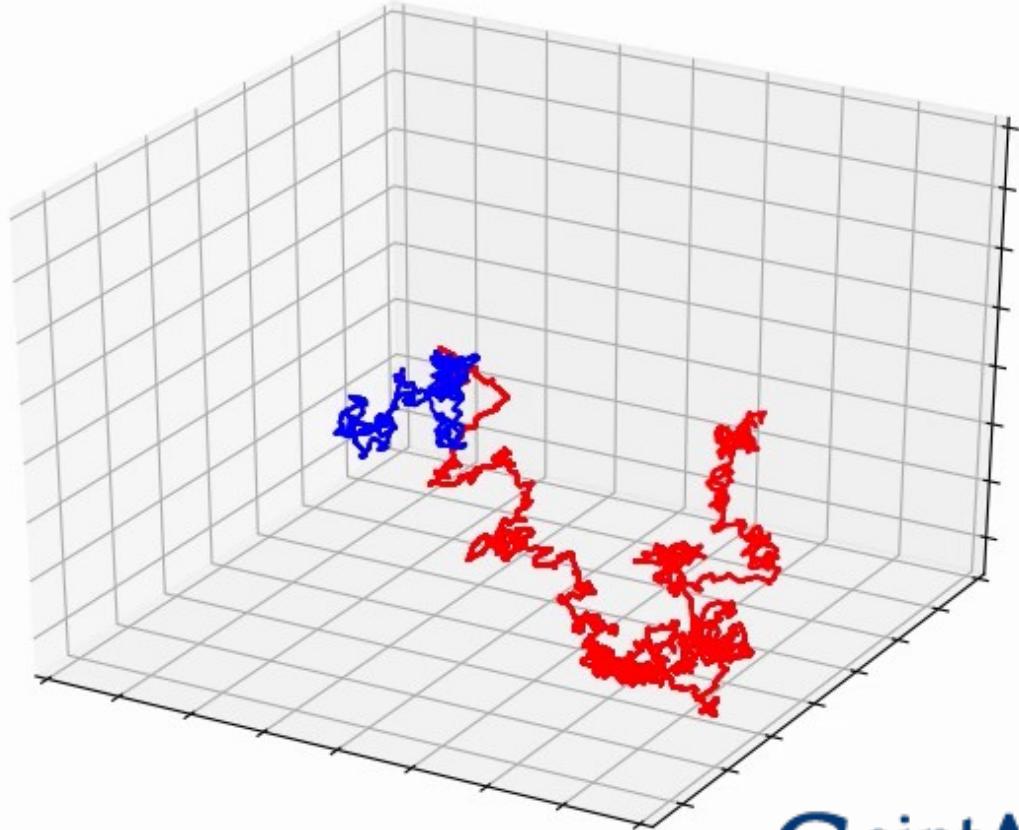




University of
St Andrews

Modelling light-tissue interactions using the Monte Carlo Radiation Transfer method

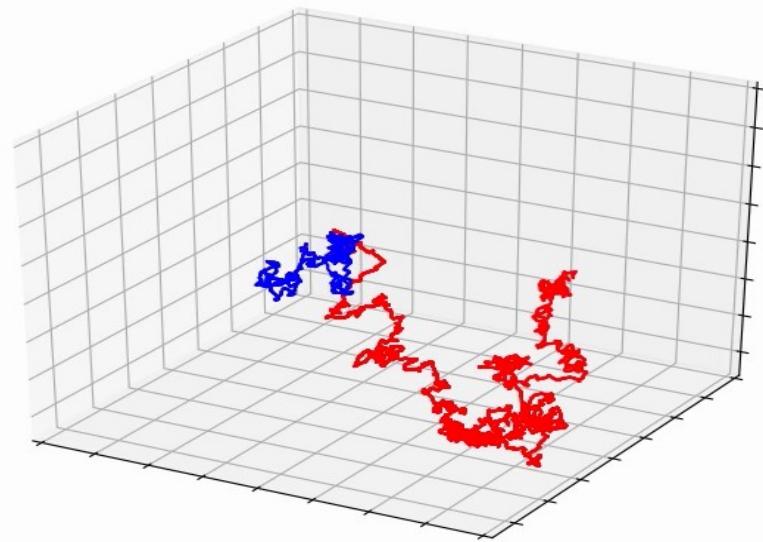
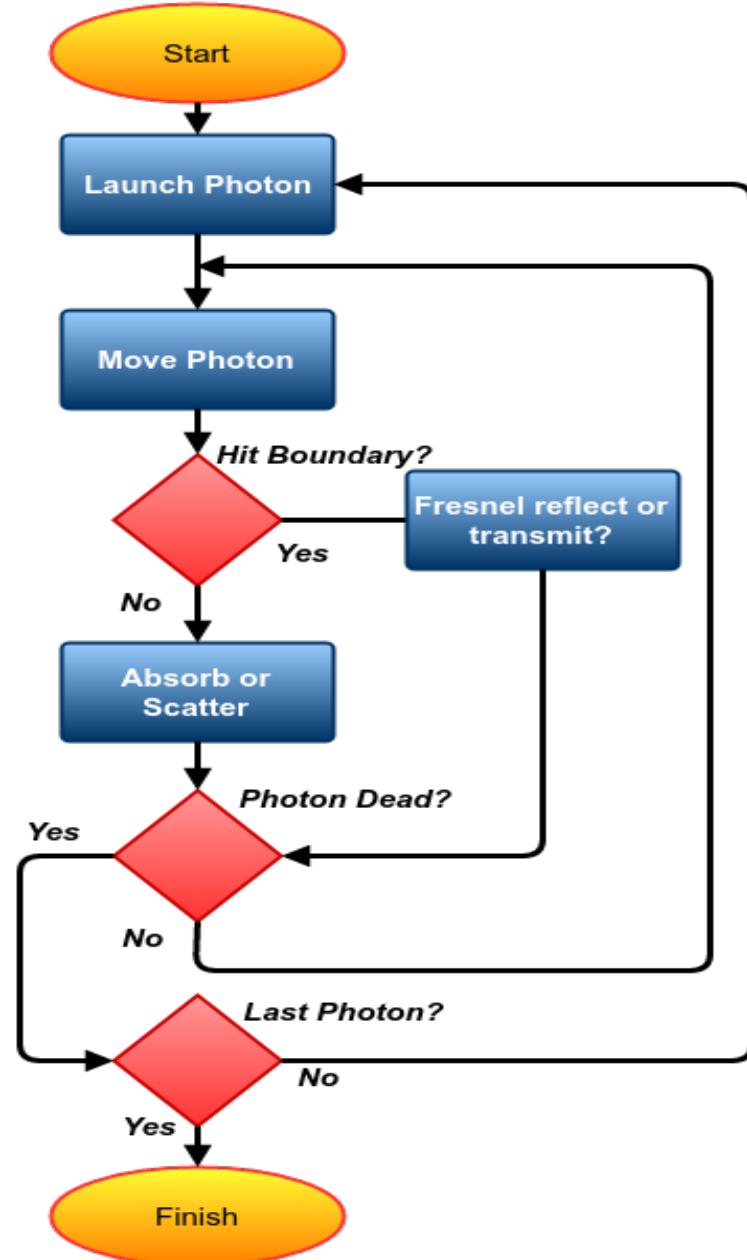


Lewis McMillan
lm959@st-andrews.ac.uk
github.com/lewisfish

Saint Andrews Monte Carlo Summer School

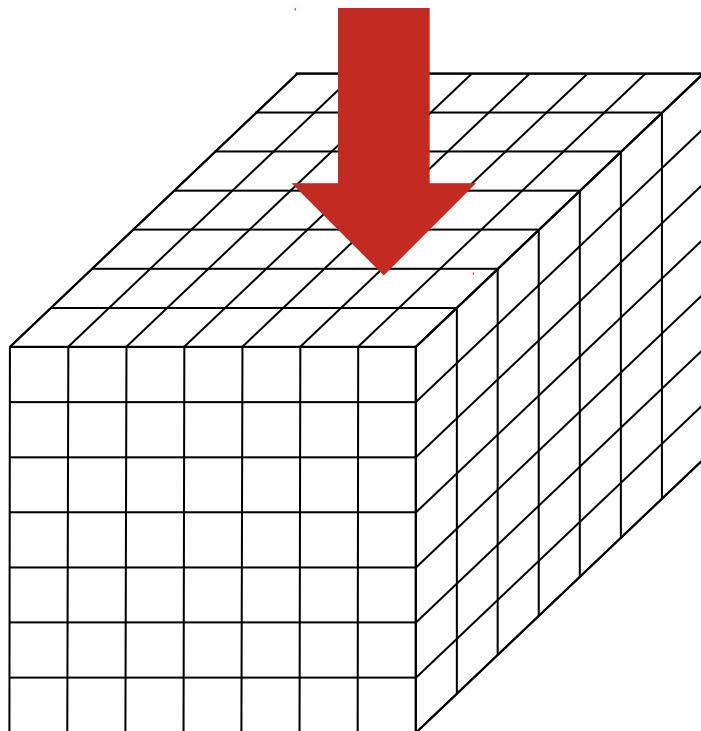
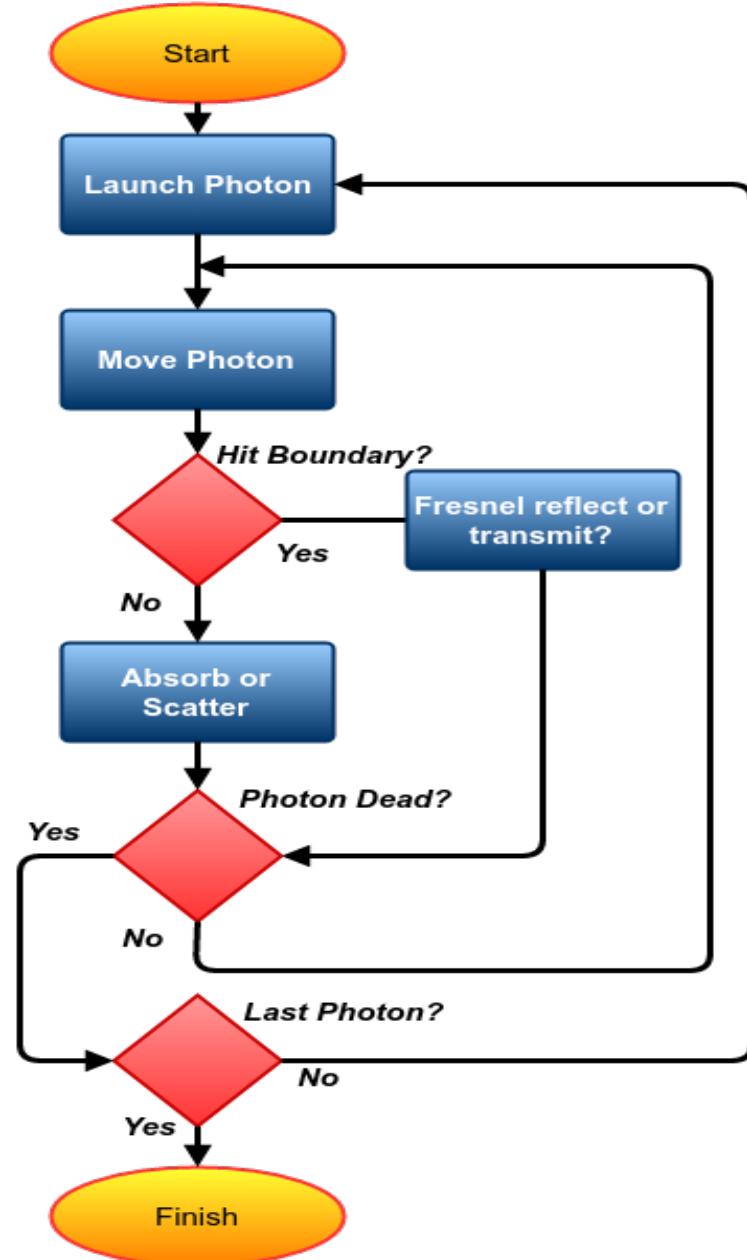
Monte Carlo Radiation Transfer

