Inverse Adding-Doubling

(Version 3-15-2)

1. `iad` program.

Here is a relatively robust command-line utility that shows how the iad and ad subroutines might be called. It suffers because it is written in `CWEB` and I used the macro expansion feature instead of creating separate functions. Oh well.

I create an empty file `iad_main.h` to simplify the Makefile

⟨ `iad_main.h`   1 ⟩ ≡

2.   All the actual output for this web file goes into `iad_main.c`

⟨ `iad_main.c` 2 ⟩ ≡
  ⟨ Include files for *main* 3 ⟩
  ⟨ print version function 19 ⟩
  ⟨ print usage function 20 ⟩
  ⟨ stringdup together function 26 ⟩
  ⟨ mystrtod function 27 ⟩
  ⟨ seconds elapsed function 28 ⟩
  ⟨ print error legend function 25 ⟩
  ⟨ what_char function 30 ⟩
  ⟨ print long error function 31 ⟩
  ⟨ print dot function 32 ⟩
  ⟨ calculate coefficients function 21 ⟩
  ⟨ parse string into array function 29 ⟩
  ⟨ print results header function 23 ⟩
  ⟨ Print results function 24 ⟩

  int *main*(**int** *argc*, **char** ∗∗*argv*)
  {
    ⟨ Declare variables for *main* 4 ⟩
    ⟨ Handle options 5 ⟩
    Initialize_Measure(&*m*);
    ⟨ Command-line changes to *m* 16 ⟩
    Initialize_Result(*m*, &*r*);
    ⟨ Command-line changes to *r* 13 ⟩
    if (*cl_forward_calc* ≠ UNINITIALIZED) {
      ⟨ Calculate and Print the Forward Calculation 6 ⟩
      exit(EXIT_SUCCESS);
    }
    ⟨ prepare file for reading 10 ⟩
    if (*process_command_line*) {
      ⟨ Count command-line measurements 18 ⟩
      ⟨ Calculate and write optical properties 11 ⟩
      exit(EXIT_SUCCESS);
    }
    if (*Read_Header*(*stdin*, &*m*, &*params*) ≡ 0) {
      start_time = *clock*( );
      while (*Read_Data_Line*(*stdin*, &*m*, &*r*, *params*) ≡ 0) {
        ⟨ Command-line changes to *m* 16 ⟩
        ⟨ Calculate and write optical properties 11 ⟩
      }
    }
    if (*cl_verbosity* > 0) *fprintf*(*stderr*, "\n\n");
    if (*any_error* ∧ *cl_verbosity* > 1) *print_error_legend*( );
    exit(EXIT_SUCCESS);
  }

3.   The first two defines are to stop Visual C++ from silly complaints

⟨ Include files for *main* 3 ⟩ ≡
#**define** _CRT_SECURE_NO_WARNINGS
#**define** _CRT_NONSTDC_NO_WARNINGS
#**define** NO_SLIDES 0
#**define** ONE_SLIDE_ON_TOP 1
#**define** TWO_IDENTICAL_SLIDES 2
#**define** ONE_SLIDE_ON_BOTTOM 3
#**define** ONE_SLIDE_NEAR_SPHERE 4
#**define** ONE_SLIDE_NOT_NEAR_SPHERE 5
#**define** MR_IS_ONLY_RD 1
#**define** MT_IS_ONLY_TD 2
#**define** NO_UNSCATTERED_LIGHT 3
#**include** <stdio.h>
#**include** <string.h>
#**include** <stdlib.h>
#**include** <unistd.h>
#**include** <time.h>
#**include** <math.h>
#**include** <ctype.h>
#**include** <errno.h>
#**include** "ad_globl.h"
#**include** "ad_prime.h"
#**include** "iad_type.h"
#**include** "iad_pub.h"
#**include** "iad_io.h"
#**include** "iad_calc.h"
#**include** "iad_util.h"
#**include** "version.h"
#**include** "mc_lost.h"
#**include** "ad_frsnl.h"

See also section 34.

This code is used in sections 2 and 33.

4.   ⟨ Declare variables for *main* 4 ⟩ ≡
   struct measure_type *m*;
   struct invert_type *r*;
   char *∗g_out_name* = Λ;
   int *c*;
   long *n_photons* = 100000;
   int *MC_MAX_iterations* = 19;
   int *any_error* = 0;
   int *process_command_line* = 0;
   int *params* = 0;
   int *cl_quadrature_points* = UNINITIALIZED;
   int *cl_verbosity* = 2;
   double *cl_forward_calc* = UNINITIALIZED;
   double *cl_default_a* = UNINITIALIZED;
   double *cl_default_g* = UNINITIALIZED;
   double *cl_default_b* = UNINITIALIZED;
   double *cl_default_mua* = UNINITIALIZED;
   double *cl_default_mus* = UNINITIALIZED;
   double *cl_tolerance* = UNINITIALIZED;
   double *cl_slide_OD* = UNINITIALIZED;
   double *cl_cos_angle* = UNINITIALIZED;
   double *cl_beam_d* = UNINITIALIZED;
   double *cl_sample_d* = UNINITIALIZED;
   double *cl_sample_n* = UNINITIALIZED;
   double *cl_slide_d* = UNINITIALIZED;
   double *cl_slide_n* = UNINITIALIZED;
   double *cl_slides* = UNINITIALIZED;
   double *cl_default_fr* = UNINITIALIZED;
   double *cl_rstd_t* = UNINITIALIZED;
   double *cl_rstd_r* = UNINITIALIZED;
   double *cl_baffle_r* = UNINITIALIZED;
   double *cl_baffle_t* = UNINITIALIZED;
   double *cl_rc_fraction* = UNINITIALIZED;
   double *cl_tc_fraction* = UNINITIALIZED;
   double *cl_lambda* = UNINITIALIZED;
   double *cl_rwall_r* = UNINITIALIZED;
   double *cl_rwall_t* = UNINITIALIZED;
   double *cl_search* = UNINITIALIZED;
   double *cl_mus0* = UNINITIALIZED;
   double *cl_musp0* = UNINITIALIZED;
   double *cl_mus0_pwr* = UNINITIALIZED;
   double *cl_mus0_lambda* = UNINITIALIZED;
   double *cl_UR1* = UNINITIALIZED;
   double *cl_UT1* = UNINITIALIZED;
   double *cl_Tc* = UNINITIALIZED;
   double *cl_method* = UNINITIALIZED;
   int *cl_num_spheres* = UNINITIALIZED;
   double *cl_sphere_one*[5] = {UNINITIALIZED, UNINITIALIZED, UNINITIALIZED, UNINITIALIZED,
       UNINITIALIZED};
   double *cl_sphere_two*[5] = {UNINITIALIZED, UNINITIALIZED, UNINITIALIZED, UNINITIALIZED,
       UNINITIALIZED};
   clock_t *start_time* = *clock*( );

char *command_line_options*[ ] = "1:2:a:A:b:B:c:C:d:D:e:E:f:F:g:G:hH:i:L:M:n:N:o:p:q:r:R:s:S:\
t:T:u:vV:x:Xz";

See also section 35.

This code is used in sections 2 and 33.

5.   use the *getopt*( ) to process options.

⟨ Handle options 5 ⟩ ≡
  while ((*c* = *getopt*(*argc*, *argv*, *command_line_options*)) ≠ EOF) {
    int *n*;
    char *cc*;
    char *∗tmp_str* = Λ;

    switch (*c*) {
    case '1': *tmp_str* = *strdup*(*optarg*);
      parse_string_into_array(*optarg*, *cl_sphere_one*, 5);
      if (*cl_sphere_one*[4] ≡ UNINITIALIZED) {
        fprintf(*stderr*, "Error␣in␣command−line␣argument␣for␣−1\n");
        fprintf(*stderr*, "␣␣␣␣the␣current␣argument␣is␣'%s'␣but␣it␣must␣have␣5␣terms:␣", *tmp_str*);
        fprintf(*stderr*, "'d_sphere␣d_sample␣d_empty␣d_detector␣r_wall'\n");
        exit(EXIT_FAILURE);
      }
      break;
    case '2': *tmp_str* = *strdup*(*optarg*);
      parse_string_into_array(*optarg*, *cl_sphere_two*, 5);
      if (*cl_sphere_two*[4] ≡ UNINITIALIZED) {
        fprintf(*stderr*, "Error␣in␣command−line␣argument␣for␣−2\n");
        fprintf(*stderr*, "␣␣␣␣the␣current␣argument␣is␣'%s'␣but␣it␣must␣have␣5␣terms:␣", *tmp_str*);
        fprintf(*stderr*, "'d_sphere␣d_sample␣d_empty␣d_detector␣r_wall'\n");
        exit(EXIT_FAILURE);
      }
      break;
    case 'a': *cl_default_a* = *my_strtod*(*optarg*);
      if (*cl_default_a* < 0 ∨ *cl_default_a* > 1) {
        fprintf(*stderr*, "Error␣in␣command−line\n");
        fprintf(*stderr*, "␣␣␣␣␣albedo␣'−a␣%s'\n", *optarg*);
        exit(EXIT_FAILURE);
      }
      break;
    case 'A': *cl_default_mua* = *my_strtod*(*optarg*);
      if (*cl_default_mua* < 0) {
        fprintf(*stderr*, "Error␣in␣command−line\n");
        fprintf(*stderr*, "␣␣␣␣␣absorption␣'−A␣%s'\n", *optarg*);
        exit(EXIT_FAILURE);
      }
      break;
    case 'b': *cl_default_b* = *my_strtod*(*optarg*);
      if (*cl_default_b* < 0) {
        fprintf(*stderr*, "Error␣in␣command−line\n");
        fprintf(*stderr*, "␣␣␣␣␣optical␣thickness␣'−b␣%s'\n", *optarg*);
        exit(EXIT_FAILURE);
      }
      break;
    case 'B': *cl_beam_d* = *my_strtod*(*optarg*);
      if (*cl_beam_d* < 0) {
        fprintf(*stderr*, "Error␣in␣command−line\n");
        fprintf(*stderr*, "␣␣␣␣␣beam␣diameter␣'−B␣%s'\n", *optarg*);
        exit(EXIT_FAILURE);
      }

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      break;
   case 'c': cl_rc_fraction = my_strtod(optarg);
      if (cl_rc_fraction < 0.0 ∨ cl_rc_fraction > 1.0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣unscattered␣refl␣fraction␣'-c␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_SUCCESS);
      }
      break;
   case 'C': cl_tc_fraction = my_strtod(optarg);
      if (cl_tc_fraction < 0.0 ∨ cl_tc_fraction > 1.0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣unscattered␣trans␣fraction␣'-C␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_SUCCESS);
      }
      break;
   case 'd': cl_sample_d = my_strtod(optarg);
      if (cl_sample_d < 0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣sample␣thickness␣'-d␣%s'\n", optarg);
         exit(EXIT_FAILURE);
      }
      break;
   case 'D': cl_slide_d = my_strtod(optarg);
      if (cl_slide_d < 0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣slide␣thickness␣'-D␣%s'\n", optarg);
         exit(EXIT_FAILURE);
      }
      break;
   case 'e': cl_tolerance = my_strtod(optarg);
      if (cl_tolerance < 0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣error␣tolerance␣'-e␣%s'\n", optarg);
         exit(EXIT_FAILURE);
      }
      break;
   case 'E': cl_slide_OD = my_strtod(optarg);
      if (cl_slide_OD < 0) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣slide␣optical␣depth␣'-E␣%s'\n", optarg);
         exit(EXIT_FAILURE);
      }
      break;
   case 'f': cl_default_fr = my_strtod(optarg);
      if (cl_default_fr < 0.0 ∨ cl_default_fr > 1.0) {
         fprintf(stderr, "Error␣in␣command-line␣argument:␣");
         fprintf(stderr, "'-f␣%s'␣The␣argument␣must␣be␣between␣0␣and␣1.\n", optarg);
         exit(EXIT_SUCCESS);
      }
      break;
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case 'F':      /* initial digit means this is mus is constant */
  if (isdigit(optarg[0])) {
    cl_default_mus = my_strtod(optarg);
    if (cl_default_mus < 0) {
      fprintf(stderr, "Error␣in␣command-line\n");
      fprintf(stderr, "␣␣␣␣␣mus␣'-F␣%s'\n", optarg);
      exit(EXIT_FAILURE);
    }
    break;
  }      /* should be a string like 'R 1000 1.2 -1.8' */
  n = sscanf(optarg, "%c␣%lf␣%lf␣%lf", &cc, &cl_mus0_lambda, &cl_mus0, &cl_mus0_pwr);
  if (n ≠ 4 ∨ (cc ≠ 'P' ∧ cc ≠ 'R')) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣bad␣-F␣option.␣'-F␣%s'\n", optarg);
    fprintf(stderr, "␣␣␣␣␣-F␣1.0␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣for␣mus␣=1.0\n");
    fprintf(stderr, "␣␣␣␣␣-F␣'P␣500␣1.0␣-1.3'␣for␣mus␣=1.0*(lambda/500)^(-1.3)\n");
    fprintf(stderr, "␣␣␣␣␣-F␣'R␣500␣1.0␣-1.3'␣for␣mus'=1.0*(lambda/500)^(-1.3)\n");
    exit(EXIT_FAILURE);
  }
  if (cc ≡ 'R' ∨ cc ≡ 'r') {
    cl_musp0 = cl_mus0;
    cl_mus0 = UNINITIALIZED;
  }
  break;
case 'g': cl_default_g = my_strtod(optarg);
  if (cl_default_g < −1 ∨ cl_default_g > 1) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣anisotropy␣'-g␣%s'\n", optarg);
    exit(EXIT_FAILURE);
  }
  break;
case 'G':
  if (optarg[0] ≡ '0') cl_slides = NO_SLIDES;
  else if (optarg[0] ≡ '2') cl_slides = TWO_IDENTICAL_SLIDES;
  else if (optarg[0] ≡ 't' ∨ optarg[0] ≡ 'T') cl_slides = ONE_SLIDE_ON_TOP;
  else if (optarg[0] ≡ 'b' ∨ optarg[0] ≡ 'B') cl_slides = ONE_SLIDE_ON_BOTTOM;
  else if (optarg[0] ≡ 'n' ∨ optarg[0] ≡ 'N') cl_slides = ONE_SLIDE_NEAR_SPHERE;
  else if (optarg[0] ≡ 'f' ∨ optarg[0] ≡ 'F') cl_slides = ONE_SLIDE_NOT_NEAR_SPHERE;
  else {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣Argument␣for␣'-G␣%s'␣must␣be␣\n", optarg);
    fprintf(stderr, "␣␣␣␣␣'t'␣---␣light␣always␣hits␣top␣slide␣first\n");
    fprintf(stderr, "␣␣␣␣␣'b'␣---␣light␣always␣hits␣bottom␣slide␣first\n");
    fprintf(stderr, "␣␣␣␣␣'n'␣---␣slide␣always␣closest␣to␣sphere\n");
    fprintf(stderr, "␣␣␣␣␣'f'␣---␣slide␣always␣farthest␣from␣sphere\n");
    exit(EXIT_FAILURE);
  }
  break;
case 'H':
  if (optarg[0] ≡ '0') {
    cl_baffle_r = 0;
    cl_baffle_t = 0;
```

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  }
  else if (optarg[0] ≡ '1') {
    cl_baffle_r = 1;
    cl_baffle_t = 0;
  }
  else if (optarg[0] ≡ '2') {
    cl_baffle_r = 0;
    cl_baffle_t = 1;
  }
  else if (optarg[0] ≡ '3') {
    cl_baffle_r = 1;
    cl_baffle_t = 1;
  }
  else {
    fprintf(stderr, "Error␣in␣command-line␣-H␣argument\n");
    fprintf(stderr, "␣␣␣␣␣argument␣is␣'%s',␣but␣", optarg);
    fprintf(stderr, "must␣be␣0,␣1,␣2,␣or␣3\n");
    exit(EXIT_FAILURE);
  }
case 'i': cl_cos_angle = my_strtod(optarg);
  if (cl_cos_angle < 0 ∨ cl_cos_angle > 90) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣incident␣angle␣'-i␣%s'\n", optarg);
    fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣90␣degrees\n");
    exit(EXIT_FAILURE);
  }
  cl_cos_angle = cos(cl_cos_angle * M_PI/180.0);
  break;
case 'L': cl_lambda = my_strtod(optarg);
  break;
case 'M': MC_MAX_iterations = (int) my_strtod(optarg);
  if (MC_MAX_iterations < 0 ∨ MC_MAX_iterations > 50) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣MC␣iterations␣'-M␣%s'\n", optarg);
    exit(EXIT_FAILURE);
  }
  break;
case 'n': cl_sample_n = my_strtod(optarg);
  if (cl_sample_n < 0.1 ∨ cl_sample_n > 10) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣slab␣index␣'-n␣%s'\n", optarg);
    exit(EXIT_FAILURE);
  }
  break;
case 'N': cl_slide_n = my_strtod(optarg);
  if (cl_slide_n < 0.1 ∨ cl_slide_n > 10) {
    fprintf(stderr, "Error␣in␣command-line\n");
    fprintf(stderr, "␣␣␣␣␣slide␣index␣'-N␣%s'\n", optarg);
    exit(EXIT_FAILURE);
  }
  break;
case 'o': g_out_name = strdup(optarg);
```

```
      break;
   case 'p': n_photons = (long) my_strtod(optarg);
      break;
   case 'q': cl_quadrature_points = (int) my_strtod(optarg);
      if (cl_quadrature_points % 4 ≠ 0) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣'−q␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣Quadrature␣points␣must␣be␣a␣multiple␣of␣4\n");
         exit(EXIT_FAILURE);
      }
      if ((cl_cos_angle ≠ UNINITIALIZED) ∧ (cl_quadrature_points % 12 ≠ 0)) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣'−q␣%s'\n", optarg);
         fprintf(stderr,
               "␣␣␣␣␣Quadrature␣points␣must␣be␣multiple␣of␣12␣for␣oblique␣incidence\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 'r': cl_UR1 = my_strtod(optarg);
      process_command_line = 1;
      if (cl_UR1 < 0 ∨ cl_UR1 > 1) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣UR1␣value␣'−r␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 'R': cl_rstd_r = my_strtod(optarg);
      if (cl_rstd_r < 0 ∨ cl_rstd_r > 1) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣Rstd␣value␣'−R␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 's': cl_search = (int) my_strtod(optarg);
      break;
   case 'S': cl_num_spheres = (int) my_strtod(optarg);
      if (cl_num_spheres ≠ 0 ∧ cl_num_spheres ≠ 1 ∧ cl_num_spheres ≠ 2) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣sphere␣number␣'−S␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣0,␣1,␣or␣2\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 't': cl_UT1 = my_strtod(optarg);
      if (cl_UT1 < 0 ∨ cl_UT1 > 1) {
         fprintf(stderr, "Error␣in␣command−line\n");
         fprintf(stderr, "␣␣␣␣␣UT1␣value␣'−t␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
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      process_command_line = 1;
      break;
   case 'T': cl_rstd_t = my_strtod(optarg);
      if (cl_rstd_t < 0 ∨ cl_rstd_t > 1) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣␣transmission␣standard␣'-T␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 'u': cl_Tc = my_strtod(optarg);
      if (cl_Tc < 0 ∨ cl_Tc > 1) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣␣unscattered␣transmission␣'-u␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      process_command_line = 1;
      break;
   case 'v': print_version(cl_verbosity);
      exit(EXIT_SUCCESS);
      break;
   case 'V': cl_verbosity = my_strtod(optarg);
      break;
   case 'w': cl_rwall_r = my_strtod(optarg);
      if (cl_rwall_r < 0 ∨ cl_rwall_r > 1) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣␣refl␣sphere␣wall␣'-w␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 'W': cl_rwall_t = my_strtod(optarg);
      if (cl_rwall_t < 0 ∨ cl_rwall_r > 1) {
         fprintf(stderr, "Error␣in␣command-line\n");
         fprintf(stderr, "␣␣␣␣␣trans␣sphere␣wall␣'-w␣%s'\n", optarg);
         fprintf(stderr, "␣␣␣␣␣must␣be␣between␣0␣and␣1\n");
         exit(EXIT_FAILURE);
      }
      break;
   case 'x': Set_Debugging((int) my_strtod(optarg));
      break;
   case 'X': cl_method = COMPARISON;
      break;
   case 'z': cl_forward_calc = 1;
      process_command_line = 1;
      break;
   default: fprintf(stderr, "unknown␣option␣'%c'\n", c);     /∗ fall through ∗/
   case 'h': print_usage();
      exit(EXIT_SUCCESS);
   }
}
```

$argc \mathrel{-}= optind;$
$argv \mathrel{+}= optind;$

This code is used in section 2.

6.   We are doing a forward calculation. We still need to set the albedo and optical depth appropriately. Obviously when the -a switch is used then the albedo should be fixed as a constant equal to $cl\_default\_a$. The other cases are less clear. If scattering and absorption are both specified, then calculate the albedo using these values. If the scattering is not specified, then we assume that the sample is an unscattering sample and therefore the albedo is zero. On the other hand, if the scattering is specified and the absorption is not, then the albedo is set to one.

⟨ Calculate and Print the Forward Calculation 6 ⟩ ≡
   if $(cl\_default\_a \equiv \text{UNINITIALIZED})$ {
      if $(cl\_default\_mus \equiv \text{UNINITIALIZED})$ $r.a = 0;$
      else if $(cl\_default\_mua \equiv \text{UNINITIALIZED})$ $r.a = 1;$
      else $r.a = cl\_default\_mus/(cl\_default\_mua + cl\_default\_mus);$
   }
   else $r.a = cl\_default\_a;$

See also sections 7, 8, and 9.

This code is used in section 2.

7.   This is slightly more tricky because there are four things that can affect the optical thickness — $cl\_default\_b$, the default mua, default mus and the thickness. If the sample thickness is unspecified, then the only reasonable thing to do is to assume that the sample is very thick. Otherwise, we use the sample thickness to calculate the optical thickness.

⟨ Calculate and Print the Forward Calculation 6 ⟩ +≡
   if $(cl\_default\_b \equiv \text{UNINITIALIZED})$ {
      if $(cl\_sample\_d \equiv \text{UNINITIALIZED})$ $r.b = \text{HUGE\_VAL};$
      else if $(r.a \equiv 0)$ {
         if $(cl\_default\_mua \equiv \text{UNINITIALIZED})$ $r.b = \text{HUGE\_VAL};$
         else $r.b = cl\_default\_mua * cl\_sample\_d;$
      }
      else {
         if $(cl\_default\_mus \equiv \text{UNINITIALIZED})$ $r.b = \text{HUGE\_VAL};$
         else $r.b = cl\_default\_mus/r.a * cl\_sample\_d;$
      }
   }
   else $r.b = cl\_default\_b;$

8.   The easiest case, use the default value or set it to zero

⟨ Calculate and Print the Forward Calculation 6 ⟩ +≡
   if $(cl\_default\_g \equiv \text{UNINITIALIZED})$ $r.g = 0;$
   else $r.g = cl\_default\_g;$

9.   ⟨ Calculate and Print the Forward Calculation 6 ⟩ +≡

 $r.slab.a = r.a;$
 $r.slab.b = r.b;$
 $r.slab.g = r.g;$
 {
  double $mu\_sp, mu\_a, m\_r, m\_t;$

  $Calculate\_MR\_MT(m, r, \text{TRUE}, \text{TRUE}, \&m\_r, \&m\_t);$
  $Calculate\_Mua\_Musp(m, r, \&mu\_sp, \&mu\_a);$
  if $(cl\_verbosity > 0)$ {
   $Write\_Header(m, r, -1);$
   $print\_results\_header(stdout);$
  }
  $print\_optical\_property\_result(stdout, m, r, m\_r, m\_t, mu\_a, mu\_sp, 0);$
 }

10.   Make sure that the file is not named '-' and warn about too many files

⟨ prepare file for reading 10 ⟩ ≡

 if $(argc > 1)$ {
  $fprintf(stderr, \texttt{"Only␣a␣single␣file␣can␣be␣processed␣at␣a␣time\n"});$
  $fprintf(stderr, \texttt{"try␣'apply␣iad␣file1␣file2␣...␣fileN'\n"});$
  $exit(\texttt{EXIT\_FAILURE});$
 }
 if $(argc \equiv 1 \wedge strcmp(argv[0], \texttt{"-"}) \neq 0)$ { /* filename exists and != "-" */
  int $n;$
  char $*base\_name, *rt\_name;$

  $base\_name = strdup(argv[0]);$
  $n = (\textbf{int})(strlen(base\_name) - strlen(\texttt{".rxt"}));$
  if $(n > 0 \wedge strstr(base\_name + n, \texttt{".rxt"}) \neq \Lambda)$ $base\_name[n] = \texttt{'\0'};$
  $rt\_name = strdup\_together(base\_name, \texttt{".rxt"});$
  if $(freopen(argv[0], \texttt{"r"}, stdin) \equiv \Lambda \wedge freopen(rt\_name, \texttt{"r"}, stdin) \equiv \Lambda)$ {
   $fprintf(stderr, \texttt{"Could␣not␣open␣either␣'%s'␣or␣'%s'\n"}, argv[0], rt\_name);$
   $exit(\texttt{EXIT\_FAILURE});$
  }
  if $(g\_out\_name \equiv \Lambda)$ $g\_out\_name = strdup\_together(base\_name, \texttt{".txt"});$
  $free(rt\_name);$
  $free(base\_name);$
  $process\_command\_line = 0;$
 }
 if $(g\_out\_name \neq \Lambda)$ {
  if $(freopen(g\_out\_name, \texttt{"w"}, stdout) \equiv \Lambda)$ {
   $fprintf(stderr, \texttt{"Could␣not␣open␣file␣'%s'␣for␣output\n"}, g\_out\_name);$
   $exit(\texttt{EXIT\_FAILURE});$
  }
 }

This code is used in section 2.

11.   Need to explicitly reset *r.search* each time through the loop, because it will get altered by the calculation process. We want to be able to let different lines have different constraints. In particular consider the file `newton.tst`. In that file the first two rows contain three real measurements and the last two have the collimated transmission explicitly set to zero — in other words there are really only two measurements.

⟨ Calculate and write optical properties 11 ⟩ ≡
```
{
   ⟨Local Variables for Calculation 12⟩
   if (Debug(DEBUG_ANY)) {
      fprintf (stderr, "\n-------------------NEXT␣DATA␣POINT--------------------\n");
      if (m.lambda ≠ 0) fprintf (stderr, "lambda=%6.1f␣", m.lambda);
      fprintf (stderr, "MR=%8.5f␣MT=%8.5f\n\n", m.m_r, m.m_t);
   }
   Initialize_Result (m, &r);
   ⟨Command-line changes to r 13⟩
   ⟨Warn and quit for bad options 17⟩
   ⟨Write Header 14⟩
   m.ur1_lost = 0;
   m.uru_lost = 0;
   m.ut1_lost = 0;
   m.utu_lost = 0;
   Inverse_RT (m, &r);
   if (r.error ≡ IAD_NO_ERROR) {
      calculate_coefficients (m, r, &LR, &LT, &mu_sp, &mu_a);
      ⟨Improve result using Monte Carlo 15⟩
   }
   print_optical_property_result (stdout, m, r, LR, LT, mu_a, mu_sp, rt_total);
   if (r.error ≠ IAD_NO_ERROR) any_error = 1;
   if (Debug(DEBUG_ANY)) print_long_error (r.error);
   else   print_dot (start_time, r.error, mc_total, TRUE, cl_verbosity);
}
```
See also section 37.

This code is used in sections 2 and 33.

12.

⟨ Local Variables for Calculation 12 ⟩ ≡
```
   static int rt_total = 0;
   static int mc_total = 0;
   double ur1 = 0;
   double ut1 = 0;
   double uru = 0;
   double utu = 0;
   double mu_a = 0;
   double mu_sp = 0;
   double LR = 0;
   double LT = 0;

   rt_total ++;
```
This code is used in section 11.

13.   ⟨ Command-line changes to r 13 ⟩ ≡
  if ($cl\_quadrature\_points \neq$ UNINITIALIZED) $r.method.quad\_pts = cl\_quadrature\_points$;
  else $r.method.quad\_pts = 8$;
  if ($cl\_default\_a \neq$ UNINITIALIZED) $r.default\_a = cl\_default\_a$;
  if ($cl\_default\_mua \neq$ UNINITIALIZED) {
    $r.default\_mua = cl\_default\_mua$;
    if ($cl\_sample\_d \neq$ UNINITIALIZED) $r.default\_ba = cl\_default\_mua * cl\_sample\_d$;
    else $r.default\_ba = cl\_default\_mua * m.slab\_thickness$;
  }
  if ($cl\_default\_b \neq$ UNINITIALIZED) $r.default\_b = cl\_default\_b$;
  if ($cl\_default\_g \neq$ UNINITIALIZED) $r.default\_g = cl\_default\_g$;
  if ($cl\_tolerance \neq$ UNINITIALIZED) {
    $r.tolerance = cl\_tolerance$;
    $r.MC\_tolerance = cl\_tolerance$;
  }
  if ($cl\_musp0 \neq$ UNINITIALIZED)
    $cl\_mus0 = (r.default\_g \neq$ UNINITIALIZED$) ?\ cl\_musp0 / (1 - r.default\_g) : cl\_musp0$;
  if ($cl\_mus0 \neq$ UNINITIALIZED $\wedge\ m.lambda \neq 0$)
    $cl\_default\_mus = cl\_mus0 * pow(m.lambda / cl\_mus0\_lambda, cl\_mus0\_pwr)$;
  if ($cl\_default\_mus \neq$ UNINITIALIZED) {
    $r.default\_mus = cl\_default\_mus$;
    if ($cl\_sample\_d \neq$ UNINITIALIZED) $r.default\_bs = cl\_default\_mus * cl\_sample\_d$;
    else $r.default\_bs = cl\_default\_mus * m.slab\_thickness$;
  }
  if ($cl\_search \neq$ UNINITIALIZED) $r.search = cl\_search$;
This code is used in sections 2 and 11.

14.   ⟨ Write Header 14 ⟩ ≡
  if ($rt\_total \equiv 1 \wedge cl\_verbosity > 0$) {
    $Write\_Header(m, r, params)$;
    if ($MC\_MAX\_iterations > 0$) {
      if ($n\_photons \geq 0$)
        $fprintf(stdout, $"#␣␣Photons␣used␣to␣estimate␣lost␣light␣=␣␣␣%ld\n"$, n_photons)$;
      else $fprintf(stdout, $"#␣␣␣␣␣␣Time␣used␣to␣estimate␣lost␣light␣=␣␣␣%ld␣ms\n"$, -n_photons)$;
    }
    else $fprintf(stdout, $"#␣␣Photons␣used␣to␣estimate␣lost␣light␣=␣␣␣0\n")$;
    $fprintf(stdout, $"#\n")$;
    $print\_results\_header(stdout)$;
  }
This code is used in section 11.

15.   Use Monte Carlo to figure out how much light leaks out. We use the sphere corrected values as the starting values and only do try Monte Carlo when spheres are used, the albedo unknown or non-zero, and there has been no error. The sphere parameters must be known because otherwise the beam size and the port size are unknown.

⟨ Improve result using Monte Carlo 15 ⟩ ≡

  if $(m.as\_r \neq 0 \land r.default\_a \neq 0)$ {

    double $mu\_sp\_last = mu\_sp$;

    double $mu\_a\_last = mu\_a$;

    if $(Debug(\texttt{DEBUG\_LOST\_LIGHT}))$ {

      $print\_results\_header(stderr)$;

      $print\_optical\_property\_result(stderr, m, r, \texttt{LR}, \texttt{LT}, mu\_a, mu\_sp, rt\_total)$;

    }

    while $(r.MC\_iterations < MC\_MAX\_iterations)$ {

      if $(Debug(\texttt{DEBUG\_ITERATIONS}))$

        $fprintf(stderr,$ `"\n−−−−−−−−−−−−␣Monte␣Carlo␣Iteration␣%d␣−−−−−−−−−−−−−−−−−\n"`,

          $r.MC\_iterations + 1)$;

      $MC\_Lost(m, r, n\_photons, \&ur1, \&ut1, \&uru, \&utu, \&m.ur1\_lost, \&m.ut1\_lost, \&m.uru\_lost,$

        $\&m.utu\_lost)$;

      $mc\_total\mathbin{++}$;

      $r.MC\_iterations\mathbin{++}$;

      $Inverse\_RT(m, \&r)$;

      $calculate\_coefficients(m, r, \&\texttt{LR}, \&\texttt{LT}, \&mu\_sp, \&mu\_a)$;

      if $(fabs(mu\_a\_last − mu\_a)/(mu\_a + 0.0001) < r.MC\_tolerance \land fabs(mu\_sp\_last − mu\_sp)/(mu\_sp +$

        $0.0001) < r.MC\_tolerance)$ **break**;

      $mu\_a\_last = mu\_a$;

      $mu\_sp\_last = mu\_sp$;

      if $(Debug(\texttt{DEBUG\_LOST\_LIGHT}))$

        $print\_optical\_property\_result(stderr, m, r, \texttt{LR}, \texttt{LT}, mu\_a, mu\_sp, rt\_total)$;

      else $print\_dot(start\_time, r.error, mc\_total, \texttt{FALSE}, cl\_verbosity)$;

      if $(r.error \neq \texttt{IAD\_NO\_ERROR})$ **break**;

    }

  }

This code is used in section 11.

16.   Stuff the command line arguments that should be constant over the entire inversion process into the measurement record and set up the result record to handle the arguments properly so that the optical properties can be determined.

⟨ Command-line changes to m 16 ⟩ ≡
  if ($cl\_cos\_angle \neq$ UNINITIALIZED) {
    $m.slab\_cos\_angle = cl\_cos\_angle$;
    if ($cl\_quadrature\_points \equiv$ UNINITIALIZED) $cl\_quadrature\_points = 12$;
    if ($cl\_quadrature\_points \neq 12 * (cl\_quadrature\_points/12)$) {
      $fprintf$($stderr$,
        "If␣you␣use␣the␣-i␣option␣to␣specify␣an␣oblique␣incidence␣angle,␣then\n");
      $fprintf$($stderr$, "the␣number␣of␣quadrature␣points␣must␣be␣a␣multiple␣of␣12\n");
      $exit$(EXIT_SUCCESS);
    }
  }
  if ($cl\_sample\_n \neq$ UNINITIALIZED) $m.slab\_index = cl\_sample\_n$;
  if ($cl\_slide\_n \neq$ UNINITIALIZED) {
    $m.slab\_bottom\_slide\_index = cl\_slide\_n$;
    $m.slab\_top\_slide\_index = cl\_slide\_n$;
  }
  if ($cl\_slide\_OD \neq$ UNINITIALIZED) {
    $m.slab\_bottom\_slide\_b = cl\_slide\_OD$;
    $m.slab\_top\_slide\_b = cl\_slide\_OD$;
  }
  if ($cl\_sample\_d \neq$ UNINITIALIZED) $m.slab\_thickness = cl\_sample\_d$;
  if ($cl\_beam\_d \neq$ UNINITIALIZED) $m.d\_beam = cl\_beam\_d$;
  if ($cl\_slide\_d \neq$ UNINITIALIZED) {
    $m.slab\_bottom\_slide\_thickness = cl\_slide\_d$;
    $m.slab\_top\_slide\_thickness = cl\_slide\_d$;
  }
  if ($cl\_slides \equiv$ NO_SLIDES) {
    $m.slab\_bottom\_slide\_index = 1.0$;
    $m.slab\_bottom\_slide\_thickness = 0.0$;
    $m.slab\_top\_slide\_index = 1.0$;
    $m.slab\_top\_slide\_thickness = 0.0$;
  }
  if ($cl\_slides \equiv$ ONE_SLIDE_ON_TOP $\lor cl\_slides \equiv$ ONE_SLIDE_NEAR_SPHERE) {
    $m.slab\_bottom\_slide\_index = 1.0$;
    $m.slab\_bottom\_slide\_thickness = 0.0$;
  }
  if ($cl\_slides \equiv$ ONE_SLIDE_ON_BOTTOM $\lor cl\_slides \equiv$ ONE_SLIDE_NOT_NEAR_SPHERE) {
    $m.slab\_top\_slide\_index = 1.0$;
    $m.slab\_top\_slide\_thickness = 0.0$;
  }
  if ($cl\_slides \equiv$ ONE_SLIDE_NEAR_SPHERE $\lor cl\_slides \equiv$ ONE_SLIDE_NOT_NEAR_SPHERE) $m.flip\_sample = 1$;
  else $m.flip\_sample = 0$;
  if ($cl\_method \neq$ UNINITIALIZED) $m.method = ($**int**$) cl\_method$;
  if ($cl\_rstd\_t \neq$ UNINITIALIZED) $m.rstd\_t = cl\_rstd\_t$;
  if ($cl\_rstd\_r \neq$ UNINITIALIZED) $m.rstd\_r = cl\_rstd\_r$;
  if ($cl\_rwall\_r \neq$ UNINITIALIZED) $m.rw\_r = cl\_rwall\_r$;
  if ($cl\_rwall\_t \neq$ UNINITIALIZED) $m.rw\_t = cl\_rwall\_t$;
  if ($cl\_sphere\_one[0] \neq$ UNINITIALIZED) {
    double d_sample_r, d_empty_r, $d\_detector\_r$;

$m.d\_sphere\_r = cl\_sphere\_one\,[0];$
$d\_sample\_r = cl\_sphere\_one\,[1];$
$d\_empty\_r = cl\_sphere\_one\,[2];$
$d\_detector\_r = cl\_sphere\_one\,[3];$
$m.rw\_r = cl\_sphere\_one\,[4];$
$m.as\_r = (d\_sample\_r\,/m.d\_sphere\_r\,/2) * (d\_sample\_r\,/m.d\_sphere\_r\,/2);$
$m.ae\_r = (d\_empty\_r\,/m.d\_sphere\_r\,/2) * (d\_empty\_r\,/m.d\_sphere\_r\,/2);$
$m.ad\_r = (d\_detector\_r\,/m.d\_sphere\_r\,/2) * (d\_detector\_r\,/m.d\_sphere\_r\,/2);$
$m.aw\_r = 1.0 - m.as\_r - m.ae\_r - m.ad\_r;$
$m.d\_sphere\_t = m.d\_sphere\_r;$
$m.as\_t = m.as\_r;$
$m.ae\_t = m.ae\_r;$
$m.ad\_t = m.ad\_r;$
$m.aw\_t = m.aw\_r;$
$m.rw\_t = m.rw\_r;$
if $(cl\_num\_spheres \equiv \texttt{UNINITIALIZED})$ $m.num\_spheres = 1;$
}
if $(cl\_sphere\_two\,[0] \neq \texttt{UNINITIALIZED})$ {
  double $d\_sample\_t, d\_empty\_t, d\_detector\_t;$

  $m.d\_sphere\_t = cl\_sphere\_two\,[0];$
  $d\_sample\_t = cl\_sphere\_two\,[1];$
  $d\_empty\_t = cl\_sphere\_two\,[2];$
  $d\_detector\_t = cl\_sphere\_two\,[3];$
  $m.rw\_t = cl\_sphere\_two\,[4];$
  $m.as\_t = (d\_sample\_t\,/m.d\_sphere\_t\,/2) * (d\_sample\_t\,/m.d\_sphere\_t\,/2);$
  $m.ae\_t = (d\_empty\_t\,/m.d\_sphere\_t\,/2) * (d\_empty\_t\,/m.d\_sphere\_t\,/2);$
  $m.ad\_t = (d\_detector\_t\,/m.d\_sphere\_t\,/2) * (d\_detector\_t\,/m.d\_sphere\_t\,/2);$
  $m.aw\_t = 1.0 - m.as\_t - m.ae\_t - m.ad\_t;$
  if $(cl\_num\_spheres \equiv \texttt{UNINITIALIZED})$ $m.num\_spheres = 2;$
}
if $(cl\_num\_spheres \neq \texttt{UNINITIALIZED})$ {
  $m.num\_spheres = (\textbf{int})\, cl\_num\_spheres;$
  if $(m.num\_spheres > 0 \wedge m.method \equiv \texttt{UNKNOWN})$ $m.method = \texttt{SUBSTITUTION};$
}
if $(cl\_rc\_fraction \neq \texttt{UNINITIALIZED})$ $m.fraction\_of\_rc\_in\_mr = cl\_rc\_fraction;$
if $(cl\_tc\_fraction \neq \texttt{UNINITIALIZED})$ $m.fraction\_of\_tc\_in\_mt = cl\_tc\_fraction;$
if $(cl\_UR1 \neq \texttt{UNINITIALIZED})$ $m.m\_r = cl\_UR1;$
if $(cl\_UT1 \neq \texttt{UNINITIALIZED})$ $m.m\_t = cl\_UT1;$
if $(cl\_Tc \neq \texttt{UNINITIALIZED})$ $m.m\_u = cl\_Tc;$
if $(cl\_default\_fr \neq \texttt{UNINITIALIZED})$ $m.f\_r = cl\_default\_fr;$
if $(cl\_baffle\_r \neq \texttt{UNINITIALIZED})$ $m.baffle\_r = cl\_baffle\_r;$
if $(cl\_baffle\_t \neq \texttt{UNINITIALIZED})$ $m.baffle\_t = cl\_baffle\_t;$
if $(cl\_lambda \neq \texttt{UNINITIALIZED})$ $m.lambda = cl\_lambda;$

This code is used in section 2.

