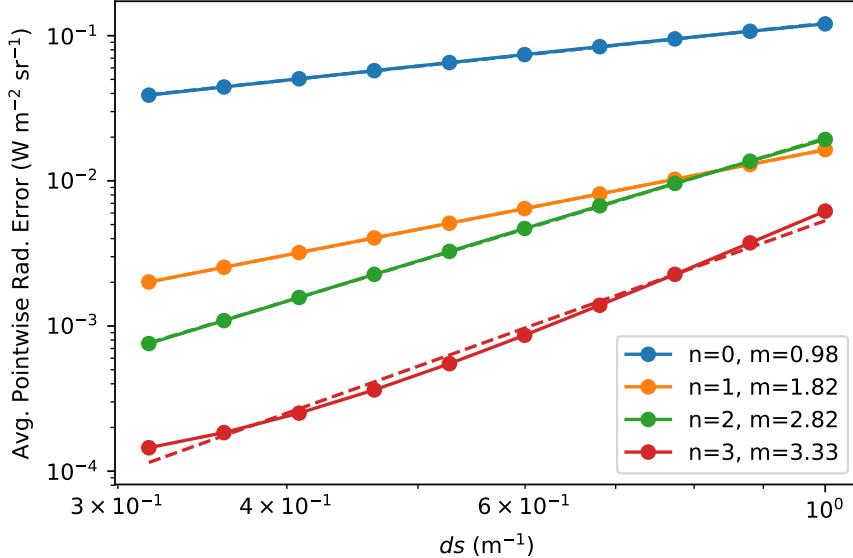


Figure 5.2: Code verification for the numerical asymptotics solution via the Method of Manufactured Solutions. A range of  $b$  values are run, using 0–3 terms in the asymptotic series. The legend shows the number of terms ( $n$ ) and the observed convergence order ( $m$ ) for each solution.

#### 5.4 Verification of Calculations

As mentioned in Section 5.2, numerical error can be estimated for realistic simulations for cases when the exact solution is not known by analyzing the convergence of a scalar functional of the numerical solution over several grid sizes. This type of error reporting is crucial for accurately communicating the trustworthiness of simulation results, and has long been a common requirement for journals in some computational fields such as computational fluid dynamics (CFD) [38].

### 5.4.1 Richardson Extrapolation

Richardson extrapolation is a technique for estimating the continuum value of a scalar functional derived from a solution to a differential equation by using values of the scalar obtained from numerical solutions on several different grids. The technique was developed by Richardson in 1912 with an application paper [32] related to a stresses on a dam, and is also known as  $h^2$  extrapolation since it was originally applied to a second order method. The basic concept is as follows.

Let the scalar of interest be called  $\phi$  and the grid spacing  $h$ . Denote the exact solution as

$$\phi_e = \lim_{h \rightarrow 0} \phi(h),$$

The crux of the technique is to assume that discretization error can be written as a linear combination of powers of  $h$ , as in a Taylor series. That is,

$$\phi - \phi_e = g_0 + g_1 h + g_2 h^2 + g_3 h^3 + \dots . \quad (5.5)$$

Assuming that a second order numerical method is used, the first two terms on the right hand side are zero. For a first order method, only the first term is necessarily zero. Of course, in a “zeroth order” method, the absolute error is bounded from below by  $|g_0|$ , and so does not approach zero as the grid is refined. “Zeroth order” methods are also known as “incorrect.”

The original technique involves numerical solutions on two grids with spacings  $h_1 < h_2$  (i.e., grid 1 is finer), from which scalars  $\phi_1$  and  $\phi_2$  are calculated. The

ratio  $r = h_2/h_1$  is called the grid refinement ratio. Then,

$$\phi_1 = \phi_e + g_2 h_1^2 + O(h^3),$$

$$\phi_2 = \phi_e + g_2 h_2^2 + O(h^3).$$

Solving for  $g_2$  yields

$$g_2 = \frac{\phi_1 - \phi_e}{h_1^2} + O(h^3),$$

so

$$\begin{aligned}\phi_1 &= \phi_e + \frac{h_2^2}{h_1^2}(\phi_1 - \phi_e) + O(h^3) \\ &= \phi_e + r^2(\phi_1 - \phi_e) + O(h^3) \\ &= \phi_e(1 - r^2) + \phi_1 r^2 + O(h^3).\end{aligned}$$

Hence, the approximate continuum solution is

$$\phi_e = \frac{\phi_2 - \phi_1 r^2}{1 - r^2} + O(h^3).$$

In essence, Richardson extrapolation allows for  $\phi$  values from two solutions from an order  $h^p$  numerical method to be combined to produce an approximation of order  $h^{p+1}$  to the continuum value of  $\phi$ .

#### 5.4.2 Generalized Richardson Extrapolation

Of course, the above equations are only approximations. In reality, higher order terms introduce noise which may distort the extrapolated value when only two grid sizes are used. In order to reduce this noise, the concept can be easily generalized to

incorporate more than two numerical solutions, as follows. From

$$\phi \approx \phi_e + g_2 h^2,$$

it is clear that  $\phi$  is approximately linear in  $h^2$ . Therefore, a simple linear fit through multiple points in  $(h^2, \phi)$  space yields  $\phi_e$  as the  $\phi$ -intercept. The slope,  $g_2$ , can be discarded. If significant noise due to outliers still distorts the extrapolated values during fitting, a robust fitting algorithm such as Huber [48] or Ridge [18] regression can help reduce the influence of outliers.

Additionally, this take on Richardson extrapolation is trivially applied to multiple dimensions. For a grid which has several resolution parameters  $h_1, h_2, \dots, h_n$  (e.g. multiple spatial dimensions, or spatial and angular grid resolutions), if the algorithm is second-order in each resolution parameter, then

$$\phi \approx \phi_e + g_{21} h_1^2 + g_{22} h_2^2 + \dots + g_{2n} h_n^2.$$

Hence, fitting a hyper-plane through several points in  $(h_1^2, h_2^2, \dots, h_n^2, \phi)$  space similarly produces  $\phi_e$  as the  $\phi$  intercept.

## CHAPTER VI

### PRACTICAL APPLICATION

This chapter deals with practical considerations when applying the previously discussed numerical algorithms to simulate the light field for realistic scenarios of kelp growing in ocean waters. In this chapter, the spatial kelp distribution model of Chapter II and the light model of Chapter III are implemented as described in Chapter IV and verified in Chapter V and applied to a realistic scenario.

The computational code must be supplied with appropriate physical parameters to emulate the particular seaweed under consideration and the optical properties of the surrounding aquatic medium. Further, the choice of algorithm between numerical asymptotics and finite difference must be made, and algorithm-specific parameters must be chosen, based on the physical situation under consideration, the computational resources available, and the desired level of accuracy in the computed light field.

Guidelines are presented in this chapter to aid the user in making these decisions, and the performance of the model is discussed. Finally, comparison is made to simpler light models, and specific differences are noted. With all of this information, a potential user may decide if and how to use the three-dimensional light model presented in this thesis.

## 6.1 Physical Parameters

In this section, physical model parameters are discussed. The primary use-case for the present model is that it is run in conjunction with a kelp growth model and ocean model which call it periodically to update the light field. In that case, those models will provide some of the necessary parameters such as the size of the kelp fronds, optical properties of the aquatic medium, and current speed as functions of depth. If the light model is run without kelp growth and ocean models, as is the case for the results in this chapter, then these parameters must be hand-picked to represent a realistic situation of interest. Other parameters external to the kelp growth and ocean models can be found in the literature, as summarized in Table 6.1 and Table 6.2. Still, some parameters remain which are not well described in the literature. In such cases, rough estimates are given or their experimental determination is discussed.

### 6.1.1 Parameters from Literature

Given here is a table of parameter values found in the literature which are used in the following sections to test this light model under realistic conditions. A few comments are in order. No values were available for the absorptance of *Saccharina latissima*, but a value for *Macrocystis pyrifera* was found. The surface irradiance from [8] was given in terms of photons per second, and was converted to  $\text{W m}^{-2}$  according to the approximate relationship in Equation (3.1).

In [31], detailed measurements of optical properties in various ocean waters are presented. A few of those measurements are reproduced here, using the same

Table 6.1: Physical parameter values.

Parameter Name	Symbol	Value(s)	Citation
Kelp absorptance	$A_k$	0.8	[13]
Water absorption coefficient	$a_w$	See Table 6.2	[31]
Scattering coefficient	$b$	See Table 6.2	[31]
Volume scattering function	$\beta$	tabulated	[31, 42]
Frond thickness	$f_t$	0.4 mm	[15]
Frond aspect ratio	$f_r$	5.0	[15]
Frond shape parameter	$f_s$	0.5	estimated
Surface solar irradiance	$I_0$	50 W m <sup>-2</sup>	[8]

site names as in the original report. There are three categories of water provided: AUTEC is from Tongue of the Ocean, Bahama Islands, and represents clear, pure water; HAOCE is from offshore southern California, and represents a more average coastal region, likely the most similar to water where kelp cultivation would occur; NUC data is from the San Diego Harbor, and represents turbid water, likely more so than one would expect to find in a seaweed farm. These values give a sense for the range of absorption and scattering coefficients that the model should be tested against. Aside from absorption and scattering coefficients, detailed tabulations of volume scattering functions are also given in [31]. While a simpler linear model is

used for the simulations in this thesis, it is recommended that future simulations interpolate the tabulated VSF from [31].

Table 6.2: Field measurement data of optical properties in the ocean [31]. The site names used in the original paper are used. AUTEC: Bahamas; HAOCE: Coastal southern California; NUC: San Diego Harbor. Absorption, scattering, and total attenuation coefficients ( $a$ ,  $b$ , and  $c = a + b$ ) and their ratios are given.

Site	$a(\text{m}^{-1})$	$b(\text{m}^{-1})$	$c(\text{m}^{-1})$	$a/c$	$b/c$
AUTEC 8	0.114	0.037	0.151	0.753	0.247
HAOCE 11	0.179	0.219	0.398	0.449	0.551
NUC 2200	0.337	1.583	1.92	0.176	0.824
NUC 2240	0.125	1.205	1.33	0.094	0.906

### 6.1.2 Frond Alignment Coefficient

The *frond alignment coefficient*,  $\eta$ , describes the dependence of frond alignment on current speed, as mentioned in Section 2.3.2. To the author's knowledge, no such parameter is available in the literature. However, similar measurements have been made in the MACROSEA project by Norvik [28] to describe the dependence of the elevation angle of the frond as a function of current speed. In that study, artificial seaweed was designed, suitable for use in fresh water laboratory flumes without

fear of degradation. Using those synthetic kelp fronds, one could perform a simple experiment to determine the frond alignment coefficient, sketched here.

Fix a taught vertical rope or rod in the center of a flume, and attach the fronds to it with a short string which acts as the stipe. To emulate the holdfast, the string should be tied tightly around the vertical rope or rod so as to prevent it from rotating at its attachment point, giving the frond a preferred orientation from which it has to bend. The preferred directions should be more or less evenly distributed. A camera should be mounted directly over the vertical rope, pointed straight down. If possible, a fluorescent dye could be applied to the tip of each frond to make their orientations more easily discernible in the recording. Turn on the flume to several current speeds, recording a video or many snapshots for each. If the fluorescent dye is applied, then a simple peak-finding image processing algorithm can be applied to locate the frond tips. By preprocessing the image to a gray scale such that the color of the dye has the highest intensity, the tip locations are located at local maxima.

Once the tip locations are determined, the azimuthal orientations can be calculated relative to the vertical line. Data from all snapshots for the same current speed can be combined, and a von Mises distribution can be fitted to the combined data, noting the best fit values of  $\mu$  and  $\kappa$ . Presumably, the best fit  $\mu$  will be in the direction of current flow. After repeating the procedure for several current speeds,  $\kappa$  can be plotted as a function of current speed. Then, an optimal value for the frond alignment coefficient  $\eta$  can be found by fitting  $\kappa = \eta\mu$  to the data. It may, of course,

turn out that this simple linear relationship does not hold, in which case a more appropriate description can be determined.

### 6.1.3 Simulation Context

In the case that the model is called by time-dependent kelp growth and ocean models, certain parameters can be passed as arguments to the light calculation subroutines to inform them of the encompassing context. Specifically, the ocean model can provide current speed and direction over depth, which is used in calculating the kelp distribution. The position of the sun and irradiance just below the surface of the water can also be provided by the ocean model, which is used to generate the surface radiance boundary condition. The ocean model should also provide an absorption coefficient for each depth layer, which may vary due to nutrient concentrations and biological specimens such as phytoplankton. The kelp growth model is expected to provide super-individual data describing the population in each depth layer. Then, Equations (4.1) and (4.2) are used to calculate length and orientation distributions, as described in Section 4.2.1.

Presumably, the ocean model uses a spatial grid much coarser than the grid required for the light model. For example, SINMOD [45] uses a minimum horizontal spatial resolution of 32 m, whereas a grid resolution on the order of centimeters is more appropriate for the light model. While the vertical resolution of the encompassing simulation is probably finer than the horizontal resolution, it may also not be sufficiently fine to use for light field calculations. Assuming that this is the case,

the depth-dependent quantities provided by the encompassing simulations are to be interpolated at the appropriate depths for the light model grid.

While it is reasonable for the ocean model to inform the light model of the surface irradiance and position of the sun, it is unlikely that a full angular radiance distribution is given. Therefore, a simplistic model is used which assigns the highest radiance value to the direction of the sun and lower values to other directions according to the difference in angle, while preserving the total irradiance from the surface. Specifically, the surface boundary condition used is

$$f(\boldsymbol{\omega}) = I_0 \frac{\exp(-D_s \cos^{-1}(\boldsymbol{\omega}_s \cdot \boldsymbol{\omega}))}{\int_{2\pi} \exp(-D_s \cos^{-1}(\boldsymbol{\omega}_s \cdot \boldsymbol{\omega})) d\boldsymbol{\omega}}, \quad (6.1)$$

where  $\boldsymbol{\omega}_s$  is the propagation direction of the sun's rays and  $D_s \in [0, \infty)$  (units  $\text{rad}^{-1}$ ) varies the sharpness of the angular distribution of surface radiance. When  $D_s = 0$ , the distribution is totally flat, while as  $D_s \rightarrow \infty$ , the distribution approaches a delta function. This can be considered a coarse description of the amount of scattering in the atmosphere, since light arrives at Earth nearly all from a single direction. A value of  $D_s = 1 \text{ rad}^{-1}$  is used for the simulations in this chapter.

#### 6.1.4 Standalone Context

The simulation results shown in the later sections of this chapter probe the light model in various ways independent of any encompassing kelp growth or ocean models, and therefore the physical parameters that they would supply must be hand-picked to represent a realistic scenario to which the light model may be applied. Therefore, the following parameter choices are made.

The depth-dependent mean kelp frond length is chosen to be

$$\mu_l(z) = l_{\max} \frac{3z^2 \exp(-z) + 1/2}{12 \exp(-2) + 1/2}, \quad (6.2)$$

which has a local maximum of  $\mu_l(2) = l_{\max}$ . The value  $l_{\max} = 6\text{ m}$  is used for the sake of agreement with [28], and the vertical number density of fronds is taken to be  $\rho_n = 120$  individuals per meter, as in [8]. The kelp frond length standard deviations are chosen to be the constant function  $\sigma_l(z) = 1\text{ m}$ . The periodic horizontal domain is  $10\text{ m} \times 10\text{ m}$ , yielding a horizontal rope density of  $D = 0.01\text{ ropes/m}^2$ . Also, the current angles are held constant over depth at  $\theta_w(z) = 0$ , as is the current speed  $v_w = 1\text{ m s}^{-1}$  with  $\eta = 1\text{ s m}^{-1}$ . For the light field,  $\omega_s = \hat{z}$  (sunlight from directly above) and  $D_s = 1\text{ rad}^{-1}$  are used.

## 6.2 Computational Expense

The choice of finite difference or numerical asymptotics and the specific parameters of each has a significant impact on both computation time and solution accuracy. The impact of the choice of algorithm and parameters on both factors is explored in this section in order to aid the reader in making these decisions.

### 6.2.1 CPU Time

Computation time is a significant consideration, especially when using the light model in the context of a time-dependent kelp growth simulation where it will be called repeatedly. The computational demand can be lessened by updating the light model only a few times per day rather than every time step. Still, accuracy must be

balanced with reasonable resource consumption. If the light model is taking as much time as all of the other aspects combined, any accuracy gained from the light field computation is likely being lost elsewhere in the model.

Also, both algorithms are parallelized using OpenMP [23], so increasing the parallelism decreases the computation time, though it does not reduce the overall resource consumption. Further, some sections of the code are necessarily serial, which reduces the effective parallelism to some degree. When using 8 threads, an average CPU usage of about 7 cores is observed over the course of the entire computation, while for 32 threads, it is around 22. The parallel efficiency decreases as thread count increases because the serial sections bias the average parallelism downward. This is not intended to discourage parallelism, only to represent it accurately; in reality, the speedup is quite noticeable when the thread count is increased.

The choice of algorithm has a significant impact on computation time. The finite difference method relies on an iterative method for solving the linear system. It runs until an error criterion is satisfied, and therefore the exact number of computations is not known ahead of time. On the other hand, the numerical asymptotics algorithm is a direct method that performs a predetermined number of calculations. The computation time of the latter is therefore more predictable.

When using the numerical asymptotics algorithm, the number of terms used in the asymptotic series has a definite impact on computation time. The leading order term involves fewer calculations than the rest since no scattering integration is performed, though the difference is minor. The following terms, however, perform an

identical number of calculations. Therefore, the  $n$  term approximation takes about  $n$  times as long as the leading order (no-scattering) approximation. Figure 6.1 shows CPU time for 32 cores for both asymptotics and finite difference for five spatial grids.

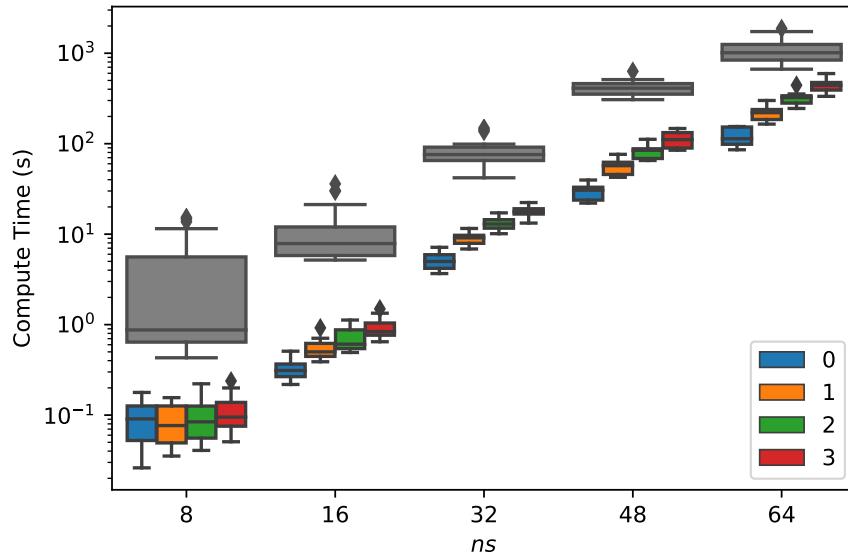


Figure 6.1: Computation time required for numerical asymptotics and finite difference algorithms over a range of spatial grid sizes using  $n_a = 10$  and 32 CPUs. Only five grid sizes are shown, with the finite difference shown in gray and numerical asymptotic algorithm for  $n = 0, \dots, 3$  terms in color for each grid. The horizontal offset within each grid size is only for visual clarity. Note the large range in compute times—small simulations take fractions of a second while large grids take upwards of a half-hour.

### 6.2.2 Memory Usage

Memory usage is perhaps the most important consideration when choosing the algorithm and grid size. While the numerical asymptotics algorithm requires only a few multiples of the memory required to store the radiance itself, the finite difference algorithm requires the generation and storage of a coefficient matrix several orders of magnitude larger than the solution vector. These memory requirements are given for a combination of spatial and angular grid sizes in Table D.1. It is worth noting that using several terms from the asymptotic series does not increase the memory usage, as the same arrays are reused between iterations.

Furthermore, the actual iterative solution of the matrix equation requires the allocation of several multiples of that amount of memory. A good approximation of the memory required to solve the linear system with GMRES (restarted every 100 iterations) is five times the memory required to store the coefficient matrix. Even for large grids, the numerical asymptotics approach has not been observed to use more than five gigabytes of memory, which is well within the memory capacity of a common modern laptop or workstation. On the other hand, the finite difference algorithm uses enormous amounts of memory, from tens of gigabytes for small to medium grids to hundreds of gigabytes for large grids. These estimates are plotted in Figure 6.2, and listed numerically in Table D.2.

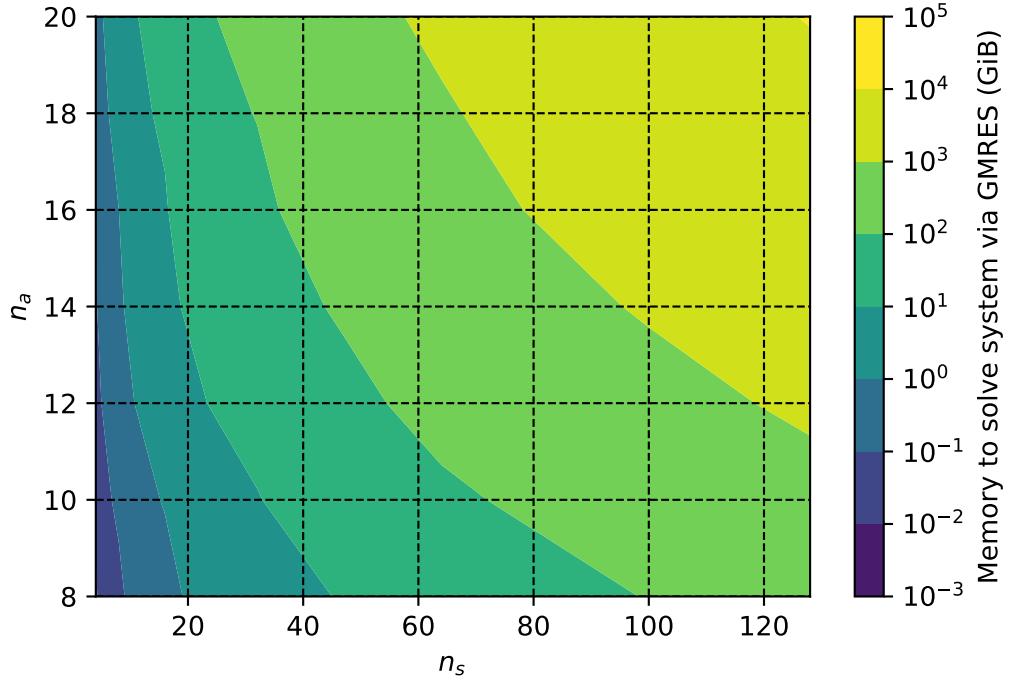


Figure 6.2: Estimated memory required to solve the linear system of equations for the finite difference algorithm using GMRES, restarted every 100 iterations. Table D.2 contains the same data in text form.

### 6.3 Grid Size and Discretization Error

The size of the spatial-angular grid is an important choice that must be made in order to balance numerical accuracy with computational cost. Since both the numerical asymptotics and finite difference algorithms are second order methods, the discretization error is proportional to the square of the grid spacing, in both the spatial and angular domains. In this section, a realistic simulation (as described in

Section 6.1.4) is performed on many grids, and the discretization error of each is estimated via Richardson Extrapolation, as described in Section 5.4.2. These error estimates allow the spatial and angular components of discretization to be isolated; rules of thumb for both grid spacings are enabled by this analysis.

### 6.3.1 Error Estimation

A set of simulations is run for a range of spatial and angular grid sizes with optical properties from Petzold’s coastal California waters (HAOCE11), listed in Table 6.2. Grid sizes of  $n_s = 32, 48, 64, 72$  and  $n_a = 4, 8, 10, 12$  are considered; one simulation is run for every combination of these values. The average irradiance over the whole domain is calculated for each simulation, which is used as the scalar metric for comparing solutions on disparate grids. The average irradiances for each simulation are plotted in Figures 6.3 and 6.4 as functions of the squared grid spacings  $ds^2$  and  $da^2$ , given by Equations (5.3) and (5.4) with  $x_{\max} - x_{\min} = y_{\max} - y_{\min} = 10$  m. All parameters aside from grid resolution are held constant, so discretization error is the only source of variation within each plot.

Notice that in Figure 6.4, the average irradiance is linear in squared grid spacing for each slice in the resolution space. This pattern holds for both the finite difference and numerical asymptotics algorithms, indicating that all of the grid sizes considered are within the asymptotic region of both methods, since the observed convergence order matches the theoretical order. This demonstrates that the aver-

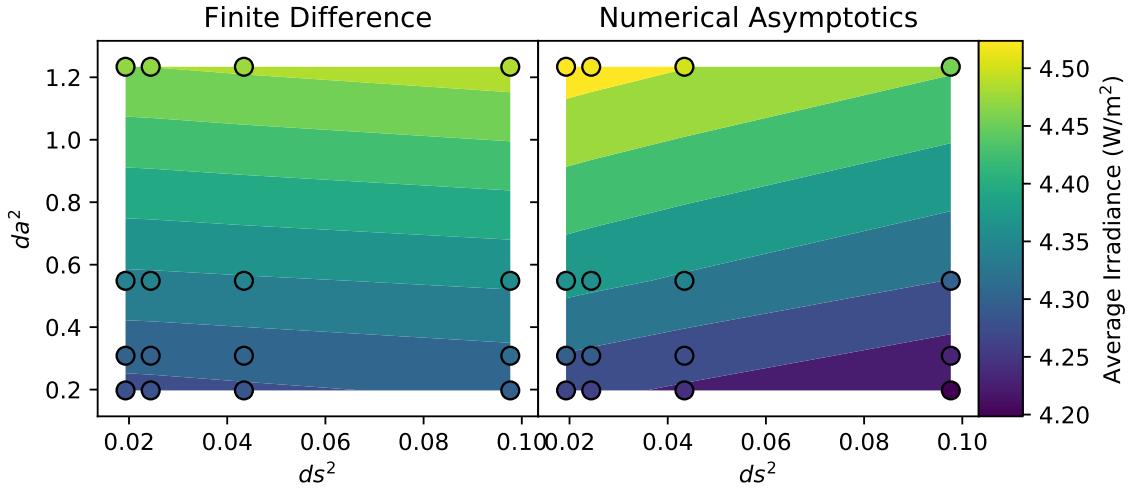


Figure 6.3: Average irradiance plotted against squared resolution for a variety of grid sizes for finite difference and numerical asymptotics with  $n = 0$ . The linear contours demonstrate that both methods are second order in both resolution parameters.

age irradiance is planar over the whole two-dimensional squared-resolution space, as shown by the parallel linear contours in Figure 6.3.

### 6.3.2 Error Prediction

The continuum value for the average irradiance is estimated via Richardson extrapolation by fitting a plane through the scalar irradiances in squared-resolution space, as described in Section 5.4.2. Values from this plane are shown in Figure 6.4 as “x”s plotted under the observed errors, shown with circles. The excellent agreement between the prediction and observation is a testament to the validity of the generalized Richardson extrapolation method in this circumstance.

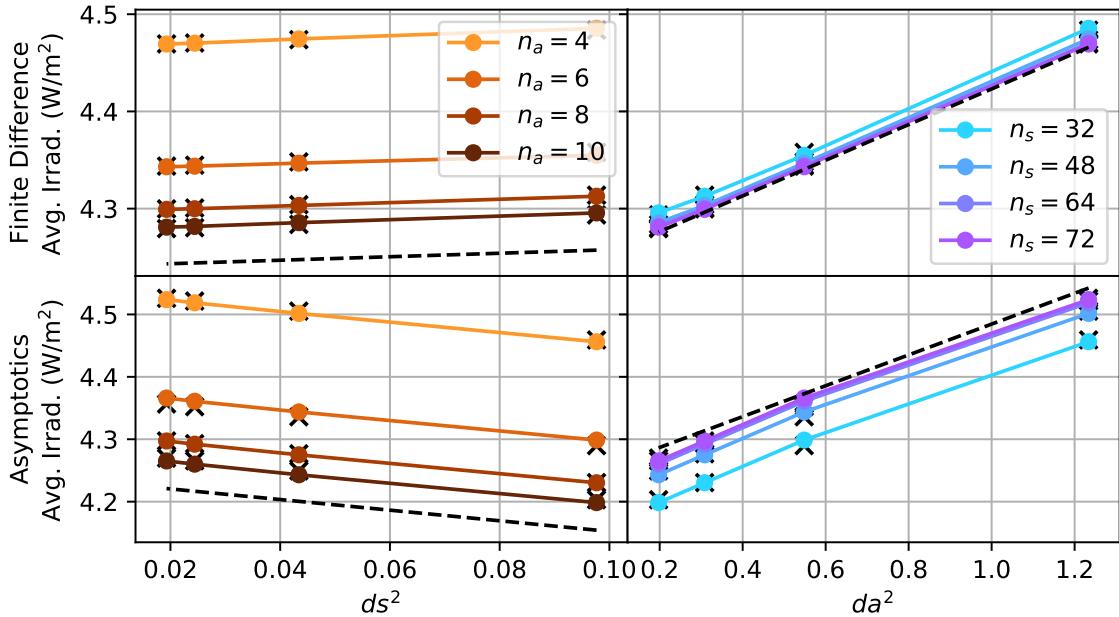


Figure 6.4: Average irradiance versus squared resolution. Each line is a 1D projection from Figure 6.4. Predicted error values are marked with “x”s, and observed error values with circles. Isolated spatial and angular components of discretization error are plotted with a dashed line on the left and right columns respectively.

Specifically, the discretization error for each algorithm is found to be

$$\begin{aligned}\varepsilon_{\text{FD}}(ds, da) &= c_{11}ds^2 + c_{12}da^2, \\ \varepsilon_{\text{asym}}(ds, da) &= c_{21}ds^2 + c_{22}da^2,\end{aligned}\tag{6.3}$$

where

$$\begin{aligned}c_{11} &= 0.180, & C_{12} &= 0.183, \\ c_{21} &= -0.851, & C_{22} &= 0.247.\end{aligned}\tag{6.4}$$

By evaluating this plane at  $ds = 0$ ,  $da = 0$ , the extrapolated continuum value of average irradiance is found. The generalized Richardson extrapolation plane

is shifted down by the continuum value to construct a model to predict discretization error as a function of grid resolution. The intersections of this model plane with the  $ds = 0$  and  $da = 0$  planes are the isolated angular and spatial components of discretization error, respectively. These isolated components of discretization error are shown in Figure 6.5 for both algorithms. This figure allows for quick estimation of the grid size necessary to achieve a given error threshold. The total discretization error for a potential grid can be found by taking the sum of the component errors for the algorithm in question.

For example, take the asymptotics algorithm with the grid  $n_s = 60$ ,  $n_a = 20$ . The asymptotics curves are orange, with the dashed line showing the angular component error and the solid line showing the spatial component. The angular discretization error for this particular grid looks to be about  $2 \times 10^{-1} \text{ W m}^{-2}$ , while the spatial discretization error is about  $3 \times 10^{-2} \text{ W m}^{-2}$ . In this case, the spatial grid is unnecessarily fine, since the angular discretization error dominates by almost an order of magnitude. In general, the components of grid size should be chosen to produce roughly similar discretization errors so as to avoid unnecessary computation.

From the other perspective, consider an overall discretization error criterion of  $\bar{\varepsilon} = 2 \times 10^{-2} \text{ W m}^{-2}$ . This can be achieved by any grid whose spatial and angular error components sum to less than  $\bar{\varepsilon}$ , but for simplicity, set both component thresholds to  $\bar{\varepsilon}_s = \bar{\varepsilon}_a = 1 \times 10^{-2} \text{ W m}^{-2}$ . By visual inspection of Figure 6.5, this seems to suggest  $n_s = 92$ ,  $n_a = 22$  for the asymptotics algorithm, or  $n_s = 42$ ,  $n_a = 20$  for the finite difference algorithm.

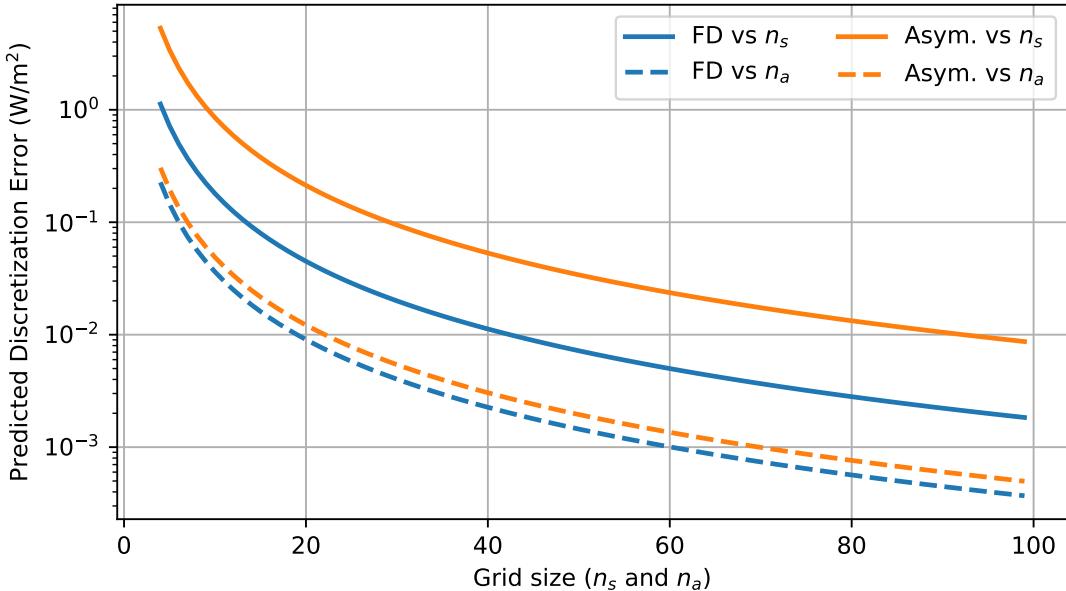


Figure 6.5: Predictions for isolated spatial and angular components of discretization error as a function of grid size for both algorithms. This figure can be used to estimate the grid sizes that each algorithm would require to meet a given error criterion. The total discretization error is the sum of the spatial and angular parts.