Uses random numbers and interaction probabilities to simulate photon propagation

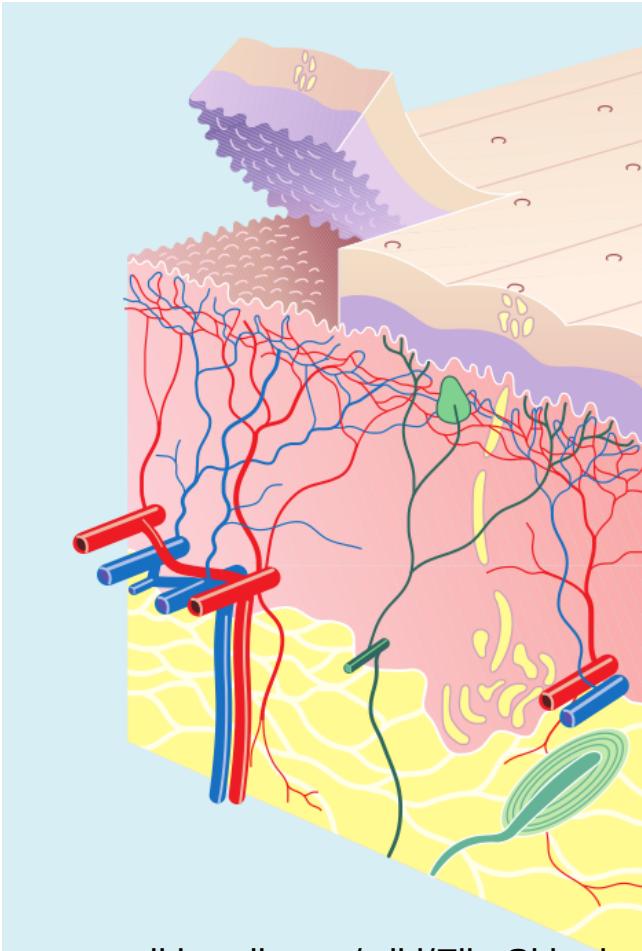


Monte Carlo Radiation Transfer

Uses random numbers and interaction probabilities to simulate photon propagation



Voxel Model

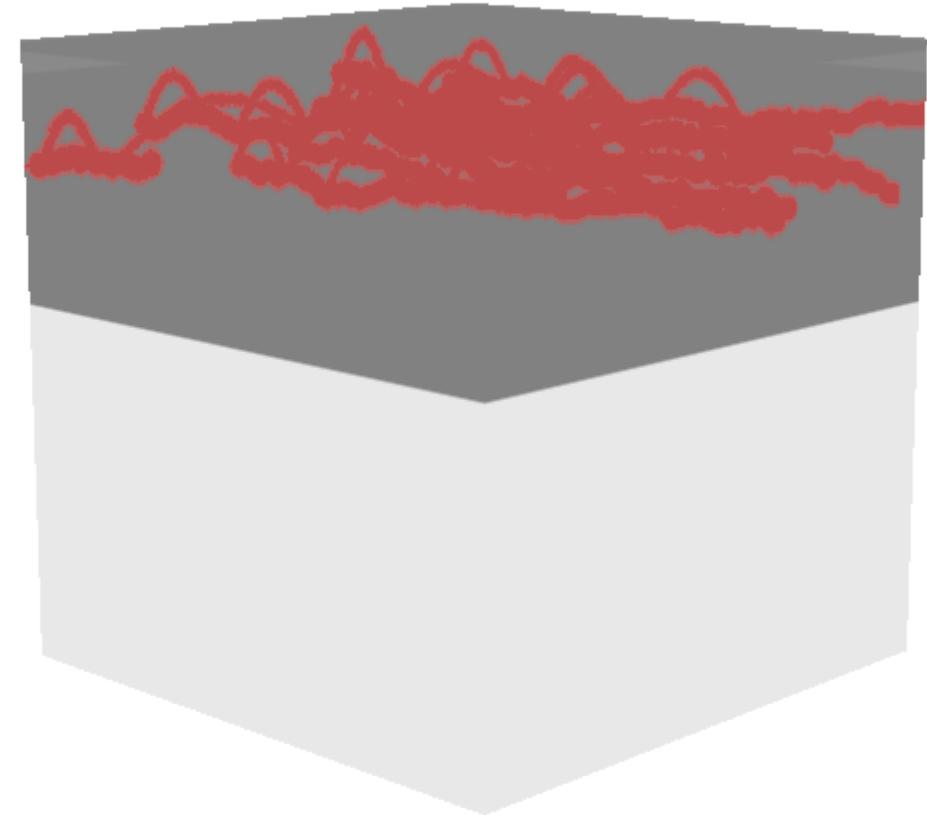
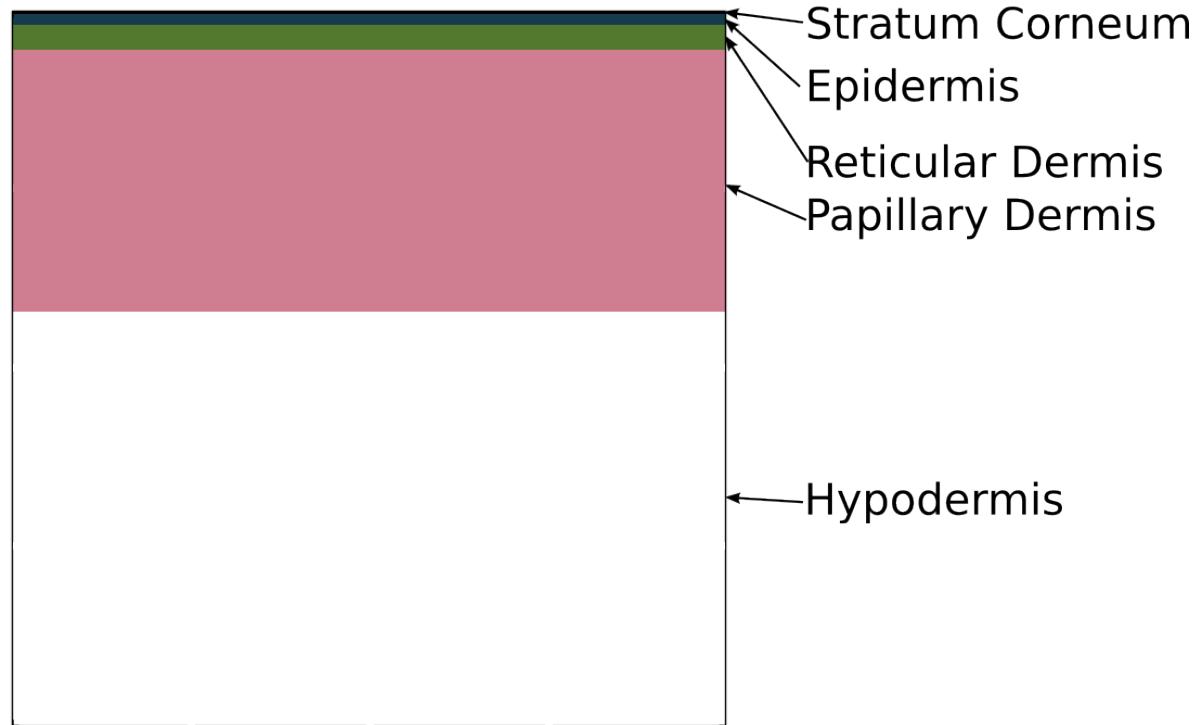