17.   ⟨Warn and quit for bad options 17⟩ ≡
  if (*cl_method* ≡ COMPARISON ∧ *m.d_sphere_r* ≠ 0 ∧ *m.as_r* ≡ 0) {
    fprintf (*stderr*, "A␣dual−beam␣measurement␣is␣specified,␣but␣no␣port␣sizes.\n");
    fprintf (*stderr*, "You␣might␣forsake␣the␣−X␣option␣and␣use␣zero␣spheres␣(which␣gives\n");
    fprintf (*stderr*, "the␣same␣result␣except␣lost␣light␣is␣not␣taken␣into␣account).\n");
    fprintf (*stderr*, "Alternatively,␣bite␣the␣bullet␣and␣enter␣your␣sphere␣parameters,\n");
    fprintf (*stderr*, "with␣the␣knowledge␣that␣only␣the␣beam␣diameter␣and␣sample␣port\n");
    fprintf (*stderr*, "diameter␣will␣be␣used␣to␣estimate␣lost␣light␣from␣the␣edges.\n");
    exit (EXIT_SUCCESS);
  }
  if (*cl_method* ≡ COMPARISON ∧ *m.num_spheres* ≡ 2) {
    fprintf (*stderr*, "A␣dual−beam␣measurement␣is␣specified,␣but␣a␣two␣sphere␣experiment\n");
    fprintf (*stderr*, "is␣specified.␣Since␣this␣seems␣impossible,␣I␣will␣make␣it\n");
    fprintf (*stderr*, "impossible␣for␣you␣unless␣you␣specify␣0␣or␣1␣sphere.\n");
    exit (EXIT_SUCCESS);
  }
  if (*cl_method* ≡ COMPARISON ∧ *m.f_r* ≠ 0) {
    fprintf (*stderr*, "A␣dual−beam␣measurement␣is␣specified,␣but␣a␣fraction␣of␣light\n");
    fprintf (*stderr*, "is␣specified␣to␣hit␣the␣sphere␣wall␣first.␣␣This␣situation\n");
    fprintf (*stderr*, "is␣not␣supported␣by␣iad.␣␣Sorry.\n");
    exit (EXIT_SUCCESS);
  }
This code is used in section 11.

18.   put the values for command line reflection and transmission into the measurement record.

⟨Count command-line measurements 18⟩ ≡
  m.num_measures = 3;
  if (*m.m_t* ≡ 0) *m.num_measures* −−;
  if (*m.m_u* ≡ 0) *m.num_measures* −−;
  params = *m.num_measures*;
  if (*m.num_measures* ≡ 3) {   /∗ need to fill slab entries to calculate the optical thickness ∗/
    struct AD_slab_type *s*;

    s.n_slab = *m.slab_index*;
    s.n_top_slide = *m.slab_top_slide_index*;
    s.n_bottom_slide = *m.slab_bottom_slide_index*;
    s.b_top_slide = *m.slab_top_slide_b*;
    s.b_bottom_slide = *m.slab_bottom_slide_b*;
    s.cos_angle = *m.slab_cos_angle*;
    cl_default_b = *What_Is_B* (*s*, *m.m_u*);
  }
This code is used in section 2.

19.   ⟨ print version function 19 ⟩ ≡

  static void *print_version* (**int** *verbosity*)

  {

    if (*verbosity* ≡ 0) {

      fprintf (*stdout*, `"%s"`, *VersionShort*);

    }

    else {

      fprintf (*stdout*, `"iad␣%s\n"`, *Version*);

      fprintf (*stdout*, `"Copyright␣1993−2024␣Scott␣Prahl,␣scott.prahl@oit.edu\n"`);

      fprintf (*stdout*, `"␣␣␣␣␣␣␣␣␣␣␣(see␣Applied␣Optics,␣32:559−568,␣1993)\n\n"`);

      fprintf (*stdout*, `"This␣is␣free␣software;␣see␣the␣source␣for␣copying␣conditions.\n"`);

      fprintf (*stdout*, `"There␣is␣no␣warranty;␣not␣even␣for␣MERCHANTABILITY␣or␣FITNESS.\n"`);

      fprintf (*stdout*, `"FOR␣A␣PARTICULAR␣PURPOSE.\n"`);

    }

  }

This code is used in section 2.

20.   ⟨ print usage function 20 ⟩ ≡
  static void *print_usage*(**void**)
  {
    fprintf(*stdout*, "iad␣%s\n\n", *Version*);
    fprintf(*stdout*, "iad␣finds␣optical␣properties␣from␣measurements\n\n");
    fprintf(*stdout*, "Usage:␣␣iad␣[options]␣input\n\n");
    fprintf(*stdout*, "Options:\n");
    fprintf(*stdout*, "␣␣-1␣'#␣#␣#␣#␣#'␣␣␣reflection␣sphere␣parameters␣\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣'d_sphere␣d␣d_sample_port␣d_empty_port␣d\
        _detector_port␣r_wall'\n");
    fprintf(*stdout*, "␣␣-2␣'#␣#␣#␣#␣#'␣␣␣transmission␣sphere␣parameters␣\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣'d_sphere␣d␣d_sample_port␣d_empty_port␣d\
        _detector_port␣r_wall'\n");
    fprintf(*stdout*, "␣␣-a␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣use␣this␣albedo␣\n");
    fprintf(*stdout*, "␣␣-A␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣use␣this␣absorption␣coefficient␣\n");
    fprintf(*stdout*, "␣␣-b␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣use␣this␣optical␣thickness␣\n");
    fprintf(*stdout*, "␣␣-B␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣beam␣diameter␣\n");
    fprintf(*stdout*, "␣␣-c␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣fraction␣of␣unscattered␣refl␣in␣MR\n");
    fprintf(*stdout*, "␣␣-C␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣fraction␣of␣unscattered␣trans␣in␣MT\n");
    fprintf(*stdout*, "␣␣-d␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣thickness␣of␣sample␣\n");
    fprintf(*stdout*, "␣␣-D␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣thickness␣of␣slide␣\n");
    fprintf(*stdout*, "␣␣-e␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣error␣tolerance␣(default␣0.0001)␣\n");
    fprintf(*stdout*, "␣␣-E␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣optical␣depth␣(=mua*D)␣for␣slides\n");
    fprintf(*stdout*,
        "␣␣-f␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣allow␣a␣fraction␣0.0-1.0␣of␣light␣to␣hit␣sphere␣wall␣first\n");
    fprintf(*stdout*, "␣␣-F␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣constrain␣scattering␣coefficient␣\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣constant:␣use␣constant␣scattering␣coefficient␣\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣'P␣lambda0␣mus0␣gamma'␣then␣mus=mus0\
        *(lambda/lambda0)^gamma\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣'R␣lambda0␣musp0␣gamma'␣␣musp=musp0*\
        (lambda/lambda0)^gamma\n");
    fprintf(*stdout*, "␣␣-g␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣scattering␣anisotropy␣(default␣0)␣\n");
    fprintf(*stdout*, "␣␣-G␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣type␣of␣boundary␣'0',␣'2',␣'t',␣'b',␣'n',␣'f'␣\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣'0'␣or␣'2'␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣---␣number␣of␣slides\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣'t'␣(top)␣or␣'b'␣(bottom)␣---␣one␣slide␣\
        that␣is␣hit␣by␣light␣first\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣'n'␣(near)␣or␣'f'␣(far)␣␣␣---␣one␣slide␣\
        position␣relative␣to␣sphere\n");
    fprintf(*stdout*, "␣␣-h␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣display␣help\n");
    fprintf(*stdout*, "␣␣-H␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣0,␣no␣baffles␣for␣R␣or␣T␣spheres\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣1,␣baffle␣for␣R␣but␣not␣for␣T␣sphere\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣2,␣baffle␣for␣T␣but␣not␣for␣R␣sphere\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣=␣3,␣baffle␣for␣both␣R␣and␣T␣spheres␣(default)\n");
    fprintf(*stdout*, "␣␣-L␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣specify␣the␣wavelength␣lambda\n");
    fprintf(*stdout*, "␣␣-M␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣number␣of␣Monte␣Carlo␣iterations\n");
    fprintf(*stdout*, "␣␣-M␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣number␣of␣Monte␣Carlo␣iterations\n");
    fprintf(*stdout*, "␣␣-n␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣specify␣index␣of␣refraction␣of␣slab\n");
    fprintf(*stdout*, "␣␣-N␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣specify␣index␣of␣refraction␣of␣slides\n");
    fprintf(*stdout*, "␣␣-o␣filename␣␣␣␣␣␣␣explicitly␣specify␣filename␣for␣output\n");
    fprintf(*stdout*, "␣␣-p␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣#␣of␣Monte␣Carlo␣photons␣(default␣100000)\n");
    fprintf(*stdout*, "␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣a␣negative␣number␣is␣max␣MC␣time␣in␣milliseconds\n");
    fprintf(*stdout*, "␣␣-q␣#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣number␣of␣quadrature␣points␣(default=8)\n");

fprintf (*stdout*, "␣␣-r␣#␣␣␣␣␣␣␣␣␣␣␣␣␣total␣reflection␣measurement\n");
fprintf (*stdout*, "␣␣-R␣#␣␣␣␣␣␣␣␣␣␣␣␣␣actual␣reflectance␣for␣100%%␣measurement␣\n");
fprintf (*stdout*, "␣␣-S␣#␣␣␣␣␣␣␣␣␣␣␣␣␣number␣of␣spheres␣used\n");
fprintf (*stdout*, "␣␣-t␣#␣␣␣␣␣␣␣␣␣␣␣␣␣total␣transmission␣measurement\n");
fprintf (*stdout*, "␣␣-T␣#␣␣␣␣␣␣␣␣␣␣␣␣␣actual␣transmission␣for␣100%%␣measurement␣\n");
fprintf (*stdout*, "␣␣-u␣#␣␣␣␣␣␣␣␣␣␣␣␣␣unscattered␣transmission␣measurement\n");
fprintf (*stdout*, "␣␣-v␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣version␣information\n");
fprintf (*stdout*, "␣␣-V␣0␣␣␣␣␣␣␣␣␣␣␣␣␣verbosity␣low␣---␣no␣output␣to␣stdout\n");
fprintf (*stdout*, "␣␣-V␣1␣␣␣␣␣␣␣␣␣␣␣␣␣verbosity␣moderate␣\n");
fprintf (*stdout*, "␣␣-V␣2␣␣␣␣␣␣␣␣␣␣␣␣␣verbosity␣high\n");
fprintf (*stdout*, "␣␣-w␣#␣␣␣␣␣␣␣␣␣␣␣␣␣wall␣reflectivity␣for␣reflection␣sphere\n");
fprintf (*stdout*, "␣␣-W␣#␣␣␣␣␣␣␣␣␣␣␣␣␣wall␣reflectivity␣for␣transmission␣sphere\n");
fprintf (*stdout*, "␣␣-x␣#␣␣␣␣␣␣␣␣␣␣␣␣␣set␣debugging␣level\n");
fprintf (*stdout*, "␣␣-X␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣dual␣beam␣configuration\n");
fprintf (*stdout*, "␣␣-z␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣do␣forward␣calculation\n");
fprintf (*stdout*, "Examples:\n");
fprintf (*stdout*, "␣␣iad␣file.rxt␣␣␣␣␣␣␣␣␣␣␣Results␣will␣be␣put␣in␣file.txt\n");
fprintf (*stdout*, "␣␣iad␣file␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Same␣as␣above\n");
fprintf (*stdout*, "␣␣iad␣-c␣0.9␣file.rxt␣␣␣␣␣␣␣Assume␣M_R␣includes␣90%%␣of␣uns\
    cattered␣reflectance\n");
fprintf (*stdout*, "␣␣iad␣-C␣0.8␣file.rxt␣␣␣␣␣␣␣Assume␣M_T␣includes␣80%%␣of␣uns\
    cattered␣transmittance\n");
fprintf (*stdout*, "␣␣iad␣-e␣0.0001␣file.rxt␣␣␣␣Better␣convergence␣to␣R␣&␣T␣values\n");
fprintf (*stdout*,
    "␣␣iad␣-f␣1.0␣file.rxt␣␣␣␣␣␣␣All␣light␣hits␣reflectance␣sphere␣wall␣first\n");
fprintf (*stdout*, "␣␣iad␣-o␣out␣file.rxt␣␣␣␣␣␣␣Calculated␣values␣in␣out\n");
fprintf (*stdout*, "␣␣iad␣-r␣0.3␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣R_total=0.3,␣b=inf,␣find␣albedo\n");
fprintf (*stdout*, "␣␣iad␣-r␣0.3␣-t␣0.4␣␣␣␣␣␣␣␣␣R_total=0.3,␣T_total=0.4,␣find␣a,b,g\n");
fprintf (*stdout*, "␣␣iad␣-r␣0.3␣-t␣0.4␣-n␣1.5␣␣R_total=0.3,␣T_total=0.4,␣n=1.5,␣find␣a,b\n");
fprintf (*stdout*, "␣␣iad␣-r␣0.3␣-t␣0.4␣␣␣␣␣␣␣␣␣R_total=0.3,␣T_total=0.4,␣find␣a,b\n");
fprintf (*stdout*, "␣␣iad␣-p␣1000␣file.rxt␣␣␣␣␣␣Only␣1000␣photons\n");
fprintf (*stdout*, "␣␣iad␣-p␣-100␣file.rxt␣␣␣␣␣␣Allow␣only␣100ms␣per␣iteration\n");
fprintf (*stdout*, "␣␣iad␣-q␣4␣file.rxt␣␣␣␣␣␣␣␣␣Four␣quadrature␣points\n");
fprintf (*stdout*, "␣␣iad␣-M␣0␣file.rxt␣␣␣␣␣␣␣␣␣No␣MC␣␣␣␣␣(iad)\n");
fprintf (*stdout*, "␣␣iad␣-M␣1␣file.rxt␣␣␣␣␣␣␣␣␣MC␣once␣␣(iad->␣MC␣->␣iad)\n");
fprintf (*stdout*, "␣␣iad␣-M␣2␣file.rxt␣␣␣␣␣␣␣␣␣MC␣twice␣(iad->␣MC␣->␣iad␣->␣MC␣->␣iad)\n");
fprintf (*stdout*, "␣␣iad␣-M␣0␣-q␣4␣file.rxt␣␣␣␣Fast␣and␣crude␣conversion\n");
fprintf (*stdout*,
    "␣␣iad␣-G␣t␣file.rxt␣␣␣␣␣␣␣␣␣␣One␣top␣slide␣with␣properties␣from␣file.rxt\n");
fprintf (*stdout*,
    "␣␣iad␣-G␣b␣-N␣1.5␣-D␣1␣file␣Use␣1␣bottom␣slide␣with␣n=1.5␣and␣thickness=1\n");
fprintf (*stdout*, "␣␣iad␣-x␣␣␣1␣file.rxt␣␣␣␣␣␣␣Show␣sphere␣and␣MC␣effects\n");
fprintf (*stdout*, "␣␣iad␣-x␣␣␣2␣file.rxt␣␣␣␣␣␣␣Show␣grid␣decisions\n");
fprintf (*stdout*, "␣␣iad␣-x␣␣␣4␣file.rxt␣␣␣␣␣␣␣Show␣interations\n");
fprintf (*stdout*, "␣␣iad␣-x␣␣␣8␣file.rxt␣␣␣␣␣␣␣Show␣lost␣light␣effects\n");
fprintf (*stdout*, "␣␣iad␣-x␣16␣file.rxt␣␣␣␣␣␣␣Show␣best␣grid␣points\n");
fprintf (*stdout*, "␣␣iad␣-x␣32␣file.rxt␣␣␣␣␣␣␣Show␣decisions␣for␣type␣of␣search\n");
fprintf (*stdout*, "␣␣iad␣-x␣64␣file.rxt␣␣␣␣␣␣␣Show␣all␣grid␣calculations\n");
fprintf (*stdout*, "␣␣iad␣-x␣128␣file.rxt␣␣␣␣␣␣␣DEBUG_EVERY_CALC\n");
fprintf (*stdout*, "␣␣iad␣-x␣255␣file.rxt␣␣␣␣␣␣␣Show␣all␣debugging␣output\n");
fprintf (*stdout*,
    "␣␣iad␣-X␣-i␣8␣file.rxt␣␣␣␣␣␣Dual␣beam␣spectrometer␣with␣8␣degree␣incidence\n\n");

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    fprintf (stdout ,
        "␣␣iad␣-z␣-a␣0.9␣-b␣1␣-i␣45␣␣Forward␣calc␣assuming␣45␣degree␣incidence\n\n");
    fprintf (stdout , "␣␣apply␣iad␣x.rxt␣y.rxt␣␣␣␣␣␣Process␣multiple␣files\n\n");
    fprintf (stdout , "Report␣bugs␣to␣<scott.prahl@oit.edu>\n\n");
  }
```

This code is used in section 2.

21.   Just figure out the damn scattering and absorption

⟨ calculate coefficients function 21 ⟩ ≡

```
  static void  Calculate_Mua_Musp(struct measure_type m, struct invert_type r, double
        *musp, double *mua )
  {
    if (r.b ≡ HUGE_VAL) {
      if (r.a ≤ 1 · 10⁻⁵) {
        *musp = 0.0;
        *mua = 1.0;
        return;
      }
      if (r.default_mus ≠ UNINITIALIZED) {
        *musp = r.default_mus * (1 − r.g);
        *mua = r.default_mus /r.a − r.default_mus;
        return;
      }
      if (r.default_mua ≠ UNINITIALIZED) {
        *musp = (r.default_mua /(1 − r.a) − r.default_mua ) * (1 − r.g);
        *mua = r.default_mua;
        return;
      }
      *musp = 1.0 − r.g;
      *mua = (1.0 − r.a)/r.a;
      return;
    }
    *musp = r.a * r.b/m.slab_thickness * (1.0 − r.g);
    *mua = (1 − r.a) * r.b/m.slab_thickness;
  }
```

See also section 22.

This code is used in section 2.

22.   This can only be called immediately after *Inverse_RT* You have been warned! Notice that *Calculate_Distance*█ does not pass any slab properties.

⟨ calculate coefficients function 21 ⟩ +≡

```
  static void calculate_coefficients(struct measure_type m, struct invert_type r, double *LR, double
        *LT, double *musp, double *mua )
  {
    double delta ;
    *LR = 0;
    *LT = 0;
    Calculate_Distance (LR, LT, &delta );
    Calculate_Mua_Musp (m, r, musp, mua );
  }
```

23. ⟨ print results header function 23 ⟩ ≡

 static void *print_results_header*(**FILE** *∗fp*)

 {

  if (*Debug*(DEBUG_LOST_LIGHT)) {

   fprintf(*fp*, "# |␣Meas␣␣␣␣␣␣M_R␣␣|␣Meas␣␣␣␣␣␣M_T␣␣|␣␣calc␣␣␣calc␣␣␣calc␣␣|");

   fprintf(*fp*, "␣␣Lost␣␣␣Lost␣␣␣Lost␣␣␣Lost␣␣|␣MC␣␣␣IAD␣␣Error\n");

   fprintf(*fp*, "#␣wave␣|␣␣M_R␣␣␣␣␣␣fit␣␣|␣␣M_T␣␣␣␣␣␣fit␣␣|␣␣mu_a␣␣␣mu_s'␣␣␣g␣␣␣␣|␣␣");

   fprintf(*fp*, "␣UR1␣␣␣␣URU␣␣␣␣UT1␣␣␣␣UTU␣␣|␣␣#␣␣␣␣␣#␣␣␣Type\n");

   fprintf(*fp*, "#␣␣nm␣␣|␣␣---␣␣␣␣␣␣---␣␣|␣␣---␣␣␣␣␣␣---␣␣|1/mm␣␣␣1/mm␣␣␣␣---␣␣|");

   fprintf(*fp*, "␣␣␣---␣␣␣␣---␣␣␣␣---␣␣␣␣---␣␣|␣---␣␣---␣␣---\n");

   fprintf(*fp*, "#--");

   fprintf(*fp*, "--\n");

  }

  else {

   fprintf(*fp*, "#␣␣␣␣␣\tMeasured␣\t␣␣␣M_R␣␣␣\tMeasured␣\t␣␣␣M_T␣␣␣\tEstimat\

    ed\tEstimated\tEstimated");

   if (*Debug*(DEBUG_LOST_LIGHT)) *fprintf*(*fp*, "\t␣␣Lost␣␣␣\t␣␣Lost␣␣␣\t␣␣Lost␣␣␣\t␣␣Lo\

    st␣␣␣\t␣␣␣MC␣␣␣␣\t␣␣␣IAD␣␣␣\t␣␣Error␣␣");

   fprintf(*fp*, "\n");

   fprintf(*fp*, "##wave\t␣␣␣M_R␣␣␣\t␣␣␣fit␣␣␣\t␣␣␣M_T␣␣␣\t␣␣␣fit␣␣␣\t␣␣mu_a␣\

    ␣␣\t␣␣mu_s'␣␣\t␣␣␣␣␣g␣␣␣␣");

   if (*Debug*(DEBUG_LOST_LIGHT)) *fprintf*(*fp*, "\t␣␣␣UR1␣␣␣\t␣␣␣URU␣␣␣\t␣␣␣UT1␣␣␣\t␣␣␣U\

    TU␣␣␣\t␣␣␣␣␣#␣␣␣␣␣\t␣␣␣␣␣#␣␣␣␣\t␣␣State␣␣");

   fprintf(*fp*, "\n");

   fprintf(*fp*, "#␣[nm]\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣1/mm␣\

    ␣␣\t␣␣1/mm␣␣␣\t␣␣[---]␣␣");

   if (*Debug*(DEBUG_LOST_LIGHT)) *fprintf*(*fp*, "\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣[-\

    --]␣␣\t␣␣[---]␣␣\t␣␣[---]␣␣\t␣␣[---]␣␣");

   fprintf(*fp*, "\n");

  }

 }

This code is used in section 2.

24.   When debugging lost light, it is handy to see how each iteration changes the calculated values for the optical properties. We do that here if we are debugging, otherwise we just print a number or something to keep the user from wondering what is going on.

⟨ Print results function 24 ⟩ ≡

  void *print_optical_property_result*(**FILE** *fp, **struct measure_type** *m*, **struct invert_type** *r*, **double**
        LR, **double** LT, **double** *mu_a*, **double** *mu_sp*, **int** *line*)

  {

    if (*Debug*(DEBUG_LOST_LIGHT)) {

      if (*m.lambda* ≠ 0) *fprintf*(*fp*, `"%6.1f␣␣␣"`, *m.lambda*);

      else *fprintf*(*fp*, `"%6d␣␣␣"`, *line*);

      if (*mu_a* ≥ 200) *mu_a* = 199.9999;

      if (*mu_sp* ≥ 1000) *mu_sp* = 999.9999;

      fprintf(*fp*, `"%6.4f␣%␣6.4f␣|␣"`, *m.m_r*, LR);

      fprintf(*fp*, `"%6.4f␣%␣6.4f␣|␣"`, *m.m_t*, LT);

      fprintf(*fp*, `"%6.3f␣"`, *mu_a*);

      fprintf(*fp*, `"%6.3f␣"`, *mu_sp*);

      fprintf(*fp*, `"%6.3f␣|"`, *r.g*);

      fprintf(*fp*, `"␣%6.4f␣%6.4f␣"`, *m.ur1_lost*, *m.uru_lost*);

      fprintf(*fp*, `"%6.4f␣%6.4f␣|␣"`, *m.ut1_lost*, *m.utu_lost*);

      fprintf(*fp*, `"%2d␣␣"`, *r.MC_iterations*);

      fprintf(*fp*, `"%3d"`, *r.AD_iterations*);

      fprintf(*fp*, `"␣␣␣␣%c␣\n"`, *what_char*(*r.error*));

    }

    else {

      if (*m.lambda* ≠ 0) *fprintf*(*fp*, `"%6.1f\t"`, *m.lambda*);

      else *fprintf*(*fp*, `"%6d\t"`, *line*);

      if (*mu_a* ≥ 200) *mu_a* = 199.9999;

      if (*mu_sp* ≥ 1000) *mu_sp* = 999.9999;

      fprintf(*fp*, `"%␣9.4f\t%␣9.4f\t"`, *m.m_r*, LR);

      fprintf(*fp*, `"%␣9.4f\t%␣9.4f\t"`, *m.m_t*, LT);

      fprintf(*fp*, `"%␣9.4f\t"`, *mu_a*);

      fprintf(*fp*, `"%␣9.4f\t"`, *mu_sp*);

      fprintf(*fp*, `"%␣9.4f\t"`, *r.g*);

      fprintf(*fp*, `"␣%c␣\n"`, *what_char*(*r.error*));

    }

    fflush(*fp*);

  }

This code is used in section 2.

25.   ⟨ print error legend function 25 ⟩ ≡
  static void *print_error_legend*(**void**)
  {
    if (*Debug*(DEBUG_ANY)) **return**;
    fprintf (*stderr*, "−−−−−−−−−−−−−−−−␣Sorry,␣but␣...␣errors␣encountered␣−−−−−−−−−−−−−−\n");
    fprintf (*stderr*, "␣␣␣*␣␣==>␣Success␣␣␣␣␣␣␣␣␣␣␣");
    fprintf (*stderr*, "␣␣0−9␣==>␣Monte␣Carlo␣Iteration\n");
    fprintf (*stderr*, "␣␣␣R␣␣==>␣M_R␣is␣too␣big␣␣␣");
    fprintf (*stderr*, "␣␣␣␣r␣␣==>␣M_R␣is␣too␣small\n");
    fprintf (*stderr*, "␣␣␣␣T␣␣==>␣M_T␣is␣too␣big␣␣␣");
    fprintf (*stderr*, "␣␣␣␣t␣␣==>␣M_T␣is␣too␣small\n");
    fprintf (*stderr*, "␣␣␣U␣␣==>␣M_U␣is␣too␣big␣␣␣");
    fprintf (*stderr*, "␣␣␣␣u␣␣==>␣M_U␣is␣too␣small\n");
    fprintf (*stderr*, "␣␣␣␣!␣␣==>␣M_R␣+␣M_T␣>␣1␣␣␣␣");
    fprintf (*stderr*, "␣␣␣␣+␣␣==>␣Did␣not␣converge\n\n");
  }

This code is used in section 2.

26.   returns a new string consisting of s+t

⟨ stringdup together function 26 ⟩ ≡
  static char ∗*strdup_together*(**char** ∗*s*, **char** ∗*t*)
  {
    char ∗*both*;
    if (*s* ≡ Λ) {
      if (*t* ≡ Λ) **return** Λ;
      return *strdup*(*t*);
    }
    if (*t* ≡ Λ) **return** *strdup*(*s*);
    both = *malloc*(*strlen*(*s*) + *strlen*(*t*) + 1);
    if (*both* ≡ Λ) *fprintf* (*stderr*, "Could␣not␣allocate␣memory␣for␣both␣strings.\n");
    strcpy(*both*, *s*);
    strcat(*both*, *t*);
    return *both*;
  }

This code is used in section 2.

27.   catch parsing errors in strtod

⟨ mystrtod function 27 ⟩ ≡
  static double my_strtod(**const char** $*str$)
  {
    char $*endptr$;
    $errno = 0$;
    double $val = strtod(str, \&endptr)$;
    if $(endptr \equiv str)$ {   /∗ No digits were found ∗/
      $fprintf(stderr, \texttt{"Error␣in␣command-line\textbackslash n"})$;
      $fprintf(stderr, \texttt{"␣␣␣␣␣No␣conversion␣could␣be␣performed␣for␣`\%s`.\textbackslash n"}, str)$;
      $exit(\texttt{EXIT\_FAILURE})$;
    }
    if $(*endptr \neq \texttt{'\textbackslash 0'})$ {   /∗ String contains extra characters after the number ∗/
      $fprintf(stderr, \texttt{"Error␣in␣command-line\textbackslash n"})$;
      $fprintf(stderr, \texttt{"␣␣␣␣␣Partial␣conversion␣of␣string␣=␣'\%s'\textbackslash n"}, str)$;
      $exit(\texttt{EXIT\_FAILURE})$;
    }
    if $(errno \equiv \texttt{ERANGE})$ {
      /∗ The converted value is out of range of representable values by a double ∗/
      $fprintf(stderr, \texttt{"Error␣in␣command-line\textbackslash n"})$;
      $printf(\texttt{"␣␣␣␣␣The␣value␣'\%s'␣is␣out␣of␣range␣of␣double.\textbackslash n"}, str)$;
      $exit(\texttt{EXIT\_FAILURE})$;
    }
    return val;
  }

This code is used in section 2.

28.   assume that start time has already been set

⟨ seconds elapsed function 28 ⟩ ≡
  static double $seconds\_elapsed$(**clock_t** $start\_time$)
  {
    clock_t $finish\_time = clock()$;
    return (**double**)$(finish\_time - start\_time)/\texttt{CLOCKS\_PER\_SEC}$;
  }

This code is used in section 2.

29.   given a string and an array, this fills the array with numbers from the string. The numbers should be separated by spaces.

Returns 0 upon successfully filling n entries, returns 1 for any error.

⟨ parse string into array function 29 ⟩ ≡
  static int *parse_string_into_array*(**char** *s, **double** *a, **int** n)
  {
    char *t, *last, *r;
    int i = 0;

    t = s;
    last = s + strlen(s);
    while (t < last) {   /* a space should mark the end of number */
      r = t;
      while (*r ≠ '␣' ∧ *r ≠ '\0') r++;
      r = '\0';   / parse the number and save it */
      if (sscanf(t, "%lf", &(a[i])) ≡ 0) **return** 1;
      i++;   /* are we done ? */
      if (i ≡ n) {
        if (a[i − 1] ≤ 0 ∨ a[i − 1] > 1) {
          fprintf(stderr,
            "Sphere␣wall␣reflectivity␣(r_w=%g)␣must␣be␣a␣fraction␣less␣than␣one.\n",
            a[i − 1]);
          exit(EXIT_FAILURE);
        }
        return 0;
      }   /* move pointer just after last number */
      t = r + 1;
    }
    return 1;
  }

This code is used in section 2.

30.   ⟨ what_char function 30 ⟩ ≡
  static char *what_char*(**int** err)
  {
    if (err ≡ IAD_NO_ERROR) **return** '*';
    if (err ≡ IAD_TOO_MANY_ITERATIONS) **return** '+';
    if (err ≡ IAD_MR_TOO_BIG) **return** 'R';
    if (err ≡ IAD_MR_TOO_SMALL) **return** 'r';
    if (err ≡ IAD_MT_TOO_BIG) **return** 'T';
    if (err ≡ IAD_MT_TOO_SMALL) **return** 't';
    if (err ≡ IAD_MU_TOO_BIG) **return** 'U';
    if (err ≡ IAD_MU_TOO_SMALL) **return** 'u';
    if (err ≡ IAD_TOO_MUCH_LIGHT) **return** '!';
    return '?';
  }

This code is used in section 2.

31. ⟨ print long error function 31 ⟩ ≡
  static void $print\_long\_error$(**int** err)
  {
    if ($err \equiv$ `IAD_TOO_MANY_ITERATIONS`) $fprintf$($stderr$, "Failed␣Search,␣too␣many␣iterations\n");
    if ($err \equiv$ `IAD_MR_TOO_BIG`) $fprintf$($stderr$, "Failed␣Search,␣M_R␣is␣too␣big\n");
    if ($err \equiv$ `IAD_MR_TOO_SMALL`) $fprintf$($stderr$, "Failed␣Search,␣M_R␣is␣too␣small\n");
    if ($err \equiv$ `IAD_MT_TOO_BIG`) $fprintf$($stderr$, "Failed␣Search,␣M_T␣is␣too␣big\n");
    if ($err \equiv$ `IAD_MT_TOO_SMALL`) $fprintf$($stderr$, "Failed␣Search,␣M_T␣is␣too␣small\n");
    if ($err \equiv$ `IAD_MU_TOO_BIG`) $fprintf$($stderr$, "Failed␣Search,␣M_U␣is␣too␣big\n");
    if ($err \equiv$ `IAD_MU_TOO_SMALL`) $fprintf$($stderr$, "Failed␣Search,␣M_U␣is␣too␣snall\n");
    if ($err \equiv$ `IAD_TOO_MUCH_LIGHT`) $fprintf$($stderr$, "Failed␣Search,␣Total␣light␣bigger␣than␣1\n");
    $fprintf$($stderr$, "\n");
  }

This code is used in section 2.

32.   The idea here is to show some intermediate output while a file is being processed.

⟨ print dot function 32 ⟩ ≡
  static void $print\_dot$(**clock_t** $start\_time$, **int** err, **int** $points$, **int** $final$, **int** $verbosity$)
  {
    static int $counter = 0$;
    $counter$ ++;
    if ($verbosity \equiv 0 \lor Debug$(`DEBUG_ANY`)) **return**;
    if ($final$) $fprintf$($stderr$, "%c", $what\_char$(err));
    else {
      $counter$ −−;
      $fprintf$($stderr$, "%1d\b", $points$ % 10);
    }
    if ($final$) {
      if ($counter$ % 50 $\equiv$ 0) {
        double $rate = ($seconds_elapsed$($start_time$)/$counter$);
        $fprintf$($stderr$, "␣␣%3d␣done␣(%5.2f␣s/pt)\n", $counter$, $rate$);
      }
      else if ($counter$ % 10 $\equiv$ 0) $fprintf$($stderr$, "␣");
    }
    $fflush$($stderr$);
  }

This code is used in section 2.

33.   Simple command-line shell program.

Here is a quick skeleton that I put together to show how the inverse adding-doubling code works. I have only cursorily tested this. If you find obvious bugs, they are probably real but should not extend beyond this code snippet.

All the output for this web file goes into `iad_main.c`

⟨ `iad_main_mus.c`   33 ⟩ ≡

  ⟨ Include files for *main* 3 ⟩

  int *main*(**int** *argc*, **char** **argv)

  {

    ⟨ Declare variables for *main* 4 ⟩

    if (*Read_Header*(&*m*, &*r*) ≡ `TRUE`) {

      ⟨ Process the header 36 ⟩

      m.num_measures = 2;

      m.m_r = 0.0;

      m.slab_thickness = 0.1;

      while (*fp* ≠ `EOF`) {

        fp = *scanf*("%lf␣%lf␣%lf␣%lf", &*lambda*, &*r.mu_a*, &*m.default_g*, &*m.m_t*);

        fp = *readln*(&*line*);

        ⟨ Calculate and write optical properties 11 ⟩

      }

    }

    exit(`EXIT_SUCCESS`);

  }

34.   ⟨ Include files for *main* 3 ⟩ +≡

#include <stdio.h>

#include <string.h>

#include <stdlib.h>

#include "ad_globl.h"

#include "iad_type.h"

#include "iad_pub.h"

#include "iad_io.h"

35.   ⟨ Declare variables for *main* 4 ⟩ +≡

  struct measure_type *m*;

  struct invert_type *r*;

  int *lines*;

  char *format1 = "␣␣␣␣R␣␣␣␣\t␣␣␣␣T␣␣␣␣\t␣␣␣␣Tc␣␣␣␣\t␣␣␣␣␣a␣␣␣␣\t␣␣␣␣␣b␣␣␣␣\t␣\
    ␣␣␣␣g␣␣␣␣\t␣␣␣␣␣!/?\n";

  char *format2 = "␣%9.5f\t␣%9.5f\t␣%9.5f\t␣%9.5f\t␣%9.5f\t␣%9.5f\t␣%9c\n";

  char *found* = '?';

  int *fp*;

  double *lambda*;

  int *line* = 1;

36.   ⟨ Process the header 36 ⟩ ≡

  m.slab_thickness = 1;

  Initialize_Result(*m*, &*r*);

  Write_Header(*m*, *r*);

  lines = 1;

  printf(*format1*, *m.m_r*, *m.m_t*, *m.m_u*, *r.a*, *r.b*, *r.g*);

This code is used in section 33.

37.   ⟨ Calculate and write optical properties 11 ⟩ +≡

 {

  $r.search = FIND\_mus$;

  $Inverse\_RT(m, \&r)$;

  if $(r.found \equiv \texttt{TRUE})$ $found = $ '!';

  else $found = $ '?';

  $printf(format2, m.m\_r, m.m\_t, m.m\_u, r.a, r.b, r.g, found)$;

  $fflush(stdout)$;

 }

38. IAD Types.   This file has no routines. It is responsible for creating the header file `iad_type.h` and nothing else.

⟨ `iad_type.h` 38 ⟩ ≡
#undef `FALSE`
#undef `TRUE`
  ⟨ Preprocessor definitions ⟩
  ⟨ Structs to export from IAD Types 41 ⟩

39.
#define `FIND_A` 0
#define `FIND_B` 1
#define `FIND_AB` 2
#define `FIND_AG` 3
#define `FIND_AUTO` 4
#define `FIND_BG` 5
#define $FIND\_BaG$ 6
#define $FIND\_BsG$ 7
#define $FIND\_Ba$ 8
#define $FIND\_Bs$ 9
#define `FIND_G` 10
#define `FIND_B_WITH_NO_ABSORPTION` 11
#define `FIND_B_WITH_NO_SCATTERING` 12
#define `RELATIVE` 0
#define `ABSOLUTE` 1
#define `COLLIMATED` 0
#define `DIFFUSE` 1
#define `FALSE` 0
#define `TRUE` 1
#define `IAD_MAX_ITERATIONS` 500

40.   Need error codes for this silly program

#**define** IAD_NO_ERROR 0
#**define** IAD_TOO_MANY_ITERATIONS 1
#**define** IAD_AS_NOT_VALID 16
#**define** IAD_AE_NOT_VALID 17
#**define** IAD_AD_NOT_VALID 18
#**define** IAD_RW_NOT_VALID 19
#**define** IAD_RD_NOT_VALID 20
#**define** IAD_RSTD_NOT_VALID 21
#**define** IAD_GAMMA_NOT_VALID 22
#**define** IAD_F_NOT_VALID 23
#**define** IAD_BAD_PHASE_FUNCTION 24
#**define** IAD_QUAD_PTS_NOT_VALID 25
#**define** IAD_BAD_G_VALUE 26
#**define** IAD_TOO_MANY_LAYERS 27
#**define** IAD_MEMORY_ERROR 28
#**define** IAD_FILE_ERROR 29
#**define** IAD_EXCESSIVE_LIGHT_LOSS 30
#**define** IAD_RT_LT_MINIMUM 31
#**define** IAD_MR_TOO_SMALL 32
#**define** IAD_MR_TOO_BIG 33
#**define** IAD_MT_TOO_SMALL 34
#**define** IAD_MT_TOO_BIG 35
#**define** IAD_MU_TOO_SMALL 36
#**define** IAD_MU_TOO_BIG 37
#**define** IAD_TOO_MUCH_LIGHT 38
#**define** IAD_TSTD_NOT_VALID 39
#**define** UNINITIALIZED -99
#**define** DEBUG_A_LITTLE 1
#**define** DEBUG_GRID 2
#**define** DEBUG_ITERATIONS 4
#**define** DEBUG_LOST_LIGHT 8
#**define** DEBUG_BEST_GUESS 16
#**define** DEBUG_SEARCH 32
#**define** DEBUG_GRID_CALC 64
#**define** DEBUG_EVERY_CALC 128
#**define** DEBUG_ANY #FFFFFFFF
#**define** UNKNOWN 0
#**define** COMPARISON 1
#**define** SUBSTITUTION 2

41.   The idea of the structure **measure_type** is collect all the information regarding a single measurement together in one spot. No information regarding how the inversion procedure is supposed to be done is contained in this structure, unlike in previous incarnations of this program.

⟨ Structs to export from IAD Types 41 ⟩ ≡

  typedef struct measure_type {
    double $slab\_index$;
    double $slab\_thickness$;
    double $slab\_top\_slide\_index$;
    double $slab\_top\_slide\_b$;
    double $slab\_top\_slide\_thickness$;
    double $slab\_bottom\_slide\_index$;
    double $slab\_bottom\_slide\_b$;
    double $slab\_bottom\_slide\_thickness$;
    double $slab\_cos\_angle$;
    int $num\_spheres$;
    int $num\_measures$;
    int $method$;
    int $flip\_sample$;
    int $baffle\_r$, $baffle\_t$;
    double d_beam;
    double $fraction\_of\_rc\_in\_mr$;
    double $fraction\_of\_tc\_in\_mt$;
    double m_r, m_t, m_u;
    double $lambda$;
    double as_r, ad_r, ae_r, aw_r, rd_r, rw_r, $rstd\_r$, f_r;
    double as_t, ad_t, ae_t, aw_t, rd_t, rw_t, $rstd\_t$;
    double $ur1\_lost$, uru_lost, $ut1\_lost$, utu_lost;
    double d_sphere_r, d_sphere_t;
  } **IAD_measure_type**;

See also sections 42 and 43.

This code is used in section 38.

42.   This describes how the inversion process should proceed and also contains the results of that inversion process.

⟨ Structs to export from IAD Types 41 ⟩ +≡

  typedef struct invert_type {

    double *a*;   /∗ the calculated albedo ∗/

    double *b*;   /∗ the calculated optical depth ∗/

    double *g*;   /∗ the calculated anisotropy ∗/

    int *found*;

    int *search*;

    int *metric*;

    double *tolerance*;

    double *MC_tolerance*;

    double *final_distance*;

    int *error*;

    struct AD_slab_type *slab*;

    struct *AD_method_type method*;

    int *AD_iterations*;

    int *MC_iterations*;

    double *default_a*;

    double *default_b*;

    double *default_g*;

    double *default_ba*;

    double *default_bs*;

    double *default_mua*;

    double *default_mus*;

  } **IAD_invert_type**;

43.   A few types that used to be enum's are now int's.

⟨ Structs to export from IAD Types 41 ⟩ +≡

  typedef int search_type;

  typedef int boolean_type;

  typedef int illumination_type;

  typedef struct guess_t {

    double *distance*;

    double *a*;

    double *b*;

    double *g*;

  } **guess_type**;

  extern double FRACTION;

44.   IAD Public.

This contains the routine *Inverse_RT* that should generally be the basic entry point into this whole mess. Call this routine with the proper values and true happiness is bound to be yours.

Altered accuracy of the standard method of root finding from 0.001 to 0.00001. Note, it really doesn't help to change the method from `ABSOLUTE` to `RELATIVE`, but I did anyway. (3/3/95)

⟨ `iad_pub.c`   44 ⟩ ≡
#include `<stdio.h>`
#include `<math.h>`
#include `"nr_util.h"`
#include `"ad_globl.h"`
#include `"ad_frsnl.h"`
#include `"iad_type.h"`
#include `"iad_util.h"`
#include `"iad_calc.h"`
#include `"iad_find.h"`
#include `"iad_pub.h"`
#include `"iad_io.h"`
#include `"stdlib.h"`
#include `"mc_lost.h"`
  ⟨ Definition for *Inverse_RT* 48 ⟩
  ⟨ Definition for *measure_OK* 54 ⟩
  ⟨ Definition for *determine_search* 61 ⟩
  ⟨ Definition for *Initialize_Result* 65 ⟩
  ⟨ Definition for *Initialize_Measure* 73 ⟩
  ⟨ Definition for *ez_Inverse_RT* 71 ⟩
  ⟨ Definition for *Spheres_Inverse_RT* 75 ⟩
  ⟨ Definition for *Spheres_Inverse_RT2* 88 ⟩
  ⟨ Definition for *Calculate_MR_MT* 82 ⟩
  ⟨ Definition for *MinMax_MR_MT* 86 ⟩
  ⟨ Definition for *Calculate_Minimum_MR* 84 ⟩

45.   All the information that needs to be written to the header file `iad_pub.h`. This eliminates the need to maintain a set of header files as well.

⟨ `iad_pub.h`   45 ⟩ ≡
  ⟨ Prototype for *Inverse_RT* 47 ⟩;
  ⟨ Prototype for *measure_OK* 53 ⟩;
  ⟨ Prototype for *determine_search* 60 ⟩;
  ⟨ Prototype for *Initialize_Result* 64 ⟩;
  ⟨ Prototype for *ez_Inverse_RT* 70 ⟩;
  ⟨ Prototype for *Initialize_Measure* 72 ⟩;
  ⟨ Prototype for *Calculate_MR_MT* 81 ⟩;
  ⟨ Prototype for *MinMax_MR_MT* 85 ⟩;
  ⟨ Prototype for *Calculate_Minimum_MR* 83 ⟩;
  ⟨ Prototype for *Spheres_Inverse_RT2* 87 ⟩;

46.   Here is the header file needed to access one interesting routine in the `libiad.so` library.

⟨ `lib_iad.h`   46 ⟩ ≡
  ⟨ Prototype for *ez_Inverse_RT* 70 ⟩;
  ⟨ Prototype for *Spheres_Inverse_RT* 74 ⟩;
  ⟨ Prototype for *Spheres_Inverse_RT2* 87 ⟩;

47. Inverse RT.   *Inverse_RT* is the main function in this whole package. You pass the variable m containing your experimentally measured values to the function *Inverse_RT*. It hopefully returns the optical properties in r that are appropriate for your experiment.

$\langle$ Prototype for *Inverse_RT* 47 $\rangle \equiv$
   void *Inverse_RT* (**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 45 and 48.

48. $\langle$ Definition for *Inverse_RT* 48 $\rangle \equiv$
  $\langle$ Prototype for *Inverse_RT* 47 $\rangle$
  {
    $r{\rightarrow}found$ = FALSE;
    if ($r{\rightarrow}search \equiv$ FIND_AUTO) $r{\rightarrow}search = determine\_search(m, *r)$;
    if ($r{\rightarrow}search \equiv$ FIND_B_WITH_NO_ABSORPTION) {
      $r{\rightarrow}default\_a = 1$;
      $r{\rightarrow}search$ = FIND_B;
    }
    if ($r{\rightarrow}search \equiv$ FIND_B_WITH_NO_SCATTERING) {
      $r{\rightarrow}default\_a = 0$;
      $r{\rightarrow}search$ = FIND_B;
    }
    $\langle$ Exit with bad input data 49 $\rangle$
    $\langle$ Find the optical properties 50 $\rangle$
    $\langle$ Print basic sphere and MC effects 51 $\rangle$
    if ($r{\rightarrow}final\_distance \leq r{\rightarrow}tolerance$) $r{\rightarrow}found$ = TRUE;
  }

This code is used in section 44.

49.   There is no sense going to all the trouble to try a multivariable minimization if the input data is bogus. So I wrote a single routine *measure_OK* to do just this.

$\langle$ Exit with bad input data 49 $\rangle \equiv$
  $r{\rightarrow}error = measure\_OK(m, *r)$;
  if ($r{\rightarrow}method.quad\_pts < 4$) $r{\rightarrow}error$ = IAD_QUAD_PTS_NOT_VALID;
  if ($r{\rightarrow}error \neq$ IAD_NO_ERROR) **return**;

This code is used in section 48.

50.   Now I fob the real work off to the unconstrained minimization routines. Ultimately, I would like to replace all these by constrained minimization routines. Actually the first five already are constrained. The real work will be improving the last five because these are 2-D minimization routines.

⟨ Find the optical properties 50 ⟩ ≡
  if (*Debug*(DEBUG_ITERATIONS)) {
    fprintf (*stderr*, "−−−−−−−−−−−−−−−␣Beginning␣New␣Search␣−−−−−−−−−−−−−−−−\n");
    fprintf (*stderr*, "␣␣␣␣␣␣␣␣␣␣␣␣");
    fprintf (*stderr*, "␣␣␣␣␣␣␣a␣␣␣␣␣␣␣␣␣␣b␣␣␣␣␣␣␣␣␣␣␣g␣␣␣|");
    fprintf (*stderr*, "␣␣␣␣␣M_R␣␣␣␣␣␣␣␣␣calc␣␣␣|");
    fprintf (*stderr*, "␣␣␣␣␣M_T␣␣␣␣␣␣␣␣␣calc␣␣␣|");
    if (*r*→*metric* ≡ RELATIVE) *fprintf* (*stderr*, "␣relative␣distance\n");
    else *fprintf* (*stderr*, "␣absolute␣distance\n");
  }
  switch (*r*→*search*) {
  case FIND_A: *U_Find_A*(*m*, *r*);
    break;
  case FIND_B: *U_Find_B*(*m*, *r*);
    break;
  case FIND_G: *U_Find_G*(*m*, *r*);
    break;
  case *FIND_Ba*: *U_Find_Ba*(*m*, *r*);
    break;
  case *FIND_Bs*: *U_Find_Bs*(*m*, *r*);
    break;
  case FIND_AB: *U_Find_AB*(*m*, *r*);
    break;
  case FIND_AG: *U_Find_AG*(*m*, *r*);
    break;
  case FIND_BG: *U_Find_BG*(*m*, *r*);
    break;
  case *FIND_BsG*: *U_Find_BsG*(*m*, *r*);
    break;
  case *FIND_BaG*: *U_Find_BaG*(*m*, *r*);
    break;
  }
  if (*Debug*(DEBUG_ITERATIONS))
    fprintf (*stderr*, "Final␣amoeba␣result␣after␣AD_iterations␣=␣%d\n", *r*→*AD_iterations*);
  if (*r*→*AD_iterations* ≥ IAD_MAX_ITERATIONS) *r*→*error* = IAD_TOO_MANY_ITERATIONS;
This code is used in section 48.

51.   This is to support -x 1

⟨ Print basic sphere and MC effects 51 ⟩ ≡

  if (*Debug*(DEBUG_A_LITTLE)) {

    double M_R, M_T;

    fprintf (*stderr*, "AD␣iterations=␣%3d␣␣␣MC␣iterations=%3d", *r→AD_iterations*, *r→MC_iterations*);

    fprintf (*stderr*, "␣␣␣␣␣␣␣␣␣␣␣␣␣a=%6.4f␣b=%8.4f␣g=%6.4f\n", *r→slab.a*, *r→slab.b*, *r→slab.g*);

    fprintf (*stderr*, "␣␣␣␣␣M_R␣loss␣␣␣␣␣␣%8.5f␣␣M_T␣loss␣␣␣␣␣␣%8.5f", *m.ur1_lost*, *m.ut1_lost*);

    if (*r→MC_iterations* ≡ 0) *fprintf* (*stderr*, "␣(␣no␣MC␣calculation␣yet)\n");

    else *fprintf* (*stderr*, "␣(␣MC␣loss␣calculation)\n");

    Calculate_MR_MT (*m*, *∗r*, FALSE, FALSE, &M_R, &M_T);

    fprintf (*stderr*, "␣␣␣␣␣M_R␣bare␣␣␣␣␣␣%8.5f␣␣M_T␣bare␣␣␣␣␣␣%8.5f", M_R, M_T);

    fprintf (*stderr*, "␣(␣−−−␣MC␣loss,␣−−−␣sphere␣effects)\n");

    Calculate_MR_MT (*m*, *∗r*, FALSE, TRUE, &M_R, &M_T);

    fprintf (*stderr*, "␣␣␣␣␣M_R␣sphere␣␣␣%8.5f␣␣M_T␣sphere␣␣␣%8.5f", M_R, M_T);

    fprintf (*stderr*, "␣(␣−−−␣MC␣loss,␣+++␣sphere␣effects)\n");

    Calculate_MR_MT (*m*, *∗r*, TRUE, FALSE, &M_R, &M_T);

    fprintf (*stderr*, "␣␣␣␣␣M_R␣mc␣␣␣␣␣␣␣␣%8.5f␣␣M_T␣mc␣␣␣␣␣␣␣␣%8.5f", M_R, M_T);

    fprintf (*stderr*, "␣(␣+++␣MC␣loss,␣−−−␣sphere␣effects)\n");

    Calculate_MR_MT (*m*, *∗r*, TRUE, TRUE, &M_R, &M_T);

    fprintf (*stderr*, "␣␣␣␣␣M_R␣both␣␣␣␣␣␣%8.5f␣␣M_T␣both␣␣␣␣␣␣%8.5f", M_R, M_T);

    fprintf (*stderr*, "␣(␣+++␣MC␣loss,␣+++␣sphere␣effects)\n");

    fprintf (*stderr*, "␣␣␣␣␣M_R␣measured␣%8.5f␣␣M_T␣measured␣%8.5f", *m.m_r*, *m.m_t*);

    fprintf (*stderr*, "␣(␣␣target␣values)\n\n");

  }

This code is used in section 48.

52. Validation.

53.   Now the question is — just what is bad data? Here's the prototype.

⟨ Prototype for *measure_OK* 53 ⟩ ≡
    int *measure_OK* (**struct measure_type** *m*, **struct invert_type** *r*)

This code is used in sections 45 and 54.

54.   It would just be nice to stop computing with bad data. This does not work in practice because it turns out that there is often bogus data in a full wavelength scan. Often the reflectance is too low for short wavelengths and at long wavelengths the detector (photomultiplier tube) does not work worth a damn.

   The two sphere checks are more complicated. For example, we can no longer categorically state that the transmittance is less than one or that the sum of the reflectance and transmittance is less than one. Instead we use the transmittance to bound the values for the reflectance — see the routine *MinMax_MR_MT* below.

⟨ Definition for *measure_OK* 54 ⟩ ≡
    ⟨ Prototype for *measure_OK* 53 ⟩
    {
        double *ru*, *tu*;
        if (*m.num_spheres* ≠ 2) {
            ⟨ Check MT for zero or one spheres 56 ⟩
            ⟨ Check MR for zero or one spheres 55 ⟩
        }
        else {
            int *error* = *MinMax_MR_MT* (*m*, *r*);
            if (*error* ≠ IAD_NO_ERROR) **return** *error*;
        }
        ⟨ Check MU 57 ⟩
        if (*m.num_spheres* ≠ 0) {
            ⟨ Check sphere parameters 58 ⟩
        }
        return IAD_NO_ERROR;
    }

This code is used in section 44.

55. The reflectance is constrained by the index of refraction of the material and the transmission. The upper bound for the reflectance is just one minus the transmittance. The specular (unscattered) reflectance from the boundaries imposes minimum for the reflectance. Obviously, the reflected light cannot be less than that from the first boundary. This might be calculated by assuming an infinite layer thickness. But we can do better.

There is a definite bound on the minimum reflectance from a sample. If you have a sample with a given transmittance m_t, the minimum reflectance possible is found by assuming that the sample does not scatter any light.

Knowledge of the indicies of refraction makes it a relatively simple matter to determine the optical thickness $b = mu\_a * d$ of the slab. The minimum reflection is obtained by including all the specular reflectances from all the surfaces.

If the default albedo has been specified as zero, then there is really no need to check MR because it is ignored.

$\langle$ Check MR for zero or one spheres $55\,\rangle \equiv$