It is important to note that the error analysis in this section has been performed for only a single set of optical properties (HAOCE11). Optical properties are sure to have some effect on grid convergence, as they affect the derivatives of the absorption field the solution, thereby impacting the accuracy of quadrature on a particular grid. Furthermore, only  $n = 0$  was tested for the asymptotics algorithm. Discretization may compound for higher-order approximations. Also, keep in mind that  $n_a$  ( $n_\phi$  in particular) must be an even number, as mentioned in Section 4.1.

## 6.4 Optical Conditions for Asymptotics

Since the asymptotic approximation is based on a Taylor series expansion around the case of no scattering, it is only valid for relatively small scattering coefficients. Extremely high-scattering scenarios are out of reach for the asymptotic approximation, and the finite difference approach must be used in those cases. Whereas in low-scattering waters, adding terms to the asymptotic series tends to decrease the error in the solution, in high-scattering situations, adding terms causes the error to diverge. Therefore, if the finite difference solution is out of the question for cases of high scattering, the leading order approximation is the best option. An in-depth analysis of the error incurred by the numerical asymptotics algorithm is presented in this section.

### 6.4.1 Raw Simulation Results

In all of the following results, the properties of the kelp are held constant while the optical properties of the water are varied. Ten values of  $a_w$  are taken at equal intervals on a linear scale from  $0.1 \text{ m}^{-1}$  to  $0.5 \text{ m}^{-1}$  (inclusive), and ten values of  $b$  are taken at even intervals on a log scale from  $0.01 \text{ m}^{-1}$  to  $1.5 \text{ m}^{-1}$  (inclusive). For each set of optical properties, numerical asymptotics is employed with 0, 1, 2, and 3 scattering events, and a finite difference calculation is performed. A spatial-angular grid size of  $72 \times 10$  is used for all calculations. Each asymptotics calculation is compared to the finite difference calculation with the same optical properties, and a pointwise error is calculated. Figure 6.6 shows this type of comparison for a single value of  $a_w$ ,

varying  $b$ . As discussed in Section 5.3.4, the order  $n$  approximation converges with roughly order  $n + 1$ . However, the figure shows that this trend does not continue indefinitely as  $b$  decreases. This is because although truncation error decreases as  $b \rightarrow 0$ , discretization error remains constant. Because of this, no results with this grid size show errors below about  $0.07 \text{ W m}^{-2}$ . Simulations with errors below this threshold are therefore discarded in order to isolate trends in the truncation error.

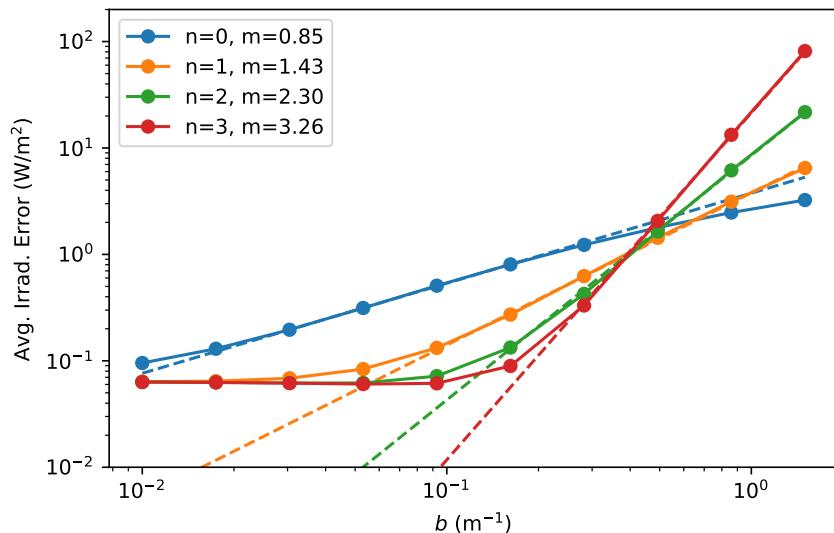


Figure 6.6: Average pointwise difference in irradiance between finite difference and asymptotics solutions for several values of  $b$  and  $n$  with constant  $a = 0.1$  in a realistic kelp scenario using a  $72 \times 10$  grid. Proper convergence of truncation error is observed between  $b = 0.1$  and  $b = 0.6$ . Below  $b = 0.1$ , discretization error dominates. Above  $b = 0.6$ , the asymptotic series diverges.

Figure 6.7 shows a different slice of the simulation results. Here,  $n = 0$  is held constant while  $a_w$  and  $b$  are plotted on the  $x$  and (log)  $y$  axes, with average

error plotted on the (log) color scale. Note that mean error does not depend only on  $b$ . Rather, errors are largest for waters with low absorption and high scattering, and lowest for low scattering, high absorption. The clear pattern in the variation of error over the  $a_w$ - $b$  domain indicates that a third parameter can be calculated from  $a_w$  and  $b$ , which is sufficient to determine the accuracy of the approximation.

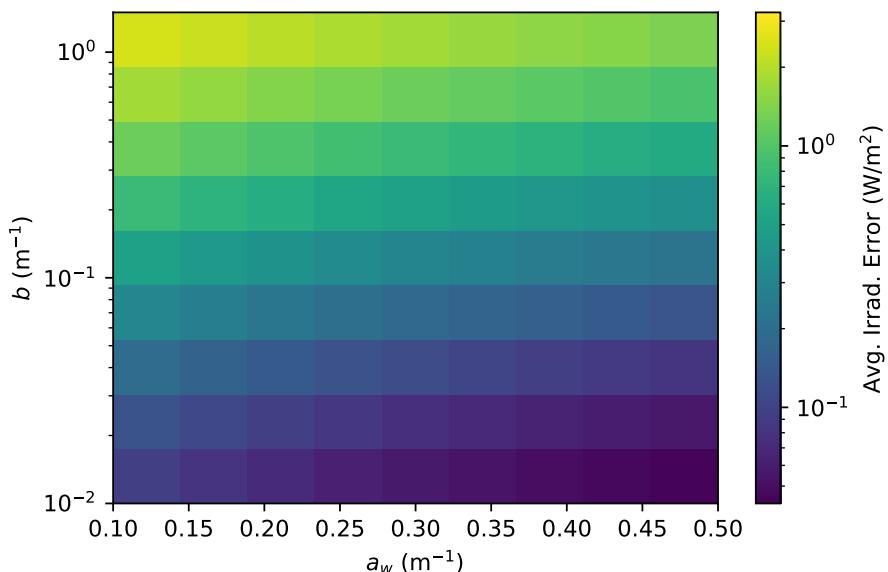


Figure 6.7: Average pointwise difference in irradiance between finite difference and asymptotics solutions for several values of  $b$  and  $a$  with constant  $n = 0$  in a realistic kelp scenario using a  $72 \times 10$  grid. Note that truncation error is smallest for low-scattering, high-absorption cases, and largest for high-scattering, low absorption.

Figure 6.8 shows a similar view of the simulation results as Figure 6.7, except that now, the different approximation orders are considered for each set of optical properties, and the order with the lowest error is found. The order of the best

approximation is shown for each case, and the error incurred by that approximation is shown on the color axis. In the upper left corner, the most difficult cases are shown. In this region, the leading order approximation is most accurate, showing that additional terms cause the solution to diverge. After a brief transition region, the three-term approximation is most accurate, in agreement with Figure 6.6.

Note that for low scattering, high absorption waters where the error is lowest, the  $n = 2$  approximation seems to perform better than  $n = 3$ . As mentioned previously, this is because a lower bound on the total error is imposed by the discretization error, as suggested by Figure 6.6. In fact, the two approximations are nearly identical; the former is only slightly better, and no conclusions about truncation error should be drawn from this part of the figure.

In actual usage, one is concerned not with finding the best approximation, but rather the cheapest one which meets some error threshold. Figure 6.9 shows the smallest value of  $n$  observed to meet discretization error targets of at most  $\bar{\varepsilon} = 1.0 \text{ W m}^{-2}$  and  $\bar{\varepsilon} = 0.1 \text{ W m}^{-2}$  in the left and right columns respectively, with the actual average error incurred shown on the color axis. In both cases, there are some optical properties for which the error threshold cannot be met for any  $n$ . This is represented by an “X” in the figure, and the error of the leading order approximation is shown in color. Note that as  $\bar{\varepsilon}$  is decreased, the error threshold cannot be satisfied for a larger set of optical properties, and where it is achievable, more scattering terms are required.

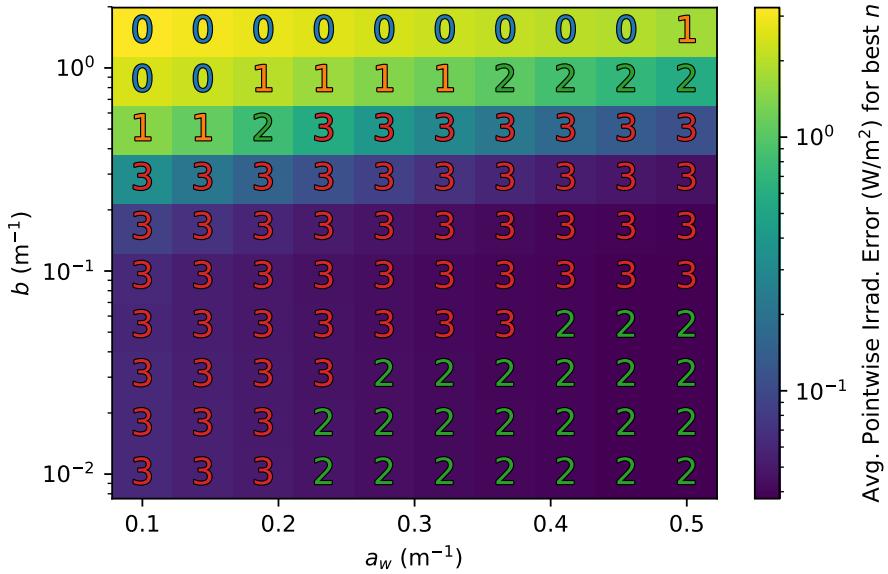


Figure 6.8: The best asymptotics solution for each  $(a_w, b)$ . The value of  $n$  used is written in each cell. For high-scattering cases, the  $n > 0$  terms diverge, so  $n = 0$  is the best approximation. For most cases,  $n = 3$  is the best. For very low-scattering cases, discretization error masks the truncation error trend.

#### 6.4.2 Truncation Error Model

Figure 6.10 concisely represents the simulation results for all optical properties and approximation orders, with error  $\varepsilon$  plotted on the vertical axis and  $b$  plotted on the color axis. In the left column,  $a_w$  is plotted on the horizontal axis. On a log-log scale, the simplicity of the relationship among these three quantities is striking. Holding  $b$  constant, a log-log linear relationship is apparent between the error  $\varepsilon$  and the absorption coefficient  $a_w$ . Meanwhile, holding  $a_w$  constant, log-uniform increases

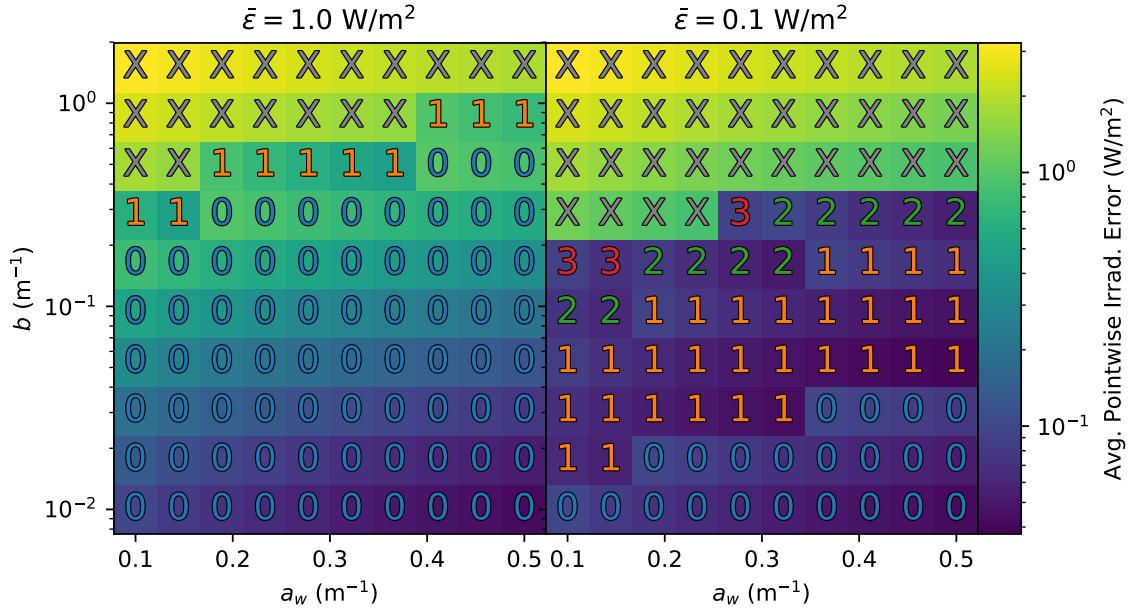


Figure 6.9: For each  $(a_w, b)$ , the smallest value of  $n$  which satisfies the error criterion shown above is printed in the cell. “X” denotes an optical situation in which the criterion cannot be met since adding further terms makes the solution less accurate, not more. As seen on the left, the  $n = 0$  solution usually suffices for moderate error criteria.

in  $b$  cause log-uniform increases in  $\varepsilon$ . That is,  $\ln \varepsilon$  seems to increase linearly with  $\ln b$  and decrease linearly with  $\ln a$ . Restated, it seems that  $\varepsilon \propto b^{d_1} / a_w^{d_2}$ .

Then, by fitting a plane to the observed values in  $(\ln a_w, \ln b, \ln \varepsilon)$  space, a continuous model can be derived for  $\varepsilon(a_w, b)$ . Performing this procedure separately for each  $n$  value yields values of  $d_1$  and  $d_2$  which appear to be independent of  $n$ . Remarkably, the fit for each order of approximation yields  $d_1 = 3/4$ ,  $d_2 = 1/2$  to within a few percent variation. The black “x”s in Figure 6.10 are the predictions of

this model, setting  $d_1 = 3/4$  and  $d_2 = 1/2$  explicitly. The accuracy of the prediction suggests the definition of a third parameter, as mentioned in Section 6.4.1,

$$\xi = \frac{b^{3/4}}{a_w^{1/2}}, \quad (6.5)$$

with the unusual units  $\text{m}^{-1/4}$ . In the right column of Figure 6.10,  $\varepsilon$  is plotted as a function of  $\xi$ . Notice that all of the results collapse onto a single line. Thus, for the sake of understanding the usefulness of the asymptotic series in approximating the true light field,  $\xi$  can be used as a single variable to characterize all waters.

In Figure 6.11,  $\varepsilon$  is plotted as a function of  $\xi$  for all combinations of  $a_w$ ,  $b$ , and  $n$ , effectively combining the right column of Figure 6.10 on a single plot. For each  $n$ , the log-log plot displays a clear linear relationship, similar to the pattern seen previously in Figures 6.6 and 5.2. However, this figure abstracts that pattern over both  $a_w$  and  $b$ , whereas previously it was seen only for  $b$ . Note that the convergence curves for all lines appear to roughly intersect at a characteristic point. That point, denoted  $(\xi^*, \varepsilon^*)$ , represents a bifurcation in the convergence behavior of the numerical asymptotics algorithm. For waters with  $\xi < \xi^*$ , accuracy improves with additional terms, whereas for  $\xi > \xi^*$ , additional terms decrease accuracy.

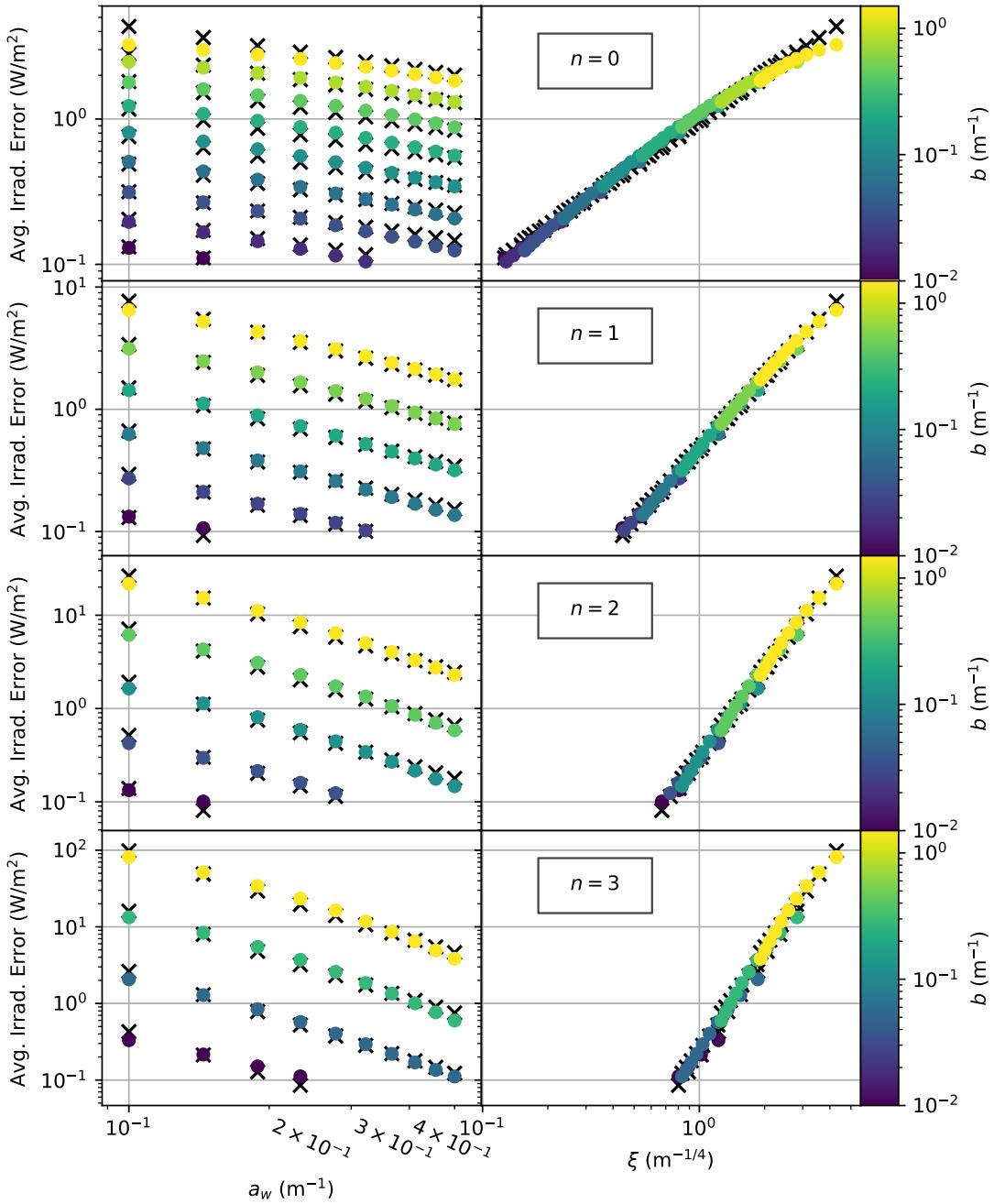


Figure 6.10: Truncation error versus  $a_w$  and  $\xi$  for each  $n$ . Simulations dominated by discretization error have been discarded. The right column shows that  $\xi$  sufficiently characterizes an optical situation for the sake of predicting truncation error of the asymptotic approximation. Errors predicted by Equation (6.7) are marked with “x”s.

In order to systematically determine  $(\xi^*, \varepsilon^*)$ , the log-log convergence curve of order  $n + 1$  is assumed to have slope  $n + 1$ , which is approximately true, at least for  $\xi < \xi^*$ . Further, it is assumed that there is a single point where all of these curves intersect. This point fully specifies the convergence curves, all other free parameters having been eliminated by the previous assumptions. Thus, the error for the order  $n$  approximation is assumed to satisfy

$$\ln(\varepsilon_n(\xi)) - \ln \varepsilon^* = (n + 1)(\ln \xi - \ln \xi^*), \quad (6.6)$$

or equivalently,

$$\varepsilon_n(\xi) = \varepsilon^* \left( \frac{\xi}{\xi^*} \right)^{n+1}. \quad (6.7)$$

Then, a residual function is constructed which accumulates squared differences between the fit functions and their corresponding data points, weighting all squared errors by  $1/\varepsilon$  in order to deem the simulations with lower errors more important since errors diverge for large  $\xi$  values and do not fit the linear function quite as well. A numerical optimization algorithm is then used to search the two dimensional parameter space for the minimizers of the residual, which produces the point  $(\xi^*, \varepsilon^*)$ . This procedure yields the result

$$\xi^* = 1.58 \text{ m}^{-1/4}, \quad (6.8)$$

$$\varepsilon^* = 1.30 \text{ W m}^{-2}, \quad (6.9)$$

as shown in Figure 6.11. Thus, waters characterized below this threshold are worth considering for solution via numerical asymptotics, whereas others are better suited for a finite difference solution.

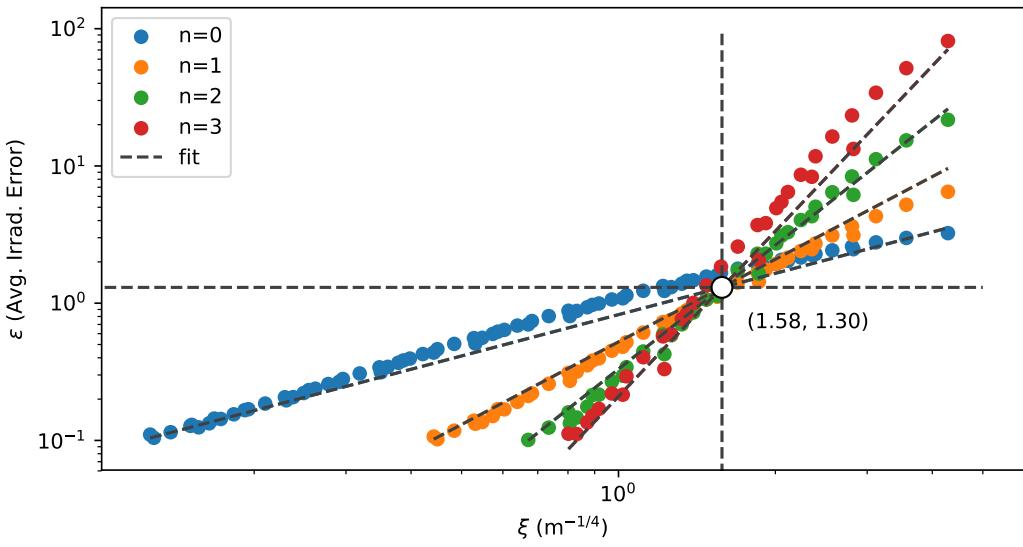


Figure 6.11: All data from the right column of 6.10 on a single plot demonstrates a characteristic  $\xi = \xi^*$  above which the asymptotic series approach is inappropriate. This observation permits a simple model for predicting truncation error.

The determination of  $\xi^*$  and  $\varepsilon^*$  marks the construction of a simple analytical model given by Equation (6.7) which predicts the errors for any set of aquatic optical properties. Figure 6.12 shows the predictions of this model for several values of  $a_w$ ,  $b$ , and  $n$ , with  $\varepsilon$  plotted on the color axis. Note that  $\xi^*$  is a contour in  $(a_w, b)$  space, and is marked on the figure with a dashed white line.  $\xi < \xi^*$  is the region to the lower right of the threshold, and  $\xi > \xi^*$  is the region to the upper left. Also note that this model and its predictions deal only with truncation error, and that discretization error distorts the actual solution accuracy, as seen in Figures 6.6 and 6.8.

This model can now be used to produce general guidelines for the choice of  $n$  given a desired error. Assuming that a maximum error  $\varepsilon = \bar{\varepsilon}$  is permissible, the minimum order of  $n$  which produces  $\varepsilon$  is desired. This order, denoted  $\bar{n}$ , can be determined by solving Equation (6.6) for  $n$  when  $\varepsilon = \bar{\varepsilon}$  and rounding up to the nearest integer. That is,

$$\bar{n} = \text{ceil} \left( \frac{\ln \bar{\varepsilon} - \ln \varepsilon^*}{\ln \xi - \ln \xi^*} - 1 \right),$$

which is equivalent almost everywhere to

$$\bar{n} = \text{floor} \left( \frac{\ln \bar{\varepsilon} - \ln \varepsilon^*}{\ln \xi - \ln \xi^*} \right). \quad (6.10)$$

Figure 6.13 shows  $\bar{n}$  up to  $\bar{n} = 3$  for  $\bar{\varepsilon} = 0.1$ ,  $\bar{\varepsilon} = 0.05$ , and  $\bar{\varepsilon} = 0.01$ . The  $\xi^*$  contour is plotted. Assuming that  $\bar{\varepsilon} < \varepsilon^*$ , if higher contours of  $\bar{n}$  were plotted, they would approach the  $\xi^*$  contour as  $\bar{n} \rightarrow \infty$  since no accuracy better than  $\varepsilon^*$  is achievable by any order approximation when  $\xi > \xi^*$ .

To summarize this analysis, once an error threshold  $\bar{\varepsilon}$  is chosen, the optical properties  $a_w$  and  $b$  determine the optimal numerical approach according to Figure 6.13 and Equation (6.10). If  $\xi^*(a_w, b) > \xi^*$ , then the finite difference algorithm should be used if possible. If memory or computation time requires the numerical asymptotics algorithm to be used, then the  $n = 0$  approximation should be used, effectively ignoring scattering in order to avoid a diverging solution.

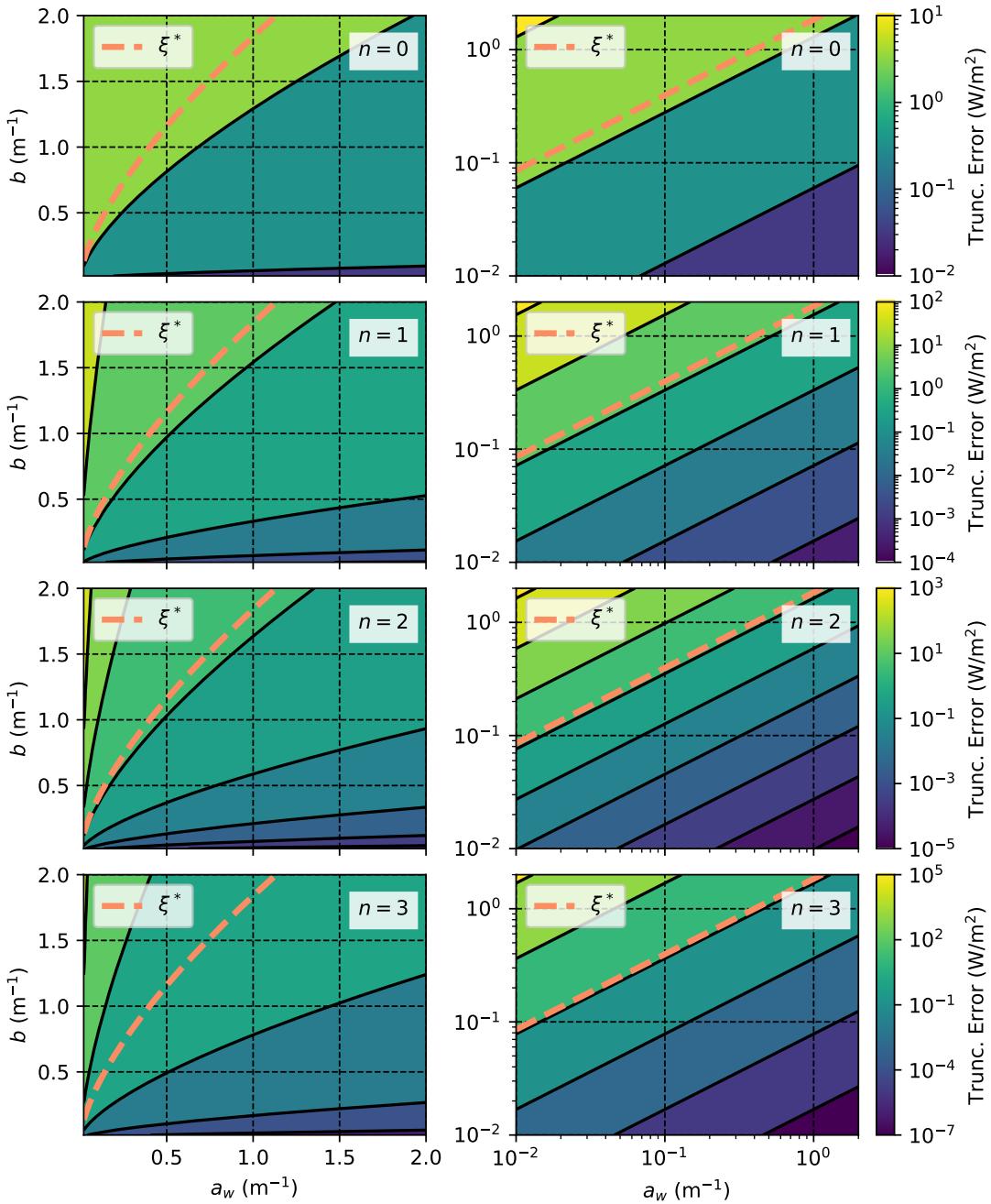


Figure 6.12: Predicted truncation error for a range of  $a_w$  and  $b$  values.  $n$  varies over plot rows. Linear-linear scale on the left, log-log scale on the right. The asymptotic series is appropriate only for  $(a_w, b)$  values to the right of the  $\xi^*$  contour.

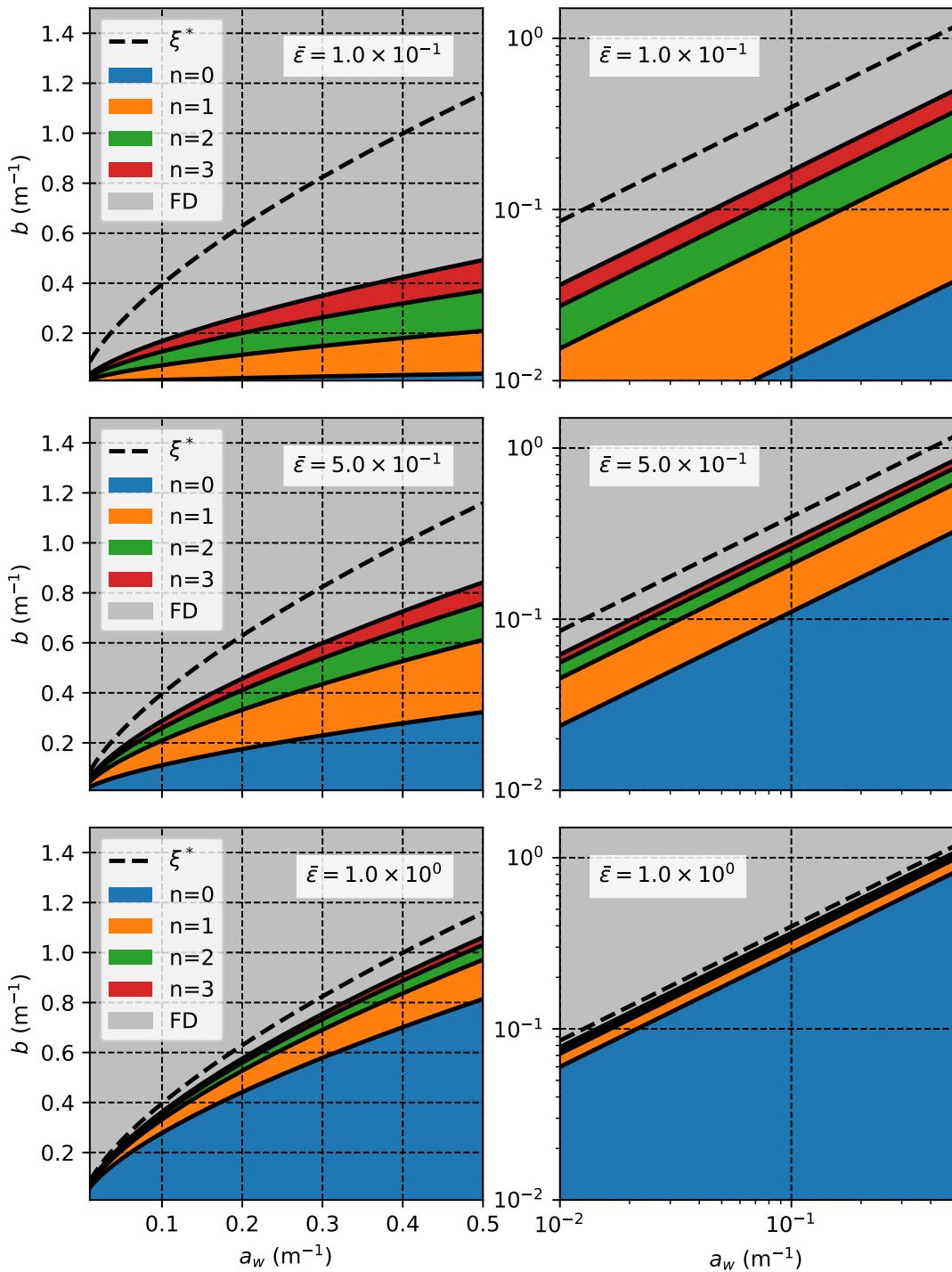


Figure 6.13: Recommended  $n = \bar{n}$  value as a function of  $(a_w, b)$  to achieve the truncation error criteria  $\bar{\varepsilon} = 0.1, 0.5$ , and  $1.0 \text{ W/m}^2$  for the three plot rows.