https://commons.wikimedia.org/wiki/File:Skin_layers.svg Hubble telescope

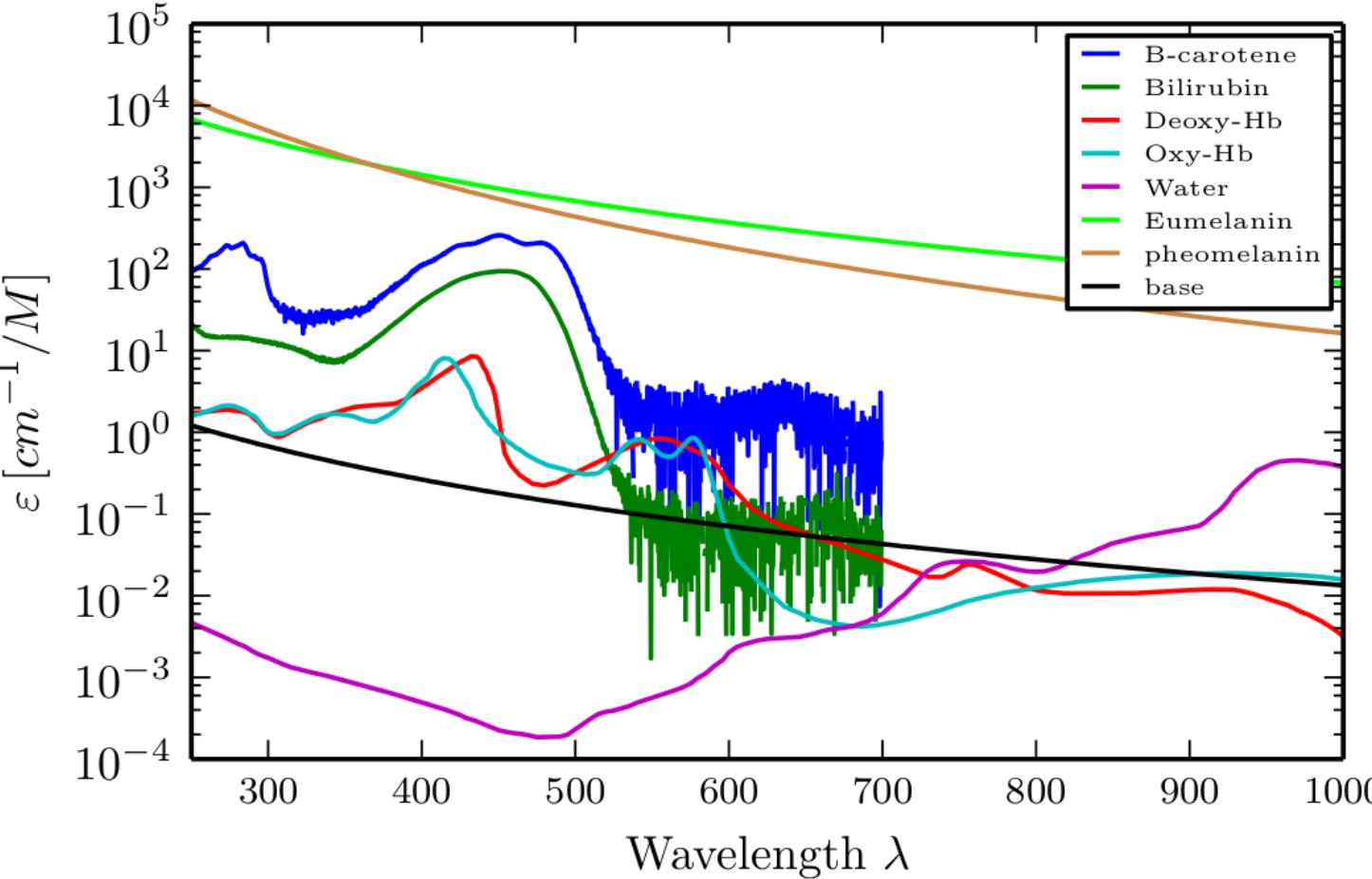


The Butterfly Nebula: NGC 6302 © HUBBLESTIE.org

Voxel Model



5 layer skin model



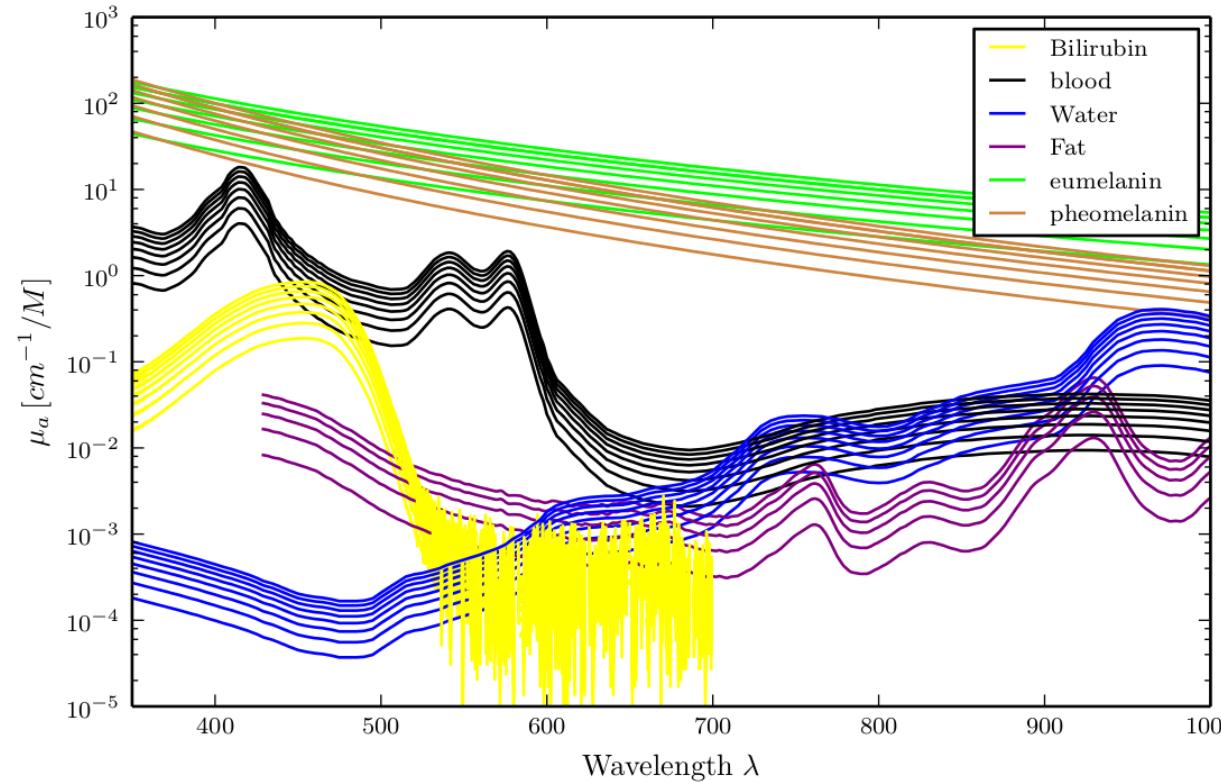
- 5 Layer skin model
- Various absorbers:
Blood, Melanin,
Bilirubin, water, fat...

$$\mu_a^{layer} = 2.3 \sum_i C_i \mathcal{E}_i + \sum_j f_{v,j} \mu_{a,j}$$

5 layer skin model

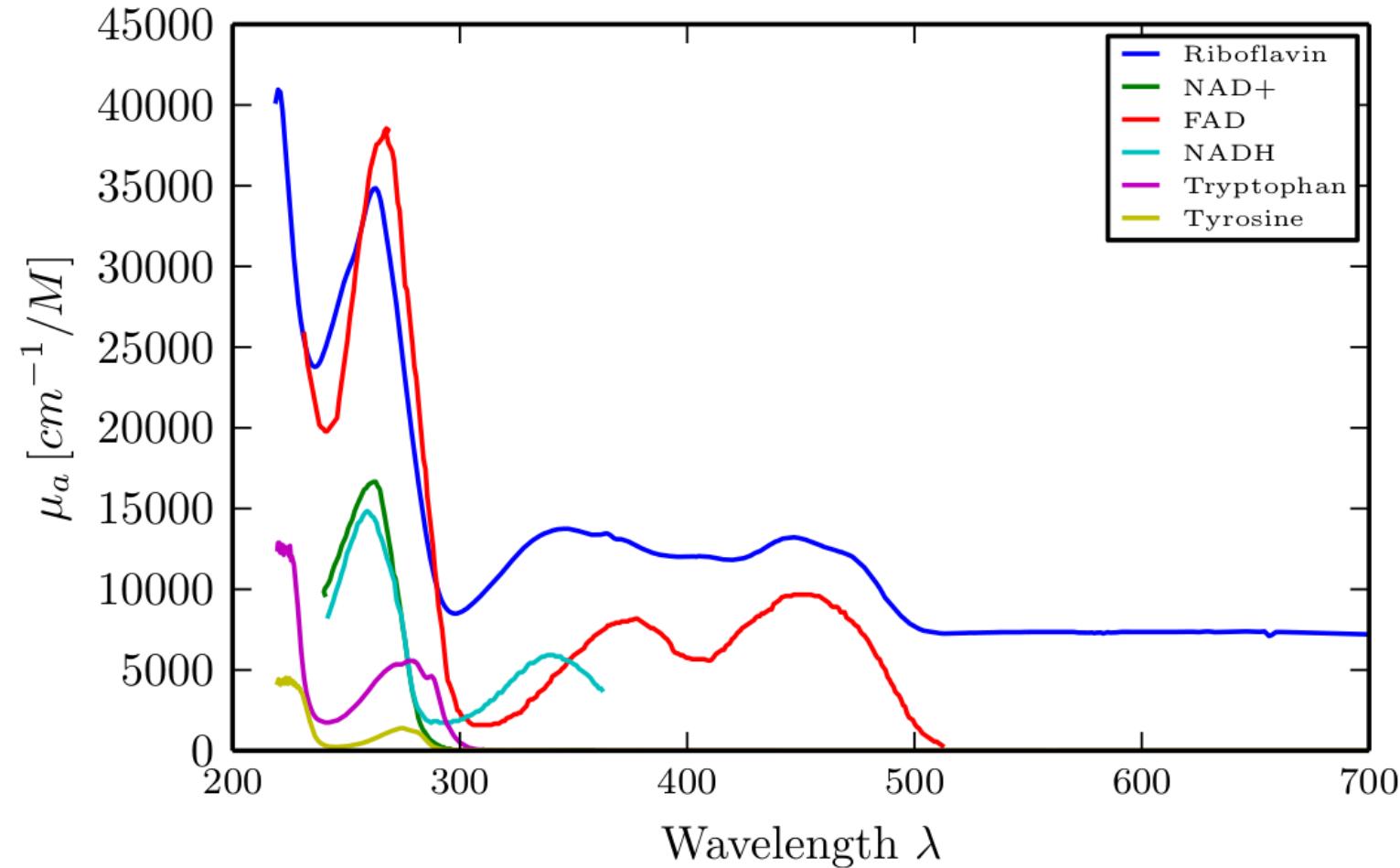
$$\begin{aligned}\mu_a^{layer} = & B S \mu_{a.oxy} + B(1 - S)\mu_{a.deoxy} + W\mu_{a.H_2O} + F\mu_{a.fat} + M\mu_{a.melansome} \\ & + 2.3 C_{bilirubin} \mathcal{E}_{bilirubin} + 2.3 C_{\beta-Carotene} \mathcal{E}_{\beta-Carotene} + A\mu_{a.baseline}\end{aligned}$$

- Vary volumes, concentrations and fractions of absorbers
- Can account for different ages and skin types



5 layer skin model

- 5 Layer skin model
- Various absorbers: Blood, Melanin, Bilirubin, water, fat...
- Various fluorophores: NADH, FAD, Riboflavin, Tyrosine...



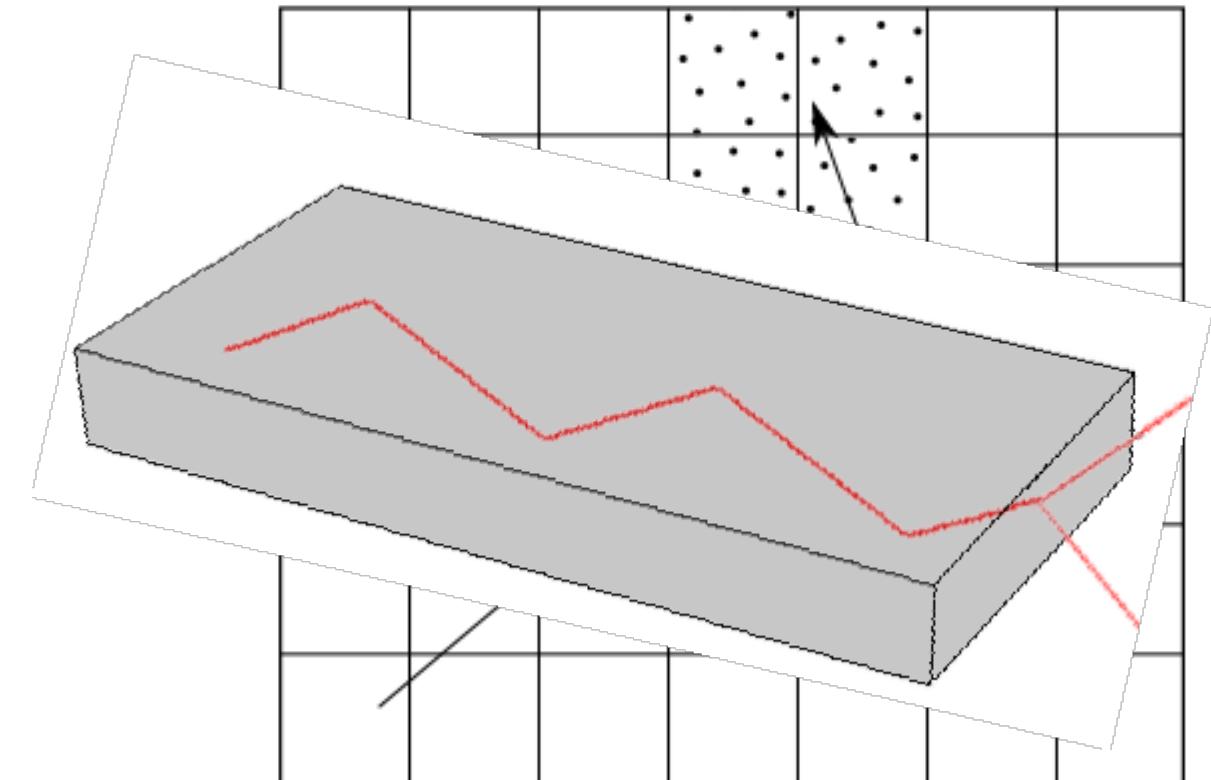
Fresnel Reflections/Refractions

- Model reflection/refraction at voxel boundaries

$$R_s = \left| \frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t} \right|^2$$

$$R_t = \left| \frac{n_1 \cos\theta_t - n_2 \cos\theta_i}{n_1 \cos\theta_t + n_2 \cos\theta_i} \right|^2$$

