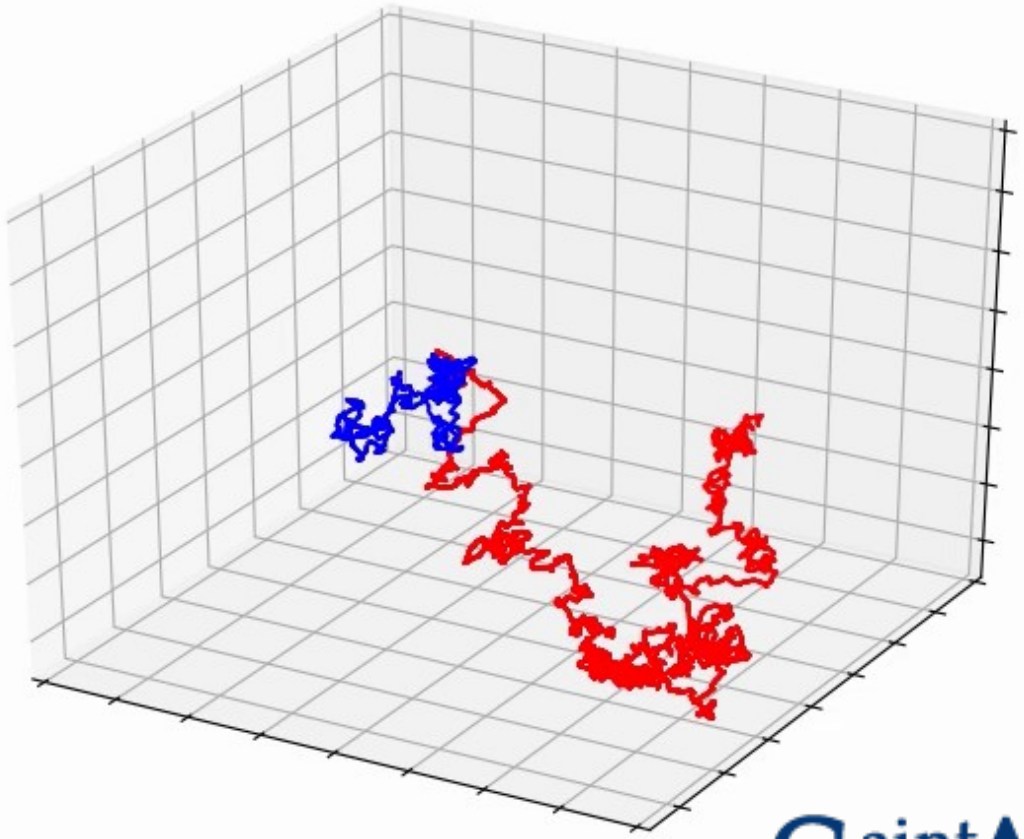
University of St Andrews

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



