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MODELLING THE LIGHT FIELD IN MACROALGAE AQUACULTURE

A Thesis

Presented to

The Graduate Faculty of The University of Akron

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

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May, 2018

MODELLING THE LIGHT FIELD IN MACROALGAE AQUACULTURE

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	Thesis
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ABSTRACT

A probabilistic model for the spatial distribution of kelp fronds is developed based on a kite-shaped geometry and simple assumptions about the motion of fronds due to water velocity. Radiative transfer theory is then applied to determine the radiation field by using the kelp model to determine optical properties of the medium. Finite difference and asymptotic solutions are explored, and behavior of the results over the parameter space is investigated. Numerical simulations to predict the lifetime biomass production of kelp plants are performed to compare our light model to the previous exponential decay model.

ACKNOWLEDGEMENTS

Acknowledgments: This project was supported in part by the National Science Foundation under Grant No. EEC-1359256, and by the Norwegian National Research Council, Project number 254883/E40.

Mentors: Shane Rogers, Department of Environmental Engineering, Clarkson University; Ole Jacob Broch, and Aleksander Handå, SINTEF Fisheries and Aquaculture, Trondheim, Norway.

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CHAPTER I

INTRODUCTION

1.1 Motivation

Given the global rise in population, efficient and innovative resource utilization is increasingly important. In particular, food and fuel are clearly in high demand. Meanwhile, growing concern for the negative environmental impacts of petroleum-based fuel is generating a market for biofuel, especially corn-based ethanol. However, corn-based ethanol has been heavily criticized for diverting land usage away from food production. At the same time, a great deal of unutilized saltwater coastline is available for both food and fuel production through seaweed cultivation. Specifically, the sugar kelp *Saccharina Latissima* is known to be a viable source of food, both for direct human consumption and for fish cultivation, as well as for biofuel production.

Furthermore, nitrogen leakage into water bodies is a significant ecological danger, and is especially relevant near large conventional agriculture facilities due to run-off from nitrogen-based fertilizers, as well as near wastewater treatment plants. As a specific example, there is a wastewater treatment plant in Boothbay Harbor, Maine which is facing increasingly demanding EPA regulations limiting the concentration of certain nutrients permissible to be released into the ocean via wastewater

treatment outfalls. In order to adhere to these stricter requirements using conventional nutrient remediation, a significant quantity of specialized equipment would be necessary, which is not currently present in the Boothbay Harbor plant. Being surrounded on all sides by water and private property, the treatment plant lacks the necessary space for the additional equipment, and would therefore need to move their entire facility to a new location in order to conform to these new nutrient regulations. As an alternative to conventional nutrient remediation techniques, the cultivation of the macroalgae Saccharina Latissima (sugar kelp) near the outfall site has been proposed. The purpose of such an undertaking would be twofold: to prevent eutrophication of the surrounding ecosystem by sequestering the nutrients in question, and to reduce the need for nutrient input, which is one of the largest costs in macroalgae cultivation.

Once grown, a variety of products can be derived from macroalgae, including biofuel, fish/cattle feed stock, and high value chemical materials such as alginate and agar. Food for human consumption is also a common product of kelp aquaculture, though it may not be ideal for a wastewater treatment application. Thus, there is an ongoing effort to investigate the feasibility, and optimal implementation of kelp farming in wastewater treatment operations.

Industrial scale macroalgae cultivation has long existed in Eastern Asia due to the popularity of seaweed in Asian cuisine. More recently, kelp aquaculture has been developing in Scandinavia and in the Northeastern United States. For example, the MACROSEA project is a four year international research collaboration funded by

the Research Council of Norway targeting "successful and predictable production of high quality biomass thereby making significant steps towards industrial macroalgae cultivation in Norway." 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. Work is underway at SINTEF, a private Norwegian research institution, to develop such models. Ole Jacob Broch is a mathematician at SINTEF, a research organization in Trondheim, Norway, who has been working to model the growth of Saccharina Latissima using SINMOD, a large-scale 3D hydrodynamical ocean model developed at SINTEF which generates data on water temperature, water velocity, light intensity, and phytoplankton concentrations among other valuable quantities [13].

One aspect of the model which has yet to be fully developed is the availability of light, considering factors such as absorption and scattering by the aquatic medium, as well as by the kelp itself. In this thesis, we contribute to this effort by developing a first-principles model of the light field in a kelp farming environment. As a first step, a model for the spatial distribution of kelp is developed. Radiative transfer theory is then applied to determine the effects of the kelp and water on the availability of light throughout the medium. We pursue a numerical finite difference solution to the Radiative Transfer Equation, and subsequently discuss asymptotic approximations which prove to be sufficiently accurate and less computationally intensive. We also provide a detailed description of the numerical solution of this model, accompanied

by source code for a FORTRAN implementation of the solution. This model can be used independently, or in conjunction with a life cycle kelp model to determine the amount of light available for photosynthesis at a single time step.



Figure 1.1: Saccharina Latissima being harvested

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 [1]. 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, simply specifying a single parameter which determines the percentage of light which 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*, with an emphasis on including more environmental parameters and a more complete description of the growth and decay of the kelp [7]. He takes into account respiration, frond decay, and most importantly for my work, sub-canopy light attenuation due to self-shading. He simply adds a coefficient to the exponential decay of light as a function of depth to represent shading from kelp fronds. He doesn't consider and radial nor 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 simplistic.

Both Anderson's and Jackson's model were carried out by numerically solving a system of differential equations over small time intervals. In 1990, M.A. Burgman and V.A. Gerard developed a stochastic population model [3]. This approach is quite different, and 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. That same year, Nyman et. al. tested a similar model in New Zealand, as well as a Markov chain model, and compared the results with experimental data [9].

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 [5, 14]. These were the some of the first models of kelp growth that did not specifically relate to Macrocystis pyrifera ("giant kelp"). Initially, there was a great deal of excitement about this species due to it's incredible size and growth rate, but difficulties in harvesting and negative environmental impacts have caused scientists to investigate other kelp species.

1.3 Background on Radiative Transfer

In terms of optical quantities, our primary interest is in the radiance at each point from all directions, which affects 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 largely unutilized in the fields of oceanography and aquaculture. Meanwhile, it has been studied extensively in two fields: stellar astrophysics and computer graphics. In its full form, radiance is a function of 3 spatial dimensions, 2 angular dimensions, and frequency, making for an incredibly complex problem. In this work, frequency is ignored, only monochromatic radiation 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 our situation, emission is negligible, owing only perhaps to some small luminescent phytoplankton or some such anomaly, and can therefore be safely ignored.

We use monochromatic radiative transfer in order to model the light field in an aqueous environment populated by vegetation. The vegetation (kelp) is modeled by a spatial probability distribution, which we assume to be given. The two quantities we seek to compute are *radiance* and *irradiance*. Radiance is the intensity of light in at a particular point in a particular direction, while irradiance is the total light intensity at a point in space, integrated over all angles. The Radiative Transfer Equation is an integro-partial differential equation for radiance, which has been used primarily in stellar astrophysics; it's application to marine biology is fairly recent [8].

Understanding the growth rate and nutrient recovery by kelp cultures has important marine biological implications. For example, recent work by our research group at Clarkson University, the University of Maine, and SINTEF Fisheries and Aquaculture is investigating kelp aquaculture as a means to recover nutrients from wastewater effluent plumes in coastal environments into a valuable biomass feedstock for many products. Current models for kelp growth place little emphasis on the way in which nearby plants shade one another. Self-shading may be a significant model feature, though, as light availability may impact the growth and composition of the kelp biomass, and thus the mixture of goods that may be derived.

1.4 Overview of Thesis

The remainder of this document is organized as follows. In Chapter 2, we develop a probabilistic model to describe the spatial distribution of kelp by assuming simple distributions for the lengths and orientations of fronds. We begin Chapter 3 with a survey of fundamental radiometric quantities and optical properties of matter. We use the spatial kelp distribution from Chapter 2 to determine optical properties of the combined water-kelp medium. We then present the Radiative Transfer Equation, an integro-partial differential equation which describes the the light field as a function of position and angle. An asymptotic expansion is explored for cases where absorption dominates scattering in the medium, such as in very clear water or high kelp den-

sity. In Chapter 4, details are given for the numerical solution of the equations from Chapters 2 and 3. Both the full finite difference solution and the asymptotic approximation are described. Next, in Chapter 5, we discuss the availability of necessary parameters in the literature. For those which are not readily available, we give rough estimates and briefly describe experimental methods for their determination. Then, in Chapter 6, we investigate the necessary grid resolution for adequate accuracy in the full finite difference solution and compare to the asymptotic approximation for a few parameter sets. Further, we determine the effect of varying a few key parameters on the light field predicted by the asymptotic approximation. Afterwards, we use the light model developed here in a full lifecycle simulation of kelp growth and compare the light field and biomass production to those predicted by a simpler 1D exponential decay light model. Finally, we conclude with Chapter 7 by giving a brief summary of the model, discuss and its performance, and suggest improvements and avenues for future work.

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, which we do in this chapter. We take a probabilistic approach to describing the kelp. We begin by describing the distribution of kelp fronds, and through algebraic manipulation, we are able to assign to each point in space a probability that kelp occupies the location.

2.1 Physical Setup

Being a salt water species, macroalgae cultivation occurs primarily in the ocean, with the exception of the initial stage of growth, where microscopic kelp spores are inoculated onto a thread in a small laboratory pool. This thread is then wrapped around a large rope, which is placed in the ocean and generally suspended by buoys in one of two configurations: horizontal or vertical. Thus far, I am primarily concerned with modeling the vertical rope case, in which the kelp plants extend radially outward from the rope in all directions, which are made up of a single frond (leaf), stipe (stem) and holdfast (root structure). We consider a rectangular grid of such vertical ropes. Plants extending from each rope will shade both themselves and their neighbors to varying degrees based on the depth of the kelp, the rope spacing, the angle of incident

light on the surface and the nature of scattering in the water. In addition, light will be naturally absorbed by the water to varying degrees as determined by the clarity of the water.



Figure 2.1: 4×4 array of vertical kelp ropes

2.2 Coordinate System

Consider the rectangular domain

$$x_{\min} \le x \le x_{\max}$$

$$y_{\min} \le y \le y_{\max}$$

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

For all three dimensional analysis, we use the absolute coordinate system defined in figure 2.2. In the following sections, it is necessary to convert between Cartesian and spherical coordinates, which we do using the relations

$$x = r \sin \phi \cos \theta,$$

$$y = r \sin \phi \sin \theta,$$

$$z = r \cos \phi.$$
(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.

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial r} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial r}$$
 (2.2)

Then, calculating derivatives from (2.1) yields

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x} \sin \phi \cos \theta + \frac{\partial f}{\partial y} \sin \phi \sin \theta + \frac{\partial f}{\partial z} \cos \phi. \tag{2.3}$$

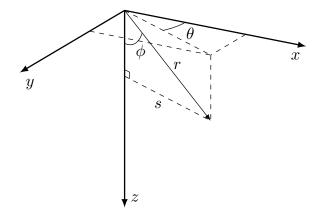


Figure 2.2: Downward-facing right-handed coordinate system with radial distance r from the origin, distance s from the z axis, zenith angle ϕ and azimuthal angle θ

2.3 Population Distributions

2.3.1 Frond Shape

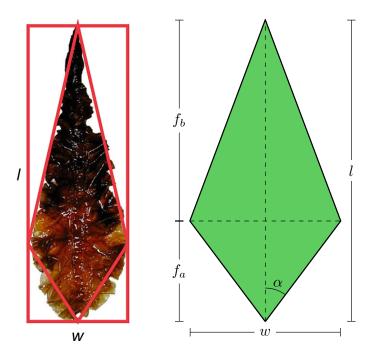


Figure 2.3: Simplified kite-shaped frond

We assume the frond is a kite with length l from base to tip, and width w from left to right. The shortest distance from the base to the diagonal connecting the left and right corners is called f_a , and the shortest distance from that diagonal to the tip is called f_b . We have

$$f_a + f_b = l (2.4)$$

When considering a whole population with varying sizes, it is more convenient to

specify ratios than absolute lengths. Let the following ratios be defined.

$$f_r = \frac{l}{w} \tag{2.5}$$

$$f_s = \frac{f_a}{f_b} \tag{2.6}$$

These ratios are assumed to be consistent among the entire population, making all fronds geometrically similar. With these definitions, the shape of the frond can be fully specified by l, f_r , and f_s . It is possible, then, to redefine w, f_a and f_b as follows from the preceding formulas.

$$w = \frac{l}{f_r} \tag{2.7}$$

$$f_a = \frac{lf_s}{1 + f_s} \tag{2.8}$$

$$f_b = \frac{l}{1 + f_s} \tag{2.9}$$

The angle α , half of the angle at the base corner, is also important in our analysis. Using the above equations,

$$\alpha = \tan^{-1} \left(\frac{2f_r f_s}{1 + f_s} \right) \tag{2.10}$$

The area of the frond is given by

$$A = \frac{lw}{2} = \frac{l^2}{2f_r}. (2.11)$$

Likewise, if the area is known, then the length is

$$l = \sqrt{2Af_r} \tag{2.12}$$

2.3.2 Length and Angle Distributions

We assume that frond lengths are normally distributed with mean μ_l and standard deviation σ_l . We assume the frond 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, μ and κ , which shift and sharpen its peak respectively, as shown in Figure 2.4. κ can be considered analogous to $1/\sigma$ in the normal distribution. Here, we use $\mu = \theta_w$ and $\kappa = v_w$. That is, in the case of zero current velocity, the frond angles are be distributed uniformly, while as current velocity increases, they become increasingly likely to be pointing in the direction of the current. Note that θ_w and v_w vary over depth.

The PDF for this distribution is

$$P_{\theta_f}(\theta_f) = \frac{\exp\left(v_w \cos(\theta_f - v_w)\right)}{2\pi I_0(v_w)} \tag{2.13}$$

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 κ approaches 0.

$$\lim_{v_m \to 0} P_{\theta_f}(\theta_f) = \frac{1}{2\pi} \,\forall \, \theta_f \in [-\pi, \pi] \tag{2.14}$$

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.

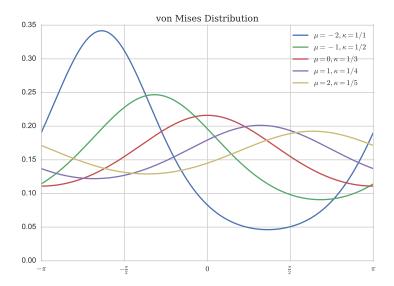


Figure 2.4: von Mises distribution for a variety of parameters

Given independent events A and B,

$$P(A \cap B) = P(A)P(B) \tag{2.15}$$

Then the probability of frond length l and frond angle θ_f coinciding is

$$P_{2D}(\theta_f, l) = P_{\theta_f}(\theta_f) \cdot L(l) \tag{2.16}$$

A contour plot of this 2D distribution for a specific set of parameters is shown in figure 2.5, where probability is represented by color in the 2D plane. Darker green represents higher probability, while lighter beige represents lower probability. In figure 2.6, 50 samples are drawn from this distribution and plotted.

It is important to note that if P_{θ_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, (2.15) would no longer hold, and it would be necessary to use the following more general relation.

$$P(A \cap B) = P(A)P(B|A) = P(B)P(B|A)$$
 (2.17)

This is currently not taken into consideration in this model.

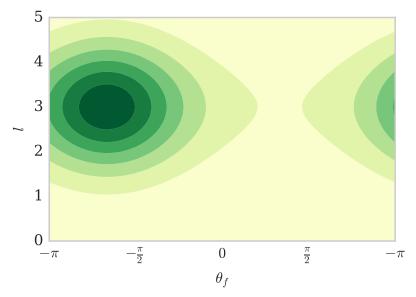


Figure 2.5: 2D length-angle probability distribution with $\theta_w = 2\pi/3, v_w = 1$

2.4 Spatial Distribution

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 and then converting to polar coordinates. Of primary interest are the edges connected to the frond tip. For convenience,

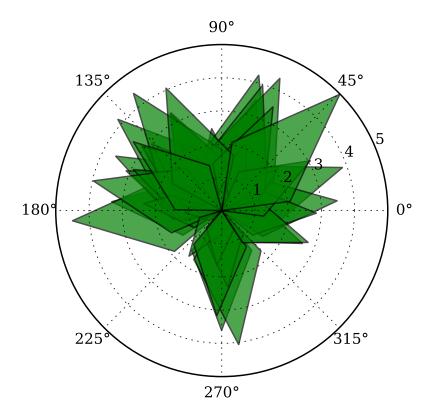


Figure 2.6: A sample of 50 kelp fronds with length and angle picked from the distribution above with $f_s = 0.5$ and $f_r = 2$.

we will use a rotated coordinate system (θ', s) such that the line connecting the base to the tip is vertical, with the base at (0,0). The Cartesian analogue of this coordinate system, (x', y'), has the following properties.

$$x' = s\cos\theta' \tag{2.18}$$

$$y' = s\sin\theta' \tag{2.19}$$

and

$$s = \sqrt{x'^2 + y'^2} \tag{2.20}$$

$$\theta' = \operatorname{atan2}(y, x) \tag{2.21}$$

2.4.2 Functional Description of Frond Edge

With this coordinate system established, we can describe the outer two edges of the frond 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

$$y'_f(x') = l - \text{sign}(x') \frac{f_b}{w/2} x'.$$
 (2.22)

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

$$s_f'(\theta') = \frac{l}{\sin \theta' + S(\theta') \frac{2f_b}{w} \cos \theta'}$$
 (2.23)

where

$$S(\theta') = \operatorname{sign}(\theta' - \pi/2) \tag{2.24}$$

Then, using the relationships in Section 2.3.1, we can rewrite the above equation in terms of our frond ratios f_s and f_r .

$$s_f'(\theta') = \frac{l}{\sin \theta' + S(\theta') \frac{2f_r}{1 + f_s} \cos \theta'}$$
 (2.25)

2.4.3 Absolute Coordinates

To generalize to a frond pointed at an angle θ_f , we will use the coordinate system (θ, s) such that

$$\theta = \theta' + \theta_f - \frac{\pi}{2} \tag{2.26}$$

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

$$s_f(\theta) = s_f' \left(\theta - \theta_f + \frac{\pi}{2} \right) \tag{2.27}$$

2.4.4 Conditions for Occupancy

Consider a fixed frond of length l at an angle θ_f . The point (θ, s) is occupied by the frond if

$$|\theta_f - \theta| < \alpha \tag{2.28}$$

and

$$s < s_f(\theta) \tag{2.29}$$

Equivalently, letting the point (θ, s) be fixed, a frond occupies the point if the following conditions are satisfied.

$$\theta - \alpha < \theta_f < \theta + \alpha \tag{2.30}$$

and

$$l > l_{min}(\theta, s) \tag{2.31}$$

where

$$l_{min}(\theta, s) = s \cdot \frac{l}{s_f(\theta)} \tag{2.32}$$

Then, considering the point to be fixed, (2.30) and (2.31) define the spacial region $R_s(\theta, s)$ called the "occupancy region for (θ, 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. $R_s(3\pi/4, 3/2)$ is shown in blue in figure 2.7 and the smallest possible occupying fronds for several values of θ_f are shown in various colors. Any frond longer than these at the same angle will also occupy the point.

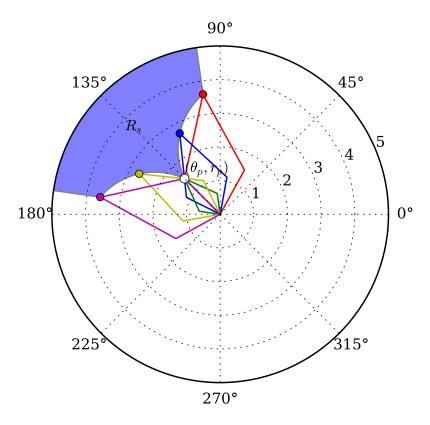


Figure 2.7: Outlines of minimum-length fronds for a variety of angles to occupy the point $(\theta, s) = (3\pi/4, 3/2)$

2.4.5 Probability of Occupancy

We are interested in the probability that, given a fixed point (θ, s) , values of l and θ_f chosen from the distributions described in Section 2.3.2 will fall in the occupancy

region. This is found by integrating P_{2D} over the occupancy region for (θ, s) , as depicted in figure 2.8.

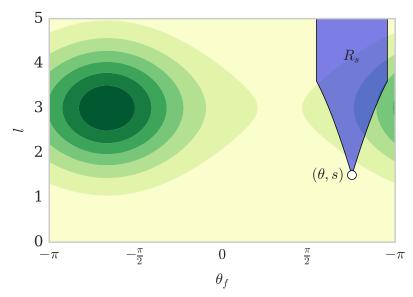


Figure 2.8: Contour plot of $P_{2D}(\theta_f, l)$ overlayed with the region in the $\theta_f - l$ plane which results in a frond occupying the point $(\theta, s) = (3\pi/4, 3/2)$

Now, integrating $P_{2D}(\theta_f, l)$ over $R_s(\theta, s)$ yields the proportion of the population occupying the point (θ, s) .

$$\tilde{P}_{k}(\theta, s, z) = \iint_{R_{s}(\theta, s)} P_{2D}(\theta_{f}, l) dl d\theta_{f}$$

$$= \int_{\theta - \alpha}^{\theta + \alpha} \int_{l_{min}(\theta_{f})}^{\infty} P_{2D}(\theta_{f}, l) dl d\theta_{f} \tag{2.33}$$

Then, multiplying \tilde{P}_k by the number of fronds in the population n of the depth layer gives the expected number of fronds occupying the point. Now, assuming a uniform thickness t for all fronds, and a thickness dz of the depth layer, we find

the proportion of the grid cell occupied by kelp to be

$$P_k = \frac{nt}{dz}\tilde{P}. (2.34)$$

Then, the effective absorption coefficient can be calculated at any point in space as

$$a(\vec{x}) = P_k(\vec{x})a_k + (1 - P_k(\vec{x}))a_w \tag{2.35}$$

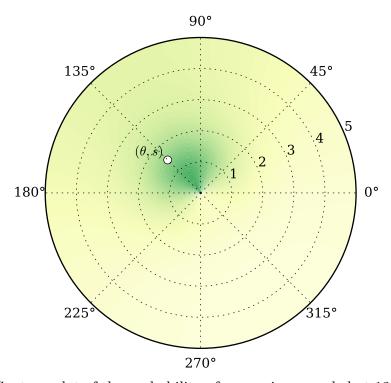


Figure 2.9: Contour plot of the probability of occupying sampled at 121 points using $\theta_f = 2\pi/3, v_w = 1$

CHAPTER III

LIGHT MODEL

Now that we have formulated the distribution of kelp throughout the medium, we introduce the radiative transfer equation, which is used to calculate the light field.

3.1 Optical Definitions

3.1.1 Radiometric Quantities

One of the most fundamental quantities in optics is radiant flux Φ , which is the has units of energy per time. The quantity of primary interest in modeling the light field is radiance L, which is defined as the radiant flux per steradian per projected surface area perpendicular to the direction of propagation of the beam. That is,

$$L = \frac{d^2\Phi}{dAd\omega} \tag{3.1}$$

Once the radiance L is calculated everywhere, the irradiance is

$$I(\vec{x}) = \int_{4\pi} L(\vec{x}, \vec{\omega}) d\omega. \tag{3.2}$$

Integrating $I(\vec{x})$, which has units W/m², over the surface of a frond, produces the power (with units W) transmitted to the frond. This is discussed further in Section 4.4.1

Irradiance can be converted to moles of photons (also called Einsteins) per second as

$$1 \,\mathrm{W/m^2} = 4.2 \,\mathrm{\mu mol \, photons/s}. \tag{3.3}$$

3.1.2 Inherent Optical Properties

We must now define a few inherent optical properties (IOPs) which depend only on the medium of propagation. These phenomena are governed by three inherent optical properties (IOPs) of the medium. The absorption coefficient $a(\vec{x})$ (units m⁻¹) defines the proportional loss of radiance per unit length. The scattering coefficient b (units m⁻¹), defines the proportional loss of radiance per unit length, and is assumed to be constant over space.

The volume scattering function (VSF) $\beta(\Delta): [-1,1] \to \mathbb{R}^+$ (units sr⁻¹) defines the probability of light scattering at any given angle from its source. Formally, given two directions $\vec{\omega}$ and $\vec{\omega}'$, $\beta(\vec{\omega} \cdot \vec{\omega}')$ is the probability density of light scattering from $\vec{\omega}$ into $\vec{\omega}'$ (or vice-versa). Of course, since a single direction subtends no solid angle, the probability of scattering occurring exactly from $\vec{\omega}$ to $\vec{\omega}'$ is 0. Rather, we say that the probability of radiance being scattered from a direction ω into an element of solid angle Ω is $\int_{\Omega} \beta(\vec{\omega} \cdot \vec{\omega}') d\vec{\omega}'$.