```
{
  double mr, mt;
  Calculate_Minimum_MR(m, r, &mr, &mt);
    /* one parameter search only needs one good measurement */
  if (r.search ≡ FIND_A ∨ r.search ≡ FIND_G ∨ r.search ≡ FIND_B ∨ r.search ≡ FIND_Bs ∨ r.search ≡
        FIND_Ba) {
    if (m.m_r < mr ∧ m.m_t ≤ 0) return IAD_MR_TOO_SMALL;
  }
  else {
    if (r.default_a ≡ UNINITIALIZED ∨ r.default_a > 0) {
      if (m.m_r < mr) return IAD_MR_TOO_SMALL;
    }
  }
}
```

This code is used in section 54.

56. The transmittance is also constrained by the index of refraction of the material. The minimum transmittance is zero, but the maximum transmittance cannot exceed the total light passing through the sample when there is no scattering or absorption. This is calculated by assuming an infinitely thin (to eliminate any scattering or absorption effects).

There is a problem when spheres are present. The estimated values for the transmittance using Sp_mu_RT are not actually limiting cases. This will require a bit of fixing, but for now that test is omitted if the number of spheres is more than zero.

$\langle$ Check MT for zero or one spheres $56\,\rangle \equiv$

```
if (m.m_t < 0) return IAD_MT_TOO_SMALL;
Sp_mu_RT_Flip(m.flip_sample, r.slab.n_top_slide, r.slab.n_slab, r.slab.n_bottom_slide, r.slab.b_top_slide, 0,
      r.slab.b_bottom_slide, r.slab.cos_angle, &ru, &tu);
if (m.num_spheres ≡ 0 ∧ m.m_t > tu) {
  fprintf(stderr, "ntop=%7.5f,␣nslab=%7.5f,␣nbottom=%7.5f\n", r.slab.n_top_slide, r.slab.n_slab,
        r.slab.n_bottom_slide);
  fprintf(stderr, "tu_max=%7.5f,␣m_t=%7.5f,␣t_std=%7.5f\n", tu, m.m_t, m.rstd_t);
  return IAD_MT_TOO_BIG;
}
```

This code is used in section 54.

57.   The unscattered transmission is now always included in the total transmittance. Therefore the unscattered transmittance must fall betwee zero and `M_T`

⟨ Check MU 57 ⟩ ≡
    if $(m.m\_u < 0)$ **return** `IAD_MU_TOO_SMALL`;
    if $(m.m\_t > 0 \wedge m.m\_u > m.m\_t)$ **return** `IAD_MU_TOO_BIG`;

This code is used in section 54.

58.   Make sure that reflection sphere parameters are reasonable

⟨ Check sphere parameters 58 ⟩ ≡
    if $(m.as\_r < 0 \vee m.as\_r \geq 0.2)$ **return** `IAD_AS_NOT_VALID`;
    if $(m.ad\_r < 0 \vee m.ad\_r \geq 0.2)$ **return** `IAD_AD_NOT_VALID`;
    if $(m.ae\_r < 0 \vee m.ae\_r \geq 0.2)$ **return** `IAD_AE_NOT_VALID`;
    if $(m.rw\_r < 0 \vee m.rw\_r > 1.0)$ **return** `IAD_RW_NOT_VALID`;
    if $(m.rd\_r < 0 \vee m.rd\_r > 1.0)$ **return** `IAD_RD_NOT_VALID`;
    if $(m.rstd\_r < 0 \vee m.rstd\_r > 1.0)$ **return** `IAD_RSTD_NOT_VALID`;
    if $(m.rstd\_t < 0 \vee m.rstd\_t > 1.0)$ **return** `IAD_TSTD_NOT_VALID`;
    if $(m.f\_r < 0 \vee m.f\_r > 1)$ **return** `IAD_F_NOT_VALID`;

See also section 59.

This code is used in section 54.

59.   Make sure that transmission sphere parameters are reasonable

⟨ Check sphere parameters 58 ⟩ +≡
    if $(m.as\_t < 0 \vee m.as\_t \geq 0.2)$ **return** `IAD_AS_NOT_VALID`;
    if $(m.ad\_t < 0 \vee m.ad\_t \geq 0.2)$ **return** `IAD_AD_NOT_VALID`;
    if $(m.ae\_t < 0 \vee m.ae\_t \geq 0.2)$ **return** `IAD_AE_NOT_VALID`;
    if $(m.rw\_t < 0 \vee m.rw\_r > 1.0)$ **return** `IAD_RW_NOT_VALID`;
    if $(m.rd\_t < 0 \vee m.rd\_t > 1.0)$ **return** `IAD_RD_NOT_VALID`;
    if $(m.rstd\_t < 0 \vee m.rstd\_t > 1.0)$ **return** `IAD_TSTD_NOT_VALID`;

60.   Searching Method.

The original idea was that this routine would automatically determine what optical parameters could be figured out from the input data. This worked fine for a long while, but I discovered that often it was convenient to constrain the optical properties in various ways. Consequently, this routine got more and more complicated.

What should be done is to figure out whether the search will be 1D or 2D and split this routine into two parts.

It would be nice to enable the user to constrain two parameters, but the infrastructure is missing at this point.

⟨ Prototype for *determine_search* 60 ⟩ ≡
  search_type *determine_search*(**struct measure_type** *m*, **struct invert_type** *r*)

This code is used in sections 45 and 61.

61.   This routine is responsible for selecting the appropriate optical properties to determine.

⟨ Definition for *determine_search* 61 ⟩ ≡
  ⟨ Prototype for *determine_search* 60 ⟩
  {
    double rt, tt, rd, td, tc, rc;
    int $search = 0$;
    int $independent = m.num\_measures$;
    if ($Debug$(DEBUG_SEARCH)) {
      $fprintf$($stderr$, "SEARCH:␣starting␣with␣%d␣measurement(s)\n", $m.num\_measures$);
      $fprintf$($stderr$, "SEARCH:␣m_r␣=␣%8.5f␣", $m.m\_r$);
      $fprintf$($stderr$, "m_t␣=␣%8.5f␣", $m.m\_t$);
      $fprintf$($stderr$, "m_u␣=␣%8.5f\n", $m.m\_u$);
    }
    $Estimate\_RT$(m, r, &rt, &tt, &rd, &rc, &td, &tc);
    if ($m.m\_u \equiv 0 \wedge independent \equiv 3$) {
      if ($Debug$(DEBUG_SEARCH)) $fprintf$($stderr$, "SEARCH:␣no␣information␣in␣tc\n");
      $independent$ −−;
    }
    if ($rd \equiv 0 \wedge independent \geq 2$) {
      if ($Debug$(DEBUG_SEARCH)) $fprintf$($stderr$, "SEARCH:␣no␣information␣in␣rd\n");
      $independent$ −−;
    }
    if ($td \equiv 0 \wedge independent \geq 2$) {
      if ($Debug$(DEBUG_SEARCH)) $fprintf$($stderr$, "SEARCH:␣no␣information␣in␣td\n");
      $independent$ −−;
    }
    if ($independent \equiv 1 \vee independent \equiv -1$) {
      ⟨ One parameter search 62 ⟩
    }
    else if ($independent \equiv 2$) {
      ⟨ Two parameter search 63 ⟩
    }   /∗ three real parameters with information! ∗/
    else {
      $search = $ FIND_AG;
    }
    if ($search \equiv$ FIND_BG $\wedge m.m\_u > 0$) $search = $ FIND_G;
    if ($Debug$(DEBUG_SEARCH)) {
      $fprintf$($stderr$, "SEARCH:␣ending␣with␣%d␣measurement(s)\n", $m.num\_measures$);
      $fprintf$($stderr$, "SEARCH:␣final␣choice␣for␣search␣=␣");
      if ($search \equiv$ FIND_A) $fprintf$($stderr$, "FIND_A\n");
      if ($search \equiv$ FIND_B) $fprintf$($stderr$, "FIND_B\n");
      if ($search \equiv$ FIND_AB) $fprintf$($stderr$, "FIND_AB\n");
      if ($search \equiv$ FIND_AG) $fprintf$($stderr$, "FIND_AG\n");
      if ($search \equiv$ FIND_AUTO) $fprintf$($stderr$, "FIND_AUTO\n");
      if ($search \equiv$ FIND_BG) $fprintf$($stderr$, "FIND_BG\n");
      if ($search \equiv FIND\_BaG$) $fprintf$($stderr$, "FIND_BaG\n");
      if ($search \equiv FIND\_BsG$) $fprintf$($stderr$, "FIND_BsG\n");
      if ($search \equiv FIND\_Ba$) $fprintf$($stderr$, "FIND_Ba\n");
      if ($search \equiv FIND\_Bs$) $fprintf$($stderr$, "FIND_Bs\n");
      if ($search \equiv$ FIND_G) $fprintf$($stderr$, "FIND_G\n");
      if ($search \equiv$ FIND_B_WITH_NO_ABSORPTION) $fprintf$($stderr$, "FIND_B_WITH_NO_ABSORPTION\n");
      if ($search \equiv$ FIND_B_WITH_NO_SCATTERING) $fprintf$($stderr$, "FIND_B_WITH_NO_SCATTERING\n");

```
    }
    return search;
  }
```
This code is used in section 44.

62. The fastest inverse problems are those in which just one measurement is known. This corresponds to a simple one-dimensional minimization problem. The only complexity is deciding exactly what should be allowed to vary. The basic assumption is that the anisotropy has been specified or will be assumed to be zero.

  If the anistropy is assumed known, then one other assumption will allow us to figure out the last parameter to solve for.

  Ultimately, if no default values are given, then we look at the value of the total transmittance. If this is zero, then we assume that the optical thickness is infinite and solve for the albedo. Otherwise we will just make a stab at solving for the optical thickness assuming the albedo is one.

⟨One parameter search 62⟩ ≡