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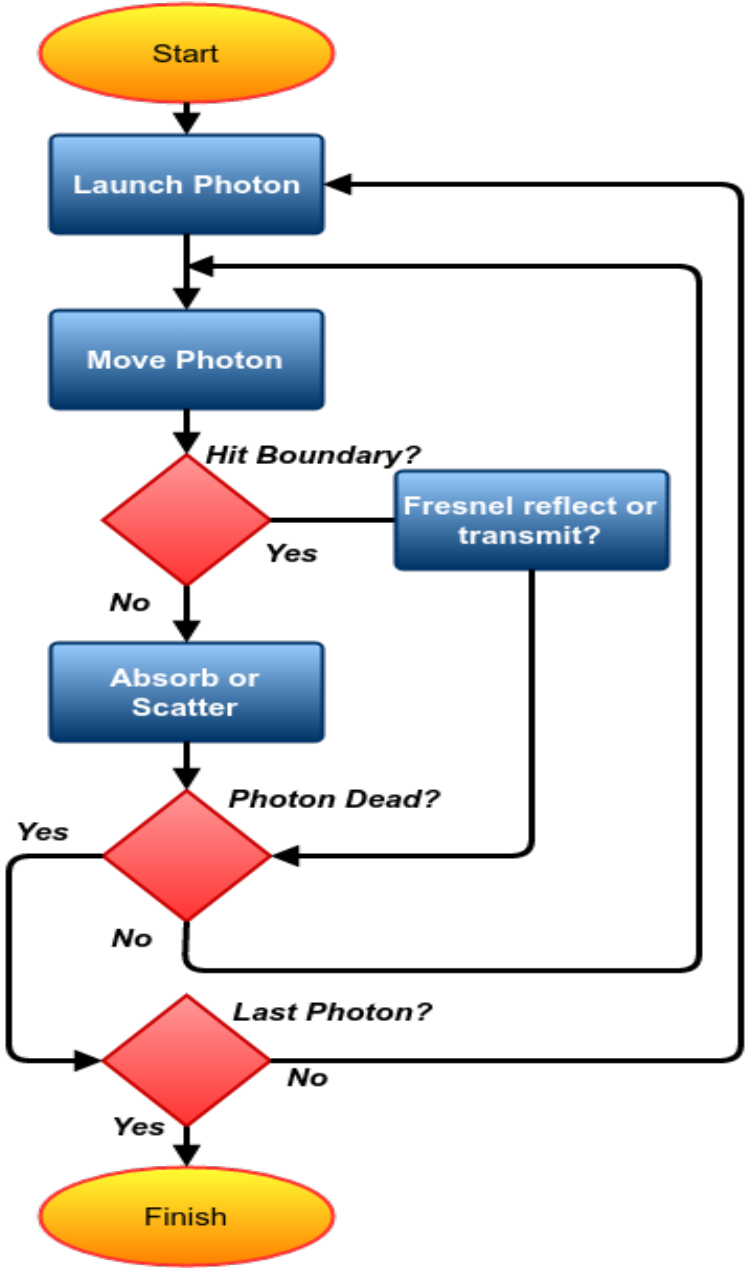
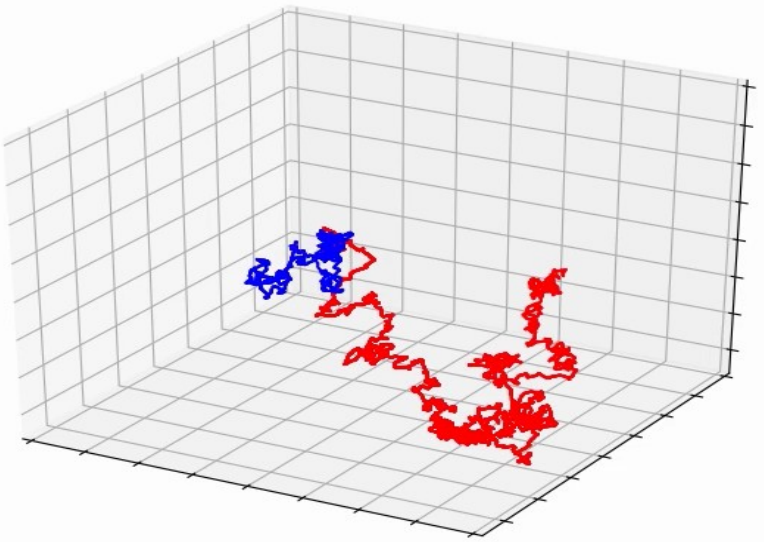
github.com/lewisfish