The VSF is normalized such that

$$\int_{-1}^{1} \beta(\Delta) \, d\Delta = \frac{1}{2\pi},\tag{3.4}$$

so that for any ω ,

$$\int_{4\pi} \beta(\vec{\omega} \cdot \vec{\omega}') \, d\vec{\omega}' = 1. \tag{3.5}$$

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

3.2 The Radiative Transfer Equation

3.2.1 Ray Notation

Consider a fixed position \vec{x} and direction $\vec{\omega}$ such that $\vec{\omega} \cdot \hat{z} \neq 0$.

Let $\vec{l}(\vec{x}, \vec{\omega}, s)$ denote the linear path containing \vec{x} with initial z coordinate given by

$$z_0 = \begin{cases} 0, & \vec{\omega} \cdot \hat{z} < 0 \\ z_{\text{max}}, & \vec{\omega} \cdot \hat{z} > 0 \end{cases}$$
 (3.6)

Then,

$$\vec{l}(\vec{x}, \vec{\omega}, s) = \frac{1}{\tilde{s}} (s\vec{x} + (\tilde{s} - s)\vec{x_0}(\vec{x}, \vec{\omega}))$$
(3.7)

where

$$\vec{x_0}(\vec{x}, \vec{\omega}) = \vec{x} - \tilde{s}\vec{\omega} \tag{3.8}$$

is the origin of the ray, and

$$\tilde{s} = \frac{\vec{x} \cdot \hat{z} - z_0}{\vec{\omega} \cdot \hat{z}} \tag{3.9}$$

is the path length from $\vec{x_0}(\vec{x}, \vec{\omega})$ to \vec{x} .

3.2.2 Colloquial Description

Denote the radiance at \vec{x} in the direction $\vec{\omega}$ by $L(\vec{x}, \vec{\omega})$. As light travels along $\vec{l}(\vec{x}, \vec{\omega}, s)$, interaction with the medium produces three 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.

3.2.3 Equation of Transfer

Then, combining these phenomena, the Radiative Transfer equation along $\vec{l}(\vec{x}, \vec{\omega})$ becomes

$$\frac{dL}{ds}(\vec{l}(\vec{x},\vec{\omega},s),\vec{\omega}) = -(a(\vec{x}) + b)L(\vec{x},\vec{\omega}) + b\int_{4\pi} \beta(\vec{\omega} \cdot \vec{\omega}')L(\vec{x}) d\omega', \tag{3.10}$$

where $\int_{4\pi}$ denotes integration over the unit sphere.

Now, we have

$$\begin{split} \frac{dL}{ds}(\vec{l}(\vec{x}, \vec{\omega}, s), \vec{\omega}) &= \frac{d\vec{l}}{ds}(\vec{x}, \vec{\omega}, s) \cdot \nabla L(\vec{x}, \vec{\omega}', \vec{\omega}) \\ &= \vec{\omega} \cdot \nabla L(\vec{x}, \vec{\omega}) \end{split}$$

Then, the general form of the Radiative Transfer Equation is

$$\vec{\omega} \cdot \nabla L(\vec{x}, \vec{\omega}) = -(a(\vec{x}) + b)L(\vec{x}, \vec{\omega}) + b \int_{4\pi} \beta(\vec{\omega} \cdot \vec{\omega}')L(\vec{x}, \vec{\omega}') d\omega'$$
 (3.11)

or, equivalently,

$$\vec{\omega} \cdot \nabla L(\vec{x}, \vec{\omega}) + a(\vec{x})L(\vec{x}, \vec{\omega}) = b \left(\int_{4\pi} \beta(\vec{\omega} \cdot \vec{\omega}')L(\vec{x}, \vec{\omega}') d\omega' - L(\vec{x}, \vec{\omega}) \right)$$
(3.12)

3.2.4 Boundary Conditions

We use periodic boundary conditions in the x and y directions.

$$L\left((x_{\min}, y, z), \vec{\omega}\right) = L\left((x_{\max}, y, z), \vec{\omega}\right) \tag{3.13}$$

$$L\left((x, y_{\min}, z), \vec{\omega}\right) = L\left((x, y_{\max}, z), \vec{\omega}\right) \tag{3.14}$$

In the z direction, we specify a spatially uniform downwelling light just under the surface of the water by a function $f(\vec{\omega})$. 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.

$$L(\vec{x_s}, \vec{\omega}) = f(\omega) \text{ if } \vec{\omega} \cdot \hat{z} > 0$$
 (3.15)

$$L(\vec{x_b}, \vec{\omega}) = 0 \text{ if } \vec{\omega} \cdot \hat{z} < 0 \tag{3.16}$$

3.3 Low-Scattering Approximation

In clear waters where absorption is more important than scattering, an asymptotic expansion can be used whereby the light field is generated through a sequence of discrete scattering events.

3.3.1 Asymptotic Expansion

Taking b to be small, we introduce the asymptotic series

$$L(\vec{x}, \vec{\omega}) = L_0(\vec{x}, \vec{\omega}) + bL_1(\vec{x}, \vec{\omega}) + b^2 L_2(\vec{x}, \vec{\omega}) + \cdots$$
 (3.17)

Then, substituting the above into the RTE,

$$\vec{\omega} \cdot \nabla \left[L_0(\vec{x}, \vec{\omega}) + bL_1(\vec{x}, \vec{\omega}) + b^2 L_2(\vec{x}, \vec{\omega}) + \cdots \right]$$

$$+ a(\vec{x}) \left[L_0(\vec{x}, \vec{\omega}) + bL_1(\vec{x}, \vec{\omega}) + b^2 L_2(\vec{x}, \vec{\omega}) + \cdots \right]$$

$$= b \left(\int_{4\pi} \beta(|\vec{\omega} - \vec{\omega}'|) \left[L_0(\vec{x}, \vec{\omega}') + bL_1(\vec{x}, \vec{\omega}') + b^2 L_2(\vec{x}, \vec{\omega}') + \cdots \right] d\vec{\omega}'$$

$$- \left[L_0(\vec{x}, \vec{\omega}) + bL_1(\vec{x}, \vec{\omega}) + b^2 L_2(\vec{x}, \vec{\omega}) + \cdots \right] \right)$$

$$(3.18)$$

Then, grouping like powers of b, we have the decoupled set of equations

:

$$\vec{\omega} \cdot \nabla L_0(\vec{x}, \vec{\omega}) + a(\vec{x})L_0(\vec{x}) = 0 \tag{3.19}$$

$$\vec{\omega} \cdot \nabla L_1(\vec{x}, \vec{\omega}) + a(\vec{x})L_1(\vec{x}) = \int_{4\pi} \beta(|\vec{\omega} - \vec{\omega}'|)L_0(\vec{x}, \vec{\omega}') d\vec{\omega}' - L_0(\vec{x}, \vec{\omega})$$
(3.20)

$$\vec{\omega} \cdot \nabla L_2(\vec{x}, \vec{\omega}) + a(\vec{x})L_2(\vec{x}) = \int_{4\pi} \beta(|\vec{\omega} - \vec{\omega}'|)L_1(\vec{x}, \vec{\omega}') d\vec{\omega}' - L_1(\vec{x}, \vec{\omega})$$
(3.21)

For boundary conditions, let x_s be a point on the surface of the domain.

$$L_0(\vec{x_s}, \vec{\omega}) + bL_1(\vec{x_s}, \vec{\omega}) + b^2 L_2(\vec{x_s}, \vec{\omega}) + \dots = \begin{cases} f(\omega), & \hat{z} \cdot \omega > 0\\ 0, & \text{otherwise,} \end{cases}$$
(3.22)

which becomes

$$L_0(\vec{x}, \vec{\omega}) = \begin{cases} f(\omega), & \hat{z} \cdot \omega > 0, \\ 0, & \text{otherwise,} \end{cases}$$
 (3.23)

$$L_1(\vec{x}, \vec{\omega}) = 0 \tag{3.24}$$

$$L_2(\vec{x}, \vec{\omega}) = 0. \tag{3.25}$$

:

3.3.2 Analytical Solution

For all $\vec{x}, \vec{\omega}$, let

$$\tilde{a}(s) = a(\vec{l}(\vec{x}, \vec{\omega}), s), \tag{3.26}$$

$$\frac{du_0}{ds}(s) + \tilde{a}(s)u_0(s) = 0, u_0(0) = f(\vec{\omega})$$
(3.27)

$$u_0(s) = f(\omega) \exp\left(-\int_0^s \tilde{a}(s) \, ds\right),\tag{3.28}$$

$$L_0(\vec{l}(\vec{x}, \vec{\omega}, s), \vec{\omega}) = u_0(s)$$
 (3.29)

$$g_n(s) = \int_{4\pi} \beta(|\vec{\omega} - \vec{\omega}'|) L_{n-1}(\vec{l}(\vec{x}, \vec{\omega}', s), \vec{\omega}') d\vec{\omega}' - L_{n-1}(\vec{l}(\vec{x}, \vec{\omega}, s), \vec{\omega})$$
(3.30)

$$\frac{du_n}{ds}(s) + \tilde{a}(s)u_n(s) = g_n(s), u_n(0) = 0$$
 (3.31)

$$u_n(s) = \int_0^s g_n(s') \exp\left(-\int_{s''}^{s'} \tilde{a}(s'') ds''\right) ds'$$
 (3.32)

$$L_n(\vec{l}(\vec{x}, \vec{\omega}, s), \vec{\omega}) = u_n(s)$$
(3.33)

CHAPTER IV

NUMERICAL SOLUTION

In this chapter, the mathematical details involved in the numerical solution of the previously described equations are presented. It is assumed that this model is run in conjunction with a model describing the growth of kelp over its life cycle, which calls this light model periodically to update the light field.

4.1 Super-Individuals

The algorithm described in this chapter has two components. First, a probabilistic description of the kelp is generated at each point in a discrete spatial grid. Second, optical properties of the resulting kelp-water medium are derived, and the light field is calculated. The first component is described here.

4.1.1 Frond Length Distribution

Rather than model each kelp frond, a subset of the population, called super-individuals, are modelled explicitly, and are considered to represent many identical individuals, as in [11]. Specifically, at each depth k, there are n super-individuals, indexed by i. Super-individual i has a frond area A_{ki} and represents n_{ki} individual fronds.

From (2.12), the frond length of the super-individual is $l_{ki} = \sqrt{2A_{ki}f_r}$. Given the super-individual data, we calculate the mean μ and standard deviation σ frond lengths using the formulas:

$$\mu_k = \frac{\sum_{i=1}^{N} l_{ki}}{\sum_{i=1}^{N} n_{ki}},\tag{4.1}$$

$$\sigma_k = \frac{\sum_{i=1}^{N} (l_{ki} - \mu_k)^2}{\sum_{i=1}^{N} n_{ki}}.$$
(4.2)

We then assume that frond lengths are normally distributed in each depth layer with mean μ_k and standard deviation σ_k .

4.2 Discrete Grid

The following is a description of the uniform, rectangular 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.

The number of grid cells in each dimension are denoted by n_x , n_y , n_z , n_θ , and n_ϕ , with uniform spacings dx, dy, dz, $d\theta$, and $d\phi$ between adjacent grid points.

The following indices are assigned to each dimension:

$$x \to i$$
 (4.3)

$$y \to j \tag{4.4}$$

$$z \to k$$
 (4.5)

$$\theta \to l$$
 (4.6)

$$\phi \to m$$
 (4.7)

It is convenient, however, to use a single index p to refer to directions $\vec{\omega}$ rather than referring to θ and ϕ separately. Then, the center of a generic grid cell will be denoted as $(x_i, y_j, z_k, \vec{\omega}_p)$, and the boundaries between adjacent grid cells will be referred to as edges. One-indexing is employed throughout this document.

4.2.1 Spatial Grid

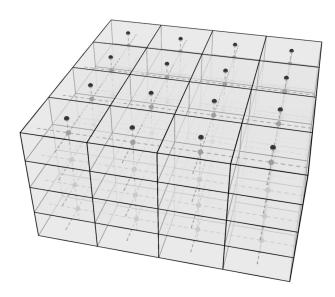


Figure 4.1: Spatial grid

$$dx = \frac{x_{\text{max}} - x_{\text{min}}}{n_x} \tag{4.8}$$

$$dy = \frac{y_{\text{max}} - y_{\text{min}}}{n_y} \tag{4.9}$$

$$dz = \frac{z_{\text{max}} - z_{\text{min}}}{n_z} \tag{4.10}$$

Denote the edges as

$$x_i^e = (i-1)x \text{ for } i = 1, \dots, n_x$$
 (4.11)

$$y_j^e = (j-1)y \text{ for } j = 1, \dots, n_y$$
 (4.12)

$$z_k^e = (k-1)z \text{ for } k = 1, \dots, n_z$$
 (4.13)

and the cell centers as

$$x_i = (i - 1/2)dx \text{ for } i = 1, \dots, n_x$$
 (4.14)

$$y_j = (j - 1/2)dy \text{ for } j = 1, \dots, n_y$$
 (4.15)

$$z_k = (k - 1/2)dz$$
 for $k = 1, \dots, n_z$ (4.16)

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

Also, note that no grid center is located on the plane z=0. The surface radiance boundary condition is treated separately.

4.2.2 Angular Grid

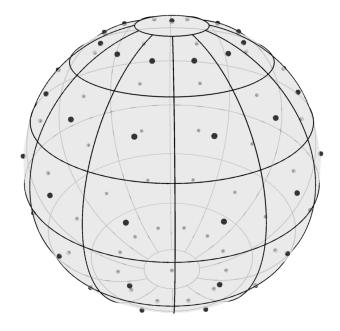


Figure 4.2: Angular grid at each point in space

Now, we define the azimuthal angle such that

$$\theta_l = (l-1)d\theta. \tag{4.17}$$

For the sake of periodicity, we need

$$\theta_1 = 0, \tag{4.18}$$

$$\theta_{n_{\theta}} = 2\pi - d\theta, \tag{4.19}$$

which requires

$$d\theta = \frac{2\pi}{n_{\theta}}. (4.20)$$

For the polar angle, we similarly let

$$\phi_m = (m-1)d\phi \tag{4.21}$$

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

$$\phi_1 = 0, \tag{4.22}$$

$$\phi_{n_{\phi}} = \pi. \tag{4.23}$$

This gives us

$$d\phi = \frac{\pi}{n_{\phi} - 1}.\tag{4.24}$$

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

$$\theta_l^e = (l - 1/2)d\theta, \qquad l = 1, \dots, n_\theta$$
 (4.25)

$$\phi_m^e = (m - 1/2)d\phi, \quad m = 1, \dots, n_\phi - 1.$$
 (4.26)

Note that while θ has its final edge following its final center, this is not the case for ϕ .

As shown in Figure 4.2, $\phi = 0$ and $\phi = \pi$, called the north (+z) and south (-z) poles respectively, are treated separately. The total number of angles considered is $n_{\vec{\omega}} = n_{\phi}n_{\theta} - 2(n_{\theta} - 1)$. Since the poles create a non-rectangular angular grid in the sense that $n_{\vec{\omega}}$ is not the product of two integers, it is advantageous to use a single variable $p = 1, \ldots, n_{\vec{\omega}}$ to index angles $\vec{\omega} = (\theta, \phi)$ such that $p \in \{2, \ldots, n_{\vec{\omega}} - 1\}$ refers to the interior of the angular grid, and p = 1 and $p = n_{\vec{\omega}}$ refer to the north and south

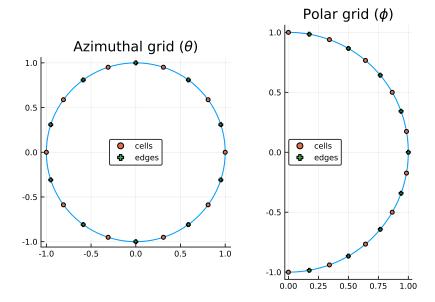


Figure 4.3: Angular grid

poles respectively. The following notation is used.

$$\hat{l}(p) = \text{mod1}(p, n_{\theta}) \tag{4.27}$$

$$\hat{m}(p) = \text{ceil}(p/n_{\theta}) + 1 \tag{4.28}$$

$$\hat{\theta}_p = \theta_{\hat{l}(p)} \tag{4.29}$$

$$\hat{\phi}_p = \phi_{\hat{m}(p)} \tag{4.30}$$

Thus, it follows that

$$p = (\hat{m}(p) - 2) n_{\theta} + \hat{l}(p). \tag{4.31}$$

Accordingly, define

$$\hat{p}(l,m) = (m-1)n_{\theta} + l. \tag{4.32}$$

Further, we refer to the angular grid cell centered at $\vec{\omega}_p$ as Ω_p , and the solid angle subtended by Ω_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 infinitessimal differential and for finite grid spacing.

For the poles, we have

$$|\Omega_1| = |\Omega_{n_{\vec{\omega}}}| = \int_{\Omega_1} d\vec{\omega} \tag{4.33}$$

$$= \int_0^{2\pi} \int_0^{d\phi/2} \sin\phi \, d\phi \, d\theta \tag{4.34}$$

$$=2\pi\cos\phi\Big|_{d\phi/2}^{0}\tag{4.35}$$

$$= 2\pi (1 - \cos(d\phi/2)) \tag{4.36}$$

And for all other angular grid cells,

$$|\Omega_p| = \int_{\Omega_p} d\vec{\omega} \tag{4.37}$$

$$= \int_{\theta_l^e}^{\theta_{l+1}^e} \int_{\phi_m^e}^{\phi_{m+1}^e} \sin(\phi) d\phi d\theta$$
 (4.38)

$$= d\theta \int_{\phi_m^e}^{\phi_{m+1}^e} \sin(\phi) d\phi \tag{4.39}$$

$$= d\theta \left(\cos(\phi_m^e) - \cos(\phi_{m+1}^e)\right). \tag{4.40}$$

4.2.3 Angular Quadrature

We assume that all quantities are constant within a spatial-angular grid cell. We therefore employ the midpoint rule for both spatial and angular integration.

Define the angular characteristic function

$$\mathcal{X}_{p}^{\Omega}(\vec{\omega}) = \begin{cases}
1, & \vec{\omega} \in \Omega_{p} \\
0, & \text{otherwise}
\end{cases}$$
(4.41)

$$\int_{4\pi} f(\vec{\omega}) d\vec{\omega} = \int_{4\pi} \sum_{p=1}^{n_{\vec{\omega}}} f_p \mathcal{X}_p^{\Omega}(\vec{\omega}) d\vec{\omega}$$
 (4.42)

$$= \sum_{p=1}^{n_{\vec{\omega}}} f_p \int_{4\pi} \mathcal{X}_p^{\Omega}(\vec{\omega}) \, d\vec{\omega}$$
 (4.43)

$$=\sum_{p=1}^{n_{\vec{\omega}}} f_p \int_{\Omega_p} d\vec{\omega} \tag{4.44}$$

$$=\sum_{p=1}^{n_{\vec{\omega}}} f_p |\Omega_p| \tag{4.45}$$

4.2.4 Scattering Integral

Specifically, we integrate β to determine the amount of light scattered between angular grid cells.

Consider two angular grid cells, Ω and Ω' . The average probability density of scattering from $\vec{\omega} \in \Omega$ to $\vec{\omega}' \in \Omega'$ (or vice versa) is

$$\beta_{pp'} = \frac{1}{|\Omega| |\Omega'|} \int_{\Omega} \int_{\Omega'} \beta(\vec{\omega} \cdot \vec{\omega}') d\vec{\omega}' d\vec{\omega}$$
 (4.46)

Denote the radiance at $(x_i, y_j, z_k, \vec{\omega}_p)$ by L_{ijkp} . Then, the total radiance scattered into Ω_p from $\Omega_{p'}$ is

$$\int_{\Omega} \int_{\Omega'} \beta(\vec{\omega} \cdot \vec{\omega}') L(\vec{x}, \vec{\omega}') d\vec{\omega}' d\vec{\omega} = L_{ijkp'} \int_{\Omega} \int_{\Omega_{p'}} \beta(\vec{\omega} \cdot \vec{\omega}') d\vec{\omega}' d\vec{\omega}$$
(4.47)

$$= \beta_{pp'} |\Omega| |\Omega'| L_{ijkp'}. \tag{4.48}$$

Hence, the average radiance scattered is $\beta_{pp'} |\Omega'| L_{ijkp'}$.

4.3 Finite Difference

We now discuss the discretization of derivatives on the spatial grid.

4.3.1 Discretization

For the spatial interior of the domain, we use the 2nd order central difference formula (CD2) to approximate the derivatives, which is

$$f'(x) = \frac{f(x+dx) - f(x-dx)}{2dx} + \mathcal{O}(dx^3).$$
 (CD2)

When applying the PDE on the upper or lower boundary, we use the forward and backward difference (FD2 and BD2) formulas respectively. Omitting $\mathcal{O}(dx^3)$, we have

$$f'(x) = \frac{-3f(x) + 4f(x + dx) - f(x + 2dx)}{2dx}$$
 (FD2)

$$f'(x) = \frac{3f(x) - 4f(x - dx) + f(x - 2dx)}{2dx}$$
 (BD2)

For the upper and lower boundaries, we need an asymmetric finite difference method. In general, the Taylor Series of a function f about x is

$$f'(x+\varepsilon) = \sum_{n=1}^{\infty} \frac{f^{(n)}(x)}{n!} \varepsilon^n$$
 (4.49)

Truncating after the first few terms, we have

$$f'(x+\varepsilon) = f(x) + f'(x)\varepsilon + \frac{f''(x)}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)$$
 (4.50)

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

$$f'(x - \frac{\varepsilon}{2}) = f(x) - \frac{f'(x)\varepsilon}{2} + \frac{f''(x)\varepsilon^2}{8} + \mathcal{O}(\varepsilon^3).$$
 (4.51)

Rearranging (4.50) produces

$$f''(x)\varepsilon^{2} = 2f(x+\varepsilon) - 2f(x) - 2f'(x)\varepsilon + \mathcal{O}(\varepsilon^{3})$$
(4.52)

Combining (4.51) with (4.52) gives

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

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

$$= \frac{4}{5}\left(2f(x) - 2f(x - \frac{\varepsilon}{2}) + \frac{f(x + \varepsilon)}{4} - \frac{f(x)}{4}\right) + \mathcal{O}(\varepsilon^3)$$

Then, dividing by ε gives

$$f'(x) = \frac{-8f(x - \frac{\varepsilon}{2}) + 7f(x) + f(x + \varepsilon)}{5\varepsilon} + \mathcal{O}(\varepsilon^2)$$
 (4.53)

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

$$f'(x) = \frac{-f(x-\varepsilon) - 7f(x) + 8f(x + \frac{\varepsilon}{2})}{5\varepsilon} + \mathcal{O}(\varepsilon^2)$$
 (4.54)

4.3.2 Difference Equation

In general, we have

$$\vec{\omega} \cdot \nabla L_p = -(a+b)L_p + \sum_{p'=1}^{n_{\vec{\omega}}} \beta_{pp'} L_{p'}. \tag{4.55}$$

$$\vec{\omega} \cdot \nabla L_p + (a + b(1 - \beta_{pp'}))L_p - \sum_{p'=1}^{n_{\vec{\omega}}} \beta_{pp'} L_{p'} = 0$$
 (4.56)

Interior:

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_{p} \cos \hat{\theta}_{p}$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_{p} \sin \hat{\theta}_{p}$$

$$+ \frac{L_{ij,k+1,p} - L_{ij,k-1,p}}{2dz} \cos \hat{\phi}_{p}$$

$$+ (a_{ijk} + b(1 - \beta_{pp'})) L_{ijkp} - \sum_{p'=1}^{n_{\bar{\omega}}} \beta_{pp'} L_{ijkp'}$$
(4.57)

Surface downwelling (BC):

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p$$

$$+ \frac{-8f_p + 7L_{ijkp} + L_{ij,k+1,p}}{5dz} \cos \hat{\phi}_p$$

$$+ (a_{ijk} + b(1 - \beta_{pp'}))L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\vec{\omega}}} \beta_{pp'} L_{ijkp'}.$$

Combining L_{ijkp} terms on the left and moving the boundary condition to the right gives

$$\frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p$$

$$+ \frac{L_{ij,k+1,p}}{5dz} \cos \hat{\phi}_p$$

$$+ (a_{ijk} + b(1 - \beta_{pp'}) + \frac{7}{5dz} \cos \hat{\phi}_p) L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\omega}} \beta_{pp'} L_{ijkp'} = \frac{8f_p}{5dz} \cos \hat{\phi}_p.$$
(4.58)

Likewise for the bottom boundary condition, we have

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_p \cos \hat{\theta}_p$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_p \sin \hat{\theta}_p$$

$$- \frac{L_{ij,k-1,p}}{5dz} \cos \hat{\phi}_p$$

$$+ (a_{ijk} + b(1 - \beta_{pp'}) - \frac{7}{5dz} \cos \hat{\phi}_p) L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\omega}} \beta_{pp'} L_{ijkp'}.$$

$$(4.59)$$

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

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_{p} \cos \hat{\theta}_{p}$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_{p} \sin \hat{\theta}_{p}$$

$$+ \frac{-3L_{ijkp} + 4L_{ij,k+1,p} - L_{ij,k+2,p}}{2dz} \cos \hat{\phi}_{p}$$

$$+ (a_{ijk} + b(1 - \beta_{pp'}))L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\omega}} \beta_{pp'} L_{ijkp'}.$$
(4.60)

Grouping L_{ijkp} terms gives

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_{p} \cos \hat{\theta}_{p}$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_{p} \sin \hat{\theta}_{p}$$

$$+ \frac{4L_{ij,k+1,p} - L_{ij,k+2,p}}{2dz} \cos \hat{\phi}_{p}$$

$$+ \left(a_{ijk} + b(1 - \beta_{pp'}) - 3\frac{\cos \hat{\phi}_{p}}{2dz}\right) L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\vec{\omega}}} \beta_{pp'} L_{ijkp'}.$$
(4.61)

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

$$0 = \frac{L_{i+1,jkp} - L_{i-1,jkp}}{2dx} \sin \hat{\phi}_{p} \cos \hat{\theta}_{p}$$

$$+ \frac{L_{i,j+1,kp} - L_{i,j-1,kp}}{2dy} \sin \hat{\phi}_{p} \sin \hat{\theta}_{p}$$

$$+ \frac{-4L_{ij,k-1,p} + L_{ij,k-2,p}}{2dz} \cos \hat{\phi}_{p}$$

$$+ \left(a_{ijk} + b(1 - \beta_{pp'}) + 3\frac{\cos \hat{\phi}_{p}}{2dz}\right) L_{ijkp}$$

$$- \sum_{p'=1}^{n_{\bar{\omega}}} \beta_{pp'} L_{ijkp'}$$
(4.62)

4.3.3 Structure of Linear System

Describe layout of matrix.