```
  if (r.default_a ≠ UNINITIALIZED) {
    if (r.default_a ≡ 0) search = FIND_B_WITH_NO_SCATTERING;
    else if (r.default_a ≡ 1) search = FIND_B_WITH_NO_ABSORPTION;
    else if (tt ≡ 0) search = FIND_G;
    else search = FIND_B;
  }
  else if (r.default_b ≠ UNINITIALIZED) search = FIND_A;
  else if (r.default_bs ≠ UNINITIALIZED) search = FIND_Ba;
  else if (r.default_ba ≠ UNINITIALIZED) search = FIND_Bs;
  else if (td ≡ 0) search = FIND_A;
  else if (rd ≡ 0) search = FIND_B_WITH_NO_SCATTERING;
  else search = FIND_B_WITH_NO_ABSORPTION;
```
This code is used in section 61.

63.   If the absorption depth $\mu_a d$ is constrained return *FIND_BsG*. Recall that I use the bizarre mnemonic $bs = \mu_s d$ here and so this means that the program will search over various values of $\mu_s d$ and g.

   If there are just two measurements then I assume that the anisotropy is not of interest and the only thing to calculate is the reduced albedo and optical thickness based on an assumed anisotropy.

⟨ Two parameter search 63 ⟩ ≡
  if $(r.default\_a \neq$ UNINITIALIZED$)$ {
    if $(r.default\_a \equiv 0)$ *search* = FIND_B;
    else if $(r.default\_g \neq$ UNINITIALIZED$)$ *search* = FIND_B;
    else *search* = FIND_BG;
  }
  else if $(r.default\_b \neq$ UNINITIALIZED$)$ {
    if $(r.default\_g \neq$ UNINITIALIZED$)$ *search* = FIND_A;
    else *search* = FIND_AG;
  }
  else if $(r.default\_ba \neq$ UNINITIALIZED$)$ {
    if $(r.default\_g \neq$ UNINITIALIZED$)$ *search* = *FIND_Bs*;
    else *search* = *FIND_BsG*;
  }
  else if $(r.default\_bs \neq$ UNINITIALIZED$)$ {
    if $(r.default\_g \neq$ UNINITIALIZED$)$ *search* = *FIND_Ba*;
    else *search* = *FIND_BaG*;
  }
  else if $(rt + tt > 1 \wedge 0 \wedge m.num\_spheres \neq 2)$ *search* = FIND_B_WITH_NO_ABSORPTION;
  else *search* = FIND_AB;
This code is used in section 61.

64.   This little routine just stuffs reasonable values into the structure we use to return the solution. This does not replace the values for *r.default_g* nor for *r.method.quad_pts*. Presumably these have been set correctly elsewhere.

⟨ Prototype for *Initialize_Result* 64 ⟩ ≡
  void *Initialize_Result*(**struct measure_type** m, **struct invert_type** $*r$)
This code is used in sections 45 and 65.

65.   ⟨ Definition for *Initialize_Result* 65 ⟩ ≡
  ⟨ Prototype for *Initialize_Result* 64 ⟩
  {
    ⟨ Fill r with reasonable values 66 ⟩
  }
This code is used in section 44.

66.   Start with the optical properties.

⟨ Fill r with reasonable values 66 ⟩ ≡
  $r{\to}a = 0.0$;
  $r{\to}b = 0.0$;
  $r{\to}g = 0.0$;
See also sections 67, 68, and 69.
This code is used in section 65.

67.   Continue with other useful stuff.

⟨ Fill r with reasonable values 66 ⟩ +≡
  r→$found$ = FALSE;
  r→$tolerance$ = 0.0001;
  r→$MC\_tolerance$ = 0.01;   /∗ percent ∗/
  r→$search$ = FIND_AUTO;
  r→$metric$ = RELATIVE;
  r→$final\_distance$ = 10;
  r→$AD\_iterations$ = 0;
  r→$MC\_iterations$ = 0;
  r→$error$ = IAD_NO_ERROR;

68.   The defaults might be handy

⟨ Fill r with reasonable values 66 ⟩ +≡
  r→$default\_a$ = UNINITIALIZED;
  r→$default\_b$ = UNINITIALIZED;
  r→$default\_g$ = UNINITIALIZED;
  r→$default\_ba$ = UNINITIALIZED;
  r→$default\_bs$ = UNINITIALIZED;
  r→$default\_mua$ = UNINITIALIZED;
  r→$default\_mus$ = UNINITIALIZED;

69.   It is necessary to set up the slab correctly so, I stuff reasonable values into this record as well.

⟨ Fill r with reasonable values 66 ⟩ +≡
  r→$slab.a$ = 0.5;
  r→$slab.b$ = 1.0;
  r→$slab.g$ = 0;
  r→$slab.phase\_function$ = HENYEY_GREENSTEIN;
  r→$slab.n\_slab$ = $m.slab\_index$;
  r→$slab.n\_top\_slide$ = $m.slab\_top\_slide\_index$;
  r→$slab.n\_bottom\_slide$ = $m.slab\_bottom\_slide\_index$;
  r→$slab.b\_top\_slide$ = $m.slab\_top\_slide\_b$;
  r→$slab.b\_bottom\_slide$ = $m.slab\_bottom\_slide\_b$;
  r→$slab.cos\_angle$ = $m.slab\_cos\_angle$;
  r→$method.a\_calc$ = 0.5;
  r→$method.b\_calc$ = 1;
  r→$method.g\_calc$ = 0.5;
  r→$method.quad\_pts$ = 8;
  r→$method.b\_thinnest$ = 1.0/32.0;

70.   EZ Inverse RT.   *ez_Inverse_RT* is a simple interface to the main function *Inverse_RT* in this package. It eliminates the need for complicated data structures so that the command line interface (as well as those to Perl and Mathematica) will be simpler. This function assumes that the reflection and transmission include specular reflection and that the transmission also include unscattered transmission.

Other assumptions are that the top and bottom slides have the same index of refraction, that the illumination is collimated. Of course no sphere parameters are included.

⟨ Prototype for *ez_Inverse_RT* 70 ⟩ ≡
   void *ez_Inverse_RT* (**double** *n*, **double** *nslide*, **double** UR1, **double** UT1, **double** *Tc*, **double** *∗a*, **double**
      ∗b, **double** *∗g*, **int** *∗error*)

This code is used in sections 45, 46, and 71.

71.   ⟨ Definition for *ez_Inverse_RT* 71 ⟩ ≡
  ⟨ Prototype for *ez_Inverse_RT* 70 ⟩
  {
    struct measure_type *m*;
    struct invert_type *r*;
    ∗a = 0;
    ∗b = HUGE_VAL;
    ∗g = 0;
    Initialize_Measure (&*m*);
    m.slab_index = *n*;
    m.slab_top_slide_index = *nslide*;
    m.slab_bottom_slide_index = *nslide*;
    m.slab_cos_angle = 1.0;
    m.num_measures = 3;
    if (UT1 ≡ 0) *m.num_measures* −−;
    if (*Tc* ≡ 0) *m.num_measures* −−;
    m.m_r = UR1;
    m.m_t = UT1;
    m.m_u = *Tc*;
    Initialize_Result (*m*, &*r*);
    r.method.quad_pts = 8;
    Inverse_RT (*m*, &*r*);
    ∗error = *r.error*;
    if (*r.error* ≡ IAD_NO_ERROR) {
      ∗a = *r.a*;
      ∗b = *r.b*;
      ∗g = *r.g*;
    }
  }

This code is used in section 44.

72.   ⟨ Prototype for *Initialize_Measure* 72 ⟩ ≡
  void *Initialize_Measure* (**struct measure_type** *∗m*)

This code is used in sections 45 and 73.

73.   ⟨ Definition for *Initialize_Measure* 73 ⟩ ≡
  ⟨ Prototype for *Initialize_Measure* 72 ⟩
  {
    double *default_sphere_d* = 8.0 ∗ 25.4;
    double *default_sample_d* = 0.0 ∗ 25.4;
    double *default_detector_d* = 0.1 ∗ 25.4;
    double *default_entrance_d* = 0.5 ∗ 25.4;
    double *sphere_area* = M_PI ∗ *default_sphere_d* ∗ *default_sphere_d*;

    m⃗slab_index = 1.0;
    m⃗slab_top_slide_index = 1.0;
    m⃗slab_top_slide_b = 0.0;
    m⃗slab_top_slide_thickness = 0.0;
    m⃗slab_bottom_slide_index = 1.0;
    m⃗slab_bottom_slide_b = 0.0;
    m⃗slab_bottom_slide_thickness = 0.0;
    m⃗slab_thickness = 1.0;
    m⃗slab_cos_angle = 1.0;
    m⃗num_spheres = 0;
    m⃗num_measures = 1;
    m⃗method = UNKNOWN;
    m⃗fraction_of_rc_in_mr = 1.0;
    m⃗fraction_of_tc_in_mt = 1.0;
    m⃗baffle_r = 1;
    m⃗baffle_t = 1;
    m⃗flip_sample = 0;
    m⃗m_r = 0.0;
    m⃗m_t = 0.0;
    m⃗m_u = 0.0;
    m⃗d_sphere_r = *default_sphere_d*;
    m⃗as_r = (M_PI ∗ *default_sample_d* ∗ *default_sample_d*/4.0)/*sphere_area*;
    m⃗ad_r = (M_PI ∗ *default_detector_d* ∗ *default_detector_d*/4.0)/*sphere_area*;
    m⃗ae_r = (M_PI ∗ *default_entrance_d* ∗ *default_entrance_d*/4.0)/*sphere_area*;
    m⃗aw_r = 1.0 − *m⃗as_r* − *m⃗ad_r* − *m⃗ae_r*;
    m⃗rd_r = 0.0;
    m⃗rw_r = 1.0;
    m⃗rstd_r = 1.0;
    m⃗f_r = 0.0;
    m⃗d_sphere_t = *default_sphere_d*;
    m⃗as_t = *m⃗as_r*;
    m⃗ad_t = *m⃗ad_r*;
    m⃗ae_t = 0;
    m⃗aw_t = 1.0 − *m⃗as_t* − *m⃗ad_t* − *m⃗ae_t*;
    m⃗rd_t = 0.0;
    m⃗rw_t = 1.0;
    m⃗rstd_t = 1.0;
    m⃗lambda = 0.0;
    m⃗d_beam = 0.0;
    m⃗ur1_lost = 0;
    m⃗uru_lost = 0;
    m⃗ut1_lost = 0;
    m⃗utu_lost = 0;
  }

This code is used in section 44.

74. To avoid interfacing with C-structures it is necessary to pass the information as arrays. Here I have divided the experiment into (1) setup, (2) reflection sphere coefficients, (3) transmission sphere coefficients, (4) measurements, and (5) results.

⟨Prototype for *Spheres_Inverse_RT* 74⟩ ≡
   void *Spheres_Inverse_RT* (**double** *∗setup*, **double** *∗analysis*, **double** *∗sphere_r*, **double** *∗sphere_t*, **double**
      ∗measurements, **double** *∗results*)

This code is used in sections 46 and 75.

75. ⟨Definition for *Spheres_Inverse_RT* 75⟩ ≡
  ⟨Prototype for *Spheres_Inverse_RT* 74⟩
  {
    struct measure_type *m*;
    struct invert_type *r*;
    long *num_photons*;
    double *ur1*, *ut1*, *uru*, *utu*;
    int *i*, *mc_runs* = 1;

    Initialize_Measure (&*m*);
    ⟨handle setup 76⟩
    ⟨handle reflection sphere 79⟩
    ⟨handle transmission sphere 80⟩
    ⟨handle measurement 78⟩
    Initialize_Result (*m*, &*r*);
    results [0] = 0;
    results [1] = 0;
    results [2] = 0;
    ⟨handle analysis 77⟩
    Inverse_RT (*m*, &*r*);
    for (*i* = 0; *i* < *mc_runs*; *i*++) {
      MC_Lost (*m*, *r*, *num_photons*, &*ur1*, &*ut1*, &*uru*, &*utu*, &*m.ur1_lost*, &*m.ut1_lost*, &*m.uru_lost*,
        &*m.utu_lost*);
      Inverse_RT (*m*, &*r*);
    }
    if (*r.error* ≡ `IAD_NO_ERROR`) {
      results [0] = (1 − *r.a*) ∗ *r.b*/*m.slab_thickness*;
      results [1] = (*r.a*) ∗ *r.b*/*m.slab_thickness*;
      results [2] = *r.g*;
    }
    results [3] = *r.error*;
  }

This code is used in section 44.

76.   These are in exactly the same order as the parameters in the .rxt header

⟨ handle setup 76 ⟩ ≡
  {
     double d_sample_r, $d\_entrance\_r$, $d\_detector\_r$;
     double d_sample_t, $d\_entrance\_t$, $d\_detector\_t$;

     $m.slab\_index = setup[0]$;
     $m.slab\_top\_slide\_index = setup[1]$;
     $m.slab\_thickness = setup[2]$;
     $m.slab\_top\_slide\_thickness = setup[3]$;
     $m.d\_beam = setup[4]$;
     $m.rstd\_r = setup[5]$;
     $m.num\_spheres = (\textbf{int})\,setup[6]$;
     $m.d\_sphere\_r = setup[7]$;
     $d\_sample\_r = setup[8]$;
     $d\_entrance\_r = setup[9]$;
     $d\_detector\_r = setup[10]$;
     $m.rw\_r = setup[11]$;
     $m.d\_sphere\_t = setup[12]$;
     $d\_sample\_t = setup[13]$;
     $d\_entrance\_t = setup[14]$;
     $d\_detector\_t = setup[15]$;
     $m.rw\_t = setup[16]$;
     $r.default\_g = setup[17]$;
     $num\_photons = (\textbf{long})\,setup[18]$;
     $m.as\_r = (d\_sample\_r / m.d\_sphere\_r / 2.0) * (d\_sample\_r / m.d\_sphere\_r / 2.0)$;
     $m.ae\_r = (d\_entrance\_r / m.d\_sphere\_r / 2.0) * (d\_entrance\_r / m.d\_sphere\_r / 2.0)$;
     $m.ad\_r = (d\_detector\_r / m.d\_sphere\_r / 2.0) * (d\_detector\_r / m.d\_sphere\_r / 2.0)$;
     $m.aw\_r = 1.0 - m.as\_r - m.ae\_r - m.ad\_r$;
     $m.as\_t = (d\_sample\_t / m.d\_sphere\_t / 2.0) * (d\_sample\_t / m.d\_sphere\_t / 2.0)$;
     $m.ae\_t = (d\_entrance\_t / m.d\_sphere\_t / 2.0) * (d\_entrance\_t / m.d\_sphere\_t / 2.0)$;
     $m.ad\_t = (d\_detector\_t / m.d\_sphere\_t / 2.0) * (d\_detector\_t / m.d\_sphere\_t / 2.0)$;
     $m.aw\_t = 1.0 - m.as\_t - m.ae\_t - m.ad\_t$;
     $m.slab\_bottom\_slide\_index = m.slab\_top\_slide\_index$;
     $m.slab\_bottom\_slide\_thickness = m.slab\_top\_slide\_thickness$;
     $fprintf(stderr, \texttt{"****}_\sqcup\texttt{executing}_\sqcup\texttt{FIXME}_\sqcup\texttt{****/n"})$;
     $m.slab\_cos\_angle = 1.0$;   /∗ FIXME ∗/
  }

This code is used in section 75.

77.   ⟨ handle analysis 77 ⟩ ≡
  $r.method.quad\_pts = (\textbf{int})\,analysis[0]$;
  $mc\_runs = (\textbf{int})\,analysis[1]$;
This code is used in section 75.

78.

⟨ handle measurement 78 ⟩ ≡
  $m.m\_r = measurements[0]$;
  $m.m\_t = measurements[1]$;
  $m.m\_u = measurements[2]$;
  $m.num\_measures = 3$;
  if $(m.m\_t \equiv 0)$ $m.num\_measures--$;
  if $(m.m\_u \equiv 0)$ $m.num\_measures--$;
This code is used in section 75.

79.

⟨ handle reflection sphere 79 ⟩ ≡
  $m.as\_r = sphere\_r[0]$;
  $m.ae\_r = sphere\_r[1]$;
  $m.ad\_r = sphere\_r[2]$;
  $m.rw\_r = sphere\_r[3]$;
  $m.rd\_r = sphere\_r[4]$;
  $m.rstd\_r = sphere\_r[5]$;
  $m.f\_r = sphere\_r[7]$;
This code is used in section 75.

80.

⟨ handle transmission sphere 80 ⟩ ≡
  $m.as\_t = sphere\_t[0]$;
  $m.ae\_t = sphere\_t[1]$;
  $m.ad\_t = sphere\_t[2]$;
  $m.rw\_t = sphere\_t[3]$;
  $m.rd\_t = sphere\_t[4]$;
  $m.rstd\_t = sphere\_t[5]$;
This code is used in section 75.

81.   I needed a routine that would calculate the values of M_R and M_T without doing the whole inversion process. It seems odd that this does not exist yet.

The values for the lost light $m.uru\_lost$ etc., should be calculated before calling this routine.

⟨ Prototype for $Calculate\_MR\_MT$ 81 ⟩ ≡
  void $Calculate\_MR\_MT$(**struct measure_type** m, **struct invert_type** r, **int** $include\_MC$, **int**
      $include\_spheres$, **double** ∗M_R, **double** ∗M_T)
This code is used in sections 45 and 82.

82. ⟨Definition for *Calculate_MR_MT* 82⟩ ≡
⟨Prototype for *Calculate_MR_MT* 81⟩
{
  double *distance*;
  struct measure_type *old_mm*;
  struct invert_type *old_rr*;
  if (¬*include_MC*) {
    m.ur1_lost = 0;
    m.ut1_lost = 0;
    m.uru_lost = 0;
    m.utu_lost = 0;
  }
  if (¬*include_spheres*) {
    m.num_spheres = 0;
  }
  Get_Calc_State(&*old_mm*, &*old_rr*);
  Set_Calc_State(*m*, *r*);
  Calculate_Distance(M_R, M_T, &*distance*);
  Set_Calc_State(*old_mm*, *old_rr*);
}

This code is used in section 44.

83. So, it turns out that the minimum measured M_R can be less than four percent for black glass! This is because the sphere efficiency is much worse for the glass than for the white standard.

⟨Prototype for *Calculate_Minimum_MR* 83⟩ ≡
  void *Calculate_Minimum_MR*(**struct measure_type** *m*, **struct invert_type** *r*, **double** *∗mr*, **double**
      ∗mt)

This code is used in sections 45 and 84.

84. ⟨Definition for *Calculate_Minimum_MR* 84⟩ ≡
⟨Prototype for *Calculate_Minimum_MR* 83⟩
{
  if (*m.m_u* > 0) *r.slab.b* = *What_Is_B*(*r.slab*, *m.m_u*);
  else if (*r.default_b* ≠ UNINITIALIZED) *r.slab.b* = *r.default_b*;
  else *r.slab.b* = HUGE_VAL;
  r.slab.a = 0;
  if (*r.default_g* ≡ UNINITIALIZED) *r.slab.g* = 0.0;
  else *r.slab.g* = *r.default_g*;
  r.a = *r.slab.a*;
  r.b = *r.slab.b*;
  r.g = *r.slab.g*;
  Calculate_MR_MT(*m*, *r*, FALSE, TRUE, *mr*, *mt*);
}

This code is used in section 44.

85.   The minimum possible value of `MR` for a given `MT` will be when the albedo is zero and the maximum value will be when the albedo is one. In the first case there will be no light loss and in the second we will assume that any light loss is neglible (to maximize `MR`).

   The second case is perhaps over-simplified. Obviously for a fixed thickness as the albedo increases, the reflectance will increase. So how does $U\_Find\_B(\,)$ work when the albedo is set to 1?

   The problem is that to calculate these values one must know the optical thickness. Fortunately with the recent addition of constrained minimization, we can do exactly this.

   The only thing that remains is to sort out the light lost effect.

⟨ Prototype for $MinMax\_MR\_MT$ 85 ⟩ ≡
   int $MinMax\_MR\_MT$(**struct measure_type** m, **struct invert_type** r)

This code is used in sections 45 and 86.

86.   ⟨ Definition for $MinMax\_MR\_MT$ 86 ⟩ ≡
   ⟨ Prototype for $MinMax\_MR\_MT$ 85 ⟩
   {
       double $distance$, $measured\_m\_r$, $min\_possible\_m\_r$, $max\_possible\_m\_r$, $temp\_m\_t$;

       if $(m.m\_r < 0)$ **return** `IAD_MR_TOO_SMALL`;
       if $(m.m\_r * m.rstd\_r > 1)$ **return** `IAD_MR_TOO_BIG`;
       if $(m.m\_t < 0)$ **return** `IAD_MT_TOO_SMALL`;
       if $(m.m\_t \equiv 0)$ **return** `IAD_NO_ERROR`;
       $measured\_m\_r = m.m\_r$;
       $m.m\_r = 0$;
       $r.search = $ `FIND_B`;
       if $(Debug(\text{DEBUG\_ITERATIONS}))$
          $fprintf(stderr, \texttt{"Determining\_minimum\_possible\_M\_R\_for\_given\_M\_T\textbackslash n"})$;
       $r.default\_a = 0$;
       $U\_Find\_B(m, \&r)$;
       $Calculate\_Distance(\&min\_possible\_m\_r, \&temp\_m\_t, \&distance)$;
       if $(measured\_m\_r < min\_possible\_m\_r)$ **return** `IAD_MR_TOO_SMALL`;
       if $(Debug(\text{DEBUG\_ITERATIONS}))$
          $fprintf(stderr, \texttt{"Determining\_maximum\_possible\_M\_R\_for\_given\_M\_T\textbackslash n"})$;
       $r.default\_a = 1.0$;
       $U\_Find\_B(m, \&r)$;
       $Calculate\_Distance(\&max\_possible\_m\_r, \&temp\_m\_t, \&distance)$;
       if $(measured\_m\_r > max\_possible\_m\_r)$ **return** `IAD_MR_TOO_BIG`;
       return `IAD_NO_ERROR`;
   }

This code is used in section 44.

87.   ⟨ Prototype for $Spheres\_Inverse\_RT2$ 87 ⟩ ≡
   void $Spheres\_Inverse\_RT2$(**double** $*sample$, **double** $*illumination$, **double** $*sphere\_r$, **double** $*sphere\_t$, **double** $*analysis$, **double** $*measurement$, **double** $*a$, **double** $*b$, **double** $*g$)

This code is used in sections 45, 46, and 88.

88.   ⟨ Definition for *Spheres_Inverse_RT2* 88 ⟩ ≡
  ⟨ Prototype for *Spheres_Inverse_RT2* 87 ⟩
  {
    struct measure_type *m*;
    struct invert_type *r*;
    long *num_photons*;
    double *ur1*, *ut1*, *uru*, *utu*;
    int *i*, *mc_runs* = 1;
    Initialize_Measure(&*m*);
    ⟨ handle2 sample 89 ⟩
    ⟨ handle2 illumination 90 ⟩
    ⟨ handle2 reflection sphere 91 ⟩
    ⟨ handle2 transmission sphere 92 ⟩
    ⟨ handle2 analysis 93 ⟩
    ⟨ handle2 measurement 94 ⟩
    Initialize_Result(*m*, &*r*);
    Inverse_RT(*m*, &*r*);
    for (*i* = 0; *i* < *mc_runs*; *i*++) {
        MC_Lost(*m*, *r*, *num_photons*, &*ur1*, &*ut1*, &*uru*, &*utu*, &*m.ur1_lost*, &*m.ut1_lost*, &*m.uru_lost*,
            &*m.utu_lost*);
        Inverse_RT(*m*, &*r*);
    }
    if (*r.error* ≡ `IAD_NO_ERROR`) {
        ∗a = *r.a*;
        ∗b = *r.b*;
        ∗g = *r.g*;
    }
  }
This code is used in section 44.

89.   Just move the values from the sample array into the right places

⟨ handle2 sample 89 ⟩ ≡
  m.slab_index = *sample*[0];
  m.slab_top_slide_index = *sample*[1];
  m.slab_bottom_slide_index = *sample*[2];
  m.slab_thickness = *sample*[3];
  m.slab_top_slide_thickness = *sample*[4];
  m.slab_bottom_slide_thickness = *sample*[5];
  m.slab_top_slide_thickness = 0;
  m.slab_bottom_slide_thickness = 0;
This code is used in section 88.

90.   Just move the values from the illumination array into the right places. Need to spend time to figure
out how to integrate items 2, 3, and 4

⟨ handle2 illumination 90 ⟩ ≡
  m.d_beam = *illumination*[0];   /∗ m.lambda = illumination[1]; ∗/
    /∗ m.specular-reflection-excluded = illumination[2]; ∗/   /∗ m.direct-transmission-excluded =
        illumination[3]; ∗/   /∗ m.diffuse-illumination = illumination[4]; ∗/
  m.num_spheres = *illumination*[5];
This code is used in section 88.

91.

$\langle$ handle2 reflection sphere $91 \rangle \equiv$

  {

    double d_sample_r, $d\_entrance\_r$, $d\_detector\_r$;

    $m.d\_sphere\_r = sphere\_r[0]$;

    $d\_sample\_r = sphere\_r[1]$;

    $d\_entrance\_r = sphere\_r[2]$;

    $d\_detector\_r = sphere\_r[3]$;

    $m.rw\_r = sphere\_r[4]$;

    $m.rd\_r = sphere\_r[5]$;

    $m.as\_r = (d\_sample\_r/m.d\_sphere\_r/2.0) * (d\_sample\_r/m.d\_sphere\_r/2.0)$;

    $m.ae\_r = (d\_entrance\_r/m.d\_sphere\_r/2.0) * (d\_entrance\_r/m.d\_sphere\_r/2.0)$;

    $m.ad\_r = (d\_detector\_r/m.d\_sphere\_r/2.0) * (d\_detector\_r/m.d\_sphere\_r/2.0)$;

    $m.aw\_r = 1.0 - m.as\_r - m.ae\_r - m.ad\_r$;

  }

This code is used in section 88.

92.

$\langle$ handle2 transmission sphere $92 \rangle \equiv$

  {

    double d_sample_t, $d\_entrance\_t$, $d\_detector\_t$;

    $m.d\_sphere\_t = sphere\_t[0]$;

    $d\_sample\_t = sphere\_t[1]$;

    $d\_entrance\_t = sphere\_t[2]$;

    $d\_detector\_t = sphere\_t[3]$;

    $m.rw\_t = sphere\_t[4]$;

    $m.rd\_t = sphere\_t[5]$;

    $m.as\_t = (d\_sample\_t/m.d\_sphere\_t/2.0) * (d\_sample\_t/m.d\_sphere\_t/2.0)$;

    $m.ae\_t = (d\_entrance\_t/m.d\_sphere\_t/2.0) * (d\_entrance\_t/m.d\_sphere\_t/2.0)$;

    $m.ad\_t = (d\_detector\_t/m.d\_sphere\_t/2.0) * (d\_detector\_t/m.d\_sphere\_t/2.0)$;

    $m.aw\_t = 1.0 - m.as\_t - m.ae\_t - m.ad\_t$;

  }

This code is used in section 88.

93.

$\langle$ handle2 analysis $93 \rangle \equiv$

  $r.method.quad\_pts = (\textbf{int})\ analysis[0]$;

  $mc\_runs = (\textbf{int})\ analysis[1]$;

  $num\_photons = (\textbf{long})\ analysis[2]$;

This code is used in section 88.

94.

$\langle$ handle2 measurement $94 \rangle \equiv$

  $m.rstd\_r = measurement[0]$;

  $m.m\_r = measurement[1]$;

  $m.m\_t = measurement[2]$;

  $m.m\_u = measurement[3]$;

  $m.num\_measures = 3$;

  if $(m.m\_t \equiv 0)\ m.num\_measures\,{-}{-}$;

  if $(m.m\_u \equiv 0)\ m.num\_measures\,{-}{-}$;

This code is used in section 88.

95.   IAD Input Output.
   The special define below is to get Visual C to suppress silly warnings.

⟨ iad_io.c 95 ⟩ ≡
#**define** _CRT_SECURE_NO_WARNINGS
#**define** MAX_LINE_LENGTH 256
   char LINE_LEGEND[MAX_LINE_LENGTH] = "";
#**include** <string.h>
#**include** <stdio.h>
#**include** <stdlib.h>
#**include** <ctype.h>
#**include** <math.h>
#**include** "ad_globl.h"
#**include** "iad_type.h"
#**include** "iad_io.h"
#**include** "iad_pub.h"
#**include** "version.h"
   ⟨ Definition for *skip_white* 106 ⟩
   ⟨ Definition for *read_number* 108 ⟩
   ⟨ Definition for *check_magic* 110 ⟩
   ⟨ Definition for *remove_whitespace* 119 ⟩
   ⟨ Definition for *remove_comment* 120 ⟩
   ⟨ Definition for *remove_first_char* 121 ⟩
   ⟨ Definition for *Read_Data_Legend* 123 ⟩
   ⟨ Definition for *Read_Data_Line_Per_Legend* 104 ⟩
   ⟨ Definition for *Read_Header* 99 ⟩
   ⟨ Definition for *Write_Header* 112 ⟩
   ⟨ Definition for *Read_Data_Line* 103 ⟩

96.   ⟨ iad_io.h 96 ⟩ ≡
   ⟨ Prototype for *Read_Header* 98 ⟩;
   ⟨ Prototype for *Write_Header* 111 ⟩;
   ⟨ Prototype for *Read_Data_Line* 102 ⟩;

97.   Reading the file header.

98.   ⟨Prototype for *Read_Header* 98⟩ ≡
  int *Read_Header*(**FILE** *∗fp*, **struct measure_type** *∗m*, **int** *∗params*)

This code is used in sections 96 and 99.

99.   Pretty straightforward stuff. The only thing that needs to be commented on is that only one slide thickness/index is specified in the file. This must be applied to both the top and bottom slides. Finally, to specify no slide, then either setting the slide index to 1.0 or the thickness to 0.0 should do the trick.

⟨Definition for *Read_Header* 99⟩ ≡
  ⟨Prototype for *Read_Header* 98⟩
  {
    double *x*;

    Initialize_Measure(*m*);
    if (*check_magic*(*fp*)) **return** 1;
    if (*read_number*(*fp*, &*m*→*slab_index*)) **return** 1;
    if (*read_number*(*fp*, &*m*→*slab_top_slide_index*)) **return** 1;
    if (*read_number*(*fp*, &*m*→*slab_thickness*)) **return** 1;
    if (*read_number*(*fp*, &*m*→*slab_top_slide_thickness*)) **return** 1;
    if (*read_number*(*fp*, &*m*→*d_beam*)) **return** 1;
    if (*m*→*slab_top_slide_thickness* ≡ 0.0) *m*→*slab_top_slide_index* = 1.0;
    if (*m*→*slab_top_slide_index* ≡ 1.0) *m*→*slab_top_slide_thickness* = 0.0;
    if (*m*→*slab_top_slide_index* ≡ 0.0) {
      m→*slab_top_slide_thickness* = 0.0;
      m→*slab_top_slide_index* = 1.0;
    }
    m→*slab_bottom_slide_index* = *m*→*slab_top_slide_index*;
    m→*slab_bottom_slide_thickness* = *m*→*slab_top_slide_thickness*;
    if (*read_number*(*fp*, &*m*→*rstd_r*)) **return** 1;
    if (*read_number*(*fp*, &*x*)) **return** 1;
    m→*num_spheres* = (**int**) *x*;
    m→*method* = SUBSTITUTION;
    ⟨Read coefficients for reflection sphere 100⟩
    ⟨Read coefficients for transmission sphere 101⟩
    x = *Read_Data_Legend*(*fp*);
    ∗params = (**int**) *x*;
    m→*num_measures* = (*∗params* ≥ 3) ? 3 : *∗params*;
    return 0;
  }

This code is used in section 95.

100. ⟨ Read coefficients for reflection sphere 100 ⟩ ≡

  {

    double d_sample_r, d_empty_r, $d\_detector\_r$;

    if ($read\_number(fp, \&m \rightarrow d\_sphere\_r)$) **return** 1;
    if ($read\_number(fp, \& d\_sample\_r)$) **return** 1;
    if ($read\_number(fp, \& d\_empty\_r)$) **return** 1;
    if ($read\_number(fp, \& d\_detector\_r)$) **return** 1;
    if ($read\_number(fp, \&m \rightarrow rw\_r)$) **return** 1;
    $m \rightarrow as\_r = (d\_sample\_r / m \rightarrow d\_sphere\_r / 2.0) * (d\_sample\_r / m \rightarrow d\_sphere\_r / 2.0)$;
    $m \rightarrow ae\_r = (d\_empty\_r / m \rightarrow d\_sphere\_r / 2.0) * (d\_empty\_r / m \rightarrow d\_sphere\_r / 2.0)$;
    $m \rightarrow ad\_r = (d\_detector\_r / m \rightarrow d\_sphere\_r / 2.0) * (d\_detector\_r / m \rightarrow d\_sphere\_r / 2.0)$;
    $m \rightarrow aw\_r = 1.0 - m \rightarrow as\_r - m \rightarrow ae\_r - m \rightarrow ad\_r$;

  }

This code is used in section 99.

101. ⟨ Read coefficients for transmission sphere 101 ⟩ ≡

  {

    double d_sample_t, d_empty_t, $d\_detector\_t$;

    if ($read\_number(fp, \&m \rightarrow d\_sphere\_t)$) **return** 1;
    if ($read\_number(fp, \& d\_sample\_t)$) **return** 1;
    if ($read\_number(fp, \& d\_empty\_t)$) **return** 1;
    if ($read\_number(fp, \& d\_detector\_t)$) **return** 1;
    if ($read\_number(fp, \&m \rightarrow rw\_t)$) **return** 1;
    $m \rightarrow as\_t = (d\_sample\_t / m \rightarrow d\_sphere\_t / 2.0) * (d\_sample\_t / m \rightarrow d\_sphere\_t / 2.0)$;
    $m \rightarrow ae\_t = (d\_empty\_t / m \rightarrow d\_sphere\_t / 2.0) * (d\_empty\_t / m \rightarrow d\_sphere\_t / 2.0)$;
    $m \rightarrow ad\_t = (d\_detector\_t / m \rightarrow d\_sphere\_t / 2.0) * (d\_detector\_t / m \rightarrow d\_sphere\_t / 2.0)$;
    $m \rightarrow aw\_t = 1.0 - m \rightarrow as\_t - m \rightarrow ae\_t - m \rightarrow ad\_t$;

  }

This code is used in section 99.

102.   Reading just one line of a data file.

This reads a line of data based on the value of *params*.

If the first number is greater than one then it is assumed to be the wavelength and is ignored. test on the first value of the line.

A non-zero value is returned upon a failure.

⟨ Prototype for *Read_Data_Line* 102 ⟩ ≡

   int *Read_Data_Line*(**FILE** *∗fp*, **struct measure_type** *∗m*, **struct invert_type** *∗r*, **int** *params*)

This code is used in sections 96 and 103.

103.   ⟨ Definition for *Read_Data_Line* 103 ⟩ ≡

  ⟨ Prototype for *Read_Data_Line* 102 ⟩

  {

    if (*strlen*(LINE_LEGEND) > 0) **return** *Read_Data_Line_Per_Legend*(*fp*, *m*, *r*, *params*);

    if (*read_number*(*fp*, &*m*→*m_r*)) **return** 1;

    if (*m*→*m_r* > 1) {

      m→*lambda* = *m*→*m_r*;

      if (*read_number*(*fp*, &*m*→*m_r*)) **return** 1;

    }

    if (*params* ≡ −1) {

      m→*m_t* = *m*→*m_r*;

      m→*m_r* = 0;

      return 0;

    }

    if (*params* ≡ 1) **return** 0;

    if (*read_number*(*fp*, &*m*→*m_t*)) **return** 1;

    if (*params* ≡ 2) **return** 0;

    if (*read_number*(*fp*, &*m*→*m_u*)) **return** 1;

    if (*params* ≡ 3) **return** 0;

    if (*read_number*(*fp*, &*m*→*rw_r*)) **return** 1;

    m→*rw_t* = *m*→*rw_r*;

    if (*params* ≡ 4) **return** 0;

    if (*read_number*(*fp*, &*m*→*rw_t*)) **return** 1;

    if (*params* ≡ 5) **return** 0;

    if (*read_number*(*fp*, &*m*→*rstd_r*)) **return** 1;

    if (*params* ≡ 6) **return** 0;

    if (*read_number*(*fp*, &*m*→*rstd_t*)) **return** 1;

    return 0;

  }

This code is used in section 95.

104. ⟨ Definition for *Read_Data_Line_Per_Legend* 104 ⟩ ≡
  int *Read_Data_Line_Per_Legend*(**FILE** ∗*fp*, **struct measure_type** ∗*m*, **struct invert_type** ∗*r*, **int**
        params)
  {
    int *count* = 0;
    double *x*;
    while (*count* < *params*) {
      if (*read_number*(*fp*, &*x*)) **return** 1;
      char *c* = LINE_LEGEND[*count*];
      if (FALSE) *fprintf*(*stderr*, "count␣=␣%2d,␣option␣=␣%c,␣value␣=␣%10.5f\n", *count*, *c*, *x*);
      switch (*c*) {
      case 'a': *r*→*default_a* = *x*;
        break;
      case 'b': *r*→*default_b* = *x*;
        break;
      case 'B': *m*→*d_beam* = *x*;
        break;
      case 'c': *m*→*fraction_of_rc_in_mr* = *x*;
        break;
      case 'C': *m*→*fraction_of_tc_in_mt* = *x*;
        break;
      case 'd': *m*→*slab_thickness* = *x*;
        break;
      case 'D': *m*→*slab_top_slide_thickness* = *x*;
        m→*slab_bottom_slide_thickness* = *x*;
        break;
      case 'e': *r*→*tolerance* = *x*;
        r→*MC_tolerance* = *x*;
        break;
      case 'g': *r*→*default_g* = *x*;
        break;
      case 'L': *m*→*lambda* = *x*;
        break;
      case 'M': *m*→*num_spheres* = (**int**) *x*;
        break;
      case 'n': *m*→*slab_index* = *x*;
        break;
      case 'N': *m*→*slab_top_slide_index* = *x*;
        m→*slab_bottom_slide_index* = *x*;
        break;
      case 'q': *r*→*method*.*quad_pts* = (**int**) *x*;
        break;
      case 'r': *m*→*m_r* = *x*;
        break;
      case 'R': *m*→*rstd_r* = *x*;
        break;
      case 't': *m*→*m_t* = *x*;
        break;
      case 'S': *m*→*num_spheres* = (**int**) *x*;
        break;
      case 'T': *m*→*rstd_t* = *x*;