Saint Andrews Monte Carlo Summer School

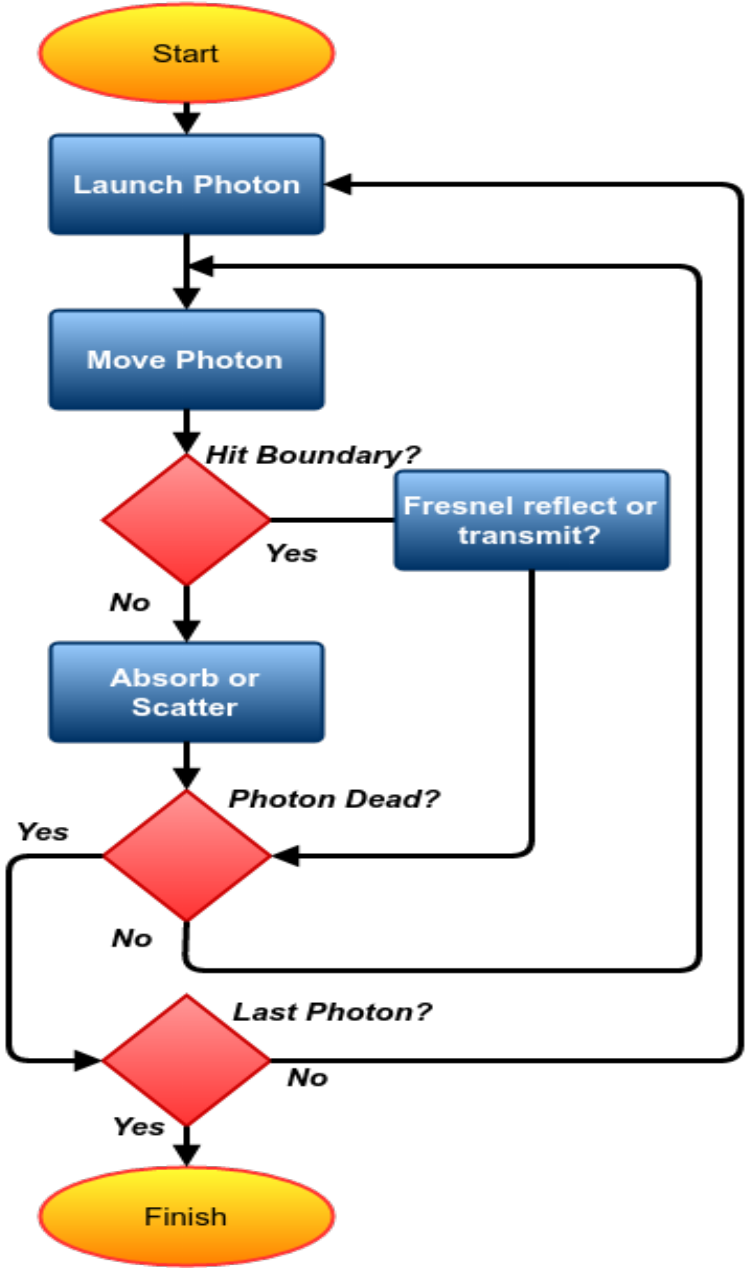
Monte Carlo Radiation Transfer



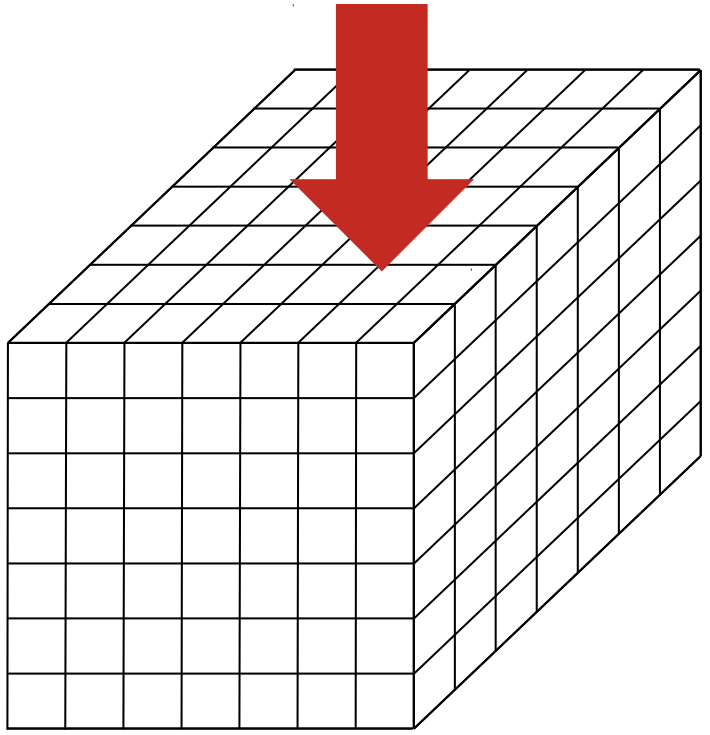
Uses random numbers and interaction probabilities to simulate photon propagation