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

Table 4.1: Breakdown of nonzero matrix elements by derivative case

Number of rows/columns: $n_x n_y n_z n_{\vec{\omega}}$

Number of nonzero RHS entries: $n_x n_y n_z/2$

Total number of nonzero matrix entries: $n_x n_y n_{\vec{\omega}} [n_z (n_{\vec{\omega}} + 6) - 1]$

4.3.4 GMRES

GMRES is a Krylov Subspace method. These work like this. Here's what's special about GMRES. Advantages. Drawbacks. Not practical for running in SINMOD.

4.4 Numerical Asymptotics

Given a position \vec{x} and direction $\vec{\omega}$, a path through the discrete grid can be constructed as described in Appendix A, from which we can extract piecewise constant variations of the path absorption coefficient, $\tilde{a}(s)$ and the effective source, $g_n(s)$ from 3.3.2. Then, we proceed as follows.

* Here are the equations for calculating the double integral over ray paths required for the asymptotics. It will hopefully make more sense once I add words to accompany the symbols.

Let

$$g_n(s) = \sum_{i=1}^{N-1} g_{ni} \mathcal{X}_i(s)$$
 (4.63)

$$\tilde{a}(s) = \sum_{i=1}^{N-1} \tilde{a}_i \mathcal{X}_i(s) \tag{4.64}$$

(4.65)

and

$$\mathcal{X}_{i}(s) = \begin{cases}
1, & a_{I} \leq s < s_{i+1} \\
0, & \text{otherwise}
\end{cases}$$
(4.66)

and $\{s_i\}_{i=1}^N$ is increasing.

Let $ds_i = s_{i+1} - s_i$.

Let $\hat{i}(s) = \min \{ i \in \{1, ..., N\} : s_i > s \}$. Let $\tilde{d}(s) = s_{\hat{i}(s)} - s$.

We have $s_1 = 0$ and $s_N = \tilde{s}$.

$$u_n(\tilde{s}) = \int_0^{\tilde{s}} g_n(s') \exp\left(-\int_{s''}^{s'} \tilde{a}(s'') \, ds''\right) \, ds'$$
 (4.67)

$$= \int_{0}^{s_{N}} \sum_{i=1}^{N-1} g_{ni} \mathcal{X}_{i}(s') \exp\left(-\int_{s''}^{s'} \sum_{j=1}^{N-1} \tilde{a}_{j} \mathcal{X}_{j}(s'') ds''\right) ds'$$
(4.68)

$$= \sum_{i=1}^{N-1} g_{ni} \int_0^{s_N} \mathcal{X}_i(s') \exp\left(-\sum_{j=1}^{N-1} \tilde{a}_j \int_{s''}^{s'} \mathcal{X}_j(s'') ds''\right) ds'$$
(4.69)

$$= \sum_{i=1}^{N-1} g_{ni} \int_{s_i}^{s_{i+1}} \exp\left(-\tilde{a}_{\hat{i}(s')-1}\tilde{d}(s') - \sum_{j=\hat{i}(s')}^{N-1} \tilde{a}_j ds_j\right) ds'$$
(4.70)

$$= \sum_{i=1}^{N-1} g_{ni} \int_{s_i}^{s_{i+1}} \exp\left(-\tilde{a}_i(s_{i+1} - s') - \sum_{j=i+1}^{N-1} \tilde{a}_j ds_j\right) ds'$$
 (4.71)

Let

$$b_i = -\tilde{a}_i s_{i+1} - \sum_{j=i+1}^{N-1} \tilde{a}_j ds_j. \tag{4.72}$$

$$u_n(\tilde{s}) = \sum_{i=1}^{N-1} g_{ni} \int_{s_i}^{s_{i+1}} \exp(\tilde{a}_i s' + b_i) ds'$$
 (4.73)

$$= \sum_{i=1}^{N-1} g_{ni} e^{b_i} \int_{s_i}^{s_{i+1}} \exp(\tilde{a}_i s') ds'$$
 (4.74)

Let

$$d_i = \int_{s_i}^{s_{i+1}} \exp\left(\tilde{a}_i s'\right) \, ds' \tag{4.75}$$

$$= \begin{cases} ds_i, & \tilde{a} = 0\\ (\exp(\tilde{a}_i s_{i+1}) - \exp(\tilde{a}_i s_i)) / \tilde{a}_i, & \text{otherwise} \end{cases}$$

$$(4.76)$$

Then,

$$u_n(\tilde{s}) = \sum_{i=1}^{N-1} g_{ni} d_i e^{b_i}$$
(4.77)

4.4.1 Perceived Irradiance

The average irradiance experienced by a kelp frond in depth layer k is

$$\tilde{I}_k = \frac{\sum_{ij} P_{ijk} I_{ijk}}{\sum_{ij} P_{ijk}} \tag{4.78}$$

The irradiance perceived by a the kelp is expected to be slightly lower than the average irradiance,

$$\bar{I}_k = \frac{\sum_{ij} I_{ijk}}{n_x n_y} \tag{4.79}$$

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.

CHAPTER V

PARAMETER VALUES

I'll describe what one would do in order to determine "frond bending coefficients", as well as optical properties of water and kelp, citing literature and reporting values obtained by others.

- 5.1 Parameters from Literature
- * More to come
- 5.2 Frond Distribution Parameters
- 5.2.1 Rotation
- 5.2.2 Lift

Parameter Name	Symbol	Value(s)	Citation	Notes	
Kelp Absorp-	A_k	0.8	[4]	Actually for	
tance				Macrocystis	
				Pyrifera	
Water absorp-	a_w	?	?	?	
tion coefficient					
Scattering coeffi-	b	0.366	[12]	Table 2, $b_{\lambda 0}$,	
cient				mean	
VSF	β	tabulated	[10, 12],	Currently using	
				Petzold	
Frond thickness	t	$0.4\mathrm{mm}$	Ole Jacob	Carina? ***	
Water absorp-	a_w	$0.03\ 1\ 1/{\rm m}$	[6]	Fig. 6, dense	
tion coefficient				cluster. Sam-	
				nanger Fjord,	
				Western Norway.	
Water scattering	a_w	$0.5~1\mathrm{1/m}$	[6]	Fig. 7, dense	
coefficient				cluster. Sam-	
				nanger Fjord,	
				Western Norway.	
Surface solar ir-	I_0	$50\mathrm{Wm^{-2}}$	[2]	Irradiance for	
radiance				maximal pho-	
		50		tosynthesis,	
		θU		converted from	

photons

Site	$a(\mathrm{m}^{-1})$	$b(\mathrm{m}^{-1})$	$c(\mathrm{m}^{-1})$	a/c	b/c
AUTEC 7	0.082	0.117	0.199	0.412	0.588
AUTEC 8	0.114	0.037	0.151	0.753	0.247
AUTEC 9	0.122	0.043	0.165	0.742	0.258
HAOCE 5	0.195	0.275	0.47	0.415	0.585
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 2040	0.366	1.824	2.19	0.167	0.833
NUC 2240	0.125	1.205	1.33	0.094	0.906
Filtered Fresh	0.093	0.009	0.102	0.907	0.093
$Filtered\ Fresh\ +\ Scat.$	0.138	0.547	0.685	0.202	0.798
Fresh + Scat. + Abs.	0.764	0.576	1.34	0.57	0.43
As Delivered	0.196	1.284	1.48	0.133	0.867
Filtered 40 min	0.188	0.407	0.595	0.315	0.685
Filtered 1hr 40 min	0.093	0.081	0.174	0.537	0.463
Filtered 18hr	0.085	0.008	0.093	0.909	0.091

Table 5.2: Petzold IOP summary [10]. I'll pull a few cases from here and point out when the asymptotic approximation will work.

CHAPTER VI

MODEL ANALYSIS

6.1 Grid Study

Run many grid sizes with GMRES, using asymptotic solution as initial guess. Compare CPU times and accuracy, assuming largest grid is "true" solution. Determine necessary grid size to achieve reasonable accuracy.

6.2 Asymptotic Convergence

Compare asymptotic solutions to GMRES with reasonable grid size as determined above. Compare CPU time and accuracy. Determine ideal number of scatters to include (number of terms in asymptotic series). Repeat for a few values of scattering coefficient.

6.3 Sensitivity Analysis

Vary parameters and measure average differences in radiance for full grid, as well as average irradance over depth.

- absorption coefficient
- scattering coefficient

- VSF
- frond bending coefficient

6.4 Kelp Cultivation Simulation

Run Ole Jacob's model with my new light model, compare:

- irrad over time for several depths
- computation time
- harvestable biomass

CHAPTER VII

CONCLUSION

We present a probabilistic model for the spatial distribution of kelp, and develop a first-principles model for the light field, considering absorption and scattering due to the water and kelp. A full finite difference solution is presented, and an asymptotic approximation based on discrete scattering events is subsequently developed.

Future work:

- Frond bending
- Horizontal kelp ropes (long lines)
- etc.

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APPENDIX A

RAY TRACING ALGORITHM

In order to evaluate a path integral through the previously described 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 $\vec{p_1} = (p_{1x}, p_{1y}, p_{1z})$ and a corresponding path $\vec{l}(\vec{x_1}, \vec{\omega}, s)$. To find the location of discontinuities in the itegrand, we first calculate the distance from its origin, $\vec{p_0} = \vec{x_0}(\vec{p_1}, \vec{\omega}) = (p_{0x}, p_{0y}, p_{0z})$ to grid edges in each dimension separately.

Given

$$x_i = p_{0x} + \frac{s_i^x}{\tilde{s}}(p_{1x} - p_{0x}) \tag{A.1}$$

$$y_j = p_{0y} + \frac{s_j^y}{\tilde{s}}(p_{1y} - p_{0y}) \tag{A.2}$$

$$z_k = p_{0z} + \frac{s_k^z}{\tilde{s}}(p_{1z} - p_{0z}) \tag{A.3}$$

we have

$$s_i^x = \tilde{s} \frac{x_i - p_{0x}}{p_{1x} - p_{0x}} \tag{A.4}$$

$$s_i^y = \tilde{s} \frac{y_i - p_{0y}}{p_{1y} - p_{0y}} \tag{A.5}$$

$$s_i^z = \tilde{s} \frac{z_i - p_{0z}}{p_{1z} - p_{0z}} \tag{A.6}$$

(A.7)

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

$$\delta_x = \operatorname{sign}(p_{0x} - p_{1x}) \tag{A.8}$$

$$\delta_y = \operatorname{sign}(p_{0y} - p_{1y}) \tag{A.9}$$

$$\delta_z = \operatorname{sign}(p_{0z} - p_{1z}) \tag{A.10}$$

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

$$\sigma_x = (\delta_x + 1)/2 \tag{A.11}$$

$$\sigma_y = (\delta_y + 1)/2 \tag{A.12}$$

$$\sigma_z = (\delta_z + 1)/2 \tag{A.13}$$

For this algorithm, we keep two sets of indices. (i, j, k) indexes the grid cell, and will be used for extracting physical quantities from each cell along the path. Meanwhile, (i^e, j^e, k^e) will index the edges between grid cells, beginning after the first cell. i.e., $i^e = 1$ 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 $\vec{p_0}$.

That is,

$$i_0 = \operatorname{ceil}\left(\frac{p_{0x} - x_{\min}}{dx}\right) \tag{A.14}$$

$$j_0 = \operatorname{ceil}\left(\frac{p_{0y} - y_{\min}}{dy}\right) \tag{A.15}$$

$$k_0 = \operatorname{ceil}\left(\frac{p_{0z} - z_{\min}}{dz}\right) \tag{A.16}$$

Then,

$$i_0^e = i_0 + \sigma_x \tag{A.17}$$

$$j_0^e = j_0 + \sigma_y \tag{A.18}$$

$$k_0^e = k_0 + \sigma_z \tag{A.19}$$

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

$$s_i^x = \hat{s} \frac{x_i^e - p_{0x}}{p_{1x} - p_{0x}} \tag{A.20}$$

$$s_j^y = \hat{s} \frac{y_j^e - p_{0y}}{p_{1y} - p_{0y}} \tag{A.21}$$

$$s_k^z = \hat{s} \frac{z_k^e - p_{0z}}{p_{1z} - p_{0z}} \tag{A.22}$$

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 that dimension. That is,

* We also track s, the path length.

Consider i, j, k fixed (denoting the current grid cell).

$$d = \operatorname{argmin}_{x,y,z} \left\{ s_i^x - s, s_j^y - s, s_k^z \right\}$$
(A.23)

* This doesn't quite make sense yet.

$$\begin{cases}
i = i + \delta_x, & \text{if } d = x \\
j = j + \delta_y, & \text{if } d = y \\
z = k + \delta_z, & \text{if } d = z
\end{cases}$$
(A.24)

and

$$\begin{cases}
i^e = i^e + \delta_x, & \text{if } d = x \\
j^e = j^e + \delta_y, & \text{if } d = y \\
z^e = k^e + \delta_z, & \text{if } d = z
\end{cases}$$
(A.25)

Then, move to the adjacent grid cell in the dimension which requires the shortest step to reach an edge. Save ds of the path through this cell. Also save abs. coef. and source.

APPENDIX B

FORTRAN CODE

The full FORTRAN implementation of the model described in this thesis. This code can be found online at:

https://github.com/OliverEvans96/kelp

https://gitlab.com/OliverEvans96/kelp

```
utils.f90
1 |! General utilities which might be useful in
      other settings
   module utils
3
   implicit none
4
   ! Constants
   double precision, parameter :: pi = 4.D0 * datan
      (1.D0)
8
   contains
9
10
   ! Determine base directory relative to current
      directory
   ! by looking for Makefile, which is in the base
11
      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 :: maxlength = numpaths *
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
       pathlengths(1) = 1
40
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
            !write(*,*) 'Checking "', tmp_path(1:
51
               pathlengths(ii)),
52
            inquire(file=tmp_path(1:pathlengths(ii))
                // '/Makefile', exist=found)
53
            ! If so, stop. Otherwise, keep looking.
            if (found) then
54
55
                getbasedir = tmp_path(1:pathlengths(
                   ii))
56
                exit
57
            end if
58
       end do
59
60
        ! If it hasn't been found, then this script
          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 \mid! Determine array size from min, max and step
```

```
69
   |! If alignment is off, array will overstep the
       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
           )
76
        ! dx - step size
77
        double precision, intent(in) :: xmin, xmax,
           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))
    end function
85
86
    ! Create array from bounds and number of
87
       elements
88
    ! xmax is not included in array
    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
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
        ! Step size
107
108
        double precision dx
109
110
        ! Calculate step size
        dx = (xmax - xmin) / imax
111
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
153
         ! INPUTS:
         ! x0 - x value at which to interpolate
154
155
        double precision, intent(in) :: x0
156
         ! xx - ordered x values at which y data is
           sampled
157
         ! yy - corresponding y values to interpolate
158
         double precision, dimension (nn), intent(in)
             :: xx,yy
159
         ! nn - length of data
160
        integer, intent(in) :: nn
161
         ! OUTPUT:
162
163
         ! interp - interpolated y value
164
        double precision interp
165
```

```
166
         ! BODY:
167
168
         ! Index of lower-adjacent data (xx(i) < x0 <
            xx(i+1)
169
         integer ii
170
         ! Slope of liine between (xx(ii),yy(ii)) and
             (xx(ii+1),yy(ii+1))
171
        double precision mm
172
173
         ! If out of bounds, then return endpoint
           value
        if (x0 < xx(1)) then
174
175
            interp = yy(1)
        else if (x0 > xx(nn)) then
176
177
            interp = yy(nn)
178
         else
179
           ! Determine ii
180
181
           do ii = 1, nn
182
               if (xx(ii) > x0) then
183
                   ! We've now gone one index too far
184
                   exit
185
               end if
186
           end do
187
188
           ! Determine whether we're on the right
              endpoint
189
           if(ii-1 < nn) then
190
               ! If this is a legitimate
                  interpolation, then
191
               ! subtract since we went one index too
                   far
192
               ii = ii - 1
193
194
               ! Calculate slope
               mm = (yy(ii+1) - yy(ii)) / (xx(ii+1) -
195
                   xx(ii))
196
197
               ! Return interpolated value
               interp = yy(ii) + mm * (x0 - xx(ii))
198
199
           else
200
               ! If we're actually interpolating the
                 right endpoint,
201
               ! then just return it.
202
               interp = yy(nn)
203
           end if
204
205
       end if
206
207
    end function
208
```

```
209
    ! Calculate unshifted position of periodic image
210
    ! Assuming xmin, xmax are extreme attainable
       values of x
211
    function shift_mod(x, xmin, xmax)
212
      double precision x, xmin, xmax
213
      double precision mod_part, shift_mod
214
      mod_part = mod(x-xmin, xmax-xmin)
215
      if (mod_part .ge. 0) then
216
         ! In this case, mod_part is distance
            between image & lower bound
217
         shift_mod = xmin + mod_part
218
      else
219
         ! In this case, mod_part is distance
            between image & upper bound
220
         shift_mod = xmax + mod_part
221
      endif
222
    end function shift_mod
223
224
    ! Bilinear interpolation on evenly spaced 2D
       grid
225
    ! Assume upper endpoint is not included and is
       identical
226
    ! to the lower endpoint, which is included.
227
    function bilinear_array_periodic(x, y, nx, ny,
       x_vals, y_vals, fun_vals)
228
      implicit none
229
      double precision x, y
230
      integer nx, ny
231
      double precision, dimension(:) :: x_vals,
         y_vals
232
      double precision, dimension(:,:) :: fun_vals
233
234
      double precision dx, dy, xmin, ymin
235
      integer i0, j0, i1, j1
236
      double precision x0, x1, y0, y1
237
      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
         i1 = i0 + 1
255
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
         y1 = y_vals(j1)
264
      else
265
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,
         y0, x1, y1, z00, z01, z10, z11)
276
    end function bilinear_array_periodic
277
278
    ! Bilinear interpolation on evenly spaced 2D
279
    ! Assume upper and lower endpoints are included
280
    function bilinear_array(x, y, x_vals, y_vals,
       fun_vals)
281
      implicit none
282
      double precision x, y
283
      double precision, dimension(:) :: x_vals,
         y_vals
284
      double precision, dimension(:,:) :: fun_vals
285
286
      double precision dx, dy, xmin, ymin
      integer i0, j0, i1, j1
287
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
      j0 = int(floor((y-ymin)/dy))+1
300
```

```
301
      i1 = i0 + 1
302
      j1 = j0 + 1
303
304
      ! Bounds checking
305
       ! if(i0 .lt. 1) then
306
            i0 = 1
            i1 = 1
307
      !
308
        else if(i1 .gt. nx) then
309
            i0 = nx
310
            i1 = nx
311
      ! endif
312
      ! if (j0 .lt. 1) then
            j0 = 1
313
            j1 = 1
314
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
         , z00, z01, z10, z11)
331
    end function bilinear_array
332
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-
       rectangle involving
336
    ! the point (x,y) and the point diagonally
       across the rectangle
337
    function bilinear(x, y, x0, y0, x1, y1, z00, z01
       , z10, z11)
338
      implicit none
      double precision x, y double precision x0, y0, x1, y1, z00, z01, z10
339
340
          , z11
341
      double precision a, b, c, d
342
      double precision bilinear
343
344
      a = (x-x0)*(y-y0)
345
      b = (x1-x)*(y-y0)
```

```
346
      c = (x-x0)*(y1-y)
347
      d = (x1-x)*(y1-y)
348
349
      bilinear = (a*z11 + b*z01 + c*z10 + d*z00) / (
         a + b + c + d
350
    end function bilinear
351
352
    ! Integrate using left endpoint rule
353
    ! Assuming the right endpoint is not included in
354
    function lep_rule(arr,dx,nn)
355
         implicit none
356
357
         ! INPUTS:
358
         ! arr - array to integrate
359
        double precision, dimension(nn) :: arr
         ! dx - array spacing (mesh size)
360
361
        double precision dx
         ! nn - length of arr
362
363
        integer, intent(in) :: nn
364
365
         ! OUTPUT:
366
         ! lep_rule - integral w/ left endpoint rule
367
        double precision lep_rule
368
369
        ! BODY:
370
371
         ! Counter
372
        integer ii
373
374
         ! Set output to zero
375
        lep_rule = 0.0d0
376
377
         ! Accumulate integral
378
        do ii = 1, nn
379
             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
      \quad \text{double precision } \, dx \\
389
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 *
            (arr(ii) + arr(ii+1))
397
      end do
398
399
    end function trap_rule_dx
400
401
    ! Integrate using trapezoid rule
402
    ! Assuming both endpoints are included in arr
403
    function trap_rule_uneven(xx, yy, nn)
404
      implicit none
405
      double precision, dimension(nn) :: xx
406
      double precision, dimension(nn) :: yy
407
      integer ii, nn
408
      double precision trap_rule_uneven
409
410
      trap_rule_uneven = 0.0d0
411
      do ii=1, nn-1
412
413
         trap_rule_uneven = trap_rule_uneven + 0.5d0
             *(xx(ii+1)-xx(ii))*(yy(ii) + yy(ii)
            +1))
414
415
    end function trap_rule_uneven
416
417
    function trap_rule_dx_uneven(dx, yy, nn)
418
      implicit none
419
      double precision, dimension(nn-1) :: dx
420
      double precision, dimension(nn) :: yy
      integer ii, nn
421
422
      double precision trap_rule_dx_uneven
423
424
      trap_rule_dx_uneven = 0.0d0
425
426
      do ii=1, nn-1
427
         trap_rule_dx_uneven = trap_rule_dx_uneven +
             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
    function midpoint_rule_halfends(dx, yy, nn)
433
       result(integral)
434
      implicit none
435
      integer ii, nn
436
      double precision, dimension(nn) :: dx, yy
437
      double precision integral
438
439
      if(nn > 1) then
        integral = .5d0 * (dx(1)*yy(1) + dx(nn)*yy(
440
           nn))
441
```

```
442
        do ii=2, nn-1
443
           integral = integral + dx(ii)*yy(ii)
444
        end do
445
      else
446
         integral = 0.d0
447
      end if
448
    end function midpoint_rule_halfends
449
450
    ! Normalize 1D array and return integral w/ left
        endpoint rule
451
    function normalize_dx(arr,dx,nn)
452
         implicit none
453
454
         ! INPUTS:
         ! arr - array to normalize
455
456
         double precision, dimension(nn) :: arr
457
         ! dx - array spacing (mesh size)
        double precision dx ! nn - length of arr
458
459
460
        integer, intent(in) :: nn
461
462
         ! OUTPUT:
463
         ! normalize - integral before normalization
           (left endpoint rule)
464
        double precision normalize_dx
465
         ! BODY:
466
467
468
         ! Calculate integral
469
        normalize_dx = lep_rule(arr,dx,nn)
470
471
         ! Normalize array
472
        arr = arr / normalize_dx
473
      end function normalize_dx
474
475
476
    ! Normalize 1D unevenly-spaced array and
477
    ! return integral w/ trapezoid rule
    ! Will not be quite accurate if rightmost
478
       endpoint is not included
479
      (Very small for VSF, so not a big deal there)
    ! Modifies yy in place
480
    function normalize_uneven(xx, yy, nn) result(
481
       norm)
482
      implicit none
483
484
      ! INPUTS:
485
      ! xx, yy - array values of data to normalize
486
      double precision, dimension(nn) :: xx, yy
487
      ! nn - length of arr
488
      integer, intent(in) :: nn
489
```

```
490
      ! OUTPUT:
491
      ! normalize - integral before normalization (
         left endpoint rule)
      double precision norm
492
493
494
      ! BODY:
495
496
      ! Calculate integral
      ! PERHAPS WE SHOULD USE TRAPEZOID RULE
497
498
      norm = trap_rule_uneven(xx, yy, nn)
499
500
      ! Normalize array
501
      yy(:) = yy(:) / norm
502
503
    end function normalize_uneven
504
505
    ! Read 2D array from file
    function read_array(filename, fmtstr, nn, mm,
506
       skiplines_in)
507
         implicit none
508
509
         ! INPUTS:
510
         ! filename - path to file to be read
511
         ! fmtstr - input format (no parentheses, don
           't specify columns)
         ! e.g. 'E10.2', not '(2E10.2)'
512
513
         character(len=*), intent(in) :: filename,
           fmtstr
514
         ! nn - Number of data rows in file
515
         ! mm - number of data columns in file
516
         integer, intent(in) :: nn, mm
517
         ! skiplines - optional - number of lines to
           skip from header
518
         integer, optional :: skiplines_in
519
         integer skiplines
520
521
         ! OUTPUT:
522
         double precision, dimension(nn,mm) ::
           read_array
523
524
         ! BODY:
525
526
         ! Row counter
527
         integer ii
528
         ! File unit number
        integer, parameter :: un = 10
! Final format to use
529
530
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), '"'
         !write(*,*) 'using format "', trim(finfmt),
538
539
540
         ! Open file
        open(unit=un, file=trim(filename), status='
541
           old', form='formatted')
542
543
        ! Skip lines if desired
544
        if (present (skiplines_in)) then
545
             skiplines = skiplines_in
             do ii = 1, skiplines
546
                 ! Read without variable ignores the
547
                    line
548
                 read(un,*)
549
             end do
550
        else
551
             skiplines = 0
552
        end if
553
554
        ! Loop through lines
555
        do ii = 1, nn
             ! Read one row at a time
556
557
             read(unit=un, fmt=trim(finfmt))
                read_array(ii,:)
558
        end do
559
560
        ! Close file
561
        close(unit=un)
562
563
    end function
564
565
    ! Print 2D array to stdout
    subroutine print_int_array(arr,nn,mm,fmtstr_in)
566
567
      implicit none
568
569
      ! INPUTS:
570
      ! arr - array to print
      integer, dimension (nn,mm), intent(in) :: arr
571
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 specify columns)
576
      ! e.g. 'E10.2', not '(2E10.2)'
577
      character(len=*), optional :: fmtstr_in
      character(len=256) fmtstr
578
579
580
      ! NO OUTPUTS
```

```
581
582
      ! BODY
583
584
      ! Row counter
      integer ii
585
      ! Final format to use
586
      character(len=256) finfmt
587
588
589
      ! Determine string format
590
      if(present(fmtstr_in)) then
591
          fmtstr = fmtstr_in
592
      else
593
         fmtstr = 'I10'
594
      end if
595
596
      ! Generate final format string
      write(finfmt,'(A,I4,A,A)') '(', mm, trim(
597
         fmtstr), ')'
598
599
      ! Loop through rows
600
      do ii = 1, nn
601
         ! Print one row at a time
602
          write(*,finfmt) 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(
           <u>in</u>) :: arr
616
         ! nn - number of data rows in file
         ! nn - number of data columns in file
617
618
         integer, intent(in) :: nn, mm
619
         ! fmtstr - output format (no parentheses,
           don't specify columns)
620
         ! e.g. 'E10.2', not '(2E10.2)'
        character(len=*), optional :: fmtstr_in
621
622
        character(len=256) fmtstr
623
624
        ! NO OUTPUTS
625
626
        ! BODY
627
628
         ! Row counter
629
        integer ii
```

```
630
         ! Final format to use
631
         character(len=256) finfmt
632
633
         ! Determine string format
634
         if(present(fmtstr_in)) then
              fmtstr = fmtstr_in
635
636
         else
637
             fmtstr = 'ES10.2'
638
         end if
639
640
         ! Generate final format string
         write(finfmt, '(A, I4, A, A)') '(', mm, trim(
641
            fmtstr), ')'
642
643
         ! Loop through rows
644
         do ii = 1, nn
645
             ! Include row number
             !write(*,'(I10)', advance='no') ii
! Print one row at a time
646
647
648
             write(*,finfmt) arr(ii,:)
649
         end do
650
651
         ! Print blank line after
         write(*,*) ','
652
653
654
    end subroutine
655
656
    ! Write 2D array to file
    subroutine write_array(arr,nn,mm,filename,
657
       fmtstr_in)
658
         implicit none
659
660
         ! INPUTS:
         ! arr - array to print
661
         double precision, dimension (nn,mm), intent(
662
            in) :: arr
         ! nn - number of data rows in file ! nn - number of data columns in file
663
664
665
         integer, intent(in) :: nn, mm
         ! filename - file to write to
666
667
         character(len=*) filename
668
         ! fmtstr - output format (no parentheses,
            don't specify columns)
669
         ! e.g. 'E10.2', not '(2E10.2)'
670
         character(len=*), optional :: fmtstr_in
671
         character(len=256) fmtstr
672
673
         ! NO OUTPUTS
674
675
         ! BODY
676
         ! Row counter
677
```

```
678
         integer ii
         ! Final format to use
679
680
        character(len=256) finfmt
681
         ! Dummy file unit to use
682
         integer, parameter :: un = 20
683
684
         ! Open file for writing
685
         open(unit=un, file=trim(filename), status='
           replace', form='formatted')
686
687
         ! Determine string format
688
         if(present(fmtstr_in)) then
689
             fmtstr = fmtstr_in
690
         else
             fmtstr = 'E10.2'
691
692
         end if
693
694
         ! Generate final format string
         write(finfmt, '(A, I4, A, A)') '(', mm, trim(
695
           fmtstr), ')'
696
697
         ! Loop through rows
698
        do ii = 1, nn
699
             ! Print one row at a time
700
             write(un,finfmt) arr(ii,:)
701
         end do
702
703
         ! Close file
704
        close(unit=un)
705
706
    end subroutine
707
708
    subroutine zeros(x, n)
709
      implicit none
710
      integer n, i
711
      double precision, dimension(n) :: x
712
      do i=1, n
713
714
          x(i) = 0
715
      end do
716
    end subroutine zeros
717
718 | end module
     sag.f90
 1 |module sag
 2 3
    use utils
    use fastgl
    implicit none
```

```
Spatial grids do not include upper endpoints.
   ! Angular grids do include upper endpoints.
9
   ! Both include lower endpoints.
10
11
   ! To use:
   ! call grid%set_bounds(...)
12
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
      procedure :: phat, lhat, mhat
39
40
      procedure :: init => angle_init ! Call after
         set_num
41
      procedure :: integrate_points =>
         angle_integrate_points
42
      procedure :: integrate_func =>
         angle_integrate_func
```

```
43
      procedure :: deinit => angle_deinit
44
   end type angle2d
45
46
   type angle_dim
47
      integer num
48
      double precision minval, maxval, prefactor
49
      double precision, dimension(:), allocatable
         :: vals, weights, sin, cos
50
    contains
51
      procedure :: set_bounds => angle_set_bounds
      procedure :: set_num => angle1d_set_num
52
      procedure :: deinit => angle1d_deinit
procedure :: integrate_points =>
53
54
         angle1d_integrate_points
55
      procedure :: integrate_func =>
         angle1d_integrate_func
      procedure :: assign_linspace =>
56
         angle1d_assign_linspace
57
      procedure :: assign_legendre
58
   end type angle_dim
59
60
   type space_dim
61
      integer num
62
      double precision minval, maxval
63
      double precision, dimension(:), allocatable
         :: vals, edges, spacing
64
    contains
65
      procedure :: integrate_points =>
         space_integrate_points
66
      procedure :: trapezoid_rule
      procedure :: set_bounds => space_set_bounds
67
      procedure :: set_num => space_set_num
68
69
      procedure :: set_uniform_spacing =>
         space_set_uniform_spacing
70
      !procedure :: set_num_from_spacing
71
      procedure :: set_uniform_spacing_from_num
72
      procedure :: set_spacing_array =>
         space_set_spacing_array
73
      procedure :: deinit => space_deinit
74
      procedure :: assign_linspace
75
   end type space_dim
76
77
   type space_angle_grid !(sag)
78
     type(space_dim) :: x, y, z
79
     type(angle2d) :: angles
80
     double precision, dimension(:), allocatable ::
         x_factor, y_factor
81
   contains
82
     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 =>
         sag_set_num_from_spacing
 87
      procedure :: set_uniform_spacing_from_num =>
         sag_set_uniform_spacing_from_num
 88
      procedure :: calculate_factors =>
         sag_calculate_factors
 89
    end type space_angle_grid
 90
 91
    contains
 92
 93
      subroutine index_list_init(indices)
 94
         class(index_list) indices
         indices%i = 1
 95
 96
         indices\%j = 1
 97
         indices%k = 1
 98
         indices\%p = 1
99
      end subroutine
100
101
      subroutine index_list_print(indices)
         class(index_list) indices
102
103
104
        write(*,*) 'i, j, k, p = ', indices%i,
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(1)
116
         class(angle2d) :: angles
117
         integer 1, p
118
         if (p .eq. 1) then
119
            1 = 1
         else if (p .eq. angles%nomega) then
120
121
            1 = 1
122
         else
123
            l = mod1(p-1, angles%ntheta)
124
       end if
125
      end function lhat
126
      function mhat(angles, p) result(m)
127
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
        end if
137
      end function mhat
138
139
      function phat(angles, 1, m) result(p)
140
        class(angle2d) :: angles
141
        integer 1, m, p
142
143
        if (m .eq. 1) then
144
145
        else if (m .eq. angles%nphi) then
146
           p = angles%nomega
147
        else
           p = (m-2)*angles%ntheta + 1 + 1
148
149
        end if
150
      end function phat
151
152
      subroutine angle_init(angles)
153
        class(angle2d) :: angles
154
        integer 1, m, p
155
        double precision area
156
157
158
        ! TODO: CONSIDER REMOVING non-p
159
        allocate(angles%theta(angles%ntheta))
        allocate(angles%phi(angles%nphi))
160
161
        allocate(angles%theta_edge(angles%ntheta))
162
        allocate(angles%phi_edge(angles%nphi-1))
163
        allocate(angles%theta_p(angles%nomega))
        allocate(angles%phi_p(angles%nomega))
164
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))
        allocate(angles%cos_phi_p(angles%nomega))
169
170
        allocate(angles%sin_phi_p(angles%nomega))
        allocate(angles%cos_theta(angles%nomega))
171
172
        allocate(angles%sin_theta(angles%nomega))
173
        allocate(angles%cos_phi(angles%nomega))
        allocate(angles%sin_phi(angles%nomega))
174
175
        allocate (angles % cos_theta_edge (angles % ntheta
176
        allocate (angles % sin_theta_edge (angles % ntheta
           ))
177
        allocate(angles%cos_phi_edge(angles%nphi-1))
        allocate(angles%sin_phi_edge(angles%nphi-1))
178
```

```
allocate (angles % cos_theta_edge_p (angles %
179
           nomega))
180
        allocate (angles%sin_theta_edge_p(angles%
           nomega))
181
        allocate (angles % cos_phi_edge_p (angles % nomega
182
        allocate(angles%sin_phi_edge_p(angles%nomega
           -1))
183
        allocate(angles%area_p(angles%nomega))
184
185
         ! Calculate spacing
        angles%dtheta = 2.d0*pi/dble(angles%ntheta)
186
        angles%dphi = pi/dble(angles%nphi-1)
187
188
        ! Create grids
189
190
        do l=1, angles%ntheta
191
            angles%theta(1) = dble(1-1)*angles%dtheta
192
            angles%cos_theta(1) = cos(angles%theta(1)
193
            angles%sin_theta(1) = sin(angles%theta(1)
194
            angles%theta_edge(1) = dble(1-0.5d0)*
              angles%dtheta
            angles%cos_theta_edge(1) = cos(angles%
195
              theta_edge(1))
196
            angles%sin_theta_edge(1) = sin(angles%
               theta_edge(1))
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))
            if (m<angles%nphi) then</pre>
203
204
               angles%phi_edge(m) = dble(m-0.5d0)*
                  angles%dphi
205
               angles%cos_phi_edge(m) = cos(angles%
                  phi_edge(m))
206
               angles%sin_phi_edge(m) = sin(angles%
                  phi_edge(m))
207
            end if
208
        end do
209
210
        ! Create p arrays
211
        do m=2, angles%nphi-1
212
           area = angles%dtheta &
213
                 * (angles%cos_phi_edge(m-1) - angles
                    %cos_phi_edge(m))
214
           do l=1, angles%ntheta
```

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

```
252
        angles%cos_theta_edge_p(p) = cos(angles%
           theta_edge_p(p))
253
        angles%sin_theta_edge_p(p) = sin(angles%
           theta_edge_p(p))
254
        angles%cos_phi_edge_p(p) = cos(angles%
           phi_edge_p(p))
255
        angles%sin_phi_edge_p(p) = sin(angles%
           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(1)
262
        angles%theta_edge_p(p) = angles%theta_edge(1
263
        angles%phi_p(p) = angles%phi(m)
264
        angles%cos_theta_p(p) = cos(angles%theta_p(p)
        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
         grid cells
272
      function angle_integrate_points(angles,
         func_vals) result(integral)
273
        class(angle2d) :: angles
274
        double precision, dimension(angles%nomega)
           :: 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) *
              func_vals(p)
282
        end do
283
284
      end function angle_integrate_points
285
286
      function angle_integrate_func(angles,
         func_callable) result(integral)
287
        class(angle2d) :: angles
288
        double precision, external :: func_callable
```

```
289
        double precision, dimension(:), allocatable
           :: func_vals
290
        double precision integral
291
        integer p
292
        double precision theta, phi
293
294
        allocate(func_vals(angles%nomega))
295
296
        do p=1, angles%nomega
297
           theta = angles%theta_p(p)
298
           phi = angles%phi_p(p)
299
            func_vals(p) = func_callable(theta, phi)
300
301
302
        integral = angles%integrate_points(func_vals
303
304
        deallocate(func_vals)
      end function angle_integrate_func
305
306
307
      subroutine angle_deinit(angles)
308
        class(angle2d) :: angles
309
        deallocate (angles %theta)
        deallocate(angles%phi)
310
311
        deallocate(angles%theta_edge)
312
        deallocate(angles%phi_edge)
313
        deallocate(angles%theta_p)
314
        deallocate(angles%phi_p)
315
        deallocate(angles%theta_edge_p)
        deallocate(angles%phi_edge_p)
316
317
        deallocate(angles%cos_theta)
318
        deallocate(angles%sin_theta)
319
        deallocate (angles %cos_phi)
320
        deallocate (angles % sin_phi)
321
        deallocate(angles%cos_theta_p)
322
        deallocate(angles%sin_theta_p)
323
        deallocate(angles%cos_phi_p)
324
        deallocate(angles%sin_phi_p)
325
        deallocate(angles%cos_theta_edge)
326
        deallocate(angles%sin_theta_edge)
327
        deallocate(angles%cos_phi_edge)
328
        deallocate (angles % sin_phi_edge)
329
        deallocate(angles%cos_theta_edge_p)
330
        deallocate(angles%sin_theta_edge_p)
        deallocate(angles%cos_phi_edge_p)
331
332
        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,
         maxval)
340
        class(angle_dim) :: angle
341
        double precision minval, maxval
342
        angle%minval = minval
343
        angle%maxval = maxval
344
      end subroutine angle_set_bounds
345
346
      subroutine angle1d_set_num(angle, num)
347
        class(angle_dim) :: angle
348
        integer num
349
        angle%num = num
350
      end subroutine angle1d_set_num
351
352
      subroutine angle1d_assign_linspace(angle)
353
        class(angle_dim) :: angle
354
        double precision spacing
355
        integer i
356
357
        spacing = (angle%maxval - angle%minval) /
           dble(angle%num)
358
        do i=1, angle%num
359
            angle%vals(i) = (i-1) * spacing
360
361
      end subroutine angle1d_assign_linspace
362
363
      ! To calculate \int_{xmin}^{xmax} f(x) dx :
      ! int = prefactor * sum(weights * f(roots))
364
      subroutine assign_legendre(angle)
365
        class(angle_dim) :: angle
366
367
        double precision root, weight, theta
368
        integer i
        ! glpair produces both x and theta, where x=
369
           cos(theta). We'll throw out theta.
370
371
        allocate(angle%vals(angle%num))
372
        allocate(angle%weights(angle%num))
373
        allocate(angle%sin(angle%num))
374
        allocate(angle%cos(angle%num))
375
376
        ! Prefactor for integration
377
        ! From change of variables
378
        angle%prefactor = (angle%maxval - angle%
           minval) / 2.d0
379
380
        do i = 1, angle%num
381
            call glpair(angle%num, i, theta, weight,
              root)
```

```
382
           call affine_transform(root, -1.d0, 1.d0,
              angle%minval, angle%maxval)
383
            angle%vals(i) = root
384
            angle%weights(i) = weight
385
            angle\%sin(i) = sin(root)
386
           angle\%cos(i) = cos(root)
387
        end do
388
389
      end subroutine assign_legendre
390
391
      ! Integrate callable function over angle via
         Gauss-Legendre quadrature
392
393
      function angle1d_integrate_func(angle,
         func_callable) result(integral)
394
        class(angle_dim) :: angle
395
        double precision, external :: func_callable
        double precision, dimension(:), allocatable
396
           :: func_vals
397
        double precision integral
398
        integer i
399
400
        allocate(func_vals(angle%num))
401
402
        do i=1, angle%num
403
           func_vals(i) = func_callable(angle%vals(i
              ))
404
        end do
405
406
        integral = angle%integrate_points(func_vals)
407
408
        deallocate(func_vals)
409
      end function angle1d_integrate_func
410
411
      ! Integrate function given function values
         sampled at legendre theta values
412
      function angle1d_integrate_points(angle,
         func_vals) result(integral)
413
        class(angle_dim) :: angle
414
        double precision, dimension(angle%num) ::
           func_vals
415
        double precision integral
416
417
        integral = angle%prefactor * sum(angle%
           weights * func_vals)
418
      end function angle1d_integrate_points
419
420
      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
         sampled at even grid points
432
      function space_integrate_points(space,
         func_vals) result(integral)
433
        class(space_dim) :: space
        double precision, dimension(space%num) ::
434
           func_vals
435
        double precision integral
436
437
        ! Encapsulate actual method for easy
           switching
438
        integral = space%trapezoid_rule(func_vals)
439
440
      end function space_integrate_points
441
442
      function trapezoid_rule(space, func_vals)
         result(integral)
        class(space_dim) :: space
443
444
        double precision, dimension(space%num) ::
           func_vals
445
        double precision integral
446
447
        integral = 0.5d0 * sum(func_vals * space%
           spacing)
448
      end function
449
450
      subroutine space_set_bounds(space, minval,
         maxval)
451
        class(space_dim) :: space
        double precision minval, maxval
452
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,
         spacing)
464
        class(space_dim) :: space
465
        double precision spacing
```