```
        break;
     case 'u': m→m_u = x;
        break;
     case 'w': m→rw_r = x;
        break;
     case 'W': m→rw_t = x;
        break;
     default: fprintf (stderr, "legend␣variable␣'%c'␣unimplemented", c);
        return 1;
     }
     count ++;
   }
   return 0;
}
```

This code is used in section 95.

105. Skip over white space and comments. It is assumed that # starts all comments and continues to the end of a line. This routine should work on files with nearly any line ending CR, LF, CRLF.

Failure is indicated by a non-zero return value.

⟨ Prototype for *skip_white* 105 ⟩ ≡
   int *skip_white* (**FILE** ∗*fp*)

This code is used in section 106.

106. ⟨ Definition for *skip_white* 106 ⟩ ≡
   ⟨ Prototype for *skip_white* 105 ⟩
   {
     int *c* = *fgetc* (*fp*);
     while (¬*feof* (*fp*)) {
        if (*isspace* (*c*)) *c* = *fgetc* (*fp*);
        else if (*c* ≡ '#') **do** *c* = *fgetc* (*fp*); **while** (¬*feof* (*fp*) ∧ *c* ≠ '\n' ∧ *c* ≠ '\r');
        else break;
     }
     if (*feof* (*fp*)) **return** 1;
     ungetc (*c*, *fp*);
     return 0;
   }

This code is used in section 95.

107. Read a single number. Return 0 if there are no problems, otherwise return 1.

⟨ Prototype for *read_number* 107 ⟩ ≡
   int *read_number* (**FILE** ∗*fp*, **double** ∗*x*)

This code is used in section 108.

108. ⟨ Definition for *read_number* 108 ⟩ ≡
   ⟨ Prototype for *read_number* 107 ⟩
   {
     if (*skip_white* (*fp*)) **return** 1;
     if (*fscanf* (*fp*, "%lf", *x*)) **return** 0;
     else return 1;
   }

This code is used in section 95.

109. Ensure that the data file is actually in the right form. Return 0 if the file has the right starting characters. Return 1 if on a failure.

⟨ Prototype for *check_magic* 109 ⟩ ≡
  int *check_magic*(**FILE** *∗fp*)

This code is used in section 110.

110. ⟨ Definition for *check_magic* 110 ⟩ ≡
  ⟨ Prototype for *check_magic* 109 ⟩
  {
    char *magic*[ ] = "IAD1";
    int *i, c*;
    for (*i* = 0; *i* < 4; *i*++) {
      c = *fgetc*(*fp*);
      if (*feof*(*fp*) ∨ *c* ≠ *magic*[*i*]) {
        fprintf(*stderr*, "Sorry,␣but␣iad␣input␣files␣must␣begin␣with␣IAD1\n");
        fprintf(*stderr*, "␣␣␣␣␣␣␣␣as␣the␣first␣four␣characters␣of␣the␣file.\n");
        fprintf(*stderr*, "␣␣␣␣␣␣␣␣Perhaps␣you␣are␣using␣an␣old␣iad␣format?\n");
        return 1;
      }
    }
    return 0;
  }

This code is used in section 95.

111.   Formatting the header information.

⟨ Prototype for *Write_Header* 111 ⟩ ≡
  void *Write_Header* (**struct measure_type** *m*, **struct invert_type** *r*, **int** *params*)

This code is used in sections 96 and 112.

112.   ⟨ Definition for *Write_Header* 112 ⟩ ≡
  ⟨ Prototype for *Write_Header* 111 ⟩
  {
    ⟨ Write slab info 113 ⟩
    ⟨ Write irradiation info 114 ⟩
    ⟨ Write general sphere info 115 ⟩
    ⟨ Write first sphere info 116 ⟩
    ⟨ Write second sphere info 117 ⟩
    ⟨ Write measure and inversion info 118 ⟩
  }

This code is used in section 95.

113.   ⟨ Write slab info 113 ⟩ ≡
  double *xx*;

  printf ("#␣Inverse␣Adding−Doubling␣%s␣\n", *Version*);
  printf ("#␣\n");
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Beam␣diameter␣=␣%7.1f␣mm\n", *m.d_beam*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Sample␣thickness␣=␣%7.3f␣mm\n", *m.slab_thickness*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Top␣slide␣thickness␣=␣%7.3f␣mm\n", *m.slab_top_slide_thickness*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Bottom␣slide␣thickness␣=␣%7.3f␣mm\n", *m.slab_bottom_slide_thickness*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣Sample␣index␣of␣refraction␣=␣%7.4f\n", *m.slab_index*);
  printf ("#␣␣␣␣␣␣␣␣␣Top␣slide␣index␣of␣refraction␣=␣%7.4f\n", *m.slab_top_slide_index*);
  printf ("#␣␣␣␣␣Bottom␣slide␣index␣of␣refraction␣=␣%7.4f\n", *m.slab_bottom_slide_index*);

This code is used in section 112.

114.   ⟨ Write irradiation info 114 ⟩ ≡
  printf ("#␣\n");

This code is used in section 112.

115.   ⟨ Write general sphere info 115 ⟩ ≡
  printf ("#␣␣Percentage␣unscattered␣refl.␣in␣M_R␣=␣%7.1f␣%%\n", *m.fraction_of_rc_in_mr* ∗ 100);
  printf ("#␣Percentage␣unscattered␣trans.␣in␣M_T␣=␣%7.1f␣%%\n", *m.fraction_of_tc_in_mt* ∗ 100);
  printf ("#␣\n");

This code is used in section 112.

116.   ⟨ Write first sphere info 116 ⟩ ≡
  printf ("#␣Reflection␣sphere");
  if (*m.baffle_r*) *printf* ("␣has␣a␣baffle␣between␣sample␣and␣detector␣");
  else *printf* ("␣has␣no␣baffle␣between␣sample␣and␣detector");
  if (*m.num_spheres* > 0) *printf* ("\n");
  else *printf* ("␣(all␣ignored␣since␣no␣spheres␣used)\n");
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sphere␣diameter␣=␣%7.1f␣mm\n", *m.d_sphere_r*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sample␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.as_r*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣empty␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.ae_r*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.ad_r*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣reflectance␣=␣%7.1f␣%%\n", *m.rd_r* * 100);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣wall␣reflectance␣=␣%7.1f␣%%\n", *m.rw_r* * 100);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣calibration␣standard␣=␣%7.1f␣%%\n", *m.rstd_r* * 100);
  printf ("#\n");
This code is used in section 112.

117.   ⟨ Write second sphere info 117 ⟩ ≡
  printf ("#␣Transmission␣sphere");
  if (*m.baffle_t*) *printf* ("␣has␣a␣baffle␣between␣sample␣and␣detector␣");
  else *printf* ("␣has␣no␣baffle␣between␣sample␣and␣detector");
  if (*m.num_spheres* > 0) *printf* ("\n");
  else *printf* ("␣(all␣ignored␣since␣no␣spheres␣used)\n");
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sphere␣diameter␣=␣%7.1f␣mm\n", *m.d_sphere_t*);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sample␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.as_t*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣empty␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.ae_t*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣port␣diameter␣=␣%7.1f␣mm\n", 2 * *m.d_sphere_r* * *sqrt*(*m.ad_t*));
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣reflectance␣=␣%7.1f␣%%\n", *m.rd_t* * 100);
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣wall␣reflectance␣=␣%7.1f␣%%", *m.rw_t* * 100);
  if (*m.ae_t* ≡ 0) *printf* ("␣(cal␣std␣since␣empty␣port␣is␣closed)");
  printf ("\n");
  printf ("#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣calibration␣standard␣=␣%7.1f␣%%", *m.rstd_t* * 100);
  if (*m.ae_t* ≡ 0) *printf* ("␣(ignored)");
  printf ("\n");
This code is used in section 112.

118.   ⟨ Write measure and inversion info 118 ⟩ ≡
  printf ("#\n");
  switch (*params*) {
  case −1: *printf* ("#␣No␣M_R␣or␣M_T␣−−␣forward␣calculation.\n");
    break;
  case 1: *printf* ("#␣Just␣M_R␣was␣measured");
    break;
  case 2: *printf* ("#␣M_R␣and␣M_T␣were␣measured");
    break;
  case 3: *printf* ("#␣M_R,␣M_T,␣and␣M_U␣were␣measured");
    break;
  case 4: *printf* ("#␣M_R,␣M_T,␣M_U,␣and␣r_w␣were␣measured");
    break;
  case 5: *printf* ("#␣M_R,␣M_T,␣M_U,␣r_w,␣and␣t_w␣were␣measured");
    break;
  case 6: *printf* ("#␣M_R,␣M_T,␣M_U,␣r_w,␣t_w,␣and␣r_std␣were␣measured");
    break;
  case 7: *printf* ("#␣M_R,␣M_T,␣M_U,␣r_w,␣t_w,␣r_std␣and␣t_std␣were␣measured");
    break;
  default: *printf* ("#␣Something␣went␣wrong␣...␣measures␣should␣be␣1␣to␣5!\n");
    break;
  }
  if (1 ≤ *params* ∧ *params* ≤ 7) {
    if (*m.flip_sample*) *printf* ("␣(sample␣flipped)␣");
    switch (*m.method*) {
    case UNKNOWN: *printf* ("␣using␣an␣unknown␣method.\n");
      break;
    case SUBSTITUTION: *printf* ("␣using␣the␣substitution␣(single-beam)␣method.\n");
      break;
    case COMPARISON: *printf* ("␣using␣the␣comparison␣(dual-beam)␣method.\n");
    }
  }
  switch (*m.num_spheres*) {
  case 0: *printf* ("#␣No␣sphere␣corrections␣were␣used");
    break;
  case 1:
    if (*m.method* ≡ COMPARISON) *printf* ("#␣No␣sphere␣corrections␣were␣needed");
    else *printf* ("#␣Single␣sphere␣corrections␣were␣used");
    break;
  case 2: *printf* ("#␣Double␣sphere␣corrections␣were␣used");
    break;
  }
  printf ("␣and␣light␣was␣incident␣at␣%d␣degrees␣from␣the␣normal",
      (**int**)(*acos*(*m.slab_cos_angle*) ∗ 57.2958));
  printf (".\n");
  switch (*r.search*) {
  case FIND_AB: *printf* ("#␣The␣inverse␣routine␣varied␣the␣albedo␣and␣optical␣depth.\n");
    printf ("#␣\n");
    xx = (*r.default_g* ≠ UNINITIALIZED) ? *r.default_g* : 0;
    printf ("#␣Default␣single␣scattering␣anisotropy␣=␣%7.3f␣\n", *xx*);
    break;
  case FIND_AG: *printf* ("#␣The␣inverse␣routine␣varied␣the␣albedo␣and␣anisotropy.\n");

$printf\,($"#␣\n"$);$

if $(r.default\_b \neq$ UNINITIALIZED$)$

  $printf\,($"#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Default␣(mu_t*d)␣=␣%7.3g\n"$, r.default\_b);$

else $printf\,($"#␣\n"$);$

break;

case FIND_AUTO: $printf\,($"#␣The␣inverse␣routine␣adapted␣to␣the␣input␣data.\n"$);$

  $printf\,($"#␣\n"$);$

  $printf\,($"#␣\n"$);$

  break;

case FIND_A: $printf\,($"#␣The␣inverse␣routine␣varied␣only␣the␣albedo.\n"$);$

  $printf\,($"#␣\n"$);$

  $xx = (r.default\_g \neq$ UNINITIALIZED$)\ ?\ r.default\_g : 0;$

  $printf\,($"#␣Default␣single␣scattering␣anisotropy␣is␣%7.3f␣"$, xx);$

  $xx = (r.default\_b \neq$ UNINITIALIZED$)\ ?\ r.default\_b :$ HUGE_VAL$;$

  $printf\,($"␣and␣(mu_t*d)␣=␣%7.3g\n"$, xx);$

  break;

case FIND_B: $printf\,($"#␣The␣inverse␣routine␣varied␣only␣the␣optical␣depth.\n"$);$

  $printf\,($"#␣\n"$);$

  $xx = (r.default\_g \neq$ UNINITIALIZED$)\ ?\ r.default\_g : 0;$

  $printf\,($"#␣Default␣single␣scattering␣anisotropy␣is␣%7.3f␣"$, xx);$

  if $(r.default\_a \neq$ UNINITIALIZED$)$ $printf\,($"and␣default␣albedo␣=␣%7.3g\n"$, r.default\_a);$

  else $printf\,($"\n"$);$

  break;

case $FIND\_Ba$: $printf\,($"#␣The␣inverse␣routine␣varied␣only␣the␣absorption.\n"$);$

  $printf\,($"#␣\n"$);$

  $xx = (r.default\_bs \neq$ UNINITIALIZED$)\ ?\ r.default\_bs : 0;$

  $printf\,($"#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Default␣(mu_s*d)␣=␣%7.3g\n"$, xx);$

  break;

case $FIND\_Bs$: $printf\,($"#␣The␣inverse␣routine␣varied␣only␣the␣scattering.\n"$);$

  $printf\,($"#␣\n"$);$

  $xx = (r.default\_ba \neq$ UNINITIALIZED$)\ ?\ r.default\_ba : 0;$

  $printf\,($"#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Default␣(mu_a*d)␣=␣%7.3g\n"$, xx);$

  break;

default: $printf\,($"#␣\n"$);$

  $printf\,($"#␣\n"$);$

  $printf\,($"#␣\n"$);$

  break;

}

$printf\,($"#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣AD␣quadrature␣points␣=␣%3d\n"$, r.method.quad\_pts);$

$printf\,($"#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣AD␣tolerance␣for␣success␣=␣%9.5f\n"$, r.tolerance);$

$printf\,($"#␣␣␣␣␣␣␣MC␣tolerance␣for␣mu_a␣and␣mu_s'␣=␣%7.3f␣%%\n"$, r.MC\_tolerance);$

This code is used in section 112.

119.   Discard white space and dashes in the legend string

⟨ Definition for *remove_whitespace* 119 ⟩ ≡
```
  void remove_whitespace(char *str)
  {
    int i, j = 0;
    for (i = 0; str[i] ≠ '\0'; i++) {
      if (¬isspace(str[i]) ∧ str[i] ≠ '−') {
        str[j++] = str[i];
      }
    }
    str[j] = '\0';
  }
```
This code is used in section 95.

120.   ⟨ Definition for *remove_comment* 120 ⟩ ≡
```
  void remove_comment(char *str)
  {
    int i;
    for (i = 0; str[i] ≠ '\0'; i++) {
      if (str[i] ≡ '#') {
        str[i] = '\0';
        break;
      }
    }
  }
```
This code is used in section 95.

121.   ⟨ Definition for *remove_first_char* 121 ⟩ ≡
```
  void remove_first_char(char *str)
  {
    int len = strlen(str);
    if (len > 0) {
      for (int i = 0; i < len; i++) {
        str[i] = str[i + 1];
      }
    }
  }
```
This code is used in section 95.

122.   ⟨ Prototype for *Read_Data_Legend* 122 ⟩ ≡
```
  int Read_Data_Legend(FILE *fp)
```
This code is used in section 123.

123.   ⟨ Definition for *Read_Data_Legend* 123 ⟩ ≡
  ⟨ Prototype for *Read_Data_Legend* 122 ⟩
  {
     int $n = 0$;

     skip_white(*fp*);
     if (*fgets*(LINE_LEGEND, MAX_LINE_LENGTH, *fp*) ≡ Λ) {
        fprintf(*stderr*, "could␣not␣read␣Data␣Legend␣String␣in␣file\n");
        exit(EXIT_FAILURE);
     }
     remove_whitespace(LINE_LEGEND);
     remove_comment(LINE_LEGEND);
     if (*isdigit*(LINE_LEGEND[0]) ∧ LINE_LEGEND[0] ≠ '0') {
        $n = $ LINE_LEGEND[0] − '0';
        remove_first_char(LINE_LEGEND);
     }
     else $n = strlen$(LINE_LEGEND);
     fprintf(*stderr*, "n=%d␣LEGEND='%s'\n", *n*, LINE_LEGEND);
     return *n*;
  }
This code is used in section 95.

124.   IAD Calculation.

⟨ `iad_calc.c`   124 ⟩ ≡

#include `<math.h>`
#include `<string.h>`
#include `<stdio.h>`
#include `<stdlib.h>`
#include `"nr_util.h"`
#include `"nr_zbrent.h"`
#include `"ad_globl.h"`
#include `"ad_frsnl.h"`
#include `"ad_prime.h"`
#include `"iad_type.h"`
#include `"iad_util.h"`
#include `"iad_calc.h"`
#define `ABIT` $1 \cdot 10^{-6}$
#define `A_COLUMN` 1
#define `B_COLUMN` 2
#define `G_COLUMN` 3
#define `URU_COLUMN` 4
#define `UTU_COLUMN` 5
#define `UR1_COLUMN` 6
#define `UT1_COLUMN` 7
#define `REFLECTION_SPHERE` 1
#define `TRANSMISSION_SPHERE` 0
#define `GRID_SIZE` 101
#define `T_TRUST_FACTOR` 1
#define `MAX_ABS_G` 0.999999
#define `SWAP`(a, b)
 {
   double $swap = (a);$
   $(a) = (b);$
   $(b) = swap;$
 }
 static int `CALCULATING_GRID` $= 0;$
 static struct **measure_type** `MM`;
 static struct **invert_type** `RR`;
 static struct **measure_type** `MGRID`;
 static struct **invert_type** `RGRID`;
 static double $** \mathit{The\_Grid} = \Lambda;$
 static double $GG\_a;$
 static double $GG\_b;$
 static double $GG\_g;$
 static double $GG\_bs;$
 static double $GG\_ba;$
 static boolean_type $\mathit{The_Grid_Initialized} = $ `FALSE`;
 static boolean_type $\mathit{The\_Grid\_Search} = -1;$
 ⟨ Definition for $\mathit{Set\_Calc\_State}$ 140 ⟩
 ⟨ Definition for $\mathit{Get\_Calc\_State}$ 142 ⟩
 ⟨ Definition for $\mathit{Same\_Calc\_State}$ 144 ⟩
 ⟨ Prototype for $\mathit{Fill\_AB\_Grid}$ 162 ⟩;
 ⟨ Prototype for $\mathit{Fill\_AG\_Grid}$ 166 ⟩;

⟨ Definition for *RT_Flip* 160 ⟩
⟨ Definition for *Allocate_Grid* 146 ⟩
⟨ Definition for *Valid_Grid* 150 ⟩
⟨ Definition for *fill_grid_entry* 161 ⟩
⟨ Definition for *Fill_Grid* 176 ⟩
⟨ Definition for *Near_Grid_Points* 158 ⟩
⟨ Definition for *Fill_AB_Grid* 163 ⟩
⟨ Definition for *Fill_AG_Grid* 167 ⟩
⟨ Definition for *Fill_BG_Grid* 170 ⟩
⟨ Definition for *Fill_BaG_Grid* 172 ⟩
⟨ Definition for *Fill_BsG_Grid* 174 ⟩
⟨ Definition for *Grid_ABG* 148 ⟩
⟨ Definition for *Gain* 129 ⟩
⟨ Definition for *Gain_11* 131 ⟩
⟨ Definition for *Gain_22* 133 ⟩
⟨ Definition for *Two_Sphere_R* 135 ⟩
⟨ Definition for *Two_Sphere_T* 137 ⟩
⟨ Definition for *Calculate_Distance_With_Corrections* 182 ⟩
⟨ Definition for *Calculate_Grid_Distance* 180 ⟩
⟨ Definition for *Calculate_Distance* 178 ⟩
⟨ Definition for *abg_distance* 156 ⟩
⟨ Definition for *Find_AG_fn* 196 ⟩
⟨ Definition for *Find_AB_fn* 198 ⟩
⟨ Definition for *Find_Ba_fn* 200 ⟩
⟨ Definition for *Find_Bs_fn* 202 ⟩
⟨ Definition for *Find_A_fn* 204 ⟩
⟨ Definition for *Find_B_fn* 206 ⟩
⟨ Definition for *Find_G_fn* 208 ⟩
⟨ Definition for *Find_BG_fn* 210 ⟩
⟨ Definition for *Find_BaG_fn* 212 ⟩
⟨ Definition for *Find_BsG_fn* 214 ⟩
⟨ Definition for *maxloss* 216 ⟩
⟨ Definition for *Max_Light_Loss* 218 ⟩

125.

⟨ iad_calc.h   125 ⟩ ≡

  ⟨ Prototype for *Gain* 128 ⟩;
  ⟨ Prototype for *Gain_11* 130 ⟩;
  ⟨ Prototype for *Gain_22* 132 ⟩;
  ⟨ Prototype for *Two_Sphere_R* 134 ⟩;
  ⟨ Prototype for *Two_Sphere_T* 136 ⟩;
  ⟨ Prototype for *Set_Calc_State* 139 ⟩;
  ⟨ Prototype for *Get_Calc_State* 141 ⟩;
  ⟨ Prototype for *Same_Calc_State* 143 ⟩;
  ⟨ Prototype for *Valid_Grid* 149 ⟩;
  ⟨ Prototype for *Allocate_Grid* 145 ⟩;
  ⟨ Prototype for *Fill_Grid* 175 ⟩;
  ⟨ Prototype for *Near_Grid_Points* 157 ⟩;
  ⟨ Prototype for *Grid_ABG* 147 ⟩;
  ⟨ Prototype for *Find_AG_fn* 195 ⟩;
  ⟨ Prototype for *Find_AB_fn* 197 ⟩;
  ⟨ Prototype for *Find_Ba_fn* 199 ⟩;
  ⟨ Prototype for *Find_Bs_fn* 201 ⟩;
  ⟨ Prototype for *Find_A_fn* 203 ⟩;
  ⟨ Prototype for *Find_B_fn* 205 ⟩;
  ⟨ Prototype for *Find_G_fn* 207 ⟩;
  ⟨ Prototype for *Find_BG_fn* 209 ⟩;
  ⟨ Prototype for *Find_BsG_fn* 213 ⟩;
  ⟨ Prototype for *Find_BaG_fn* 211 ⟩;
  ⟨ Prototype for *Fill_BG_Grid* 169 ⟩;
  ⟨ Prototype for *Fill_BsG_Grid* 173 ⟩;
  ⟨ Prototype for *Fill_BaG_Grid* 171 ⟩;
  ⟨ Prototype for *Calculate_Distance_With_Corrections* 181 ⟩;
  ⟨ Prototype for *Calculate_Distance* 177 ⟩;
  ⟨ Prototype for *Calculate_Grid_Distance* 179 ⟩;
  ⟨ Prototype for *abg_distance* 155 ⟩;
  ⟨ Prototype for *maxloss* 215 ⟩;
  ⟨ Prototype for *Max_Light_Loss* 217 ⟩;
  ⟨ Prototype for *RT_Flip* 159 ⟩;

126. Initialization.

The functions in this file assume that the local variables `MM` and `RR` have been initialized appropriately. The variable `MM` contains all the information about how a particular experiment was done. The structure `RR` contains the data structure that is passed to the adding-doubling routines as well as the number of quadrature points.

127.   Gain.

Assume that a sphere is illuminated with diffuse light having a power P. This light will undergo multiple reflections in the sphere walls that will increase the power falling on the detector.

The gain on the detector due to integrating sphere effects varies with the presence of a baffle between the sample and the detector. If a baffle is present then

$$G_{\text{no baffle}}(r_s) = \frac{1}{1 - a_w r_w - a_d r_d - a_s r_s}$$

or with a baffle as

$$G_{\text{baffle}}(r_s) = \frac{1}{1 - a_w r_w - r_w(1 - a_e)(a_d r_d + a_s r_s)}$$

For a black sphere the gain does not depend on the diffuse reflectivity of the sample and is unity. $G(r_s) = 1$, which is easily verified by setting $r_w = 0$.

128. $\langle$ Prototype for $Gain$ 128 $\rangle \equiv$
  double $Gain(\textbf{int } sphere, \textbf{struct measure\_type } m, \textbf{double } \texttt{URU})$
This code is used in sections 125 and 129.

129. $\langle$ Definition for $Gain$ 129 $\rangle \equiv$
  $\langle$ Prototype for $Gain$ 128 $\rangle$
  {
    double $G, denom$;
    if $(sphere \equiv \texttt{REFLECTION\_SPHERE})$ {
      if $(m.baffle\_r)$ $denom = 1.0 - m.rw\_r * (m.aw\_r + (1 - m.ae\_r) * (m.ad\_r * m.rd\_r + m.as\_r * \texttt{URU}))$;
      else $denom = 1.0 - m.aw\_r * m.rw\_r - m.ad\_r * m.rd\_r - m.as\_r * \texttt{URU}$;
    }
    else {
      if $(m.baffle\_t)$ $denom = 1.0 - m.rw\_t * (m.aw\_t + (1 - m.ae\_t) * (m.ad\_t * m.rd\_t + m.as\_t * \texttt{URU}))$;
      else $denom = 1.0 - m.aw\_t * m.rw\_t - m.ad\_t * m.rd\_t - m.as\_t * \texttt{URU}$;
    }
    $G = 1.0/denom$;
    return G;
  }
This code is used in section 124.

130.   The gain for light on the detector in the first sphere for diffuse light starting in that same sphere is defined as

$$G_{1 \to 1}(r_s, t_s) \equiv \frac{P_{1 \to 1}(r_s, t_s)/A_d}{P/A}$$

then the full expression for the gain is

$$G_{1 \to 1}(r_s, t_s) = \frac{G(r_s)}{1 - a_s a_s' r_w r_w'(1 - a_e)(1 - a_e')G(r_s)G'(r_s)t_s^2}$$

$\langle$ Prototype for $Gain\_11$ 130 $\rangle \equiv$
  double $Gain\_11(\textbf{struct measure\_type } m, \textbf{double } \texttt{URU}, \textbf{double } tdiffuse)$
This code is used in sections 125 and 131.

131.   ⟨ Definition for *Gain_11* 131 ⟩ ≡
⟨ Prototype for *Gain_11* 130 ⟩
{
    double G, GP, G11;

    $G = Gain(\texttt{REFLECTION\_SPHERE}, m, \texttt{URU})$;
    $\texttt{GP} = Gain(\texttt{TRANSMISSION\_SPHERE}, m, \texttt{URU})$;
    $\texttt{G11} = G/(1 - m.as\_r * m.as\_t * m.aw\_r * m.aw\_t * (1 - m.ae\_r) * (1 - m.ae\_t) * G * \texttt{GP} * \textit{tdiffuse} * \textit{tdiffuse})$;
    return G11;
}

This code is used in section 124.

132.   Similarly, when the light starts in the second sphere, the gain for light on the detector in the second sphere $G_{2\to 2}$ is found by switching all primed variables to unprimed. Thus $G_{2\to 1}(r_s, t_s)$ is

$$G_{2\to 2}(r_s, t_s) = \frac{G'(r_s)}{1 - a_s a'_s r_w r'_w (1 - a_e)(1 - a'_e) G(r_s) G'(r_s) t_s^2}$$

⟨ Prototype for *Gain_22* 132 ⟩ ≡
    double *Gain_22*(**struct measure_type** m, **double** URU, **double** *tdiffuse*)

This code is used in sections 125 and 133.

133.   ⟨ Definition for *Gain_22* 133 ⟩ ≡
⟨ Prototype for *Gain_22* 132 ⟩
{
    double G, GP, G22;

    $G = Gain(\texttt{REFLECTION\_SPHERE}, m, \texttt{URU})$;
    $\texttt{GP} = Gain(\texttt{TRANSMISSION\_SPHERE}, m, \texttt{URU})$;
    $\texttt{G22} = \texttt{GP}/(1 - m.as\_r * m.as\_t * m.aw\_r * m.aw\_t * (1 - m.ae\_r) * (1 - m.ae\_t) * G * \texttt{GP} * \textit{tdiffuse} * \textit{tdiffuse})$;
    return G22;
}

This code is used in section 124.

134.   The reflected power for two spheres makes use of the formulas for *Gain_11* above.

The light on the detector in the reflection (first) sphere arises from three sources: the fraction of light directly reflected off the sphere wall $f r_w^2 (1 - a_e) P$, the fraction of light reflected by the sample $(1 - f) r_s^{\text{direct}} r_w^2 (1 - a_e) P$, and the light transmitted through the sample $(1 - f) t_s^{\text{direct}} r'_w (1 - a'_e) P$,

$$
\begin{aligned}
R(r_s^{\text{direct}}, r_s, t_s^{\text{direct}}, t_s) = {} & G_{1\to 1}(r_s, t_s) \cdot a_d (1 - a_e) r_w^2 f P \\
& + G_{1\to 1}(r_s, t_s) \cdot a_d (1 - a_e) r_w (1 - f) r_s^{\text{direct}} P \\
& + G_{2\to 1}(r_s, t_s) \cdot a_d (1 - a'_e) r'_w (1 - f) t_s^{\text{direct}} P
\end{aligned}
$$

which simplifies slightly to

$$
\begin{aligned}
R(r_s^{\text{direct}}, r_s, t_s^{\text{direct}}, t_s) = {} & a_d (1 - a_e) r_w P \cdot G_{1\to 1}(r_s, t_s) \\
& \times \left[(1 - f) r_s^{\text{direct}} + f r_w + (1 - f) a'_s (1 - a'_e) r'_w t_s^{\text{direct}} t_s G'(r_s) \right]
\end{aligned}
$$

⟨ Prototype for *Two_Sphere_R* 134 ⟩ ≡
    double *Two_Sphere_R*(**struct measure_type** m, **double** UR1, **double** URU, **double** UT1, **double** UTU)

This code is used in sections 125 and 135.

135. ⟨Definition for *Two_Sphere_R* 135⟩ ≡
  ⟨Prototype for *Two_Sphere_R* 134⟩
  {
    double x, GP;

    GP = $Gain$(TRANSMISSION_SPHERE, m, URU);
    $x = m.ad\_r * (1 - m.ae\_r) * m.rw\_r * Gain\_11 (m, \text{URU}, \text{UTU});$
    $x \mathrel{*}= (1 - m.f\_r) * \text{UR1} + m.rw\_r * m.f\_r + (1 - m.f\_r) * m.as\_t * (1 - m.ae\_t) * m.rw\_t * \text{UT1} * \text{UTU} * \text{GP};$
    return x;
  }

This code is used in section 124.

136. For the power on the detector in the transmission (second) sphere we have the same three sources. The only difference is that the subscripts on the gain terms now indicate that the light ends up in the second sphere

$$T(r_s^{\text{direct}}, r_s, t_s^{\text{direct}}, t_s) = G_{1\to 2}(r_s, t_s) \cdot a_d'(1 - a_e)r_w^2 fP$$
$$+ G_{1\to 2}(r_s, t_s) \cdot a_d'(1 - a_e)r_w(1 - f)r_s^{\text{direct}} P$$
$$+ G_{2\to 2}(r_s, t_s) \cdot a_d'(1 - a_e')r_w'(1 - f)t_s^{\text{direct}} P$$

or

$$T(r_s^{\text{direct}}, r_s, t_s^{\text{direct}}, t_s) = a_d'(1 - a_e')r_w'P \cdot G_{2\to 2}(r_s, t_s)$$
$$\times \left[(1 - f)t_s^{\text{direct}} + (1 - a_e)r_w a_s t_s (f r_w + (1 - f)r_s^{\text{direct}})G(r_s) \right]$$

⟨Prototype for *Two_Sphere_T* 136⟩ ≡
  double *Two_Sphere_T*(**struct measure_type** m, **double** UR1, **double** URU, **double** UT1, **double** UTU)
This code is used in sections 125 and 137.

137. ⟨Definition for *Two_Sphere_T* 137⟩ ≡
  ⟨Prototype for *Two_Sphere_T* 136⟩
  {
    double x, G;

    $G = Gain$(REFLECTION_SPHERE, m, URU);
    $x = m.ad\_t * (1 - m.ae\_t) * m.rw\_t * Gain\_22 (m, \text{URU}, \text{UTU});$
    $x \mathrel{*}= (1 - m.f\_r) * \text{UT1} + (1 - m.ae\_r) * m.rw\_r * m.as\_r * \text{UTU} * (m.f\_r * m.rw\_r + (1 - m.f\_r) * \text{UR1}) * G;$
    return x;
  }

This code is used in section 124.

138.   Grid Routines.   There is a long story associated with these routines. I spent a lot of time trying to find an empirical function to allow a guess at a starting value for the inversion routine. Basically nothing worked very well. There were too many special cases and what not. So I decided to calculate a whole bunch of reflection and transmission values and keep their associated optical properties linked nearby.

I did the very simplest thing. I just allocate a matrix that is five columns wide. Then I fill every row with a calculated set of optical properties and observables. The distribution of values that I use could certainly use some work, but they currently work.

SO... how does this thing work anyway? There are two possible grids one for calculations requiring the program to find the albedo and the optical depth (a and b) and one to find the albedo and anisotropy (a and g). These grids must be allocated and initialized before use.

139.   This is a pretty important routine that should have some explanation. The reason that it exists, is that we need some 'out-of-band' information during the minimization process. Since the light transport calculation depends on all sorts of stuff (e.g., the sphere parameters) and the minimization routines just vary one or two parameters this information needs to be put somewhere.

I chose the global variables MM and RR to save things in.

The bottom line is that you cannot do a light transport calculation without calling this routine first.

⟨ Prototype for *Set_Calc_State* 139 ⟩ ≡
  void *Set_Calc_State*(**struct measure_type** m, **struct invert_type** r)

This code is used in sections 125 and 140.

140.   ⟨ Definition for *Set_Calc_State* 140 ⟩ ≡
  ⟨ Prototype for *Set_Calc_State* 139 ⟩
  {
    memcpy(&MM, &m, **sizeof**(**struct measure_type**));
    memcpy(&RR, &r, **sizeof**(**struct invert_type**));
  }

This code is used in section 124.

141.   The inverse of the previous routine. Note that you must have space for the parameters m and r already allocated.

⟨ Prototype for *Get_Calc_State* 141 ⟩ ≡
  void *Get_Calc_State*(**struct measure_type** $*m$, **struct invert_type** $*r$)

This code is used in sections 125 and 142.

142.   ⟨ Definition for *Get_Calc_State* 142 ⟩ ≡
  ⟨ Prototype for *Get_Calc_State* 141 ⟩
  {
    memcpy(m, &MM, **sizeof**(**struct measure_type**));
    memcpy(r, &RR, **sizeof**(**struct invert_type**));
  }

This code is used in section 124.

143.   The inverse of the previous routine. Note that you must have space for the parameters m and r already allocated.

⟨ Prototype for *Same_Calc_State* 143 ⟩ ≡
  boolean_type *Same_Calc_State*(**struct measure_type** m, **struct invert_type** r)

This code is used in sections 125 and 144.

144. ⟨Definition for *Same_Calc_State* 144⟩ ≡
  ⟨Prototype for *Same_Calc_State* 143⟩
  {
    if (*The_Grid* ≡ Λ) **return** FALSE;
    if (¬ *The_Grid_Initialized*) **return** FALSE;
    if (*r.search* ≠ RR.*search*) **return** FALSE;
    if (*r.method.quad_pts* ≠ RR.*method.quad_pts*) **return** FALSE;
    if (*r.slab.a* ≠ RR.*slab.a*) **return** FALSE;
    if (*r.slab.b* ≠ RR.*slab.b*) **return** FALSE;
    if (*r.slab.g* ≠ RR.*slab.g*) **return** FALSE;
    if (*r.slab.phase_function* ≠ RR.*slab.phase_function*) **return** FALSE;
    if (*r.slab.n_slab* ≠ RR.*slab.n_slab*) **return** FALSE;
    if (*r.slab.n_top_slide* ≠ RR.*slab.n_top_slide*) **return** FALSE;
    if (*r.slab.n_bottom_slide* ≠ RR.*slab.n_bottom_slide*) **return** FALSE;
    if (*r.slab.b_top_slide* ≠ RR.*slab.b_top_slide*) **return** FALSE;
    if (*r.slab.b_bottom_slide* ≠ RR.*slab.b_bottom_slide*) **return** FALSE;
    if (*r.slab.cos_angle* ≠ RR.*slab.cos_angle*) **return** FALSE;
    if ((*m.num_measures* ≡ 3) ∧ (*m.m_u* ≠ MGRID.*m_u*)) **return** (FALSE);
    return TRUE;
  }
This code is used in section 124.

145. ⟨Prototype for *Allocate_Grid* 145⟩ ≡
  void *Allocate_Grid*(**search_type** *s*)
This code is used in sections 125 and 146.

146. ⟨Definition for *Allocate_Grid* 146⟩ ≡
  ⟨Prototype for *Allocate_Grid* 145⟩
  {
    (**void**) *s*;
    The_Grid = *dmatrix*(0, GRID_SIZE ∗ GRID_SIZE, 1, 7);
    if (*The_Grid* ≡ Λ) *AD_error*("unable␣to␣allocate␣the␣grid␣matrix");
    The_Grid_Initialized = FALSE;
  }
This code is used in section 124.

147. This routine will return the *a*, *b*, and *g* values for a particular row in the grid.
⟨Prototype for *Grid_ABG* 147⟩ ≡
  void *Grid_ABG*(**int** *i*, **int** *j*, **guess_type** ∗*guess*)
This code is used in sections 125 and 148.

148. ⟨ Definition for *Grid_ABG* 148 ⟩ ≡
  ⟨ Prototype for *Grid_ABG* 147 ⟩
  {
    if $(0 \le i \wedge i < \texttt{GRID\_SIZE} \wedge 0 \le j \wedge j < \texttt{GRID\_SIZE})$ {
      $guess \text{-} a = The\_Grid[\texttt{GRID\_SIZE} * i + j][\texttt{A\_COLUMN}];$
      $guess \text{-} b = The\_Grid[\texttt{GRID\_SIZE} * i + j][\texttt{B\_COLUMN}];$
      $guess \text{-} g = The\_Grid[\texttt{GRID\_SIZE} * i + j][\texttt{G\_COLUMN}];$
      $guess \text{-} distance = Calculate\_Grid\_Distance(i, j);$
    }
    else {
      $guess \text{-} a = 0.5;$
      $guess \text{-} b = 0.5;$
      $guess \text{-} g = 0.5;$
      $guess \text{-} distance = 999;$
    }
  }

This code is used in section 124.

149. This routine is used to figure out if the current grid is valid. This can fail for several reasons. First the grid may not have been allocated. Or it may not have been initialized. The boundary conditions may have changed. The number or values of the sphere parameters may have changed. It is tedious, but straightforward to check these cases out.

  If this routine returns true, then it is a pretty good bet that the values in the current grid can be used to guess the next starting set of values.

⟨ Prototype for *Valid_Grid* 149 ⟩ ≡
  boolean_type *Valid_Grid*(**struct measure_type** *m*, **search_type** *s*)

This code is used in sections 125 and 150.

150. ⟨ Definition for *Valid_Grid* 150 ⟩ ≡
  ⟨ Prototype for *Valid_Grid* 149 ⟩
  {
    ⟨ Tests for invalid grid 151 ⟩
    return (TRUE);
  }

This code is used in section 124.

151. First check are to test if the grid has ever been filled

⟨ Tests for invalid grid 151 ⟩ ≡
  if (*The_Grid* ≡ Λ) {
    if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Fill␣because␣NULL\n");
    return (FALSE);
  }
  if (¬*The_Grid_Initialized*) {
    if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Fill␣because␣not␣initialized\n");
    return (FALSE);
  }

See also sections 152, 153, and 154.

This code is used in section 150.

152.   If the type of search has changed then report the grid as invalid

⟨ Tests for invalid grid 151 ⟩ +≡
  if (*The_Grid_Search* ≠ *s*) {
    if (*Debug*(DEBUG_GRID)) *fprintf* (*stderr*, "GRID:␣Fill␣because␣search␣type␣changed\n");
    return (FALSE);
  }

153.   Compare the *m.m_u* value only if there are three measurements

⟨ Tests for invalid grid 151 ⟩ +≡
  if ((*m.num_measures* ≡ 3) ∧ (*m.m_u* ≠ MGRID.*m_u*)) {
    if (*Debug*(DEBUG_GRID)) *fprintf* (*stderr*, "GRID:␣Fill␣because␣unscattered␣light␣changed\n");
    return (FALSE);
  }

154.   Make sure that the boundary conditions have not changed.

⟨ Tests for invalid grid 151 ⟩ +≡
  if (*m.slab_index* ≠ MGRID.*slab_index*) {
    if (*Debug*(DEBUG_GRID))
      fprintf (*stderr*, "GRID:␣Fill␣because␣slab␣refractive␣index␣changed\n");
    return (FALSE);
  }
  if (*m.slab_cos_angle* ≠ MGRID.*slab_cos_angle*) {
    if (*Debug*(DEBUG_GRID)) *fprintf* (*stderr*, "GRID:␣Fill␣because␣light␣angle␣changed\n");
    return (FALSE);
  }
  if (*m.slab_top_slide_index* ≠ MGRID.*slab_top_slide_index*) {
    if (*Debug*(DEBUG_GRID)) *fprintf* (*stderr*, "GRID:␣Fill␣because␣top␣slide␣index␣changed\n");
    return (FALSE);
  }
  if (*m.slab_bottom_slide_index* ≠ MGRID.*slab_bottom_slide_index*) {
    if (*Debug*(DEBUG_GRID)) *fprintf* (*stderr*, "GRID:␣Fill␣because␣bottom␣slide␣index␣changed\n");
    return (FALSE);
  }

155.   Routine to just figure out the distance to a particular a, b, g point

⟨ Prototype for *abg_distance* 155 ⟩ ≡
  void *abg_distance*(**double** *a*, **double** *b*, **double** *g*, **guess_type** *∗guess*)
This code is used in sections 125 and 156.

156.   ⟨ Definition for *abg_distance* 156 ⟩ ≡
  ⟨ Prototype for *abg_distance* 155 ⟩
  {
    double m_r, m_t, *distance*;
    struct measure_type *old_mm*;
    struct invert_type *old_rr*;

    Get_Calc_State(&*old_mm*, &*old_rr*);
    RR.*slab*.$a = a$;
    RR.*slab*.$b = b$;
    RR.*slab*.$g = g$;
    Calculate_Distance(&m_r, &m_t, &*distance*);
    Set_Calc_State(*old_mm*, *old_rr*);
    guess→$a = a$;
    guess→$b = b$;
    guess→$g = g$;
    guess→*distance* = *distance*;
  }

This code is used in section 124.

157.   This just searches through the grid to find the minimum entry and returns the optical properties of that entry. The smallest, the next smallest, and the third smallest values are returned.

  This has been rewritten to use *Calculate_Distance_With_Corrections* so that changes in sphere parameters won't necessitate recalculating the grid.

  ⟨ Prototype for *Near_Grid_Points* 157 ⟩ ≡
    void *Near_Grid_Points*(**double** r, **double** t, **search_type** s, **int** ∗*i_min*, **int** ∗*j_min*)

This code is used in sections 125 and 158.

158. ⟨ Definition for *Near_Grid_Points* 158 ⟩ ≡
  ⟨ Prototype for *Near_Grid_Points* 157 ⟩
  {
    int *i*, *j*;
    double *fval*;
    double *smallest* = 10.0;
    struct measure_type *old_mm*;
    struct invert_type *old_rr*;

    (**void**) *r*;
    (**void**) *t*;
    (**void**) *s*;
    if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Finding␣best␣grid␣points\n");
    Get_Calc_State(&*old_mm*, &*old_rr*);
    ∗i_min = 0;
    ∗j_min = 0;
    for (*i* = 0; *i* < GRID_SIZE; *i*++) {
      for (*j* = 0; *j* < GRID_SIZE; *j*++) {
        CALCULATING_GRID = 1;
        fval = *Calculate_Grid_Distance*(*i*, *j*);
        CALCULATING_GRID = 0;
        if (*fval* < *smallest*) {
          ∗i_min = *i*;
          ∗j_min = *j*;
          smallest = *fval*;
        }
      }
    }
    Set_Calc_State(*old_mm*, *old_rr*);
  }

This code is used in section 124.

159. Routine to incorporate flipping of sample if needed. This is pretty simple. The assumption is that flipping is handled relative to the reflection side of the sphere. Thus even when flipping is needed, the usual call to RT( ) will result in the correct values for the reflectances. The transmission values can then be calculated by swapping the top and bottom slides.

Technically, the value of slab should be **const** but it is not so that we don't pay a copying overhead whenever *flip* is false (the usual case).

⟨ Prototype for *RT_Flip* 159 ⟩ ≡
  void *RT_Flip*(**int** *flip*, **int** *n*, **struct AD_slab_type** *∗slab*, **double** *∗UR1*, **double** *∗UT1*, **double**
      ∗URU, **double** *∗UTU*)

This code is used in sections 125 and 160.

160.   ⟨ Definition for *RT_Flip* 160 ⟩ ≡
  ⟨ Prototype for *RT_Flip* 159 ⟩
  {
    double *correct_UR1*, *correct_URU*;

    RT(*n*, *slab*, UR1, UT1, URU, UTU);
    if (*flip*) {
      correct_UR1 = ∗UR1;
      correct_URU = ∗URU;
      SWAP(*slab*→*n_top_slide*, *slab*→*n_bottom_slide*)SWAP(*slab*→*b_top_slide*, *slab*→*b_bottom_slide*)RT(*n*, *slab*, UR1,
          UT1, URU, UTU);
      SWAP(*slab*→*n_top_slide*, *slab*→*n_bottom_slide*)SWAP(*slab*→*b_top_slide*,
          slab→*b_bottom_slide*) ∗ UR1 = *correct_UR1*;
      ∗URU = *correct_URU*;
    }
  }

This code is used in section 124.

161.   Simple routine to put values into the grid

Presumes that RR.*slab* is properly set up.

⟨ Definition for *fill_grid_entry* 161 ⟩ ≡

```
static void fill_grid_entry(int i, int j)
{
    double ur1, ut1, uru, utu;
    if (RR.slab.b ≤ 1 · 10⁻⁶) RR.slab.b = 1 · 10⁻⁶;
    if (Debug(DEBUG_GRID_CALC) ∧ i ≡ 0 ∧ j ≡ 0) {
        fprintf(stderr, "+␣␣␣i␣␣␣j␣");
        fprintf(stderr, "␣␣␣␣␣␣␣a␣␣␣␣␣␣␣␣␣␣b␣␣␣␣␣␣␣␣␣␣␣g␣␣␣␣␣|");
        fprintf(stderr, "␣␣␣␣␣␣M_R␣␣␣␣␣␣␣␣␣grid␣␣|");
        fprintf(stderr, "␣␣␣␣␣M_T␣␣␣␣␣␣␣␣␣␣grid\n");
    }
    if (Debug(DEBUG_EVERY_CALC)) {
        if (¬CALCULATING_GRID)
            fprintf(stderr, "a=%8.5f␣b=%10.5f␣g=%8.5f␣", RR.slab.a, RR.slab.b, RR.slab.g);
        else {
            if (j ≡ 0) fprintf(stderr, ".");
            if (i + 1 ≡ GRID_SIZE ∧ j ≡ 0) fprintf(stderr, "\n");
        }
    }
    RT_Flip(MM.flip_sample, RR.method.quad_pts, &RR.slab, &ur1, &ut1, &uru, &utu);
    if (Debug(DEBUG_EVERY_CALC) ∧ ¬CALCULATING_GRID)
        fprintf(stderr, "ur1=%8.5f␣ut1=%8.5f\n", ur1, ut1);
    The_Grid[GRID_SIZE * i + j][A_COLUMN] = RR.slab.a;
    The_Grid[GRID_SIZE * i + j][B_COLUMN] = RR.slab.b;
    The_Grid[GRID_SIZE * i + j][G_COLUMN] = RR.slab.g;
    The_Grid[GRID_SIZE * i + j][UR1_COLUMN] = ur1;
    The_Grid[GRID_SIZE * i + j][UT1_COLUMN] = ut1;
    The_Grid[GRID_SIZE * i + j][URU_COLUMN] = uru;
    The_Grid[GRID_SIZE * i + j][UTU_COLUMN] = utu;
    if (Debug(DEBUG_GRID_CALC)) {
        fprintf(stderr, "+␣%3d␣%3d␣", i, j);
        fprintf(stderr, "%10.5f␣%10.5f␣%10.5f␣|", RR.slab.a, RR.slab.b, RR.slab.g);
        fprintf(stderr, "%10.5f␣%10.5f␣|", MM.m_r, uru);
        fprintf(stderr, "%10.5f␣%10.5f␣\n", MM.m_t, utu);
    }
}
```

This code is used in section 124.

162.   This routine fills the grid with a proper set of values. With a little work, this routine could be made much faster by (1) only generating the phase function matrix once, (2) Making only one pass through the array for each albedo value, i.e., using the matrix left over from $b = 1$ to generate the solution for $b = 2$. Unfortunately this would require a complete revision of the *Calculate_Distance* routine. Fortunately, this routine should only need to be calculated once at the beginning of each run.

⟨ Prototype for *Fill_AB_Grid* 162 ⟩ ≡