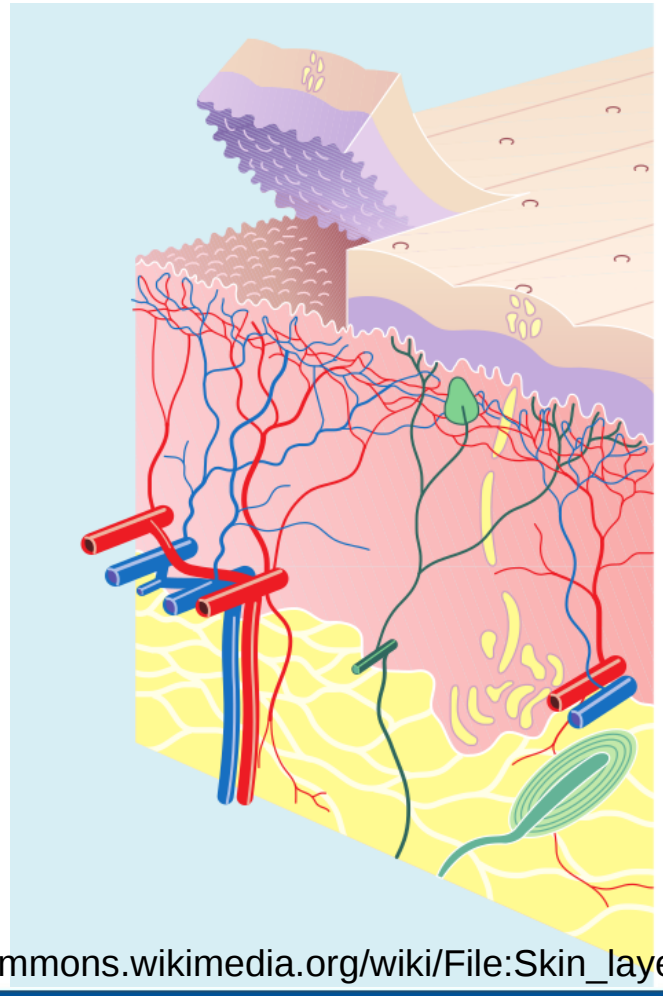
Monte Carlo Radiation Transfer



Uses random numbers and interaction probabilities to simulate photon propagation



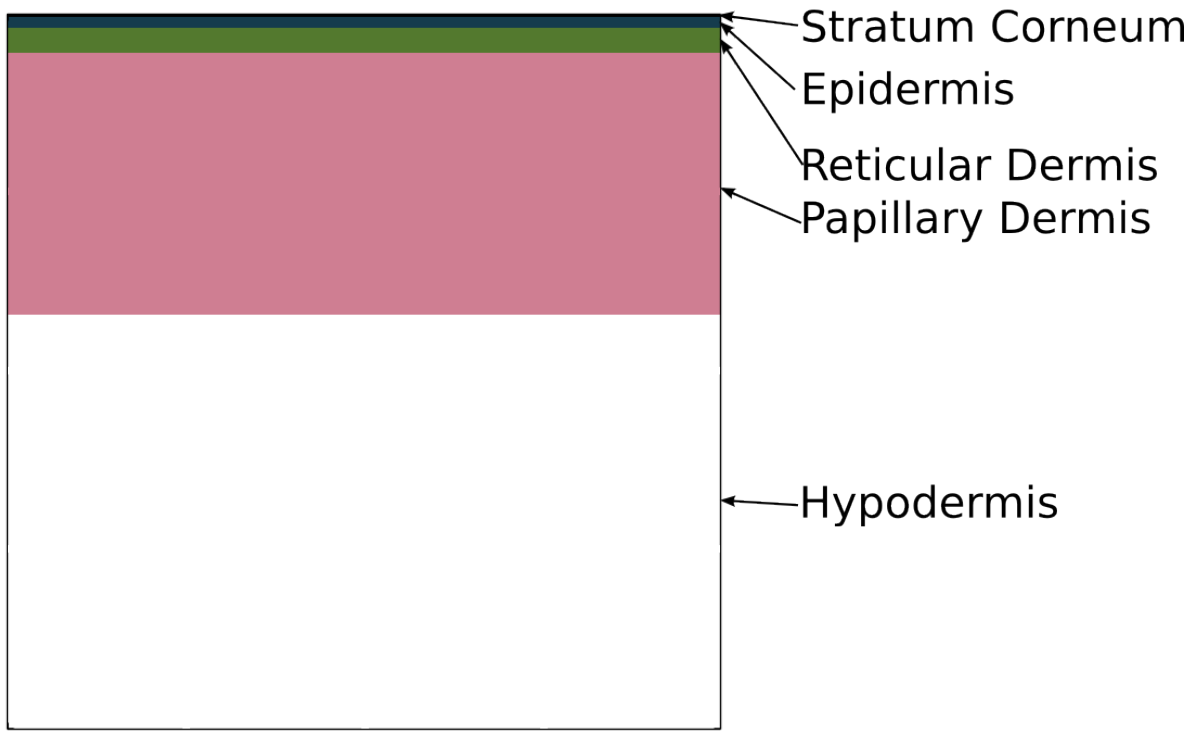