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

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

```
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
           multiplied
562
        ! in order to calculate distance traveled in
            t.he
563
        ! (x, y) direction along a ray in the (theta
            , phi)
564
        ! direction
565
        class(space_angle_grid) :: grid
566
        integer p, nomega
567
        double precision theta, phi
568
569
        nomega = grid%angles%nomega
570
571
        allocate(grid%x_factor(nomega))
572
        allocate(grid%y_factor(nomega))
573
574
        do p=1, nomega
575
           theta = grid%angles%theta_p(p)
           phi = grid%angles%phi_p(p)
576
577
           grid%x_factor(p) = tan(phi) * cos(theta)
578
           grid%y_factor(p) = tan(phi) * sin(theta)
579
        end do
580
581
      end subroutine sag_calculate_factors
582
583
      subroutine sag_set_uniform_spacing_from_num(
         grid)
584
        class(space_angle_grid) :: grid
585
        call grid%x%set_uniform_spacing_from_num()
586
        call grid%y%set_uniform_spacing_from_num()
587
        call grid%z%set_uniform_spacing_from_num()
588
      end subroutine
         sag_set_uniform_spacing_from_num
589
590
      ! subroutine sag_set_num_from_spacing(grid)
591
          class(space_angle_grid) :: grid
592
          call grid%x%set_num_from_spacing()
593
          call grid%y%set_num_from_spacing()
594
          call grid%z%set_num_from_spacing()
595
596
      ! end subroutine sag_set_num_from_spacing
597
598
      subroutine sag_deinit(grid)
599
        class(space_angle_grid) :: grid
```

```
call grid%x%deinit()
600
        call grid%y%deinit()
601
        call grid%z%deinit()
602
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
         , ymax]
610
      subroutine affine_transform(x, xmin, xmax,
         ymin, ymax)
611
        double precision x, xmin, xmax, ymin, ymax
612
        x = ymin + (ymax - ymin)/(xmax - xmin) * (x-xmin)
613
      end subroutine affine_transform
614
615
      function num_from_spacing(xmin, xmax, dx)
         result(n)
616
        double precision xmin, xmax, dx
617
        integer n
        n = floor( (xmax - xmin) / dx )
618
619
      end function num_from_spacing
620
621
      function spacing_from_num(xmin, xmax, nx)
         result(dx)
622
        double precision xmin, xmax, dx
623
        integer nx
        dx = (xmax - xmin) / dble(nx)
624
625
      end function spacing_from_num
626 | end module sag
     kelp3d.f90
    ! Kelp 3D
    ! Oliver Evans
 3
    ! 8/31/2017
 4
 5
    ! Given superindividual/water current data at
       each depth, generate kelp distribution at
       each point in 3D space
 6
 7
    module kelp3d
 8
 9
    use kelp_context
10
11
    implicit none
12
13
    contains
14
```

```
subroutine generate_grid(xmin, xmax, nx, ymin,
      ymax, ny, zmin, zmax, nz, ntheta, nphi, grid,
       p_kelp)
16
     double precision xmin, xmax, ymin, ymax, zmin,
     integer nx, ny, nz, ntheta, nphi
17
18
     type(space_angle_grid) grid
19
     double precision, dimension(:,:,:),
        allocatable :: p_kelp
20
21
     call grid%set_bounds(xmin, xmax, ymin, ymax,
        zmin, zmax)
22
     call grid%set_num(nx, ny, nz, ntheta, nphi)
23
24
     allocate(p_kelp(nx,ny,nz))
25
26
   end subroutine generate_grid
27
   subroutine kelp3d_deinit(grid, rope, p_kelp)
28
29
     type(space_angle_grid) grid
30
     type(rope_state) rope
31
     double precision, dimension(:,:,:),
        allocatable :: p_kelp
32
     call rope%deinit()
33
     call grid%deinit()
     deallocate(p_kelp)
34
   end subroutine kelp3d_deinit
35
36
37
   subroutine calculate_kelp_on_grid(grid, p_kelp,
      frond, rope, quadrature_degree)
38
     type(space_angle_grid), intent(in) :: grid
     type(frond_shape), intent(in) :: frond
39
     type(rope_state), intent(in) :: rope
40
41
     type(point3d) point
42
     integer, intent(in) :: quadrature_degree
43
     double precision, dimension(grid%x%num, grid%y
        %num, grid%z%num) :: p_kelp
44
     type (depth_state) depth
45
46
     integer i, j, k, nx, ny, nz
47
     double precision x, y, z
48
49
     nx = grid%x%num
50
     ny = grid%y%num
51
     nz = grid%z%num
52
53
     do k=1, nz
       z = grid%z%vals(k)
54
55
       call depth%set_depth(rope, grid, k)
56
       do i=1, nx
```

```
57
         x = grid%x%vals(i)
58
         do j=1, ny
59
           y = grid%y%vals(j)
60
           call point%set_cart(x, y, z)
           p_kelp(i, j, k) = kelp_proportion(point,
61
               frond, grid, depth,
              quadrature_degree)
62
            !p_kelp(i, j, k) = prob_kelp(point,
              frond, depth, quadrature_degree)
63
        end do
64
       end do
65
     end do
66
   end subroutine calculate_kelp_on_grid
67
68
   subroutine shading_region_limits(theta_low_lim,
      theta_high_lim, point, frond)
69
     type(point3d), intent(in) :: point
70
     type(frond_shape), intent(in) :: frond
71
     double precision, intent(out) :: theta_low_lim
        , theta_high_lim
72
73
     theta_low_lim = point%theta - frond%alpha
74
     theta_high_lim = point%theta + frond%alpha
75
   end subroutine shading_region_limits
76
77
   function prob_kelp(point, frond, depth,
      quadrature_degree)
   ! P_s(theta_p, r_p) - This is the proportion of
78
      the population of this depth layer which can
      be found in this Cartesian grid cell.
     type(point3d), intent(in) :: point
79
80
     type(frond_shape), intent(in) :: frond
     type(depth_state), intent(in) :: depth
81
82
     integer, intent(in) :: quadrature_degree
83
     double precision prob_kelp
84
     double precision theta_low_lim, theta_high_lim
85
86
     call shading_region_limits(theta_low_lim,
        theta_high_lim, point, frond)
87
     prob_kelp = integrate_ps(theta_low_lim,
        theta_high_lim, quadrature_degree, point,
        frond, depth)
88
   end function prob_kelp
89
90
  | function kelp_proportion(point, frond, grid,
      depth, quadrature_degree)
91
     ! This is the proportion of the volume of the
        Cartesian grid cell occupied by kelp
     type(point3d), intent(in) :: point
92
93
     type(frond_shape), intent(in) :: frond
```

```
94
      type(depth_state), intent(in) :: depth
      type(space_angle_grid), intent(in) :: grid
95
96
      integer, intent(in) :: quadrature_degree
97
      double precision p_k, n, t, dz
98
      double precision kelp_proportion
99
100
      n = depth%num_fronds
101
      dz = grid%z%spacing(depth%depth_layer)
      t = frond%ft
102
103
      !write(*,*) 'KELP PROPORTION'
      !write(*,*) 'n=', n
104
      !write(*,*) 'dz=', dz
105
      !write(*,*) 't=', t
106
      !write(*,*) 'coef=', n*t/dz
107
      p_k = prob_kelp(point, frond, depth,
108
         quadrature_degree)
109
      kelp_proportion = n*t/dz * p_k
110
    end function kelp_proportion
111
112
    function integrate_ps(theta_low_lim,
       theta_high_lim, quadrature_degree, point,
       frond, depth) result(integral)
      type(point3d), intent(in) :: point
113
114
      type(frond_shape), intent(in) :: frond
115
      double precision, intent(in) :: theta_low_lim,
          theta_high_lim
116
      integer, intent(in) :: quadrature_degree
117
      type(depth_state), intent(in) :: depth
118
      double precision integral
119
      double precision, dimension(:), allocatable ::
          integrand_vals
120
      integer i
121
122
      type(angle_dim) :: theta_f
123
      call theta_f%set_bounds(theta_low_lim,
         theta_high_lim)
124
      call theta_f%set_num(quadrature_degree)
125
      call theta_f%assign_legendre()
126
127
      allocate(integrand_vals(theta_f%num))
128
129
      do i=1, theta_f%num
130
        integrand_vals(i) = ps_integrand(theta_f%
           vals(i), point, frond, depth)
131
      end do
132
133
      integral = theta_f%integrate_points(
         integrand_vals)
134
135
      deallocate(integrand_vals)
```

```
call theta_f%deinit()
136
137
138
    end function integrate_ps
139
140
    function ps_integrand(theta_f, point, frond,
       depth)
141
      type(point3d), intent(in) :: point
142
      type(frond_shape), intent(in) :: frond
143
      type(depth_state), intent(in) :: depth
144
      double precision theta_f, l_min
145
      double precision angular_part, length_part
146
      double precision ps_integrand
147
148
      l_min = min_shading_length(theta_f, point,
         frond)
149
150
      angular_part = depth%angle_distribution_pdf(
         theta_f)
151
      length_part = 1 - depth%
         length_distribution_cdf(l_min)
152
153
      ps_integrand = angular_part * length_part
154
    end function ps_integrand
155
156
157
    function min_shading_length(theta_f, point,
       frond) result(1 min)
    ! L_min(\theta)
158
159
      type(point3d), intent(in) :: point
160
      type(frond_shape), intent(in) :: frond
      double precision, intent(in) :: theta_f
double precision l_min
161
162
163
      double precision tpp
164
      double precision frond_frac
165
166
      ! tpp === theta_p_prime
167
      tpp = point%theta - theta_f + pi / 2.d0
      frond_frac = 2.d0 * frond%fr / (1.d0 + frond%
168
         fs)
169
      l_min = point%r * (sin(tpp) + angular_sign(tpp)
         ) * frond_frac * cos(tpp))
170
    end function min_shading_length
171
172
    ! function frond_edge(theta, theta_f, L, fs, fr)
173
   |! r_f(\theta)|
174
        double precision, intent(in) :: theta,
       theta_f, L, fs, fr
175
        double precision, intent(out) :: frond_edge
176
177
   1.1
        frond_edge = relative_frond_edge(theta -
       theta_f + pi/2.d0)
```

```
178
179
    ! end function frond_edge
180
181
   |! function relative_frond_edge(theta_prime, L,
       fs, fr)
    ! ! r_f '(\theta')
182
183
        double precision, intent(in) :: theta_prime,
        L, fs, fr
184
        double precision, intent(out) ::
       relative_frond_edge
185
186
        relative_frond_edge = L / (sin(theta_prime)
       + angular_sign(theta_prime * alpha(fs, fr) *
       cos(theta_prime)))
187
    ! end function relative_frond_edge
188
189
    function angular_sign(theta_prime)
190
    ! S(\theta')
191
      double precision, intent(in) :: theta_prime
192
      double precision angular_sign
193
194
      ! This seems to be incorrect in summary.pdf as
          of 9/9/18
195
      ! In the report, it's written as sgn(
         theta_print - pi/2.d0)
196
      ! This results in L_min < 0 - not good!
197
      angular_sign = sgn(pi/2.d0 - theta_prime)
198
    end function angular_sign
199
200 end module kelp3d
    rte_sparse_matrices.f90
 1 |module rte_sparse_matrices
    use sag
 3
    use kelp_context
    use mgmres
 5
    !use hdf5_utils
 6
    implicit none
 7
 8
    type solver_params
 9
       integer maxiter_inner, maxiter_outer
       double precision tol_abs, tol_rel
10
11
    end type solver_params
12
    type rte_mat
13
14
       type(space_angle_grid) grid
15
       type(optical_properties) iops
16
       type(solver_params) params
17
       integer nx, ny, nz, nomega
18
       integer i, j, k, p
```

```
19
      integer nonzero, n_total
20
      integer x_block_size, y_block_size,
         z_block_size, omega_block_size
21
22
      double precision, dimension(:), allocatable
         :: surface_vals
23
      ! A stored in coordinate form in row, col,
24
         data
25
      integer, dimension(:), allocatable :: row,
         col
26
      double precision, dimension(:), allocatable
         :: data
27
      ! b and x stored in rhs in full form
28
      double precision, dimension(:), allocatable
         :: rhs, sol
29
30
      ! Pointer to solver subroutine
31
      ! Set to mgmres by default
32
      procedure(solver_interface), pointer, nopass
         :: solver => mgmres_st
33
34
    contains
35
      procedure :: init => mat_init
36
      procedure :: deinit => mat_deinit
37
      procedure :: calculate_size
38
      procedure :: set_solver_params =>
         mat_set_solver_params
      procedure :: assign => mat_assign
39
40
      procedure :: add => mat_add
41
      procedure :: assign_rhs => mat_assign_rhs
42
      !procedure :: store_index => mat_store_index
43
      !procedure :: find_index => mat_find_index
44
      procedure :: set_bc => mat_set_bc
45
      procedure :: solve => mat_solve
46
      procedure :: ind => mat_ind
47
      !procedure :: to_hdf => mat_to_hdf
48
      procedure attenuate
49
      procedure angular_integral
50
51
      ! Derivative subroutines
52
      procedure x_cd2
53
      procedure x_cd2_first
      procedure x_cd2_last
54
55
      procedure y_cd2
56
      procedure y_cd2_first
57
      procedure y_cd2_last
58
      procedure z_cd2
59
      procedure z_fd2
60
      procedure z_bd2
61
      procedure z_surface_bc
62
      procedure z_bottom_bc
63
```

```
64
    end type rte_mat
65
66
    interface
       ! Define interface for external procedure
67
68
       ! https://stackoverflow.com/questions
          /8549415/how-to-declare-the-interface-
          section-for-a-procedure-argument-which-in-
          turn-ref
69
       subroutine solver_interface(n_total, nonzero,
           row, col, data, &
70
             sol, rhs, maxiter_outer, maxiter_inner,
71
            tol_abs, tol_rel)
72
         integer :: n_total, nonzero
73
         integer, dimension(nonzero) :: row, col
         double precision, dimension(nonzero) ::
74
            data
75
         double precision, dimension(nonzero) :: sol
76
         double precision, dimension(n_total) :: rhs
77
         integer :: maxiter_outer, maxiter_inner
78
         double precision :: tol_abs, tol_rel
79
       end subroutine solver_interface
80
    end interface
81
82
    contains
83
84
      subroutine mat_init(mat, grid, iops)
85
        class(rte_mat) mat
86
        type(space_angle_grid) grid
87
        type(optical_properties) iops
88
        integer nnz, n_total
89
90
        mat%grid = grid
91
        mat%iops = iops
92
93
        call mat%calculate_size()
94
95
        n_total = mat%n_total
96
        nnz = mat%nonzero
        allocate(mat%surface_vals(grid%angles%nomega
97
           ))
98
        allocate(mat%row(nnz))
99
        allocate(mat%col(nnz))
100
        allocate(mat%data(nnz))
101
        allocate(mat%rhs(n_total))
102
        allocate(mat%sol(n_total))
103
        call zeros(mat%rhs, n_total)
104
105
        call zeros(mat%sol, n_total)
106
      end subroutine mat_init
107
```

```
108
109
      subroutine mat_deinit(mat)
        class(rte_mat) mat
110
        deallocate(mat%row)
111
112
        deallocate(mat%col)
113
        deallocate (mat %data)
        deallocate(mat%rhs)
114
        deallocate(mat%sol)
115
        deallocate(mat%surface_vals)
116
117
      end subroutine mat_deinit
118
119
      subroutine calculate_size(mat)
120
        class(rte_mat) mat
121
        integer nx, ny, nz, nomega
122
123
        nx = mat%grid%x%num
124
        ny = mat%grid%y%num
125
        nz = mat%grid%z%num
126
        nomega = mat%grid%angles%nomega
127
128
        !mat%nonzero = nx * ny * ntheta * nphi * ( (
           nz-1) * (6 + ntheta * nphi) + 1)
129
        mat%nonzero = nx * ny * nomega * (nz * (
           nomega + 6) - 1)
130
        mat%n_total = nx * ny * nz * nomega
131
132
        !mat%theta_block_size = 1
133
        !mat%phi_block_size = mat%theta_block_size *
            ntheta
134
        mat%omega_block_size = 1
        mat%y_block_size = mat%omega_block_size *
135
           nomega
136
        mat%x_block_size = mat%y_block_size * ny
137
        mat%z_block_size = mat%x_block_size * nx
138
139
      end subroutine calculate_size
140
141
       subroutine mat_to_hdf(mat,filename)
         class(rte_mat) mat
142
   !
143
         character(len=*) filename
144
         call write_coo(filename, mat%row, mat%col,
       mat%data, mat%nonzero)
145
       end subroutine mat_to_hdf
146
147
      subroutine mat_set_bc(mat, bc)
148
        class(rte_mat) mat
149
        class(boundary_condition) bc
150
        integer p
151
152
        do p=1, mat%grid%angles%nomega/2
```

```
mat%surface_vals(p) = bc%bc_grid(p)
153
154
        end do
155
      end subroutine mat_set_bc
156
157
      subroutine mat_solve(mat)
158
        class(rte_mat) mat
159
        type(solver_params) params
160
161
        params = mat%params
162
163
        write(*,*) 'mat%n_total =', mat%n_total
        write(*,*) 'mat%nonzero =', mat%nonzero
164
        write(*,*) 'size(mat%row) =', size(mat%row)
165
166
        write(*,*) 'size(mat%col) =', size(mat%col)
        write(*,*) 'size(mat%data) =', size(mat%data
167
168
        write(*,*) 'size(mat%sol) =', size(mat%sol)
        write(*,*) 'size(mat%rhs) =', size(mat%rhs)
169
170
        write(*,*) 'params%maxiter_outer =', params%
           maxiter_outer
        write(*,*) 'params%maxiter_inner =', params%
171
           maxiter_inner
172
        write(*,*) 'params%tol_rel =', params%
           tol_rel
173
        write(*,*) 'params%tol_abs =', params%
           tol_abs
        ! open(unit=1, file='row.txt')
174
        ! open(unit=2, file='col.txt')
175
        ! open(unit=3, file='data.txt')
176
177
        ! open(unit=4, file='rhs.txt')
        ! open(unit=5, file='sol.txt')
178
179
        ! write(1,*) mat%row
        ! write(2,*) mat%col
180
181
        ! write(3,*) mat%data
182
        ! write(4,*) mat%rhs
183
        ! close(1)
184
185
        ! close(2)
186
        ! close(3)
187
        ! close(4)
188
        call mat%solver(mat%n_total, mat%nonzero, &
189
190
             mat%row, mat%col, mat%data, mat%sol,
                mat%rhs, &
191
              params%maxiter_outer, params%
                maxiter_inner, &
192
             params%tol_abs, params%tol_rel)
193
        ! write(5,*) mat%sol
194
195
        ! close(5)
```

```
196
197
      end subroutine mat_solve
198
199
      subroutine mat_set_solver_params(mat,
         maxiter_outer, &
200
           maxiter_inner, tol_abs, tol_rel)
201
        class(rte_mat) mat
202
        integer maxiter_outer, maxiter_inner
203
        double precision tol_abs, tol_rel
204
205
        mat%params%maxiter_outer = maxiter_outer
206
        mat%params%maxiter_inner = maxiter_inner
207
        mat%params%tol_abs = tol_abs
208
        mat%params%tol_rel = tol_rel
      end subroutine mat_set_solver_params
209
210
211
      function mat_ind(mat, i, j, k, p) result(ind)
212
        ! Assuming var ordering: z, x, y, omega
213
        class(rte_mat) mat
214
        integer i, j, k, p
215
        integer ind
216
217
        ind = (i-1) * mat%x_block_size + (j-1) * mat
           %v_block_size + &
218
              (k-1) * mat%z_block_size + p * mat%
                 omega_block_size
219
      end function mat_ind
220
221
      subroutine mat_assign(mat, row_num, ent, val,
222
        ! It's assumed that this is the only time
           this entry is defined
223
        class(rte_mat) mat
224
        double precision val
225
        integer i, j, k, p
226
        integer row_num, ent
227
228
        mat%row(ent) = row_num
229
        mat%col(ent) = mat%ind(i, j, k, p)
230
        mat%data(ent) = val
231
232
        ent = ent + 1
233
      end subroutine mat_assign
234
235
      subroutine mat_add(mat, repeat_ent, val)
236
        ! Use this when you know that this entry has
            already been assigned
        ! and you'd like to add this value to the
237
           existing value.
238
239
        class(rte_mat) mat
```

```
240
        double precision val
241
        integer repeat_ent
242
243
        ! Entry number where value is already stored
244
        mat%data(repeat_ent) = mat%data(repeat_ent)
           + val
245
      end subroutine mat_add
246
247
      subroutine mat_assign_rhs(mat, row_num, data)
248
        class(rte mat) mat
249
        double precision data
250
        integer row_num
251
252
        mat%rhs(row_num) = data
253
      end subroutine mat_assign_rhs
254
255
      ! subroutine mat_store_index(mat, row_num,
         col num)
256
          ! Remember where we stored information for
          this matrix element
257
          class(rte mat) mat
258
          integer row_num, col_num
259
          !mat%index_map(row_num, col_num) = mat%ent
260
      ! end subroutine
261
262
      ! function mat_find_index(mat, row_num,
         col_num) result(index)
          ! Find the position in row, col, data
263
         where this entry
264
          ! is defined.
265
          class(rte_mat) mat
266
          integer row_num, col_num, index
267
268
          index = mat%index_map(row_num, col_num)
269
270
          ! This took up 95% of execution time.
271
          ! Only search up to most recently assigned
          index
272
          ! do index=1, mat%ent-1
273
                if( (mat%row(index) .eq. row_num) .
         and. (mat%col(index) .eq. col_num)) then
274
          1
                   exit
275
                end if
276
          ! end do
277
      ! end function mat_find_index
278
279
      subroutine attenuate(mat, indices, repeat_ent)
280
        ! Has to be called after angular_integral
281
        ! Because they both write to the same matrix
            entry
282
        ! And adding here is more efficient than a
           conditional
```

```
283
        ! in the angular loop.
284
        class(rte_mat) mat
285
        double precision attenuation
286
        type(index_list) indices
        double precision aa, bb
287
288
        integer repeat_ent
289
290
        aa = mat%iops%abs_grid(indices%i, indices%j,
            indices%k)
        bb = mat%iops%scat
291
292
        attenuation = aa + bb
293
294
        call mat%add(repeat_ent, attenuation)
295
      end subroutine attenuate
296
297
      subroutine x_cd2(mat, indices, row_num, ent)
298
        class(rte_mat) mat
299
        double precision val, dx
300
        type(index_list) indices
301
        integer i, j, k, p
302
        integer row_num, ent
303
304
        i = indices%i
305
        j = indices%;
306
        k = indices%k
307
        p = indices%p
308
309
        dx = mat%grid%x%spacing(1)
310
311
        val = mat%grid%angles%sin_phi_p(p) &
312
              * mat%grid%angles%cos_theta_p(p) / (2.
                 d0 * dx
313
314
        call mat%assign(row_num,ent,-val,i-1,j,k,p)
315
        call mat%assign(row_num,ent,val,i+1,j,k,p)
316
      end subroutine x_cd2
317
318
      subroutine x_cd2_first(mat, indices, row_num,
        class(rte_mat) mat
319
320
        double precision val, dx
321
        integer nx
322
        type(index_list) indices
323
        integer i, j, k, p
324
        integer row_num, ent
325
326
        i = indices%i
327
        j = indices%j
328
        k = indices%k
329
        p = indices%p
330
```

```
dx = mat%grid%x%spacing(1)
331
332
        nx = mat%grid%x%num
333
334
        val = mat%grid%angles%sin_phi_p(p) &
335
              * mat%grid%angles%cos_theta_p(p) / (2.
                 d0 * dx
336
337
        call mat%assign(row_num,ent,-val,nx,j,k,p)
338
        call mat%assign(row_num,ent,val,i+1,j,k,p)
339
      end subroutine x_cd2_first
340
341
      subroutine x_cd2_last(mat, indices, row_num,
         ent)
342
        class(rte_mat) mat
343
        double precision val, dx
344
        type(index_list) indices
345
        integer i, j, k, p
346
        integer row_num, ent
347
348
        i = indices%i
349
        j = indices%j
350
        k = indices%k
351
        p = indices%p
352
353
        dx = mat%grid%x%spacing(1)
354
355
        val = mat%grid%angles%sin_phi_p(p) &
356
              * mat%grid%angles%cos_theta_p(p) / (2.
                 d0 * dx)
357
358
        call mat%assign(row_num,ent,-val,i-1,j,k,p)
359
        call mat%assign(row_num,ent,val,1,j,k,p)
      end subroutine x_cd2_last
360
361
362
      subroutine y_cd2(mat, indices, row_num, ent)
363
        class(rte_mat) mat
364
        double precision val, dy
365
        type(index_list) indices
366
        integer i, j, k, p
367
        integer row_num, ent
368
369
        i = indices%i
370
        j = indices%j
371
        k = indices%k
372
        p = indices%p
373
374
        dy = mat%grid%y%spacing(1)
375
376
        val = mat%grid%angles%sin_phi_p(p) &
```

```
377
              * mat%grid%angles%sin_theta_p(p) / (2.
                 d0 * dy)
378
379
        call mat%assign(row_num,ent,-val,i,j-1,k,p)
380
        call mat%assign(row_num,ent,val,i,j+1,k,p)
381
      end subroutine y_cd2
382
383
      subroutine y_cd2_first(mat, indices, row_num,
         ent)
384
        class(rte_mat) mat
385
        double precision val, dy
386
        integer ny
387
        type(index_list) indices
388
        integer i, j, k, p
389
        integer row_num, ent
390
391
        i = indices%i
        j = indices%i
392
393
        k = indices%k
394
        p = indices%p
395
396
        dy = mat%grid%y%spacing(1)
397
        ny = mat%grid%y%num
398
399
        val = mat%grid%angles%sin_phi_p(p) &
400
              * mat%grid%angles%sin_theta_p(p) / (2.
                 d0 * dy)
401
402
        call mat%assign(row_num,ent,-val,i,ny,k,p)
403
        call mat%assign(row_num,ent,val,i,j+1,k,p)
404
      end subroutine y_cd2_first
405
406
      subroutine y_cd2_last(mat, indices, row_num,
         ent)
407
        class(rte_mat) mat
        double precision val, dy
408
409
        type(index_list) indices
410
        integer i, j, k, p
411
        integer row_num, ent
412
413
        i = indices%i
        j = indices%i
414
415
        k = indices%k
416
        p = indices%p
417
        dy = mat%grid%y%spacing(1)
418
419
420
        val = mat%grid%angles%sin_phi_p(p) &
421
              * mat%grid%angles%sin_theta_p(p) / (2.
                 d0 * dy
```

```
422
423
        call mat%assign(row_num,ent,-val,i,j-1,k,p)
424
        call mat%assign(row_num,ent,val,i,1,k,p)
      end subroutine y_cd2_last
425
426
427
      subroutine z_cd2(mat, indices, row_num, ent)
428
        class(rte_mat) mat
429
        double precision val, dz
430
        type(index_list) indices
431
        integer i, j, k, p
        integer row_num, ent
432
433
434
        i = indices%i
        j = indices%j
435
        k = indices%k
436
437
        p = indices%p
438
439
        dz = mat%grid%z%spacing(indices%k)
440
441
        val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
442
443
        call mat%assign(row_num,ent,-val,i,j,k-1,p)
444
        call mat%assign(row_num,ent,val,i,j,k+1,p)
445
      end subroutine z_cd2
446
447
      subroutine z_fd2(mat, indices, row_num, ent,
         repeat_ent)
448
        ! Has to be called after angular_integral
449
        ! Because they both write to the same matrix
            entry
450
        ! And adding here is more efficient than a
           conditional
451
        ! in the angular loop.
452
        class(rte_mat) mat
        double precision val, val1, val2, val3, dz
453
454
        type(index_list) indices
455
        integer i, j, k, p
        integer row_num, ent, repeat_ent
456
457
458
        i = indices%i
        j = indices%i
459
        k = indices%k
460
461
        p = indices%p
462
463
        dz = mat%grid%z%spacing(indices%k)
464
465
        val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
            dz)
466
        val1 = -3.d0 * val
467
```

```
468
        val2 = 4.d0 * val
469
        val3 = -val
470
471
        call mat%add(repeat_ent, val1)
472
        call mat%assign(row_num,ent,val2,i,j,k+1,p)
473
        call mat%assign(row_num,ent,val3,i,j,k+2,p)
474
      end subroutine z_fd2
475
476
      subroutine z_bd2(mat, indices, row_num, ent,
         repeat_ent)
477
         ! Has to be called after angular_integral
478
         ! Because they both write to the same matrix
479
         ! And adding here is more efficient than a
           conditional
480
         ! in the angular loop.
481
        class(rte_mat) mat
482
        double precision val, val1, val2, val3, dz
483
        type(index_list) indices
484
        integer i, j, k, p
485
        integer row_num, ent, repeat_ent
486
487
        i = indices%i
488
        j = indices%j
489
        k = indices%k
490
        p = indices%p
491
492
        dz = mat%grid%z%spacing(indices%k)
493
494
        val = mat%grid%angles%cos_phi_p(p) / (2.d0 *
            dz)
495
496
        val1 = 3.d0 * val
497
        val2 = -4.d0 * val
498
        val3 = val
499
500
        call mat%add(repeat_ent, val1)
501
        call mat%assign(row_num,ent,val2,i,j,k-1,p)
502
        call mat%assign(row_num,ent,val3,i,j,k-2,p)
503
      end subroutine z_bd2
504
505
      subroutine angular_integral(mat, indices,
         row_num, ent)
506
        class(rte_mat) mat
507
         ! Primed angular integration variables
508
        integer pp
509
        double precision val
510
        type(index_list) indices
511
        integer row_num, ent
512
513
        ! Interior
```

```
do pp=1, mat%grid%angles%nomega
514
515
            ! TODO: Make sure I don't have p and pp
              backwards
516
           val = -mat%iops%scat * mat%iops%
              vsf_integral(indices%p, pp)
           call mat%assign(row_num, ent, val,
517
              indices%i, indices%j, indices%k, pp)
518
        end do
519
      end subroutine angular_integral
520
521
      subroutine z_surface_bc(mat, indices, row_num,
          ent, repeat_ent)
522
        class(rte_mat) mat
523
        double precision bc_val
524
        type(index_list) indices
525
        double precision val1, val2, dz
526
        integer row_num, ent, repeat_ent
527
528
        dz = mat%grid%z%spacing(1)
529
530
        val1 = mat%grid%angles%cos_phi_p(indices%p)
           / (5.d0 * dz)
        val2 = 7.d0 * val1
531
532
        bc_val = 8.d0 * val1 * mat%surface_vals(
           indices%p)
533
534
        call mat%assign(row_num,ent,val1,indices%i,
           indices%j,2,indices%p)
535
        call mat%add(repeat_ent, val2)
536
        call mat%assign_rhs(row_num, bc_val)
537
538
      end subroutine z_surface_bc
539
540
        subroutine z_bottom_bc(mat, indices, row_num
           , ent, repeat_ent)
        class(rte_mat) mat
541
542
        type(index_list) indices
543
        double precision val1, val2, dz
544
        integer nz
545
        integer row_num, ent, repeat_ent
546
547
        dz = mat%grid%z%spacing(1)
548
        nz = mat%grid%z%num
549
550
        val1 = -mat%grid%angles%cos_phi_p(indices%p)
            / (5.d0 * dz)
551
        val2 = 7.d0 * val1
552
553
        call mat%assign(row_num, ent, val1, indices%i,
           indices%j,nz-1,indices%p)
554
        call mat%add(repeat_ent, val2)