```
void Fill_AB_Grid(struct measure_type m, struct invert_type r)
```

This code is used in sections 124 and 163.

163.   ⟨ Definition for *Fill_AB_Grid* 163 ⟩ ≡
  ⟨ Prototype for *Fill_AB_Grid* 162 ⟩
  {
    int *i, j*;
    double *a*;
    double *min_b* = −8;   /∗ exp(-10) is smallest thickness ∗/
    double *max_b* = +8;   /∗ exp(+8) is greatest thickness ∗/
    if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Filling␣AB␣grid\n");
    if (*The_Grid* ≡ Λ) *Allocate_Grid*(*r.search*);
    ⟨ Zero *GG* 168 ⟩
    Set_Calc_State(*m, r*);
    GG_g = RR.*slab.g*;
    for (*i* = 0; *i* < GRID_SIZE; *i*++) {
      double *x* = (**double**)*i*/(GRID_SIZE − 1.0);
      RR.*slab.b* = *exp*(*min_b* + (*max_b* − *min_b*) ∗ *x*);
      for (*j* = 0; *j* < GRID_SIZE; *j*++) {
        ⟨ Generate next albedo using j 165 ⟩
        fill_grid_entry(*i, j*);
      }
    }
    The_Grid_Initialized = TRUE;
    The_Grid_Search = FIND_AB;
  }

This code is used in section 124.

164.   Now it seems that I must be a bit more subtle in choosing the range of albedos to use in the grid. Originally I just spaced them according to

$$a = 1 - \left[\frac{j-1}{n-1}\right]^3$$

where $1 \le j \le n$. Long ago it seems that I based things only on the square of the bracketed term, but I seem to remember that I was forced to change it from a square to a cube to get more global convergence.

So why am I rewriting this? Well, because it works very poorly for samples with small albedos. For example, when $n = 11$ then the values chosen for a are (1, .999, .992, .973, .936, .875, .784, .657, .488, .271, 0). Clearly very skewed towards high albedos.

I am considering a two part division. I'm not too sure how it should go. Let the first half be uniformly divided and the last half follow the cubic scheme given above. The list of values should then be (1, .996, .968, .892, 0.744, .5, .4, .3, .2, .1, 0).

Maybe it would be best if I just went back to a quadratic term. Who knows?

In the **if** statement below, note that it could read $j \ge k$ and still generate the same results.

⟨ Nonworking code 164 ⟩ ≡
  k = *floor*((GRID_SIZE − 1)/2);
  if (*j* > *k*) {
    a = 0.5 ∗ (1 − (*j* − *k* − 1)/(GRID_SIZE − *k* − 1));
    RR.*slab.a* = *a*;
  }
  else {
    a = (*j* − 1.0)/(GRID_SIZE − *k* − 1);
    RR.*slab.a* = 1.0 − *a* ∗ *a* ∗ *a*/2;
  }

165.   Here is heuristic that seems to work well

⟨ Generate next albedo using j 165 ⟩ ≡
  $a = (\textbf{double})\, j/(\texttt{GRID\_SIZE} - 1.0)$;
  $\text{RR}.slab.a = (1.0 - a * a) * (1.0 - a) + (1.0 - a) * (1.0 - a) * a$;

This code is used in sections 163 and 167.

166.   This is quite similar to *Fill_AB_Grid*, with the exception of the little shuffle I do at the beginning to figure out the optical thickness to use. The problem is that the optical thickness may not be known. If it is known then the only way that we could have gotten here is if the user dictated `FIND_AG` and specified b and only provided two measurements. Otherwise, the user must have made three measurements and the optical depth can be figured out from $m.m\_u$.

This routine could also be improved by not recalculating the anisotropy matrix for every point. But this would only end up being a minor performance enhancement if it were fixed.

⟨ Prototype for *Fill_AG_Grid* 166 ⟩ ≡
  void *Fill_AG_Grid*(**struct measure_type** m, **struct invert_type** r)

This code is used in sections 124 and 167.

167.   ⟨ Definition for *Fill_AG_Grid* 167 ⟩ ≡
  ⟨ Prototype for *Fill_AG_Grid* 166 ⟩
  {
    int i, j;
    double a;
    if (*Debug*(`DEBUG_GRID`)) *fprintf*(*stderr*, "GRID:␣Filling␣AG␣grid\n");
    if (*The_Grid* ≡ Λ) *Allocate_Grid*(*r.search*);
    ⟨ Zero *GG* 168 ⟩
    Set_Calc_State(m, r);
    $GG\_b = r.slab.b$;
    for ($i = 0$; $i < $ `GRID_SIZE`; $i{+}{+}$) {
      $\text{RR}.slab.g = \texttt{MAX\_ABS\_G} * (2.0 * i/(\texttt{GRID\_SIZE} - 1.0) - 1.0)$;
      for ($j = 0$; $j < $ `GRID_SIZE`; $j{+}{+}$) {
        ⟨ Generate next albedo using j 165 ⟩
        fill_grid_entry(i, j);
      }
    }
    The_Grid_Initialized = `TRUE`;
    The_Grid_Search = `FIND_AG`;
  }

This code is used in section 124.

168.

⟨ Zero *GG* 168 ⟩ ≡
  $GG\_a = 0.0$;
  $GG\_b = 0.0$;
  $GG\_g = 0.0$;
  $GG\_bs = 0.0$;
  $GG\_ba = 0.0$;

This code is used in sections 163, 167, 170, 172, and 174.

169.   This is quite similar to *Fill_AB_Grid*, with the exception of the that the albedo is held fixed while *b* and *g* are varied.

This routine could also be improved by not recalculating the anisotropy matrix for every point. But this would only end up being a minor performance enhancement if it were fixed.

⟨ Prototype for *Fill_BG_Grid* 169 ⟩ ≡
 void *Fill_BG_Grid*(**struct measure_type** *m*, **struct invert_type** *r*)

This code is used in sections 125 and 170.

170.   ⟨ Definition for *Fill_BG_Grid* 170 ⟩ ≡
 ⟨ Prototype for *Fill_BG_Grid* 169 ⟩
 {
  int *i, j*;
  if (*The_Grid* ≡ Λ) *Allocate_Grid*(*r.search*);
  ⟨ Zero *GG* 168 ⟩
  if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Filling␣BG␣grid\n");
  Set_Calc_State(*m, r*);
  RR.*slab*.*b* = 1.0/32.0;
  RR.*slab*.*a* = RR.*default_a*;
  GG_a = RR.*slab*.*a*;
  for (*i* = 0; *i* < GRID_SIZE; *i*++) {
   RR.*slab*.*b* *= 2;
   for (*j* = 0; *j* < GRID_SIZE; *j*++) {
    RR.*slab*.*g* = MAX_ABS_G * (2.0 * *j*/(GRID_SIZE − 1.0) − 1.0);
    fill_grid_entry(*i, j*);
   }
  }
  The_Grid_Initialized = TRUE;
  The_Grid_Search = FIND_BG;
 }

This code is used in section 124.

171.   This is quite similar to *Fill_BG_Grid*, with the exception of the that the $b_s = \mu_s d$ is held fixed. Here *b* and *g* are varied on the usual grid, but the albedo is forced to take whatever value is needed to ensure that the scattering constant remains fixed.

⟨ Prototype for *Fill_BaG_Grid* 171 ⟩ ≡
 void *Fill_BaG_Grid*(**struct measure_type** *m*, **struct invert_type** *r*)

This code is used in sections 125 and 172.

172.   ⟨ Definition for *Fill_BaG_Grid* 172 ⟩ ≡
  ⟨ Prototype for *Fill_BaG_Grid* 171 ⟩
  {
    int i, j;
    double bs, ba;
    if (*The_Grid* ≡ Λ) *Allocate_Grid*(*r.search*);
    ⟨ Zero *GG* 168 ⟩
    if (*Debug*(DEBUG_GRID)) *fprintf*(*stderr*, "GRID:␣Filling␣BaG␣grid\n");
    Set_Calc_State(*m, r*);
    $ba = 1.0/32.0$;
    $bs = \mathtt{RR}.default\_bs$;
    $GG\_bs = bs$;
    for ($i = 0$; $i < \mathtt{GRID\_SIZE}$; $i{+}{+}$) {
      $ba \mathrel{*}= 2$;
      $ba = exp((\textbf{double}) i/(\mathtt{GRID\_SIZE} - 1.0) * log(1024.0))/16.0$;
      $\mathtt{RR}.slab.b = ba + bs$;
      if ($\mathtt{RR}.slab.b > 0$) $\mathtt{RR}.slab.a = bs/\mathtt{RR}.slab.b$;
      else $\mathtt{RR}.slab.a = 0$;
      for ($j = 0$; $j < \mathtt{GRID\_SIZE}$; $j{+}{+}$) {
        $\mathtt{RR}.slab.g = \mathtt{MAX\_ABS\_G} * (2.0 * j/(\mathtt{GRID\_SIZE} - 1.0) - 1.0)$;
        fill_grid_entry(i, j);
      }
    }
    The_Grid_Initialized = TRUE;
    The_Grid_Search = *FIND_BaG*;
  }
This code is used in section 124.

173.   Very similiar to the above routine. The value of $b_a = \mu_a d$ is held constant.

⟨ Prototype for *Fill_BsG_Grid* 173 ⟩ ≡
  void *Fill_BsG_Grid*(**struct measure_type** m, **struct invert_type** r)
This code is used in sections 125 and 174.

174.   ⟨ Definition for *Fill_BsG_Grid* 174 ⟩ ≡
  ⟨ Prototype for *Fill_BsG_Grid* 173 ⟩
  {
     int i, j;
     double bs, ba;
     if (*The_Grid* ≡ Λ) *Allocate_Grid*(*r.search*);
     ⟨ Zero *GG* 168 ⟩
     Set_Calc_State(*m, r*);
     $bs = 1.0/32.0$;
     $ba = $ RR.*default_ba*;
     $GG\_ba = ba$;
     for ($i = 0$; $i < $ GRID_SIZE; $i{+}{+}$) {
        $bs \mathrel{*}= 2$;
        RR.*slab.b* = $ba + bs$;
        if (RR.*slab.b* > 0) RR.*slab.a* = $bs/$RR.*slab.b*;
        else RR.*slab.a* = 0;
        for ($j = 0$; $j < $ GRID_SIZE; $j{+}{+}$) {
           RR.*slab.g* = MAX_ABS_G $* (2.0 * j/($GRID_SIZE$ - 1.0) - 1.0)$;
           fill_grid_entry(i, j);
        }
     }
     The_Grid_Initialized = TRUE;
     The_Grid_Search = *FIND_BsG*;
  }
This code is used in section 124.

175.   ⟨ Prototype for *Fill_Grid* 175 ⟩ ≡
  void *Fill_Grid*(**struct measure_type** *m*, **struct invert_type** *r*, **int** *force_new*)
This code is used in sections 125 and 176.

176.   ⟨ Definition for *Fill_Grid* 176 ⟩ ≡
  ⟨ Prototype for *Fill_Grid* 175 ⟩
  {
     if (*force_new* ∨ ¬*Same_Calc_State*(*m, r*)) {
        switch (*r.search*) {
        case FIND_AB: *Fill_AB_Grid*(*m, r*);
           break;
        case FIND_AG: *Fill_AG_Grid*(*m, r*);
           break;
        case FIND_BG: *Fill_BG_Grid*(*m, r*);
           break;
        case *FIND_BaG*: *Fill_BaG_Grid*(*m, r*);
           break;
        case *FIND_BsG*: *Fill_BsG_Grid*(*m, r*);
           break;
        default: *AD_error*("Attempt␣to␣fill␣grid␣for␣unknown␣search␣case.");
        }
     }
     Get_Calc_State(&MGRID, &RGRID);
  }
This code is used in section 124.

177.   Calculating R and T.

Calculate_Distance returns the distance between the measured values in MM and the calculated values for the current guess at the optical properties. It assumes that the everything in the local variables MM and RR have been set appropriately.

⟨ Prototype for *Calculate_Distance* 177 ⟩ ≡
    void *Calculate_Distance*(**double** ∗M_R, **double** ∗M_T, **double** ∗*deviation*)

This code is used in sections 125 and 178.

178.   ⟨ Definition for *Calculate_Distance* 178 ⟩ ≡
  ⟨ Prototype for *Calculate_Distance* 177 ⟩
  {
      double *Rc*, *Tc*, *ur1*, *ut1*, *uru*, *utu*;

      if (RR.*slab*.*b* ≤ 1 · 10⁻⁶) RR.*slab*.*b* = 1 · 10⁻⁶;
      RT_Flip(MM.*flip_sample*, RR.*method*.*quad_pts*, &RR.*slab*, &*ur1*, &*ut1*, &*uru*, &*utu*);
      Sp_mu_RT_Flip(MM.*flip_sample*, RR.*slab*.*n_top_slide*, RR.*slab*.*n_slab*, RR.*slab*.*n_bottom_slide*,
          RR.*slab*.*b_top_slide*, RR.*slab*.*b*, RR.*slab*.*b_bottom_slide*, RR.*slab*.*cos_angle*, &*Rc*, &*Tc*);
      if ((¬CALCULATING_GRID ∧ *Debug*(DEBUG_ITERATIONS)) ∨ (CALCULATING_GRID ∧
          Debug(DEBUG_GRID_CALC))) *fprintf*(*stderr*, "␣␣␣␣␣␣␣␣␣");
      Calculate_Distance_With_Corrections(*ur1*, *ut1*, *Rc*, *Tc*, *uru*, *utu*, M_R, M_T, *deviation*);
  }

This code is used in section 124.

179.   ⟨ Prototype for *Calculate_Grid_Distance* 179 ⟩ ≡
    double *Calculate_Grid_Distance*(**int** *i*, **int** *j*)

This code is used in sections 125 and 180.

180. ⟨Definition for *Calculate_Grid_Distance* 180⟩ ≡
  ⟨Prototype for *Calculate_Grid_Distance* 179⟩
  {
    double *ur1*, *ut1*, *uru*, *utu*, *Rc*, *Tc*, *b*, *dev*, LR, LT;
    if (*Debug*(DEBUG_GRID_CALC) ∧ *i* ≡ 0 ∧ *j* ≡ 0) {
      fprintf(*stderr*, "+␣␣␣i␣␣␣j␣");
      fprintf(*stderr*, "␣␣␣␣␣␣a␣␣␣␣␣␣␣␣␣␣b␣␣␣␣␣␣␣␣␣␣g␣␣␣␣␣|");
      fprintf(*stderr*, "␣␣␣␣␣M_R␣␣␣␣␣␣␣␣grid␣␣␣|");
      fprintf(*stderr*, "␣␣␣␣␣M_T␣␣␣␣␣␣␣␣␣grid␣␣␣|␣␣distance\n");
    }
    if (*Debug*(DEBUG_GRID_CALC)) *fprintf*(*stderr*, "g␣%3d␣%3d␣", *i*, *j*);
    b = *The_Grid*[GRID_SIZE ∗ *i* + *j*][B_COLUMN];
    ur1 = *The_Grid*[GRID_SIZE ∗ *i* + *j*][UR1_COLUMN];
    ut1 = *The_Grid*[GRID_SIZE ∗ *i* + *j*][UT1_COLUMN];
    uru = *The_Grid*[GRID_SIZE ∗ *i* + *j*][URU_COLUMN];
    utu = *The_Grid*[GRID_SIZE ∗ *i* + *j*][UTU_COLUMN];
    RR.*slab*.*a* = *The_Grid*[GRID_SIZE ∗ *i* + *j*][A_COLUMN];
    RR.*slab*.*b* = *The_Grid*[GRID_SIZE ∗ *i* + *j*][B_COLUMN];
    RR.*slab*.*g* = *The_Grid*[GRID_SIZE ∗ *i* + *j*][G_COLUMN];
    Sp_mu_RT_Flip(MM.*flip_sample*, RR.*slab*.*n_top_slide*, RR.*slab*.*n_slab*, RR.*slab*.*n_bottom_slide*,
        RR.*slab*.*b_top_slide*, *b*, RR.*slab*.*b_bottom_slide*, RR.*slab*.*cos_angle*, &*Rc*, &*Tc*);
    CALCULATING_GRID = 1;
    Calculate_Distance_With_Corrections(*ur1*, *ut1*, *Rc*, *Tc*, *uru*, *utu*, &LR, &LT, &*dev*);
    CALCULATING_GRID = 0;
    return *dev*;
  }

This code is used in section 124.

181. This is the routine that actually finds the distance. I have factored this part out so that it can be used in the *Near_Grid_Points* routine.

Rc and *Tc* refer to the unscattered (collimated) reflection and transmission.

The only tricky part is to remember that the we are trying to match the measured values. The measured values are affected by sphere parameters and light loss. Since the values UR1 and UT1 are for an infinite slab sample with no light loss, the light loss out the edges must be subtracted. It is these values that are used with the sphere formulas to convert the modified UR1 and UT1 to values for ∗M_R and ∗M_T.

⟨Prototype for *Calculate_Distance_With_Corrections* 181⟩ ≡
  void *Calculate_Distance_With_Corrections*(**double** UR1, **double** UT1, **double** *Rc*, **double** *Tc*, **double**
      URU, **double** UTU, **double** ∗M_R, **double** ∗M_T, **double** ∗*dev*)

This code is used in sections 125 and 182.

182. ⟨Definition for *Calculate_Distance_With_Corrections* 182⟩ ≡
  ⟨Prototype for *Calculate_Distance_With_Corrections* 181⟩
  {
    ⟨Determine calculated light to be used 183⟩
    switch (MM.*num_spheres*) {
    case 0: ⟨Calc M_R and M_T for no spheres 185⟩
      break;
    case 1:
      if (MM.*method* ≡ COMPARISON) {
        ⟨Calc M_R and M_T for dual beam sphere 189⟩
      }
      else {
        ⟨Calc M_R and M_T for single beam sphere 186⟩
      }
      break;
    case 2: ⟨Calc M_R and M_T for two spheres 190⟩
      break;
    default: *fprintf*(*stderr*, "Bad␣number␣of␣spheres␣=␣%d\n", MM.*num_spheres*);
      exit(EXIT_FAILURE);
    }
    ⟨Calculate the deviation 191⟩
    ⟨Print diagnostics 194⟩
  }

This code is used in section 124.

183. The calculated values for M_R and M_T must be adapted to match the measurements. The diffuse light URU and UTU are used to determine the gain from the sphere. They're only modified by the lost light calculation. All values can become slightly negative because the Monte Carlo is noisy. Negative values are set to zero.

⟨Determine calculated light to be used 183⟩ ≡
  double *UR1_calc*, *UT1_calc*, *URU_calc*, *UTU_calc*;

  $URU_calc = $ URU $-$ MM.*uru_lost*;
  if ($URU\_calc < 0$) $URU\_calc = 0$;
  $UTU_calc = $ UTU $-$ MM.*utu_lost*;
  if ($UTU\_calc < 0$) $UTU\_calc = 0$;

See also section 184.

This code is used in section 182.

184. The measurements for UR1 and UT1 need to be modified to accommodate light that misses the detector either because it is intentionally not collected (unscattered light) or it leaks out (lost light). Since none of the light that leaks out could be unscattered light, these two are independent of one another.

The code allows for some of the light to hit the sphere wall first; these effects are accounted for in the sphere code below.

⟨Determine calculated light to be used 183⟩ +≡
  $UR1_calc = $ UR1 $- (1.0 - $ MM.*fraction_of_rc_in_mr*$) * Rc - $ MM.*ur1_lost*;
  if ($UR1\_calc < 0$) $UR1\_calc = 0$;
  $UT1_calc = $ UT1 $- (1.0 - $ MM.*fraction_of_tc_in_mt*$) * Tc - $ MM.*ut1_lost*;
  if ($UT1\_calc < 0$) $UT1\_calc = 0$;

185.   When no spheres are used, then no corrections can or need to be made. The lost light estimates in MM.*ur1_lost* and MM.*ut1_lost* should be zero and so the values for *UR1_calc* and *UT1_calc* properly account for the presence or absence of unscattered light.

⟨ Calc M_R and M_T for no spheres 185 ⟩ ≡
```
{
    *M_R = UR1_calc;
    *M_T = UT1_calc;
}
```
This code is used in section 182.

186.   In a reflection experiment, some fraction f of the incident light P_i might hit the wall first. Thus the incident power on the sample is $(1-f)P_i$ and the incident power on the sphere wall will be fP_i. The diffuse reflection entering the sphere depends on the presence of a baffle.

If a baffle is present then

$$P_d = [a_d(1-a_e)r_w P_i] \cdot (r_s^{\text{direct}} * (1-f) + r_w f) \cdot G(r_s)$$

and when there is no baffle

$$P_d = [a_d P_i] \cdot (r_s^{\text{direct}} * (1-f) + r_w f) \cdot G(r_s)$$

Since the quantities in square brackets are identical for $R(r_s^{\text{direct}}, r_s)$, $R(0,0)$, and $R(r_{\text{std}}, r_{\text{std}})$. Consequently they cancel out when calculating the normalized reflection measurement

$$M_R = r_{\text{std}} \cdot \frac{R(r_s^{\text{direct}}, r_s) - R(0,0)}{R(r_{\text{std}}, r_{\text{std}}) - R(0,0)}$$

This leads to the following code for M_R

⟨ Calc M_R and M_T for single beam sphere 186 ⟩ ≡
```
double P_std, P, P_0, G, G_0, G_std;
int tmp;

G_0 = Gain(REFLECTION_SPHERE, MM, 0.0);
G = Gain(REFLECTION_SPHERE, MM, URU_calc);
G_std = Gain(REFLECTION_SPHERE, MM, MM.rstd_r);
P = G * (UR1_calc * (1 − MM.f_r) + MM.f_r * MM.rw_r);
P_std = G_std * (MM.rstd_r * (1 − MM.f_r) + MM.f_r * MM.rw_r);
P_0 = G_0 * (MM.f_r * MM.rw_r);
*M_R = MM.rstd_r * (P − P_0)/(P_std − P_0);
```
See also section 188.

This code is used in section 182.

187.   In a transmission experiment, the calculations are simpler and harder. First, the value of $T(0,0) = 0$ because computationally, there is no dark noise in the detector nor any possible light leakage from the outside into the sphere. This simplifies

$$M_T = r_0 \cdot \frac{T(t_s^{\text{direct}}, r_s) - T(0,0)}{T(t_{\text{std}}, r_{\text{std}}) - T(0,0)}$$

to

$$M_T = r_0 \cdot \frac{T(t_s^{\text{direct}}, r_s)}{T(t_{\text{std}}, r_{\text{std}})}$$

where r_0 might be r_{std} or r_w for the transmission sphere.

We do not need to worry about some fraction of the incident light P_i hitting the sphere wall before interacting with the sample.

Finally, if the transmission sphere has a baffle present for the sample measurement, then it is no longer in the right place and diffuse light entering the sphere is just $[a_d P_i] r_0$

When a baffle is present then the light falling on the detector in a transmission experiment is

$$P_d = T(t_s^{\text{direct}}, r_s) = [a_d P_i](1 - a_e) r_w t_s^{\text{direct}} G(r_s)$$

and with no baffle present

$$P_d = T(t_s^{\text{direct}}, r_s) = [a_d P_i] t_s^{\text{direct}} G(r_s)$$

188.   The normalization $T(t_{\mathrm{std}}, r_{\mathrm{std}})$ can be measured in two ways.

When transmission measurements are made, typically the empty port (the one that let the light into the sphere for the reflection measurement) is filled with a white port cover whose reflectance matches the rest of the sphere. In this case, the natural way to make the standard transmission measurement is to shine the beam through the empty sample port onto the back side of the sphere. If the baffle was properly placed for the transmission experiment (between the sample port and the detector) then the calibration transmission measurement is now made in a sphere without a baffle. In addition, the beam is diffused only after bouncing off the sphere wall. Therefore the power falling on the detector is

$$P_{\mathrm{std}} = T(1.0, r_w) = [a_d P_i] r_w G(0)$$

An alternate method is when there is an empty port in the sphere (perhaps to allow the unscattered light to leave). In any case, the calibration measurement is done by removing the sample and placing the calibration standare in what used to be the empty port. In this case, the roles of the sample and empty ports have switched. Consequently, the areas of the sample and empty ports must be swapped before the gain is calculated.

$$P_{\mathrm{std}} = T(1.0, r_{\mathrm{std}}) = [a_d P_i] r_{\mathrm{std}} G(r_{\mathrm{std}})$$

Note that r_w or r_{std} in P_{std} term cancel with r_0 when calculating M_T. Further, the quantities $a_d P_i$ also cancel.

$\langle$ Calc `M_R` and `M_T` for single beam sphere $186 \rangle + \equiv$
  $P = UT1\_calc * Gain(\texttt{TRANSMISSION\_SPHERE}, \texttt{MM}, URU\_calc);$
  if $(\texttt{MM}.baffle\_t)$ $P *= (1 - \texttt{MM}.ae\_t) * \texttt{MM}.rw\_t;$
  $tmp = \texttt{MM}.baffle\_t;$
  $\texttt{MM}.baffle\_t = \texttt{FALSE};$
  if $(\texttt{MM}.ae\_t \equiv 0)$ {
    $P\_std = Gain(\texttt{TRANSMISSION\_SPHERE}, \texttt{MM}, 0);$
  }
  else {
    $\texttt{SWAP}(\texttt{MM}.ae\_t, \texttt{MM}.as\_t);$
    $P\_std = Gain(\texttt{TRANSMISSION\_SPHERE}, \texttt{MM}, \texttt{MM}.rstd\_t);$
    $\texttt{SWAP}(\texttt{MM}.ae\_t, \texttt{MM}.as\_t);$
  }
  $\texttt{MM}.baffle\_t = tmp;$
  $*\texttt{M\_T} = P/P\_std;$

189.   The dual beam case is different because the sphere efficiency is equivalent for measurement of light hitting the sample first or hitting the reference standard first. The dual beam measurement should report the ratio of these two reflectance measurements, thereby eliminating the need to calculate the sphere gain.

The only correction that needs to be made have already been made, namely subtracting the `UR1` or `UT1` lost light and also accounting for whether or not unscattered light is collected.

Originally, I had a bunch of calculations trying to account for light that hits the sphere wall first. Since the exact details of how a dual beam spectrometer reports its measurements is unknown, it makes no sense to try and account for it.

$\langle$ Calc `M_R` and `M_T` for dual beam sphere $189 \rangle \equiv$
  {
    $*\texttt{M\_R} = UR1\_calc;$
    $*\texttt{M\_T} = UT1\_calc;$
  }
This code is used in section 182.

190. When two integrating spheres are present then the double integrating sphere formulas are slightly more complicated.

The normalized sphere measurements for two spheres are

$$M_R = \frac{R(r_s^{\,\text{direct}}, r_s, t_s^{\,\text{direct}}, t_s) - R(0,0,0,0)}{R(r_\text{std}, r_\text{std}, 0, 0) - R(0,0,0,0)}$$

and

$$M_T = \frac{T(r_s^{\,\text{direct}}, r_s, t_s^{\,\text{direct}}, t_s) - T(0,0,0,0)}{T(0,0,1,1) - T(0,0,0,0)}$$

Note that R_0 and T_0 will be zero unless one has explicitly set the fraction $m.f\_r$ or $m.f\_t$ to be non-zero.

⟨ Calc M_R and M_T for two spheres 190 ⟩ ≡

```
{
    double R_0, T_0;
    R_0 = Two_Sphere_R(MM, 0, 0, 0, 0);
    T_0 = Two_Sphere_T(MM, 0, 0, 0, 0);
    *M_R = MM.rstd_r * (Two_Sphere_R(MM, UR1_calc, URU_calc, UT1_calc,
        UTU_calc) − R_0)/(Two_Sphere_R(MM, MM.rstd_r, MM.rstd_r, 0, 0) − R_0);
    *M_T = (Two_Sphere_T(MM, UR1_calc, URU_calc, UT1_calc, UTU_calc) − T_0)/(Two_Sphere_T(MM, 0, 0,
        1, 1) − T_0);
}
```

This code is used in section 182.

191. There are at least three things that need to be considered here. First, the number of measurements. Second, is the metric is relative or absolute. And third, is the albedo fixed at zero which means that the transmission measurement should be used instead of the reflection measurement.

⟨ Calculate the deviation 191 ⟩ ≡

```
if (RR.search ≡ FIND_A ∨ RR.search ≡ FIND_G ∨ RR.search ≡ FIND_B ∨ RR.search ≡ FIND_Bs ∨ RR.search ≡
        FIND_Ba) {
    ⟨ One parameter deviation 192 ⟩
}
else {
    ⟨ Two parameter deviation 193 ⟩
}
```

This code is used in section 182.

192. This part was slightly tricky. The crux of the problem was to decide if the transmission or the reflection was trustworthy. After looking a bunches of measurements, I decided that the transmission measurement was almost always more reliable. So when there is just a single measurement known, then use the total transmission if it exists.

⟨ One parameter deviation 192 ⟩ ≡

```
if (MM.m_t > 0) {
    if (RR.metric ≡ RELATIVE) *dev = fabs(MM.m_t − *M_T)/(MM.m_t + ABIT);
    else *dev = fabs(MM.m_t − *M_T);
}
else {
    if (RR.metric ≡ RELATIVE) *dev = fabs(MM.m_r − *M_R)/(MM.m_r + ABIT);
    else *dev = fabs(MM.m_r − *M_R);
}
```

This code is used in section 191.

193.   This stuff happens when we are doing two parameter searches. In these cases there should be information in both R and T. The distance should be calculated using the deviation from both. The albedo stuff might be able to be take out. We'll see.

⟨ Two parameter deviation 193 ⟩ ≡
```
  if (RR.metric ≡ RELATIVE) {
    if (MM.m_t > ABIT) *dev = T_TRUST_FACTOR * fabs(MM.m_t − *M_T)/(UTU_calc + ABIT);
    if (RR.default_a ≠ 0) {
      *dev += fabs(MM.m_r − *M_R)/(URU_calc + ABIT);
    }
  }
  else {
    *dev = T_TRUST_FACTOR * fabs(MM.m_t − *M_T);
    if (RR.default_a ≠ 0)  *dev += fabs(MM.m_r − *M_R);
  }
```
This code is used in section 191.

194.   This is here so that I can figure out why the program is not converging. This is a little convoluted so that the global constants at the top of this file interact properly.

⟨ Print diagnostics 194 ⟩ ≡
```
  if ((Debug(DEBUG_ITERATIONS) ∧ ¬CALCULATING_GRID) ∨
        (Debug(DEBUG_GRID_CALC) ∧ CALCULATING_GRID)) {
    fprintf(stderr, "%10.5f␣%10.5f␣%10.5f␣|", RR.slab.a, RR.slab.b, RR.slab.g);
    fprintf(stderr, "␣%10.5f␣%10.5f␣|", MM.m_r, *M_R);
    fprintf(stderr, "␣%10.5f␣%10.5f␣|", MM.m_t, *M_T);
    fprintf(stderr, "%10.3f\n", *dev);
  }
```
This code is used in section 182.

195.   ⟨ Prototype for Find_AG_fn 195 ⟩ ≡
double Find_AG_fn(**double** x[])

This code is used in sections 125 and 196.

196.   ⟨ Definition for Find_AG_fn 196 ⟩ ≡
⟨ Prototype for Find_AG_fn 195 ⟩
```
  {
    double m_r, m_t, deviation;
    RR.slab.a = acalc2a(x[1]);
    RR.slab.g = gcalc2g(x[2]);
    Calculate_Distance(&m_r, &m_t, &deviation);
    return deviation;
  }
```
This code is used in section 124.

197.   ⟨ Prototype for Find_AB_fn 197 ⟩ ≡
double Find_AB_fn(**double** x[])

This code is used in sections 125 and 198.

198.   ⟨Definition for *Find_AB_fn* 198⟩ ≡
  ⟨Prototype for *Find_AB_fn* 197⟩
  {
    double m_r, m_t, *deviation*;
    RR.*slab*.*a* = *acalc2a*(*x*[1]);
    RR.*slab*.*b* = *bcalc2b*(*x*[2]);
    Calculate_Distance(&m_r, &m_t, &*deviation*);
    return *deviation*;
  }

This code is used in section 124.

199.   ⟨Prototype for *Find_Ba_fn* 199⟩ ≡
  double *Find_Ba_fn*(**double** *x*)

This code is used in sections 125 and 200.

200.   This is tricky only because the value in RR.*slab*.*b* is used to hold the value of *bs* or $d \cdot \mu_s$. It must be switched to the correct value for the optical thickness and then switched back at the end of the routine.

⟨Definition for *Find_Ba_fn* 200⟩ ≡
  ⟨Prototype for *Find_Ba_fn* 199⟩
  {
    double m_r, m_t, *deviation*, *ba*, *bs*;
    bs = RR.*slab*.*b*;
    ba = *bcalc2b*(*x*);
    RR.*slab*.*b* = *ba* + *bs*;   /∗ unswindle ∗/
    RR.*slab*.*a* = *bs*/(*ba* + *bs*);
    Calculate_Distance(&m_r, &m_t, &*deviation*);
    RR.*slab*.*b* = *bs*;   /∗ swindle ∗/
    return *deviation*;
  }

This code is used in section 124.

201.   See the comments for the *Find_Ba_fn* routine above. Play the same trick but use *ba*.

⟨Prototype for *Find_Bs_fn* 201⟩ ≡
  double *Find_Bs_fn*(**double** *x*)

This code is used in sections 125 and 202.

202.   ⟨Definition for *Find_Bs_fn* 202⟩ ≡
  ⟨Prototype for *Find_Bs_fn* 201⟩
  {
    double m_r, m_t, *deviation*, *ba*, *bs*;
    ba = RR.*slab*.*b*;   /∗ unswindle ∗/
    bs = *bcalc2b*(*x*);
    RR.*slab*.*b* = *ba* + *bs*;
    RR.*slab*.*a* = *bs*/(*ba* + *bs*);
    Calculate_Distance(&m_r, &m_t, &*deviation*);
    RR.*slab*.*b* = *ba*;   /∗ swindle ∗/
    return *deviation*;
  }

This code is used in section 124.

203.   ⟨ Prototype for $Find\_A\_fn$ 203 ⟩ ≡
   double $Find\_A\_fn($**double** $x)$
This code is used in sections 125 and 204.

204.   ⟨ Definition for $Find\_A\_fn$ 204 ⟩ ≡
   ⟨ Prototype for $Find\_A\_fn$ 203 ⟩
   {
      double $m\_r, m\_t, deviation$;
      RR.$slab.a = acalc2a(x)$;
      $Calculate\_Distance(\&m\_r, \&m\_t, \&deviation)$;
      return $deviation$;
   }
This code is used in section 124.

205.   ⟨ Prototype for $Find\_B\_fn$ 205 ⟩ ≡
   double $Find\_B\_fn($**double** $x)$
This code is used in sections 125 and 206.

206.   ⟨ Definition for $Find\_B\_fn$ 206 ⟩ ≡
   ⟨ Prototype for $Find\_B\_fn$ 205 ⟩
   {
      double $m\_r, m\_t, deviation$;
      RR.$slab.b = bcalc2b(x)$;
      $Calculate\_Distance(\&m\_r, \&m\_t, \&deviation)$;
      return $deviation$;
   }
This code is used in section 124.

207.   ⟨ Prototype for $Find\_G\_fn$ 207 ⟩ ≡
   double $Find\_G\_fn($**double** $x)$
This code is used in sections 125 and 208.

208.   ⟨ Definition for $Find\_G\_fn$ 208 ⟩ ≡
   ⟨ Prototype for $Find\_G\_fn$ 207 ⟩
   {
      double $m\_r, m\_t, deviation$;
      RR.$slab.g = gcalc2g(x)$;
      $Calculate\_Distance(\&m\_r, \&m\_t, \&deviation)$;
      return $deviation$;
   }
This code is used in section 124.

209.   ⟨ Prototype for $Find\_BG\_fn$ 209 ⟩ ≡
   double $Find\_BG\_fn($**double** $x[\,])$
This code is used in sections 125 and 210.

210.   ⟨ Definition for *Find_BG_fn* 210 ⟩ ≡
  ⟨ Prototype for *Find_BG_fn* 209 ⟩
  {
    double *m_r*, *m_t*, *deviation*;
    RR.*slab*.*b* = *bcalc2b*(*x*[1]);
    RR.*slab*.*g* = *gcalc2g*(*x*[2]);
    RR.*slab*.*a* = RR.*default_a*;
    Calculate_Distance(&*m_r*, &*m_t*, &*deviation*);
    return *deviation*;
  }

This code is used in section 124.

211.   For this function the first term $x[1]$ will contain the value of $\mu_s d$, the second term will contain the anisotropy. Of course the first term is in the bizarre calculation space and needs to be translated back into normal terms before use. We just at the scattering back on and voilá we have a useable value for the optical depth.

⟨ Prototype for *Find_BaG_fn* 211 ⟩ ≡
  double *Find_BaG_fn*(**double** *x*[ ])

This code is used in sections 125 and 212.

212.   ⟨ Definition for *Find_BaG_fn* 212 ⟩ ≡
  ⟨ Prototype for *Find_BaG_fn* 211 ⟩
  {
    double *m_r*, *m_t*, *deviation*;
    RR.*slab*.*b* = *bcalc2b*(*x*[1]) + RR.*default_bs*;
    if (RR.*slab*.*b* ≤ 0) RR.*slab*.*a* = 0;
    else RR.*slab*.*a* = RR.*default_bs*/RR.*slab*.*b*;
    RR.*slab*.*g* = *gcalc2g*(*x*[2]);
    Calculate_Distance(&*m_r*, &*m_t*, &*deviation*);
    return *deviation*;
  }

This code is used in section 124.

213.   ⟨ Prototype for *Find_BsG_fn* 213 ⟩ ≡
  double *Find_BsG_fn*(**double** *x*[ ])

This code is used in sections 125 and 214.

214.   ⟨ Definition for *Find_BsG_fn* 214 ⟩ ≡
  ⟨ Prototype for *Find_BsG_fn* 213 ⟩
  {
    double *m_r*, *m_t*, *deviation*;
    RR.*slab*.*b* = *bcalc2b*(*x*[1]) + RR.*default_ba*;
    if (RR.*slab*.*b* ≤ 0) RR.*slab*.*a* = 0;
    else RR.*slab*.*a* = 1.0 − RR.*default_ba*/RR.*slab*.*b*;
    RR.*slab*.*g* = *gcalc2g*(*x*[2]);
    Calculate_Distance(&*m_r*, &*m_t*, &*deviation*);
    return *deviation*;
  }

This code is used in section 124.

215.   Routine to figure out if the light loss exceeds what is physically possible. Returns the descrepancy betwreent the current values and the maximum possible values for the the measurements m_r and m_t.

⟨ Prototype for *maxloss* 215 ⟩ ≡
  double *maxloss* (**double** f)

This code is used in sections 125 and 216.

216.   ⟨ Definition for *maxloss* 216 ⟩ ≡
  ⟨ Prototype for *maxloss* 215 ⟩
  {
    struct measure_type m_old ;
    struct invert_type r_old ;
    double $m\_r, m\_t, deviation$;

    $Get\_Calc\_State(\&m\_old, \&r\_old)$;
    $\mathtt{RR}.slab.a = 1.0$;
    $\mathtt{MM}.ur1\_lost \mathrel{*}= f$;
    $\mathtt{MM}.ut1\_lost \mathrel{*}= f$;
    $Calculate\_Distance(\&m\_r, \&m\_t, \&deviation)$;
    $Set\_Calc\_State(m\_old, r\_old)$;
    $deviation = ((\mathtt{MM}.m\_r + \mathtt{MM}.m\_t) - (m\_r + m\_t))$;
    return *deviation* ;
  }

This code is used in section 124.

217.   This checks the two light loss values $ur1\_loss$ and $ut1\_loss$ to see if they exceed what is physically possible. If they do, then these values are replaced by a couple that are the maximum possible for the current values in m and r.

⟨ Prototype for *Max_Light_Loss* 217 ⟩ ≡
  void *Max_Light_Loss* (**struct measure_type** m, **struct invert_type** r, **double** $*ur1\_loss$, **double** $*ut1\_loss$)

This code is used in sections 125 and 218.

218.   ⟨ Definition for Max_Light_Loss 218 ⟩ ≡
  ⟨ Prototype for Max_Light_Loss 217 ⟩
  {
    struct measure_type m_old;
    struct invert_type r_old;

    $*ur1\_loss = m.ur1\_lost$;
    $*ut1\_loss = m.ut1\_lost$;
    if $(Debug(\texttt{DEBUG\_LOST\_LIGHT}))$
      $fprintf(stderr, \texttt{"\\nlost␣before␣ur1=\%7.5f,␣ut1=\%7.5f\\n"}, *ur1\_loss, *ut1\_loss)$;
    $Get\_Calc\_State(\&m\_old, \&r\_old)$;
    $Set\_Calc\_State(m, r)$;
    if $(maxloss(1.0) * maxloss(0.0) < 0)$ {
      double $frac$;

      $frac = zbrent(maxloss, 0.00, 1.0, 0.001)$;
      $*ur1\_loss = m.ur1\_lost * frac$;
      $*ut1\_loss = m.ut1\_lost * frac$;
    }
    $Set\_Calc\_State(m\_old, r\_old)$;
    if $(Debug(\texttt{DEBUG\_LOST\_LIGHT}))$
      $fprintf(stderr, \texttt{"lost␣after␣␣ur1=\%7.5f,␣ut1=\%7.5f\\n"}, *ur1\_loss, *ut1\_loss)$;
  }
This code is used in section 124.

219.   this is currently unused

$\langle$ Unused diffusion fragment 219 $\rangle \equiv$

  typedef struct {

    double f;

    double $aprime$;

    double $bprime$;

    double $gprime$;

    double $boundary\_method$;

    double n_top;

    double n_bottom;

    double $slide\_top$;

    double $slide\_bottom$;

    double `F0`;

    double $depth$;

    double $Exact\_coll\_flag$;

  } **slabtype**;

  static void `DE_RT`(**int** $nfluxes$, **AD_slab_type** $slab$, **double** $*$`UR1`, **double** $*$`UT1`, **double** $*$`URU`, **double**

       $*$`UTU`)

  {

    slabtype s;

    double rp, tp, rs, ts;

    $s.f = slab.g * slab.g$;

    $s.gprime = slab.g/(1 + slab.g)$;

    $s.aprime = (1 - s.f) * slab.a/(1 - slab.a * s.f)$;

    $s.bprime = (1 - slab.a * s.f) * slab.b$;

    $s.boundary\_method = Egan$;

    $s.n\_top = slab.n\_slab$;

    $s.n\_bottom = slab.n\_slab$;

    $s.slide\_top = slab.n\_top\_slide$;

    $s.slide\_bottom = slab.n\_bottom\_slide$;

    $s.$`F0`$ = 1/$`M_PI`;

    $s.depth = 0.0$;

    $s.Exact_coll_flag = $ `FALSE`;

    if (`MM`.$illumination \equiv collimated$) {

      $compute\_R\_and\_T(\&s, 1.0, \&rp, \&rs, \&tp, \&ts)$;

      $*$`UR1`$ = rp + rs$;

      $*$`UT1`$ = tp + ts$;

      $*$`URU`$ = 0.0$;

      $*$`UTU`$ = 0.0$;

      return;

    }

    $quad\_Dif\_Calc\_R\_and\_T(\&s, \&rp, \&rs, \&tp, \&ts)$;

    $*$`URU`$ = rp + rs$;

    $*$`UTU`$ = tp + ts$;

    $*$`UR1`$ = 0.0$;

    $*$`UT1`$ = 0.0$;

  }

220. IAD Find. March 1995. Incorporated the *quick_guess* algorithm for low albedos.

⟨ `iad_find.c` 220 ⟩ ≡
#**include** `<math.h>`
#**include** `<stdio.h>`
#**include** `<stdlib.h>`
#**include** `"ad_globl.h"`
#**include** `"nr_util.h"`
#**include** `"nr_mnbrk.h"`
#**include** `"nr_brent.h"`
#**include** `"nr_amoeb.h"`
#**include** `"iad_type.h"`
#**include** `"iad_util.h"`
#**include** `"iad_calc.h"`
#**include** `"iad_find.h"`
#**define** `NUMBER_OF_GUESSES` 10
  guess_type *guess* [`NUMBER_OF_GUESSES`];

  int *compare_guesses* (**const void** ∗*p1*, **const void** ∗*p2*)
  {
    guess_type ∗*g1* = (**guess_type** ∗) *p1*;
    guess_type ∗*g2* = (**guess_type** ∗) *p2*;

    if (*g1*→*distance* < *g2*→*distance*) **return** −1;
    else if (*g1*→*distance* ≡ *g2*→*distance*) **return** 0;
    else return 1;
  }
  ⟨ Definition for *U_Find_Ba* 234 ⟩
  ⟨ Definition for *U_Find_Bs* 232 ⟩
  ⟨ Definition for *U_Find_A* 236 ⟩
  ⟨ Definition for *U_Find_B* 240 ⟩
  ⟨ Definition for *U_Find_G* 238 ⟩
  ⟨ Definition for *U_Find_AG* 243 ⟩
  ⟨ Definition for *U_Find_AB* 223 ⟩
  ⟨ Definition for *U_Find_BG* 248 ⟩
  ⟨ Definition for *U_Find_BaG* 254 ⟩
  ⟨ Definition for *U_Find_BsG* 259 ⟩

221. All the information that needs to be written to the header file `iad_find.h`. This eliminates the need to maintain a set of header files as well.

⟨ `iad_find.h` 221 ⟩ ≡
  ⟨ Prototype for *U_Find_Ba* 233 ⟩;
  ⟨ Prototype for *U_Find_Bs* 231 ⟩;
  ⟨ Prototype for *U_Find_A* 235 ⟩;
  ⟨ Prototype for *U_Find_B* 239 ⟩;
  ⟨ Prototype for *U_Find_G* 237 ⟩;
  ⟨ Prototype for *U_Find_AG* 242 ⟩;
  ⟨ Prototype for *U_Find_AB* 222 ⟩;
  ⟨ Prototype for *U_Find_BG* 247 ⟩;
  ⟨ Prototype for *U_Find_BaG* 253 ⟩;
  ⟨ Prototype for *U_Find_BsG* 258 ⟩;

222.   Fixed Anisotropy.
This is the most common case.

⟨ Prototype for *U_Find_AB* 222 ⟩ ≡
   void *U_Find_AB*(**struct measure_type** *m*, **struct invert_type** *∗r*)
This code is used in sections 221 and 223.

223.   ⟨ Definition for *U_Find_AB* 223 ⟩ ≡
   ⟨ Prototype for *U_Find_AB* 222 ⟩
   {
      ⟨ Allocate local simplex variables 224 ⟩
      if (*Debug*(DEBUG_SEARCH)) {
         fprintf(*stderr*, "SEARCH:␣Using␣U_Find_AB()");
         fprintf(*stderr*, "␣(mu=%6.4f)", *r→slab.cos_angle*);
         if (*r→default_g* ≠ UNINITIALIZED) *fprintf*(*stderr*, "␣␣default_g␣=␣%8.5f", *r→default_g*);
         fprintf(*stderr*, "\n");
      }
      r→slab.g = (*r→default_g* ≡ UNINITIALIZED) ? 0 : *r→default_g*;
      Set_Calc_State(*m*, *∗r*);
      ⟨ Get the initial *a*, *b*, and *g* 225 ⟩
      ⟨ Initialize the nodes of the *a* and *b* simplex 226 ⟩
      ⟨ Evaluate the *a* and *b* simplex at the nodes 227 ⟩
      amoeba(*p*, *y*, 2, *r→tolerance*, *Find_AB_fn*, &*r→AD_iterations*);
      ⟨ Choose the best node of the *a* and *b* simplex 228 ⟩
      ⟨ Free simplex data structures 230 ⟩
      ⟨ Put final values in result 229 ⟩
   }
This code is used in section 220.

224.   To use the simplex algorithm, we need to vectors and a matrix.

⟨ Allocate local simplex variables 224 ⟩ ≡
   int *i*, *i_best*, *j_best*;
   double *∗x*, *∗y*, *∗∗p*;
   x = *dvector*(1, 2);
   y = *dvector*(1, 3);
   p = *dmatrix*(1, 3, 1, 2);
This code is used in sections 223, 243, 248, 254, and 259.

225.   Just get the optimal optical properties to start the search process.

I had to add the line that tests to make sure the albedo is greater than 0.2 because the grid just does not work so well in this case. The problem is that for low albedos there is really very little information about the anisotropy available. This change was also made in the analagous code for a and b.

⟨ Get the initial a, b, and g 225 ⟩ ≡
```
  {      /* double a3,b3,g3; */
    size_t count = NUMBER_OF_GUESSES;      /* distance to last result */