Voxel Model

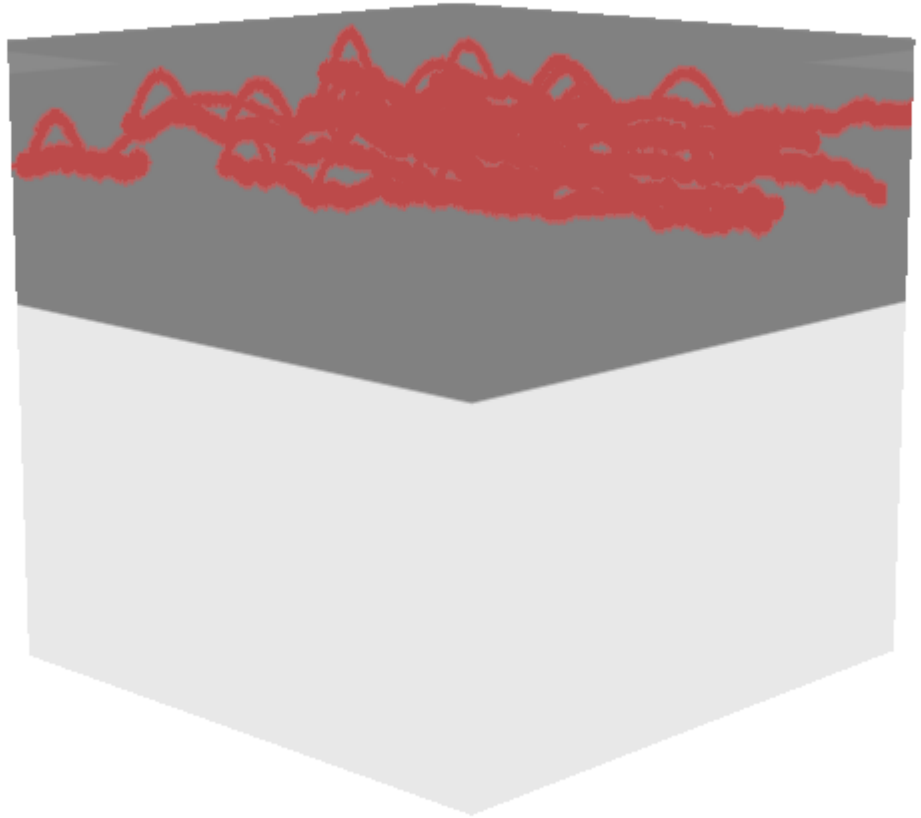


https://commons.wikimedia.org/wiki/File:Skin_layers.svg

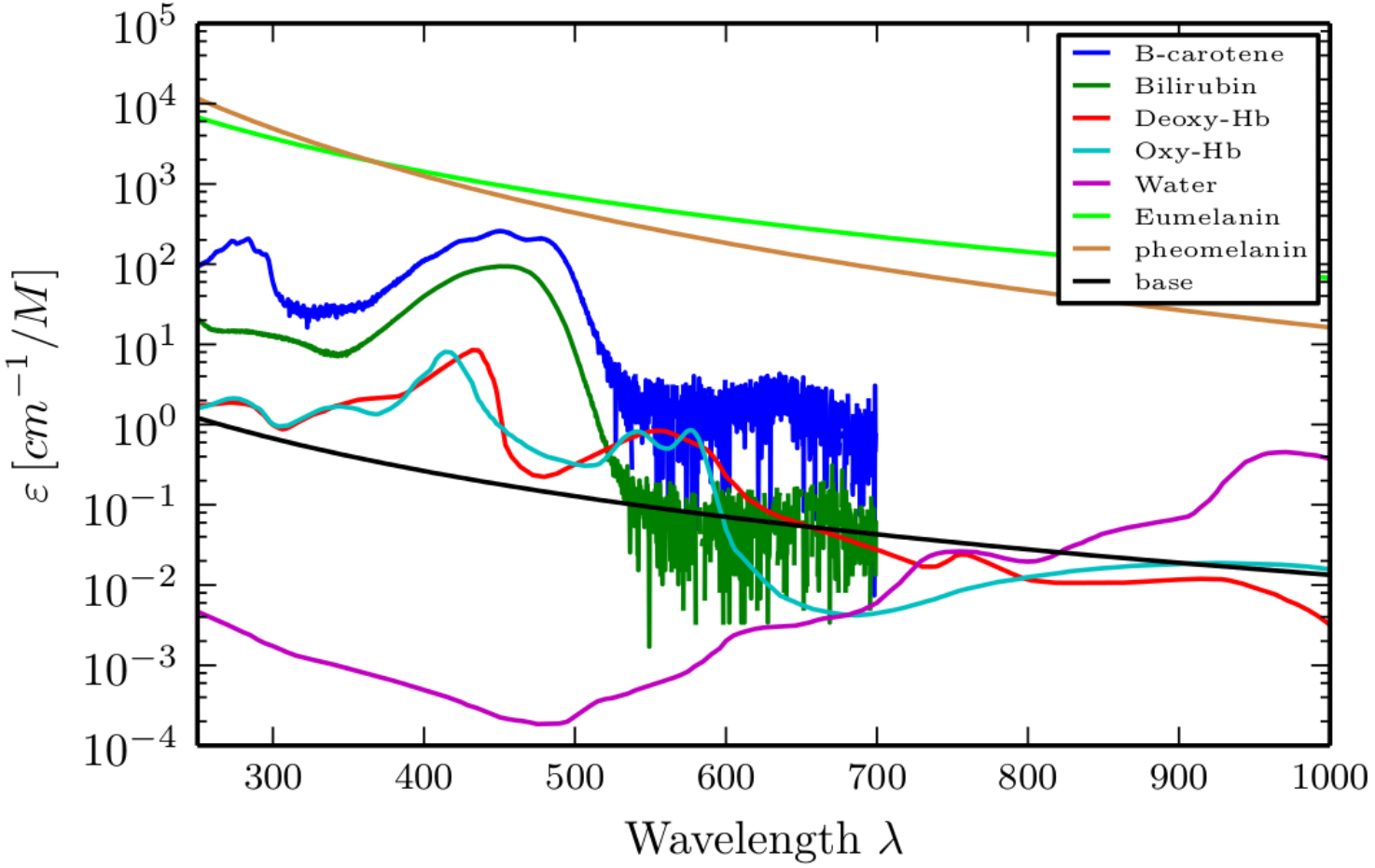
Hubble telescope

Voxel Model


Stratum Corneum