```

```
555
556
      end subroutine z_bottom_bc
557
558
      ! Finite difference wrappers
559
560
        subroutine wrap_x_cd2(mat, indices)
561
          type(rte_mat) mat
562
          type(index_list) indices
563
          call mat%x_cd2(indices)
564
      ! end subroutine wrap_x_cd2
565
566
       subroutine wrap_x_cd2_last(mat, indices)
567
          type(rte_mat) mat
568
          type(index_list) indices
569
          call mat%x_cd2_last(indices)
570
      ! end subroutine wrap_x_cd2_last
571
      ! subroutine wrap_x_cd2_first(mat, indices)
572
573
          type(rte_mat) mat
574
          type(index_list) indices
575
          call mat%x_cd2_first(indices)
576
      ! end subroutine wrap_x_cd2_first
577
578
       subroutine wrap_y_cd2(mat, indices)
579
          type(rte_mat) mat
580
          type(index_list) indices
581
          call mat%y_cd2(indices)
582
      ! end subroutine wrap_y_cd2
583
      ! subroutine wrap_y_cd2_last(mat, indices)
584
585
          type(rte_mat) mat
586
          type(index_list) indices
587
          call mat%y_cd2_last(indices)
588
      ! end subroutine wrap_y_cd2_last
589
590
      ! subroutine wrap_y_cd2_first(mat, indices)
591
          type(rte_mat) mat
592
          type(index_list) indices
593
          call mat%y_cd2_first(indices)
594
      ! end subroutine wrap_y_cd2_first
595
596
      ! subroutine wrap_z_cd2(mat, indices)
597
          type(rte_mat) mat
598
          type(index_list) indices
599
          call mat%z_cd2(indices)
600
      ! end subroutine wrap_z_cd2
601
602 | end module rte_sparse_matrices
```

```
module rte3d
   use kelp_context
   use rte_sparse_matrices
   use light_context
5
   implicit none
6
   interface
8
      subroutine deriv_interface(mat, indices,
         row_num, ent)
9
        use rte_sparse_matrices
10
        class(rte_mat) mat
11
        type(index_list) indices
12
        integer row_num, ent
13
      end subroutine deriv_interface
14
      subroutine angle_loop_interface(mat, indices,
          ddx, ddy)
15
        use rte_sparse_matrices
        import deriv_interface
16
17
        type(space_angle_grid) grid
18
        type(rte_mat) mat
19
        type(index_list) indices
        procedure(deriv_interface) :: ddx, ddy
20
21
      end subroutine angle_loop_interface
22
   end interface
23
24
   contains
25
26
   subroutine whole_space_loop(mat, indices)
27
     type(rte_mat) mat
28
     type(index_list) indices
29
     integer i, j, k
30
31
     procedure(deriv_interface), pointer :: ddx,
32
     procedure(angle_loop_interface), pointer ::
        angle_loop
33
34
     !$ integer omp_get_num_procs
35
     !$ integer num_threads_z, num_threads_x,
        num_threads_y
36
37
     ! Enable nested parallelism
38
     !$ call omp_set_nested(.true.)
39
40
     ! Use nz procs for outer loop,
41
     ! or num_procs if num_procs < nz
42
     ! Divide the rest of the tasks as appropriate
43
44
     !$ num_threads_z = min(omp_get_num_procs(),
        mat%grid%z%num)
45
     !$ num_threads_x = min( &
```

```
omp_get_num_procs()/num_threads_z, &
46
47
     !$
            mat%grid%x%num)
     !$ num_threads_y = min( &
48
            omp_get_num_procs()/(num_threads_z*
49
        num_threads_x), &
50
           mat%grid%y%num)
     ! $
51
52
     !$ write(*,*) 'num_procs =', omp_get_num_procs
53
     !$ write(*,*) 'ntz =', num_threads_z
     !$ write(*,*) 'ntx =', num_threads_x
54
     !$ write(*,*) 'nty =', num_threads_y
55
56
57
     !$omp parallel do default(none) shared(mat) &
58
     !$omp private(ddx,ddy,angle_loop, k, i, j)
        private(indices) &
59
     !$omp shared(num_threads_x,num_threads_y,
        num_threads_z) &
60
     !$omp num_threads(num_threads_z) if(
        num_threads_z .gt. 1)
61
     do k=1, mat%grid%z%num
        write(*,*) 'k =', k
62
63
        indices %k = k
64
        if (k .eq. 1) then
65
            angle_loop => surface_angle_loop
66
        else if (k .eq. mat % grid % z % num) then
67
            angle_loop => bottom_angle_loop
68
69
            angle_loop => interior_angle_loop
70
        end if
71
72
         !$omp parallel do default(none) shared(mat)
            private(i,j) &
73
         !$omp firstprivate(indices,angle_loop, k)
           private(ddx,ddy) &
74
         !$omp shared(num_threads_x,num_threads_y,
           num_threads_z) &
75
         !$omp num_threads(num_threads_x) if(
           num_threads_x .gt. 1)
        do i=1, mat%grid%x%num
76
77
            indices%i = i
78
            if(indices%i .eq. 1) then
79
               ddx => x_cd2_first
80
            else if(indices%i .eq. mat%grid%x%num)
               then
81
               ddx => x_cd2_last
82
            else
83
               ddx => x_cd2
84
            end if
```

```
85
             !$omp parallel do default(none) shared(
               mat) private(j) &
86
             !$omp firstprivate(indices,ddx,ddy,
                angle_loop, i, k) &
87
             !$omp shared(num_threads_x,num_threads_y
                , num_threads_z) &
88
             !$omp num_threads(num_threads_y) if(
                num_threads_y .gt. 1)
89
             do j=1, mat%grid%y%num
90
                indices\%j = j
91
                if(indices%j .eq. 1) then
92
                   ddy => y_cd2_first
93
                else if(indices%j .eq. mat%grid%y%num
                   ) then
94
                   ddy => y_cd2_last
95
                else
96
                   ddy => y_cd2
97
                end if
98
99
                call angle_loop(mat, indices, ddx,
100
             end do
101
             !$omp end parallel do
102
         end do
         !$omp end parallel do
103
104
      end do
105
      !$omp end parallel do
106
    end subroutine whole_space_loop
107
108
    function calculate_start_ent(grid, indices)
       result (ent)
      type(space_angle_grid) grid
109
110
      type(index_list) indices
111
      integer ent
      integer boundary_nnz, interior_nnz
112
113
      integer num_boundary, num_interior
114
      integer num_this_x, num_this_z
115
116
      ! Nonzero matrix entries for an surface or
         bottom spatial grid cell
117
      ! Definitely an integer since nomega is even
118
      boundary_nnz = grid%angles%nomega * (2 * grid%
         angles%nomega + 11) / 2
      ! Nonzero matrix entries for an interior
119
         spatial grid cell
120
      interior_nnz = grid%angles%nomega * (grid%
         angles%nomega + 6)
121
122
      ! Order: z, x, y, omega
123
      ! Total number traversed so far in each
         spatial category
```

```
124
125
      num_this_x = indices%j - 1
126
      ! depth layer
127
      num_this_z = (indices%i - 1) * grid%y%num +
         num_this_x
128
129
      ! Calculate number of spatial grid cells of
         each type which have
130
      ! already been traversed up to this point
131
      if (indices %k .eq. 1) then
132
         num_boundary = num_this_z
         num_interior = 0
133
134
      else if (indices%k .eq. grid%z%num) then
135
         num_boundary = (grid%x%num * grid%y%num) +
            num_this_z
136
         num_interior = (grid%z%num-2) * grid%x%num
            * grid%y%num
137
      else
138
         num_boundary = grid%x%num * grid%y%num
139
         num_interior = num_this_z + (indices%k-2) *
             grid%x%num * grid%y%num
      end if
140
141
142
      ent = num_boundary * boundary_nnz +
         num_interior * interior_nnz + 1
143
    end function calculate_start_ent
144
145
    function calculate_repeat_ent(ent, p) result(
       repeat_ent)
      integer ent, p, repeat_ent
146
147
      ! Entry number for row=mat%ind(i,j,k,p), col=
         mat%ind(i,j,k,p),
148
      ! which will be modified multiple times in
         this matrix row
149
      repeat_ent = ent + p - 1
150
    end function calculate_repeat_ent
151
152
    subroutine interior_angle_loop(mat, indices, ddx
       , ddy)
153
      type(rte_mat) mat
154
      type(index_list) indices
155
      procedure(deriv_interface) :: ddx, ddy
      integer p
156
      integer ent, repeat_ent
157
158
      integer row_num
159
      ! Determine which matrix row to start at
160
161
      ent = calculate_start_ent(mat%grid, indices)
162
      indices\%p = 1
163
      row_num = mat%ind(indices%i, indices%j,
         indices%k, indices%p)
```

```
164
165
      do p=1, mat%grid%angles%nomega
166
         indices\%p = p
167
         repeat_ent = calculate_repeat_ent(ent, p)
168
         call mat%angular_integral(indices, row_num,
             ent)
169
         call ddx(mat, indices, row_num, ent)
170
         call ddy(mat, indices, row_num, ent)
         call mat%z_cd2(indices, row_num, ent)
171
172
         call mat%attenuate(indices, repeat_ent)
173
         row_num = row_num + 1
174
      end do
175
    end subroutine
176
177
    subroutine surface_angle_loop(mat, indices, ddx,
        ddy)
178
      type(rte_mat) mat
179
      type(index_list) indices
180
      integer p
      procedure(deriv_interface) :: ddx, ddy
181
182
      integer ent, repeat_ent
      integer row_num
183
184
185
      ! Determine which matrix row to start at
186
      ent = calculate_start_ent(mat%grid, indices)
187
      indices\%p = 1
188
      row_num = mat%ind(indices%i, indices%j,
         indices%k, indices%p)
189
190
      ! Downwelling
191
      do p=1, mat%grid%angles%nomega / 2
         indices%p = p
192
193
         repeat_ent = calculate_repeat_ent(ent, p)
194
         call mat%angular_integral(indices, row_num,
             ent)
195
         call ddx(mat, indices, row_num, ent)
196
         call ddy(mat, indices, row_num, ent)
197
         call mat%z_surface_bc(indices, row_num, ent
            , repeat_ent)
198
         call mat%attenuate(indices, repeat_ent)
199
         row_num = row_num + 1
200
      end do
201
      ! Upwelling
      do p=mat%grid%angles%nomega/2+1, mat%grid%
202
         angles%nomega
203
         indices\%p = p
204
         repeat_ent = calculate_repeat_ent(ent, p)
205
         call mat%angular_integral(indices, row_num,
             ent)
         call ddx(mat, indices, row_num, ent)
206
```

```
207
         call ddy(mat, indices, row_num, ent)
208
         call mat%z_fd2(indices, row_num, ent,
            repeat_ent)
209
         call mat%attenuate(indices, repeat_ent)
210
         row_num = row_num + 1
211
      end do
212
    end subroutine surface_angle_loop
213
214
    subroutine bottom_angle_loop(mat, indices, ddx,
       ddy)
215
      type(rte_mat) mat
216
      type(index_list) indices
217
      integer p
218
      integer row_num, ent, repeat_ent
219
      procedure(deriv_interface) :: ddx, ddy
220
221
      ! Determine which matrix row to start at
222
      ent = calculate_start_ent(mat%grid, indices)
223
      indices\%p = 1
      row_num = mat%ind(indices%i, indices%j,
224
         indices%k, indices%p)
225
226
      ! Downwelling
      do p=1, mat%grid%angles%nomega/2
227
228
         indices\%p = p
229
         repeat_ent = calculate_repeat_ent(ent, p)
230
         call mat%angular_integral(indices, row_num,
231
         call ddx(mat, indices, row_num, ent)
232
         call ddy(mat, indices, row_num, ent)
233
         call mat%z_bd2(indices, row_num, ent,
            repeat_ent)
234
         call mat%attenuate(indices, repeat_ent)
235
         row_num = row_num + 1
236
      end do
237
      ! Upwelling
238
      do p=mat%grid%angles%nomega/2+1, mat%grid%
         angles%nomega
239
         indices\%p = p
240
         repeat_ent = calculate_repeat_ent(ent, p)
241
         call mat%angular_integral(indices, row_num,
             ent)
242
         call ddx(mat, indices, row_num, ent)
243
         call ddy(mat, indices, row_num, ent)
244
         call mat%z_bottom_bc(indices, row_num, ent,
             repeat_ent)
245
         call mat%attenuate(indices, repeat_ent)
246
         row_num = row_num + 1
247
      end do
248
   end subroutine bottom_angle_loop
```

```
249
250
    subroutine gen_matrix(mat)
251
      type(rte_mat) mat
252
      type(index_list) indices
253
254
      call indices%init()
255
256
      call whole_space_loop(mat, indices)
257
      ! call surface_space_loop(mat, indices)
258
      ! call interior_space_loop(mat, indices)
259
      ! call bottom_space_loop(mat, indices)
260
    end subroutine gen_matrix
261
262
    subroutine rte3d_deinit(mat, iops, light)
263
      type(rte_mat) mat
264
      type(optical_properties) iops
265
      type(light_state) light
266
267
      call mat%deinit()
268
      call iops%deinit()
269
      call light%deinit()
270
    end subroutine
271
272 | end module rte3d
    kelp_context.f90
    module kelp_context
    use sag
    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
      procedure :: set_shape => frond_set_shape
19
      procedure :: calculate_angles =>
20
         frond_calculate_angles
21
    end type frond_shape
22
23
    type rope_state
24
       integer nz
```

```
double precision, dimension(:), allocatable
25
         :: frond_lengths, frond_stds, num_fronds,
         water_speeds, water_angles
26
   contains
27
       procedure :: init => rope_init
28
       procedure :: deinit => rope_deinit
29
   end type rope_state
30
31
   type depth_state
32
      double precision frond_length, frond_std,
         num_fronds, water_speeds, water_angles,
         depth
33
      integer depth_layer
34
   contains
35
      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
         :: vsf_angles, vsf_vals, vsf_cos
      double precision, dimension(:), allocatable
44
         :: abs_water
45
      double precision abs_kelp, vsf_scat_coef,
      ! On x, y, z grid - including water & kelp.
46
47
      double precision, dimension(:,:,:),
         allocatable :: abs_grid
48
      ! On theta, phi, theta_prime, phi_prime grid
49
      double precision, dimension(:,:), allocatable
          :: vsf, vsf_integral
50
    contains
51
      procedure :: init => iop_init
52
      procedure :: calculate_coef_grids
      procedure :: load_vsf
53
      procedure :: eval_vsf
54
55
      procedure :: calc_vsf_on_grid
56
      procedure :: deinit => iop_deinit
57
      procedure :: vsf_from_function
58
   end type optical_properties
59
60
   type boundary_condition
61
      double precision IO, decay, theta_s, phi_s
62
      type(space_angle_grid) grid
63
      double precision, dimension(:), allocatable
         :: bc_grid
64
    contains
65
      procedure :: bc_gaussian
66
      procedure :: init => bc_init
67
      procedure :: deinit => bc_deinit
```

```
68
    end type boundary_condition
69
70
    contains
71
72
      function bc_gaussian(bc, theta, phi)
        class(boundary_condition) bc
73
74
        double precision theta, phi, diff
75
        double precision bc_gaussian
76
        diff = angle_diff_3d(theta, phi, bc%theta_s,
            bc%phi_s)
77
        bc_gaussian = exp(-bc%decay * diff)
78
      end function bc_gaussian
79
80
      subroutine bc_init(bc, grid, theta_s, phi_s,
         decay, IO)
81
        class(boundary_condition) bc
82
        type(space_angle_grid) grid
        double precision theta_s, phi_s, decay, IO
83
84
        integer p
85
        double precision theta, phi
86
87
        allocate(bc%bc_grid(grid%angles%nomega))
88
89
        bc%theta_s = theta_s
        bc%phi_s = phi_s
90
91
        bc%decay = decay
92
        bc\%I0 = I0
93
94
        ! Only set BC for downwelling light
95
        do p=1, grid%angles%nomega/2
96
           theta = grid%angles%theta_p(p)
97
           phi = grid%angles%phi_p(p)
98
           bc%bc_grid(p) = bc%bc_gaussian(theta, phi
              )
99
        end do
100
        ! Zero upwelling light specified at surface
101
        do p=grid%angles%nomega/2+1, grid%angles%
           nomega
102
           bc\%bc\_grid(p) = 0.d0
        end do
103
104
105
        ! Normalize
106
        bc%bc_grid = bc%I0 * bc%bc_grid &
107
              / grid%angles%integrate_points(bc%
                bc_grid)
108
109
      end subroutine bc_init
110
      subroutine bc_deinit(bc)
111
112
        class(boundary_condition) bc
        deallocate(bc%bc_grid)
113
```

```
114
        end subroutine
115
116
      subroutine point_set_cart(point, x, y, z)
117
        class(point3d) :: point
        double precision x, y, z
118
119
        point%x = x
120
        point %y = y
121
        point %z = z
122
        call point%cartesian_to_polar()
123
      end subroutine point_set_cart
124
125
      subroutine point_set_cyl(point, theta, r, z)
126
        class(point3d) :: point
127
        double precision theta, r, z
128
        point%theta = theta
129
        point%r = r
130
        point %z = z
131
        call point%polar_to_cartesian()
132
      end subroutine point_set_cyl
133
134
      subroutine polar_to_cartesian(point)
135
        class(point3d) :: point
136
        point%x = point%r*cos(point%theta)
137
        point%y = point%r*sin(point%theta)
138
      end subroutine polar_to_cartesian
139
140
      subroutine cartesian_to_polar(point)
141
        class(point3d) :: point
        point%r = sqrt(point%x**2 + point%y**2)
142
143
        point%theta = atan2(point%y, point%x)
      end subroutine cartesian_to_polar
144
145
146
      subroutine frond_set_shape(frond, fs, fr, ft)
147
        class(frond_shape) frond
148
        double precision fs, fr, ft
149
        frond\%fs = fs
150
        frond\%fr = fr
        frond%ft = ft
151
152
        call frond%calculate_angles()
153
      end subroutine frond_set_shape
154
155
      subroutine frond_calculate_angles(frond)
        class(frond_shape) frond
156
157
        frond%tan_alpha = 2.d0*frond%fs*frond%fr /
           (1.d0 + frond\%fs)
158
        frond%alpha = atan(frond%tan_alpha)
159
      end subroutine
160
161
      subroutine iop_init(iops, grid)
162
        class(optical_properties) iops
```

```
type(space_angle_grid) grid
163
164
165
        iops%grid = grid
166
167
        ! Assume that these are preallocated and
           passed to function
168
        ! Nevermind, don't assume this.
169
        allocate(iops%abs_water(grid%z%num))
170
171
        ! Assume that these must be allocated here
172
        allocate(iops%vsf_angles(iops%num_vsf))
        allocate(iops%vsf_vals(iops%num_vsf))
173
174
        allocate(iops%vsf_cos(iops%num_vsf))
175
        allocate(iops%vsf(grid%angles%nomega,grid%
           angles%nomega))
176
        allocate(iops%vsf_integral(grid%angles%
           nomega, grid%angles%nomega))
177
        allocate(iops%abs_grid(grid%x%num, grid%y%
           num, grid%z%num))
178
      end subroutine iop_init
179
180
      subroutine calculate_coef_grids(iops, p_kelp)
181
        class(optical_properties) iops
182
        double precision, dimension(:,:,:) :: p_kelp
183
184
        integer k
185
186
        ! Allow water IOPs to vary over depth
187
        do k=1, iops%grid%z%num
188
          iops%abs_grid(:,:,k) = (iops%abs_kelp -
             iops%abs_water(k)) * p_kelp(:,:,k) +
             iops%abs_water(k)
189
       end do
190
191
      end subroutine calculate_coef_grids
192
193
194
      subroutine load_vsf(iops, filename, fmtstr)
195
        class(optical_properties) :: iops
196
        character(len=*) :: filename, fmtstr
197
        double precision, dimension(:,:),
           allocatable :: tmp_2d_arr
198
        integer num_rows, num_cols, skiplines_in
199
200
        ! First column is the angle at which the
           measurement is taken
201
        ! Second column is the value of the VSF at
           that angle
202
        num_rows = iops%num_vsf
203
        num_cols = 2
```

```
204
        skiplines_in = 1 ! Ignore comment on first
           line
205
206
        allocate(tmp_2d_arr(num_rows, num_cols))
207
        tmp_2d_arr = read_array(filename, fmtstr,
208
           num_rows, num_cols, skiplines_in)
209
        iops%vsf_angles = tmp_2d_arr(:,1)
210
        iops%vsf_vals = tmp_2d_arr(:,2)
211
212
        ! write(*,*) 'vsf_angles = ', iops%
           vsf_angles
213
        ! write(*,*) 'vsf_vals = ', iops%vsf_vals
214
215
        ! Pre-evaluate for all pair of angles
216
        call iops%calc_vsf_on_grid()
217
      end subroutine load_vsf
218
219
      function eval_vsf(iops, theta)
220
        class(optical_properties) iops
221
        double precision theta
222
        double precision eval_vsf
223
        ! No need to set vsf(0) = 0.
224
        ! It's the area under the curve that matters
           , not the value.
225
        eval_vsf = interp(theta, iops%vsf_angles,
           iops%vsf_vals, iops%num_vsf)
226
227
      end function eval_vsf
228
229
      subroutine rope_init(rope, grid)
230
        class(rope_state) :: rope
231
        type(space_angle_grid) :: grid
232
233
        rope%nz = grid%z%num
234
        allocate(rope%frond_lengths(rope%nz))
235
        allocate(rope%frond_stds(rope%nz))
236
        allocate(rope%water_speeds(rope%nz))
237
        allocate(rope%water_angles(rope%nz))
238
        allocate(rope%num_fronds(rope%nz))
239
      end subroutine rope_init
240
241
      subroutine rope_deinit(rope)
242
        class(rope_state) rope
243
        deallocate(rope%frond_lengths)
244
        deallocate(rope%frond_stds)
245
        deallocate(rope%water_speeds)
246
        deallocate(rope%water_angles)
247
        deallocate(rope%num_fronds)
248
      end subroutine rope_deinit
```

```
249
250
      subroutine set_depth(depth, rope, grid,
         depth_layer)
251
        class(depth_state) depth
252
        type(rope_state) rope
253
        type(space_angle_grid) grid
254
        integer depth_layer
255
256
        depth%frond_length = rope%frond_lengths(
           depth_layer)
257
        depth%frond_std = rope%frond_stds(
           depth_layer)
258
        depth%water_speeds = rope%water_speeds(
           depth_layer)
259
        depth%water_angles = rope%water_angles(
           depth_layer)
260
        depth%num_fronds = rope%num_fronds(
           depth_layer)
261
        depth%depth_layer = depth_layer
        depth%depth = grid%z%vals(depth_layer)
262
263
      end subroutine set_depth
264
265
      function length_distribution_cdf(depth, L)
         result(output)
266
        ! C_L(L)
267
        class(depth_state) depth
268
        double precision L, L_mean, L_std
269
        double precision output
270
271
        L_mean = depth%frond_length
272
        L_std = depth%frond_std
273
274
        call normal_cdf(L, L_mean, L_std, output)
275
      end function length_distribution_cdf
276
277
      function angle_distribution_pdf(depth, theta_f
         ) result(output)
278
        ! P_{\theta_f}(\theta_f)
279
        class(depth_state) depth
280
        double precision theta_f, v_w, theta_w
281
        double precision output
282
        double precision diff
283
284
        v_w = depth%water_speeds
285
        theta_w = depth%water_angles
286
287
        ! von_mises_pdf is only defined on [-pi, pi]
288
        ! So take difference of angles and input
           into
        ! von_mises dist. centered & x=0.
289
```

```
290
291
        diff = angle_diff_2d(theta_f, theta_w)
292
293
        call von_mises_pdf(diff, 0.d0, v_w, output)
294
      end function angle_distribution_pdf
295
296
      function angle_mod(theta) result(mod_theta)
297
        ! Shift theta to the interval [-pi, pi]
        ! which is where von_mises_pdf is defined.
298
299
300
        double precision theta, mod_theta
301
302
        mod\_theta = mod(theta + pi, 2.d0*pi) - pi
303
      end function angle_mod
304
305
      function angle_diff_2d(theta1, theta2) result(
         diff)
306
        ! Shortest difference between two angles
           which may be
307
        ! in different periods.
308
        double precision theta1, theta2, diff
309
        double precision modt1, modt2
310
311
        ! Shift to [0, 2*pi]
312
        modt1 = mod(theta1, 2*pi)
313
        modt2 = mod(theta2, 2*pi)
314
315
        ! https://gamedev.stackexchange.com/
           questions/4467/comparing-angles-and-
           working-out-the-difference
316
317
        diff = pi - abs(abs(modt1-modt2) - pi)
318
      end function angle_diff_2d
319
320
      function angle_diff_3d(theta, phi, theta_prime
           phi_prime) result(diff)
321
        ! Angle between two vectors in spherical
           coordinates
322
        double precision theta, phi, theta_prime,
           phi_prime
323
        double precision alpha, diff
324
325
        ! Faster, but produces lots of NaNs (at
           least in Python)
326
        !alpha = sin(theta)*sin(theta_prime)*cos(
           theta-theta_prime) + cos(phi)*cos(
           phi_prime)
327
328
329
        ! Slower, but more accurate
        alpha = (sin(phi)*sin(phi_prime) &
330
```

```
331
          * (cos(theta)*cos(theta_prime) + sin(theta
             )*sin(theta_prime)) &
332
          + cos(phi)*cos(phi_prime))
333
334
        ! Avoid out-of-bounds errors due to rounding
335
        alpha = min(1.d0, alpha)
336
        alpha = max(-1.d0, alpha)
337
338
        diff = acos(alpha)
339
      end function angle_diff_3d
340
341
      subroutine vsf_from_function(iops, func)
342
        class(optical_properties) iops
343
        double precision, external :: func
344
        integer i
345
        type(angle_dim) :: angle1d
346
347
        call angle1d%set_bounds(-1.d0, 1.d0)
348
        call angle1d%set_num(iops%num_vsf)
        call angle1d%assign_legendre()
349
350
351
        iops%vsf_angles(:) = acos(angle1d%vals(:))
352
        do i=1, iops%num_vsf
353
            iops%vsf_vals(i) = func(iops%vsf_angles(i
              ))
354
        end do
355
356
        call iops%calc_vsf_on_grid()
357
358
        call angle1d%deinit()
359
      end subroutine vsf_from_function
360
361
      subroutine calc_vsf_on_grid(iops)
362
        class(optical_properties) iops
363
        double precision th, ph, thp, php
        integer p, pp
364
        integer nomega
365
366
        double precision norm
367
368
        nomega = iops%grid%angles%nomega
369
370
        ! Calculate cos VSF
371
        iops%vsf_cos = cos(iops%vsf_angles)
372
373
        ! Normalize cos VSF to 1/(2pi) on [-1, 1]
374
        iops%vsf_scat_coef = abs(trap_rule_uneven(
           iops%vsf_cos, iops%vsf_vals, iops%num_vsf
           ))
375
        iops%vsf_vals(:) = iops%vsf_vals(:) / (2*pi
           * iops%vsf_scat_coef)
376
```

```
377
         ! write(*,*) 'norm = ', iops%vsf_scat_coef
        ! write(*,*) 'now: ', trap_rule_uneven(iops%
378
           vsf_cos, iops%vsf_vals, iops%num_vsf)
        ! write(*,*) 'cos: ', iops%vsf_cos
! write(*,*) 'vals: ', iops%vsf_vals
379
380
381
382
        do p=1, nomega
383
            th = iops%grid%angles%theta_p(p)
384
            ph = iops%grid%angles%phi_p(p)
385
              pp=1, nomega
386
               thp = iops%grid%angles%theta_p(pp)
387
               php = iops%grid%angles%phi_p(pp)
388
               ! TODO: Might be better to calculate
                  average scattering
389
               ! from angular cell rather than only
                  using center
               iops%vsf(p, pp) = iops%eval_vsf(
390
                  angle_diff_3d(th,ph,thp,php))
391
            end do
392
393
            ! Normalize each row of VSF (midpoint
               rule)
394
            norm = sum(iops%vsf(p,:) * iops%grid%
               angles%area_p(:))
395
            iops%vsf(p,:) = iops%vsf(p,:) / norm
396
397
            ! % / meter light scattered from cell pp
               into direction p.
398
            ! TODO: Could integrate VSF instead of
               just using value at center
399
            iops%vsf_integral(p, :) = iops%vsf(p, :)
400
                 * iops%grid%angles%area_p(:)
401
            !write(*,*) 'vsf_integral (beta_pp)', p,
               ' = ', iops%vsf_integral(p, :)
402
        end do
403
404
         ! Normalize VSF on unit sphere w.r.t. north
405
         !iops%vsf_scat_coef = sum(iops%vsf(1,:) *
           iops%grid%angles%area_p)
406
         !iops%vsf = iops%vsf / iops%vsf_scat_coef
407
         !iops%vsf_integral = iops%vsf_integral /
           iops%vsf_scat_coef
408
      end subroutine calc_vsf_on_grid
409
410
      subroutine iop_deinit(iops)
411
        class(optical_properties) iops
412
        deallocate(iops%vsf_angles)
        deallocate(iops%vsf_vals)
413
```

```
414
         deallocate(iops%vsf_cos)
415
         deallocate(iops%vsf)
416
         deallocate(iops%vsf_integral)
417
         deallocate(iops%abs_water)
418
         deallocate(iops%abs_grid)
419
420
      end subroutine iop_deinit
421
422 | end module kelp_context
     light_context.f90
    module light_context
 2
3
      use sag
      use rte_sparse_matrices
 4
       !use hdf5
 5
      implicit none
 6
 7
      type light_state
 8
          double precision, dimension(:,:,:),
             allocatable :: irradiance
 9
          double precision, dimension(:,:,:,:),
             allocatable :: radiance
 10
          type(space_angle_grid) :: grid
 11
          type(rte_mat) :: mat
 12
        contains
 13
          procedure :: init => light_init
          procedure :: init_grid => light_init_grid
procedure :: calculate_radiance
 14
 15
 16
          procedure :: calculate_irradiance
 17
          procedure :: deinit => light_deinit
 18
          !procedure :: to_hdf => light_to_hdf
 19
      end type light_state
 20
 21
    contains
 22
 23
       ! Init for use with mat
 24
      subroutine light_init(light, mat)
 25
         class(light_state) light
 26
         type(rte_mat) mat
 27
         integer nx, ny, nz, nomega
 28
 29
         light%mat = mat
 30
         light%grid = mat%grid
 31
 32
        nx = light%grid%x%num
 33
        ny = light%grid%y%num
 34
        nz = light%grid%z%num
 35
        nomega = light%grid%angles%nomega
 36
 37
         allocate(light%irradiance(nx, ny, nz))
```

```
38
        allocate(light%radiance(nx, ny, nz, nomega))
39
     end subroutine light_init
40
41
     ! Init for use without mat
42
     subroutine light_init_grid(light, grid)
43
        class(light_state) light
44
       type(space_angle_grid) grid
45
       integer nx, ny, nz, nomega
46
47
       light%grid = grid
48
49
       nx = light%grid%x%num
50
       ny = light%grid%y%num
51
       nz = light%grid%z%num
52
       nomega = light%grid%angles%nomega
53
54
       allocate(light%irradiance(nx, ny, nz))
55
        allocate(light%radiance(nx, ny, nz, nomega))
56
     end subroutine light_init_grid
57
58
     subroutine calculate_radiance(light)
59
       class(light_state) light
       integer i, j, k, p
integer nx, ny, nz, nomega
60
61
62
        integer index