    abg_distance(r→slab.a, r→slab.b, r→slab.g, &(guess[0]));
    if (¬Valid_Grid(m, r→search))  Fill_Grid(m, *r, 1);      /* distance to nearest grid point */
    Near_Grid_Points(m.m_r, m.m_t, r→search, &i_best, &j_best);
    Grid_ABG(i_best, j_best, &(guess[1]));
    Grid_ABG(i_best + 1, j_best, &(guess[2]));
    Grid_ABG(i_best − 1, j_best, &(guess[3]));
    Grid_ABG(i_best, j_best + 1, &(guess[4]));
    Grid_ABG(i_best, j_best − 1, &(guess[5]));
    Grid_ABG(i_best + 1, j_best + 1, &(guess[6]));
    Grid_ABG(i_best − 1, j_best − 1, &(guess[7]));
    Grid_ABG(i_best + 1, j_best − 1, &(guess[8]));
    Grid_ABG(i_best − 1, j_best + 1, &(guess[9]));
    qsort((void *) guess, count, sizeof(guess_type), compare_guesses);
    if (Debug(DEBUG_BEST_GUESS)) {
      int k;

      fprintf(stderr, "BEST:␣GRID␣GUESSES\n");
      fprintf(stderr, "BEST:␣␣k␣␣␣␣␣␣␣albedo␣␣␣␣␣␣␣␣␣␣␣␣b␣␣␣␣␣␣␣␣␣␣␣␣g␣␣␣␣distance\n");
      for (k = 0;  k ≤ 6;  k++) {
        fprintf(stderr, "BEST:%3d␣␣", k);
        fprintf(stderr, "%10.5f␣", guess[k].a);
        fprintf(stderr, "%10.5f␣", guess[k].b);
        fprintf(stderr, "%10.5f␣", guess[k].g);
        fprintf(stderr, "%10.5f\n", guess[k].distance);
      }
    }
  }
```

226.   ⟨Initialize the nodes of the a and b simplex 226⟩ ≡
  {
    int k, kk;
    $p[1][1] = a2acalc(guess[0].a)$;
    $p[1][2] = b2bcalc(guess[0].b)$;
    for $(k = 1; \ k < 7; \ k{+}{+})$ {
      if $(guess[0].a \neq guess[k].a)$ **break**;
    }
    $p[2][1] = a2acalc(guess[k].a)$;
    $p[2][2] = b2bcalc(guess[k].b)$;
    for $(kk = 1; \ kk < 7; \ kk{+}{+})$ {
      if $(k \equiv kk)$ **continue**;
      if $(guess[0].b \neq guess[kk].b \vee guess[k].b \neq guess[kk].b)$ **break**;
    }
    $p[3][1] = a2acalc(guess[kk].a)$;
    $p[3][2] = b2bcalc(guess[kk].b)$;
    if $(Debug(\texttt{DEBUG\_BEST\_GUESS}))$ {
      $fprintf(stderr,$ "−−−\n"$)$;
      $fprintf(stderr,$ "BEST:␣<1>␣"$)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[0].a)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[0].b)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[0].g)$;
      $fprintf(stderr,$ "%10.5f\n"$, guess[0].distance)$;
      $fprintf(stderr,$ "BEST:␣<2>␣"$)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[k].a)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[k].b)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[k].g)$;
      $fprintf(stderr,$ "%10.5f\n"$, guess[k].distance)$;
      $fprintf(stderr,$ "BEST:␣<3>␣"$)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[kk].a)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[kk].b)$;
      $fprintf(stderr,$ "%10.5f␣"$, guess[kk].g)$;
      $fprintf(stderr,$ "%10.5f\n"$, guess[kk].distance)$;
      $fprintf(stderr,$ "\n"$)$;
    }
  }

This code is used in section 223.

227.   ⟨Evaluate the a and b simplex at the nodes 227⟩ ≡
  for $(i = 1; \ i \leq 3; \ i{+}{+})$ {
    $x[1] = p[i][1]$;
    $x[2] = p[i][2]$;
    $y[i] = Find\_AB\_fn(x)$;
  }

This code is used in section 223.

228.   ⟨ Choose the best node of the a and b simplex 228 ⟩ ≡
 $r\text{→}final\_distance = 10;$
 for $(i = 1;\ i \leq 3;\ i\text{++})$ {
  if $(y[i] < r\text{→}final\_distance)$ {
   $r\text{→}slab.a = acalc2a(p[i][1]);$
   $r\text{→}slab.b = bcalc2b(p[i][2]);$
   $r\text{→}final\_distance = y[i];$
  }
 }

This code is used in section 223.

229.   ⟨ Put final values in result 229 ⟩ ≡
 $r\text{→}a = r\text{→}slab.a;$
 $r\text{→}b = r\text{→}slab.b;$
 $r\text{→}g = r\text{→}slab.g;$
 $r\text{→}found = (r\text{→}tolerance \leq r\text{→}final\_distance);$
 $Set\_Calc\_State(m, *r);$

This code is used in sections 223, 232, 234, 236, 238, 240, 243, 248, 254, and 259.

230.   Since we allocated these puppies, we got to get rid of them.

⟨ Free simplex data structures 230 ⟩ ≡
 $free\_dvector(x, 1, 2);$
 $free\_dvector(y, 1, 3);$
 $free\_dmatrix(p, 1, 3, 1, 2);$

This code is used in sections 223, 243, 248, 254, and 259.

231. Fixed Absorption and Anisotropy.   Typically, this routine is called when the absorption coefficient is known, the anisotropy is known, and the physical thickness of the sample is known. This routine calculates the varies the scattering coefficient until the measurements are matched.

This was written for Ted Moffitt to analyze some intralipid data. We wanted to know what the scattering coefficient of the Intralipid was and made total transmission measurements through a sample with a fixed physical thickness. We did not make reflection measurements because the light source diverged too much, and we could not make reflection measurements easily.

In retrospect, we could have made URU measurements by illuminating the wall of the integrating sphere. However, these diffuse type of measurements are very difficult to make accurately.

This is tricky only because the value in $slab.b$ is used to hold the value of ba or $d \cdot \mu_a$ when the $Find\_Bs\_fn$ is used.

⟨ Prototype for U_Find_Bs 231 ⟩ ≡
  void U_Find_Bs(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 232.

232.   ⟨ Definition for U_Find_Bs 232 ⟩ ≡
  ⟨ Prototype for U_Find_Bs 231 ⟩
  {
    double $ax, bx, cx, fa, fb, fc, bs$;
    if ($Debug$(DEBUG_SEARCH)) {
      $fprintf$($stderr$, "SEARCH:␣Using␣U_Find_Bs()");
      $fprintf$($stderr$, "␣(mu=%6.4f)", $r{\rightarrow}slab.cos\_angle$);
      if ($r{\rightarrow}default\_ba \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_ba␣=␣%8.5f", $r{\rightarrow}default\_ba$);
      if ($r{\rightarrow}default\_g \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_g␣=␣%8.5f", $r{\rightarrow}default\_g$);
      $fprintf$($stderr$, "\n");
    }
    if ($m.m\_t \equiv 0$) {
      $r{\rightarrow}slab.b =$ HUGE_VAL;
      U_Find_A(m, r);
      return;
    }
    $r{\rightarrow}slab.a = 0$;
    $r{\rightarrow}slab.g = (r{\rightarrow}default\_g \equiv$ UNINITIALIZED$)$? $0 : r{\rightarrow}default\_g$;
    $r{\rightarrow}slab.b = (r{\rightarrow}default\_ba \equiv$ UNINITIALIZED$)$? HUGE_VAL $: r{\rightarrow}default\_ba$;
    Set_Calc_State($m, *r$);   /∗ store ba in RR.slab.b ∗/
    $ax = b2bcalc$(0.1);   /∗ first try for bs ∗/
    $bx = b2bcalc$(1.0);
    $mnbrak$($\&ax, \&bx, \&cx, \&fa, \&fb, \&fc, Find\_Bs\_fn$);
    $r{\rightarrow}final\_distance = brent$($ax, bx, cx, Find\_Bs\_fn, r{\rightarrow}tolerance, \&bs$);   /∗ recover true values ∗/
    $r{\rightarrow}slab.a = bcalc2b(bs)/(bcalc2b(bs) + r{\rightarrow}slab.b)$;
    $r{\rightarrow}slab.b = bcalc2b(bs) + r{\rightarrow}slab.b$;
    ⟨ Put final values in result 229 ⟩
  }

This code is used in section 220.

233.   Fixed Absorption and Scattering.   Typically, this routine is called when the scattering coefficient is known, the anisotropy is known, and the physical thickness of the sample is known. This routine calculates the varies the absorption coefficient until the measurements are matched.

This is tricky only because the value in $slab.b$ is used to hold the value of bs or $d \cdot \mu_s$ when the $Find\_Ba\_fn$ is used.

⟨ Prototype for U_Find_Ba 233 ⟩ ≡
    void U_Find_Ba(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 234.

**234.   ** ⟨ Definition for U_Find_Ba 234 ⟩ ≡
    ⟨ Prototype for U_Find_Ba 233 ⟩
    {
        double $ax, bx, cx, fa, fb, fc, ba$;
        if ($Debug$(DEBUG_SEARCH)) {
            $fprintf$($stderr$, "SEARCH:␣Using␣U_Find_Bs()");
            $fprintf$($stderr$, "␣(mu=%6.4f)", r→$slab.cos\_angle$);
            if (r→$default\_bs \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_bs␣=␣%8.5f", r→$default\_bs$);
            if (r→$default\_g \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_g␣=␣%8.5f", r→$default\_g$);
            $fprintf$($stderr$, "\n");
        }
        r→$slab.a = 0$;
        r→$slab.g = (r$→$default\_g \equiv$ UNINITIALIZED) ? 0 : r→$default\_g$;
        r→$slab.b = (r$→$default\_bs \equiv$ UNINITIALIZED) ? HUGE_VAL : r→$default\_bs$;
        if ($m.m\_t \equiv 0$) {
            r→$slab.b =$ HUGE_VAL;
            U_Find_A(m, r);
            return;
        }
        Set_Calc_State($m, *r$);   /* store bs in RR.slab.b */
        $ax = b2bcalc(0.1)$;   /* first try for ba */
        $bx = b2bcalc(1.0)$;
        $mnbrak$(&ax, &bx, &cx, &fa, &fb, &fc, $Find\_Ba\_fn$);
        r→$final\_distance = brent(ax, bx, cx, Find\_Ba\_fn, r$→$tolerance, $&$ba$);   /* recover true values */
        r→$slab.a = (r$→$slab.b)/(bcalc2b(ba) + r$→$slab.b)$;
        r→$slab.b = bcalc2b(ba) + r$→$slab.b$;   /* actual value of b */
        ⟨ Put final values in result 229 ⟩
    }

This code is used in section 220.

235. Fixed Optical Depth and Anisotropy.   Typically, this routine is called when the optical thickness is assumed infinite. However, it may also be called when the optical thickness is assumed to be fixed at a particular value. Typically the only reasonable situation for this to occur is when the diffuse transmission is non-zero but the collimated transmission is zero. If this is the case then there is no information in the collimated transmission measurement and there is no sense even using it because the slab is not infinitely thick.

⟨ Prototype for U_Find_A 235 ⟩ ≡
>   **void** U_Find_A(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 236.

236.   ⟨ Definition for U_Find_A 236 ⟩ ≡
>   ⟨ Prototype for U_Find_A 235 ⟩
>   {
>   **double** Rt, Tt, Rd, Rc, Td, Tc;
>   **if** ($Debug$(DEBUG_SEARCH)) {
> $fprintf$($stderr$, "SEARCH:␣Using␣U_Find_A()");
> $fprintf$($stderr$, "␣(mu=%6.4f)", r→$slab.cos\_angle$);
>   **if** (r→$default\_b$ ≠ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_b␣=␣%8.5f", r→$default\_b$);
>   **if** (r→$default\_g$ ≠ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_g␣=␣%8.5f", r→$default\_g$);
> $fprintf$($stderr$, "\n");
>   }
> $Estimate\_RT$($m, *r, \&Rt, \&Tt, \&Rd, \&Rc, \&Td, \&Tc$);
> r→$slab.g$ = (r→$default\_g$ ≡ UNINITIALIZED) ? 0 : r→$default\_g$;
> r→$slab.b$ = (r→$default\_b$ ≡ UNINITIALIZED) ? HUGE_VAL : r→$default\_b$;
> r→$slab.a$ = 0.0;
> r→$final\_distance$ = 0.0;
> Set_Calc_State($m, *r$);
>   **if** ($Rt > 0.99999$) {
> r→$final\_distance$ = $Find\_A\_fn$($a2acalc$(1.0));
> r→$slab.a$ = 1.0;
>   }
>   **else** {
>   **double** $x, ax, bx, cx, fa, fb, fc$;
> ax = $a2acalc$(0.3);
> bx = $a2acalc$(0.5);
> $mnbrak$($\&ax, \&bx, \&cx, \&fa, \&fb, \&fc, Find\_A\_fn$);
> r→$final\_distance$ = $brent$($ax, bx, cx, Find\_A\_fn, r$→$tolerance, \&x$);
> r→$slab.a$ = $acalc2a$(x);
>   }
>   ⟨ Put final values in result 229 ⟩
>   }

This code is used in section 220.

237. Fixed Optical Depth and Albedo.

⟨ Prototype for *U_Find_G* 237 ⟩ ≡
  void *U_Find_G*(**struct measure_type** *m*, **struct invert_type** *∗r*)

This code is used in sections 221 and 238.

238.   ⟨ Definition for *U_Find_G* 238 ⟩ ≡
  ⟨ Prototype for *U_Find_G* 237 ⟩
  {
    double *Rt*, *Tt*, *Rd*, *Rc*, *Td*, *Tc*;
    double *x*, *ax*, *bx*, *cx*, *fa*, *fb*, *fc*;
    if (*Debug*(DEBUG_SEARCH)) {
      fprintf(*stderr*, "SEARCH:␣Using␣U_Find_G()");
      fprintf(*stderr*, "␣(mu=%6.4f)", *r→slab.cos_angle*);
      if (*r→default_a* ≠ UNINITIALIZED) *fprintf*(*stderr*, "␣␣default_a␣=␣%8.5f", *r→default_a*);
      if (*r→default_b* ≠ UNINITIALIZED) *fprintf*(*stderr*, "␣␣default_b␣=␣%8.5f", *r→default_b*);
      fprintf(*stderr*, "\n");
    }
    Estimate_RT(*m*, *∗r*, &*Rt*, &*Tt*, &*Rd*, &*Rc*, &*Td*, &*Tc*);
    r→slab.a = (*r→default_a* ≡ UNINITIALIZED) ? 0.5 : *r→default_a*;
    if (*r→default_b* ≠ UNINITIALIZED) *r→slab.b* = *r→default_b*;
    else if (*m.m_u* > 0) *r→slab.b* = *What_Is_B*(*r→slab*, *m.m_u*);
    else *r→slab.b* = HUGE_VAL;
    r→slab.g = 0.0;
    r→final_distance = 0.0;
    Set_Calc_State(*m*, *∗r*);
    ax = *g2gcalc*(−0.99);
    bx = *g2gcalc*(0.99);
    mnbrak(&*ax*, &*bx*, &*cx*, &*fa*, &*fb*, &*fc*, *Find_G_fn*);
    r→final_distance = *brent*(*ax*, *bx*, *cx*, *Find_G_fn*, *r→tolerance*, &*x*);
    r→slab.g = *gcalc2g*(*x*);
    Set_Calc_State(*m*, *∗r*);
    ⟨ Put final values in result 229 ⟩
  }

This code is used in section 220.

239.   Fixed Anisotropy and Albedo.   This routine can be called in three different situations: (1) the albedo is zero, (2) the albedo is one, or (3) the albedo is fixed at a default value. I calculate the individual reflections and transmissions to establish which of these cases we happen to have.

⟨ Prototype for U_Find_B 239 ⟩ ≡
  void U_Find_B(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 240.

240.   ⟨ Definition for U_Find_B 240 ⟩ ≡
  ⟨ Prototype for U_Find_B 239 ⟩
  {
    double Rt, Tt, Rd, Rc, Td, Tc;
    if ($Debug$(DEBUG_SEARCH)) {
      $fprintf$($stderr$, "SEARCH:␣Using␣U_Find_B()");
      $fprintf$($stderr$, "␣(mu=%6.4f)", $r{\rightarrow}slab.cos\_angle$);
      if ($r{\rightarrow}default\_a \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_a␣=␣%8.5f", $r{\rightarrow}default\_a$);
      if ($r{\rightarrow}default\_g \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_g␣=␣%8.5f", $r{\rightarrow}default\_g$);
      $fprintf$($stderr$, "\n");
    }
    $Estimate\_RT$($m, *r, \&Rt, \&Tt, \&Rd, \&Rc, \&Td, \&Tc$);
    $r{\rightarrow}slab.g = (r{\rightarrow}default\_g \equiv$ UNINITIALIZED$)\,?\,0 : r{\rightarrow}default\_g$;
    $r{\rightarrow}slab.a = (r{\rightarrow}default\_a \equiv$ UNINITIALIZED$)\,?\,0 : r{\rightarrow}default\_a$;
    $r{\rightarrow}slab.b = 0.5$;
    $r{\rightarrow}final\_distance = 0.0$;
    Set_Calc_State($m, *r$);
    ⟨ Iteratively solve for b 241 ⟩
    ⟨ Put final values in result 229 ⟩
  }

This code is used in section 220.

241.   This could be improved tremendously. I just don't want to mess with it at the moment.

⟨ Iteratively solve for b 241 ⟩ ≡
  {
    double $x, ax, bx, cx, fa, fb, fc$;
    $ax = b2bcalc(0.1)$;
    $bx = b2bcalc(10)$;
    $mnbrak$($\&ax, \&bx, \&cx, \&fa, \&fb, \&fc, Find\_B\_fn$);
    $r{\rightarrow}final\_distance = brent$($ax, bx, cx, Find\_B\_fn, r{\rightarrow}tolerance, \&x$);
    $r{\rightarrow}slab.b = bcalc2b(x)$;
    Set_Calc_State($m, *r$);
  }

This code is used in section 240.

242. Fixed Optical Depth.

We can get here a couple of different ways.

First there can be three real measurements, i.e., t_c is not zero, in this case we want to fix b based on the t_c measurement.

Second, we can get here if a default value for b has been set.

Otherwise, we really should not be here. Just set $b = 1$ and calculate away.

$\langle$ Prototype for U_Find_AG 242 $\rangle \equiv$
  void U_Find_AG(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 243.

243. $\langle$ Definition for U_Find_AG 243 $\rangle \equiv$
  $\langle$ Prototype for U_Find_AG 242 $\rangle$
  {
    $\langle$ Allocate local simplex variables 224 $\rangle$
    if $(Debug(\texttt{DEBUG\_SEARCH}))$ {
      $fprintf(stderr, \texttt{"SEARCH:}\_\texttt{Using}\_\texttt{U\_Find\_AG()"});$
      $fprintf(stderr, \texttt{"}\_\texttt{(mu=\%6.4f)"}, r\rightarrow slab.cos\_angle);$
      if $(r\rightarrow default\_b \neq \texttt{UNINITIALIZED})$ $fprintf(stderr, \texttt{"}\_\_\texttt{default\_b}\_=\_\texttt{\%8.5f"}, r\rightarrow default\_b);$
      $fprintf(stderr, \texttt{"\textbackslash n"});$
    }
    if $(m.num\_measures \equiv 3)$ $r\rightarrow slab.b = What\_Is\_B(r\rightarrow slab, m.m\_u);$
    else if $(r\rightarrow default\_b \equiv \texttt{UNINITIALIZED})$ $r\rightarrow slab.b = 1;$
    else $r\rightarrow slab.b = r\rightarrow default\_b;$
    $Set\_Calc\_State(m, *r);$
    $\langle$ Get the initial a, b, and g 225 $\rangle$
    $\langle$ Initialize the nodes of the a and g simplex 244 $\rangle$
    $\langle$ Evaluate the a and g simplex at the nodes 245 $\rangle$
    $amoeba(p, y, 2, r\rightarrow tolerance, Find\_AG\_fn, \&r\rightarrow AD\_iterations);$
    $\langle$ Choose the best node of the a and g simplex 246 $\rangle$
    $\langle$ Free simplex data structures 230 $\rangle$
    $\langle$ Put final values in result 229 $\rangle$
  }

This code is used in section 220.

244. ⟨Initialize the nodes of the a and g simplex 244⟩ ≡
```
{
    int k, kk;
    p[1][1] = a2acalc(guess[0].a);
    p[1][2] = g2gcalc(guess[0].g);
    for (k = 1; k < 7; k++) {
        if (guess[0].a ≠ guess[k].a) break;
    }
    p[2][1] = a2acalc(guess[k].a);
    p[2][2] = g2gcalc(guess[k].g);
    for (kk = 1; kk < 7; kk++) {
        if (kk ≡ k) continue;
        if (guess[0].g ≠ guess[kk].g ∨ guess[k].g ≠ guess[kk].g) break;
    }
    p[3][1] = a2acalc(guess[kk].a);
    p[3][2] = g2gcalc(guess[kk].g);
    if (Debug(DEBUG_BEST_GUESS)) {
        fprintf(stderr, "−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−\n");
        fprintf(stderr, "BEST:␣<1>␣");
        fprintf(stderr, "%10.5f␣", guess[0].a);
        fprintf(stderr, "%10.5f␣", guess[0].b);
        fprintf(stderr, "%10.5f␣", guess[0].g);
        fprintf(stderr, "%10.5f\n", guess[0].distance);
        fprintf(stderr, "BEST:␣<2>␣");
        fprintf(stderr, "%10.5f␣", guess[k].a);
        fprintf(stderr, "%10.5f␣", guess[k].b);
        fprintf(stderr, "%10.5f␣", guess[k].g);
        fprintf(stderr, "%10.5f\n", guess[k].distance);
        fprintf(stderr, "BEST:␣<3>␣");
        fprintf(stderr, "%10.5f␣", guess[kk].a);
        fprintf(stderr, "%10.5f␣", guess[kk].b);
        fprintf(stderr, "%10.5f␣", guess[kk].g);
        fprintf(stderr, "%10.5f\n", guess[kk].distance);
        fprintf(stderr, "\n");
    }
}
```
This code is used in section 243.

245. ⟨Evaluate the a and g simplex at the nodes 245⟩ ≡
```
for (i = 1; i ≤ 3; i++) {
    x[1] = p[i][1];
    x[2] = p[i][2];
    y[i] = Find_AG_fn(x);
}
```
This code is used in section 243.

246.   Here we find the node of the simplex that gave the best result and save that one. At the same time
we save the whole simplex for later use if needed.

⟨ Choose the best node of the a and g simplex 246 ⟩ ≡
　r→$final\_distance = 10$;
　　for $(i = 1;\ i \leq 3;\ i\mathord{+}\mathord{+})$ {
　　　if $(y[i] < r\text{→}final\_distance)$ {
　　　　r→$slab.a = acalc2a(p[i][1])$;
　　　　r→$slab.g = gcalc2g(p[i][2])$;
　　　　r→$final\_distance = y[i]$;
　　　}
　　}
This code is used in section 243.

247. Fixed Albedo.   Here the optical depth and the anisotropy are varied (for a fixed albedo).

⟨ Prototype for *U_Find_BG* 247 ⟩ ≡
    void *U_Find_BG*(**struct measure_type** *m*, **struct invert_type** *∗r*)

This code is used in sections 221 and 248.

248.   ⟨ Definition for *U_Find_BG* 248 ⟩ ≡
    ⟨ Prototype for *U_Find_BG* 247 ⟩
    {
        ⟨ Allocate local simplex variables 224 ⟩
        if (*Debug*(DEBUG_SEARCH)) {
            fprintf(*stderr*, "SEARCH:␣Using␣U_Find_BG()");
            fprintf(*stderr*, "␣(mu=%6.4f)", *r→slab.cos_angle*);
            if (*r→default_a* ≠ UNINITIALIZED) *fprintf*(*stderr*, "␣␣default_a␣=␣%8.5f", *r→default_a*);
            fprintf(*stderr*, "\n");
        }
        r→slab.a = (*r→default_a* ≡ UNINITIALIZED) ? 0 : *r→default_a*;
        Set_Calc_State(*m*, *∗r*);
        ⟨ Get the initial *a*, *b*, and *g* 225 ⟩
        ⟨ Initialize the nodes of the *b* and *g* simplex 250 ⟩
        ⟨ Evaluate the *bg* simplex at the nodes 251 ⟩
        amoeba(*p*, *y*, 2, *r→tolerance*, *Find_BG_fn*, &*r→AD_iterations*);
        ⟨ Choose the best node of the *b* and *g* simplex 252 ⟩
        ⟨ Free simplex data structures 230 ⟩
        ⟨ Put final values in result 229 ⟩
    }

This code is used in section 220.

249.   A very simple start for variation of *b* and *g*. This should work fine for the cases in which the absorption or scattering are fixed.

250.   ⟨Initialize the nodes of the b and g simplex 250⟩ ≡

```
{
   int k, kk;
   p[1][1] = b2bcalc(guess[0].b);
   p[1][2] = g2gcalc(guess[0].g);
   for (k = 1; k < 7; k++) {
      if (guess[0].b ≠ guess[k].b) break;
   }
   p[2][1] = b2bcalc(guess[k].b);
   p[2][2] = g2gcalc(guess[k].g);
   for (kk = 1; kk < 7; kk++) {
      if (kk ≡ k) continue;
      if (guess[0].g ≠ guess[kk].g ∨ guess[k].g ≠ guess[kk].g) break;
   }
   p[3][1] = b2bcalc(guess[kk].b);
   p[3][2] = g2gcalc(guess[kk].g);
   if (Debug(DEBUG_BEST_GUESS)) {
      fprintf(stderr, "−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−\n");
      fprintf(stderr, "BEST:␣<1>␣");
      fprintf(stderr, "%10.5f␣", guess[0].a);
      fprintf(stderr, "%10.5f␣", guess[0].b);
      fprintf(stderr, "%10.5f␣", guess[0].g);
      fprintf(stderr, "%10.5f\n", guess[0].distance);
      fprintf(stderr, "BEST:␣<2>␣");
      fprintf(stderr, "%10.5f␣", guess[k].a);
      fprintf(stderr, "%10.5f␣", guess[k].b);
      fprintf(stderr, "%10.5f␣", guess[k].g);
      fprintf(stderr, "%10.5f\n", guess[k].distance);
      fprintf(stderr, "BEST:␣<3>␣");
      fprintf(stderr, "%10.5f␣", guess[kk].a);
      fprintf(stderr, "%10.5f␣", guess[kk].b);
      fprintf(stderr, "%10.5f␣", guess[kk].g);
      fprintf(stderr, "%10.5f\n", guess[kk].distance);
      fprintf(stderr, "\n");
   }
}
```

This code is used in section 248.

251.   ⟨Evaluate the bg simplex at the nodes 251⟩ ≡