Epidermis
Reticular Dermis
Papillary Dermis
Hypodermis



5 layer skin model



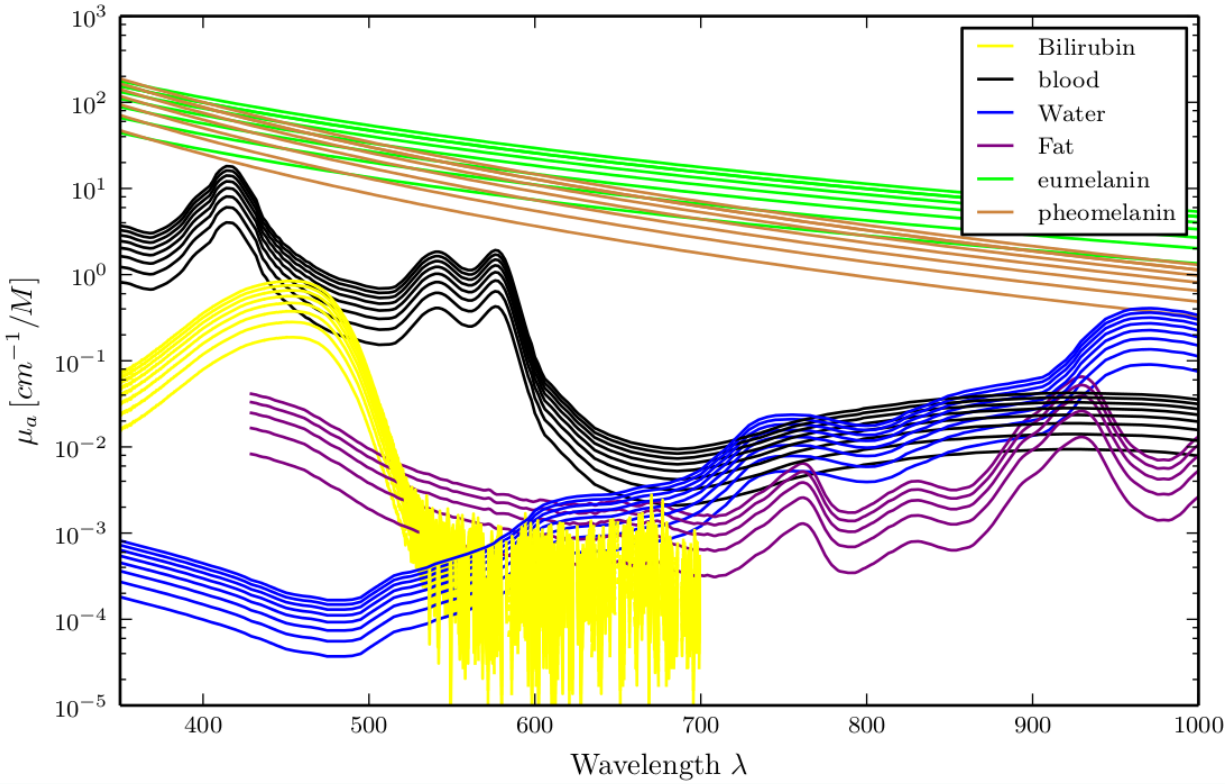
- 5 Layer skin model
- Various absorbers: Blood, Melanin, Bilirubin, water, fat...