$$R = \frac{1}{2}(R_s + R_p)$$



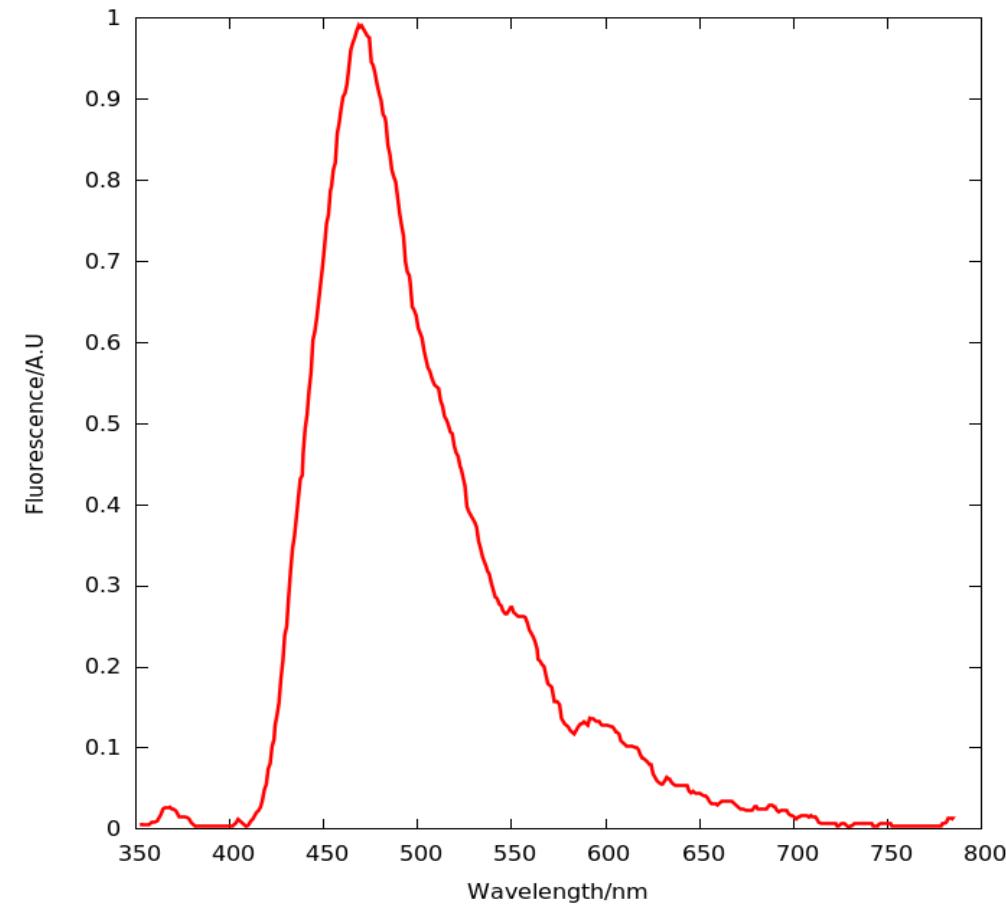
Motivation

- Cardiovascular disease one of the largest causes of death
- Traditional factors do not fully explain incidence of disease
- Research towards novel biomarkers



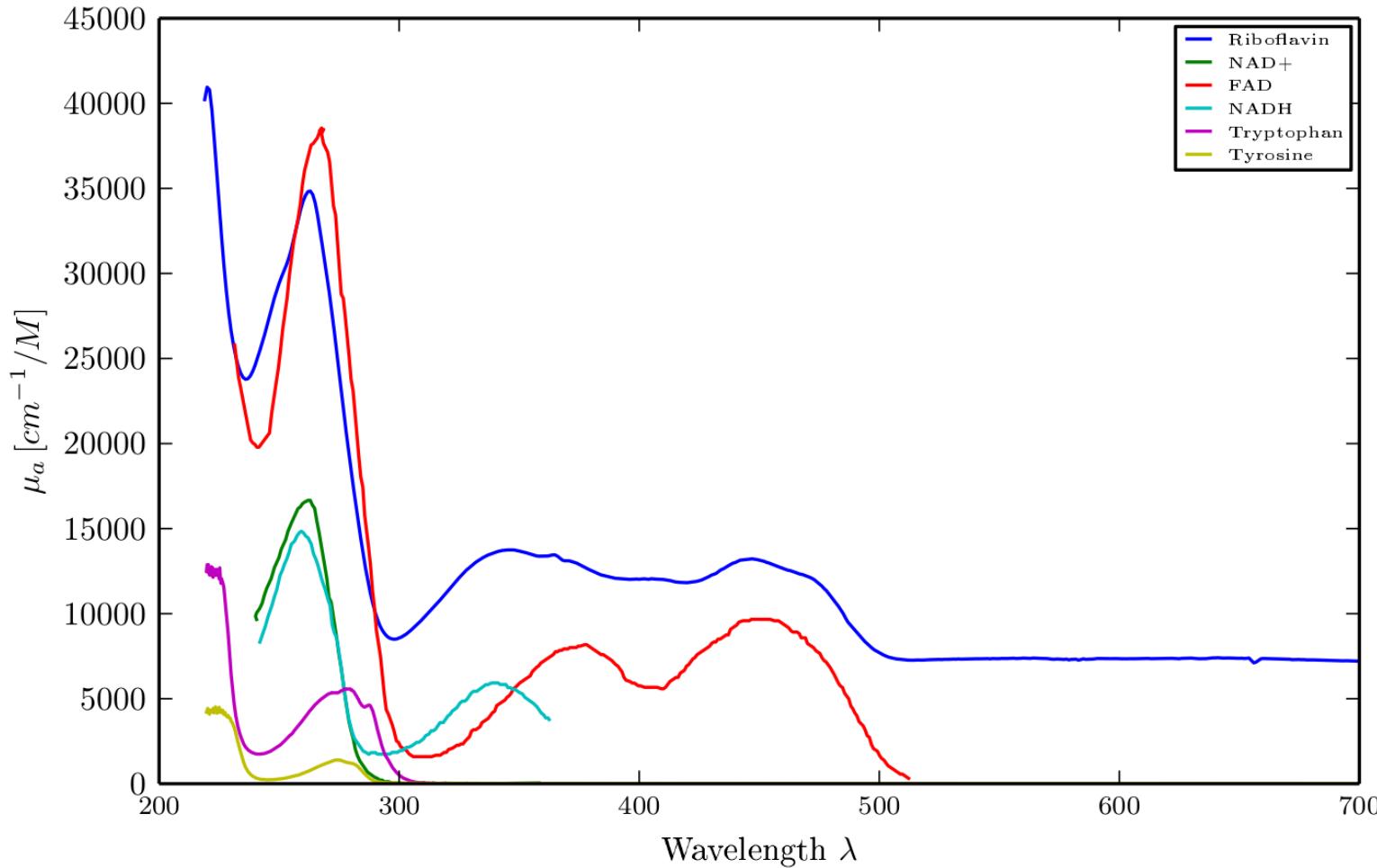
Motivation

- Collaboration Ninewells/Dundee University
- Microvascular dysfunction
- Investigate biomarkers related to oxidative stress

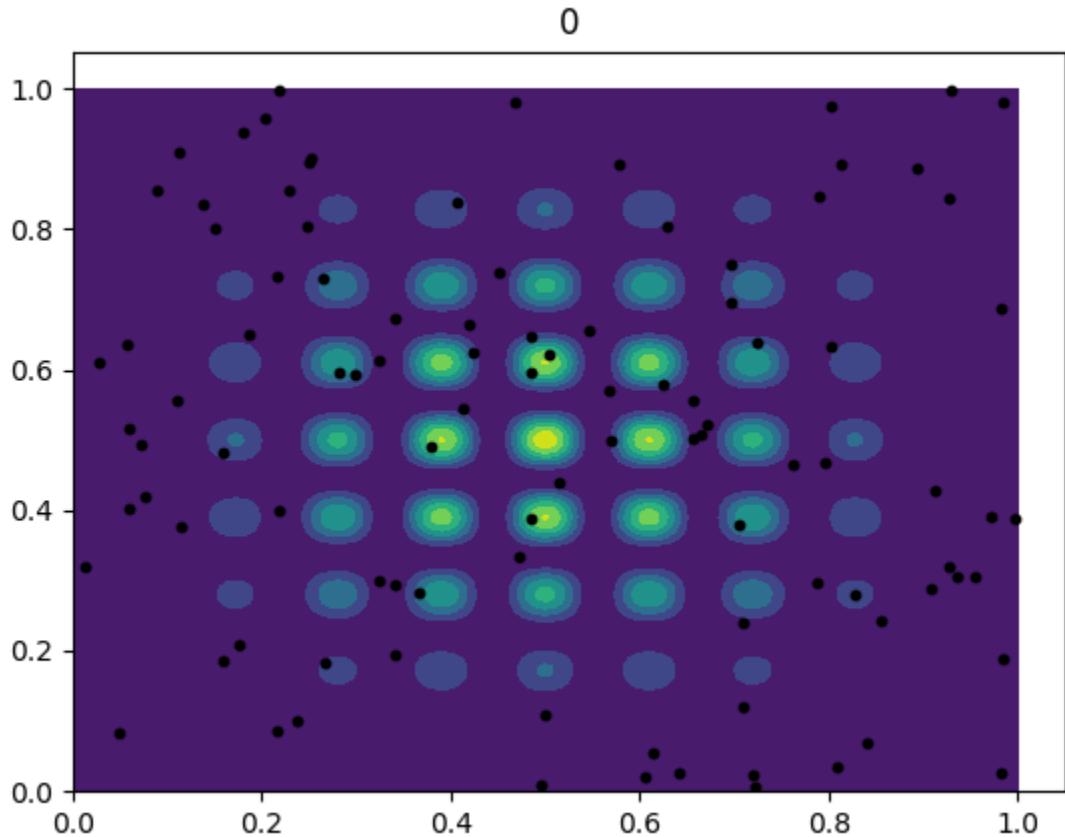
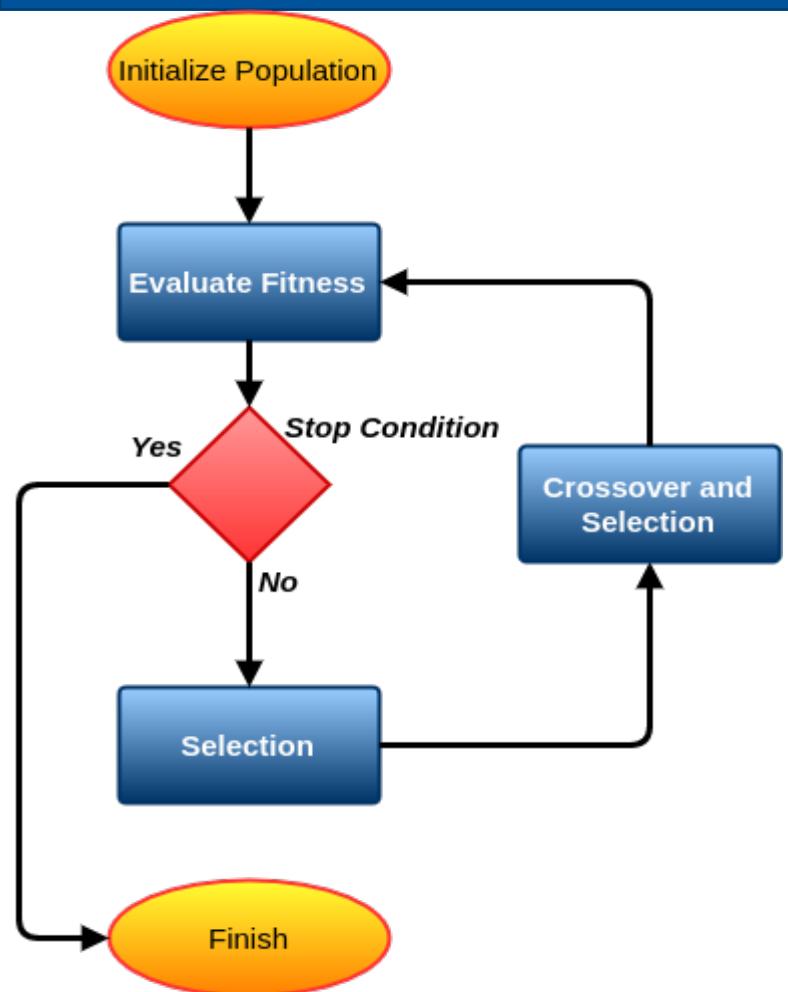