If  $\bar{n} > 3$  (i.e., the gray region between  $\xi^*$  and  $\bar{n} = 3$ ), it is theoretically possible to achieve the desired accuracy in this region by continuing to add terms, however, this is not recommended since the closer  $\xi$  is to  $\xi^*$ , the more likely it is that higher order terms will cause the solution to diverge due to some unexpected deviation in the actual performance of the algorithm from the theoretical error model presented here. As a compromise,  $n = 2$  or  $n = 3$  could be used in this region to balance the severity of divergence in the case of failure with the improved accuracy of the solution in the case of successful convergence. Finally, in any of the easier regions defined by  $\bar{n} \leq 3$ , the optimal trade-off between accuracy and computation time is achieved by using  $n = \bar{n}(a_w, b)$ .

## 6.5 Comparison to Other Light Models

Now that recommendations have been given for the choice of solution method, with the computational cost and accuracy of each having been discussed, all that remains is to compare the solutions obtained from the model presented in this thesis to other available models for the light field. Two simple models are used; in both cases, the number of calculations can be counted on two hands, whereas the model of this thesis involves many millions of calculations. Whether the insight gained from the more complex model is worth the computational expense depends on the purpose of the calculation, and is a decision for the reader to make according to their best judgment for the situation.

### 6.5.1 Simpler Models

The first model is the simplest conceivable light model—exponential attenuation with a constant absorption coefficient  $a = a_w$ . That is, the simplest solution is to ignore the kelp entirely. Of course, a depth-dependent absorption coefficient is likely to be used in a real simulation, but for the sake of the comparison, a constant  $a_w$  is maintained. The irradiance in this case is simply

$$I(z) = \exp(-a_w z). \quad (6.11)$$

The second light model, presented in [8], accounts for the kelp by adding a depth-dependent term to the absorption coefficient related to the area and spatial density of the seaweed. The model is described by

$$\frac{dI}{dz} = - \left( a_w + k_{\text{kelp}}(z) \right), \quad (6.12)$$

$$k_{\text{kelp}}(z) = - \ln(1 - A_k(1 - (1 - AD)^{\rho_f(z)})), \quad (6.13)$$

where  $A_k = 0.7$  is the kelp absorptance,  $D = 0.01$  ropes/m<sup>2</sup> is the number of vertical kelp ropes per ocean surface area,  $A(z)$  is the average area of the kelp fronds per meter vertical rope, and  $\rho_f = 120$  fronds/m is the number of kelp fronds per vertical meter of rope. Then,

$$D = \frac{1}{(x_{\max} - x_{\min})(y_{\max} - y_{\min})}, \quad (6.14)$$

and the mean frond  $A$  is calculated from the mean frond length according to Equation (2.6) as

$$A = \frac{\mu_l^2}{2f_r}. \quad (6.15)$$

Once  $k_{\text{kelp}}(z)$  is calculated according to Equation (6.13), then the solution of Equation (6.12) is a simplified version of Equation (3.12) with  $\tilde{a}(z) = a_w + k_{\text{kelp}}(z)$  and  $\tilde{\sigma}_0 = 0$ . The solution is therefore the analogous simplification of Equation (3.13), namely

$$I(z) = I_0 \exp \left( -a_w z - \int_0^z k_{\text{kelp}}(z') dz' \right). \quad (6.16)$$

### 6.5.2 Description of Comparison

In Figure 6.15, the light model of this thesis is compared to simpler models under the conditions described in Section 6.1.4 with the optical properties of coastal California (HAOCE11 from Table 6.2). In the figure, the first model described in this chapter, which ignores the kelp entirely, is labeled “No Kelp.” The second model, which uses an additional term in the absorption coefficient to describe the kelp, is labeled “Simple Kelp.” From the 3D model of this thesis, the average irradiance and perceived irradiance calculated from a finite difference solution on a  $72 \times 10$  grid are plotted. As described in Section 3.1.2, the perceived irradiance is a weighted average of the irradiance over the kelp distribution, whereas the average irradiance is weighted evenly over the entire horizontal domain.

Both quantities are plotted with error bands calculated via Richardson extrapolation. The calculation was performed for all combinations of  $n_s = 32, 48, 64, 72$  and  $n_a = 6, 8, 10$ , and the average and perceived irradiances calculated from those solutions were cubically interpolated at many  $z$  values. Then, the standard 2D Richardson extrapolation procedure was applied independently for each  $z$ , using the

interpolated irradiance value at that  $z$  as the scalar to extrapolate, as described in Section 5.4.2. The plotted curves are the irradiances from the  $72 \times 10$  grid. The error bands are three times the estimated error in order to make the estimate conservative, as recommended by [33]. For a detailed procedure for error reporting in numerical simulations, see [1].

### 6.5.3 Comparison: Irradiance Curves

First, note that the no-kelp model predicts the highest light levels throughout the domain, as should be expected since it ignores the dominant source of attenuation. The simple kelp model agrees with the no-kelp model at the surface, but then reduces quickly once the kelp, which has a maximum frond length at  $z = 2$ , becomes sufficiently dense. At the bottom of the domain where there is little kelp remaining, the two curves are seen to be parallel in the log-linear scale, showing that the absorption coefficients are roughly equal, as at the surface. The average irradiance 3D model appears to agree quite well with the simple kelp model, especially near the surface and bottom, where both models are approximately reduced to the first model. In the  $z = 2$  region where the most kelp is present, though, the 3D model predicts higher absorption than the simpler 1D model. However, between  $z = 3$  and  $z = 4$ , the light in the 3D kelp model attenuates more slowly than the 1D model, perhaps because light is able to penetrate the water in regions where the kelp is not present, and the multitude of angles in which the light travels allow some of the rays to reach even the lower depths without being absorbed by the kelp.

The perceived irradiance is clearly much lower than the average irradiance and the other models. This makes sense, as the light is dimmest in the regions of highest kelp density, and the perceived irradiance weights these regions the highest, practically ignoring the edges of the domain where light is absorbed only by the water; these regions skew the average irradiance upward, and are not actually representative of the light field where photosynthesis is occurring. From this point of view, it seems that the other two light models significantly overestimate the amount of light available where it actually of interest.

Note that the 3D model does not predict the lowest light fields everywhere; the average irradiance is observed to be larger than the no-kelp irradiance in the second plot in Figure 6.15. This is due to the effect of scattering shifting light from lower in the domain closer to the surface. This tendency for scattering to insulate the upper region of the water may prove to be important in understanding how photosynthesis near the ocean's surface differs from photosynthesis at depth.

#### 6.5.4 Comparison: Total Radiant Flux

Figure 6.14 shows the total radiant flux in Watts predicted by each model, calculated by integrating each depth-dependent light field over the vertical domain, *weighted by the frond area density* (total frond area per vertical meter). While not exactly analogous, total radiant flux can be regarded as a rough proxy for the amount of photosynthesis occurring in the entire kelp population at all depths. Reducing the entire

light field to an interpretable scalar is quite useful, as it summarizes the magnitude of the difference between the four light models.

The radiant flux predicted by the 3D average irradiance is just 13% of the flux disregarding kelp, and 57% of the simple kelp flux. Meanwhile, the perceived irradiance predicts only 3% the flux of the no-kelp model and 11% the flux of the simple kelp model. Even among the 3D models, using the perceived irradiance predicts 19% the flux of the average irradiance. Calculating the perceived irradiance is possible only because the 3D spatial kelp distribution is known, which is a unique feature of this model. The large degree of these differences in model predictions highlight the importance of considering this spatial distribution.

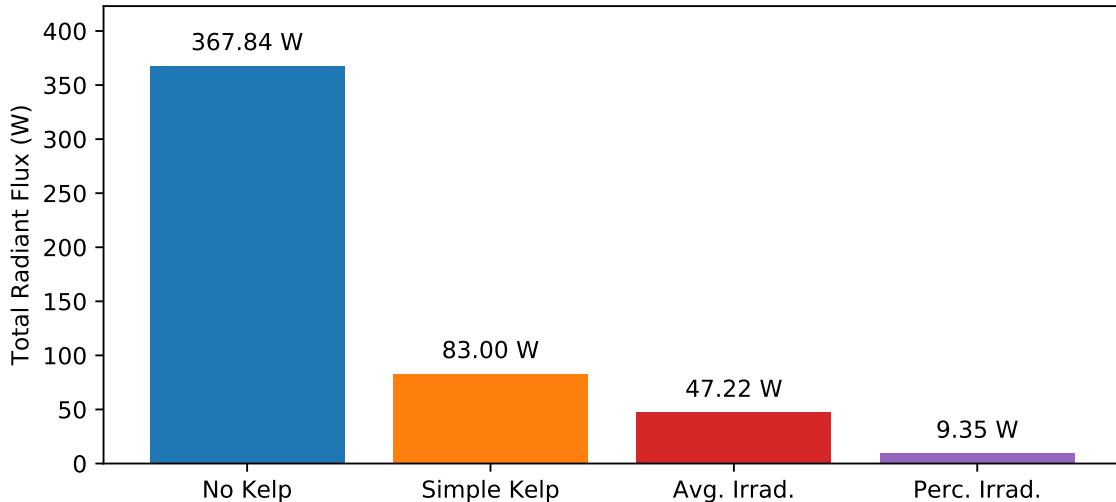


Figure 6.14: Total radiant flux in Watts through kelp predicted by each model. The magnitude of the differences highlight the importance of considering the three-dimensional spatial kelp distribution.

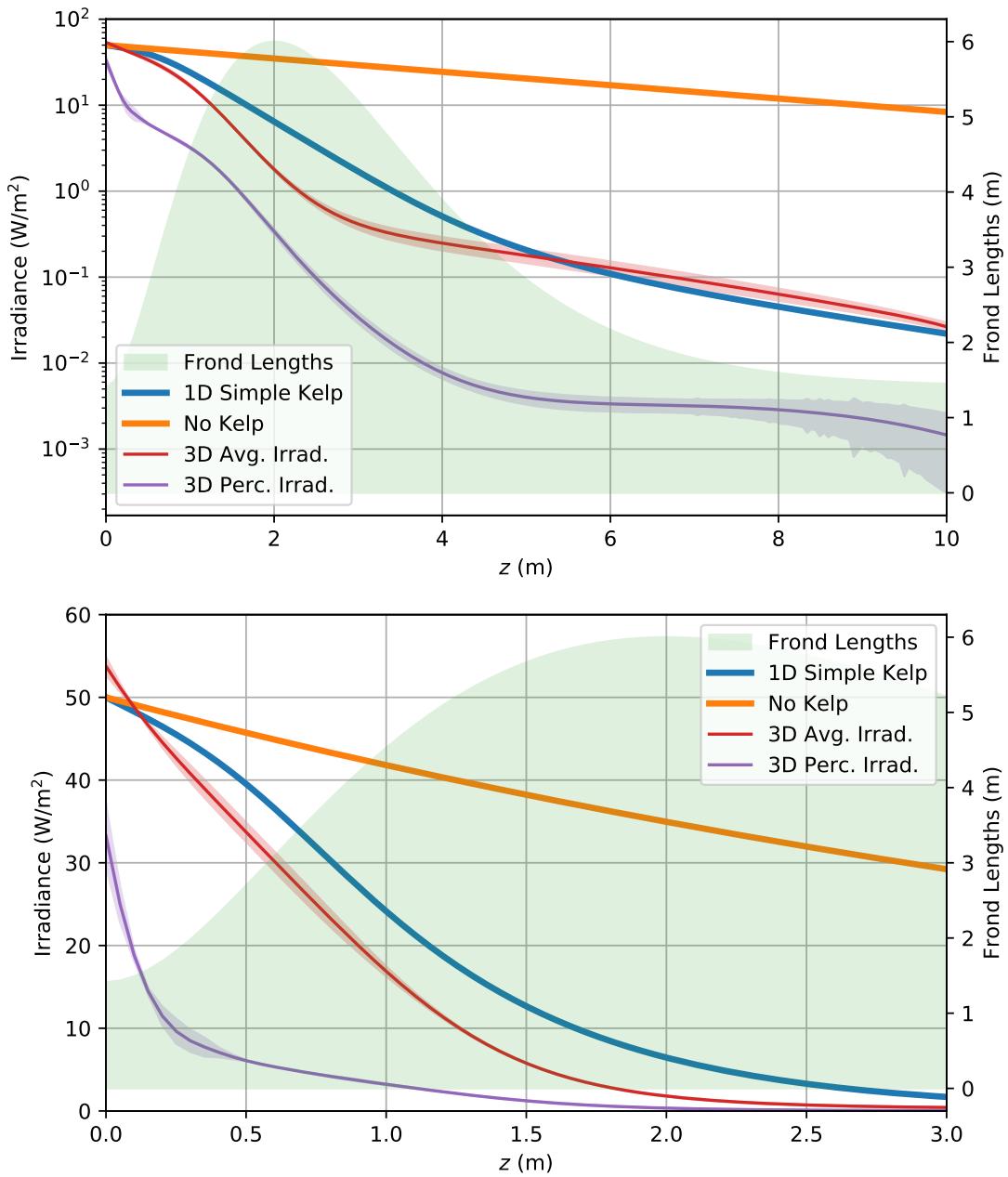


Figure 6.15: Average irradiance and perceived irradiance from finite difference compared to simpler light models for the case of coastal California water (HAOCE11) with realistic kelp growth. Frond lengths over depth are shown on the right-hand axis. Estimated discretization error is shown by error bands for perceived irradiance and average irradiance. Note the different scales in the two plots.

## CHAPTER VII

### CONCLUSION

This thesis presents a model for the light field in a vertical-rope kelp farming operation, emphasizing the effect of the seaweed itself on the overall light field. A three-dimensional model for the spatial distribution of the seaweed is developed, which then informs the absorption field of the combined seaweed-water medium. This absorption field is then used as a coefficient in the monochromatic radiative transfer equation, which calculates the full light field over all positions and angles in the domain, accounting for both attenuation and scattering in the medium.

Two numerical solution techniques are presented: finite difference and numerical asymptotics. The finite difference approach is applicable to any type of water, although it can be prohibitively expensive in terms of CPU time, and even more so in terms of memory usage. On the other hand, the numerical asymptotics algorithm is much cheaper computationally by both measures, though it is only accurate for low-scattering scenarios. Within the appropriate range of optical properties of the aquatic medium, the accuracy and computation time of the solution can be tuned by choosing the number of terms to include in the asymptotic series.

When compared to simpler one-dimensional models for the light field, the model presented in this thesis is found to predict lower light levels. This is expected,

as the full three-dimensional model considers self-shading due to the kelp in greater detail than the others. Further, the average irradiance as a function of depth predicted by the three-dimensional model is found to agree fairly well with a simpler model for kelp shading. However, the average irradiance considers areas of low shading far from the kelp which are irrelevant to photosynthesis. When the light field is examined only in the regions where kelp is actually growing, much less light is predicted. This indicates that simpler models may be overestimating the amount of light available for photosynthesis, which would, in light-limited situations involving high kelp density or low nutrient concentration, predict unrealistically large overall biomass yields in a time-dependent kelp growth simulation.

## 7.1 Model Summary

The following is a summary of the primary assumptions used in the formulation of the model. The assumptions are vast simplifications from the real system, and leave plenty of room for future improvement.

- All fronds in the population are congruent kites of equal, uniform thickness.
- Fronds are perfectly flat and horizontal.
- Fronds emanate from an infinitely thin, perfectly vertical rope, with no stipe.
- Population frond lengths are normally distributed in each depth layer.
- Fronds are oriented according to a von Mises distribution whose sharpness is proportional to current velocity and independent of frond length.

- The absorption coefficient of the aquatic medium depends only on depth.
- All fronds in the population have the same absorptance.
- The scattering coefficient is constant and equal for both kelp and water.
- Only volumetric optical effects, not surface effects, are considered.
- Frequency dependence is neglected.

## 7.2 Future Work

As with any scientific or mathematical investigation, many new opportunities for exploration have arisen from the development of this model, including improvements to the mathematical model itself, improvements to its numerical solution, and its application to answer real-world questions about kelp cultivation. Certainly, the exploration of any of the ideas presented here will lead to many more opportunities for future inquiry and so on *ad infinitum*, as is the nature of knowledge creation.

### 7.2.1 Model Improvements

Many aspects of the model have room for future improvement. The most pressing is probably the development of a model for long-lines, which is more popular in practice than the vertical lines studied here. The implementation of long-lines may prove to be closely related to allowing non-horizontal frond orientation. This could be improved in a straightforward way by including some probability distribution for

the angular elevation as a function of current speed, similar to the study performed in [28].

The cost of implementing polar rotation is that depth layers are no longer isolated. Rather than integrating the two dimensional length-orientation distribution from Section 2.3.3 to calculate the spatial kelp distribution, it would be necessary to perform a triple integral which includes the elevation distribution. Since frond elevation and azimuthal orientation are both related to current velocity, the assumption of independent distributions would have to be abandoned, as mentioned at the end of Section 2.3.3. Considering non-kite frond shapes, as well as out-of-plane bending may also improve the spatial description of the seaweed, though would pose major implementation challenges.

Improved parameter estimation is also important, especially the frond alignment coefficient  $\eta$ . Better values for the frond absorptance  $A_k$  and thickness  $f_t$  would also be advantageous. Further, it may be worthwhile to consider how the  $A_k$  and  $f_t$  vary within a single frond, over depth, and over the life cycle of the kelp plant.

Additionally, the light model itself has a few opportunities for improvement. At present, the scattering coefficient is taken to be constant over the whole domain. In reality, kelp and water have different scattering properties, which should be considered in the same way that the absorption field is presently determined by Equation (2.20). This poses an additional challenge for the numerical asymptotics solution, as the asymptotic expansion must be taken in terms of a scalar parameter. Perhaps the maximum value  $\bar{b}$  of the scattering field  $b(\mathbf{x}, \bar{b})$  could be used, which of course

would require that  $b$  be expanded in terms of  $\bar{b}$  as is currently done with  $L$  and  $\sigma$  in Equations (3.3.1) and (3.3.1) respectively.

Also, it is important to note that in reality, photosynthesis is a frequency-dependent process, and a frequency-dependent light model may therefore significantly improve seasonal growth predictions. This suggests that inelastic (a.k.a. Raman) scattering also be considered, whereby light changes not only direction but also frequency during a scattering event. Of course, frequency-dependence adds another dimension to the already five-dimensional simulation, which may push a numerical solution beyond the capability of modern computers.

Finally, a major outstanding task is the experimental validation of the model presented in this thesis. Chapter V deals with ensuring that the numerical algorithms presented here *solve the equations right*, but it remains to be shown whether they *solve the right equations*. Comparison with experimental data is an essential step in developing and refining computation models, and is sure to provide insight into potential improvements.

### 7.2.2 Numerical Improvements

Aside from improvements of the mathematical model, plenty of improvements to the numerical solution are possible. Perhaps the most important and achievable such improvement the following specific modification to the numerical asymptotics algorithm which is likely to speed up the solution by several orders of magnitude. At present, the numerical asymptotics algorithm considers each spatial-angular grid

point, determines the ray path back to its intersection with the domain boundary, and solves Equation (3.14) via Equation (4.7) over the full ray path in order to determine the effects of absorption and scattering since the previous term in the asymptotic series. Rather than integrate the full ray for each grid point, it may be possible to implement a much cheaper local algorithm which solves Equation (3.14) only between adjacent grid cells. At present, computation time is a far greater bottleneck than memory usage for the asymptotic approximation. If this algorithmic improvement indeed speeds up the computation considerably, it would make solutions feasible on much larger grids than are currently within reach.

A somewhat similar modification is available for the finite difference solution which would make larger grids achievable. However, this does not actually involve an algorithmic improvement, nor does it involve reducing the total CPU time or memory allocation required for computation. Rather, it involves distributing the computational load between computers in a way that is not currently implemented. As mentioned in Section 4.5.4, the finite difference linear system is presently solved by the multithreaded GMRES algorithm provided by the LIS package. While multithreading can only achieve parallelism within a single process on a single machine, LIS also makes available MPI implementations of its parallel algorithms. MPI is a protocol which facilitates work-sharing between processes either on the same machine or over a network. Therefore, using the MPI environment permits the coefficient matrix to be divided and stored in a distributed fashion on several nodes within a cluster, which, depending on the computational resources available, is likely to drastically

increase the grid sizes available for computation. However, network communication is often significantly slower than inter-thread communication. Therefore, unless a high-speed fiber-optic network is used, the MPI environment is likely to require a sacrifice in terms of computation time for the sake of the increased memory capacity. None of this has yet been explored in the context of this project, and is ripe for exploration in future work.

Another potential improvement, though not likely to have as significant of an impact as the two above, is to restructure the angular grid to use a more accurate quadrature, which would reduce the necessary number of angular grid points to achieve a particular level of accuracy, and therefore reduce the required computation time and memory allocation. Among the possible options are the Lebedev grid and “spherical  $t$ -design”[2, 5, 6]. In fact, many other numerical algorithms altogether are available for solving the radiative transfer equation, including finite element methods and Monte Carlo methods among others.

### 7.2.3 Application to Seaweed Cultivation

The final and perhaps most interesting and useful avenue for future work is the application of the 3D light model developed in this thesis to answer real questions about seaweed cultivation. While there are many ways in which the model and its numerical solution can be improved, a working implementation is now available, and should be taken advantage of! In particular, this light model is well-suited for use in a time-dependent growth model such as [8], as discussed in Section 6.1.3. For

example, one line of questioning which naturally arises related to light modeling is “How does the placement of kelp cultivation ropes affect the potential biomass cultivation potential of a given area? What is the optimal rope spacing to maximize said production?” These type of questions are particularly natural to investigate with this light model, as the use of periodic boundary equates domain width and rope spacing.

Also, as mentioned in Chapter I, the growth of seaweed near WWTP ocean outfalls has been proposed for nutrient remediation of the aquatic ecosystem. One concern which arises from this proposal is whether the optical conditions near the WWTP are suitable for kelp cultivation. Therefore, modeling the optical properties of such water as a function of nutrient concentrations in order to run appropriate kelp growth simulations may prove valuable for addressing such concerns. Similar inquiry may be worthwhile when considering kelp cultivation in close proximity to other potential sources of turbidity such as salmon farms [7] or other forms of aquaculture.

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## APPENDICES

## APPENDIX A

### GRID DETAILS

The width of the spatial grid cells in each dimension are

$$dx = \frac{x_{\max} - x_{\min}}{n_x},$$

$$dy = \frac{y_{\max} - y_{\min}}{n_y},$$

$$dz = \frac{z_{\max} - z_{\min}}{n_z}.$$

and the cell centers as

$$x_i = (i - 1/2)dx \text{ for } i = 1, \dots, n_x,$$

$$y_j = (j - 1/2)dy \text{ for } j = 1, \dots, n_y,$$

$$z_k = (k - 1/2)dz \text{ for } k = 1, \dots, n_z.$$

Denote the edges as

$$x_i^e = (i - 1)dx \text{ for } i = 1, \dots, n_x,$$

$$y_j^e = (j - 1)dy \text{ for } j = 1, \dots, n_y,$$

$$z_k^e = (k - 1)dz \text{ for } k = 1, \dots, n_z.$$

Note that in this convention, there are the same number of edges and cells, and edges precede centers.

Now, we define the azimuthal angle such that

$$\theta_l = (l - 1)d\theta.$$

For the sake of periodicity, we need

$$\theta_1 = 0,$$

$$\theta_{n_\theta} = 2\pi - d\theta,$$

which requires

$$d\theta = \frac{2\pi}{n_\theta}.$$

For the polar angle, we similarly let

$$\phi_m = (m - 1)d\phi.$$

Since the polar azimuthal is not periodic, we also store the endpoint, so

$$\phi_1 = 0,$$

$$\phi_{n_\phi} = \pi.$$

This gives us

$$d\phi = \frac{\pi}{n_\phi - 1}.$$

It is also useful to define the edges between angular grid cells as

$$\theta_l^e = (l - 1/2)d\theta, \quad l = 1, \dots, n_\theta \quad (\text{A.1})$$

$$\phi_m^e = (m - 1/2)d\phi, \quad m = 1, \dots, n_\phi - 1. \quad (\text{A.2})$$

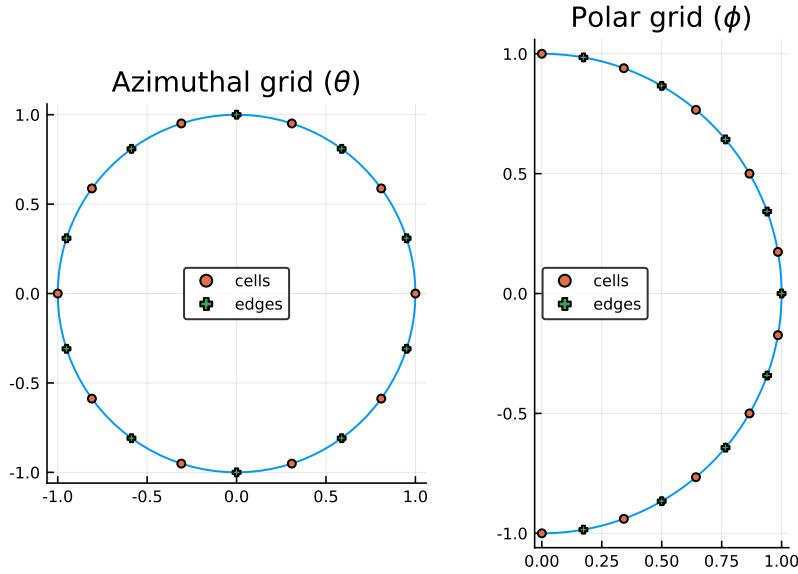


Figure A.1: Angular grid cell centers and edges.

Note that while  $\theta$  has its final edge following its final center, this is not the case for  $\phi$ , as seen in Figure A.1. Because angles are indexed by a single integer  $p$ , there is a one-to-one relationship between an integer  $p$  and a pair  $(l, m)$ . The relationships are

$$\hat{l}(p) = \text{mod1}(p, n_\theta),$$

$$\hat{m}(p) = \text{ceil}(p/n_\theta) + 1,$$

$$p = (\hat{m}(p) - 2) n_\theta + \hat{l}(p).$$

Accordingly, define

$$\hat{\theta}_p = \theta_{\hat{l}(p)},$$

$$\hat{\phi}_p = \phi_{\hat{m}(p)},$$

$$\hat{p}(l, m) = (m - 1)n_\theta + l.$$

We refer to the angular grid cell centered at  $\omega_p$  as  $\Omega_p$ , and the solid angle subtended by  $\Omega_p$  is denoted  $|\Omega_p|$ . The areas of the grid cells are calculated as follows. Note that there is a temporary abuse of notation in that the same symbols ( $d\theta$  and  $d\phi$ ) are being used for infinitesimal differential and for finite grid spacing. For the poles, we have

$$\begin{aligned} |\Omega_1| = |\Omega_{n_\omega}| &= \int_{\Omega_1} d\omega \\ &= \int_0^{2\pi} \int_0^{d\phi/2} \sin \phi \, d\phi \, d\theta \\ &= 2\pi \cos \phi \Big|_{d\phi/2}^0 \\ &= 2\pi(1 - \cos(d\phi/2)). \end{aligned}$$

For all other angular grid cells,

$$\begin{aligned} |\Omega_p| &= \int_{\Omega_p} d\omega \\ &= \int_{\theta_l^e}^{\theta_{l+1}^e} \int_{\phi_m^e}^{\phi_{m+1}^e} \sin(\phi) \, d\phi \, d\theta \\ &= d\theta \int_{\phi_m^e}^{\phi_{m+1}^e} \sin(\phi) \, d\phi \\ &= d\theta (\cos(\phi_m^e) - \cos(\phi_{m+1}^e)). \end{aligned}$$

## APPENDIX B

### RAY TRACING ALGORITHM

In order to evaluate a path integral through the discrete grid, it is first necessary to construct a one-dimensional piecewise constant integrand which is discontinuous at unevenly spaced points corresponding to the intersections between the path and edges in the spatial grid.

Consider a grid center  $\mathbf{p}_1 = (p_{1x}, p_{1y}, p_{1z})$  and a corresponding path  $\mathbf{l}(\mathbf{x}_1, \omega, s)$ . To find the location of discontinuities in the integrand, we first calculate the distance from its origin,  $\mathbf{p}_0 = \mathbf{x}_0(\mathbf{p}_1, \omega) = (p_{0x}, p_{0y}, p_{0z})$  (as in (3.5)) to grid edges in each dimension separately. Given

$$x_i = p_{0x} + \frac{s_i^x}{\tilde{s}}(p_{1x} - p_{0x}), \quad (\text{B.1})$$

$$y_j = p_{0y} + \frac{s_j^y}{\tilde{s}}(p_{1y} - p_{0y}), \quad (\text{B.2})$$

$$z_k = p_{0z} + \frac{s_k^z}{\tilde{s}}(p_{1z} - p_{0z}), \quad (\text{B.3})$$

the path lengths at which the ray intersects with edges in each dimension are calculated to be

$$s_i^x = \tilde{s} \frac{x_i - p_{0x}}{p_{1x} - p_{0x}}, \quad (\text{B.4})$$

$$s_i^y = \tilde{s} \frac{y_i - p_{0y}}{p_{1y} - p_{0y}}, \quad (\text{B.5})$$

$$s_i^z = \tilde{s} \frac{z_i - p_{0z}}{p_{1z} - p_{0z}}. \quad (\text{B.6})$$

We also keep a variable for each dimension specifying whether the ray increases or decreases in the dimension. Let

$$\delta_x = \text{sign}(p_{0x} - p_{1x}), \quad (\text{B.7})$$

$$\delta_y = \text{sign}(p_{0y} - p_{1y}), \quad (\text{B.8})$$

$$\delta_z = \text{sign}(p_{0z} - p_{1z}). \quad (\text{B.9})$$

For convenience, we also store a closely related quantity,  $\sigma$  with a value 1 for increasing rays and 0 for decreasing rays in each dimension

$$\sigma_x = (\delta_x + 1)/2, \quad (\text{B.10})$$

$$\sigma_y = (\delta_y + 1)/2, \quad (\text{B.11})$$

$$\sigma_z = (\delta_z + 1)/2, \quad (\text{B.12})$$

simply as a boolean value to track of the ray direction.

For this algorithm, we keep two sets of indices.  $(i, j, k)$  indexes the grid cell, and is used for extracting physical quantities from each cell along the path. Meanwhile,  $(i^e, j^e, k^e)$  indexes the edges between grid cells, beginning after the first cell. That is,  $i^e = 1$  refers not to the plane  $x = x_{\min}$ , but to  $x = x_{\min} + dx$ .

Let  $(i_0, j_0, k_0)$  be the indices of the grid cell containing  $\mathbf{p}_0$ . That is,

$$i_0 = \text{ceil} \left( \frac{p_{0x} - x_{\min}}{dx} \right), \quad (\text{B.13})$$

$$j_0 = \text{ceil} \left( \frac{p_{0y} - y_{\min}}{dy} \right), \quad (\text{B.14})$$

$$k_0 = \text{ceil} \left( \frac{p_{0z} - z_{\min}}{dz} \right). \quad (\text{B.15})$$

Then,

$$i_0^e = i_0 + \sigma_x, \quad (\text{B.16})$$

$$j_0^e = j_0 + \sigma_y, \quad (\text{B.17})$$

$$k_0^e = k_0 + \sigma_z. \quad (\text{B.18})$$

Now, we calculate the distance from  $p_0$  along the path to edges in each dimension.

$$s_i^x = \hat{s} \frac{x_i^e - p_{0x}}{p_{1x} - p_{0x}}, \quad (\text{B.19})$$

$$s_j^y = \hat{s} \frac{y_j^e - p_{0y}}{p_{1y} - p_{0y}}, \quad (\text{B.20})$$

$$s_k^z = \hat{s} \frac{z_k^e - p_{0z}}{p_{1z} - p_{0z}}. \quad (\text{B.21})$$

For each grid cell, we check the path lengths required to cross the next  $x$ ,  $y$ , and  $z$  edge-planes. Then, we move to the next grid cell in whichever dimension is crossed soonest. As each cell is traversed, the absorption coefficient and effective source are saved for use in the ray integral for the numerical calculation of the asymptotic approximation. For full implementation details, see the `traverse_ray` subroutine in `asymptotics.f90` in Appendix E.

## APPENDIX C

### SYNTHETIC DATA

In order to perform code verification via the Method of Manufactured solutions, analytical functions for radiance, absorption coefficient, and volume scattering function must be chosen which are simple to evaluate, are differentiable, and satisfy the constraints imposed by the algorithm implementation that are listed in Section 5.3.2.