63
64
       nx = light%grid%x%num
65
       ny = light%grid%y%num
66
       nz = light%grid%z%num
67
       nomega = light%grid%angles%nomega
68
69
       index = 1
70
        ! Set initial guess from provided radiance
71
72
        ! Traverse solution vector in order
73
        ! so as to avoid calculating index
       do k=1, nz
74
75
           do i=1, nx
76
               do j=1, ny
77
                 do p=1, nomega
78
                     light%mat%sol(index) = light%
                        radiance(i,j,k,p)
                     index = index + 1
79
80
                 end do
81
              end do
82
           end do
83
       end do
84
85
        !call light%mat%initial_guess()
86
87
        ! Solve (MGMRES)
```

```
88
        call light%mat%solve()
 89
 90
        index = 1
 91
 92
         ! Extract solution
 93
        do k=1, nz
            do i=1, nx
 94
 95
               do j=1, ny
 96
                  do p=1, nomega
 97
                      light%radiance(i,j,k,p) = light%
                         mat%sol(index)
 98
                      index = index + 1
99
                  end do
100
               end do
101
            end do
102
         end do
103
      end subroutine calculate_radiance
104
105
      subroutine calculate_irradiance(light)
106
         class(light_state) light
107
         integer i, j, k
108
         integer nx, ny, nz
109
         double precision, dimension(light%grid%
           angles%nomega) :: tmp_rad
110
111
        nx = light%grid%x%num
112
        ny = light%grid%y%num
113
        nz = light%grid%z%num
114
115
        do i=1, nx
116
            do j=1, ny
117
               do k=1, nz
118
                   ! Use temporary array to avoid
                     creating one
119
                    implicitly at every spatial grid
                     point
                  tmp_rad = light%radiance(i,j,k,:)
120
121
                  light%irradiance(i,j,k) = &
122
                        light%grid%angles%
                           integrate_points(tmp_rad)
123
               end do
124
            end do
125
        end do
126
127
      end subroutine calculate_irradiance
128
129
       subroutine light_to_hdf(light, radfile,
       irradfile)
130
          class(light_state) light
131
   11
          character(len=*) radfile
132
    1
          character(len=*) irradfile
133
   !
```

```
134 \mid !
         call hdf_write_radiance(radfile, light%
       radiance, light%grid)
135
         call hdf_write_irradiance(irradfile, light%
       irradiance, light%grid)
136
       end subroutine light_to_hdf
137
138
      subroutine light_deinit(light)
139
        class(light_state) light
140
141
        deallocate(light%irradiance)
        deallocate(light%radiance)
142
143
      end subroutine light_deinit
144 | end module
     asymptotics.f90
    module asymptotics
 2
      use kelp_context
 3
      !use rte_sparse_matrices
 4
      !use light_context
 5
      implicit none
 6
      contains
 7
      subroutine calculate_light_with_scattering(
         grid, bc, iops, radiance, num_scatters)
 9
        type(space_angle_grid) grid
10
        type(boundary_condition) bc
11
        type(optical_properties) iops
12
        double precision, dimension(:,:,:,:) ::
           radiance
13
        double precision, dimension(:,:,:,:),
           allocatable :: source
14
        integer num_scatters
15
        integer nx, ny, nz, nomega
16
        integer max_cells
17
18
        double precision, dimension(:), allocatable
           :: path_length, path_spacing, a_tilde, gn
19
20
        nx = grid%x%num
21
        ny = grid%y%num
22
        nz = grid%z%num
23
        nomega = grid%angles%nomega
24
25
        max_cells = calculate_max_cells(grid)
26
27
        allocate(path_length(max_cells+1))
        allocate(path_spacing(max_cells))
28
29
        allocate(a_tilde(max_cells))
30
        allocate(gn(max_cells))
31
        allocate(source(nx, ny, nz, nomega))
```

```
32
33
       call calculate_light_before_scattering(grid,
           bc, iops, source, radiance, path_length,
           path_spacing, a_tilde, gn)
34
35
       if (num_scatters .gt. 0) then
36
          call calculate_light_after_scattering(&
37
                grid, iops, source, radiance, &
                num_scatters, path_length,
38
                   path_spacing, &
39
                a_tilde, gn)
40
       end if
41
42
       deallocate(path_length)
43
       deallocate(path_spacing)
44
       deallocate(a_tilde)
45
       deallocate(gn)
46
       deallocate(source)
47
     end subroutine calculate_light_with_scattering
48
49
     subroutine calculate_light_before_scattering(
        grid, bc, iops, source, radiance,
        path_length, path_spacing, a_tilde, gn)
50
       type(space_angle_grid) grid
51
       type(boundary_condition) bc
52
       type(optical_properties) iops
53
       double precision, dimension(:,:,:,:) ::
          radiance, source
54
       double precision, dimension(:) ::
          path_length, path_spacing, a_tilde, gn
55
       integer i, j, k, p
56
57
       ! !$ integer omp_get_num_procs
58
       ! !$ integer num_threads_z, num_threads_x
59
60
       !! Enable nested parallelism
61
       ! !$ call omp_set_nested(.true.)
62
63
       !! Use nz procs for outer loop,
64
       ! ! or num_procs if num_procs < nz
65
       ! ! Divide the rest of the tasks as
          appropriate
66
67
       ! !$ num_threads_z = min(omp_get_num_procs()
          , grid%z%num)
68
         !$ num_threads_x = min( &
69
       !!$
                omp_get_num_procs()/num_threads_z, &
70
                grid%x%num)
       !!$
71
72
       ! !$omp parallel do default(none) private(i,
          j,k,p) &
```

```
73
        ! !$omp shared(grid,iops,radiance,bc,
           num_threads_x) &
74
        ! !$omp private(source, path_length,
           path_spacing,a_tilde,gn) &
75
        ! !$omp num_threads(num_threads_z) if(
           num_threads_z .gt. 1)
76
        do k=1, grid%z%num
77
            ! !$omp parallel do default(none) private
              (i,j,p) &
            ! !$omp firstprivate(k) shared(grid,iops,
78
              radiance, bc) &
            ! !$omp private(source,path_length,
79
              path_spacing,a_tilde,gn) &
80
            ! !$omp num_threads(num_threads_x) if(
              num_threads_x .gt. 1)
           do i=1, grid%x%num
81
82
               do j=1, grid%y%num
                  do p=1, grid%angles%nomega/2
83
84
                     ! Downwelling light
85
                     call
                        attenuate_light_from_surface
86
                         grid, iops, source, i, j, k,
                             р,&
87
                         radiance, path_length,
                            path_spacing,&
88
                         a_tilde, gn, bc)
89
90
                     ! No upwelling light before
                        scattering
91
                     radiance(i,j,k,p+grid%angles%
                        nomega/2) = 0.d0
92
                  end do
93
               end do
94
           end do
95
            ! !$omp end parallel do
96
         end do
97
         ! !$omp end parallel do
98
      end subroutine
         calculate_light_before_scattering
99
100
      subroutine attenuate_light_from_surface(&
101
           grid, iops, source, i, j, k, p, radiance,
102
           path_length, path_spacing, a_tilde, gn,
              bc)
103
        type(space_angle_grid) grid
104
        type(boundary_condition) bc
105
        type(optical_properties) iops
```

```
double precision, dimension(:,:,:,:) ::
106
           radiance, source
107
        double precision, dimension(:) ::
           path_length, path_spacing, a_tilde, gn
108
        integer i, j, k, p
        integer num_cells
109
110
        double precision atten
111
112
        ! Don't need gn here, so just ignore it
113
        call traverse_ray(grid, iops, source, i, j,
           k, p, path_length, path_spacing, a_tilde,
            gn, num_cells)
114
115
        ! Start with surface bc and attenuate along
116
        atten = sum(path_spacing(1:num_cells) *
           a_tilde(1:num_cells))
117
        ! Avoid underflow
118
        if (atten .lt. 100.d0) then
119
           radiance(i,j,k,p) = bc\%bc\_grid(p) * exp(-
              atten)
120
121
           radiance(i,j,k,p) = 0.d0
122
        end if
123
124
      end subroutine attenuate_light_from_surface
125
126
      subroutine calculate_light_after_scattering(
         grid, iops, source, radiance,&
127
           num_scatters, path_length, path_spacing,
              a_tilde, gn)
128
        type(space_angle_grid) grid
129
        type(optical_properties) iops
130
        double precision, dimension(:,:,:,:) ::
           radiance, source
131
        integer num_scatters
132
        double precision, dimension(:) ::
           path_length, path_spacing, a_tilde, gn
133
        double precision, dimension(:,:,:,:),
           allocatable :: rad_scatter
134
        integer n
135
        double precision bb
136
137
        allocate(rad_scatter(grid%x%num, grid%y%num,
            grid%z%num, grid%angles%nomega))
138
        rad_scatter = radiance
        bb = iops%scat
139
140
141
        do n=1, num_scatters
142
           write(*,*) 'scatter #', n
143
           call scatter(grid, iops, source,
```

```
rad_scatter, path_length, path_spacing
               a_tilde, gn)
144
           radiance = radiance + bb**n * rad_scatter
145
        end do
146
147
        deallocate(rad_scatter)
148
      end subroutine
         calculate_light_after_scattering
149
150
      ! Perform one scattering event
151
      subroutine scatter(grid, iops, source,
         rad_scatter, path_length, path_spacing,
         a_tilde, gn)
152
        type(space_angle_grid) grid
153
        type(optical_properties) iops
154
        double precision, dimension(:,:,:,:) ::
           rad_scatter, source
155
        double precision, dimension(:,:,:,:),
           allocatable :: scatter_integral
156
        double precision, dimension(:) ::
           path_length, path_spacing, a_tilde, gn
157
        integer nx, ny, nz, nomega
158
159
        nx = grid%x%num
160
        ny = grid%y%num
        nz = grid%z%num
161
162
        nomega = grid%angles%nomega
163
164
        allocate(scatter_integral(nx, ny, nz, nomega
165
166
        call calculate_source(grid, iops,
           rad_scatter, source, scatter_integral)
167
        call advect_light(grid, iops, source,
           rad_scatter, path_length, path_spacing,
           a_tilde, gn)
168
169
        deallocate(scatter_integral)
170
      end subroutine scatter
171
172
      ! Calculate source from no-scatter or previous
          scattering layer
173
      subroutine calculate_source(grid, iops,
         rad_scatter, source, scatter_integral)
174
        type(space_angle_grid) grid
175
        type(optical_properties) iops
176
        double precision, dimension(:,:,:,:) ::
           rad_scatter
177
        double precision, dimension(:,:,:,:) ::
           source
```

```
double precision, dimension(:,:,:,:) ::
178
           scatter_integral
179
        type(index_list) indices
180
        integer nx, ny, nz, nomega
181
        integer i, j, k, p
182
183
        !$ integer omp_get_num_procs
184
        !$ integer num_threads_z, num_threads_x
185
186
        nx = grid%x%num
187
        ny = grid%y%num
188
        nz = grid%z%num
189
        nomega = grid%angles%nomega
190
191
        ! Enable nested parallelism
192
        !$ call omp_set_nested(.true.)
193
194
        ! Use nz procs for outer loop,
195
        ! or num_procs if num_procs < nz
        ! Divide the rest of the tasks as
196
           appropriate
197
198
        !$ num_threads_z = min(omp_get_num_procs(),
           grid%z%num)
199
        !$ num_threads_x = min( &
200
               omp_get_num_procs()/num_threads_z, &
201
        ! $
               grid%x%num)
202
203
        !$omp parallel do default(none) private(
           indices) &
204
        !$omp private(i,j,k,p) shared(nx,ny,nz,
           nomega) &
205
        !$omp shared(iops, rad_scatter,
           scatter_integral) &
206
        !$omp shared(num_threads_x) &
207
        !$omp num_threads(num_threads_z) if(
           num_threads_z .gt. 1)
208
        do k=1, nz
209
            indices%k = k
210
            !$omp parallel do default(none)
              firstprivate(indices,k) &
211
            !$omp private(i,j,p) shared(nx,ny,nz,
              nomega) &
212
            !$omp shared(iops, rad_scatter,
              scatter_integral) &
213
            !$omp num_threads(num_threads_x) if(
              num_threads_x .gt. 1)
214
           do i=1, nx
215
              indices%i = i
216
              do j=1, ny
```

```
217
                  indices\%j = j
218
                  do p=1, nomega
219
                     indices\%p = p
220
                     call calculate_scatter_integral
221
                         iops, rad_scatter,&
222
                         scatter_integral,&
223
                          indices)
224
                  end do
225
               end do
226
           end do
            !$omp end parallel do
227
228
229
        !$omp end parallel do
230
231
        source(:,:,:) = -rad_scatter(:,:,:) +
           scatter_integral(:,:,:,:)
232
233
        write(*,*) 'source: ', sum(source)/size(
           source), minval(source), maxval(source)
234
235
      end subroutine calculate_source
236
237
      subroutine calculate_scatter_integral(iops,
         rad_scatter, scatter_integral, indices)
238
        type(optical_properties) iops
239
        double precision, dimension(:,:,:,:) ::
           rad_scatter, scatter_integral
240
        type(index_list) indices
241
242
        scatter_integral(indices%i,indices%j,indices
           %k,indices%p) &
243
             = sum(iops%vsf_integral(indices%p, :) &
244
              * rad_scatter(&
245
                indices%i,&
246
                indices%j,&
247
                indices%k,:))
248
249
      end subroutine calculate_scatter_integral
250
251
      subroutine advect_light(grid, iops, source,
         rad_scatter, path_length, path_spacing,
         a_tilde, gn)
252
        type(space_angle_grid) grid
253
        type(optical_properties) iops
254
        double precision, dimension(:,:,:,:) ::
           rad_scatter, source
255
        double precision, dimension(:) ::
           path_length, path_spacing, a_tilde, gn
256
        integer i, j, k, p
257
```

```
258
        !$ integer omp_get_num_procs
259
        !$ integer num_threads_z, num_threads_x
260
261
        ! Enable nested parallelism
262
        !$ call omp_set_nested(.true.)
263
264
        ! Use nz procs for outer loop,
265
         ! or num_procs if num_procs < nz
266
        ! Divide the rest of the tasks as
           appropriate
267
268
        !$ num_threads_z = min(omp_get_num_procs(),
           grid%z%num)
269
        !$ num_threads_x = min( &
270
        ! $
               omp_get_num_procs()/num_threads_z, &
271
        !$
               grid%x%num)
272
273
         !$omp parallel do default(none) &
274
         !$omp private(i,j,k,p) &
275
         !$omp shared(rad_scatter, source, grid, iops,
           num_threads_x) &
276
         !$omp private(path_length,path_spacing,
           a_tilde,gn) &
277
        !$omp num_threads(num_threads_z) if(
           num_threads_z .gt. 1)
278
        do k=1, grid%z%num
279
            !$omp parallel do default(none) &
280
            !$omp firstprivate(k) private(i,j,p) &
281
            !$omp shared(rad_scatter, source, grid, iops
282
            !$omp private(path_length,path_spacing,
              a_tilde,gn) &
283
            !$omp num_threads(num_threads_x) if(
              num_threads_x .gt. 1)
284
           do i=1, grid%x%num
285
              do j=1, grid%y%num
286
                  do p=1, grid%angles%nomega
                     call integrate_ray(grid, iops,
287
                        source,&
288
                           rad_scatter, path_length,
                              path_spacing,&
289
                           a_tilde, gn, i, j, k, p)
290
                 end do
291
               end do
292
           end do
293
            !$omp end parallel do
294
        end do
295
        !$omp end parallel do
296
      end subroutine advect_light
297
```

```
298
      ! New algorithm, double integral over
         piecewise-constant 1d funcs
299
      subroutine integrate_ray(grid, iops, source,
         rad_scatter, path_length, path_spacing,
         a_{tilde}, gn, i, j, k, p)
300
        type(space_angle_grid) :: grid
301
        type(optical_properties) :: iops
302
        double precision, dimension(:,:,:,:) ::
           source
303
        double precision, dimension(:,:,:,:) ::
           rad_scatter
304
        integer :: i, j, k, p
        ! The following are only passed to avoid
305
           unnecessary allocation
306
        double precision, dimension(:) ::
           path_length, path_spacing, a_tilde, gn
307
        integer num_cells
308
309
        call traverse_ray(grid, iops, source, i, j,
           k, p, path_length, path_spacing, a_tilde,
            gn, num_cells)
310
        rad_scatter(i,j,k,p) =
           calculate_ray_integral(num_cells,
           path_length, path_spacing, a_tilde, gn)
311
      end subroutine integrate_ray
312
313
      function calculate_ray_integral(num_cells, s,
         ds, a_tilde, gn) result(integral)
        ! Double integral which accumulates all
314
           scattered light along the path
315
        ! via an angular integral and attenuates it
           by integrating along the path
316
        integer :: num_cells
317
        double precision, dimension(num_cells) :: ds
           , a_tilde, gn
        double precision, dimension(num_cells+1) ::
318
319
        double precision :: integral
320
        double precision bi, di
321
        integer i, j
322
323
        integral = 0
324
        do i=1, num_cells
325
           bi = -a_tilde(i)*s(i+1)
326
           do j=i+1, num_cells
327
              bi = bi - a_tilde(j)*ds(j)
328
           end do
329
330
           ! WARNING: This will overflow if a_tilde
              is too large.
331
           if(a_tilde(i) .eq. 0) then
```

```
332
               di = ds(i)
333
            else
334
               di = (exp(a_tilde(i)*s(i+1))-exp(
                  a_tilde(i)*s(i))/a_tilde(i)
335
            end if
336
337
            integral = integral + gn(i)*di * exp(bi)
338
         end do
339
340
      end function calculate_ray_integral
341
342
      ! Calculate maximum number of cells a path
         through the grid could take
343
      ! This is a loose upper bound
344
      function calculate_max_cells(grid) result(
         max_cells)
345
         type(space_angle_grid) :: grid
346
         integer :: max_cells
347
        double precision dx, dy, zrange, phi_middle
348
349
         ! Angle that will have the longest ray
350
        phi_middle = grid%angles%phi(grid%angles%
           nphi/2
351
        dx = grid%x%spacing(1)
352
        dy = grid%y%spacing(1)
353
        zrange = grid%z%maxval - grid%z%minval
354
355
        \max_{\text{cells}} = \text{grid} \%z \% \text{num} + \text{ceiling} ((1/dx+1/dy))
           *zrange*tan(phi_middle))
356
      end function calculate_max_cells
357
358
      ! Traverse from surface or bottom to point (xi
         , yj, zk)
359
       ! in the direction omega_p, extracting path
         lengths (ds) and
360
      ! function values (f) along the way,
361
      ! as well as number of cells traversed (n).
362
      subroutine traverse_ray(grid, iops, source, i,
          j, k, p, s_array, ds, a_tilde, gn,
         num_cells)
363
        type(space_angle_grid) :: grid
364
         type(optical_properties) :: iops
365
         double precision, dimension(:,:,:,:) ::
            source
366
         integer :: i, j, k, p
367
         double precision, dimension(:) :: s_array,
           ds, a_tilde, gn
368
         integer :: num_cells
369
370
         integer t
371
         double precision p0x, p0y, p0z
```

```
372
        double precision p1x, p1y, p1z
373
        double precision z0
374
        double precision s_tilde, s
375
        integer dir_x, dir_y, dir_z
376
        integer shift_x, shift_y, shift_z
        integer cell_x, cell_y, cell_z
377
378
        integer edge_x, edge_y, edge_z
        integer first_x, last_x, first_y, last_y,
379
           last_z
380
        double precision s_next_x, s_next_y,
           s_next_z, s_next
381
        double precision x_factor, y_factor,
           z_factor
382
        double precision ds_x, ds_y
383
        double precision, dimension(grid%z%num) ::
           ds z
384
        double precision smx, smy
385
386
        ! Divide by these numbers to get path
           separation
387
        ! from separation in individual dimensions
388
        x_factor = grid%angles%sin_phi_p(p) * grid%
           angles%cos_theta_p(p)
389
        y_factor = grid%angles%sin_phi_p(p) * grid%
           angles%sin_theta_p(p)
390
        z_factor = grid%angles%cos_phi_p(p)
391
392
        ! Destination point
393
        p1x = grid%x%vals(i)
        ply = grid%y%vals(j)
394
395
        p1z = grid%z%vals(k)
396
397
        !write(*,*) 'START PATH.'
        !write(*,*) 'ijk = ', i, j, k
398
399
400
        ! Direction
401
        if (p.le. grid%angles%nomega/2) then
402
            Downwelling light originates from
              surface
403
           z0 = grid%z%minval
404
           dir_z = 1
405
        else
406
            ! Upwelling light originates from bottom
407
           z0 = grid%z%maxval
408
           dir_z = -1
409
        end if
410
411
        ! Total path length from origin to
           destination
412
        ! (sign is correct for upwelling and
           downwelling)
```

```
413
        s_tilde = (p1z - z0)/grid%angles%cos_phi_p(p
           )
414
415
         ! Path spacings between edge intersections
           in each dimension
416
         ! Set to 2*s_tilde if infinite in this
           dimension so that it's unreachable
417
         ! Assume x & y spacings are uniform,
418
         ! so it's okay to just use the first value.
419
        if(x_factor .eq. 0) then
420
            ds_x = 2*s_tilde
421
        else
422
            ds_x = abs(grid%x%spacing(1)/x_factor)
423
        end if
424
        if (y_factor .eq. 0) then
425
            ds_y = 2*s_tilde
426
427
            ds_y = abs(grid\%y\%spacing(1)/y_factor)
428
        end if
429
430
         ! This one is an array because z spacing can
            vary
431
         ! z_factor should never be 0, because the
           ray will never
432
         ! reach the surface or bottom.
433
        ds_z(1:grid%z%num) = dir_z * grid%z%spacing
            (1:grid%z%num)/z_factor
434
435
        ! Origin point
436
        p0x = p1x - s_{tilde} * x_{factor}
        pOy = p1y - s_tilde * y_factor
437
438
        p0z = p1z - s\_tilde * z\_factor
439
440
        ! Direction of ray in each dimension. 1 \Rightarrow
           increasing. -1 => decreasing.
441
        dir_x = int(sgn(p1x-p0x))
442
        dir_y = int(sgn(p1y-p0y))
443
444
        ! Shifts
445
        ! Conversion from cell_inds to edge_inds
446
         ! merge is fortran's ternary operator
447
        shift_x = merge(1,0,dir_x>0)
448
        shift_y = merge(1,0,dir_y>0)
449
        shift_z = merge(1,0,dir_z>0)
450
451
         ! Indices for cell containing origin point
452
        cell_x = floor((p0x-grid%x%minval)/grid%x%
           spacing(1)) + 1
453
        cell_y = floor((p0y-grid%y%minval)/grid%y%
           spacing(1)) + 1
454
         ! x and y may be in periodic image, so shift
            back.
```

```
455
        cell_x = mod1(cell_x, grid%x%num)
456
        cell_y = mod1(cell_y, grid%y%num)
457
458
        ! z starts at top or bottom depending on
           direction.
459
        if(dir_z > 0) then
            cell_z = 1
460
461
462
            cell_z = grid%z%num
463
        end if
464
465
        ! Edge indices preceeding starting cells
466
        edge_x = mod1(cell_x + shift_x, grid%x%num)
467
        edge_y = mod1(cell_y + shift_y, grid%y%num)
468
        edge_z = mod1(cell_z + shift_z, grid%z%num)
469
         ! First and last cells given direction
470
471
        if (dir_x .gt. 0) then
472
            first_x = 1
473
            last_x = grid%x%num
        else
474
475
            first_x = grid%x%num
476
            last_x = 1
477
        end if
478
        if(dir_y .gt. 0) then
479
            first_y = 1
480
            last_y = grid%y%num
481
        else
482
            first_y = grid%y%num
483
            last_y = 1
484
        end if
485
        if(dir_z .gt. 0) then
486
            last_z = grid%z%num
487
        else
488
            last_z = 1
489
        end if
490
491
        ! Calculate periodic images
492
        smx = shift_mod(p0x, grid%x%minval, grid%x%
           maxval)
493
        smy = shift_mod(p0y, grid%y%minval, grid%y%
           maxval)
494
495
         ! Path length to next edge plane in each
           dimension
496
        if (abs(x_factor) .lt. 1.d-10) then
497
            ! Will never cross, so set above total
              path length
498
            s_next_x = 2*s_tilde
499
        else if (cell_x .eq. last_x) then
```

```
500
            ! If starts out at last cell, then
              compare to periodic image
            s_next_x = (grid%x%edges(first_x) + dir_x
501
               * (grid%x%maxval - grid%x%minval)&
502
                 - smx) / x_factor
503
        else
504
            ! Otherwise, just compare to next cell
505
            s_next_x = (grid%x%edges(edge_x) - smx) /
               x factor
506
        end if
507
508
        ! Path length to next edge plane in each
           dimension
509
        if (abs(y_factor) .lt. 1.d-10) then
510
            ! Will never cross, so set above total
              path length
511
            s_next_y = 2*s_tilde
512
        else if(cell_y .eq. last_y) then
513
            ! If starts out at last cell, then
              compare to periodic image
514
            s_next_y = (grid%y%edges(first_y) + dir_y
                * (grid%y%maxval - grid%y%minval)&
515
                 - smy) / y_factor
516
        else
517
            ! Otherwise, just compare to next cell
            s_next_y = (grid%y%edges(edge_y) - smy) /
518
               y_factor
        end if
519
520
521
        s_next_z = ds_z(cell_z)
522
523
        ! Initialize path
524
        s = 0.d0
525
        s_{array}(1) = 0.d0
526
527
        ! Start with t=0 so that we can increment
           before storing,
528
        ! so that t will be the number of grid cells
            at the end of the loop.
529
        t = 0
530
531
        ! s is the beginning of the current cell,
532
        ! s_next is the end of the current cell.
533
        do while (s .lt. s_tilde)
534
           ! Move cell counter
535
           t = t + 1
536
537
            ! Extract function values
538
            a_tilde(t) = iops%abs_grid(cell_x, cell_y
               cell_z)
539
           gn(t) = source(cell_x, cell_y, cell_z, p)
540
```

```
541
           !write(*,*) ''
542
           !write(*,*) 's_next_x = ', s_next_x
           !write(*,*) 's_next_y = ', s_next_y
543
            !write(*,*) 's_next_z = ', s_next_z
544
545
           !write(*,*) 'theta, phi =', grid%angles%
              theta_p(p)*180.d0/pi, grid%angles%
              phi_p(p)*180.d0/pi
            !write(*,*) 's = ', s, '/', s_tilde
546
            !write(*,*) 'cell_z =', cell_z, '/', grid
547
              %z%num
548
            !write(*,*) 's_next_z =', s_next_z
            !write(*,*) 'last_z =', last_z
549
550
           !write(*,*) 'new'
551
           ! Move to next cell in path
552
553
           if(s_next_x .le. min(s_next_y, s_next_z))
               then
554
               ! x edge is closest
555
               s_next = s_next_x
556
557
               ! Increment indices (periodic)
558
               cell_x = mod1(cell_x + dir_x, grid%x%
                  num)
559
               edge_x = mod1(edge_x + dir_x, grid%x%
                 num)
560
561
               ! x intersection after the one at s=
                  s_next
562
               s_next_x = s_next + ds_x
563
564
           else if (s_next_y .le. min(s_next_x,
              s_next_z)) then
565
               ! y edge is closest
566
               s_next = s_next_y
567
568
               ! Increment indices (periodic)
569
               cell_y = mod1(cell_y + dir_y, grid%y%
                  num)
570
               edge_y = mod1(edge_y + dir_y, grid%y%
                 num)
571
572
               ! y intersection after the one at s=
                  s_next
573
               s_next_y = s_next + ds_y
574
575
           else if(s_next_z .le. min(s_next_x,
              s_next_y)) then
576
               ! z edge is closest
577
               s_next = s_next_z
578
579
               ! Increment indices
```

```
581
               edge_z = edge_z + dir_z
582
583
               !write(*,*) 'z edge, s_next =', s_next
584
585
               ! z intersection after the one at s=
                  s_next
586
               if(cell_z .lt. last_z) then
587
                  ! Only look ahead if we aren't at
                     the end
588
                  s_next_z = s_next + ds_z(cell_z)
589
               else
590
                  ! Otherwise, no need to continue.
591
                  ! this is our final destination.
592
                   exit
593
                  s_next_z = 2*s_tilde
594
                  !write(*,*) 'end. s_next_z =',
                     s_next_z
595
               end if
596
597
            end if
598
599
            ! Cut off early if this is the end
            ! This will be the last cell traversed if
600
                s_next >= s_tilde
601
            s_next = min(s_tilde, s_next)
602
603
            ! Store path length
604
            s_{array}(t+1) = s_{next}
605
            ! Extract path length from same cell as
               function vals
606
            ds(t) = s_next - s
607
608
            ! Update path length
            s = s_next
609
610
        end do
611
         ! Return number of cells traversed
612
613
        num_cells = t
614
615
      end subroutine traverse_ray
616 end module asymptotics
     light_interface.f90
   |module light_interface_module
 1
 2
      use rte3d
 3
      use kelp3d
 4
      use asymptotics
 5
      implicit none
 6
 7
    contains
      subroutine full_light_calculations( &
```