Autofluorescence

- No literature values of concentration of fluorophores

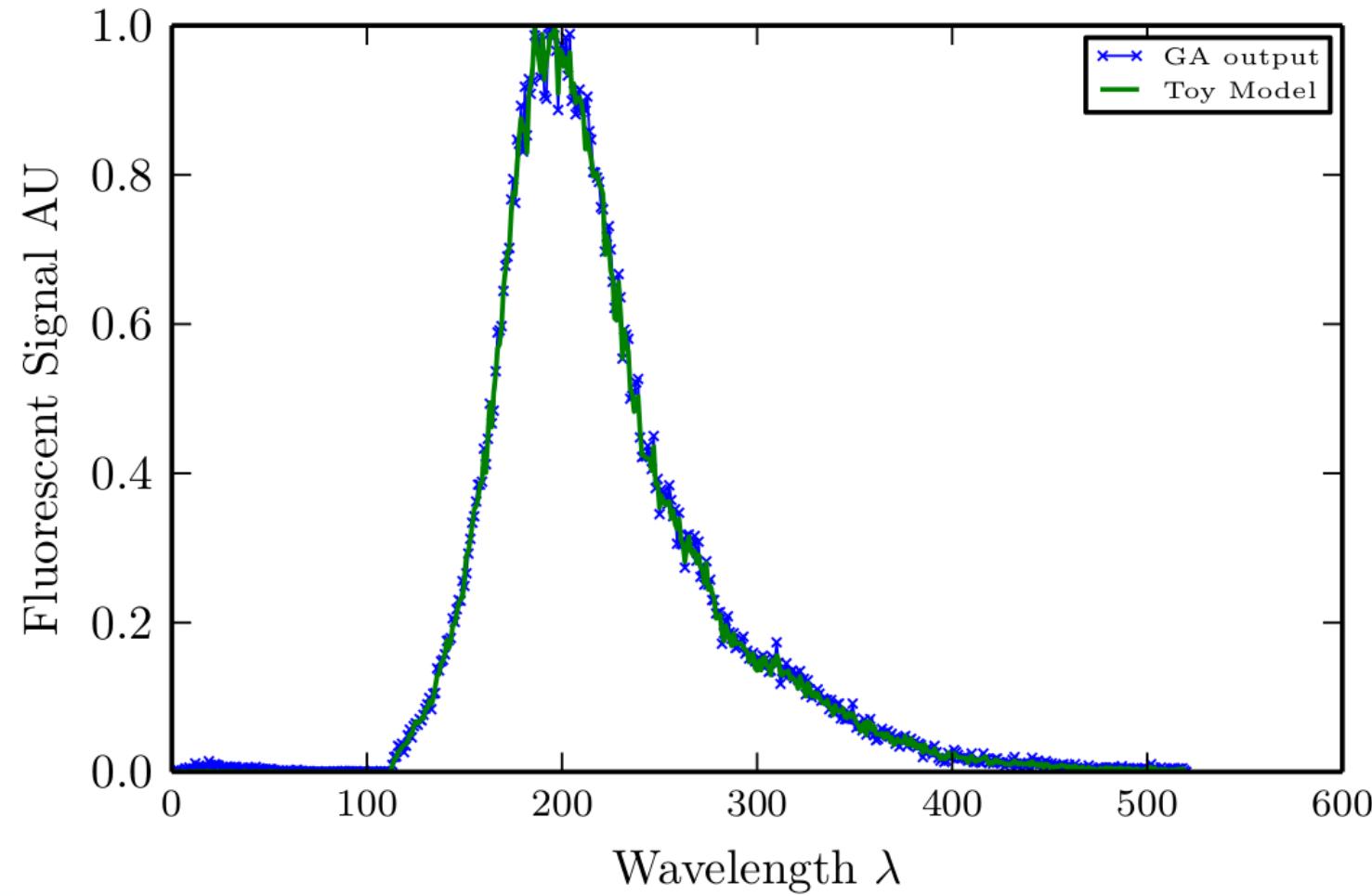


Genetic Algorithms

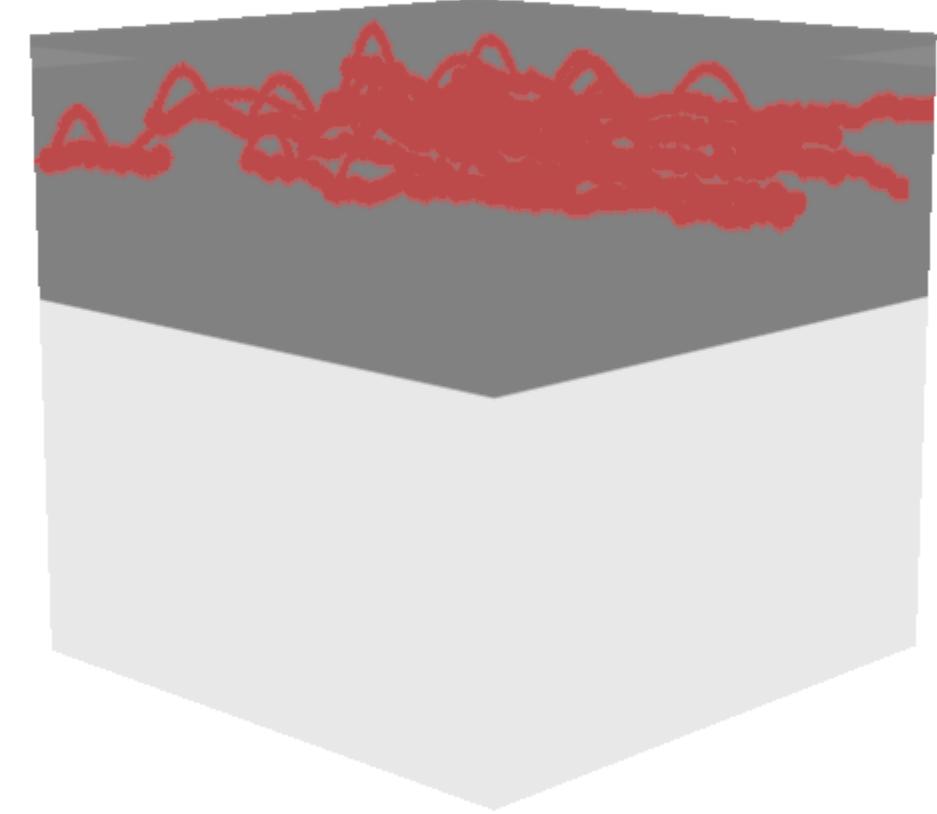


?g{ ^ | C#cl]Et sK

Genetic Algorithm

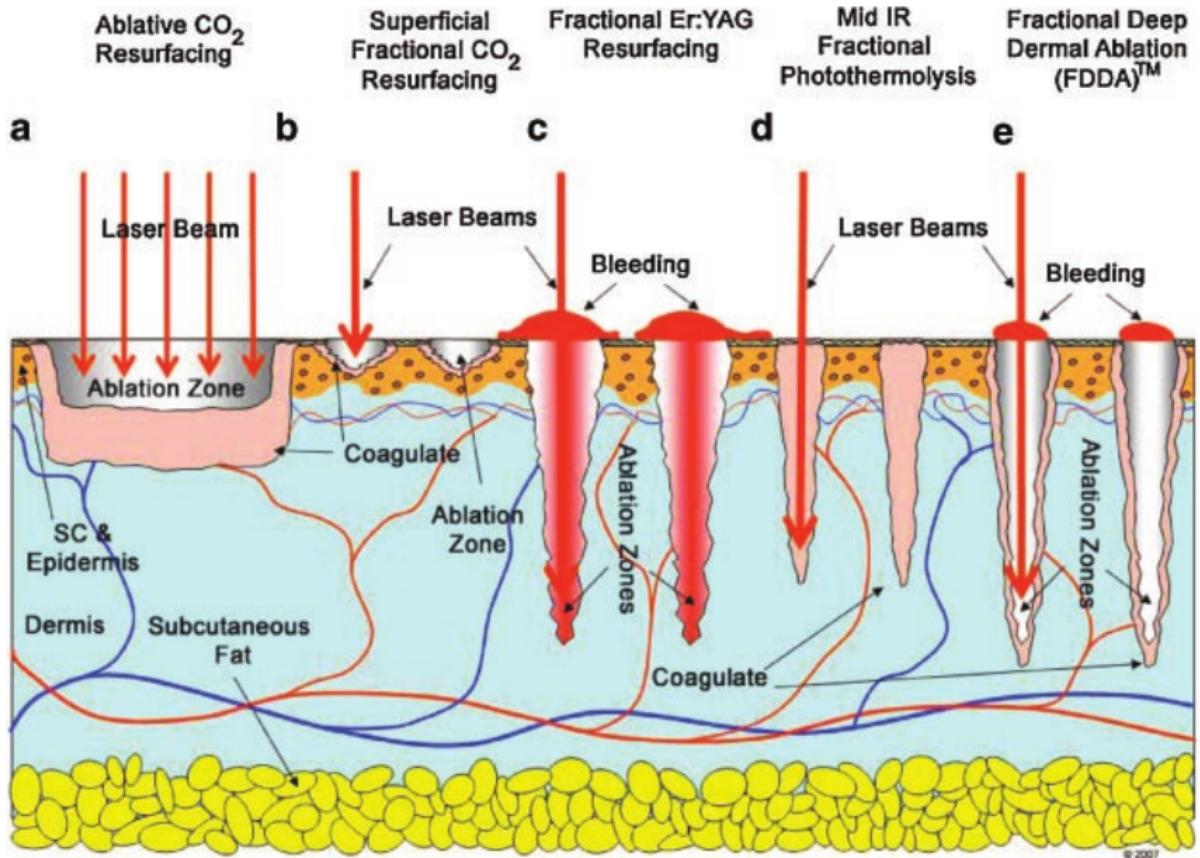


Laser Doppler flowmetry

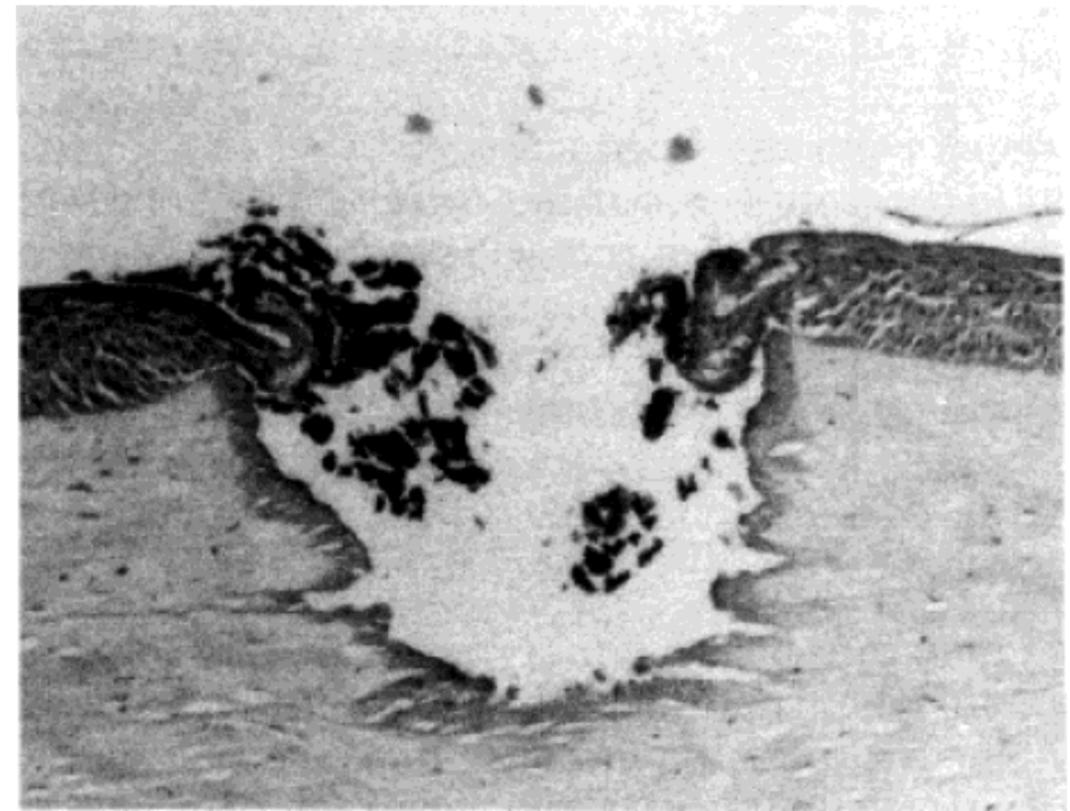


Laser Doppler flowmetry

Tissue Ablation



Rahman et al. *Lasers in surgery* (2009)