The functions chosen to meet the above conditions are

$$L(x, y, z, \theta, \phi) = \alpha (\sin(\phi + \theta) + 1) \\ \cdot \left( z \left( \sin\left(\frac{2\pi x}{\alpha}\right) + \sin\left(\frac{2\pi y}{\alpha}\right) \right) + 1 \right) \\ \cdot \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right), \quad (C.1)$$

$$a(x, y, z) = \sin\left(\frac{2\pi x}{\alpha}\right) + \sin\left(\frac{2\pi y}{\alpha}\right) + \tanh(-\gamma + z) + 5, \quad (C.2)$$

$$\beta(\Delta) = \frac{\Delta + 1}{4\pi}, \quad (C.3)$$

where  $\alpha = x_{max} - x_{min} = y_{max} - y_{min}$  is the domain width, and  $\gamma = z_{max} - z_{min}$  is the domain depth. Using the python package Sympy [24], the boundary conditions

and source function are calculated to be

$$f(\theta, \phi) = \alpha (-\gamma + 1) (\sin(\phi + \theta) + 1), \quad (C.4)$$

$$\begin{aligned} \sigma(x, y, z, \theta, \phi) = & \alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) (\sin(\phi + \theta) + 1) \\ & \cdot \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right) \left( b + \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) + \tanh(-\gamma + z) + 5 \right) \\ & - b \left[ \frac{\alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) \left( \frac{\sin(\phi)\sin(\theta)}{3} + \frac{\cos(\phi)}{3} \right) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right)}{4\pi} \right. \\ & - \frac{\alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right)}{4\pi} \\ & \cdot \left( -\frac{\pi \sin(\phi) \sin(\theta)}{2} - \frac{\sin(\phi) \sin(\theta)}{3} - \frac{\cos(\phi)}{3} \right) \\ & - \frac{\alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right)}{4\pi} \\ & \cdot \left( \frac{\sin(\phi) \sin(\theta)}{3} - \frac{2\pi \sin(\phi) \cos(\theta)}{3} + \frac{\cos(\phi)}{3} - 2\pi \right) \\ & + \frac{\alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right)}{4\pi} \\ & \cdot \left( -\frac{\pi \sin(\phi) \sin(\theta)}{2} - \frac{\sin(\phi) \sin(\theta)}{3} + \frac{2\pi \sin(\phi) \cos(\theta)}{3} - \frac{\cos(\phi)}{3} + 2\pi \right) \Big] \\ & + 2\pi z (\sin(\phi + \theta) + 1) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right) \sin(\phi) \sin(\theta) \cos \left( \frac{2\pi y}{\alpha} \right) \\ & + 2\pi z (\sin(\phi + \theta) + 1) \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right) \sin(\phi) \cos(\theta) \cos \left( \frac{2\pi x}{\alpha} \right) \\ & + \left[ \alpha \left( z \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) + 1 \right) \right. \\ & \cdot \left( \frac{(-b-1)(-\tanh^2((b+1)(\gamma-z))+1)}{\tanh(\gamma(b+1))} + 1 \right) (\sin(\phi + \theta) + 1) \\ & + \alpha \left( \sin \left( \frac{2\pi x}{\alpha} \right) + \sin \left( \frac{2\pi y}{\alpha} \right) \right) (\sin(\phi + \theta) + 1) \\ & \cdot \left. \left( -\gamma + z + \frac{\tanh((b+1)(\gamma-z))}{\tanh(\gamma(b+1))} \right) \right] \cos(\phi). \end{aligned} \quad (C.5)$$

## APPENDIX D

### MEMORY USAGE

The number of elements in the finite difference coefficient matrix is given by Equation (4.14). Assuming that double precision floating point numbers are used, the number of bytes required to store the matrix values is found by multiplying the result of (4.14) by 8 bytes per number. These values are listed in Table D.1.

Since the matrix is sparse, the indices of the elements must also be stored. Due to the large number of elements involved, long integers must be used as indices, which also require 8 bytes to store. The exact amount of memory required depends on the storage scheme, which in this case is the Compressed Sparse Row (CSR) format provided by LIS [27]. Furthermore, the iterative method required to calculate a solution to the matrix equation allocates additional working arrays. From personal experience, the memory requirement for LIS solution via GMRES, restarted every 100 iterations, is well-estimated by multiplying the values in Table D.1 by 5. These solution memory estimates are listed in Table D.2.

Table D.1: Memory to store one copy of the finite difference coefficient matrix.  $n_s$  varies over rows and  $n_a$  over columns.

$n_s \backslash n_a$	8	10	12	14	16	18	20
4	1.36 MiB	3.51 MiB	7.61 MiB	14.59 MiB	25.57 MiB	41.88 MiB	65 MiB
8	10.91 MiB	28.15 MiB	60.94 MiB	116.79 MiB	204.7 MiB	335.17 MiB	520.2 MiB
16	87.4 MiB	225.34 MiB	487.76 MiB	934.67 MiB	1.6 GiB	2.62 GiB	4.06 GiB
32	699.61 MiB	1.76 GiB	3.81 GiB	7.3 GiB	12.8 GiB	20.95 GiB	32.52 GiB
48	2.31 GiB	5.94 GiB	12.87 GiB	24.65 GiB	43.2 GiB	70.73 GiB	109.76 GiB
64	5.47 GiB	14.09 GiB	30.5 GiB	58.43 GiB	102.4 GiB	167.65 GiB	260.18 GiB
72	7.78 GiB	20.06 GiB	43.42 GiB	83.2 GiB	145.8 GiB	238.7 GiB	370.45 GiB
100	20.86 GiB	53.76 GiB	116.34 GiB	222.91 GiB	390.63 GiB	639.54 GiB	992.51 GiB
128	43.74 GiB	112.74 GiB	243.99 GiB	467.48 GiB	819.22 GiB	1.31 TiB	2.03 TiB

Table D.2: Memory to solve the linear system of equations with GMRES restarted every 100 iterations. This seems to require about five times the memory required to store the matrix. In the table,  $n_s$  varies over rows, and  $n_a$  over columns.

$n_a \backslash n_s$	8	10	12	14	16	18	20
4	6.81 MiB	17.57 MiB	38.05 MiB	72.94 MiB	127.87 MiB	209.39 MiB	325.01 MiB
8	54.57 MiB	140.74 MiB	304.7 MiB	583.96 MiB	1023.51 MiB	1.64 GiB	2.54 GiB
16	437.01 MiB	1.1 GiB	2.38 GiB	4.56 GiB	8 GiB	13.1 GiB	20.32 GiB
32	3.42 GiB	8.81 GiB	19.06 GiB	36.52 GiB	64 GiB	104.77 GiB	162.6 GiB
48	11.53 GiB	29.72 GiB	64.33 GiB	123.25 GiB	215.99 GiB	353.63 GiB	548.8 GiB
64	27.34 GiB	70.46 GiB	152.48 GiB	292.16 GiB	512 GiB	838.24 GiB	1.27 TiB
72	38.92 GiB	100.32 GiB	217.11 GiB	415.99 GiB	729 GiB	1.17 TiB	1.81 TiB
100	104.29 GiB	268.79 GiB	581.7 GiB	1.09 TiB	1.91 TiB	3.12 TiB	4.85 TiB
128	218.72 GiB	563.7 GiB	1.19 TiB	2.28 TiB	4 TiB	6.55 TiB	10.16 TiB

## APPENDIX E

### FORTRAN CODE

The full Fortran implementation of the model described in this thesis! The main subroutine is listed first: `light_interface.f90/full_light_calculations`. The electronic version of this code, as well as supplemental analysis can be found online at the following URLs:

<https://github.com/OliverEvans96/swdlyt>

<https://gitlab.com/OliverEvans96/swdlyt>

<https://gitlab.nautilus.optiputer.net/OliverEvans96/swdlyt>

Please don't hesitate to get in touch to discuss the code or any part of the model! You can reach me at `oliverevans96@gmail.com`. I commend you for making it this far, and good luck in all of your endeavors!

```
light_interface.f90
1 module light_interface
2   use rte3d
3   use kelp3d
4   use asymptotics
5   implicit none
6
7 contains
8   subroutine full_light_calculations( &
9     ! OPTICAL PROPERTIES
10    absorptance_kelp, & ! NOT THE SAME AS
11    ABSORPTION COEFFICIENT
12    abs_water, &
13    scat, &
```

```

13    num_vsf, &
14    vsf_file, &
15    ! SUNLIGHT
16    solar_zenith, &
17    solar_azimuthal, &
18    surface_irrad, &
19    ! KELP &
20    num_si, &
21    si_area, &
22    si_ind, &
23    frond_thickness, &
24    frond_aspect_ratio, &
25    frond_shape_ratio, &
26    ! WATER CURRENT
27    current_speeds, &
28    current_angles, &
29    ! SPACING
30    rope_spacing, &
31    depth_spacing, &
32    ! SOLVER PARAMETERS
33    nx, &
34    ny, &
35    nz, &
36    ntheta, &
37    nphi, &
38    fd_flag, &
39    num_scatters, &
40    num_threads, &
41    ! FINAL RESULTS
42    perceived_irrad, &
43    avg_irrad)
44
45    implicit none
46
47    ! OPTICAL PROPERTIES
48    integer, intent(in) :: nx, ny, nz, ntheta,
49                           nphi
50    ! Absorption and scattering coefficients
51    double precision, intent(in) :::
52                           absorptance_kelp, scat
53    double precision, dimension(nz), intent(in)
54                           :: abs_water
55    ! Volume scattering function
56    integer, intent(in) :: num_vsf
57    character(len=*) :: vsf_file
58    !double precision, dimension(num_vsf),
59                           intent(int) :: vsf_angles
60    !double precision, dimension(num_vsf),
61                           intent(int) :: vsf_vals
62
63    ! SUNLIGHT
64    double precision, intent(in) :: solar_zenith

```

```

60   double precision, intent(in) ::  
      solar_azimuthal  
61   double precision, intent(in) ::  
      surface_irrad  
62  
63 ! KELP  
64 ! Number of Superindividuals in each depth  
   level  
65 integer, intent(in) :: num_si  
66 ! si_area(i,j) = area of superindividual j  
   at depth i  
67 double precision, dimension(nz, num_si),  
      intent(in) :: si_area  
68 ! si_ind(i,j) = number of individuals  
   represented by superindividual j at depth  
   i  
69 double precision, dimension(nz, num_si),  
      intent(in) :: si_ind  
70 ! Thickness of each frond  
71 double precision, intent(in) ::  
      frond_thickness  
72 ! Ratio of length to width (0,infty)  
73 double precision, intent(in) ::  
      frond_aspect_ratio  
74 ! Rescaled position of greatest width (0=  
   base, 1=tip)  
75 double precision, intent(in) ::  
      frond_shape_ratio  
76  
77 ! WATER CURRENT  
78 double precision, dimension(nz), intent(in)  
      :: current_speeds  
79 double precision, dimension(nz), intent(in)  
      :: current_angles  
80  
81 ! SPACING  
82 ! Horizontal distance between vertical kelp  
   ropes = domain width  
83 double precision, intent(in) :: rope_spacing  
84 ! dz, varies over depth  
85 double precision, dimension(nz), intent(in)  
      :: depth_spacing  
86 ! SOLVER PARAMETERS  
87 ! Whether to use the finite difference  
   algorithm (otherwise, just asymptotics.)  
88 logical, intent(in) :: fd_flag  
89 ! Number of scattering events for  
   asymptotics. Use 0 if fd_flag = true.  
90 integer, intent(in) :: num_scatters  
91 ! Number of OMP threads to use for parallel  
   subroutines

```

```

92   integer, intent(in) :: num_threads
93   character*(256) :: lis_opts
94   integer :: lis_iter
95   double precision :: lis_time, lis_resid
96
97   ! FINAL RESULT
98   real, dimension(nz), intent(out) :: 
99     avg_irrad, perceived_irrad
100
101 ! -----
102
103   double precision xmin, xmax, ymin, ymax,
104     zmin, zmax
105   character(len=5), parameter :: fmtstr = 'E13
106     .4'
107   !double precision, dimension(num_vsf) :: 
108     vsf_angles, vsf_vals
109   double precision decay
110   integer quadrature_degree
111   ! Number of periodic images of the domain to
112     consider for kelp distribution
113   integer :: n_images
114
115   type(space_angle_grid) grid
116   type(rte_mat) mat
117   type(optical_properties) iops
118   type(light_state) light
119   type(rope_state) rope
120   type(frond_shape) frond
121   type(boundary_condition) bc
122
123   double precision, dimension(:, :, :, :),
124     :: pop_length_means, pop_length_stds
125   ! Number of fronds in each depth layer
126   double precision, dimension(:, :, :, :),
127     :: num_fronds
128   double precision, dimension(:, :, :, :, :),
129     :: allocatable :: p_kelp
130   double precision, dimension(nx, ny, nz,
131     ntheta*(nphi-2)+2) :: radiance
132   double precision, dimension(:, :, :, :, :),
133     :: allocatable :: source
134
135   write(*,*) 'Light calculation'
136
137   allocate(pop_length_means(nz))
138   allocate(pop_length_stds(nz))
139   allocate(num_fronds(nz))
140   allocate(p_kelp(nx, ny, nz))
141
142   xmin = -rope_spacing/2

```

```

133      xmax = rope_spacing/2
134
135      ymin = -rope_spacing/2
136      ymax = rope_spacing/2
137
138      zmin = 0.d0
139      zmax = sum(depth_spacing)
140
141      write(*,*) 'Grid'
142      call grid%set_bounds(xmin, xmax, ymin, ymax,
143                             zmin, zmax)
144      call grid%set_num(nx, ny, nz, ntheta, nphi)
145      call grid%init()
146      !call grid%set_uniform_spacing_from_num()
147      call grid%z%set_spacing_array(depth_spacing)
148
149      allocate(source( &
150                  grid%x%num, &
151                  grid%y%num, &
152                  grid%z%num, &
153                  grid%angles%omega))
154
155      ! Initialize source to zero
156      source(:,:,:,:,:) = 0.d0
157
158      call rope%init(grid)
159
160      write(*,*) 'Rope'
161      ! Calculate kelp distribution
162      call calculate_length_dist_from_superinds( &
163                                              nz, &
164                                              num_si, &
165                                              si_area, &
166                                              si_ind, &
167                                              frond_aspect_ratio, &
168                                              num_fronds, &
169                                              pop_length_means, &
170                                              pop_length_stds)
171
172      rope%frond_lengths = pop_length_means
173      rope%frond_stds = pop_length_stds
174      rope%num_fronds = num_fronds
175      rope%water_speeds = current_speeds
176      rope%water_angles = current_angles
177
178      write(*,*) 'frond_lengths = ', rope%
179      frond_lengths
178      write(*,*) 'frond_stds = ', rope%frond_stds
179      write(*,*) 'num_fronds = ', rope%num_fronds

```

```

180 |     write(*,*) 'water_speeds = ', rope%
|         water_speeds
181 |     write(*,*) 'water_angles = ', rope%
|         water_angles
182 |     write(*,*) 'Frond'
183 |
184 | ! INIT FROND
185 | call frond%set_shape(frond_shape_ratio,
|         frond_aspect_ratio, frond_thickness)
186 | write(*,*) 'ft = ', frond%ft
187 | ! CALCULATE KELP
188 | quadrature_degree = 100
189 | n_images = 2
190 | call calculate_kelp_on_grid(grid, p_kelp,
|         frond, rope, quadrature_degree, n_images,
|         num_threads)
191 | ! INIT IOPS
192 | iops%num_vsf = num_vsf
193 | call iops%init(grid)
194 | write(*,*) 'IOPs'
195 | iops%abs_kelp = absorptance_kelp /
|         frond_thickness
196 | iops%abs_water = abs_water
197 | iops%scat = scat
198 |
199 | !write(*,*) 'iop init'
200 | !iops%vsf_angles = vsf_angles
201 | !iops%vsf_vals = vsf_vals
202 | write(*,*) 'Load VSF'
203 | call iops%load_vsf(vsf_file, fmtstr)
204 |
205 | ! load_vsf already calls calc_vsf_on_grid
206 | !call iops%calc_vsf_on_grid()
207 | write(*,*) 'Calculate kelp coef. grid.'
208 | call iops%calculate_coef_grids(p_kelp)
209 |
210 | !write(*,*) 'BC'
211 | decay = 1.d0 ! Determines drop-off in
|         surface BC as a func of angle diff from (
|             theta_s, phi_s)
212 | write(*,*) 'Init BC'
213 | write(*,*) 'IO = ', surface_irrad
214 | write(*,*) 'phi_s = ', solar_zenith
215 | write(*,*) 'theta_s = ', solar_azimuthal
216 | write(*,*) 'decay = ', decay
217 | call bc%init(grid, solar_azimuthal,
|             solar_zenith, decay, surface_irrad)
218 | write(*,*) 'bc%IO = ', bc%IO
219 | write(*,*) 'bc%phi_s = ', bc%phi_s
220 | write(*,*) 'bc%theta_s = ', bc%theta_s

```

```

221 |     write(*,*) 'bc%decay = ', bc%decay
222 |     !write(*,*) 'bc'
223 |     !write(*,*) bc%bc_grid
224 |     call write_vec(bc%bc_grid, grid%angles%
225 |                     nomega/2, "bc.txt")
226 |     call write_array(iops%abs_grid(:, ny/2, :), nx
227 |                         , nz, "abs.txt")
228 |
229 |     if(num_scatters .ge. 0) then
230 |         write(*,*) 'Calculate asymptotic light
231 |                     field'
232 |         call calculate_asymptotic_light_field(&
233 |                     grid, bc, iops, source, &
234 |                     radiance, num_scatters, num_threads
235 |                     )
236 |
237 |     if(fd_flag) then
238 |
239 |         ! INIT MAT
240 |         write(*,*) 'FD Sparse Matrix'
241 |         ! Set boundary condition
242 |         call mat%init(grid, iops)
243 |         call mat%set_bc(bc)
244 |         call gen_matrix(mat, num_threads)
245 |
246 |         ! Set solver options
247 |         if(num_scatters .ge. 0) then
248 |             mat%initx_zeros = .false.
249 |         else
250 |             mat%initx_zeros = .true.
251 |         end if
252 |         lis_opts = '-i gmres -restart 100'
253 |         call mat%set_solver_opts(trim(lis_opts))
254 |
255 |         ! Initialize & set initial guess
256 |         write(*,*) 'Light init'
257 |         call light%init(mat)
258 |         light%radiance = radiance
259 |
260 |         ! Solve system
261 |         write(*,*) 'Calculate Radiance'
262 |         call light%calculate_radiance()
263 |
264 |         call mat%get_solver_stats(lis_iter,
265 |                                     lis_time, lis_resid)
266 |         call mat%deinit()

```

```

267      call light%init_grid(grid)
268      light%radiance = radiance
269  endif
270
271  write(*,*) 'Irrad'
272  call light%calculate_irradiance()
273 ! Calculate output variables
274  call calculate_average_irradiance(grid,
275      light, avg_irrad)
276  call calculate_perceived_irradiance(grid,
277      p_kelp, &
278          perceived_irrad, light%irradiance)
279
280 !write(*,*) 'vsf_angles = ', iops%vsf_angles
281 !write(*,*) 'vsf_vals = ', iops%vsf_vals
282 !write(*,*) 'vsf_norm = ', grid%
283     integrate_angle_2d(iops%vsf(1,1,:,:))
284
285 !0w7rite(*,*) 'abs_water = ', abs_water
286 ! write(*,*) 'scat_water = ', scat_water
287 !write(*,*) 'kelp '
288 !write(*,*) p_kelp(:,:,,:)
289
290 !write(*,*) 'irrad'
291 !write(*,*) light%irradiance
292
293 call write_array(p_kelp(:,ny/2,:), nx, nz, "
294     kelp.txt")
295 call write_array(light%irradiance(:,ny/2,:), nx, nz, "irrad.txt")
296
297 write(*,*) 'avg_irrad = ', avg_irrad
298 write(*,*) 'perceived_irrad = ',
299     perceived_irrad
300
301 write(*,*) 'deinit',
302 call bc%deinit()
303 !write(*,*) 'a'
304 call iops%deinit()
305 !write(*,*) 'b'
306 call light%deinit()
307 !write(*,*) 'c'
308 call rope%deinit()
309 !write(*,*) 'd'
310 call grid%deinit()
311 !write(*,*) 'e'
312
313 deallocate(pop_length_means)
314 deallocate(pop_length_stds)
315 deallocate(num_fronds)

```

```

311      deallocate(p_kelp)
312
313      !write(*,*) 'done'
314 end subroutine full_light_calculations
315
316 subroutine
317     calculate_length_dist_from_superinds( &
318     nz,  &
319     num_si,  &
320     si_area,  &
321     si_ind,  &
322     frond_aspect_ratio,  &
323     num_fronds,  &
324     pop_length_means,  &
325     pop_length_stds)
326
327 implicit none
328
329 ! Number of depth levels
330 integer, intent(in) :: nz
331 ! Number of Superindividuals in each depth
332 ! level
333 integer, intent(in) :: num_si
334 ! si_area(i,j) = area of superindividual j
335 ! at depth i
336 double precision, dimension(nz, num_si),
337 ! intent(in) :: si_area
338 ! si_area(i,j) = number of individuals
339 ! represented by superindividual j at depth
340 ! i
341 double precision, dimension(nz, num_si),
342 ! intent(in) :: si_ind
343 double precision, intent(in) :::
344 ! frond_aspect_ratio
345
346 double precision, dimension(nz), intent(out)
347 ! :: num_fronds
348 ! Population mean area at each depth level
349 double precision, dimension(nz), intent(out)
350 ! :: pop_length_means
351 ! Population area standard deviation at each
352 ! depth level
353 double precision, dimension(nz), intent(out)
354 ! :: pop_length_stds
355
356 !-----
357
358 integer i, k
359 ! Numerators for mean and std
360 double precision mean_num, std_num
361 ! Convert area to length

```

```

350   double precision , dimension(num_si) :: si_length
351
352   do k=1, nz
353     mean_num = 0.d0
354     std_num = 0.d0
355     num_fronds(k) = 0
356
357   do i=1, num_si
358     si_length(i) = sqrt(2.d0*
359       frond_aspect_ratio*si_area(k,i))
360     mean_num = mean_num + si_length(i)
361     num_fronds(k) = num_fronds(k) + si_ind
362       (k,i)
363   end do
364
365   pop_length_means(k) = mean_num /
366     num_fronds(k)
367
368   do i=1, num_si
369     std_num = std_num + (si_length(i) -
370       pop_length_means(k))**2
371   end do
372
373   pop_length_stds(k) = std_num / (
374     num_fronds(k) - 1)
375
376   end do
377
378   end subroutine calculate_length_dist_from_superinds
379
380   subroutine calculate_average_irradiance(grid,
381     light, avg_irrad)
382     type(space_angle_grid) grid
383     type(light_state) light
384     real, dimension(:) :: avg_irrad
385     integer k, nx, ny, nz
386
387     nx = grid%x%num
388     ny = grid%y%num
389     nz = grid%z%num
390
391     do k=1, nz
392       avg_irrad(k) = real(sum(light%irradiance
393         (:,:,k)) / nx / ny)
394     end do
395   end subroutine calculate_average_irradiance
396
397   subroutine calculate_perceived_irradiance(grid,
398     p_kelp, &

```

```

391     perceived_irrad, irradiance)
392 type(space_angle_grid) grid
393 double precision, dimension(:,:,:) :: p_kelp
394 real, dimension(:) :: perceived_irrad
395 double precision, dimension(:,:,:) :::
396     irradiance
397 double precision total_kelp
398 integer center_i1, center_i2, center_j1,
399     center_j2
400
401     ! Calculate the average irradiance
402     ! experienced over the frond.
403     ! Has same units as irradiance.
404     ! If no kelp, then just take the irradiance
405     ! at the center
406     ! of the grid.
407 do k=1, grid%z%num
408     total_kelp = sum(p_kelp(:,:,k))
409     if(total_kelp .eq. 0) then
410         center_i1 = int(ceiling(grid%x%num /
411                         2.d0))
412         center_j1 = int(ceiling(grid%y%num /
413                         2.d0))
414         ! For even grid, use average of center
415         ! two cells
416         ! For odd grid, just use center cell
417         if(mod(grid%x%num, 2) .eq. 0) then
418             center_i2 = center_i1 + 1
419         else
420             center_i2 = center_i1
421         end if
422         if(mod(grid%y%num, 2) .eq. 0) then
423             center_j2 = center_j1 + 1
424         else
425             center_j2 = center_j1
426         end if
427
428         ! Irradiance at the center of the grid
429         ! (at the rope)
430         perceived_irrad(k) = real(sum(
431             irradiance( &
432                 center_i1:center_i2, &
433                 center_j1:center_j2, k)) &
434                 / ((center_i2-center_i1+1) * (
435                     center_j2-center_j1+1)))
436     else
437         ! Average irradiance weighted by kelp
438         ! distribution

```

```

431     perceived_irrad(k) = real( &
432         sum(p_kelp(:,:,k)*irradiance(:,:,k
433             )) &
434             / total_kelp)
435     end if
436     end do
437 end subroutine calculate_perceived_irradiance
438
439 end module light_interface

```

asymptotics.f90

```

1 module asymptotics
2   use kelp_context
3   !use rte_sparse_matrices
4   !use light_context
5   implicit none
6   contains
7
8   subroutine calculate_asymptotic_light_field(
9     grid, bc, iops, source, radiance,
10    num_scatters, num_threads)
11   type(space_angle_grid) grid
12   type(boundary_condition) bc
13   type(optical_properties) iops
14   double precision, dimension(:,:,:,:,:) :: radiance
15   double precision, dimension(:,:,:,:,:) ,
16     allocatable :: rad_scatter
17   double precision, dimension(:,:,:,:,:) :: source
18   integer num_scatters
19   integer nx, ny, nz, nomega
20   integer max_cells
21   integer n
22   logical bc_flag
23   integer num_threads
24
25   double precision bb
26
27   double precision, dimension(:), allocatable
28     :: path_length, path_spacing, a_tilde, gn
29
30   nx = grid%x%num
31   ny = grid%y%num
32   nz = grid%z%num
33   nomega = grid%angles%nomega
34
35   max_cells = calculate_max_cells(grid)

```

```

33 |     allocate(path_length(max_cells+1))
34 |     allocate(path_spacing(max_cells))
35 |     allocate(a_tilde(max_cells))
36 |     allocate(gn(max_cells))
37 |     allocate(rad_scatter(grid%x%num, grid%y%num,
38 |                           grid%z%num, grid%angles%nomega))
39 |
40 |     write(*,*) 'before'
41 |     write(*,*) 'min radiance =', minval(radiance
42 |               )
43 |     write(*,*) 'max radiance =', maxval(radiance
44 |               )
45 |     write(*,*) 'mean radiance =', sum(radiance)/
46 |               size(radiance)
47 |
48 |     write(*,*) 'advect source + bc'
49 |     bc_flag = .true.
50 |     call advect_light( &
51 |                         grid, iops, source, radiance, &
52 |                         path_length, path_spacing, &
53 |                         a_tilde, gn, bc_flag, num_threads, bc)
54 |
55 |     write(*,*) 'after'
56 |     write(*,*) 'min radiance =', minval(radiance
57 |               )
58 |     write(*,*) 'max radiance =', maxval(radiance
59 |               )
60 |     write(*,*) 'mean radiance =', sum(radiance)/
61 |               size(radiance)
62 |
63 |     rad_scatter = radiance
64 |     bb = iops%scat
65 |
66 |     do n=1, num_scatters
67 |         write(*,*) 'scatter #', n
68 |         call scatter(grid, iops, source,
69 |                       rad_scatter, path_length, path_spacing
70 |                       , a_tilde, gn, num_threads)
71 |         radiance = radiance + bb**n * rad_scatter
72 |     end do
73 |
74 |     write(*,*) 'asymptotics complete'
75 |
76 |     deallocate(path_length)
77 |     deallocate(path_spacing)
78 |     deallocate(a_tilde)
79 |     deallocate(gn)
80 |     deallocate(rad_scatter)
81 |
82 | end subroutine
83 | calculate_asymptotic_light_field

```

```

73
74 subroutine calculate_asymptotic_light_field_expanded_source(&
75     grid, bc, iops, source, &
76     source_expansion, radiance, &
77     num_scatters, num_threads)
78 type(space_angle_grid) grid
79 type(boundary_condition) bc
80 type(optical_properties) iops
81 double precision, dimension(:,:,:,:,:) :: radiance
82 double precision, dimension(:,:,:,:,:) :: source_expansion
83 integer num_scatters
84 integer nx, ny, nz, nomega
85 integer max_cells
86 integer n
87 logical bc_flag
88 integer num_threads
89
90 double precision bb
91
92 double precision, dimension(:, allocatable
93     :: path_length, path_spacing, a_tilde, gn
94 double precision, dimension(:, :, :, :),
95     allocatable :: source
96 double precision, dimension(:, :, :, :),
97     allocatable :: rad_scatter
98 double precision, dimension(:, :, :, :),
99     allocatable :: scatter_integral
100
101 nx = grid%x%num
102 ny = grid%y%num
103 nz = grid%z%num
104 nomega = grid%angles%nomega
105 max_cells = calculate_max_cells(grid)
106
107 allocate(path_length(max_cells+1))
108 allocate(path_spacing(max_cells))
109 allocate(a_tilde(max_cells))
110 allocate(gn(max_cells))
111 allocate(rad_scatter(grid%x%num, grid%y%num,
112     grid%z%num, grid%angles%nomega))
113 allocate(scatter_integral(nx, ny, nz, nomega
    ))
114
115 write(*,*) 'advect source + bc'
116 bc_flag = .true.
117 call advect_light( &

```

```

114      grid, iops, source_expansion(:,:,:,:,1)
115      , radiance, &
116      path_length, path_spacing, &
117      a_tilde, gn, bc_flag, num_threads, bc)
118 ! Disable BC for scattering advection
119 bc_flag = .false.
120
121 rad_scatter = radiance
122 bb = iops%scat
123
124 do n=1, num_scatters
125     write(*,*) 'scatter #', n
126     call calculate_scatter_source(grid, iops,
127         rad_scatter, source, scatter_integral
128         , num_threads)
129     source = source + source_expansion
130         (:,:,:,:,n+1)
131     call advect_light(grid, iops, source,
132         rad_scatter, path_length, path_spacing
133         , a_tilde, gn, bc_flag, num_threads)
134
135     radiance = radiance + bb**n * rad_scatter
136
137 end do
138
139 write(*,*) 'asymptotics complete'
140
141 deallocate(path_length)
142 deallocate(path_spacing)
143 deallocate(a_tilde)
144 deallocate(gn)
145 deallocate(rad_scatter)
146 deallocate(scatter_integral)
147 end subroutine
148     calculate_asymptotic_light_field_expanded_source
149
150 ! Add attenuated surface light to existing
151     radiance
152 subroutine advect_surface_bc(&
153     i, j, k, p, radiance, &
154     path_spacing, num_cells, a_tilde, bc)
155 type(boundary_condition) bc
156 double precision, dimension(:,:,:,:,:) :::
157     radiance
158 double precision, dimension(:) :::
159     path_spacing, a_tilde
160 integer i, j, k, p
161 integer num_cells
162 double precision atten
163
```

```

154     atten = sum(path_spacing(1:num_cells) *
155                  a_tilde(1:num_cells))
156      ! Avoid underflow
157      if(atten .lt. 100.d0) then
158          radiance(i,j,k,p) = radiance(i,j,k,p) +
159                      bc%bc_grid(p) * exp(-atten)
160      end if
161  end subroutine advect_surface_bc
162
163  ! Perform one scattering event
164  subroutine scatter(grid, iops, source,
165                     rad_scatter, path_length, path_spacing,
166                     a_tilde, gn, num_threads)
167    type(space_angle_grid) grid
168    type(optical_properties) iops
169    double precision, dimension(:,:,:,:,:) :::
170                  rad_scatter, source
171    double precision, dimension(:,:,:,:,:) :::
172                  allocatable :: scatter_integral
173    double precision, dimension(:) :::
174                  path_length, path_spacing, a_tilde, gn
175    integer nx, ny, nz, nomega
176    logical bc_flag
177    integer num_threads
178
179    nx = grid%x%num
180    ny = grid%y%num
181    nz = grid%z%num
182    nomega = grid%angles%nomega
183    bc_flag = .false.
184
185    allocate(scatter_integral(nx, ny, nz, nomega
186                            ))
187
188    call calculate_scatter_source(grid, iops,
189                                rad_scatter, source, scatter_integral,
190                                num_threads)
191    call advect_light(grid, iops, source,
192                      rad_scatter, path_length, path_spacing,
193                      a_tilde, gn, bc_flag, num_threads)
194
195    deallocate(scatter_integral)
196  end subroutine scatter
197
198  ! Calculate source from no-scatter or previous
199  ! scattering layer
200  subroutine calculate_scatter_source(grid, iops
201                                         , rad_scatter, source, scatter_integral,
202                                         num_threads)
203    type(space_angle_grid) grid
204    type(optical_properties) iops

```

```

190 |     double precision, dimension(:,:,:,:,:) :: 
191 |         rad_scatter
192 |     double precision, dimension(:,:,:,:,:) :: 
193 |         source
194 |     double precision, dimension(:,:,:,:,:) :: 
195 |         scatter_integral
196 | type(index_list) indices
197 | integer nx, ny, nz, nomega
198 | integer i, j, k, p
199 | integer num_threads
200 |
201 | nx = grid%x%num
202 | ny = grid%y%num
203 | nz = grid%z%num
204 | nomega = grid%angles%nomega
205 |
206 | !$omp parallel do default(none) private(
207 |     indices) &
208 |     !$omp private(i,j,k,p) shared(nx,ny,nz,
209 |         nomega) &
210 |     !$omp shared(iops, rad_scatter,
211 |         scatter_integral) &
212 |     !$omp num_threads(num_threads) collapse(2)
213 |
214 | do k=1, nz
215 |     do i=1, nx
216 |         indices%k = k
217 |         indices%i = i
218 |         do j=1, ny
219 |             indices%j = j
220 |             do p=1, nomega
221 |                 indices%p = p
222 |                 call calculate_scatter_integral
223 |                     (&
224 |                         iops, rad_scatter,&
225 |                         scatter_integral,&
226 |                         indices)
227 |             end do
228 |         end do
229 |     end do
230 | !$omp end parallel do
231 | source(:,:,:,:,:) = -rad_scatter(:,:,:,:,:) +
232 |                         scatter_integral(:,:,:,:,:)
233 |
234 | write(*,*) 'source min: ', minval(source)