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

5 layer skin model

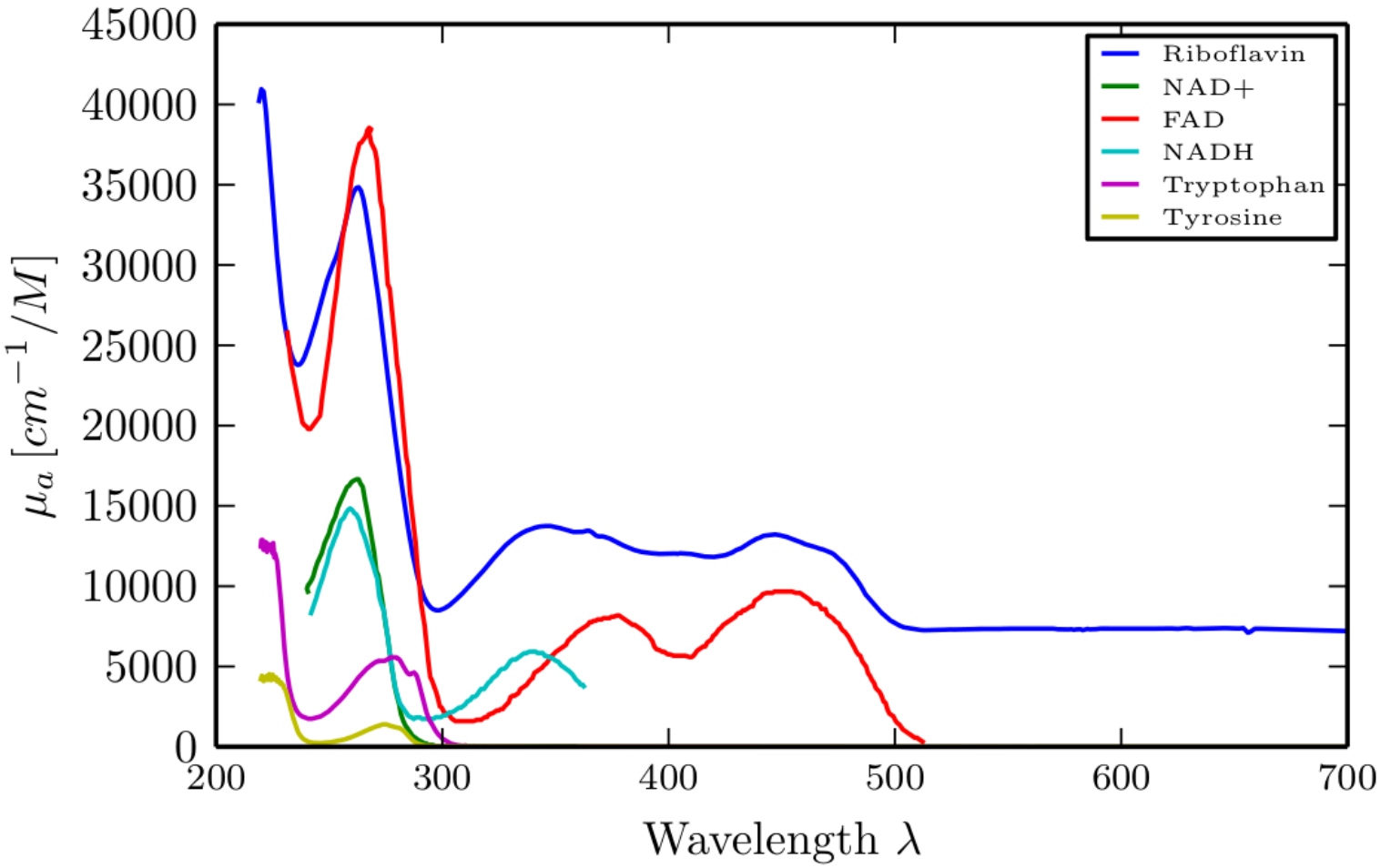
$$\mu_a^{layer} = B\,S\,\mu_{a.oxy} + B(1-S)\mu_{a.deoxy} + W\,\mu_{a.H_2O} + F\,\mu_{a.fat} + M\,\mu_{a.melansome} + 2.3\,C_{bilirubin}\mathcal{E}_{bilirubin} + 2.3\,C_{\beta-Carotene}\mathcal{E}_{\beta-Carotene} + A\,\mu_{a.baseline}$$