 $cell_z = cell_z + dir_z$

580

```
! OPTICAL PROPERTIES
10
        absorptance_kelp, & ! NOT THE SAME AS
          ABSORPTION COEFFICIENT
11
       abs_water, &
12
       scat, &
       num_vsf, &
13
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
       num_scatters, &
39
        ! FINAL RESULTS
40
       perceived_irrad, &
41
       avg_irrad)
42
43
        implicit none
44
45
        ! OPTICAL PROPERTIES
46
        integer, intent(in) :: nx, ny, nz, ntheta,
47
        ! Absorption and scattering coefficients
48
        double precision, intent(in) ::
          absorptance_kelp, scat
49
       double precision, dimension(nz), intent(in)
           :: abs_water
50
        ! Volume scattering function
51
        integer, intent(in) :: num_vsf
52
        character(len=*) :: vsf_file
53
        !double precision, dimension(num_vsf),
           intent(int) :: vsf_angles
54
        !double precision, dimension(num_vsf),
           intent(int) :: vsf_vals
```

```
55
56
       ! SUNLIGHT
57
       double precision, intent(in) :: solar_zenith
       double precision, intent(in) ::
58
          solar_azimuthal
59
       double precision, intent(in) ::
          surface_irrad
60
61
       ! KELP
62
       ! Number of Superindividuals in each depth
63
       integer, intent(in) :: num_si
64
       ! si_area(i,j) = area of superindividual j
          at depth i
65
       double precision, dimension(nz, num_si),
          intent(in) :: si_area
       ! si_ind(i,j) = number of inidividuals
66
          represented by superindividual j at depth
           i
67
       double precision, dimension(nz, num_si),
          intent(in) :: si_ind
68
       ! Thickness of each frond
69
       double precision, intent(in) ::
          frond_thickness
70
       ! Ratio of length to width (0, infty)
71
       double precision, intent(in) ::
          frond_aspect_ratio
72
       ! Rescaled position of greatest width (0=
          base, 1=tip)
73
       double precision, intent(in) ::
          frond_shape_ratio
74
       ! WATER CURRENT
75
76
       double precision, dimension(nz), intent(in)
          :: current_speeds
77
       double precision, dimension(nz), intent(in)
          :: current_angles
78
79
       ! SPACING
80
       double precision, intent(in) :: rope_spacing
       double precision, dimension(nz), intent(in)
81
          :: depth_spacing
82
       ! SOLVER PARAMETERS
83
       integer, intent(in) :: num_scatters
84
85
       ! FINAL RESULT
86
       real, dimension(nz), intent(out) ::
          avg_irrad, perceived_irrad
87
       ! -----!
88
89
```

```
90
        double precision xmin, xmax, ymin, ymax,
           zmin, zmax
91
        character(len=5), parameter :: fmtstr = 'E13
92
        !double precision, dimension(num_vsf) ::
           vsf_angles, vsf_vals
93
        double precision max_rad, decay
94
        integer quadrature_degree
95
96
        type(space_angle_grid) grid
97
        type(optical_properties) iops
98
        type(light_state) light
99
        type(rope_state) rope
100
        type(frond_shape) frond
101
        type(boundary_condition) bc
102
103
        double precision, dimension(:), allocatable
           :: pop_length_means, pop_length_stds
104
        ! Number of fronds in each depth layer
105
        double precision, dimension(:), allocatable
           :: num_fronds
        double precision, dimension(:,:,:),
106
           allocatable :: p_kelp
107
108
        write(*,*) 'Light calculation'
109
        allocate(pop_length_means(nz))
110
111
        allocate(pop_length_stds(nz))
112
        allocate(num_fronds(nz))
113
        allocate(p_kelp(nx, ny, nz))
114
115
        xmin = -rope_spacing/2
116
        xmax = rope_spacing/2
117
118
        ymin = -rope_spacing/2
119
        ymax = rope_spacing/2
120
121
        zmin = 0.d0
122
        zmax = sum(depth_spacing)
123
124
        write(*,*) 'Grid'
125
        call grid%set_bounds(xmin, xmax, ymin, ymax,
            zmin. zmax)
126
        call grid%set_num(nx, ny, nz, ntheta, nphi)
127
        call grid%init()
128
        !call grid%set_uniform_spacing_from_num()
129
        call grid%z%set_spacing_array(depth_spacing)
130
131
        call rope%init(grid)
132
```

```
133
        write(*,*) 'Rope'
134
        ! Calculate kelp distribution
135
        call calculate_length_dist_from_superinds( &
136
        nz, &
137
        num_si, &
138
        si_area, &
139
        si_ind, &
140
        frond_aspect_ratio, &
141
        num_fronds, &
142
        pop_length_means, &
143
        pop_length_stds)
144
145
        rope%frond_lengths = pop_length_means
        rope%frond_stds = pop_length_stds
146
147
        rope%num_fronds = num_fronds
148
        rope%water_speeds = current_speeds
149
        rope%water_angles = current_angles
150
151
        write(*,*) 'frond_lengths =', rope%
           frond_lengths
152
        write(*,*) 'frond_stds
                                  =', rope%frond_stds
        write(*,*) 'num_fronds
153
                                  =', rope%num_fronds
        write(*,*) 'water_speeds =', rope%
154
           water_speeds
155
        write(*,*) 'water_angles =', rope%
           water_angles
156
157
        write(*,*) 'Frond'
        ! INIT FROND
158
        call frond%set_shape(frond_shape_ratio,
159
           frond_aspect_ratio, frond_thickness)
160
        ! CALCULATE KELP
161
        quadrature_degree = 5
        call calculate_kelp_on_grid(grid, p_kelp,
162
           frond, rope, quadrature_degree)
163
        ! INIT IOPS
164
        iops%num_vsf = num_vsf
165
        call iops%init(grid)
        write(*,*) 'IOPs'
166
167
        iops%abs_kelp = absorptance_kelp /
           frond_thickness
168
        iops%abs_water = abs_water
169
        iops%scat = scat
170
171
        !write(*,*) 'iop init'
172
        !iops%vsf_angles = vsf_angles
        !iops%vsf_vals = vsf_vals
173
174
        call iops%load_vsf(vsf_file, fmtstr)
175
176
        ! load_vsf already calls calc_vsf_on_grid
177
        !call iops%calc_vsf_on_grid()
```

```
178
        call iops%calculate_coef_grids(p_kelp)
179
         !write(*,*) 'BC'
180
181
        max_rad = 1.d0 ! Doesn't matter because we'
           ll rescale
182
        decay = 1.d0 ! Does matter, but maybe not
           much. Determines drop-off from angle
183
         call bc%init(grid, solar_zenith,
           solar_azimuthal, decay, max_rad)
184
         ! Rescale surface radiance to match surface
           irradiance
185
        bc%bc_grid = bc%bc_grid * surface_irrad /
           grid%angles%integrate_points(bc%bc_grid)
186
187
        write(*,*) 'bc'
188
        write(*,*) bc%bc_grid
189
         ! write(*,*) 'bc'
190
         ! do i=1, grid%y%num
191
192
               write(*,'(10F15.3)') bc%bc_grid(i,:)
193
         ! end do
194
195
        call light%init_grid(grid)
196
197
        write(*,*) 'Scatter'
198
         call calculate_light_with_scattering(grid,
           bc, iops, light%radiance, num_scatters)
199
200
        write(*,*) 'Irrad'
201
        call light%calculate_irradiance()
202
203
         ! Calculate output variables
204
        call calculate_average_irradiance(grid,
           light, avg_irrad)
205
         call calculate_perceived_irrad(grid, p_kelp,
206
              perceived_irrad, light%irradiance)
207
         !write(*,*) 'vsf_angles = ', iops%vsf_angles
!write(*,*) 'vsf_vals = ', iops%vsf_vals
208
209
         !write(*,*) 'vsf norm = ', grid%
210
            integrate_angle_2d(iops%vsf(1,1,:,:))
211
212
         ! write(*,*) 'abs_water = ', abs_water
         ! write(*,*) 'scat_water = ', scat_water
213
        write(*,*) 'kelp '
214
215
        write(*,*) p_kelp(:,:,:)
216
        write(*,*) 'ft =', frond%ft
217
        write(*,*) 'irrad'
218
```

```
219
        write(*,*) light%irradiance
220
221
        write(*,*) 'avg_irrad = ', avg_irrad
222
        write(*,*) 'perceived_irrad = ',
           perceived_irrad
223
224
        write(*,*) 'deinit'
225
        call bc%deinit()
226
        !write(*,*) 'a'
227
        call iops%deinit()
228
        !write(*,*) 'b'
229
        call light%deinit()
230
        !write(*,*) 'c'
231
        call rope%deinit()
232
        !write(*,*) 'd'
233
        call grid%deinit()
234
        !write(*,*) 'e'
235
236
        deallocate(pop_length_means)
237
        deallocate(pop_length_stds)
238
        deallocate(num_fronds)
239
        deallocate(p_kelp)
240
241
        !write(*,*) 'done'
242
      end subroutine full_light_calculations
243
244
      subroutine
         calculate_length_dist_from_superinds( &
245
        nz, &
246
        num_si, &
247
        si_area, &
248
        si_ind, &
249
        frond_aspect_ratio, &
250
        num_fronds, &
251
        pop_length_means, &
252
        pop_length_stds)
253
254
        implicit none
255
256
        ! Number of depth levels
257
        integer, intent(in) :: nz
258
         ! Number of Superindividuals in each depth
           level
259
        integer, intent(in) :: num_si
260
         ! si_area(i,j) = area of superindividual j
           at depth i
261
        double precision, dimension(nz, num_si),
           intent(in) :: si_area
262
         ! si_area(i,j) = number of inidividuals
           represented by superindividual j at depth
```

```
double precision, dimension(nz, num_si),
263
           intent(in) :: si_ind
264
        double precision, intent(in) ::
           frond_aspect_ratio
265
266
        double precision, dimension(nz), intent(out)
            :: num_fronds
267
        ! Population mean area at each depth level
268
        double precision, dimension(nz), intent(out)
            :: pop_length_means
269
        ! Population area standard deviation at each
            depth level
270
        double precision, dimension(nz), intent(out)
            :: pop_length_stds
271
272
        ! ----!
273
274
        integer i, k
275
        ! Numerators for mean and std
276
        double precision mean_num, std_num
277
        ! Convert area to length
278
        double precision, dimension(num_si) ::
           si_length
279
280
        do k=1, nz
281
           mean_num = 0.d0
282
           std_num = 0.d0
283
           num_fronds(k) = 0
284
285
           do i=1, num_si
286
               si_length(i) = sqrt(2.d0*)
                  frond_aspect_ratio*si_area(k,i))
287
               mean_num = mean_num + si_length(i)
288
               num_fronds(k) = num_fronds(k) + si_ind
                  (k,i)
289
           end do
290
291
           pop_length_means(k) = mean_num /
              num_fronds(k)
292
293
           do i=1, num_si
294
               std_num = std_num + (si_length(i) -
                  pop_length_means(k))**2
295
           end do
296
297
           pop_length_stds(k) = std_num / (
              num_fronds(k) - 1)
298
299
        end do
300
301
      end subroutine
         calculate_length_dist_from_superinds
```

```
302
303
      subroutine calculate_average_irradiance(grid,
         light, avg_irrad)
        type(space_angle_grid) grid
304
305
        type(light_state) light
306
        real, dimension(:) :: avg_irrad
        integer k, nx, ny, nz
307
308
309
        nx = grid%x%num
310
        ny = grid%y%num
311
        nz = grid%z%num
312
313
        do k=1, nz
314
           avg_irrad(k) = real(sum(light%irradiance)
              (:,:,k)) / nx / ny)
315
316
      end subroutine calculate_average_irradiance
317
318
      subroutine calculate_perceived_irrad(grid,
         p_kelp, &
319
           perceived_irrad, irradiance)
320
        type(space_angle_grid) grid
321
        double precision, dimension(:,:,:) :: p_kelp
322
        real, dimension(:) :: perceived_irrad
        double precision, dimension(:,:,:) ::
323
           irradiance
324
325
        integer k
326
327
        ! Calculate the average irradiance
           experienced over the frond.
328
        ! Has same units as irradiance.
329
        do k=1, grid%z%num
330
           perceived_irrad(k) = real( &
331
                 sum(p_kelp(:,:,k)*irradiance(:,:,k))
332
                 / sum(p_kelp(:,:,k)))
333
        end do
334
335
      end subroutine calculate_perceived_irrad
336
    end module light_interface_module
337
```