```

```

232     write(*,*) 'source max: ', maxval(source)
233     write(*,*) 'source mean: ', sum(source)/size
234     (source)
235 end subroutine calculate_scatter_source
236
237 subroutine calculate_scatter_integral(iops,
238     rad_scatter, scatter_integral, indices)
239     type(optical_properties) iops
240     double precision, dimension(:,:,:,:) :::
241         rad_scatter, scatter_integral
242     type(index_list) indices
243
244     scatter_integral(indices%i,indices%j,indices
245         %k,indices%p) &
246         = sum(iops%vsf_integral(indices%p, :) &
247             * rad_scatter(&
248                 indices%i,&
249                 indices%j,&
250                 indices%k,:))
251
252 end subroutine calculate_scatter_integral
253
254 subroutine advect_light(grid, iops, source,
255     rad_scatter, path_length, path_spacing,
256     a_tilde, gn, bc_flag, num_threads, bc)
257     type(space_angle_grid) grid
258     type(optical_properties) iops
259     double precision, dimension(:,:,:,:) :::
260         rad_scatter, source
261     double precision, dimension(:) :::
262         path_length, path_spacing, a_tilde, gn
263     logical bc_flag
264     type(boundary_condition), intent(in),
265         optional :: bc
266     integer i, j, k, p
267     integer num_threads
268
269 !$omp parallel do default(none) &
270 !$omp private(i,j,k,p) &
271 !$omp shared(rad_scatter,source,grid,iops,
272     bc_flag,bc) &
273 !$omp private(path_length,path_spacing,
274     a_tilde,gn) &
275 !$omp num_threads(num_threads) collapse(2)
276 do k=1, grid%z%num
277     do i=1, grid%x%num
278         do j=1, grid%y%num
279             do p=1, grid%angles%omega

```

```

270      call integrate_ray(grid, iops,
271                          source,&
272                          rad_scatter, path_length,
273                          path_spacing,&
274                          a_tilde, gn, i, j, k, p,
275                          bc_flag, bc)
276          end do
277      end do
278  !$omp end parallel do
279 end subroutine advect_light
280
281 ! New algorithm, double integral over
282 ! piecewise-constant 1d funcs
283 subroutine integrate_ray(grid, iops, source,
284                         rad_scatter, path_length, path_spacing,
285                         a_tilde, gn, i, j, k, p, bc_flag, bc)
286 type(space_angle_grid) :: grid
287 type(optical_properties) :: iops
288 double precision, dimension(:,:,:,:,:) :: source
289 double precision, dimension(:,:,:,:,:) :: rad_scatter
290 integer :: i, j, k, p
291 ! The following are only passed to avoid
292 ! unnecessary allocation
293 double precision, dimension(:) :: path_length, path_spacing, a_tilde, gn
294 logical bc_flag
295 type(boundary_condition), intent(in),
296     optional :: bc
297
298 integer num_cells
299
300 call traverse_ray(grid, iops, source, i, j,
301                   k, p, path_length, path_spacing, a_tilde,
302                   gn, num_cells)
303 rad_scatter(i,j,k,p) =
304     calculate_ray_integral(num_cells,
305                           path_length, path_spacing, a_tilde, gn)
306
307 if(bc_flag .and. p .le. grid%angles%omega
308 /2) then
309     call advect_surface_bc(&
310                           i, j, k, p, rad_scatter, &
311                           path_spacing, num_cells, &
312                           a_tilde, bc)
313 end if
314
315 ! if((i .eq. 1) &

```

```

305      ! . and. (j . eq. 1) &
306      ! . and. (k . eq. grid%z%num/2) &
307      ! . and. ( &
308      ! (p . eq. 1) . or. (p . eq. grid%angles%
309      ! nomega) &
310      ! )) then
311      !     write(*,*) 'ray (', i, ', ', j, ', ', k
312      !     , ', ', p, ', ')
313      !     write(*,*) 'num_cells = ', num_cells
314      !     write(*,*) 'path_spacing:'
315      !     write(*,*) path_spacing(1:num_cells)
316      !     write(*,*) 'path_length:'
317      !     write(*,*) path_length(1:num_cells+1)
318      !     write(*,*) 'a_tilde:'
319      !     write(*,*) a_tilde(1:num_cells)
320      !     write(*,*) 'gn:'
321      !     write(*,*) gn(1:num_cells)
322      !     write(*,*)
323      ! end if
324
325  end subroutine integrate_ray
326
326  function calculate_ray_integral(num_cells, s,
327      ds, a_tilde, gn) result(integral)
327  ! Double integral which accumulates all
328  ! scattered light along the path
328  ! via an angular integral and attenuates it
328  ! by integrating along the path
329  integer :: num_cells
330  double precision, dimension(num_cells) :: ds
330      , a_tilde, gn
331  double precision, dimension(num_cells+1) :: s
332  double precision :: integral
333  double precision bi, di_exp_bi
334  double precision cutoff
335  integer i, j
336
337  ! Maximum absorption coefficient suitable
337  ! for numerical computation
338  cutoff = 10.d0
339
340  integral = 0
341  do i=1, num_cells
342      bi = -a_tilde(i)*s(i+1)
343      do j=i+1, num_cells
344          bi = bi - a_tilde(j)*ds(j)
345      end do
346

```

```

347      ! In this case, so much absorption has
348      ! occurred
349      ! previously on the path that we don't
350      ! need
351      ! to continue, and we might get underflow
352      ! if we do.
353      if(bi .lt. -100.d0) then
354          di_exp_bi = 0.d0
355      else
356
357          ! Without this conditional, overflow
358          ! occurs.
359          ! Which is unnecessary, because large
360          ! absorption
361          ! means very small light added to the
362          ! ray
363          ! at this grid cell.
364          if(a_tilde(i) .lt. cutoff) then
365              if(a_tilde(i) .eq. 0) then
366                  di_exp_bi = ds(i) * exp(bi)
367              else
368                  ! In an attempt to avoid
369                  ! overflow
370                  ! and reduce compute time,
371                  ! I'm combining exponentials.
372                  ! di*exp(bi) -> di_exp_bi
373                  di_exp_bi = (exp(a_tilde(i)*s(i)
374                      +1) + bi) - exp(a_tilde(i)*s(
375                          i) + bi))/a_tilde(i)
376              end if
377              integral = integral + gn(i)*
378                  di_exp_bi
379          end if
380      end if
381  end do
382
383  end function calculate_ray_integral
384
385  ! Calculate maximum number of cells a path
386  ! through the grid could take
387  ! This is a loose upper bound
388  function calculate_max_cells(grid) result(
389      max_cells)
390      type(space_angle_grid) :: grid
391      integer :: max_cells
392      double precision dx, dy, zrange, phi_middle
393
394      ! Angle that will have the longest ray
395      phi_middle = grid%angles%phi(grid%angles%
396          nphi/2)
397      dx = grid%x%spacing(1)
398      dy = grid%y%spacing(1)

```

```

386     zrange = grid%z%maxval - grid%z%minval
387
388     max_cells = grid%z%num + ceiling((1/dx+1/dy)
389         *zrange*tan(phi_middle))
390 end function calculate_max_cells
391
392 ! Traverse from surface or bottom to point (xi
393     , yj, zk)
394 ! in the direction omega_p, extracting path
395     lengths (ds) and
396 ! function values (f) along the way,
397 ! as well as number of cells traversed (n).
398 subroutine traverse_ray(grid, iops, source, i,
399     j, k, p, s_array, ds, a_tilde, gn,
400     num_cells)
401     type(space_angle_grid) :: grid
402     type(optical_properties) :: iops
403     double precision, dimension(:,:,:,:,:) :: source
404     integer :: i, j, k, p
405     double precision, dimension(:) :: s_array,
406     ds, a_tilde, gn
407     integer :: num_cells
408
409     integer t
410     double precision p0x, p0y, p0z
411     double precision p1x, p1y, p1z
412     double precision z0
413     double precision s_tilde, s
414     integer dir_x, dir_y, dir_z
415     integer shift_x, shift_y
416     integer cell_x, cell_y, cell_z
417     integer edge_x, edge_y
418     integer first_x, last_x, first_y, last_y,
419         last_z
420     double precision s_next_x, s_next_y,
421         s_next_z, s_next
422     double precision x_factor, y_factor,
423         z_factor
424     double precision ds_x, ds_y
425     double precision, dimension(grid%z%num) :: ds_z
426     double precision smx, smy
427
428     ! Divide by these numbers to get path
429     separation
430     ! from separation in individual dimensions
431     x_factor = grid%angles%sin_phi_p(p) * grid%
432         angles%cos_theta_p(p)
433     y_factor = grid%angles%sin_phi_p(p) * grid%
434         angles%sin_theta_p(p)
435     z_factor = grid%angles%cos_phi_p(p)

```

```

424
425 ! Destination point
426 p1x = grid%x%vals(i)
427 p1y = grid%y%vals(j)
428 p1z = grid%z%vals(k)
429
430 ! write(*,*) 'START PATH.'
431 ! write(*,*) 'ijk = ', i, j, k
432
433 ! Direction
434 if(p .le. grid%angles%nomega/2) then
435     ! Downwelling light originates from
        surface
436     z0 = grid%z%minval
437     dir_z = 1
438 else
439     ! Upwelling light originates from bottom
440     z0 = grid%z%maxval
441     dir_z = -1
442 end if
443
444 ! Total path length from origin to
        destination
445 ! (sign is correct for upwelling and
        downwelling)
446 s_tilde = (p1z - z0)/grid%angles%cos_phi_p(p
        )
447
448 ! Path spacings between edge intersections
        in each dimension
449 ! Set to 2*s_tilde if infinite in this
        dimension so that it's unreachable
450 ! (e.g., if ray is parallel to x axis, then
        no x intersection will occur.)
451 ! Assume x & y spacings are uniform,
452 ! so it's okay to just use the first value.
453 if(x_factor .eq. 0) then
454     ds_x = 2*s_tilde
455 else
456     ds_x = abs(grid%x%spacing(1)/x_factor)
457 end if
458 if(y_factor .eq. 0) then
459     ds_y = 2*s_tilde
460 else
461     ds_y = abs(grid%y%spacing(1)/y_factor)
462 end if
463
464 ! This one is an array because z spacing can
        vary
465 ! z_factor should never be 0,
466 ! because the ray is then horizontal
467 ! and infinite in length.

```

```

468 ! z_factor != 0 is ensured when nphi is even
469 .
470 ds_z(1:grid%z%num) = dir_z * grid%z%spacing
471     (1:grid%z%num)/z_factor
472 !
473 ! Origin point
474 p0x = p1x - s_tilde * x_factor
475 p0y = p1y - s_tilde * y_factor
476 p0z = p1z - s_tilde * z_factor
477 !
478 ! Direction of ray in each dimension. 1 =>
479     increasing. -1 => decreasing.
480 dir_x = int(sgn(p1x-p0x))
481 dir_y = int(sgn(p1y-p0y))
482 !
483 ! Shifts
484 ! Conversion from cell_inds to edge_inds
485 ! merge is fortran's ternary operator
486 shift_x = merge(1,0,dir_x>0)
487 shift_y = merge(1,0,dir_y>0)
488 !
489 ! Indices for cell containing origin point
490 cell_x = floor((p0x-grid%x%minval)/grid%x%
491     spacing(1)) + 1
492 cell_y = floor((p0y-grid%y%minval)/grid%y%
493     spacing(1)) + 1
494 ! x and y may be in periodic image, so shift
495     back.
496 cell_x = mod1(cell_x, grid%x%num)
497 cell_y = mod1(cell_y, grid%y%num)
498 !
499 ! z starts at top or bottom depending on
500     direction.
501 if(dir_z > 0) then
502     cell_z = 1
503 else
504     cell_z = grid%z%num
505 end if
506 !
507 ! Edge indices preceding starting cells
508 edge_x = mod1(cell_x + shift_x, grid%x%num)
509 edge_y = mod1(cell_y + shift_y, grid%y%num)
510 !
511 ! First and last cells in each
512 if(dir_x .gt. 0) then
513     first_x = 1
514     last_x = grid%x%num
515 else
516     first_x = grid%x%num
517     last_x = 1
518 end if

```

```

512     if(dir_y .gt. 0) then
513         first_y = 1
514         last_y = grid%y%num
515     else
516         first_y = grid%y%num
517         last_y = 1
518     end if
519     if(dir_z .gt. 0) then
520         last_z = grid%z%num
521     else
522         last_z = 1
523     end if
524
525     ! Calculate periodic images
526     smx = shift_mod(p0x, grid%x%minval, grid%x%
527                     maxval)
527     smy = shift_mod(p0y, grid%y%minval, grid%y%
528                     maxval)
529
530     ! Path length to next edge plane in each
531     ! dimension
532     if(abs(x_factor) .lt. 1.d-10) then
533         ! Will never cross, so set above total
534         ! path length
535         s_next_x = 2*s_tilde
536     else if(cell_x .eq. last_x) then
537         ! If starts out at last cell, then
538         ! compare to periodic image
539         s_next_x = (grid%x%edges(first_x) + dir_x
540                     * (grid%x%maxval - grid%x%minval)&
541                     - smx) / x_factor
542     else
543         ! Otherwise, just compare to next cell
544         s_next_x = (grid%x%edges(edge_x) - smx) /
545                     x_factor
546     end if
547
548     ! Path length to next edge plane in each
549     ! dimension
550     if(abs(y_factor) .lt. 1.d-10) then
551         ! Will never cross, so set above total
552         ! path length
553         s_next_y = 2*s_tilde
554     else if(cell_y .eq. last_y) then
555         ! If starts out at last cell, then
556         ! compare to periodic image
557         s_next_y = (grid%y%edges(first_y) + dir_y
558                     * (grid%y%maxval - grid%y%minval)&
559                     - smy) / y_factor
560     else
561         ! Otherwise, just compare to next cell

```

```

552     s_next_y = (grid%y%edges(edge_y) - smy) /
553         y_factor
554 end if
555
556 s_next_z = ds_z(cell_z)
557
558 ! Initialize path
559 s = 0.d0
560 s_array(1) = 0.d0
561
562 ! Start with t=0 so that we can increment
563     before storing,
564 ! so that t will be the number of grid cells
565     at the end of the loop.
566 t = 0
567
568 ! s is the beginning of the current cell,
569 ! s_next is the end of the current cell.
570 do while (s .lt. s_tilde)
571     ! Move cell counter
572     t = t + 1
573
574     ! Extract function values
575     a_tilde(t) = iops%abs_grid(cell_x, cell_y
576             , cell_z)
577     gn(t) = source(cell_x, cell_y, cell_z, p)
578
579     !write(*,*) ''
580     !write(*,*) 's_next_x = ', s_next_x
581     !write(*,*) 's_next_y = ', s_next_y
582     !write(*,*) 's_next_z = ', s_next_z
583     !write(*,*) 'theta, phi =', grid%angles%
584             theta_p(p)*180.d0/pi, grid%angles%
585             phi_p(p)*180.d0/pi
586     !write(*,*) 's = ', s, '/', s_tilde
587     !write(*,*) 'cell_z =', cell_z, '/', grid
588             %z%num
589     !write(*,*) 's_next_z =', s_next_z
590     !write(*,*) 'last_z =', last_z
591     !write(*,*) 'new'
592
593     ! Move to next cell in path
594     if(s_next_x .le. min(s_next_y, s_next_z))
595         then
596             ! x edge is closest
597             s_next = s_next_x
598
599             ! Increment indices (periodic)
600             cell_x = mod1(cell_x + dir_x, grid%x%
601                         num)

```

```

593     edge_x = mod1(edge_x + dir_x, grid%x%
      num)
594
595     ! x intersection after the one at s=
      s_next
596     s_next_x = s_next + ds_x
597
598   else if (s_next_y .le. min(s_next_x,
      s_next_z)) then
599     ! y edge is closest
600     s_next = s_next_y
601
602     ! Increment indices (periodic)
603     cell_y = mod1(cell_y + dir_y, grid%y%
      num)
604     edge_y = mod1(edge_y + dir_y, grid%y%
      num)
605
606     ! y intersection after the one at s=
      s_next
607     s_next_y = s_next + ds_y
608
609   else if (s_next_z .le. min(s_next_x,
      s_next_y)) then
610     ! z edge is closest
611     s_next = s_next_z
612
613     ! Increment indices
614     cell_z = cell_z + dir_z
615
616     ! write(*,*) 'z edge, s_next =', s_next
617
618     ! z intersection after the one at s=
      s_next
619     if(dir_z * (last_z - cell_z) .gt. 0)
      then
        ! Only look ahead if we aren't at
        the end
        s_next_z = s_next + ds_z(cell_z)
620     else
        ! Otherwise, no need to continue.
        ! this is our final destination.
        ! exit
        s_next_z = 2*s_tilde
        ! write(*,*) 'end. s_next_z =',
          s_next_z
621     end if
622
623   end if
624
625   ! Cut off early if this is the end

```

```

633      ! This will be the last cell traversed if
634      s_next >= s_tilde
635      s_next = min(s_tilde, s_next)
636      ! Store path length
637      s_array(t+1) = s_next
638      ! Extract path length from same cell as
639      ! function vals
640      ds(t) = s_next - s
641      ! Update path length
642      s = s_next
643    end do
644
645    ! Return number of cells traversed
646    num_cells = t
647
648  end subroutine traverse_ray
649 end module asymptotics

```

rte\_sparse\_matrices.f90

```

1 module rte_sparse_matrices
2 use sag
3 use kelp_context
4 use mgmres
5 use type_consts
6 !use hdf5_utils
7 ! Use 64-bit integers for LIS
8 ! Necessary for FD solution w/ large matrices
9 #define LONG_LONG
10 #include "lisf.h"
11 implicit none
12
13 type solver_opts
14   integer maxiter_inner, maxiter_outer
15   double precision tol_abs, tol_rel
16 end type solver_opts
17
18 type rte_mat
19   type(space_angle_grid) grid
20   type(optical_properties) iops
21   type(solver_opts) params
22   integer nx, ny, nz, nomega
23   integer i, j, k, p
24   integer(index_kind) nonzero, n_total
25   integer x_block_size, y_block_size,
26         z_block_size, omega_block_size
27   double precision, dimension(:), allocatable
28         :: surface_vals

```

```

29 ! CSR format
30 ! http://www.scipy-lectures.org/advanced/
31     scipy_sparse/csr_matrix.html
32 ! with LIS method 2 (LIS manual, p.19)
33 integer(index_kind), dimension(:),
34     allocatable :: ptr, col
35 double precision, dimension(:), allocatable
36     :: data
37
38 ! Lis Matrix and vectors
39 LIS_MATRIX A
40 LIS_VECTOR b, x
41 LIS_SOLVER solver
42 LIS_INTEGER ierr
43 character(len=1024) solver_opts
44 logical initx_zeros
45
46 ! Pointer to solver subroutine
47 ! Set to mgmres by default
48 !procedure(solver_interface), pointer, nopass
49     :: solver => mgmres_st
50
51 contains
52 procedure :: init => mat_init
53 procedure :: deinit => mat_deinit
54 procedure :: calculate_size
55 procedure :: set_solver_opts =>
56     mat_set_solver_opts
57 procedure :: set_row => mat_set_row
58 procedure :: assign => mat_assign
59 procedure :: add => mat_add
60 procedure :: assign_rhs => mat_assign_rhs
61 procedure :: add_rhs => mat_add_rhs
62 !procedure :: store_index => mat_store_index
63 !procedure :: find_index => mat_find_index
64 procedure :: set_bc => mat_set_bc
65 procedure :: solve => mat_solve
66 procedure :: get_solver_stats
67 procedure :: ind => mat_ind
68 !procedure :: to_hdf => mat_to_hdf
69 procedure :: attenuate
70 procedure :: angular_integral
71 procedure :: add_source
72
73 ! Derivative subroutines
74 procedure x_cd2
75 procedure x_cd2_first
76 procedure x_cd2_last
77 procedure y_cd2
78 procedure y_cd2_first
79 procedure y_cd2_last
80 procedure z_cd2
81 procedure z_fd2

```

```

77   procedure z_bd2
78   procedure z_surface_bc
79   procedure z_bottom_bc
80
81 end type rte_mat
82
83 interface
84   ! Define interface for external procedure
85   ! https://stackoverflow.com/questions/8549415/how-to-declare-the-interface-section-for-a-procedure-argument-which-in-turn-ref
86   subroutine solver_interface(n_total, nonzero,
87     row, col, data, &
88     sol, rhs, maxiter_outer, maxiter_inner,
89     &
90     tol_abs, tol_rel)
91   use type_consts
92   integer(index_kind) :: n_total, nonzero
93   integer, dimension(nonzero) :: row, col
94   double precision, dimension(nonzero) :: data
95   double precision, dimension(nonzero) :: sol
96   double precision, dimension(n_total) :: rhs
97   integer :: maxiter_outer, maxiter_inner
98   double precision :: tol_abs, tol_rel
99   end subroutine solver_interface
100 end interface
101
102 contains
103
104   subroutine mat_init(mat, grid, iops)
105     class(rte_mat) mat
106     type(space_angle_grid) grid
107     type(optical_properties) iops
108     integer(index_kind) nnz, n_total
109
110     LIS_INTEGER comm_world
111
112     mat%grid = grid
113     mat%iops = iops
114
115     call mat%calculate_size()
116
117     mat%solver_opts = ''
118     mat% ierr = 0
119
120     n_total = mat%n_total
121     nnz = mat%nonzero

```

```

122
123     write(*,*) 'lis_init'
124     call lis_initialize(mat% ierr)
125
126     call lis_solver_create(mat% solver, mat% ierr)
127
128     call lis_matrix_create(comm_world, mat% A,
129                           mat% ierr)
130     call lis_vector_create(comm_world, mat% b,
131                           mat% ierr)
132     call lis_vector_create(comm_world, mat% x,
133                           mat% ierr)
134
135     call lis_matrix_set_size(mat% A, n_total,
136                               n_total, mat% ierr)
137     call lis_vector_set_size(mat% b, n_total,
138                               n_total, mat% ierr)
139     call lis_vector_set_size(mat% x, n_total,
140                               n_total, mat% ierr)
141
142     call lis_vector_set_all(0.0d0, mat% x, mat%
143                             ierr)
144     call lis_vector_set_all(0.0d0, mat% b, mat%
145                             ierr)
146
147     if(mat% ierr .ne. 0) then
148         write(*,*) 'INIT ERR: ', mat% ierr
149         call exit(1)
150     end if
151
152     ! CSR Format
153     ! http://www.scipy-lectures.org/advanced/scipy\_sparse/csr\_matrix.html
154
155     write(*,*) 'Allocate CSR arrays'
156     allocate(mat% ptr(n_total+1))
157     allocate(mat% col(nnz))
158     allocate(mat% data(nnz))
159     allocate(mat% surface_vals(grid% angles% nomega
160                                ))
161
162     mat% ptr(n_total+1) = nnz
163 end subroutine mat_init
164
165 subroutine mat_deinit(mat)
166     class(rte_mat) mat
167
168     call lis_matrix_destroy(mat% A, mat% ierr)
169     call lis_vector_destroy(mat% b, mat% ierr)
170     call lis_vector_destroy(mat% x, mat% ierr)

```

```

161 |     call lis_solver_destroy(mat%solver, mat% ierr
162 |     )
163 |     call lis_finalize(mat% ierr)
164 |     if(mat% ierr .ne. 0) then
165 |       write(*,*) 'DEINIT ERR: ', mat% ierr
166 |       call exit(1)
167 |     end if
168 |
169 |     deallocate(mat%ptr)
170 |     deallocate(mat%col)
171 |     deallocate(mat%data)
172 |     deallocate(mat%surface_vals)
173 |   end subroutine mat_deinit
174 |
175 |   subroutine calculate_size(mat)
176 |     class(rte_mat) mat
177 |     integer(index_kind) nx, ny, nz, nomega
178 |
179 |     nx = mat%grid%x%num
180 |     ny = mat%grid%y%num
181 |     nz = mat%grid%z%num
182 |     nomega = mat%grid%angles%nomega
183 |
184 |     !mat%nonzero = nx * ny * ntheta * nphi * ( (
185 |       nz-1) * (6 + ntheta * nphi) + 1)
186 |     mat%nonzero = nx * ny * nomega * (nz * (
187 |       nomega + 6) - 1)
188 |     mat%n_total = nx * ny * nz * nomega
189 |     write(*,*) 'nnz = ', mat%nonzero
190 |     write(*,*) 'n_total = ', mat%n_total
191 |
192 |     !mat%theta_block_size = 1
193 |     !mat%phi_block_size = mat%theta_block_size *
194 |       ntheta
195 |     mat%omega_block_size = 1
196 |     mat%y_block_size = int(mat%omega_block_size *
197 |       nomega)
198 |     mat%x_block_size = int(mat%y_block_size * ny
199 |       )
200 |     mat%z_block_size = int(mat%x_block_size * nx
201 |       )
202 |   end subroutine calculate_size
203 |
204 |   subroutine mat_to_hdf(mat, filename)
205 |     class(rte_mat) mat
206 |     character(len=*) filename
207 |     call write_coo(filename, mat%row, mat%col,
208 |       mat%data, mat%nonzero)

```

```

203 !   end subroutine mat_to_hdf
204
205 subroutine mat_set_bc(mat, bc)
206   class(rte_mat) mat
207   class(boundary_condition) bc
208   integer p
209
210   do p=1, mat%grid%angles%nomega/2
211     mat%surface_vals(p) = bc%bc_grid(p)
212   end do
213 end subroutine mat_set_bc
214
215 subroutine mat_solve(mat)
216   class(rte_mat) mat
217   character(len=64) init_opt
218
219   ! write(*,*) 'mat%n_total =', mat%n_total
220   ! write(*,*) 'mat%nonzero =', mat%nonzero
221   ! open(unit=1, file='ptr.txt')
222   ! open(unit=2, file='col.txt')
223   ! open(unit=3, file='data.txt')
224   ! write(1,*) mat%ptr
225   ! write(2,*) mat%col
226   ! write(3,*) mat%data
227   ! close(1)
228   ! close(2)
229   ! close(3)
230
231   ! Create matrix
232   write(*,*) 'LIS Set CSR'
233   call lis_matrix_set_csr(mat%nonzero, mat%ptr
234     , mat%col, mat%data, mat%A, mat% ierr)
235   write(*,*) 'LIS Assemble'
236   call lis_matrix_assemble(mat%A, mat% ierr)
237
238   ! Set solver options
239   if(mat%initx_zeros) then
240     init_opt = "-initx_zeros true -print out"
241   else
242     init_opt = "-initx_zeros false -print out"
243   end if
244
245   write(*,*) 'LIS set solver options'
246   write(*,*) 'opt: ', trim(init_opt)
247   call lis_solver_set_option(init_opt, mat%
248     solver, mat% ierr)
249   if(len(trim(mat%solver_opts)) .gt. 0) then

```

```

248      write(*,*) 'opt: ', trim(mat%solver_opts
249      )
250      call lis_solver_set_option(mat%
251          solver_opts, mat%solver, mat% ierr)
252  end if
253 ! Solve
254 write(*,*) 'LIS Solve'
255 call lis_solve(mat%A, mat%b, mat%x, mat%
256     solver, mat% ierr)
257 write(*,*) 'LIS Solve done'
258
259 subroutine mat_solve
260
261 subroutine get_solver_stats(mat, lis_iter,
262     lis_time, lis_resid)
263 class(rte_mat) mat
264 integer lis_iter
265 double precision lis_time
266 double precision lis_resid
267
268 call lis_solver_get_iter(mat%solver,
269     lis_iter, mat% ierr)
270 call lis_solver_get_time(mat%solver,
271     lis_time, mat% ierr)
272 call lis_solver_get_residualnorm(mat%solver,
273     lis_resid, mat% ierr)
274 end subroutine get_solver_stats
275
276 subroutine mat_set_solver_opts(mat,
277     solver_opts)
278 class(rte_mat) mat
279 character(len=*) solver_opts
280 mat%solver_opts = solver_opts
281 end subroutine mat_set_solver_opts
282
283 function mat_ind(mat, i, j, k, p) result(ind)
284 ! Assuming var ordering: z, x, y, omega
285 class(rte_mat) mat
286 integer i, j, k, p
287 integer(index_kind) ind
288
289 ind = (i-1) * mat%x_block_size + (j-1) * mat%
290     %y_block_size + &
291     (k-1) * mat%z_block_size + p * mat%
292     omega_block_size
293 end function mat_ind
294
295 subroutine mat_set_row(mat, ent, row_num)
296 ! Start new row for CSR format

```

```

288     class(rte_mat) mat
289     integer(index_kind) ent, row_num
290     ! 0-indexing for LIS
291     mat%ptr(row_num) = ent - 1
292 end subroutine mat_set_row
293
294 subroutine mat_assign(mat, ent, val, i, j, k,
295   p)
296   ! It's assumed that this is the first time
297   ! this entry is defined
298   class(rte_mat) mat
299   double precision val
300   integer i, j, k, p
301   integer(index_kind) ent
302
303   ! LIS method 2 (LIS manual, p. 19) requires
304   ! 0-indexing
305   mat%col(ent) = mat%ind(i, j, k, p) - 1
306   mat%data(ent) = val
307
308   ent = ent + 1
309 end subroutine mat_assign
310
311 subroutine mat_add(mat, repeat_ent, val)
312   ! Use this when you know that this entry has
313   ! already been assigned
314   ! and you'd like to add this value to the
315   ! existing value.
316
317   class(rte_mat) mat
318   double precision val
319   integer(index_kind) repeat_ent
320
321   ! Entry number where value is already stored
322   mat%data(repeat_ent) = mat%data(repeat_ent)
323   + val
324 end subroutine mat_add
325
326 subroutine mat_assign_rhs(mat, row_num, data)
327   class(rte_mat) mat
328   double precision data
329   integer(index_kind) row_num
330
331   call lis_vector_set_value(LIS_INS_VALUE,
332     row_num, data, mat%b, mat%ierr)
333   if(mat%ierr .ne. 0) then
334     write(*,*) 'RHS ERR: ', mat%ierr
335     call exit(1)
336   end if
337 end subroutine mat_assign_rhs

```

```

332  subroutine mat_add_rhs(mat, row_num, data)
333    class(rte_mat) mat
334    double precision data
335    integer(index_kind) row_num
336
337    call lis_vector_set_value(LIS_ADD_VALUE,
338      row_num, data, mat%b, mat% ierr)
339    if(mat% ierr .ne. 0) then
340      write(*,*) 'RHS ERR: ', mat% ierr
341      call exit(1)
342    end if
343  end subroutine mat_add_rhs
344
345 ! subroutine mat_store_index(mat, row_num,
346 !   col_num)
347 !   ! Remember where we stored information for
348 !   ! this matrix element
349 !   ! class(rte_mat) mat
350 !   ! integer row_num, col_num
351 !   ! mat%index_map(row_num, col_num) = mat%ent
352 ! end subroutine
353
354 ! function mat_find_index(mat, row_num,
355 !   col_num) result(index)
356 !   ! Find the position in row, col, data
357 !   ! where this entry
358 !   ! is defined.
359 !   ! class(rte_mat) mat
360 !   ! integer row_num, col_num, index
361 !   ! index = mat%index_map(row_num, col_num)
362
363 !   ! This took up 95% of execution time.
364 !   ! Only search up to most recently assigned
365 !   ! index
366 !   ! do index=1, mat%ent-1
367 !     ! if( (mat%row(index) .eq. row_num) .
368 !       and. (mat%col(index) .eq. col_num)) then
369 !       ! exit
370 !       ! end if
371 !   ! end do
372 ! end function mat_find_index
373
374 subroutine attenuate(mat, indices, repeat_ent)
375 ! Has to be called after angular_integral
376 ! Because they both write to the same matrix
377 ! entry
378 ! And adding here is more efficient than a
379 ! conditional
380 ! in the angular loop.
381 class(rte_mat) mat

```

```

374      double precision attenuation
375      type(index_list) indices
376      double precision aa, bb
377      integer(index_kind) repeat_ent
378
379      aa = mat%iops%abs_grid(indices%i, indices%j,
380                               indices%k)
380      bb = mat%iops%scat
381      attenuation = aa + bb
382
383      call mat%add(repeat_ent, attenuation)
384 end subroutine attenuate
385
386 subroutine add_source(mat, indices, row_num)
387 ! Has to be called after angular_integral
388 ! Because they both write to the same matrix
389 ! entry
390 ! And adding here is more efficient than a
391 ! conditional
392 ! in the angular loop.
393 class(rte_mat) mat
394 type(index_list) indices
395 integer(index_kind) row_num
396 double precision source_val
397
398 source_val = mat%iops%source_grid(indices%i,
399                                     indices%j, indices%k, indices%p)
400
401 call mat%add_rhs(row_num, source_val)
402 end subroutine add_source
403
404 subroutine x_cd2(mat, indices, ent)
405 class(rte_mat) mat
406 double precision val, dx
407 type(index_list) indices
408 integer i, j, k, p
409 integer(index_kind) ent
410
411 i = indices%i
412 j = indices%j
413 k = indices%k
414 p = indices%p
415
416 dx = mat%grid%x%spacing(1)
417
418 val = mat%grid%angles%sin_phi_p(p) &
419      * mat%grid%angles%cos_theta_p(p) / (2.
420      d0 * dx)
421
422 call mat%assign(ent, -val, i-1, j, k, p)
423 call mat%assign(ent, val, i+1, j, k, p)