```
for (i = 1; i ≤ 3; i++) {
   x[1] = p[i][1];
   x[2] = p[i][2];
   y[i] = Find_BG_fn(x);
}
```

This code is used in section 248.

252.   Here we find the node of the simplex that gave the best result and save that one. At the same time we save the whole simplex for later use if needed.

⟨ Choose the best node of the b and g simplex 252 ⟩ ≡
  $r{\rightarrow}final\_distance = 10;$
  for $(i = 1;\ i \leq 3;\ i{+}{+})$ {
    if $(y[i] < r{\rightarrow}final\_distance)$ {
      $r{\rightarrow}slab.b = bcalc2b(p[i][1]);$
      $r{\rightarrow}slab.g = gcalc2g(p[i][2]);$
      $r{\rightarrow}final\_distance = y[i];$
    }
  }

This code is used in section 248.

253.   Fixed Scattering.   Here I assume that a constant b_s,

$$b_s = \mu_s d$$

where d is the physical thickness of the sample and μ_s is of course the absorption coefficient. This is just like U_Find_BG except that $b_a = \mu_a d$ is varied instead of b.

⟨ Prototype for U_Find_BaG 253 ⟩ ≡
   void U_Find_BaG(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 254.

254.   ⟨ Definition for U_Find_BaG 254 ⟩ ≡
  ⟨ Prototype for U_Find_BaG 253 ⟩
  {
    ⟨ Allocate local simplex variables 224 ⟩
    $Set\_Calc\_State(m, *r)$;
    ⟨ Get the initial a, b, and g 225 ⟩
    ⟨ Initialize the nodes of the ba and g simplex 255 ⟩
    ⟨ Evaluate the BaG simplex at the nodes 256 ⟩
    $amoeba(p, y, 2, r \rightarrow tolerance, Find\_BaG\_fn, \&r \rightarrow AD\_iterations)$;
    ⟨ Choose the best node of the ba and g simplex 257 ⟩
    ⟨ Free simplex data structures 230 ⟩
    ⟨ Put final values in result 229 ⟩
  }

This code is used in section 220.

255.   ⟨ Initialize the nodes of the ba and g simplex 255 ⟩ ≡
  if $(guess[0].b > r \rightarrow default\_bs)$ {
    $p[1][1] = b2bcalc(guess[0].b - r \rightarrow default\_bs)$;
    $p[2][1] = b2bcalc(2 * (guess[0].b - r \rightarrow default\_bs))$;
    $p[3][1] = p[1][1]$;
  }
  else {
    $p[1][1] = b2bcalc(0.0001)$;
    $p[2][1] = b2bcalc(0.001)$;
    $p[3][1] = p[1][1]$;
  }
  $p[1][2] = g2gcalc(guess[0].g)$;
  $p[2][2] = p[1][2]$;
  $p[3][2] = g2gcalc(0.9 * guess[0].g + 0.05)$;

This code is used in section 254.

256.   ⟨ Evaluate the BaG simplex at the nodes 256 ⟩ ≡
  for $(i = 1; \ i \leq 3; \ i\texttt{++})$ {
    $x[1] = p[i][1]$;
    $x[2] = p[i][2]$;
    $y[i] = Find\_BaG\_fn(x)$;
  }

This code is used in section 254.

257.   Here we find the node of the simplex that gave the best result and save that one. At the same time
we save the whole simplex for later use if needed.

⟨ Choose the best node of the *ba* and *g* simplex 257 ⟩ ≡
  $r→final\_distance = 10$;
  for $(i = 1;\ i \leq 3;\ i\text{++})$ {
    if $(y[i] < r→final\_distance)$ {
      $r→slab.b = bcalc2b(p[i][1]) + r→default\_bs$;
      $r→slab.a = r→default\_bs/r→slab.b$;
      $r→slab.g = gcalc2g(p[i][2])$;
      $r→final\_distance = y[i]$;
    }
  }

This code is used in section 254.

258.   Fixed Absorption.   Here I assume that a constant b_a,

$$b_a = \mu_a d$$

where d is the physical thickness of the sample and μ_a is of course the absorption coefficient. This is just like U_Find_BG except that $b_s = \mu_s d$ is varied instead of b.

⟨Prototype for U_Find_BsG 258⟩ ≡
   void U_Find_BsG(**struct measure_type** m, **struct invert_type** $*r$)

This code is used in sections 221 and 259.

259.   ⟨Definition for U_Find_BsG 259⟩ ≡
   ⟨Prototype for U_Find_BsG 258⟩
   {
      ⟨Allocate local simplex variables 224⟩
      if ($Debug$(DEBUG_SEARCH)) {
         $fprintf$($stderr$, "SEARCH:␣Using␣U_Find_BsG()");
         $fprintf$($stderr$, "␣(mu=%6.4f)", r→$slab.cos\_angle$);
         if (r→$default\_ba \neq$ UNINITIALIZED) $fprintf$($stderr$, "␣␣default_ba␣=␣%8.5f", r→$default\_ba$);
         $fprintf$($stderr$, "\n");
      }
      Set_Calc_State(m, $*r$);
      ⟨Get the initial a, b, and g 225⟩
      ⟨Initialize the nodes of the bs and g simplex 260⟩
      ⟨Evaluate the BsG simplex at the nodes 261⟩
      $amoeba$(p, y, 2, r→$tolerance$, $Find\_BsG\_fn$, &r→$AD\_iterations$);
      ⟨Choose the best node of the bs and g simplex 262⟩
      ⟨Free simplex data structures 230⟩
      ⟨Put final values in result 229⟩
   }

This code is used in section 220.

260.   ⟨Initialize the nodes of the bs and g simplex 260⟩ ≡
   $p[1][1] = b2bcalc$($guess[0].b - r$→$default\_ba$);
   $p[1][2] = g2gcalc$($guess[0].g$);
   $p[2][1] = b2bcalc$($2 * guess[0].b - 2 * r$→$default\_ba$);
   $p[2][2] = p[1][2]$;
   $p[3][1] = p[1][1]$;
   $p[3][2] = g2gcalc$($0.9 * guess[0].g + 0.05$);

This code is used in section 259.

261.   ⟨Evaluate the BsG simplex at the nodes 261⟩ ≡
   for ($i = 1$; $i \leq 3$; i++) {
      $x[1] = p[i][1]$;
      $x[2] = p[i][2]$;
      $y[i] = Find\_BsG\_fn$(x);
   }

This code is used in section 259.

262. ⟨Choose the best node of the *bs* and *g* simplex 262⟩ ≡

$r{\rightarrow}final\_distance = 10;$
$\textbf{for } (i = 1; \ i \leq 3; \ i{+}{+}) \ \{$
$\quad \textbf{if } (y[i] < r{\rightarrow}final\_distance) \ \{$
$\qquad r{\rightarrow}slab.b = bcalc2b(p[i][1]) + r{\rightarrow}default\_ba;$
$\qquad r{\rightarrow}slab.a = 1 - r{\rightarrow}default\_ba/r{\rightarrow}slab.b;$
$\qquad r{\rightarrow}slab.g = gcalc2g(p[i][2]);$
$\qquad r{\rightarrow}final\_distance = y[i];$
$\quad \}$
$\}$

This code is used in section 259.

263. IAD Utilities.
   March 1995. Reincluded *quick_guess* code.

⟨ `iad_util.c` 263 ⟩ ≡
#include `<math.h>`
#include `<float.h>`
#include `<stdio.h>`
#include `"nr_util.h"`
#include `"ad_globl.h"`
#include `"ad_frsnl.h"`
#include `"ad_bound.h"`
#include `"iad_type.h"`
#include `"iad_calc.h"`
#include `"iad_pub.h"`
#include `"iad_util.h"`
   unsigned long $g\_util\_debugging = 0$;
   ⟨ Preprocessor definitions ⟩

   ⟨ Definition for *What_Is_B* 266 ⟩
   ⟨ Definition for *Estimate_RT* 272 ⟩
   ⟨ Definition for *a2acalc* 279 ⟩
   ⟨ Definition for *acalc2a* 281 ⟩
   ⟨ Definition for *g2gcalc* 283 ⟩
   ⟨ Definition for *gcalc2g* 285 ⟩
   ⟨ Definition for *b2bcalc* 287 ⟩
   ⟨ Definition for *bcalc2b* 289 ⟩
   ⟨ Definition for *twoprime* 291 ⟩
   ⟨ Definition for *twounprime* 293 ⟩
   ⟨ Definition for *abgg2ab* 295 ⟩
   ⟨ Definition for *abgb2ag* 297 ⟩
   ⟨ Definition for *quick_guess* 304 ⟩
   ⟨ Definition for *Set_Debugging* 317 ⟩
   ⟨ Definition for *Debug* 319 ⟩
   ⟨ Definition for *Print_Invert_Type* 321 ⟩
   ⟨ Definition for *Print_Measure_Type* 323 ⟩

264. ⟨ `iad_util.h` 264 ⟩ ≡
   ⟨ Prototype for *What_Is_B* 265 ⟩;
   ⟨ Prototype for *Estimate_RT* 271 ⟩;
   ⟨ Prototype for *a2acalc* 278 ⟩;
   ⟨ Prototype for *acalc2a* 280 ⟩;
   ⟨ Prototype for *g2gcalc* 282 ⟩;
   ⟨ Prototype for *gcalc2g* 284 ⟩;
   ⟨ Prototype for *b2bcalc* 286 ⟩;
   ⟨ Prototype for *bcalc2b* 288 ⟩;
   ⟨ Prototype for *twoprime* 290 ⟩;
   ⟨ Prototype for *twounprime* 292 ⟩;
   ⟨ Prototype for *abgg2ab* 294 ⟩;
   ⟨ Prototype for *abgb2ag* 296 ⟩;
   ⟨ Prototype for *quick_guess* 303 ⟩;
   ⟨ Prototype for *Set_Debugging* 316 ⟩;
   ⟨ Prototype for *Debug* 318 ⟩;
   ⟨ Prototype for *Print_Invert_Type* 320 ⟩;
   ⟨ Prototype for *Print_Measure_Type* 322 ⟩;

265.   Finding optical thickness.

This routine figures out what the optical thickness of a slab based on the index of refraction of the slab and the amount of collimated light that gets through it.

It should be pointed out right here in the front that this routine does not work for diffuse irradiance, but then the whole concept of estimating the optical depth for diffuse irradiance is bogus anyway.

In version 1.3 changed all error output to *stderr*. Version 1.4 included cases involving absorption in the boundaries.

#**define** `BIG_A_VALUE`   999999.0
#**define** `SMALL_A_VALUE`   0.000001

⟨ Prototype for *What_Is_B* 265 ⟩ ≡
   double *What_Is_B*(**struct AD_slab_type** *slab*, **double** *Tc*)

This code is used in sections 264 and 266.

266.   ⟨ Definition for *What_Is_B* 266 ⟩ ≡
   ⟨ Prototype for *What_Is_B* 265 ⟩
   {
      double *r1*, *r2*, *t1*, *t2*, *mu_in_slab*;

      ⟨ Calculate specular reflection and transmission 267 ⟩
      ⟨ Check for bad values of *Tc* 268 ⟩
      ⟨ Solve if multiple internal reflections are not present 269 ⟩
      ⟨ Find thickness when multiple internal reflections are present 270 ⟩
   }

This code is used in section 263.

267.   The first thing to do is to find the specular reflection for light interacting with the top and bottom air-glass-sample interfaces. I make a simple check to ensure that the the indices are different before calculating the bottom reflection. Most of the time the *r1* ≡ *r2*, but there are always those annoying special cases.

⟨ Calculate specular reflection and transmission 267 ⟩ ≡
   Absorbing_Glass_RT(1.0, *slab.n_top_slide*, *slab.n_slab*, *slab.cos_angle*, *slab.b_top_slide*, &*r1*, &*t1*);
   mu_in_slab = *Cos_Snell*(1.0, *slab.cos_angle*, *slab.n_slab*);
   Absorbing_Glass_RT(*slab.n_slab*, *slab.n_bottom_slide*, 1.0, *mu_in_slab*, *slab.b_bottom_slide*, &*r2*, &*t2*);

This code is used in section 266.

268.   Bad values for the unscattered transmission are those that are non-positive, those greater than one, and those greater than are possible in a non-absorbing medium, i.e.,

$$T_c > \frac{t_1 t_2}{1 - r_1 r_2}$$

Since this routine has no way to report errors, I just set the optical thickness to the natural values in these cases.

⟨ Check for bad values of *Tc* 268 ⟩ ≡
   if (*Tc* ≤ 0) **return** (`HUGE_VAL`);
   if (*Tc* ≥ *t1* * *t2*/(1 − *r1* * *r2*)) **return** (0.001);

This code is used in section 266.

269.   If either *r1* or *r2* $\equiv 0$ then things are very simple because the sample does not sustain multiple internal reflections and the unscattered transmission is

$$T_c = t_1 t_2 \exp(-b/\nu)$$

where b is the optical thickness and ν is *slab.cos_angle*. Clearly,

$$b = -\nu \ln \left(\frac{T_c}{t_1 t_2} \right)$$

$\langle$ Solve if multiple internal reflections are not present 269 $\rangle \equiv$
    if $(r1 \equiv 0 \vee r2 \equiv 0)$ **return** $(-slab.cos\_angle * log(Tc/t1/t2))$;
This code is used in section 266.

270.   Well I kept putting it off, but now comes the time to solve the following equation for b

$$T_c = \frac{t_1 t_2 \exp(-b)}{1 - r_1 r_2 \exp(-2b)}$$

We note immediately that this is a quadratic equation in $x = \exp(-b)$.

$$r_1 r_2 T_c x^2 + t_1 t_2 x - T_c = 0$$

Sufficient tests have been made above to ensure that none of the coefficients are exactly zero. However, it is clear that the leading quadratic term has a much smaller coefficient than the other two. Since r_1 and r_2 are typically about four percent the product is roughly 10^{-3}. The collimated transmission can be very small and this makes things even worse. A further complication is that we need to choose the only positive root.

Now the roots of $ax^2 + bx + c = 0$ can be found using the standard quadratic formula,

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

This is very bad for small values of a. Instead I use

$$q = -\frac{1}{2} \left[b + \operatorname{sgn}(b) \sqrt{b^2 - 4ac} \right]$$

with the two roots

$$x = \frac{q}{a} \qquad \text{and} \qquad x = \frac{c}{q}$$

Substituting our coefficients

$$q = -\frac{1}{2} \left[t_1 t_2 + \sqrt{t_1^2 t_2^2 + 4 r_1 r_2 T_c^2} \right]$$

With some algebra, this can be shown to be

$$q = -t_1 t_2 \left[1 + \frac{r_1 r_2 T_c^2}{t_1^2 t_2^2} + \cdots \right]$$

The only positive root is $x = -T_c/q$. Therefore

$$x = \frac{2 T_c}{t_1 t_2 + \sqrt{t_1^2 t_2^2 + 4 r_1 r_2 T_c^2}}$$

(Not very pretty, but straightforward enough.)

$\langle$ Find thickness when multiple internal reflections are present 270 $\rangle \equiv$
```
  {
    double B;
    B = t1 * t2;
    return (-slab.cos_angle * log(2 * Tc/(B + sqrt(B * B + 4 * Tc * Tc * r1 * r2))));
  }
```
This code is used in section 266.

271.   Estimating R and T.

In several places, it is useful to know an *estimate* for the values of the reflection and transmission of the sample based on the measurements. This routine provides such an estimate, but it currently ignores anything corrections that might be made for the integrating spheres.

Good values are only really obtainable when $num\_measures \equiv 3$, otherwise we need to make pretty strong assumptions about the reflection and transmission values. If $num\_measures < 3$, then we will assume that no collimated light makes it all the way through the sample. The specular reflection is then just that for a semi-infinite sample and $Tc = 0$. If $num\_measures \equiv 1$, then Td is also set to zero.

rt	total reflection
rc	primary or specular reflection
rd	diffuse or scattered reflection
tt	total transmission
tp	primary or unscattered transmission
td	diffuse or scattered transmission

⟨ Prototype for *Estimate_RT* 271 ⟩ ≡
    void *Estimate_RT* (**struct measure_type** m, **struct invert_type** r, **double** $*rt$, **double** $*tt$, **double** $*rd$, **double** $*rc$, **double** $*td$, **double** $*tc$)

This code is used in sections 264 and 272.

**272.   ** ⟨ Definition for *Estimate_RT* 272 ⟩ ≡
    ⟨ Prototype for *Estimate_RT* 271 ⟩
    {
        ⟨ Calculate the unscattered transmission and reflection 273 ⟩
        ⟨ Estimate the backscattered reflection 274 ⟩
        ⟨ Estimate the scattered transmission 275 ⟩
        ⟨ Debug info for estimate RT 276 ⟩
    }

This code is used in section 263.

**273.   ** If there are three measurements then the specular reflection can be calculated pretty well. If there are fewer then the unscattered transmission is assumed to be zero. This is not necessarily the case, but after all, this routine only makes estimates of the various reflection and transmission quantities.

If there are three measurements, the optical thickness of the sample is required. Of course if there are three measurements then the illumination must be collimated and we can call *What_Is_B* to find out the optical thickness. We pass this value to a routine in the `fresnel.h` unit and sit back and wait.

All the above is true if sphere corrections are not needed. Now, we just fob this off on another function.

⟨ Calculate the unscattered transmission and reflection 273 ⟩ ≡
    Calculate_Minimum_MR (m, r, rc, tc);

This code is used in section 272.

274.   Finding the diffuse reflection is now just a matter of checking whether V1% contains the specular reflection from the sample or not and then just adding or subtracting the specular reflection as appropriate.

⟨ Estimate the backscattered reflection 274 ⟩ ≡
```
  if (m.fraction_of_rc_in_mr) {
    *rt = m.m_r;
    *rd = *rt − m.fraction_of_rc_in_mr * (*rc);
    if (*rd < 0) {
      *rd = 0;
      *rc = *rt;
    }
  }
  else {
    *rd = m.m_r;
    *rt = *rd + *rc;
  }
```
This code is used in section 272.

275.   The transmission values follow in much the same way as the diffuse reflection values — just subtract the specular transmission from the total transmission.

⟨ Estimate the scattered transmission 275 ⟩ ≡
```
  if (m.num_measures ≡ 1) {
    *tt = 0.0;
    *td = 0.0;
  }
  else if (m.fraction_of_tc_in_mt) {
    *tt = m.m_t;
    *td = *tt − *tc;
    if (*td < 0) {
      *tc = *tt;
      *td = 0;
    }
  }
  else {
    *td = m.m_t;
    *tt = *td + *tc;
  }
```
This code is used in section 272.

276.   Collect debugging info here

⟨ Debug info for estimate RT 276 ⟩ ≡
```
  if (Debug(DEBUG_SEARCH)) {
    fprintf(stderr, "SEARCH:␣r_t␣=␣%8.5f␣", *rt);
    fprintf(stderr, "r_d␣=␣%8.5f␣", *rd);
    fprintf(stderr, "r_u␣=␣%8.5f\n", *rc);
    fprintf(stderr, "SEARCH:␣t_t␣=␣%8.5f␣", *tt);
    fprintf(stderr, "t_d␣=␣%8.5f␣", *td);
    fprintf(stderr, "t_u␣=␣%8.5f\n", *tc);
  }
```
This code is used in section 272.

277.   Transforming properties.   Routines to convert optical properties to calculation space and back.

278.   *a2acalc* is used for the albedo transformations according to

$$a_{calc} = \frac{2a - 1}{a(1 - a)}$$

Care is taken to avoid division by zero. Why was this function chosen? Well mostly because it maps the region between $[0, 1] \rightarrow (-\infty, +\infty)$.

$\langle$ Prototype for *a2acalc* 278 $\rangle \equiv$
  double *a2acalc*(**double** *a*)

This code is used in sections 264 and 279.

279. $\langle$ Definition for *a2acalc* 279 $\rangle \equiv$
  $\langle$ Prototype for *a2acalc* 278 $\rangle$
  {
    if $(a \leq 0)$ **return** $-$`BIG_A_VALUE`;
    if $(a \geq 1)$ **return** `BIG_A_VALUE`;
    return $((2 * a - 1)/a/(1 - a))$;
  }

This code is used in section 263.

280.   *acalc2a* is used for the albedo transformations Now when we solve

$$a_c alc = \frac{2a - 1}{a(1 - a)}$$

we obtain the quadratic equation

$$a_{calc} a^2 + (2 - a_{calc})a - 1 = 0$$

The only root of this equation between zero and one is

$$a = \frac{-2 + a_{calc} + \sqrt{a_{calc}^2 + 4}}{2a_{calc}}$$

I suppose that I should spend the time to recast this using the more appropriate numerical solutions of the quadratic equation, but this worked and I will leave it as it is for now.

$\langle$ Prototype for *acalc2a* 280 $\rangle \equiv$
  double *acalc2a*(**double** *acalc*)

This code is used in sections 264 and 281.

281. $\langle$ Definition for *acalc2a* 281 $\rangle \equiv$
  $\langle$ Prototype for *acalc2a* 280 $\rangle$
  {
    if $(acalc \equiv$ `BIG_A_VALUE`$)$ **return** 1.0;
    else if $(acalc \equiv -$`BIG_A_VALUE`$)$ **return** 0.0;
    else if $(fabs(acalc) <$ `SMALL_A_VALUE`$)$ **return** 0.5;
    else return $((-2 + acalc + sqrt(acalc * acalc + 4))/(2 * acalc))$;
  }

This code is used in section 263.

282.   *g2gcalc* is used for the anisotropy transformations according to

$$g_{calc} = \frac{g}{1 + |g|}$$

which maps $(-1, 1) \rightarrow (-\infty, +\infty)$.

⟨ Prototype for *g2gcalc* 282 ⟩ ≡
  double *g2gcalc*(**double** *g*)

This code is used in sections 264 and 283.

283.   ⟨ Definition for *g2gcalc* 283 ⟩ ≡
  ⟨ Prototype for *g2gcalc* 282 ⟩
  {
    if $(g \leq -0.99999)$ **return** $(-\texttt{HUGE\_VAL})$;
    if $(g \geq 0.99999)$ **return** $(\texttt{HUGE\_VAL})$;
    return $(g/(1 - fabs(g)))$;
  }

This code is used in section 263.

284.   *gcalc2g* is used for the anisotropy transformations it is the inverse of *g2gcalc*. The relation is

$$g = \frac{g_{calc}}{1 + |g_{calc}|}$$

⟨ Prototype for *gcalc2g* 284 ⟩ ≡
  double *gcalc2g*(**double** *gcalc*)

This code is used in sections 264 and 285.

285.   ⟨ Definition for *gcalc2g* 285 ⟩ ≡
  ⟨ Prototype for *gcalc2g* 284 ⟩
  {
    if $(gcalc \equiv -\texttt{HUGE\_VAL})$ **return** -0.99999;
    if $(gcalc \equiv \texttt{HUGE\_VAL})$ **return** 0.99999;
    return $(gcalc/(1 + fabs(gcalc)))$;
  }

This code is used in section 263.

286.   *b2bcalc* is used for the optical depth transformations it is the inverse of *bcalc2b*. The relation is

$$b_{calc} = \ln(b)$$

The only caveats are to ensure that I don't take the logarithm of something big or non-positive.

⟨ Prototype for *b2bcalc* 286 ⟩ ≡
  double *b2bcalc*(**double** *b*)

This code is used in sections 264 and 287.

287.   ⟨Definition for *b2bcalc* 287⟩ ≡
  ⟨Prototype for *b2bcalc* 286⟩
  {
    if ($b \equiv$ HUGE_VAL) **return** HUGE_VAL;
    if ($b \leq 0$) **return** 0.0;
    return ($log(b)$);
  }
This code is used in section 263.

288.   *bcalc2b* is used for the anisotropy transformations it is the inverse of *b2bcalc*. The relation is

$$b = \exp(b_{calc})$$

The only tricky part is to ensure that I don't exponentiate something big and get an overflow error. In ANSI C the maximum value for x such that 10^x is in the range of representable finite floating point numbers (for doubles) is given by DBL_MAX_10_EXP. Thus if we want to know if

$$e^{b_{calc}} > 10^x$$

or

$$b_{calc} > x \ln(10) \approx 2.3x$$

and this is the criterion that I use.

⟨Prototype for *bcalc2b* 288⟩ ≡
  double *bcalc2b*(**double** *bcalc*)
This code is used in sections 264 and 289.

289.   ⟨Definition for *bcalc2b* 289⟩ ≡
  ⟨Prototype for *bcalc2b* 288⟩
  {
    if ($bcalc \equiv$ HUGE_VAL) **return** HUGE_VAL;
    if ($bcalc > 2.3 *$ DBL_MAX_10_EXP) **return** HUGE_VAL;
    return ($exp(bcalc)$);
  }
This code is used in section 263.

290.   *twoprime* converts the true albedo a, optical depth b to the reduced albedo ap and reduced optical depth bp that correspond to $g = 0$.

⟨Prototype for *twoprime* 290⟩ ≡
  void *twoprime*(**double** a, **double** b, **double** g, **double** $*ap$, **double** $*bp$)
This code is used in sections 264 and 291.

291.   ⟨Definition for *twoprime* 291⟩ ≡
  ⟨Prototype for *twoprime* 290⟩
  {
    if ($a \equiv 1 \wedge g \equiv 1$) $*ap = 0.0$;
    else $*ap = (1 - g) * a/(1 - a * g)$;
    if ($b \equiv$ HUGE_VAL) $*bp =$ HUGE_VAL;
    else $*bp = (1 - a * g) * b$;
  }
This code is used in section 263.

292.   *twounprime* converts the reduced albedo *ap* and reduced optical depth *bp* (for $g = 0$) to the true albedo *a* and optical depth *b* for an anisotropy *g*.

⟨ Prototype for *twounprime* 292 ⟩ ≡
  void *twounprime*(**double** *ap*, **double** *bp*, **double** *g*, **double** *∗a*, **double** *∗b*)
This code is used in sections 264 and 293.

293.   ⟨ Definition for *twounprime* 293 ⟩ ≡
  ⟨ Prototype for *twounprime* 292 ⟩
  {
    $*a = ap/(1 - g + ap * g)$;
    if $(bp \equiv$ HUGE_VAL$)$ $*b =$ HUGE_VAL;
    else $*b = (1 + ap * g/(1 - g)) * bp$;
  }
This code is used in section 263.

294.   *abgg2ab* assume *a*, *b*, *g*, and *g1* are given this does the similarity translation that you would expect it should by converting it to the reduced optical properties and then transforming back using the new value of *g*

⟨ Prototype for *abgg2ab* 294 ⟩ ≡
  void *abgg2ab*(**double** *a1*, **double** *b1*, **double** *g1*, **double** *g2*, **double** *∗a2*, **double** *∗b2*)
This code is used in sections 264 and 295.

295.   ⟨ Definition for *abgg2ab* 295 ⟩ ≡
  ⟨ Prototype for *abgg2ab* 294 ⟩
  {
    double *a*, *b*;
    twoprime(*a1*, *b1*, *g1*, &*a*, &*b*);
    twounprime(*a*, *b*, *g2*, *a2*, *b2*);
  }
This code is used in section 263.

296.   *abgb2ag* translates reduced optical properties to unreduced values assuming that the new optical thickness is given i.e., *a1* and *b1* are a' and b' for $g = 0$. This routine then finds the appropriate anisotropy and albedo which correspond to an optical thickness *b2*.

  If both *b1* and *b2* are zero then just assume $g = 0$ for the unreduced values.

⟨ Prototype for *abgb2ag* 296 ⟩ ≡
  void *abgb2ag*(**double** *a1*, **double** *b1*, **double** *b2*, **double** *∗a2*, **double** *∗g2*)
This code is used in sections 264 and 297.

297.   ⟨ Definition for *abgb2ag* 297 ⟩ ≡
  ⟨ Prototype for *abgb2ag* 296 ⟩
  {
    if $(b1 \equiv 0 \vee b2 \equiv 0)$ {
      $*a2 = a1$;
      $*g2 = 0$;
    }
    if $(b2 < b1)$ $b2 = b1$;
    if $(a1 \equiv 0)$ $*a2 = 0.0$;
    else {
      if $(a1 \equiv 1)$ $*a2 = 1.0$;
      else {
        if $(b1 \equiv 0 \vee b2 \equiv \texttt{HUGE\_VAL})$ $*a2 = a1$;
        else $*a2 = 1 + b1/b2 * (a1 - 1)$;
      }
    }
    if $(*a2 \equiv 0 \vee b2 \equiv 0 \vee b2 \equiv \texttt{HUGE\_VAL})$ $*g2 = 0.5$;
    else $*g2 = (1 - b1/b2)/(*a2)$;
  }
This code is used in section 263.

298. Guessing an inverse.

This routine is not used anymore.

⟨ Prototype for *slow_guess* 298 ⟩ ≡

   void *slow_guess*(**struct measure_type** *m*, **struct invert_type** *∗r*, **double** *∗a*, **double** *∗b*, **double** *∗g*)

This code is used in section 299.

299. ⟨ Definition for *slow_guess* 299 ⟩ ≡

  ⟨ Prototype for *slow_guess* 298 ⟩

  {

    double *fmin* = 10.0;

    double *fval*;

    double *∗x*;

    x = *dvector*(1, 2);

    switch (*r*→*search*) {

    case FIND_A: ⟨ Slow guess for *a* alone 300 ⟩

      break;

    case FIND_B: ⟨ Slow guess for *b* alone 301 ⟩

      break;

    case FIND_AB: **case** FIND_AG: ⟨ Slow guess for *a* and *b* or *a* and *g* 302 ⟩

      break;

    }

    ∗a = *r*→*slab*.*a*;

    ∗b = *r*→*slab*.*b*;

    ∗g = *r*→*slab*.*g*;

    free_dvector(*x*, 1, 2);

  }

300. ⟨ Slow guess for *a* alone 300 ⟩ ≡

  r→*slab*.*b* = HUGE_VAL;

  r→*slab*.*g* = *r*→*default_g*;

  Set_Calc_State(*m*, *∗r*);

  for (*r*→*slab*.*a* = 0.0; *r*→*slab*.*a* ≤ 1.0; *r*→*slab*.*a* += 0.1) {

    fval = *Find_A_fn*(*a2acalc*(*r*→*slab*.*a*));

    if (*fval* < *fmin*) {

      r→*a* = *r*→*slab*.*a*;

      fmin = *fval*;

    }

  }

  r→*slab*.*a* = *r*→*a*;

This code is used in section 299.

301.   Presumably the only time that this will need to be called is when the albedo is fixed or is one. For now, I'll just assume that it is one.

⟨ Slow guess for b alone 301 ⟩ ≡
  $r{\rightarrow}slab.a = 1;$
  $r{\rightarrow}slab.g = r{\rightarrow}default\_g;$
  $Set\_Calc\_State(m, *r);$
  for $(r{\rightarrow}slab.b = 1/32.0; \ r{\rightarrow}slab.b \leq 32; \ r{\rightarrow}slab.b \mathrel{*}= 2)$ {
    $fval = Find\_B\_fn(b2bcalc(r{\rightarrow}slab.b));$
    if $(fval < fmin)$ {
      $r{\rightarrow}b = r{\rightarrow}slab.b;$
      $fmin = fval;$
    }
  }
  $r{\rightarrow}slab.b = r{\rightarrow}b;$
This code is used in section 299.

302.   ⟨ Slow guess for a and b or a and g 302 ⟩ ≡
  {
    double $min\_a, min\_b, min\_g;$
    if $(\neg Valid\_Grid(m, r{\rightarrow}search)) \ Fill\_Grid(m, *r);$
    $Near\_Grid\_Points(m.m\_r, m.m\_t, r{\rightarrow}search, \&min\_a, \&min\_b, \&min\_g);$
    $r{\rightarrow}slab.a = min\_a;$
    $r{\rightarrow}slab.b = min\_b;$
    $r{\rightarrow}slab.g = min\_g;$
  }
This code is used in section 299.

303.   ⟨ Prototype for $quick\_guess$ 303 ⟩ ≡
  void $quick\_guess($**struct measure_type** $m,$ **struct invert_type** $r,$ **double** $*a,$ **double** $*b,$ **double** $*g)$
This code is used in sections 264 and 304.

304.   ⟨ Definition for $quick\_guess$ 304 ⟩ ≡
  ⟨ Prototype for $quick\_guess$ 303 ⟩
  {
    double $\mathtt{UR1}, \mathtt{UT1}, rd, td, tc, rc, bprime, aprime, alpha, beta, logr;$
    $Estimate\_RT(m, r, \&\mathtt{UR1}, \&\mathtt{UT1}, \&rd, \&rc, \&td, \&tc);$
    ⟨ Estimate $aprime$ 305 ⟩
    switch $(m.num\_measures)$ {
    case 1: ⟨ Guess when only reflection is known 307 ⟩
      break;
    case 2: ⟨ Guess when reflection and transmission are known 308 ⟩
      break;
    case 3: ⟨ Guess when all three measurements are known 309 ⟩
      break;
    }
    ⟨ Clean up guesses 314 ⟩
  }
This code is used in section 263.

305.   ⟨Estimate *aprime* 305⟩ ≡
  if (UT1 ≡ 1) *aprime* = 1.0;
  else if $(rd/(1 − \text{UT1}) ≥ 0.1)$ {
      double $tmp = (1 − rd − \text{UT1})/(1 − \text{UT1})$;
      $aprime = 1 − 4.0/9.0 * tmp * tmp$;
  }
  else if $(rd < 0.05 ∧ \text{UT1} < 0.4)$ $aprime = 1 − (1 − 10 * rd) * (1 − 10 * rd)$;
  else if $(rd < 0.1 ∧ \text{UT1} < 0.4)$ $aprime = 0.5 + (rd − 0.05) * 4$;
  else {
      double $tmp = (1 − 4 * rd − \text{UT1})/(1 − \text{UT1})$;
      $aprime = 1 − tmp * tmp$;
  }
This code is used in section 304.

306.   ⟨Estimate *bprime* 306⟩ ≡
  if $(rd < 0.01)$ {
      $bprime = What\_Is\_B(r.slab, \text{UT1})$;
      $fprintf(stderr, \texttt{"low␣rd<0.01!␣ut1=\%f␣aprime=\%f␣bprime=\%f\\n"}, \text{UT1}, aprime, bprime)$;
  }
  else if (UT1 ≤ 0) $bprime = \texttt{HUGE\_VAL}$;
  else if (UT1 > 0.1) $bprime = 2 * exp(5 * (rd − \text{UT1}) * log(2.0))$;
  else {
      $alpha = 1/log(0.05/1.0)$;
      $beta = log(1.0)/log(0.05/1.0)$;
      $logr = log(\text{UR1})$;
      $bprime = log(\text{UT1}) − beta * log(0.05) + beta * logr$;
      $bprime /= alpha * log(0.05) − alpha * logr − 1$;
  }
This code is used in sections 308, 312, and 313.

307.

⟨Guess when only reflection is known 307⟩ ≡
  $*g = r.default\_g$;
  $*a = aprime/(1 − *g + aprime * (*g))$;
  $*b = \texttt{HUGE\_VAL}$;
This code is used in section 304.

308.   ⟨Guess when reflection and transmission are known 308⟩ ≡
  ⟨Estimate *bprime* 306⟩
  $*g = r.default\_g$;
  $*a = aprime/(1 − *g + aprime * *g)$;
  $*b = bprime/(1 − *a * *g)$;
This code is used in section 304.

309.   ⟨ Guess when all three measurements are known 309 ⟩ ≡
  switch (*r.search*) {
  case FIND_A: ⟨ Guess when finding albedo 310 ⟩
    break;
  case FIND_B: ⟨ Guess when finding optical depth 311 ⟩
    break;
  case FIND_AB: ⟨ Guess when finding the albedo and optical depth 312 ⟩
    break;
  case FIND_AG: ⟨ Guess when finding anisotropy and albedo 313 ⟩
    break;
  }
This code is used in section 304.

310.
⟨ Guess when finding albedo 310 ⟩ ≡
  $*g = r.default\_g$;
  $*a = aprime/(1 - *g + aprime * *g)$;
  $*b = What\_Is\_B(r.slab, m.m\_u)$;
This code is used in section 309.

311.
⟨ Guess when finding optical depth 311 ⟩ ≡
  $*g = r.default\_g$;
  $*a = 0.0$;
  $*b = What\_Is\_B(r.slab, m.m\_u)$;
This code is used in section 309.

312.
⟨ Guess when finding the albedo and optical depth 312 ⟩ ≡
  $*g = r.default\_g$;
  if ($*g \equiv 1$) $*a = 0.0$;
  else $*a = aprime/(1 - *g + aprime * *g)$;
  ⟨ Estimate *bprime* 306 ⟩
  if ($bprime \equiv$ HUGE_VAL $\vee *a * *g \equiv 1$) $*b = $ HUGE_VAL;
  else $*b = bprime/(1 - *a * *g)$;
This code is used in section 309.

313.
⟨ Guess when finding anisotropy and albedo 313 ⟩ ≡
  $*b = What\_Is\_B(r.slab, m.m\_u)$;
  if ($*b \equiv$ HUGE_VAL $\vee *b \equiv 0$) {
    $*a = aprime$;
    $*g = r.default\_g$;
  }
  else {
    ⟨ Estimate *bprime* 306 ⟩
    $*a = 1 + bprime * (aprime - 1)/(*b)$;
    if ($*a < 0.1$) $*g = 0.0$;
    else $*g = (1 - bprime/(*b))/(*a)$;
  }
This code is used in section 309.

314.

$\langle\,$ Clean up guesses $314\,\rangle \equiv$

   if $(*a < 0)$ $*a = 0.0;$

   if $(*g < 0)$ $*g = 0.0;$

   else if $(*g \geq 1)$ $*g = 0.5;$

This code is used in section 304.

315. Some debugging stuff.

316. ⟨ Prototype for *Set_Debugging* 316 ⟩ ≡
  void *Set_Debugging*(**unsigned long** *debug_level*)

This code is used in sections 264 and 317.

317.
⟨ Definition for *Set_Debugging* 317 ⟩ ≡
  ⟨ Prototype for *Set_Debugging* 316 ⟩
  {
    g_util_debugging = *debug_level*;
  }

This code is used in section 263.

318.
⟨ Prototype for *Debug* 318 ⟩ ≡
  int *Debug*(**unsigned long** *mask*)

This code is used in sections 264 and 319.

319.
⟨ Definition for *Debug* 319 ⟩ ≡
  ⟨ Prototype for *Debug* 318 ⟩
  {
    if (*g_util_debugging* & *mask*) **return** 1;
    else return 0;
  }

This code is used in section 263.

320.
⟨ Prototype for *Print_Invert_Type* 320 ⟩ ≡
  void *Print_Invert_Type*(**struct invert_type** *r*)

This code is used in sections 264 and 321.

321.
⟨ Definition for *Print_Invert_Type* 321 ⟩ ≡
  ⟨ Prototype for *Print_Invert_Type* 320 ⟩
  {
    fprintf(*stderr*, "\n");
    fprintf(*stderr*, "default␣␣a=%10.5f␣␣␣b=%10.5f␣␣␣␣␣g=%10.5f\n", *r.default_a*, *r.default_b*, *r.default_g*);
    fprintf(*stderr*, "slab␣␣␣␣␣␣a=%10.5f␣␣␣b=%10.5f␣␣␣␣␣g=%10.5f\n", *r.slab.a*, *r.slab.b*, *r.slab.g*);
    fprintf(*stderr*, "n␣␣␣␣␣␣␣top=%10.5f␣mid=%10.5f␣␣bot=%10.5f\n", *r.slab.n_top_slide*, *r.slab.n_slab*,
        r.slab.n_bottom_slide);
    fprintf(*stderr*, "thick␣␣top=%10.5f␣cos=%10.5f␣␣bot=%10.5f\n", *r.slab.b_top_slide*, *r.slab.cos_angle*,
        r.slab.b_bottom_slide);
    fprintf(*stderr*, "search␣=␣%d␣quadrature␣points␣=␣%d\n", *r.search*, *r.method.quad_pts*);
  }

This code is used in section 263.

322.

⟨ Prototype for *Print_Measure_Type* 322 ⟩ ≡
  void *Print_Measure_Type*(**struct measure_type** *m*)

This code is used in sections 264 and 323.

323.

⟨ Definition for *Print_Measure_Type* 323 ⟩ ≡
  ⟨ Prototype for *Print_Measure_Type* 322 ⟩
  {
    fprintf(*stderr*, "\n");
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Beam␣diameter␣=␣%7.1f␣mm\n", *m.d_beam*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Sample␣thickness␣=␣%7.1f␣mm\n", *m.slab_thickness*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Top␣slide␣thickness␣=␣%7.1f␣mm\n",
        m.slab_top_slide_thickness);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣Bottom␣slide␣thickness␣=␣%7.1f␣mm\n",
        m.slab_bottom_slide_thickness);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣Sample␣index␣of␣refraction␣=␣%7.3f\n", *m.slab_index*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣Top␣slide␣index␣of␣refraction␣=␣%7.3f\n", *m.slab_top_slide_index*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣Bottom␣slide␣index␣of␣refraction␣=␣%7.3f\n", *m.slab_bottom_slide_index*);
    fprintf(*stderr*, "#␣␣␣␣␣Fraction␣unscattered␣light␣in␣M_R␣=␣%7.1f␣%%\n",
        m.fraction_of_rc_in_mr ∗ 100);
    fprintf(*stderr*, "#␣␣␣␣␣Fraction␣unscattered␣light␣in␣M_T␣=␣%7.1f␣%%\n",
        m.fraction_of_tc_in_mt ∗ 100);
    fprintf(*stderr*, "#␣\n");
    fprintf(*stderr*, "#␣Reflection␣sphere\n");
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sphere␣diameter␣=␣%7.1f␣mm\n", *m.d_sphere_r*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣sample␣port␣diameter␣=␣%7.1f␣mm\n",
        2 ∗ *m.d_sphere_r* ∗ *sqrt*(*m.as_r*));
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣entrance␣port␣diameter␣=␣%7.1f␣mm\n",
        2 ∗ *m.d_sphere_r* ∗ *sqrt*(*m.ae_r*));
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣port␣diameter␣=␣%7.1f␣mm\n",
        2 ∗ *m.d_sphere_r* ∗ *sqrt*(*m.ad_r*));
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣wall␣reflectance␣=␣%7.1f␣%%\n", *m.rw_r* ∗ 100);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣standard␣reflectance␣=␣%7.1f␣%%\n", *m.rstd_r* ∗ 100);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣detector␣reflectance␣=␣%7.1f␣%%\n", *m.rd_r* ∗ 100);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣spheres␣=␣%7d\n", *m.num_spheres*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣measures␣=␣%7d\n", *m.num_measures*);
    fprintf(*stderr*, "#␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣␣method␣=␣%7d\n", *m.method*);
    fprintf(*stderr*, "area_r␣as=%10.5f␣␣ad=%10.5f␣␣␣␣ae=%10.5f␣␣aw=%10.5f\n", *m.as_r*, *m.ad_r*,
        m.ae_r, *m.aw_r*);
    fprintf(*stderr*, "refls␣␣rd=%10.5f␣␣rw=%10.5f␣␣rstd=%10.5f␣␣␣␣f=%10.5f\n", *m.rd_r*, *m.rw_r*,
        m.rstd_r, *m.f_r*);
    fprintf(*stderr*, "area_t␣as=%10.5f␣␣ad=%10.5f␣␣␣␣␣ae=%10.5f␣␣aw=%10.5f\n", *m.as_t*, *m.ad_t*,
        m.ae_t, *m.aw_t*);
    fprintf(*stderr*, "refls␣␣rd=%10.5f␣␣rw=%10.5f␣␣rstd=%10.5f\n", *m.rd_t*, *m.rw_t*, *m.rstd_t*);
    fprintf(*stderr*, "lost␣␣ur1=%10.5f␣ut1=%10.5f␣␣␣uru=%10.5f␣␣utu=%10.5f\n", *m.ur1_lost*,
        m.ut1_lost, *m.utu_lost*, *m.utu_lost*);
  }

This code is used in section 263.

324. Index.   Here is a cross-reference table for the inverse adding-doubling program. All sections in which an identifier is used are listed with that identifier, except that reserved words are indexed only when they appear in format definitions, and the appearances of identifiers in section names are not indexed. Underlined entries correspond to where the identifier was declared. Error messages and a few other things like "ASCII code dependencies" are indexed here too.

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