J. Cummings et al. *Applied Optics* (1993)

Tissue Ablation



Before



After



V. Madan, ukdermatologist.co.uk

www.st-andrews.ac.uk

Modelling Tissue Ablation

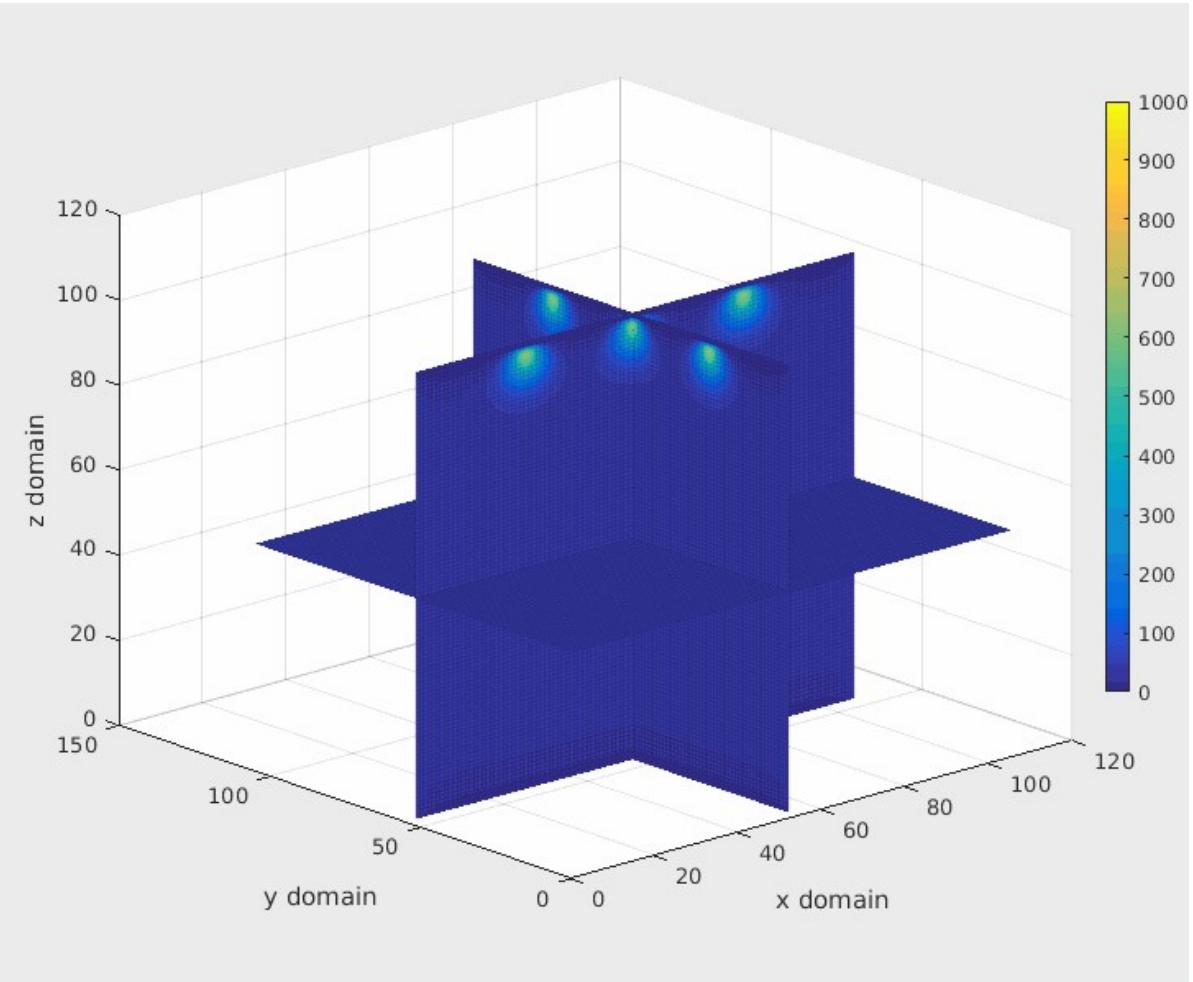
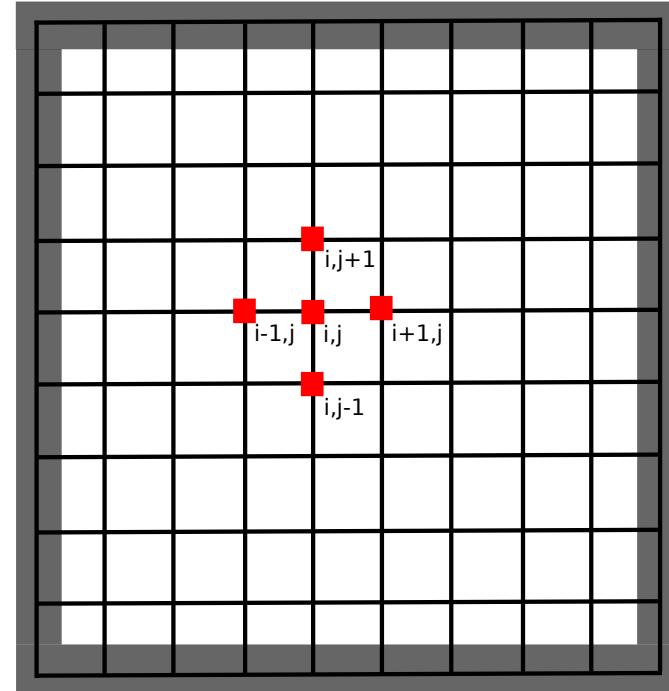
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + S$$

$$S = -hA(T_\infty - T) - \sigma\varepsilon A(T_\infty^4 - T^4) + \dot{q}$$

Convective	Radiative	Laser heat source
------------	-----------	-------------------

Modelling Tissue Ablation

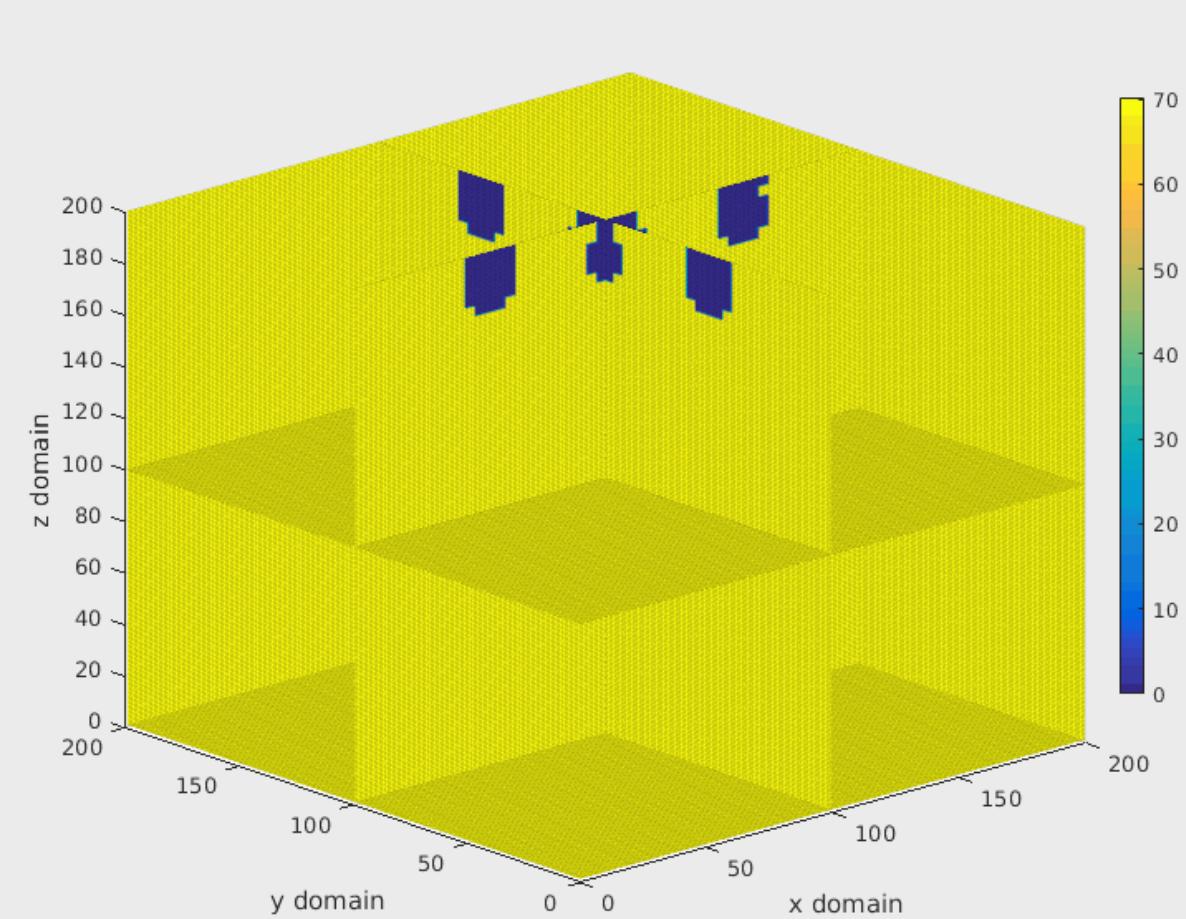
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + S$$