```

```

420  end subroutine x_cd2
421
422  subroutine x_cd2_first(mat, indices, ent)
423      class(rte_mat) mat
424      double precision val, dx
425      integer nx
426      type(index_list) indices
427      integer i, j, k, p
428      integer(index_kind) ent
429
430      i = indices%i
431      j = indices%j
432      k = indices%k
433      p = indices%p
434
435      dx = mat%grid%x%spacing(1)
436      nx = mat%grid%x%num
437
438      val = mat%grid%angles%sin_phi_p(p) &
439          * mat%grid%angles%cos_theta_p(p) / (2.
440              d0 * dx)
441
442      call mat%assign(ent,-val,nx,j,k,p)
443      call mat%assign(ent,val,i+1,j,k,p)
444  end subroutine x_cd2_first
445
446  subroutine x_cd2_last(mat, indices, ent)
447      class(rte_mat) mat
448      double precision val, dx
449      type(index_list) indices
450      integer i, j, k, p
451      integer(index_kind) ent
452
453      i = indices%i
454      j = indices%j
455      k = indices%k
456      p = indices%p
457
458      dx = mat%grid%x%spacing(1)
459
460      val = mat%grid%angles%sin_phi_p(p) &
461          * mat%grid%angles%cos_theta_p(p) / (2.
462              d0 * dx)
463
464      call mat%assign(ent,-val,i-1,j,k,p)
465      call mat%assign(ent,val,1,j,k,p)
466  end subroutine x_cd2_last
467
468  subroutine y_cd2(mat, indices, ent)
469      class(rte_mat) mat

```

```

468 |     double precision val, dy
469 |     type(index_list) indices
470 |     integer i, j, k, p
471 |     integer(index_kind) ent
472 |
473 |     i = indices%i
474 |     j = indices%j
475 |     k = indices%k
476 |     p = indices%p
477 |
478 |     dy = mat%grid%y%spacing(1)
479 |
480 |     val = mat%grid%angles%sin_phi_p(p) &
481 |           * mat%grid%angles%sin_theta_p(p) / (2.
482 |                                         d0 * dy)
483 |
484 |     call mat%assign(ent,-val,i,j-1,k,p)
485 |     call mat%assign(ent,val,i,j+1,k,p)
486 | end subroutine y_cd2
487 |
488 | subroutine y_cd2_first(mat, indices, ent)
489 |   class(rte_mat) mat
490 |   double precision val, dy
491 |   integer ny
492 |   type(index_list) indices
493 |   integer i, j, k, p
494 |   integer(index_kind) ent
495 |
496 |   i = indices%i
497 |   j = indices%j
498 |   k = indices%k
499 |   p = indices%p
500 |
501 |   dy = mat%grid%y%spacing(1)
502 |   ny = mat%grid%y%num
503 |
504 |   val = mat%grid%angles%sin_phi_p(p) &
505 |         * mat%grid%angles%sin_theta_p(p) / (2.
506 |                                         d0 * dy)
507 |
508 |   call mat%assign(ent,-val,i,ny,k,p)
509 |   call mat%assign(ent,val,i,j+1,k,p)
510 | end subroutine y_cd2_first
511 |
512 | subroutine y_cd2_last(mat, indices, ent)
513 |   class(rte_mat) mat
514 |   double precision val, dy
515 |   type(index_list) indices

```

```

516
517     i = indices%i
518     j = indices%j
519     k = indices%k
520     p = indices%p
521
522     dy = mat%grid%y%spacing(1)
523
524     val = mat%grid%angles%sin_phi_p(p) &
525           * mat%grid%angles%sin_theta_p(p) / (2.
526             d0 * dy)
527
528     call mat%assign(ent,-val,i,j-1,k,p)
529     call mat%assign(ent,val,i,1,k,p)
530   end subroutine y_cd2_last
531
532   subroutine z_cd2(mat, indices, ent)
533     class(rte_mat) mat
534     double precision val, dz
535     type(index_list) indices
536     integer i, j, k, p
537     integer(index_kind) ent
538
539     i = indices%i
540     j = indices%j
541     k = indices%k
542     p = indices%p
543
544     dz = mat%grid%z%spacing(indices%k)
545
546     val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
547       dz)
548
549     call mat%assign(ent,-val,i,j,k-1,p)
550     call mat%assign(ent,val,i,j,k+1,p)
551   end subroutine z_cd2
552
553   subroutine z_fd2(mat, indices, ent, repeat_ent
554     )
555     ! Has to be called after angular_integral
556     ! Because they both write to the same matrix
557     ! entry
558     ! And adding here is more efficient than a
559     ! conditional
560     ! in the angular loop.
561     class(rte_mat) mat
562     double precision val, val1, val2, val3, dz
563     type(index_list) indices
564     integer i, j, k, p
565     integer(index_kind) ent, repeat_ent

```

```

562 |     i = indices%i
563 |     j = indices%j
564 |     k = indices%k
565 |     p = indices%p
566 |
567 |     dz = mat%grid%z%spacing(indices%k)
568 |
569 |     val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
570 |         dz)
571 |     val1 = -3.d0 * val
572 |     val2 = 4.d0 * val
573 |     val3 = -val
574 |
575 |     call mat%add(repeat_ent, val1)
576 |     call mat%assign(ent, val2, i, j, k+1, p)
577 |     call mat%assign(ent, val3, i, j, k+2, p)
578 end subroutine z_fd2
579
580 subroutine z_bd2(mat, indices, ent, repeat_ent
581 )
582 ! Has to be called after angular_integral
583 ! Because they both write to the same matrix
584 ! entry
585 ! And adding here is more efficient than a
586 ! conditional
587 ! in the angular loop.
588 class(rte_mat) mat
589 double precision val, val1, val2, val3, dz
590 type(index_list) indices
591 integer i, j, k, p
592 integer(index_kind) ent, repeat_ent
593
594 i = indices%i
595 j = indices%j
596 k = indices%k
597 p = indices%p
598
599 dz = mat%grid%z%spacing(indices%k)
600
601 val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
602 |         dz)
603
604 val1 = 3.d0 * val
605 val2 = -4.d0 * val
606 val3 = val
607
608 call mat%add(repeat_ent, val1)
609 call mat%assign(ent, val2, i, j, k-1, p)
610 call mat%assign(ent, val3, i, j, k-2, p)
611
612 end subroutine z_bd2

```

```

608
609 subroutine angular_integral(mat, indices, ent)
610   class(rte_mat) mat
611   ! Primed angular integration variables
612   integer pp
613   double precision val
614   type(index_list) indices
615   integer(index_kind) ent
616
617   do pp=1, mat%grid%angles%nomega
618     val = -mat%iops%scat * mat%iops%
619       vsf_integral(indices%p, pp)
620     call mat%assign(ent, val, indices%i,
621                   indices%j, indices%k, pp)
622   end do
623 end subroutine angular_integral
624
625 subroutine z_surface_bc(mat, indices, row_num,
626   ent, repeat_ent)
627   class(rte_mat) mat
628   double precision bc_val
629   type(index_list) indices
630   double precision val1, val2, dz
631   integer(index_kind) row_num, ent, repeat_ent
632
633   dz = mat%grid%z%spacing(1)
634
635   val1 = mat%grid%angles%cos_phi_p(indices%p)
636     / (3.d0 * dz)
637   val2 = 3.d0 * val1
638   bc_val = 4.d0 * val1 * mat%surface_vals(
639     indices%p)
640
641   call mat%assign(ent, val1, indices%i, indices%j
642     , 2, indices%p)
643   call mat%add(repeat_ent, val2)
644   call mat%assign_rhs(row_num, bc_val)
645 end subroutine z_surface_bc
646
647 subroutine z_bottom_bc(mat, indices, ent,
648   repeat_ent)
649   class(rte_mat) mat
650   type(index_list) indices
651   double precision val1, val2, dz
652   integer nz
653   integer(index_kind) ent, repeat_ent
654
655   dz = mat%grid%z%spacing(1)
656   nz = mat%grid%z%num

```

```

651   val1 = -mat%grid%angles%cos_phi_p(indices%p)
652     / (3.d0 * dz)
653   val2 = 3.d0 * val1
654
655   call mat%assign(ent, val1, indices%i, indices%j
656     , nz-1, indices%p)
657   call mat%add(repeat_ent, val2)
658 end subroutine z_bottom_bc
659
660 end module rte_sparse_matrices

```

```

kelp_context.f90

1 module kelp_context
2 use sag
3 use prob
4 implicit none
5
6 ! Point in cylindrical coordinates
7 type point3d
8   double precision x, y, z, theta, r
9 contains
10  procedure :: set_cart => point_set_cart
11  procedure :: set_cyl => point_set_cyl
12  procedure :: cartesian_to_polar
13  procedure :: polar_to_cartesian
14 end type point3d
15
16 type frond_shape
17   double precision fs, fr, tan_alpha, alpha, ft
18 contains
19  procedure :: set_shape => frond_set_shape
20  procedure :: calculate_angles =>
21    frond_calculate_angles
22 end type frond_shape
23
24 type rope_state
25   integer nz
26   double precision, dimension(:), allocatable
27     :: frond_lengths, frond_stds, num_fronds,
28       water_speeds, water_angles
29 contains
30  procedure :: init => rope_init
31  procedure :: deinit => rope_deinit
32 end type rope_state
33
34 type depth_state
35   double precision frond_length, frond_std,
36     num_fronds, water_speeds, water_angles,
37     depth
38   integer depth_layer
39 contains
40  procedure :: set_depth

```

```

36     procedure :: length_distribution_cdf
37     procedure :: angle_distribution_pdf
38 end type depth_state
39
40 type optical_properties
41     integer num_vsf
42     type(space_angle_grid) grid
43     double precision, dimension(:), allocatable
44         :: vsf_angles, vsf_vals
45     double precision, dimension(:), allocatable
46         :: abs_water
47     double precision abs_kelp, scat
48     ! On x, y, z grid - including water & kelp.
49     double precision, dimension(:,:,:,:),
50         allocatable :: abs_grid
51     double precision, dimension(:,:,:,:),
52         allocatable :: source_grid
53     ! On theta, phi, theta_prime, phi_prime grid
54     double precision, dimension(:, :, :), allocatable
55         :: vsf, vsf_integral
56 contains
57     procedure :: init => iop_init
58     procedure :: calculate_coef_grids
59     procedure :: zero_source => iop_zero_source
60     procedure :: set_source => iop_set_source
61     procedure :: load_vsf
62     procedure :: eval_vsf
63     procedure :: calc_vsf_on_grid
64     procedure :: deinit => iop_deinit
65     procedure :: vsf_from_function
66 end type optical_properties
67
68 type boundary_condition
69     double precision I0, decay, theta_s, phi_s
70     type(space_angle_grid) grid
71     double precision, dimension(:), allocatable
72         :: bc_grid
73 contains
74     procedure :: bc_gaussian
75     procedure :: init => bc_init
76     procedure :: deinit => bc_deinit
77 end type boundary_condition
78
79 contains
80     function bc_gaussian(bc, theta, phi)
81         class(boundary_condition) bc
82         double precision theta, phi, diff
83         double precision bc_gaussian
84         diff = angle_diff_3d(theta, phi, bc%theta_s,
85             bc%phi_s)
86         bc_gaussian = exp(-bc%decay * diff)

```

```

81  end function bc_gaussian
82
83 subroutine bc_init(bc, grid, theta_s, phi_s,
84     decay, I0)
85     class(boundary_condition) bc
86     type(space_angle_grid) grid
87     double precision theta_s, phi_s, decay, I0
88     integer p
89     double precision theta, phi
90     double precision bc_norm
91     double precision, allocatable, dimension(:)
92         :: whole_bc_grid
93     integer nomega
94
95     nomega = grid%angles%nomega
96
97     allocate(bc%bc_grid(nomega/2))
98     allocate(whole_bc_grid(nomega))
99
100    bc%theta_s = theta_s
101    bc%phi_s = phi_s
102    bc%decay = decay
103    bc%I0 = I0
104
105    ! Only set BC for downwelling light
106    do p=1, nomega/2
107        theta = grid%angles%theta_p(p)
108        phi = grid%angles%phi_p(p)
109        bc%bc_grid(p) = bc%bc_gaussian(theta, phi)
110    end do
111
112    ! Normalize
113    ! Use 'whole_bc_grid' because angular
114    ! integration
115    ! subroutine requires all angles to have
116    ! values,
117    ! but 'bc%bc_grid' only has downwelling
118    ! values.
119    ! Use zeros for upwelling.
120    whole_bc_grid(1:nomega/2) = bc%bc_grid
121    whole_bc_grid(nomega/2+1:nomega) = 0
122    bc_norm = grid%angles%integrate_points(
123        whole_bc_grid)
124    bc%bc_grid = bc%I0 * bc%bc_grid / bc_norm
125
126 end subroutine bc_init
127
128 subroutine bc_deinit(bc)
129     class(boundary_condition) bc
130     deallocate(bc%bc_grid)
131
132 end subroutine

```

```

125
126 subroutine point_set_cart(point, x, y, z)
127   class(point3d) :: point
128   double precision x, y, z
129   point%x = x
130   point%y = y
131   point%z = z
132   call point%cartesian_to_polar()
133 end subroutine point_set_cart
134
135 subroutine point_set_cyl(point, theta, r, z)
136   class(point3d) :: point
137   double precision theta, r, z
138   point%theta = theta
139   point%r = r
140   point%z = z
141   call point%polar_to_cartesian()
142 end subroutine point_set_cyl
143
144 subroutine polar_to_cartesian(point)
145   class(point3d) :: point
146   point%x = point%r*cos(point%theta)
147   point%y = point%r*sin(point%theta)
148 end subroutine polar_to_cartesian
149
150 subroutine cartesian_to_polar(point)
151   class(point3d) :: point
152   point%r = sqrt(point%x**2 + point%y**2)
153   point%theta = atan2(point%y, point%x)
154 end subroutine cartesian_to_polar
155
156 subroutine frond_set_shape(frond, fs, fr, ft)
157   class(frond_shape) frond
158   double precision fs, fr, ft
159   frond%fs = fs
160   frond%fr = fr
161   frond%ft = ft
162   call frond%calculate_angles()
163 end subroutine frond_set_shape
164
165 subroutine frond_calculate_angles(frond)
166   class(frond_shape) frond
167   frond%tan_alpha = 2.d0*frond%fs*frond%fr /
168     (1.d0 + frond%fs)
169   frond%alpha = atan(frond%tan_alpha)
170 end subroutine
171
172 subroutine iop_init(iops, grid)
173   class(optical_properties) iops
174   type(space_angle_grid) grid

```

```

174      iops%grid = grid
175
176      ! Assume that these are preallocated and
177      ! passed to function
178      ! Nevermind, don't assume this.
179      allocate(iops%abs_water(grid%z%num))
180
181      ! Assume that these must be allocated here
182      ! NOTE: vsf_angles are defined on [0, pi].
183      ! (not on [-1, 1])
184      allocate(iops%vsf_angles(iops%num_vsf))
185      allocate(iops%vsf_vals(iops%num_vsf))
186      allocate(iops%vsf(grid%angles%nomega,grid%
187      angles%nomega))
188      allocate(iops%vsf_integral(grid%angles%
189      nomega,grid%angles%nomega))
190      allocate(iops%abs_grid(grid%x%num, grid%y%
191      num, grid%z%num))
192      allocate(iops%source_grid(grid%x%num, grid%y%
193      %num, grid%z%num, grid%angles%nomega))
194
195      call iops%zero_source()
196      end subroutine iop_init
197
198      subroutine iop_zero_source(iops)
199      class(optical_properties) iops
200
201      iops%source_grid = 0
202      end subroutine iop_zero_source
203
204      subroutine iop_set_source(iops, source)
205      class(optical_properties) iops
206      double precision, dimension(:,:,:,:,:) :::
207      source
208
209      iops%source_grid = source
210      end subroutine iop_set_source
211
212      subroutine calculate_coef_grids(iops, p_kelp)
213      class(optical_properties) iops
214      double precision, dimension(:,:,:,:) ::: p_kelp
215
216      integer k
217
218      ! Allow water IOPs to vary over depth
219      do k=1, iops%grid%z%num
220          iops%abs_grid(:,:,k) = (iops%abs_kelp -
221          iops%abs_water(k)) * p_kelp(:,:,k) +
222          iops%abs_water(k)

```

```

216    end do
217
218 end subroutine calculate_coef_grids
219
220
221 subroutine load_vsf(iops, filename, fmtstr)
222   class(optical_properties) :: iops
223   character(len=*) :: filename, fmtstr
224   double precision, dimension(:, :),
225             allocatable :: tmp_2d_arr
226   integer num_rows, num_cols, skip_lines_in
227
228   ! First column is the angle at which the
229   ! measurement is taken
230   ! Second column is the value of the VSF at
231   ! that angle
232   num_rows = iops%num_vsf
233   num_cols = 2
234   skip_lines_in = 1 ! Ignore comment on first
235   ! line
236
237   allocate(tmp_2d_arr(num_rows, num_cols))
238
239   tmp_2d_arr = read_array(filename, fmtstr,
240                           num_rows, num_cols, skip_lines_in)
241   iops%vsf_angles = tmp_2d_arr(:, 1)
242   iops%vsf_vals = tmp_2d_arr(:, 2)
243
244   ! write(*,*) 'vsf_angles = ', iops%
245   ! vsf_angles
246   ! write(*,*) 'vsf_vals = ', iops%vsf_vals
247
248   ! Pre-evaluate for all pair of angles
249   call iops%calc_vsf_on_grid()
250
251 end subroutine load_vsf
252
253 function eval_vsf(iops, theta)
254   class(optical_properties) iops
255   double precision theta
256   double precision eval_vsf
257
258   ! No need to set vsf(0) = 0.
259   ! It's the area under the curve that matters
260   ! , not the value.
261   eval_vsf = interp(theta, iops%vsf_angles,
262                     iops%vsf_vals, iops%num_vsf)
263
264 end function eval_vsf
265
266 subroutine rope_init(rope, grid)
267   class(rope_state) :: rope
268   type(space_angle_grid) :: grid

```

```

259
260     rope%nz = grid%z%num
261     allocate(rope%frond_lengths(rope%nz))
262     allocate(rope%frond_stds(rope%nz))
263     allocate(rope%water_speeds(rope%nz))
264     allocate(rope%water_angles(rope%nz))
265     allocate(rope%num_fronds(rope%nz))
266 end subroutine rope_init
267
268 subroutine rope_deinit(rope)
269     class(rope_state) rope
270     deallocate(rope%frond_lengths)
271     deallocate(rope%frond_stds)
272     deallocate(rope%water_speeds)
273     deallocate(rope%water_angles)
274     deallocate(rope%num_fronds)
275 end subroutine rope_deinit
276
277 subroutine set_depth(depth, rope, grid,
278                      depth_layer)
279     class(depth_state) depth
280     type(rope_state) rope
281     type(space_angle_grid) grid
282     integer depth_layer
283
284     depth%frond_length = rope%frond_lengths(
285                               depth_layer)
286     depth%frond_std = rope%frond_stds(
287                               depth_layer)
288     depth%water_speeds = rope%water_speeds(
289                               depth_layer)
290     depth%water_angles = rope%water_angles(
291                               depth_layer)
292     depth%num_fronds = rope%num_fronds(
293                               depth_layer)
294     depth%depth_layer = depth_layer
295     depth%depth = grid%z%vals(depth_layer)
296 end subroutine set_depth
297
298 function length_distribution_cdf(depth, L)
299     result(output)
300 ! C_L(L)
301     class(depth_state) depth
302     double precision L, L_mean, L_std
303     double precision output
304
305     L_mean = depth%frond_length
306     L_std = depth%frond_std
307
308     call normal_cdf(L, L_mean, L_std, output)

```

```

302 | end function length_distribution_cdf
303 |
304 | function angle_distribution_pdf(depth, theta_f
305 |   ) result(output)
306 |   ! P_{\theta_f}(\theta_f)
307 |   class(depth_state) depth
308 |   double precision theta_f, v_w, theta_w
309 |   double precision output
310 |   double precision diff
311 |
312 |   v_w = depth%water_speeds
313 |   theta_w = depth%water_angles
314 |
315 |   ! von_mises_pdf is only defined on [-pi, pi]
316 |   ! So take difference of angles and input
317 |   ! into
318 |   ! von_mises dist. centered & x=0.
319 |
320 |   call von_mises_pdf(diff, 0.d0, v_w, output)
321 | end function angle_distribution_pdf
322 |
323 | function angle_mod(theta) result(mod_theta)
324 |   ! Shift theta to the interval [-pi, pi]
325 |   ! which is where von_mises_pdf is defined.
326 |
327 |   double precision theta, mod_theta
328 |
329 |   mod_theta = mod(theta + pi, 2.d0*pi) - pi
330 | end function angle_mod
331 |
332 | function angle_diff_2d(theta1, theta2) result(
333 |   diff)
334 |   ! Shortest difference between two angles
335 |   ! which may be
336 |   ! in different periods.
337 |   double precision theta1, theta2, diff
338 |   double precision modt1, modt2
339 |
340 |   ! Shift to [0, 2*pi]
341 |   modt1 = mod(theta1, 2*pi)
342 |   modt2 = mod(theta2, 2*pi)
343 |
344 |   ! https://gamedev.stackexchange.com/questions/4467/comparing-angles-and-working-out-the-difference
345 |
346 |   diff = pi - abs(abs(modt1-modt2) - pi)
end function angle_diff_2d

```

```

347  function angle_diff_3d(theta, phi, theta_prime
348      , phi_prime) result(diff)
349      ! Angle between two vectors in spherical
350      ! coordinates
351      double precision theta, phi, theta_prime,
352          phi_prime
353      double precision alpha, diff
354
355
356      ! Faster, but produces lots of NaNs (at
357      ! least in Python)
358      !alpha = sin(theta)*sin(theta_prime)*cos(
359      !    theta-theta_prime) + cos(phi)*cos(
360      !    phi_prime)
361
362      ! Slower, but more accurate
363      alpha = (sin(phi)*sin(phi_prime) &
364          * (cos(theta)*cos(theta_prime) + sin(theta)
365              )*sin(theta_prime)) &
366          + cos(phi)*cos(phi_prime))
367
368      ! Avoid out-of-bounds errors due to rounding
369      alpha = min(1.d0, alpha)
370      alpha = max(-1.d0, alpha)
371
372      diff = acos(alpha)
373  end function angle_diff_3d
374
375 subroutine vsf_from_function(iops, func)
376     class(optical_properties) iops
377     double precision, external :: func
378     integer i
379     type(angle_dim) :: angle1d
380
381     call angle1d%set_bounds(-1.d0, 1.d0)
382     call angle1d%set_num(iops%num_vsf)
383     call angle1d%assign_legendre()
384
385     iops%vsf_angles(:) = acos(angle1d%vals(:))
386     do i=1, iops%num_vsf
387         iops%vsf_vals(i) = func(iops%vsf_angles(i
388             ))
389     end do
390
391     call iops%calc_vsf_on_grid()
392
393     call angle1d%deinit()
394  end subroutine vsf_from_function
395
396 subroutine calc_vsf_on_grid(iops)
397     class(optical_properties) iops

```

```

390   double precision th, ph, thp, php
391   integer p, pp
392   integer nomega
393   double precision norm
394
395   nomega = iops%grid%angles%nomega
396
397   do p=1, nomega
398     th = iops%grid%angles%theta_p(p)
399     ph = iops%grid%angles%phi_p(p)
400     do pp=1, nomega
401       thp = iops%grid%angles%theta_p(pp)
402       php = iops%grid%angles%phi_p(pp)
403       iops%vsf(p, pp) = iops%eval_vsf(
404         angle_diff_3d(th,ph,thp,php))
405     end do
406
407     ! Normalize each row of VSF (midpoint
408     ! rule)
409     norm = sum(iops%vsf(p,:) * iops%grid%
410               angles%area_p(:))
411     iops%vsf(p,:) = iops%vsf(p,:) / norm
412
413     ! % / meter light scattered
414     ! from cell pp (2nd ind.) into direction
415     ! p (1st ind.).
416     iops%vsf_integral(p, :) = iops%vsf(p, :)
417     &
418     * iops%grid%angles%area_p(:)
419     !write(*,*) 'vsf_integral (beta_pp)', p,
420     !      , iops%vsf_integral(p, : )
421   end do
422 end subroutine calc_vsf_on_grid
423
424 subroutine iop_deinit(iops)
425   class(optical_properties) iops
426   deallocate(iops%vsf_angles)
427   deallocate(iops%vsf_vals)
428   deallocate(iops%vsf)
429   deallocate(iops%vsf_integral)
430   deallocate(iops%abs_water)
431   deallocate(iops%abs_grid)
432   deallocate(iops%source_grid)
433
434 end subroutine iop_deinit
435
436 end module kelp_context

```

light\_context.f90

```

1 module light_context
2 ! Use 64-bit integers for LIS
3 ! Necessary for FD solution w/ large matrices
4 #define LONG__LONG
5 #include "lisf.h"
6 use sag
7 use rte_sparse_matrices
8 !use hdf5
9 implicit none
10
11 type light_state
12     double precision, dimension(:,:,:,:),
13         allocatable :: irradiance
14     double precision, dimension(:,:,:,:,:),
15         allocatable :: radiance
16     type(space_angle_grid) :: grid
17     type(rte_mat) :: mat
18 contains
19     procedure :: init => light_init
20     procedure :: init_grid => light_init_grid
21     procedure :: calculate_radiance
22     procedure :: calculate_irradiance =>
23         light_calculate_irradiance
24     procedure :: deinit => light_deinit
25     !procedure :: to_hdf => light_to_hdf
26 end type light_state
27
28 contains
29
30 ! Init for use with mat
31 subroutine light_init(light, mat)
32     class(light_state) light
33     type(rte_mat) mat
34     integer nx, ny, nz, nomega
35
36     light%mat = mat
37     light%grid = mat%grid
38
39     nx = light%grid%x%num
40     ny = light%grid%y%num
41     nz = light%grid%z%num
42     nomega = light%grid%angles%nomega
43
44     allocate(light%irradiance(nx, ny, nz))
45     allocate(light%radiance(nx, ny, nz, nomega))
46 end subroutine light_init
47
48 ! Init for use without mat
49 subroutine light_init_grid(light, grid)
50     class(light_state) light
51     type(space_angle_grid) grid
52     integer nx, ny, nz, nomega

```

```

50
51     light%grid = grid
52
53     nx = light%grid%x%num
54     ny = light%grid%y%num
55     nz = light%grid%z%num
56     nomega = light%grid%angles%nomega
57
58     allocate(light%irradiance(nx, ny, nz))
59     allocate(light%radiance(nx, ny, nz, nomega))
60 end subroutine light_init_grid
61
62 subroutine calculate_radiance(light)
63     class(light_state) light
64     integer i, j, k, p
65     integer nx, ny, nz, nomega
66     integer(index_kind) index
67     LIS_INTEGER lis_test_int
68
69     nx = light%grid%x%num
70     ny = light%grid%y%num
71     nz = light%grid%z%num
72     nomega = light%grid%angles%nomega
73
74     ! call lis_vector_get_size(light%mat%x, ln,
75     !                               gn)
76
77     ! write(*,*) 'ln = ', ln
78     ! write(*,*) 'gn = ', gn
79
80     index = 1
81
82     write(*,*) 'Set matrix values'
83     write(*,*) 'index_kind = ', storage_size(
84     !                                         index)
85     write(*,*) 'lis_kind = ', storage_size(
86     !                                         lis_test_int)
87     ! Set initial guess from provided radiance
88     ! Traverse solution vector in order
89     ! so as to avoid calculating index
90     do k=1, nz
91         do i=1, nx
92             do j=1, ny
93                 do p=1, nomega
94                     call lis_vector_set_value(
95                         LIS_INS_VALUE, index, &
96                         light%radiance(i,j,k,p),
97                         light%mat%x, light%mat%
98                         ierr)
99
100            if(light%mat%ierr .ne. 0) then

```

```

94      write(*,*) 'IG ERROR:', light
95      %mat% ierr
96      end if
97      index = index + 1
98      end do
99      end do
100     end do
101    end do
102
103   !call light%mat%initial_guess()
104
105   ! Solve (LIS)
106   write(*,*) 'Solve matrix'
107   call light%mat%solve()
108
109   index = 1
110
111   write(*,*) 'Extract solution'
112   ! Extract solution
113   do k=1, nz
114     do i=1, nx
115       do j=1, ny
116         do p=1, nomega
117           call lis_vector_get_value(light%
118             mat%x, index, &
119               light%radiance(i,j,k,p),
120               light%mat% ierr)
121           if(light%mat% ierr .ne. 0) then
122             write(*,*) 'EXTRACT ERROR:',
123               light%mat% ierr
124           end if
125           index = index + 1
126         end do
127       end do
128     end do
129   end do
130
131   subroutine calculate_radiance
132
133   subroutine light_calculate_irradiance(light)
134     class(light_state) light
135     integer i, j, k
136     integer nx, ny, nz
137     double precision, dimension(light%grid%
138       angles%nomega) :: tmp_rad
139
140     nx = light%grid%x%num
141     ny = light%grid%y%num
142     nz = light%grid%z%num
143
144     do i=1, nx

```

```

140   do j=1, ny
141     do k=1, nz
142       ! Use temporary array to avoid
143       ! creating one
144       ! implicitly at every spatial grid
145       ! point
146       tmp_rad = light%radiance(i,j,k,:)
147       light%irradiance(i,j,k) = &
148         light%grid%angles%
149           integrate_points(tmp_rad)
150     end do
151   end do
152 end do
153
154 end subroutine light_calculate_irradiance
155
156 ! subroutine light_to_hdf(light, radfile,
157 !   irradfile)
158 !   class(light_state) light
159 !   character(len=*) radfile
160 !   character(len=*) irradfile
161 !
162 !   call hdf_write_radiance(radfile, light%
163 !     radiance, light%grid)
164 !   call hdf_write_irradiance(irradfile, light%
165 !     irradiance, light%grid)
166 ! end subroutine light_to_hdf
167
168 subroutine light_deinit(light)
169   class(light_state) light
170
171   deallocate(light%irradiance)
172   deallocate(light%radiance)
173 end subroutine light_deinit
174
175 end module

```

rte3d.f90

```

1 module rte3d
2 use kelp_context
3 use rte_sparse_matrices
4 use light_context
5 use type_consts
6 implicit none
7
8 interface
9   subroutine deriv_interface(mat, indices, ent)
10    use rte_sparse_matrices
11    use type_consts
12    class(rte_mat) mat
13    type(index_list) indices

```

```

14     integer(index_kind) ent
15 end subroutine deriv_interface
16 subroutine angle_loop_interface(mat, indices,
17     ddx, ddy)
18     use rte_sparse_matrices
19     import deriv_interface
20     type(space_angle_grid) grid
21     type(rte_mat) mat
22     type(index_list) indices
23     procedure(deriv_interface) :: ddx, ddy
24 end subroutine angle_loop_interface
25 end interface
26 contains
27
28 subroutine whole_space_loop(mat, indices,
29     num_threads)
30     type(rte_mat) mat
31     type(index_list) indices
32     integer i, j, k
33     integer num_threads
34
35     procedure(deriv_interface), pointer :: ddx,
36         ddy
37     procedure(angle_loop_interface), pointer :::
38         angle_loop
39
40 !$omp parallel do default(none) shared(mat) &
41 !$omp private(ddx,ddy,angle_loop, k, i, j)
42     private(indices) &
43 !$omp num_threads(num_threads) collapse(3)
44 do k=1, mat%grid%z%num
45     do i=1, mat%grid%x%num
46         do j=1, mat%grid%y%num
47             indices%k = k
48             if(k .eq. 1) then
49                 angle_loop => surface_angle_loop
50             else if(k .eq. mat%grid%z%num) then
51                 angle_loop => bottom_angle_loop
52             else
53                 angle_loop => interior_angle_loop
54             end if
55
56             indices%i = i
57             if(indices%i .eq. 1) then
58                 ddx => x_cd2_first
59             else if(indices%i .eq. mat%grid%x%num
60 ) then
61                 ddx => x_cd2_last
62             else
63                 ddx => x_cd2

```

```

59         end if
60
61         indices%j = j
62         if(indices%j .eq. 1) then
63             ddy => y_cd2_first
64         else if(indices%j .eq. mat%grid%y%num
65             ) then
66             ddy => y_cd2_last
67         else
68             ddy => y_cd2
69         end if
70
71         call angle_loop(mat, indices, ddx,
72                         ddy)
73     end do
74 end do
75 !$omp end parallel do
76 end subroutine whole_space_loop
77
77 function calculate_start_ent(grid, indices)
78     result(ent)
79     type(space_angle_grid) grid
80     type(index_list) indices
81     integer(index_kind) ent
82     integer(index_kind) boundary_nnz, interior_nnz
83     integer(index_kind) num_boundary, num_interior
84     integer(index_kind) num_this_x, num_this_z
85
85     ! Nonzero matrix entries for an surface or
86     ! bottom spatial grid cell
87     ! Definitely an integer since nomega is even
88     boundary_nnz = grid%angles%nomega * (2 * grid%
89     angles%nomega + 11) / 2
88     ! Nonzero matrix entries for an interior
89     ! spatial grid cell
90     interior_nnz = grid%angles%nomega * (grid%
90     angles%nomega + 6)
91
91     ! Order: z, x, y, omega
92     ! Total number traversed so far in each
92     ! spatial category
93     ! row
94     num_this_x = indices%j - 1
95     ! depth layer
96     num_this_z = (indices%i - 1) * grid%y%num +
96     num_this_x
97
98     ! Calculate number of spatial grid cells of
98     ! each type which have
99     ! already been traversed up to this point

```

```

100 |     if(indices%k .eq. 1) then
101 |         num_boundary = num_this_z
102 |         num_interior = 0
103 |     else if(indices%k .eq. grid%z%num) then
104 |         num_boundary = (grid%x%num * grid%y%num) +
105 |             num_this_z
106 |         num_interior = (grid%z%num-2) * grid%x%num
107 |             * grid%y%num
108 |     else
109 |         num_boundary = grid%x%num * grid%y%num
110 |         num_interior = num_this_z + (indices%k-2) *
111 |             grid%x%num * grid%y%num
112 |     end if
113 |
114 |     ent = num_boundary * boundary_nnz +
115 |           num_interior * interior_nnz + 1
116 | end function calculate_start_ent
117 |
118 | function calculate_repeat_ent(ent, p) result(
119 |     repeat_ent)
120 |     integer p
121 |     integer(index_kind) ent, repeat_ent
122 |     ! Entry number for row=mat%ind(i,j,k,p), col=
123 |         mat%ind(i,j,k,p),
124 |     ! which will be modified multiple times in
125 |         this matrix row
126 |     repeat_ent = ent + p - 1
127 | end function calculate_repeat_ent
128 |
129 subroutine interior_angle_loop(mat, indices, ddx,
130 |     , ddy)
131 |     type(rte_mat) mat
132 |     type(index_list) indices
133 |     procedure(deriv_interface) :: ddx, ddy
134 |     integer p
135 |     integer(index_kind) ent, repeat_ent
136 |     integer(index_kind) row_num
137 |
138 |     ! Determine which matrix row to start at
139 |     ent = calculate_start_ent(mat%grid, indices)
140 |     indices%p = 1
141 |     row_num = mat%ind(indices%i, indices%j,
142 |         indices%k, indices%p)
143 |
144 |     do p=1, mat%grid%angles%nomega
145 |         indices%p = p
146 |         repeat_ent = calculate_repeat_ent(ent, p)
147 |         call mat%set_row(ent, row_num)
148 |         call mat%angular_integral(indices, ent)
149 |         call ddx(mat, indices, ent)

```

```

141 |     call ddy(mat, indices, ent)
142 |     call mat%z_cd2(indices, ent)
143 |     call mat%attenuate(indices, repeat_ent)
144 |     call mat%add_source(indices, row_num)
145 |     row_num = row_num + 1
146 |   end do
147 end subroutine
148
149 subroutine surface_angle_loop(mat, indices, ddx,
150 |     ddy)
150 type(rte_mat) mat
151 type(index_list) indices
152 integer p
153 procedure(deriv_interface) :: ddx, ddy
154 integer(index_kind) ent, repeat_ent
155 integer(index_kind) row_num
156
157 ! Determine which matrix row to start at
158 ent = calculate_start_ent(mat%grid, indices)
159 indices%p = 1
160 row_num = mat%ind(indices%i, indices%j,
161 |     indices%k, indices%p)
161
162 ! Downwelling
163 do p=1, mat%grid%angles%nomega / 2
164 |     indices%p = p
165 |     repeat_ent = calculate_repeat_ent(ent, p)
166 |     call mat%set_row(ent, row_num)
167 |     call mat%angular_integral(indices, ent)
168 |     call ddx(mat, indices, ent)
169 |     call ddy(mat, indices, ent)
170 |     call mat%z_surface_bc(indices, row_num, ent
171 |         , repeat_ent)
172 |     call mat%attenuate(indices, repeat_ent)
173 |     call mat%add_source(indices, row_num)
174 |     row_num = row_num + 1
174 end do
175 ! Upwelling
176 do p=mat%grid%angles%nomega/2+1, mat%grid%
177 |     angles%nomega
178 |     indices%p = p
179 |     repeat_ent = calculate_repeat_ent(ent, p)
180 |     call mat%set_row(ent, row_num)
181 |     call mat%angular_integral(indices, ent)
182 |     call ddx(mat, indices, ent)
183 |     call ddy(mat, indices, ent)
184 |     call mat%z_fd2(indices, ent, repeat_ent)
185 |     call mat%attenuate(indices, repeat_ent)
186 |     call mat%add_source(indices, row_num)
186 |     row_num = row_num + 1

```

```

187     end do
188 end subroutine surface_angle_loop
189
190 subroutine bottom_angle_loop(mat, indices, ddx,
191     ddy)
192     type(rte_mat) mat
193     type(index_list) indices
194     integer p
195     integer(index_kind) row_num, ent, repeat_ent
196     procedure(deriv_interface) :: ddx, ddy
197
198 ! Determine which matrix row to start at
199 ent = calculate_start_ent(mat%grid, indices)
200 indices%p = 1
201 row_num = mat%ind(indices%i, indices%j,
202     indices%k, indices%p)
203
204 ! Downwelling
205 do p=1, mat%grid%angles%nomega/2
206     indices%p = p
207     repeat_ent = calculate_repeat_ent(ent, p)
208     call mat%set_row(ent, row_num)
209     call mat%angular_integral(indices, ent)
210     call ddx(mat, indices, ent)
211     call ddy(mat, indices, ent)
212     call mat%z_bd2(indices, ent, repeat_ent)
213     call mat%attenuate(indices, repeat_ent)
214     call mat%add_source(indices, row_num)
215     row_num = row_num + 1
216 end do
217 ! Upwelling
218 do p=mat%grid%angles%nomega/2+1, mat%grid%
219     angles%nomega
220     indices%p = p
221     repeat_ent = calculate_repeat_ent(ent, p)
222     call mat%set_row(ent, row_num)
223     call mat%angular_integral(indices, ent)
224     call ddx(mat, indices, ent)
225     call ddy(mat, indices, ent)
226     call mat%z_bottom_bc(indices, ent,
227         repeat_ent)
228     call mat%attenuate(indices, repeat_ent)
229     call mat%add_source(indices, row_num)
230     row_num = row_num + 1
231 end do
232 end subroutine bottom_angle_loop
233
234 subroutine gen_matrix(mat, num_threads)
235     type(rte_mat) mat
236     type(index_list) indices

```

```

233     integer num_threads
234
235     call indices%init()
236
237     call whole_space_loop(mat, indices,
238         num_threads)
239     ! call surface_space_loop(mat, indices)
240     ! call interior_space_loop(mat, indices)
241     ! call bottom_space_loop(mat, indices)
242   end subroutine gen_matrix
243
244   subroutine rte3d_deinit(mat, iops, light)
245     type(rte_mat) mat
246     type(optical_properties) iops
247     type(light_state) light
248
249     call mat%deinit()
250     call iops%deinit()
251     call light%deinit()
252   end subroutine
253
254 end module rte3d

```

kelp3d.f90

```

1 ! Kelp 3D
2 ! Oliver Evans
3 ! 8/31/2017
4
5 ! Given superindividual/water current data at
6 ! each depth, generate kelp distribution at
7 ! each point in 3D space
8
9 module kelp3d
10
11 use kelp_context
12
13 implicit none
14
15 contains
16
17 subroutine generate_grid(xmin, xmax, nx, ymin,
18     ymax, ny, zmin, zmax, nz, ntheta, nphi, grid,
19     p_kelp)
20   double precision xmin, xmax, ymin, ymax, zmin,
21       zmax
22   integer nx, ny, nz, ntheta, nphi
23   type(space_angle_grid) grid
24   double precision, dimension(:,:,:),
25       allocatable :: p_kelp

```

```

21 |     call grid%set_bounds(xmin, xmax, ymin, ymax,
22 |                           zmin, zmax)
23 |     call grid%set_num(nx, ny, nz, ntheta, nphi)
24 |     allocate(p_kelp(nx,ny,nz))
25 |
26 end subroutine generate_grid
27
28 subroutine kelp3d_deinit(grid, rope, p_kelp)
29   type(space_angle_grid) grid
30   type(rope_state) rope
31   double precision, dimension(:,:,:,:),
32     allocatable :: p_kelp
33   call rope%deinit()
34   call grid%deinit()
35   deallocate(p_kelp)
36 end subroutine kelp3d_deinit
37
38 subroutine calculate_kelp_on_grid(grid, p_kelp,
39   frond, rope, quadrature_degree, n_images,
40   num_threads)
41   type(space_angle_grid), intent(in) :: grid
42   type(frond_shape), intent(in) :: frond
43   type(rope_state), intent(in) :: rope
44   type(point3d) point
45   integer, intent(in) :: quadrature_degree
46   integer, optional :: n_images
47   double precision, dimension(grid%x%num, grid%y
48     %num, grid%z%num) :: p_kelp
49   type(depth_state) depth
50   integer num_threads
51
52   integer i, j, k, nx, ny, nz
53   double precision x, y, z
54   ! Number of periodic images
55   ! to consider in each horizontal direction
56   ! for kelp distribution
57   ! n_images=1 => 3x3 meta-grid
58   ! n_images=2 => 5x5 meta-grid (only necessary
59   ! for very dense kelp ropes)
60   integer im_i, im_j
61   double precision x_width, y_width
62
63   x_width = grid%x%maxval - grid%x%minval
64   y_width = grid%y%maxval - grid%y%minval
65
66   if(.not. present(n_images)) then
67     n_images = 1
68   end if
69
70   nx = grid%x%num

```

```

66   ny = grid%y%num
67   nz = grid%z%num
68
69   p_kelp(:,:,:,:) = 0
70
71   !$omp parallel do default(shared) private(x,y,
72   z) &
73   !$omp firstprivate(point,depth) &
74   !$omp private(i,j,k,im_i,im_j) shared(nx,ny,nz
75   ,n_images) &
76   !$omp shared(frond,rope,grid,quadrature_degree
77   ) &
78   !$omp shared(p_kelp,x_width,y_width) &
79   !$omp num_threads(num_threads) collapse(3) &
80   !$omp schedule(dynamic, 10) ! 10 grid points
81   per thread
82   do k=1, nz
83     do i=1, nx
84       do j=1, ny
85         z = grid%z%vals(k)
86         call depth%set_depth(rope, grid, k)
87         do im_i=-n_images, n_images
88           x = im_i*x_width + grid%x%vals(i)
89           do im_j=-n_images, n_images
90             y = im_j*y_width + grid%y%vals(j)
91             call point%set_cart(x, y, z)
92             p_kelp(i, j, k) = p_kelp(i,j,k) +
93               kelp_proportion(point, frond
94               , grid, depth,
95               quadrature_degree)
96           end do
97         end do
98       end do
99     end do
100   end do
101
102   !$omp end do
103 end subroutine calculate_kelp_on_grid
104
105 subroutine shading_region_limits(theta_low_lim,
106   theta_high_lim, point, frond)
107   type(point3d), intent(in) :: point
108   type(frond_shape), intent(in) :: frond
109   double precision, intent(out) :: theta_low_lim
110   , theta_high_lim
111
112   theta_low_lim = point%theta - frond%alpha
113   theta_high_lim = point%theta + frond%alpha
114 end subroutine shading_region_limits
115

```

```

107 | function prob_kelp(point, frond, depth,
108 |   quadrature_degree)
109 | ! P_s(theta_p, r_p) - This is the proportion of
110 |   the population of this depth layer which can
111 |   be found in this Cartesian grid cell.
112 | type(point3d), intent(in) :: point
113 | type(frond_shape), intent(in) :: frond
114 | type(depth_state), intent(in) :: depth
115 | integer, intent(in) :: quadrature_degree
116 | double precision prob_kelp
117 | double precision theta_low_lim, theta_high_lim
118 |
119 | call shading_region_limits(theta_low_lim,
120 |   theta_high_lim, point, frond)
121 | prob_kelp = integrate_ps(theta_low_lim,
122 |   theta_high_lim, quadrature_degree, point,
123 |   frond, depth)
124 | end function prob_kelp
125 |
126 | function kelp_proportion(point, frond, grid,
127 |   depth, quadrature_degree)
128 | ! This is the proportion of the volume of the
129 |   Cartesian grid cell occupied by kelp
130 | type(point3d), intent(in) :: point
131 | type(frond_shape), intent(in) :: frond
132 | type(depth_state), intent(in) :: depth
133 | type(space_angle_grid), intent(in) :: grid
134 | integer, intent(in) :: quadrature_degree
135 | double precision p_k, n, t, dz
136 | double precision kelp_proportion
137 |
138 | n = depth%num_fronds
139 | dz = grid%z%spacing(depth%depth_layer)
140 | t = frond%ft
141 | !write(*,*) 'KELP PROPORTION'
142 | !write(*,*) 'n=', n
143 | !write(*,*) 'dz=', dz
144 | !write(*,*) 't=', t
145 | !write(*,*) 'coef=', n*t/dz
146 | p_k = prob_kelp(point, frond, depth,
147 |   quadrature_degree)
148 | kelp_proportion = n*t/dz * p_k
149 | end function kelp_proportion
150 |
151 | function integrate_ps(theta_low_lim,
152 |   theta_high_lim, quadrature_degree, point,
153 |   frond, depth) result(integral)
154 | type(point3d), intent(in) :: point
155 | type(frond_shape), intent(in) :: frond

```

```

145  double precision, intent(in) :: theta_low_lim,
146      theta_high_lim
147  integer, intent(in) :: quadrature_degree
148  type(depth_state), intent(in) :: depth
149  double precision integral
150  double precision, dimension(:), allocatable :: 
151      integrand_vals
152  integer i
153
154  type(angle_dim) :: theta_f
155  call theta_f%set_bounds(theta_low_lim,
156      theta_high_lim)
157  call theta_f%set_num(quadrature_degree)
158  call theta_f%assign_legendre()
159
160  allocate(integrand_vals(theta_f%num))
161
162  do i=1, theta_f%num
163      integrand_vals(i) = ps_integrand(theta_f%
164          vals(i), point, frond, depth)
165  end do
166
167  integral = theta_f%integrate_points(
168      integrand_vals)
169
170  deallocate(integrand_vals)
171  call theta_f%deinit()
172
173  end function integrate_ps
174
175  function ps_integrand(theta_f, point, frond,
176      depth)
177      type(point3d), intent(in) :: point
178      type(frond_shape), intent(in) :: frond
179      type(depth_state), intent(in) :: depth
180      double precision theta_f, l_min
181      double precision angular_part, length_part
182      double precision ps_integrand
183
184      l_min = min_shading_length(theta_f, point,
185          frond)
186
187      angular_part = depth%angle_distribution_pdf(
188          theta_f)
189      length_part = 1 - depth%
190          length_distribution_cdf(l_min)
191
192      ps_integrand = angular_part * length_part
193  end function ps_integrand

```

```

186 | function min_shading_length(theta_f , point ,
187 |   frond) result(l_min)
188 ! L_min(\theta)
189 type(point3d), intent(in) :: point
190 type(frond_shape), intent(in) :: frond
191 double precision, intent(in) :: theta_f
192 double precision l_min
193 double precision tpp
194 double precision frond_frac
195 ! tpp === theta_p_prime
196 tpp = point%theta - theta_f + pi / 2.d0
197 frond_frac = 2.d0 * frond%fr / (1.d0 + frond%
198   fs)
199 l_min = point%r * (sin(tpp) + angular_sign(tpp
200   ) * frond_frac * cos(tpp))
201 end function min_shading_length
202
203 ! function frond_edge(theta, theta_f, L, fs, fr)
204 ! ! r_f(\theta)
205 !   double precision, intent(in) :: theta,
206 !   theta_f, L, fs, fr
207 !   double precision, intent(out) :: frond_edge
208 !
209 !   frond_edge = relative_frond_edge(theta -
210   theta_f + pi/2.d0)
211 !
212 ! end function frond_edge
213
214 ! function relative_frond_edge(theta_prime, L,
215 !   fs, fr)
216 ! ! r_f'(\theta')
217 !   double precision, intent(in) :: theta_prime,
218 !   L, fs, fr
219 !   double precision, intent(out) :: :
220 !   relative_frond_edge
221 !
222 !   relative_frond_edge = L / (sin(theta_prime)
223 !     + angular_sign(theta_prime * alpha(fs, fr) *
224 !       cos(theta_prime)))
225 ! end function relative_frond_edge
226
227 function angular_sign(theta_prime)
228 ! S(\theta')
229   double precision, intent(in) :: theta_prime
230   double precision angular_sign
231
232 ! This seems to be incorrect in summary.pdf as
233   of 9/9/18

```

```

224 ! In the report, it's written as sgn(
225     theta_print - pi/2.d0)
226 ! This results in L_min < 0 - not good!
227 angular_sign = sgn(pi/2.d0 - theta_prime)
228 end function angular_sign
229
230 subroutine gaussian_blur_2d(A, sigma, dx, dy, nk
231     , num_threads)
232 ! 2D Gaussian blur (periodic BC) with std
233     sigma
234 ! with kernel radius of nk (full size (2*nk+1)
235     x(2*nk+1))
236 ! applied to matrix A with element spacings dx
237     and dy.
238 double precision, intent(inout), dimension(:, :
239     ) :: A
240 double precision, intent(in) :: sigma, dx, dy
241 ! kernel half width
242 integer, intent(in) :: nk
243 ! kernel full width
244 integer kw
245 integer num_threads
246
247 ! A matrix size
248 integer nx, ny
249
250 ! indices
251 integer i1, j1
252 integer i2, j2
253 integer i, j
254 ! kernel
255 double precision, dimension(:, :, :), allocatable
256     :: k
257 ! output matrix
258 double precision, dimension(:, :, :), allocatable
259     :: B
260 ! kernel independent variables
261 double precision x, y
262
263 if(sigma > 0) then
264     nx = size(A, 1)
265     ny = size(A, 2)
266
267     kw = 2*nk + 1
268
269     allocate(B(nx, ny))
270     allocate(k(kw, kw))
271     !write(*,*) 'creating kernel', sigma, nk
272     ! Create kernel
273     do i1=-nk, nk
274         x = i1*dx
275         i = i1+nk+1

```

```

268      do j1=-nk, nk
269          y = j1*dy
270          j = j1+nk+1
271          k(i,j) = exp(-(x**2+y**2)/(2*sigma**2))
272      end do
273
274  end do
275 ! normalize kernel
276 k = k / sum(k)
277
278 ! write(*,*) 'convolving'
279 ! convolve
280 !$omp parallel do default(private) private(x
281             ,y) &
282             !$omp private(i,j,i1,j1,i2,j2) shared(nx,ny,
283             nk,kw) &
284             !$omp shared(A,B,k) &
285             !$omp num_threads(num_threads) collapse(2) &
286             !$omp schedule(dynamic, 10) ! 10 grid points
287             per thread
288 do i1=1, nx
289     do j1=1, ny
290         B(i1, j1) = 0
291         do i2=1, kw
292             do j2=1, kw
293                 i = mod1(i1 - nk + i2 - 1, nx)
294                 j = mod1(j1 - nk + j2 - 1, ny)
295                 B(i1, j1) = B(i1, j1) + k(i2, j2)
296                     * A(i, j)
297             end do
298         end do
299     end do
300 !omp end parallel do
301 !write(*,*) 'done convolving'
302
303 ! Update original matrix
304 A(:,:) = B(:,:)
305 deallocate(k)
306 deallocate(B)
307 !write(*,*) 'gb2d done.'
308 end if
309 end subroutine gaussian_blur_2d
310
311 end module kelp3d

```

sag.f90

```

1 | module sag
2 | use utils

```

```

3 | use fastgl
4 |
5 | implicit none
6 |
7 | ! Spatial grids do not include upper endpoints.
8 | ! Angular grids do include upper endpoints.
9 | ! Both include lower endpoints.
10 |
11 | ! To use:
12 | ! call grid%set_bounds(...)
13 | ! call grid%set_num(...) (or set_uniform_spacing
|   )
14 | ! call grid%init()
15 | ! ...
16 | ! call grid%deinit()
17 |
18 |!integer, parameter :: pi = 3.141592653589793D
|   +00
19 |
20 |type index_list
21 |  integer i, j, k, p
22 |contains
23 |  procedure :: init => index_list_init
24 |  procedure :: print => index_list_print
25 |end type index_list
26 |
27 |type angle2d
28 |  integer ntheta, nphi, nomega
29 |  double precision dtheta, dphi
30 |  double precision, dimension(:), allocatable
|    :: theta, phi, theta_edge, phi_edge
31 |  double precision, dimension(:), allocatable
|    :: theta_p, phi_p, theta_edge_p,
|      phi_edge_p
32 |  double precision, dimension(:), allocatable
|    :: cos_theta, sin_theta, cos_phi, sin_phi
33 |  double precision, dimension(:), allocatable
|    :: cos_theta_edge, sin_theta_edge,
|      cos_phi_edge, sin_phi_edge
34 |  double precision, dimension(:), allocatable
|    :: cos_theta_p, sin_theta_p, cos_phi_p,
|      sin_phi_p
35 |  double precision, dimension(:), allocatable
|    :: cos_theta_edge_p, sin_theta_edge_p,
|      cos_phi_edge_p, sin_phi_edge_p
36 |  double precision, dimension(:), allocatable
|    :: area_p
37 |contains
38 |  procedure :: set_num => angle_set_num
39 |  procedure :: phat, lhat, mhat
40 |  procedure :: init => angle_init ! Call after
|    set_num

```

```

41   procedure :: integrate_points =>
42     angle_integrate_points
43   procedure :: integrate_func =>
44     angle_integrate_func
45   procedure :: deinit => angle_deinit
46 end type angle2d
47
48 type angle_dim
49   integer num
50   double precision minval, maxval, prefactor
51   double precision, dimension(:), allocatable
52     :: vals, weights, sin, cos
53 contains
54   procedure :: set_bounds => angle_set_bounds
55   procedure :: set_num => angle1d_set_num
56   procedure :: deinit => angle1d_deinit
57   procedure :: integrate_points =>
58     angle1d_integrate_points
59   procedure :: integrate_func =>
60     angle1d_integrate_func
61   procedure :: assign_linspace =>
62     angle1d_assign_linspace
63   procedure :: assign_legendre
64 end type angle_dim
65
66 type space_dim
67   integer num
68   double precision minval, maxval
69   double precision, dimension(:), allocatable
70     :: vals, edges, spacing
71 contains
72   procedure :: integrate_points =>
73     space_integrate_points
74   procedure :: trapezoid_rule
75   procedure :: set_bounds => space_set_bounds
76   procedure :: set_num => space_set_num
77   procedure :: set_uniform_spacing =>
78     space_set_uniform_spacing
79   !procedure :: set_num_from_spacing
80   procedure :: set_uniform_spacing_from_num
81   procedure :: set_spacing_array =>
82     space_set_spacing_array
83   procedure :: deinit => space_deinit
84   procedure :: assign_linspace
85 end type space_dim
86
87 type space_angle_grid !(sag)
88   type(space_dim) :: x, y, z
89   type(angle2d) :: angles
90   double precision, dimension(:), allocatable :: 
91     x_factor, y_factor
92 contains
93   procedure :: set_bounds => sag_set_bounds

```

```

83   procedure :: set_num => sag_set_num
84   procedure :: init => sag_init
85   procedure :: deinit => sag_deinit
86   !procedure :: set_num_from_spacing =>
87     sag_set_num_from_spacing
87   procedure :: set_uniform_spacing_from_num =>
88     sag_set_uniform_spacing_from_num
88   procedure :: calculate_factors =>
89     sag_calculate_factors
89 end type space_angle_grid
90
91 contains
92
93   subroutine index_list_init(indices)
94     class(index_list) indices
95     indices%i = 1
96     indices%j = 1
97     indices%k = 1
98     indices%p = 1
99   end subroutine
100
101  subroutine index_list_print(indices)
102    class(index_list) indices
103
104    write(*,*) 'i, j, k, p =', indices%i,
105      indices%j, indices%k, indices%p
105  end subroutine index_list_print
106
107  subroutine angle_set_num(angles, ntheta, nphi)
108    class(angle2d) :: angles
109    integer ntheta, nphi
110    angles%ntheta = ntheta
111    angles%nphi = nphi
112    angles%nomega = ntheta*(nphi-2) + 2
113  end subroutine angle_set_num
114
115  function lhat(angles, p) result(l)
116    class(angle2d) :: angles
117    integer l, p
118    if(p .eq. 1) then
119      l = 1
120    else if(p .eq. angles%nomega) then
121      l = 1
122    else
123      l = mod1(p-1, angles%ntheta)
124    end if
125  end function lhat
126
127  function mhat(angles, p) result(m)
128    class(angle2d) :: angles
129    integer m, p

```

```

130 |     if(p .eq. 1) then
131 |         m = 1
132 |     else if(p .eq. angles%nomega) then
133 |         m = angles%nphi
134 |     else
135 |         m = ceiling(dble(p-1)/dble(angles%ntheta)
136 |                         ) + 1
137 |     end if
138 | end function mhat
139 |
140 | function phat(angles, l, m) result(p)
141 |     class(angle2d) :: angles
142 |     integer l, m, p
143 |
144 |     if(m .eq. 1) then
145 |         p = 1
146 |     else if(m .eq. angles%nphi) then
147 |         p = angles%nomega
148 |     else
149 |         p = (m-2)*angles%ntheta + l + 1
150 |     end if
151 | end function phat
152 |
153 | subroutine angle_init(angles)
154 |     class(angle2d) :: angles
155 |     integer l, m, p
156 |     double precision area
157 |
158 |     ! TODO: CONSIDER REMOVING non-p
159 |     allocate(angles%theta(angles%ntheta))
160 |     allocate(angles%phi(angles%nphi))
161 |     allocate(angles%theta_edge(angles%ntheta))
162 |     allocate(angles%phi_edge(angles%nphi-1))
163 |     allocate(angles%theta_p(angles%nomega))
164 |     allocate(angles%phi_p(angles%nomega))
165 |     allocate(angles%theta_edge_p(angles%nomega))
166 |     allocate(angles%phi_edge_p(angles%nomega))
167 |     allocate(angles%cos_theta_p(angles%nomega))
168 |     allocate(angles%sin_theta_p(angles%nomega))
169 |     allocate(angles%cos_phi_p(angles%nomega))
170 |     allocate(angles%sin_phi_p(angles%nomega))
171 |     allocate(angles%cos_theta(angles%nomega))
172 |     allocate(angles%sin_theta(angles%nomega))
173 |     allocate(angles%cos_phi(angles%nomega))
174 |     allocate(angles%sin_phi(angles%nomega))
175 |     allocate(angles%cos_theta_edge(angles%ntheta
176 |                         ))
177 |     allocate(angles%sin_theta_edge(angles%ntheta
178 |                         ))

```

```

177 |     allocate(angles%cos_phi_edge(angles%nphi-1))
178 |     allocate(angles%sin_phi_edge(angles%nphi-1))
179 |     allocate(angles%cos_theta_edge_p(angles%
180 |         nomega))
180 |     allocate(angles%sin_theta_edge_p(angles%
181 |         nomega))
181 |     allocate(angles%cos_phi_edge_p(angles%nomega
182 |         -1))
182 |     allocate(angles%sin_phi_edge_p(angles%nomega
183 |         -1))
183 |     allocate(angles%area_p(angles%nomega))
184 |
185 | ! Calculate spacing
186 | angles%dtheta = 2.d0*pi/dble(angles%ntheta)
187 | angles%dphi = pi/dble(angles%nphi-1)
188 |
189 | ! Create grids
190 | do l=1, angles%ntheta
191 |     angles%theta(l) = dble(l-1)*angles%dtheta
192 |     angles%cos_theta(l) = cos(angles%theta(l)
193 |         )
193 |     angles%sin_theta(l) = sin(angles%theta(l)
194 |         )
194 |     angles%theta_edge(l) = dble(l-0.5d0)*
195 |         angles%dtheta
195 |     angles%cos_theta_edge(l) = cos(angles%
196 |         theta_edge(l))
196 |     angles%sin_theta_edge(l) = sin(angles%
197 |         theta_edge(l))
197 | end do
198 |
199 | do m=1, angles%nphi
200 |     angles%phi(m) = dble(m-1.d0)*angles%dphi
201 |     angles%cos_phi(m) = cos(angles%phi(m))
202 |     angles%sin_phi(m) = sin(angles%phi(m))
203 |     if(m<angles%nphi) then
204 |         angles%phi_edge(m) = dble(m-0.5d0)*
205 |             angles%dphi
205 |         angles%cos_phi_edge(m) = cos(angles%
206 |             phi_edge(m))
206 |         angles%sin_phi_edge(m) = sin(angles%
207 |             phi_edge(m))
207 |     end if
208 | end do
209 |
210 | ! Create p arrays
211 | do m=2, angles%nphi-1
211 |     area = angles%dtheta &

```

```

213      * (angles%cos_phi_edge(m-1) - angles
214          %cos_phi_edge(m))
215  do l=1, angles%ntheta
216      p = angles%phat(l, m)
217
218      angles%theta_p(p) = angles%theta(1)
219      angles%phi_p(p) = angles%phi(m)
220      angles%theta_edge_p(p) = angles%
221          theta_edge(1)
222      angles%phi_edge_p(p) = angles%phi_edge
223          (m)
224
225      angles%cos_theta_p(p) = cos(angles%
226          theta_p(p))
227      angles%sin_theta_p(p) = sin(angles%
228          theta_p(p))
229      angles%cos_phi_p(p) = cos(angles%phi_p
230          (p))
231      angles%sin_phi_p(p) = sin(angles%phi_p
232          (p))
233
234      angles%cos_theta_edge_p(p) = cos(
235          angles%theta_edge_p(p))
236      angles%sin_theta_edge_p(p) = sin(
237          angles%theta_edge_p(p))
238      angles%cos_phi_edge_p(p) = cos(angles%
239          phi_edge_p(p))
240      angles%sin_phi_edge_p(p) = sin(angles%
241          phi_edge_p(p))
242
243      angles%area_p(p) = area
244  end do
245  end do
246
247 ! Poles
248 l=1
249 area = 2.d0*pi*(1.d0-cos(angles%dphi/2.d0))
250
251 ! North Pole
252 p = 1
253 m=1
254 angles%theta_p(p) = angles%theta(1)
255 angles%theta_edge_p(p) = angles%theta_edge(1
256 )
257 angles%phi_p(p) = angles%phi(m)
258 ! phi_edge_p only defined up to nphi-1.
259 angles%phi_edge_p(p) = angles%phi_edge(m)
260 angles%cos_theta_p(p) = cos(angles%theta_p(p
261 )))

```

```

249 |     angles%sin_theta_p(p) = sin(angles%theta_p(p
250 |         ))
250 |     angles%cos_phi_p(p) = cos(angles%phi_p(p))
251 |     angles%sin_phi_p(p) = sin(angles%phi_p(p))
252 |     angles%cos_theta_edge_p(p) = cos(angles%
252 |         theta_edge_p(p))
253 |     angles%sin_theta_edge_p(p) = sin(angles%
253 |         theta_edge_p(p))
254 |     angles%cos_phi_edge_p(p) = cos(angles%
254 |         phi_edge_p(p))
255 |     angles%sin_phi_edge_p(p) = sin(angles%
255 |         phi_edge_p(p))
256 |     angles%area_p(p) = area
257 |
258 | ! South Pole
259 | p = angles%nomega
260 | m = angles%nphi
261 | angles%theta_p(p) = angles%theta(l)
262 | angles%theta_edge_p(p) = angles%theta_edge(l
262 |     )
263 | angles%phi_p(p) = angles%phi(m)
264 | angles%cos_theta_p(p) = cos(angles%theta_p(p
264 |     ))
265 | angles%sin_theta_p(p) = sin(angles%theta_p(p
265 |     ))
266 | angles%cos_phi_p(p) = cos(angles%phi_p(p))
267 | angles%sin_phi_p(p) = sin(angles%phi_p(p))
268 | angles%area_p(p) = area
269 | end subroutine angle_init
270 |
271 | ! Integrate function given function values at
271 |     grid cells
272 | function angle_integrate_points(angles ,
272 |     func_vals) result(integral)
273 | class(angle2d) :: angles
274 | double precision , dimension(angles%nomega)
274 |     :: func_vals
275 | double precision integral
276 | integer p
277 |
278 | integral = 0.d0
279 |
280 | do p=1 , angles%nomega
281 |     integral = integral + angles%area_p(p) *
281 |         func_vals(p)
282 | end do
283 |
284 | end function angle_integrate_points
285 |

```

```

286 |     function angle_integrate_func(angles ,
287 |         func_callable) result(integral)
288 |     class(angle2d) :: angles
289 |     double precision, external :: func_callable
290 |     double precision, dimension(:), allocatable
291 |         :: func_vals
292 |     double precision integral
293 |     integer p
294 |     double precision theta, phi
295 |
296 |     allocate(func_vals(angles%nomega))
297 |
298 |     do p=1, angles%nomega
299 |         theta = angles%theta_p(p)
300 |         phi = angles%phi_p(p)
301 |         func_vals(p) = func_callable(theta, phi)
302 |     end do
303 |
304 |     integral = angles%integrate_points(func_vals
305 | )
306 |
307 |     deallocate(func_vals)
308 | end function angle_integrate_func
309 |
310 | subroutine angle_deinit(angles)
311 |     class(angle2d) :: angles
312 |     deallocate(angles%theta)
313 |     deallocate(angles%phi)
314 |     deallocate(angles%theta_edge)
315 |     deallocate(angles%phi_edge)
316 |     deallocate(angles%theta_p)
317 |     deallocate(angles%phi_p)
318 |     deallocate(angles%theta_edge_p)
319 |     deallocate(angles%phi_edge_p)
320 |     deallocate(angles%cos_theta)
321 |     deallocate(angles%sin_theta)
322 |     deallocate(angles%cos_phi)
323 |     deallocate(angles%sin_phi)
324 |     deallocate(angles%cos_theta_p)
325 |     deallocate(angles%sin_theta_p)
326 |     deallocate(angles%cos_phi_p)
327 |     deallocate(angles%sin_phi_p)
328 |     deallocate(angles%cos_theta_edge)
329 |     deallocate(angles%sin_theta_edge)
330 |     deallocate(angles%cos_phi_edge)
331 |     deallocate(angles%sin_phi_edge)
332 |     deallocate(angles%cos_theta_edge_p)
333 |     deallocate(angles%sin_theta_edge_p)
334 |     deallocate(angles%cos_phi_edge_p)
335 |     deallocate(angles%sin_phi_edge_p)