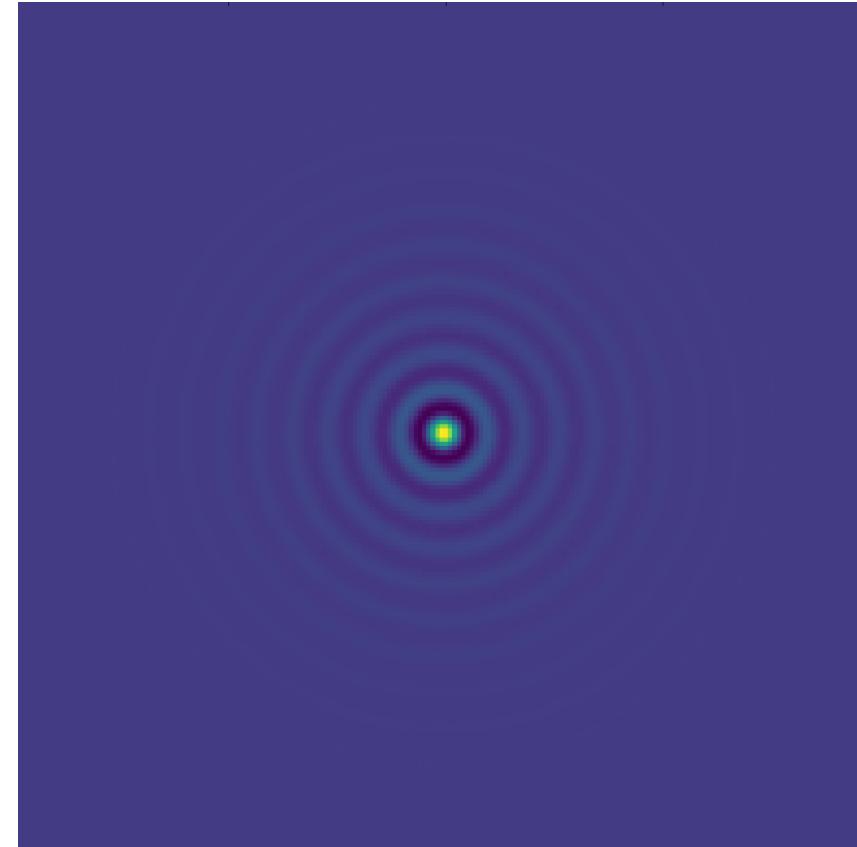
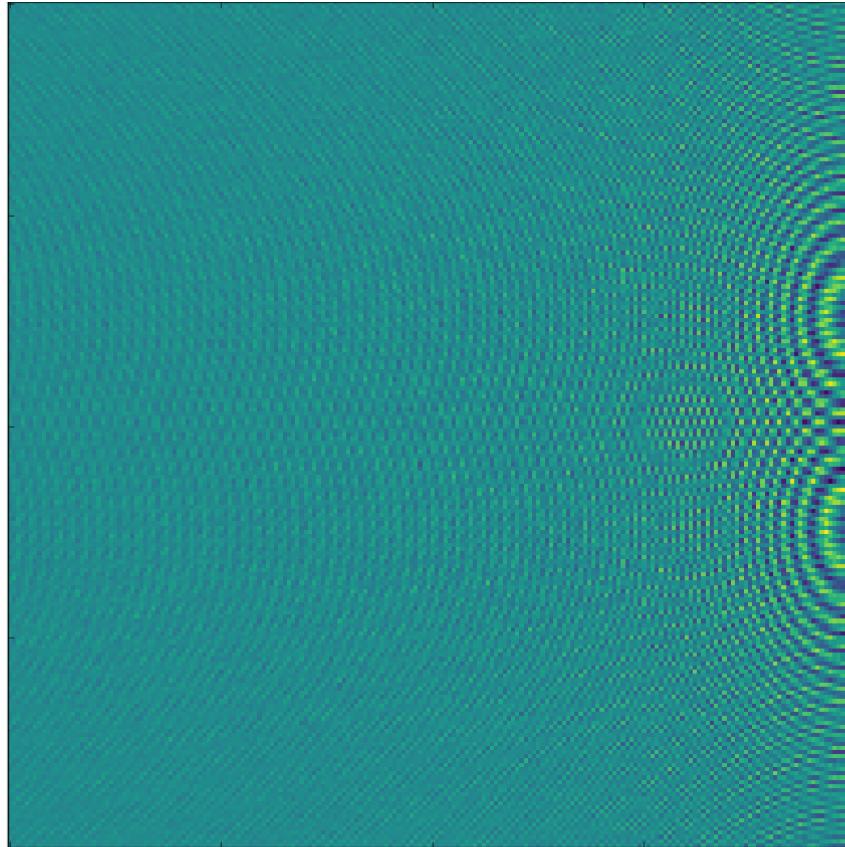
Modelling Tissue Ablation

$$\Omega(t) = \int_{t_0}^{t_f} A e^{-\frac{\Delta E}{RT}} dT$$

- Arrhenius damage model
- Taken from chemistry
- Used widely in literature for tissue damage



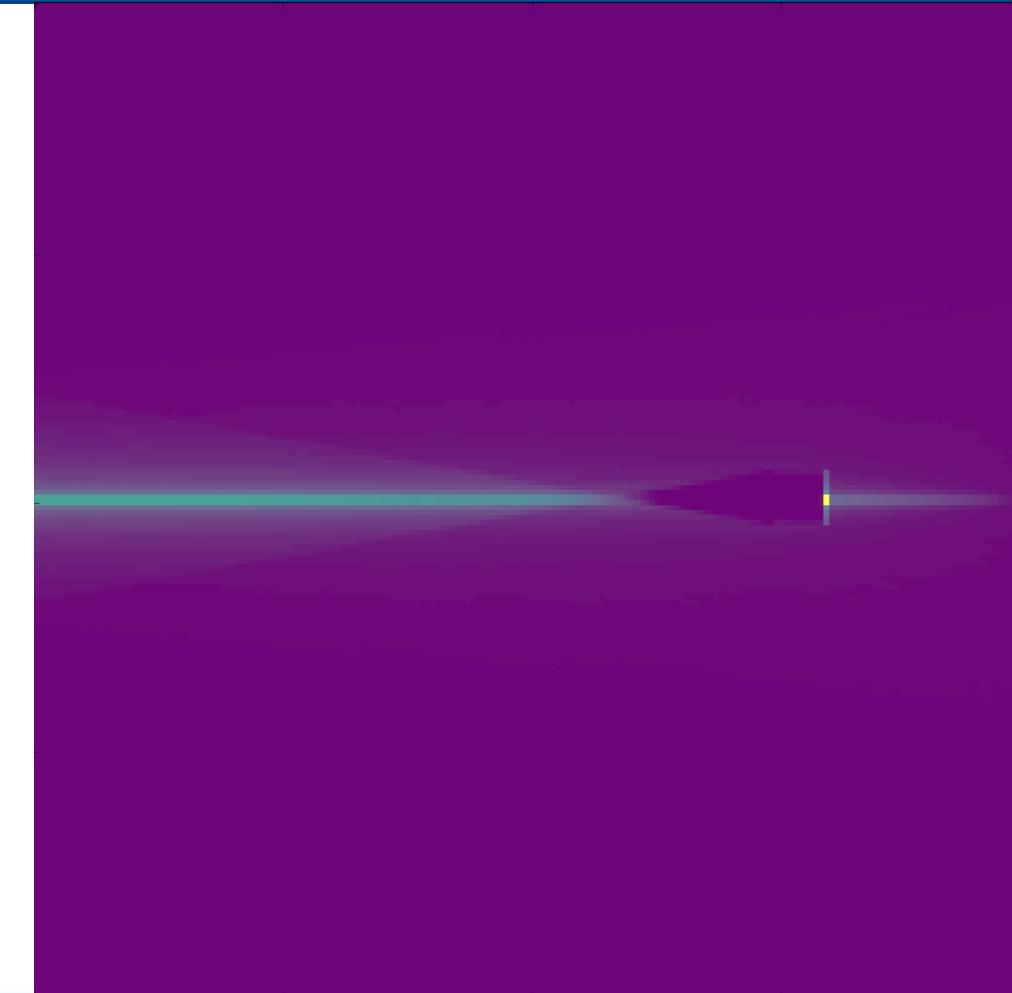
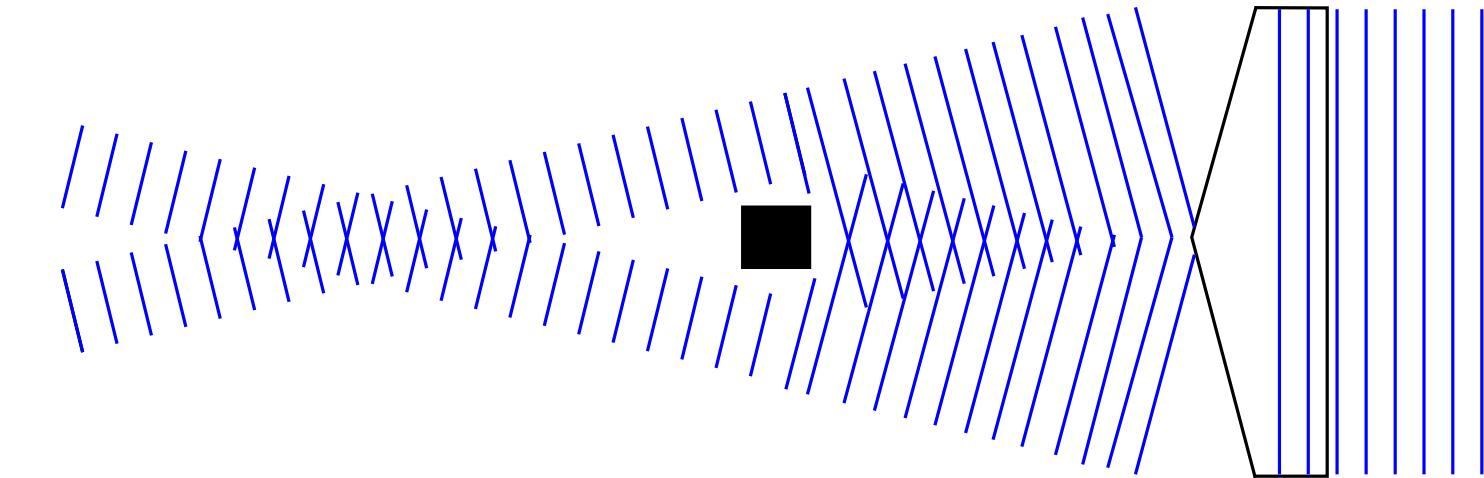
Phase Monte Carlo



- Track phase of ‘ballistic’ photons
- Recover some of the wave behavior of photons

$$\varphi = \cos\left(\frac{2\pi d}{\lambda}\right)$$

Phase Monte Carlo



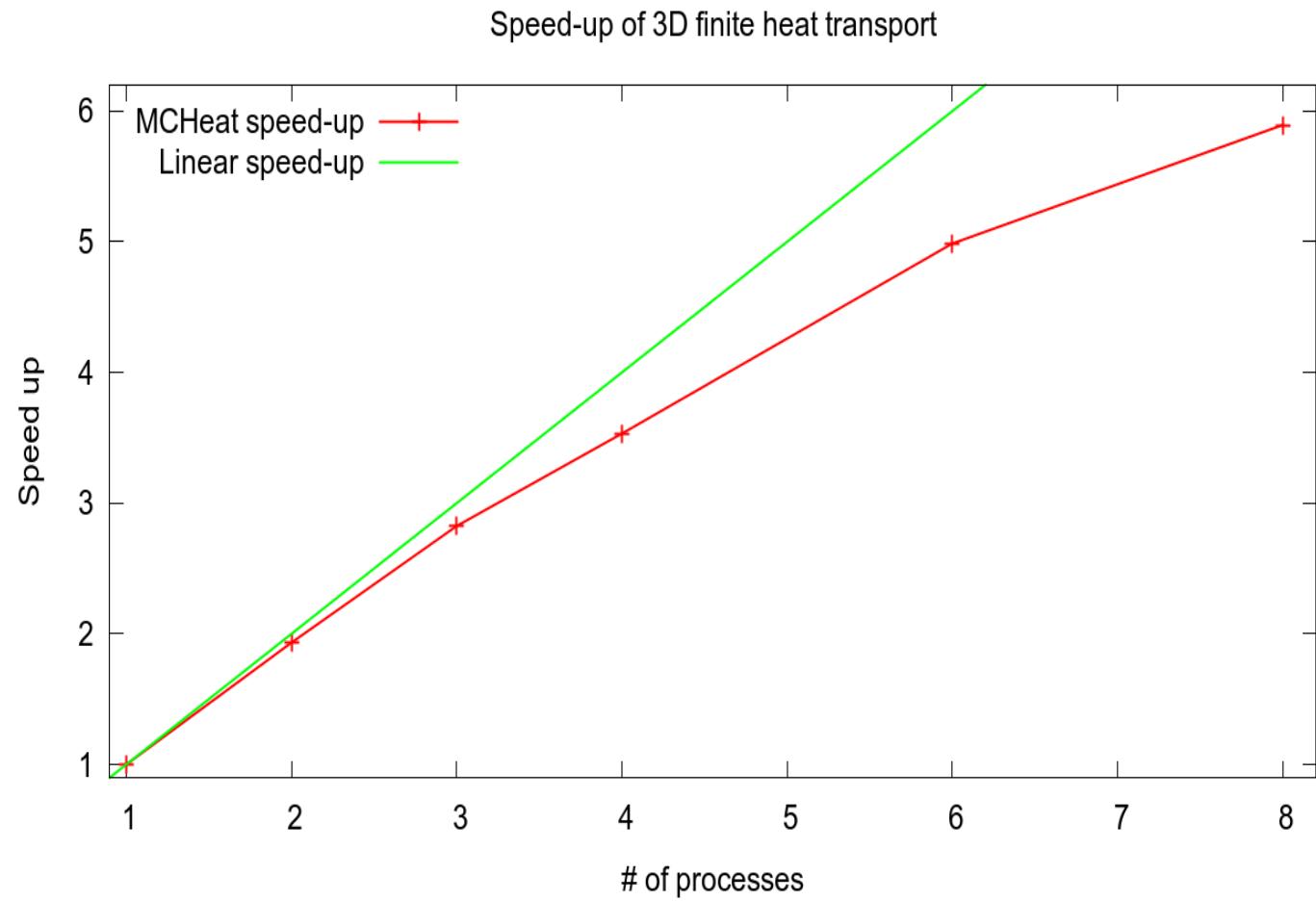
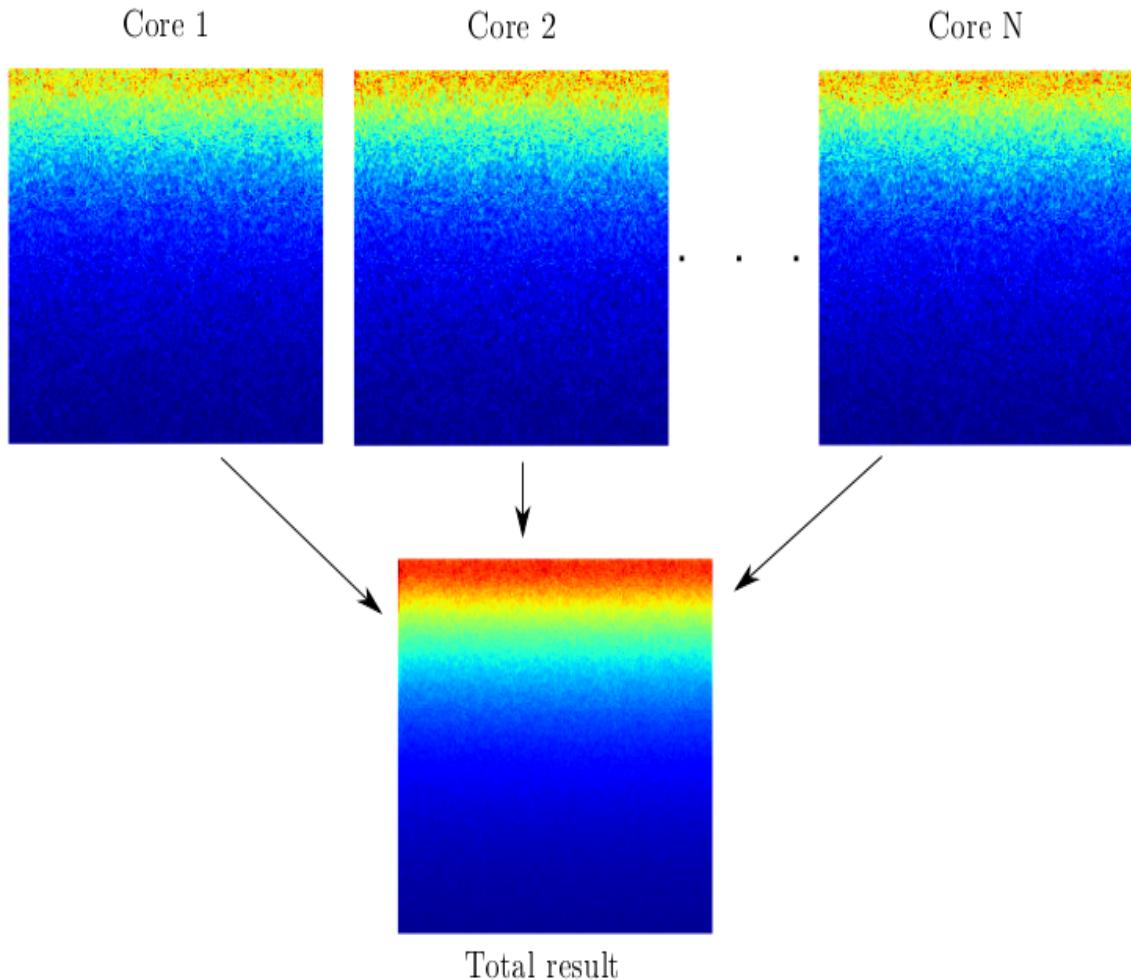
Parallelisation

- Monte Carlo is classed as embarrassingly parallel
- Easy (most of the time...) to parallelise a MCRT code
- Various libraries: Openmpi, Intel Mpi, Cray Mpi...
- In various languages: Fortran, C, Python, MATLAB, R...



Openmpi

Parallelisation



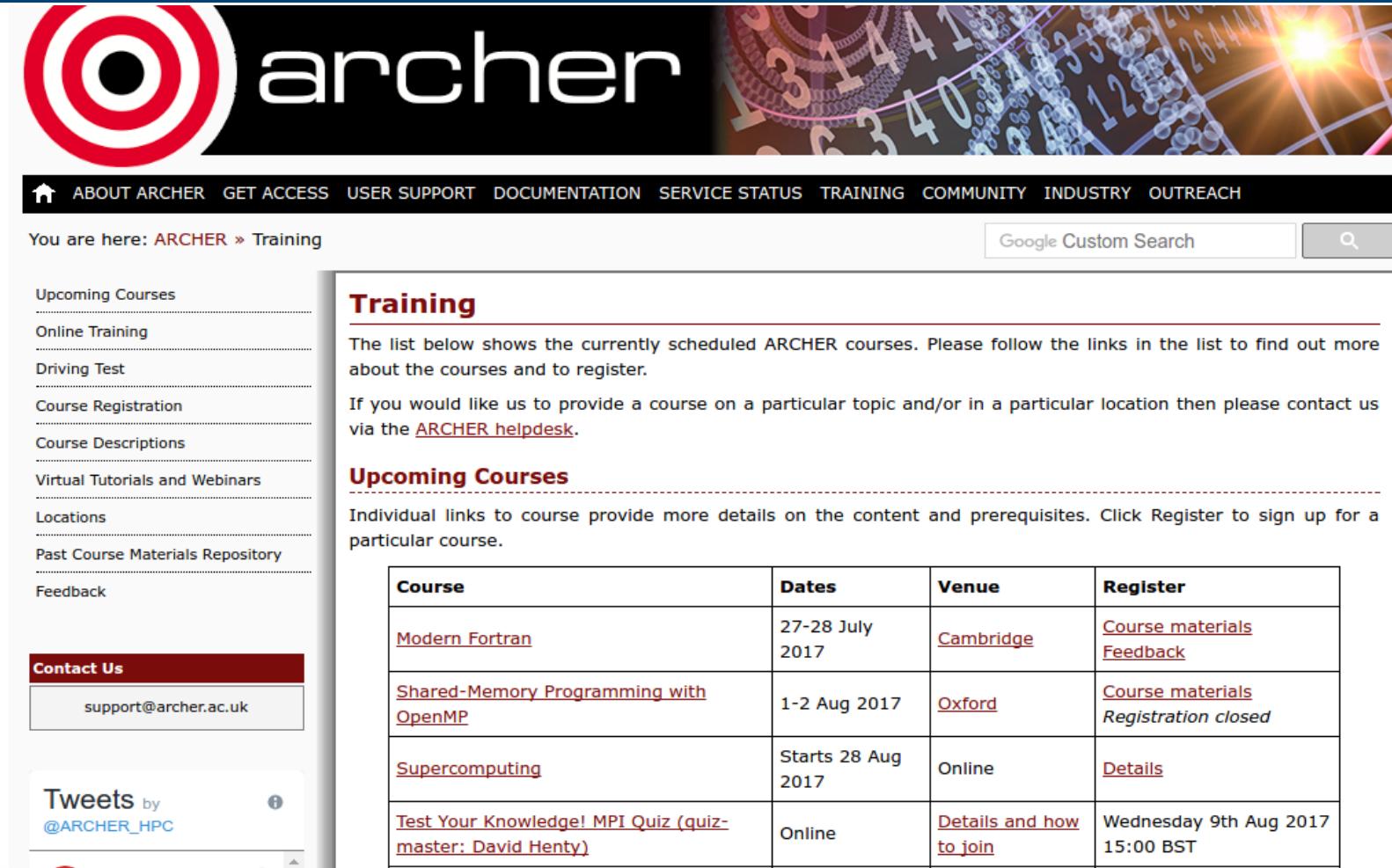
mpi_example.f90

```
1 program mpiexample
2
3     use mpi          !older mpi module
4     !use mpi_f08    !newer mpi module with derived types in place of everything is an integer
5
6     implicit none
7
8     integer, parameter :: n=200
9     integer :: error, comm, numproc, id, size_fluence, master
10    real    :: fluence(n,n,n), fluenceGLOBAL(n,n,n)
11
12    !setup variables for readability|
13    comm = mpi_comm_world
14    master = 0
15
16    !initialise mpi
17    call mpi_init(error)
18    !get number of processes
19    call mpi_comm_size(comm, numproc, error)
20    !get id of current process
21    call mpi_comm_rank(comm, id, error)
22
23
24        !do monte carlo
25        !
26        !
27        !
28        !
29        !
30        !
31
32    size_fluence = n * n * n
33
34    !sum all fluence arrays and give result to master process
35    call mpi_reduce(fluence, fluenceGLOBAL, size_fluence, mpi_real, mpi_sum, master, comm, error)
36
37    !finalize mpi
38    call mpi_finalize(error)
39
40 end program mpiexample
```

MPI Training

- EPCC summer school + other courses around country
- Basic and Advanced MPI courses
- OpenMP available as well
- Free time on Archer (#73 fastest supercomputer*)

*top500.org June 2017



The screenshot shows the ARCHER website's training page. At the top is a large red and white target logo followed by the word "archer". Below the header is a navigation bar with links: ABOUT ARCHER, GET ACCESS, USER SUPPORT, DOCUMENTATION, SERVICE STATUS, TRAINING, COMMUNITY, INDUSTRY, and OUTREACH. A search bar labeled "Google Custom Search" is also present. The main content area has a banner with a globe and numbers. It includes a sidebar with links for Upcoming Courses, Online Training, Driving Test, Course Registration, Course Descriptions, Virtual Tutorials and Webinars, Locations, Past Course Materials Repository, and Feedback. A "Contact Us" box contains the email support@archer.ac.uk. A "Tweets by @ARCHER_HPC" feed is also shown. The main content area is titled "Training" and describes currently scheduled courses. It includes a "Upcoming Courses" table:

Course	Dates	Venue	Register
Modern Fortran	27-28 July 2017	Cambridge	Course materials Feedback
Shared-Memory Programming with OpenMP	1-2 Aug 2017	Oxford	Course materials Registration closed
Supercomputing	Starts 28 Aug 2017	Online	Details
Test Your Knowledge! MPI Quiz (quiz-master: David Henty)	Online	Details and how to join	Wednesday 9th Aug 2017 15:00 BST

Further work

- Better tissue damage model
- Determine fluorescent source
- More work on LDF + autofluorescence
- Adaptive mesh grids
- All code available at github.com/lewisfish



(all in Fortran...)