```

```

333      deallocate(angles%area_p)
334  end subroutine angle_deinit
335
336
337  !!! ANGLE 1D !!!
338
339  subroutine angle_set_bounds(angle, minval,
340      maxval)
341      class(angle_dim) :: angle
342      double precision minval, maxval
343      angle%minval = minval
344      angle%maxval = maxval
345  end subroutine angle_set_bounds
346
347  subroutine angle1d_set_num(angle, num)
348      class(angle_dim) :: angle
349      integer num
350      angle%num = num
351  end subroutine angle1d_set_num
352
353  subroutine angle1d_assign_linspace(angle)
354      class(angle_dim) :: angle
355      double precision spacing
356      integer i
357
358      spacing = (angle%maxval - angle%minval) /
359          dble(angle%num)
360      do i=1, angle%num
361          angle%vals(i) = (i-1) * spacing
362      end do
363  end subroutine angle1d_assign_linspace
364
365  ! To calculate  $\int_{xmin}^{xmax} f(x) dx$  :
366  ! int = prefactor * sum(weights * f(roots))
367  subroutine assign_legendre(angle)
368      class(angle_dim) :: angle
369      double precision root, weight, theta
370      integer i
371      ! glpair produces both x and theta, where x=
372          cos(theta). We'll throw out theta.
373
374      allocate(angle%vals(angle%num))
375      allocate(angle%weights(angle%num))
376      allocate(angle%sin(angle%num))
377      allocate(angle%cos(angle%num))
378
379      ! Prefactor for integration
380      ! From change of variables
381      angle%prefactor = (angle%maxval - angle%
382          minval) / 2.d0

```

```

380 |     do i = 1, angle%num
381 |         call glpair(angle%num, i, theta, weight,
382 |                         root)
383 |         call affine_transform(root, -1.d0, 1.d0,
384 |                         angle%minval, angle%maxval)
385 |         angle%vals(i) = root
386 |         angle%weights(i) = weight
387 |         angle%sin(i) = sin(root)
388 |         angle%cos(i) = cos(root)
389 |     end do
390 |
391 | end subroutine assign_legendre
392 |
393 ! Integrate callable function over angle via
394 ! Gauss-Legendre quadrature
395 |
396 function angle1d_integrate_func(angle,
397     func_callable) result(integral)
398 class(angle_dim) :: angle
399 double precision, external :: func_callable
400 double precision, dimension(:), allocatable
401 :: func_vals
402 double precision integral
403 integer i
404 |
405 allocate(func_vals(angle%num))
406 |
407 do i=1, angle%num
408     func_vals(i) = func_callable(angle%vals(i))
409 end do
410 |
411 integral = angle%integrate_points(func_vals)
412 |
413 deallocate(func_vals)
414 end function angle1d_integrate_func
415 |
416 ! Integrate function given function values
417 ! sampled at legendre theta values
418 function angle1d_integrate_points(angle,
419     func_vals) result(integral)
420 class(angle_dim) :: angle
421 double precision, dimension(angle%num) ::
422     func_vals
423 double precision integral
424 |
425 integral = angle%prefactor * sum(angle%
426     weights * func_vals)
427 end function angle1d_integrate_points
428 |
429 subroutine angle1d_deinit(angle)

```

```

421     class(angle_dim) :: angle
422     deallocate(angle%vals)
423     deallocate(angle%weights)
424     deallocate(angle%sin)
425     deallocate(angle%cos)
426 end subroutine angle1d_deinit
427
428
429 !! SPACE !!
430
431 ! Integrate function given function values
432 ! sampled at even grid points
432 function space_integrate_points(space,
433     func_vals) result(integral)
433     class(space_dim) :: space
434     double precision, dimension(space%num) :::
434         func_vals
435     double precision integral
436
437 ! Encapsulate actual method for easy
437 ! switching
438     integral = space%trapezoid_rule(func_vals)
439
440 end function space_integrate_points
441
442 function trapezoid_rule(space, func_vals)
442     result(integral)
443     class(space_dim) :: space
444     double precision, dimension(space%num) :::
444         func_vals
445     double precision integral
446
447     integral = 0.5d0 * sum(func_vals * space%
447         spacing)
448 end function
449
450 subroutine space_set_bounds(space, minval,
450     maxval)
451     class(space_dim) :: space
452     double precision minval, maxval
453     space%minval = minval
454     space%maxval = maxval
455 end subroutine space_set_bounds
456
457 subroutine space_set_num(space, num)
458     class(space_dim) :: space
459     integer num
460     space%num = num
461 end subroutine space_set_num
462
```

```

463  subroutine space_set_uniform_spacing(space ,
464      spacing)
465      class(space_dim) :: space
466      double precision spacing
467      integer k
468      do k=1, space%num
469          space%spacing(k) = spacing
470      end do
471  end subroutine space_set_uniform_spacing
472
473  subroutine space_set_spacing_array(space ,
474      spacing)
475      class(space_dim) :: space
476      double precision , dimension(space%num) :: :
477          spacing
478      space%spacing = spacing
479  end subroutine space_set_spacing_array
480
481  subroutine assign_linspace(space)
482      class(space_dim) :: space
483      double precision spacing
484      integer i
485
486      allocate(space%vals(space%num))
487      allocate(space%edges(space%num))
488      allocate(space%spacing(space%num))
489
490      spacing = spacing_from_num(space%minval ,
491          space%maxval , space%num)
492      call space%set_uniform_spacing(spacing)
493
494      do i=1, space%num
495          space%edges(i) = space%minval + dble(i-1)
496              * space%spacing(i)
497          space%vals(i) = space%minval + dble(i-0.5
498              d0) * space%spacing(i)
499      end do
500
501  end subroutine assign_linspace
502
503  subroutine set_uniform_spacing_from_num(space)
504      ! Create evenly spaced grid (linspace)
505      class(space_dim) :: space
506      double precision spacing
507
508      spacing = spacing_from_num(space%minval ,
509          space%maxval , space%num)
510      call space%set_uniform_spacing(spacing)
511
512  end subroutine set_uniform_spacing_from_num

```

```

507 ! subroutine set_num_from_spacing(space)
508 !   class(space_dim) :: space
509 !   !space%num = num_from_spacing(space%minval
510 ! , space%maxval, space%spacing)
511 ! end subroutine set_num_from_spacing
512
513 subroutine space_deinit(space)
514   class(space_dim) :: space
515   deallocate(space%vals)
516   deallocate(space%edges)
517   deallocate(space%spacing)
518 end subroutine space_deinit
519
520 !! SAG !!
521
522 subroutine sag_set_bounds(grid, xmin, xmax,
523   ymin, ymax, zmin, zmax)
524   class(space_angle_grid) :: grid
525   double precision xmin, xmax, ymin, ymax,
526     zmin, zmax
527
528   call grid%x%set_bounds(xmin, xmax)
529   call grid%y%set_bounds(ymin, ymax)
530   call grid%z%set_bounds(zmin, zmax)
531 end subroutine sag_set_bounds
532
533 subroutine sag_set_uniform_spacing(grid, dx,
534   dy, dz)
535   class(space_angle_grid) :: grid
536   double precision dx, dy, dz
537
538   call grid%x%set_uniform_spacing(dx)
539   call grid%y%set_uniform_spacing(dy)
540   call grid%z%set_uniform_spacing(dz)
541
542 end subroutine sag_set_uniform_spacing
543
544 subroutine sag_set_num(grid, nx, ny, nz,
545   ntheta, nphi)
546   class(space_angle_grid) :: grid
547   integer nx, ny, nz, ntheta, nphi
548
549   call grid%x%set_num(nx)
550   call grid%y%set_num(ny)
551   call grid%z%set_num(nz)
552
553   call grid%angles%set_num(ntheta, nphi)
554
555 end subroutine sag_set_num
556
557 subroutine sag_init(grid)
558   class(space_angle_grid) :: grid
559
560   call grid%x%assign_linspace()

```

```

552 |     call grid%y%assign_linspace()
553 |     call grid%z%assign_linspace()
554 |
555 |     call grid%angles%init()
556 |     call grid%calculate_factors()
557 |
558 end subroutine sag_init
559
560 subroutine sag_calculate_factors(grid)
561 ! Factors by which depth difference is
562 ! multiplied
563 ! in order to calculate distance traveled in
564 ! the
565 ! (x, y) direction along a ray in the (theta
566 ! , phi)
567 ! direction
568 class(space_angle_grid) :: grid
569 integer p, nomega
570 double precision theta, phi
571
572 nomega = grid%angles%nomega
573
574 allocate(grid%x_factor(nomega))
575 allocate(grid%y_factor(nomega))
576
577 do p=1, nomega
578     theta = grid%angles%theta_p(p)
579     phi = grid%angles%phi_p(p)
580     grid%x_factor(p) = tan(phi) * cos(theta)
581     grid%y_factor(p) = tan(phi) * sin(theta)
582 end do
583
584 end subroutine sag_calculate_factors
585
586 subroutine sag_set_uniform_spacing_from_num(
587     grid)
588 class(space_angle_grid) :: grid
589 call grid%x%set_uniform_spacing_from_num()
590 call grid%y%set_uniform_spacing_from_num()
591 call grid%z%set_uniform_spacing_from_num()
592 end subroutine
593 sag_set_uniform_spacing_from_num
594
595 ! subroutine sag_set_num_from_spacing(grid)
596 !     class(space_angle_grid) :: grid
597 !     call grid%x%set_num_from_spacing()
598 !     call grid%y%set_num_from_spacing()
599 !     call grid%z%set_num_from_spacing()
600
601 ! end subroutine sag_set_num_from_spacing

```

```

598  subroutine sag_deinit(grid)
599    class(space_angle_grid) :: grid
600    call grid%x%deinit()
601    call grid%y%deinit()
602    call grid%z%deinit()
603    call grid%angles%deinit()
604
605    deallocate(grid%x_factor)
606    deallocate(grid%y_factor)
607  end subroutine sag_deinit
608
609 ! Affine shift on x from [xmin, xmax] to [ymin
610 , ymax]
610 subroutine affine_transform(x, xmin, xmax,
611   ymin, ymax)
611   double precision x, xmin, xmax, ymin, ymax
612   x = ymin + (ymax-ymin)/(xmax-xmin) * (x-xmin
613   )
613 end subroutine affine_transform
614
615 function num_from_spacing(xmin, xmax, dx)
616   result(n)
616   double precision xmin, xmax, dx
617   integer n
618   n = floor( (xmax - xmin) / dx )
619 end function num_from_spacing
620
621 function spacing_from_num(xmin, xmax, nx)
622   result(dx)
622   double precision xmin, xmax, dx
623   integer nx
624   dx = (xmax - xmin) / dble(nx)
625 end function spacing_from_num
626 end module sag

```

```

utils.f90
1 ! General utilities which might be useful in
2   other settings
3 module utils
4 implicit none
5
6 ! Constants
7 double precision, parameter :: pi = 4.D0 * datan
8   (1.D0)
9
10 contains
11
12 ! Determine base directory relative to current
13   directory

```

```

11 ! by looking for Makefile, which is in the base
   dir
12 ! Assuming that this is executed from within the
   git repo.
13 function getbasedir()
14   implicit none
15
16   ! INPUTS:
17   ! Number of paths to check
18   integer, parameter :: numpaths = 3
19   ! Maximum length of path names
20   integer, parameter :: maxlenlength = numpaths *
      2 - 1
21   ! Paths to check for Makefile
22   character(len=maxlength), parameter,
      dimension(numpaths) :: check_paths &
23   = (/ '.', '..', '..', '..', '/..../' /)
24   ! Temporary path string
25   character(len=maxlength) tmp_path
26   ! Whether Makefile has been found yet
27   logical found
28   ! Path counter
29   integer ii
30   ! Lengths of paths
31   integer, dimension(numpaths) :: pathlengths
32
33   ! OUTPUT:
34   ! getbasedir - relative path to base
      directory
35   ! Will either return '.', '..', or '..../..
36   character(len=maxlength) getbasedir
37
38
39   ! Determine length of each path
40   pathlengths(1) = 1
41   do ii = 2, numpaths
42     pathlengths(ii) = 2 + 3 * (ii - 2)
43   end do
44
45   ! Loop through paths
46   do ii = 1, numpaths
47     ! Determine this path
48     tmp_path = check_paths(ii)
49
50     ! Check whether Makefile is in this
      directory
51     !write(*,*) 'Checking ', tmp_path(1:
      pathlengths(ii)), ''
52     inquire(file=tmp_path(1:pathlengths(ii))
      // '/Makefile', exist=found)
53     ! If so, stop. Otherwise, keep looking.
54     if(found) then

```

```

55      getbasedir = tmp_path(1:pathlengths(
56          ii))
57      exit
58    end if
59  end do
59
60 ! If it hasn't been found, then this script
61 ! was probably called
61 ! from outside of the repository.
62 if(.not. found) then
63   write(*,*) 'BASE DIR NOT FOUND.'
64 end if
65
66 end function
67
68 ! Determine array size from min, max and step
69 ! If alignment is off, array will overstep the
70 ! maximum
70 function bnd2max(xmin,xmax,dx)
71   implicit none
72
73   ! INPUTS:
74   ! xmin - minimum x value in array
75   ! xmax - maximum x value in array (inclusive
75     )
76   ! dx - step size
77   double precision, intent(in) :: xmin, xmax,
77       dx
78
79   ! OUTPUT:
80   ! step2max - maximum index of array
81 integer bnd2max
82
83   ! Calculate array size
84   bnd2max = int(ceiling((xmax-xmin)/dx))
85 end function
86
87 ! Create array from bounds and number of
87 ! elements
88 ! xmax is not included in array
89 function bnd2arr(xmin,xmax,imax)
90   implicit none
91
92   ! INPUTS:
93   ! xmin - minimum x value in array
94   ! xmax - maximum x value in array (exclusive
94     )
95   double precision, intent(in) :: xmin, xmax
96   ! imax - number of elements in array
97   integer imax
98
99   ! OUTPUT:

```

```

100 ! bnd2arr - array to generate
101 double precision, dimension(imax) :: bnd2arr
102
103 ! BODY:
104
105 ! Counter
106 integer ii
107 ! Step size
108 double precision dx
109
110 ! Calculate step size
111 dx = (xmax - xmin) / imax
112
113 ! Generate array
114 do ii = 1, imax
115     bnd2arr(ii) = xmin + (ii-1) * dx
116 end do
117
118 end function
119
120 function mod1(i, n)
121     implicit none
122     integer i, n, m
123     integer mod1
124
125     m = modulo(i, n)
126
127     if(m .eq. 0) then
128         mod1 = n
129     else
130         mod1 = m
131     end if
132
133 end function mod1
134
135 function sgn_int(x)
136     integer x, sgn_int
137     ! Standard signum function
138     sgn_int = sign(1,x)
139     if(x .eq. 0.) sgn_int = 0
140 end function sgn_int
141
142 function sgn(x)
143     double precision x, sgn
144     ! Standard signum function
145     sgn = sign(1.d0,x)
146     if(x .eq. 0.) sgn = 0
147 end function sgn
148
149 ! Interpolate single point from 1D data
150 function interp(x0,xx,yy,nn)
151     implicit none

```

```

152      ! INPUTS:
153      ! x0 - x value at which to interpolate
154      double precision, intent(in) :: x0
155      ! xx - ordered x values at which y data is
156      ! sampled
157      ! yy - corresponding y values to interpolate
158      double precision, dimension (nn), intent(in)
159      :: xx,yy
160      ! nn - length of data
161      integer, intent(in) :: nn
162
163      ! OUTPUT:
164      ! interp - interpolated y value
165      double precision interp
166
167      ! BODY:
168
169      ! Index of lower-adjacent data (xx(i) < x0 <
170      ! xx(i+1))
171      integer ii
172      ! Slope of liine between (xx(ii),yy(ii)) and
173      ! (xx(ii+1),yy(ii+1))
174      double precision mm
175
176      ! If out of bounds, then return endpoint
177      ! value
178      if (x0 < xx(1)) then
179          interp = yy(1)
180      else if (x0 > xx(nn)) then
181          interp = yy(nn)
182      else
183
184          ! Determine ii
185          do ii = 1, nn
186              if (xx(ii) > x0) then
187                  ! We've now gone one index too far
188                  .
189                  exit
190              end if
191          end do
192
193          ! Determine whether we're on the right
194          ! endpoint
195          if(ii-1 < nn) then
196              ! If this is a legitimate
197              ! interpolation, then
198              ! subtract since we went one index too
199              ! far
200              ii = ii - 1
201
202          ! Calculate slope

```

```

195     mm = (yy(ii+1) - yy(ii)) / (xx(ii+1) -
196                                 xx(ii))
197
198         ! Return interpolated value
199         interp = yy(ii) + mm * (x0 - xx(ii))
200
201     else
202         ! If we're actually interpolating the
203         ! right endpoint,
204         ! then just return it.
205         interp = yy(nn)
206     end if
207
208
209 end function
210
211 ! Calculate unshifted position of periodic image
212 ! Assuming xmin, xmax are extreme attainable
213 ! values of x
214 function shift_mod(x, xmin, xmax)
215     double precision x, xmin, xmax
216     double precision mod_part, shift_mod
217     mod_part = mod(x-xmin, xmax-xmin)
218     if(mod_part .ge. 0) then
219         ! In this case, mod_part is distance
220         ! between image & lower bound
221         shift_mod = xmin + mod_part
222     else
223         ! In this case, mod_part is distance
224         ! between image & upper bound
225         shift_mod = xmax + mod_part
226     endif
227 end function shift_mod
228
229 ! Bilinear interpolation on evenly spaced 2D
230 ! grid
231 ! Assume upper endpoint is not included and is
232 ! identical
233 ! to the lower endpoint, which is included.
234 function bilinear_array_periodic(x, y, nx, ny,
235     x_vals, y_vals, fun_vals)
236     implicit none
237     double precision x, y
238     integer nx, ny
239     double precision, dimension(:) :: x_vals,
240                           y_vals
241     double precision, dimension(:, :) :: fun_vals
242
243     double precision dx, dy, xmin, ymin
244     integer i0, j0, i1, j1
245     double precision x0, x1, y0, y1
246     double precision z00, z10, z01, z11

```

```

238
239     double precision bilinear_array_periodic
240
241     xmin = x_vals(1)
242     ymin = y_vals(1)
243     dx = x_vals(2) - x_vals(1)
244     dy = y_vals(2) - y_vals(1)
245
246     ! Add 1 for one-indexing
247     i0 = int(floor((x-xmin)/dx))+1
248     j0 = int(floor((y-ymin)/dy))+1
249
250     x0 = x_vals(i0)
251     y0 = y_vals(j0)
252
253     ! Periodic wrap
254     if(i0 .lt. nx) then
255         i1 = i0 + 1
256         x1 = x_vals(i1)
257     else
258         i1 = 1
259         x1 = x_vals(nx) + dx
260     endif
261
262     if(j0 .lt. ny) then
263         j1 = j0 + 1
264         y1 = y_vals(j1)
265     else
266         j1 = 1
267         y1 = y_vals(ny) + dy
268     endif
269
270     z00 = fun_vals(i0,j0)
271     z10 = fun_vals(i1,j0)
272     z01 = fun_vals(i0,j1)
273     z11 = fun_vals(i1,j1)
274
275     bilinear_array_periodic = bilinear(x, y, x0,
276                                         y0, x1, y1, z00, z01, z10, z11)
276 end function bilinear_array_periodic
277
278 ! Bilinear interpolation on evenly spaced 2D
279 ! grid
280 ! Assume upper and lower endpoints are included
280 function bilinear_array(x, y, x_vals, y_vals,
281                         fun_vals)
282     implicit none
282     double precision x, y
283     double precision, dimension(:) :: x_vals,
284                                     y_vals
284     double precision, dimension(:, :) :: fun_vals

```

```

285
286  double precision dx, dy, xmin, ymin
287  integer i0, j0, i1, j1
288  double precision x0, x1, y0, y1
289  double precision z00, z10, z01, z11
290
291  double precision bilinear_array
292
293  xmin = x_vals(1)
294  ymin = y_vals(1)
295  dx = x_vals(2) - x_vals(1)
296  dy = y_vals(2) - y_vals(1)
297
298  ! Add 1 for one-indexing
299  i0 = int(floor((x-xmin)/dx))+1
300  j0 = int(floor((y-ymin)/dy))+1
301  i1 = i0 + 1
302  j1 = j0 + 1
303
304  ! Bounds checking
305  ! if(i0 .lt. 1) then
306  !   i0 = 1
307  !   i1 = 1
308  ! else if(i1 .gt. nx) then
309  !   i0 = nx
310  !   i1 = nx
311  ! endif
312  ! if(j0 .lt. 1) then
313  !   j0 = 1
314  !   j1 = 1
315  ! else if(j1 .gt. ny) then
316  !   j0 = ny
317  !   j1 = ny
318  ! endif
319
320  x0 = x_vals(i0)
321  x1 = x_vals(i1)
322  y0 = y_vals(j0)
323  y1 = y_vals(j1)
324
325  z00 = fun_vals(i0,j0)
326  z10 = fun_vals(i1,j0)
327  z01 = fun_vals(i0,j1)
328  z11 = fun_vals(i1,j1)
329
330  bilinear_array = bilinear(x, y, x0, y0, x1, y1
331  , z00, z01, z10, z11)
332 end function bilinear_array
333 ! ilinear interpolation of a function of two
     variables

```

```

334 ! over a rectangle of points.
335 ! Weight each point by the area of the sub-
336 ! rectangle involving
337 ! the point (x,y) and the point diagonally
338 ! across the rectangle
339 function bilinear(x, y, x0, y0, x1, y1, z00, z01
340 , z10, z11)
341 implicit none
342 double precision x, y
343 double precision x0, y0, x1, y1, z00, z01, z10
344 , z11
345 double precision a, b, c, d
346 double precision bilinear
347
348 a = (x-x0)*(y-y0)
349 b = (x1-x)*(y-y0)
350 c = (x-x0)*(y1-y)
351 d = (x1-x)*(y1-y)
352
353 bilinear = (a*z11 + b*z01 + c*z10 + d*z00) / (
354 a + b + c + d)
355 end function bilinear
356
357 ! Integrate using left endpoint rule
358 ! Assuming the right endpoint is not included in
359 ! arr
360 function lep_rule(arr,dx,nn)
361 implicit none
362
363 ! INPUTS:
364 ! arr - array to integrate
365 double precision, dimension(nn) :: arr
366 ! dx - array spacing (mesh size)
367 double precision dx
368 ! nn - length of arr
369 integer, intent(in) :: nn
370
371 ! OUTPUT:
372 ! lep_rule - integral w/ left endpoint rule
373 double precision lep_rule
374
375 ! BODY:
376
377 ! Counter
378 integer ii
379
380 ! Set output to zero
381 lep_rule = 0.0d0
382
383 ! Accumulate integral
384 do ii = 1, nn
385     lep_rule = lep_rule + arr(ii) * dx

```

```

380     end do
381
382 end function
383
384 ! Integrate using trapezoid rule
385 ! Assuming both endpoints are included in arr
386 function trap_rule_dx(arr, dx, nn)
387     implicit none
388     double precision, dimension(nn) :: arr
389     double precision dx
390     integer ii, nn
391     double precision trap_rule_dx
392
393     trap_rule_dx = 0.0d0
394
395     do ii=1, nn-1
396         trap_rule_dx = trap_rule_dx + 0.5d0 * dx *
397             (arr(ii) + arr(ii+1))
398     end do
399
400 end function trap_rule_dx
401
402 ! Integrate using trapezoid rule
403 ! Assuming both endpoints are included in arr
404 function trap_rule_uneven(xx, yy, nn)
405     implicit none
406     double precision, dimension(nn) :: xx
407     double precision, dimension(nn) :: yy
408     integer ii, nn
409     double precision trap_rule_uneven
410
411     trap_rule_uneven = 0.0d0
412
413     do ii=1, nn-1
414         trap_rule_uneven = trap_rule_uneven + 0.5d0
415             * (xx(ii+1)-xx(ii)) * (yy(ii) + yy(ii
416             +1))
417     end do
418 end function trap_rule_uneven
419
420 function trap_rule_dx_uneven(dx, yy, nn)
421     implicit none
422     double precision, dimension(nn-1) :: dx
423     double precision, dimension(nn) :: yy
424     integer ii, nn
425     double precision trap_rule_dx_uneven
426
427     trap_rule_dx_uneven = 0.0d0
428
429     do ii=1, nn-1
430         trap_rule_dx_uneven = trap_rule_dx_uneven +
431             0.5d0 * dx(ii) * (yy(ii) + yy(ii+1))

```

```

428     end do
429 end function trap_rule_dx_uneven
430
431 ! Integrate using midpoint rule
432 ! First and last bins, only use inner half
433 function midpoint_rule_halfends(dx, yy, nn)
434     result(integral)
435     implicit none
436     integer ii, nn
437     double precision, dimension(nn) :: dx, yy
438     double precision integral
439
440     if(nn > 1) then
441         integral = .5d0 * (dx(1)*yy(1) + dx(nn)*yy(
442             nn))
443
444         do ii=2, nn-1
445             integral = integral + dx(ii)*yy(ii)
446         end do
447     else
448         integral = 0.d0
449     end if
450 end function midpoint_rule_halfends
451
452 ! Normalize 1D array and return integral w/ left
453 ! endpoint rule
454 function normalize_dx(arr,dx,nn)
455     implicit none
456
457     ! INPUTS:
458     ! arr - array to normalize
459     double precision, dimension(nn) :: arr
460     ! dx - array spacing (mesh size)
461     double precision dx
462     ! nn - length of arr
463     integer, intent(in) :: nn
464
465     ! OUTPUT:
466     ! normalize - integral before normalization
467     ! (left endpoint rule)
468     double precision normalize_dx
469
470     ! BODY:
471
472     ! Calculate integral
473     normalize_dx = lep_rule(arr,dx,nn)
474
475     ! Normalize array
476     arr = arr / normalize_dx
477
478 end function normalize_dx

```

```

476 ! Normalize 1D unevenly-spaced array and
477 ! return integral w/ trapezoid rule
478 ! Will not be quite accurate if rightmost
479 ! endpoint is not included
480 ! (Very small for VSF, so not a big deal there)
481 ! Modifies yy in place
482 function normalize_uneven(xx, yy, nn) result(
483     norm)
484 implicit none
485
486 ! INPUTS:
487 ! xx, yy - array values of data to normalize
488 double precision, dimension(nn) :: xx, yy
489 ! nn - length of arr
490 integer, intent(in) :: nn
491
492 ! OUTPUT:
493 ! normalize - integral before normalization (
494 !     left endpoint rule)
495 double precision norm
496
497 ! BODY:
498
499 ! Calculate integral
500 ! PERHAPS WE SHOULD USE TRAPEZOID RULE
501 norm = trap_rule_uneven(xx, yy, nn)
502
503 ! Normalize array
504 yy(:) = yy(:) / norm
505
506 end function normalize_uneven
507
508 ! Read 2D array from file
509 function read_array(filename, fmtstr, nn, mm,
510     skiplines_in)
511     implicit none
512
513     ! INPUTS:
514     ! filename - path to file to be read
515     ! fmtstr - input format (no parentheses, don
516     !     't specify columns)
517     ! e.g. 'E10.2', not '(2E10.2)'
518     character(len=*), intent(in) :: filename,
519         fmtstr
520     ! nn - Number of data rows in file
521     ! mm - number of data columns in file
522     integer, intent(in) :: nn, mm
523     ! skiplines - optional - number of lines to
524     !     skip from header
525     integer, optional :: skiplines_in
526     integer skiplines

```

```

521 ! OUTPUT:
522 double precision, dimension(nn,mm) :: 
      read_array
523
524 ! BODY:
525
526 ! Row counter
527 integer ii
528 ! File unit number
529 integer, parameter :: un = 10
530 ! Final format to use
531 character(len=256) finfmt
532
533 ! Generate final format string
534 write(finfmt,'(A,I1,A,A)' ) '(', mm, fmtstr,
      ')
535
536 ! Print message
537 !write(*,*) 'Reading data from "', trim(
      filename), '",'
538 !write(*,*) 'using format "', trim(finfmt),
      '",'
539
540 ! Open file
541 open(unit=un, file=trim(filename), status='
      old', form='formatted')
542
543 ! Skip lines if desired
544 if(present(skiplines_in)) then
545     skiplines = skiplines_in
546     do ii = 1, skiplines
547         ! Read without variable ignores the
            line
            read(un,*)
        end do
548 else
549     skiplines = 0
550 end if
551
552 ! Loop through lines
553 do ii = 1, nn
554     ! Read one row at a time
555     read(unit=un, fmt=trim(finfmt))
556         read_array(ii,:)
557     end do
558
559 ! Close file
560 close(unit=un)
561
562 end function
563
564 ! Print 2D array to stdout

```

```

566 subroutine print_int_array(arr,nn,mm,fmtstr_in)
567     implicit none
568
569     ! INPUTS:
570     ! arr - array to print
571     integer, dimension (nn,mm), intent(in) :: arr
572     ! nn - number of data rows in file
573     ! nn - number of data columns in file
574     integer, intent(in) :: nn, mm
575     ! fmtstr - output format (no parentheses, don't
576     ! specify columns)
577     ! e.g. 'E10.2', not '(2E10.2)'
578     character(len=*), optional :: fmtstr_in
579     character(len=256) fmtstr
580
581     ! NO OUTPUTS
582
583     ! BODY
584
585     ! Row counter
586     integer ii
587     ! Final format to use
588     character(len=256) finfmt
589
590     ! Determine string format
591     if(present(fmtstr_in)) then
592         fmtstr = fmtstr_in
593     else
594         fmtstr = 'I10'
595     end if
596
597     ! Generate final format string
598     write(finfo, '(A,I4,A,A)') '(', mm, trim(
599     ! Loop through rows
600     do ii = 1, nn
601         ! Print one row at a time
602         write(*,finfo) arr(ii,:)
603     end do
604
605     ! Print blank line after
606     write(*,*) ''
607
608 end subroutine print_int_array
609
610 subroutine print_array(arr,nn,mm,fmtstr_in)
611     implicit none
612
613     ! INPUTS:
614     ! arr - array to print

```

```

615      double precision, dimension (nn,mm), intent(
616          in) :: arr
617      ! nn - number of data rows in file
618      ! nn - number of data columns in file
619      integer, intent(in) :: nn, mm
620      ! fmtstr - output format (no parentheses,
621      ! don't specify columns)
622      ! e.g. 'E10.2', not '(2E10.2)'
623      character(len=*) , optional :: fmtstr_in
624      character(len=256) fmtstr
625
626      ! NO OUTPUTS
627
628      ! BODY
629
630      ! Row counter
631      integer ii
632      ! Final format to use
633      character(len=256) finfmt
634
635      ! Determine string format
636      if(present(fmtstr_in)) then
637          fmtstr = fmtstr_in
638      else
639          fmtstr = 'ES10.2'
640      end if
641
642      ! Generate final format string
643      write(finfmt,'(A,I4,A,A)') '(', mm, trim(
644          fmtstr), ')'
645
646      ! Loop through rows
647      do ii = 1, nn
648          ! Include row number
649          ! write(*, '(I10)', advance='no') ii
650          ! Print one row at a time
651          write(*,finfmt) arr(ii,:)
652      end do
653
654      ! Print blank line after
655      write(*,*) ''
656
657      ! Write 1D array to file
658      subroutine write_vec(arr,nn,filename,fmtstr_in)
659          implicit none
660
661          ! INPUTS:
662          ! arr - array to print
663          double precision, dimension (nn), intent(in)
664              :: arr

```

```

663      ! nn - number of data rows in file
664      ! nn - number of data columns in file
665      integer, intent(in) :: nn
666      ! filename - file to write to
667      character(len=*) filename
668      ! fmtstr - output format (no parentheses,
669      !   don't specify columns)
670      ! e.g. 'E10.2', not '(2E10.2)'
671      character(len=*), optional :: fmtstr_in
672      character(len=256) fmtstr
673
674      ! NO OUTPUTS
675
676      ! BODY
677
678      ! Row counter
679      integer ii
680      ! Final format to use
681      character(len=256) finfmt
682      ! Dummy file unit to use
683      integer, parameter :: un = 20
684
685      ! Open file for writing
686      open(unit=un, file=trim(filename), status='
687          replace', form='formatted')
688
689      ! Determine string format
690      if(present(fmtstr_in)) then
691          fmtstr = fmtstr_in
692      else
693          fmtstr = 'E10.2'
694      end if
695
696      ! Generate final format string
697      write(finfmt,'(A,A,A)') '(', trim(fmtstr), '
698      ! Loop through rows
699      do ii = 1, nn
700          ! Print entry per row
701          write(un,finfmt) arr(ii)
702      end do
703
704      ! Close file
705      close(unit=un)
706
707      end subroutine
708
709      ! Write 2D array to file
710      subroutine write_array(arr,nn,mm,filename,
711          fmtstr_in)
712          implicit none

```

```

711      ! INPUTS:
712      ! arr - array to print
713      double precision, dimension (nn,mm), intent(
714          in) :: arr
715      ! nn - number of data rows in file
716      ! nn - number of data columns in file
717      integer, intent(in) :: nn, mm
718      ! filename - file to write to
719      character(len=*) filename
720      ! fmtstr - output format (no parentheses,
721      !           don't specify columns)
722      ! e.g. 'E10.2', not '(2E10.2)'
723      character(len=*), optional :: fmtstr_in
724      character(len=256) fmtstr
725
726      ! NO OUTPUTS
727
728      ! BODY
729
730      ! Row counter
731      integer ii
732      ! Final format to use
733      character(len=256) finfmt
734      ! Dummy file unit to use
735      integer, parameter :: un = 20
736
737      ! Open file for writing
738      open(unit=un, file=trim(filename), status='
739          replace', form='formatted')
740
741      ! Determine string format
742      if(present(fmtstr_in)) then
743          fmtstr = fmtstr_in
744      else
745          fmtstr = 'E10.2'
746      end if
747
748      ! Generate final format string
749      write(finfo, '(A,I4,A,A)') '(', mm, trim(
750          fmtstr), ')'
751
752      ! Loop through rows
753      do ii = 1, nn
754          ! Print one row at a time
755          write(un,finfo) arr(ii,:)
756      end do
757
758      ! Close file
759      close(unit=un)
760
761  end subroutine

```

```
759 |
760 | subroutine zeros(x, n)
761 |   implicit none
762 |   integer n, i
763 |   double precision, dimension(n) :: x
764 |
765 |   do i=1, n
766 |     x(i) = 0
767 |   end do
768 | end subroutine zeros
769 |
770 | end module
```