- 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...



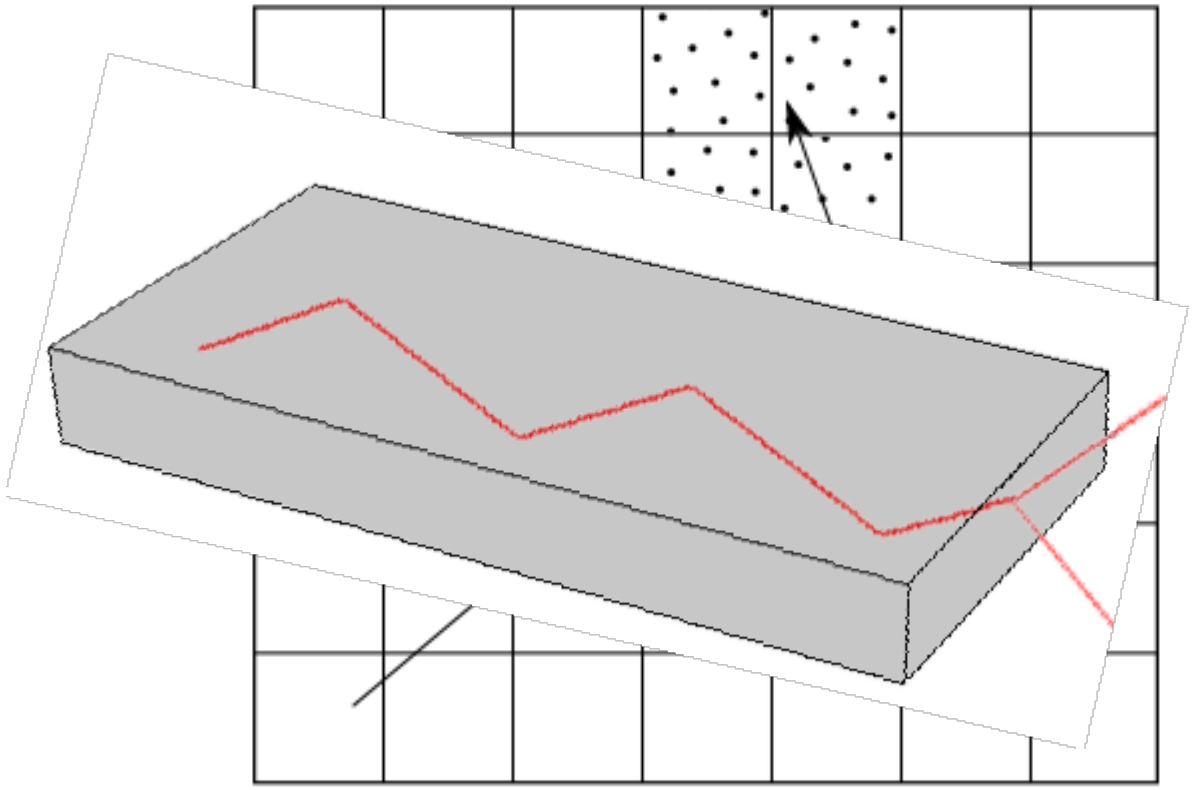
Fresnel Reflections/Refractions

- Model reflection/refraction at voxel boundaries

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

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

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

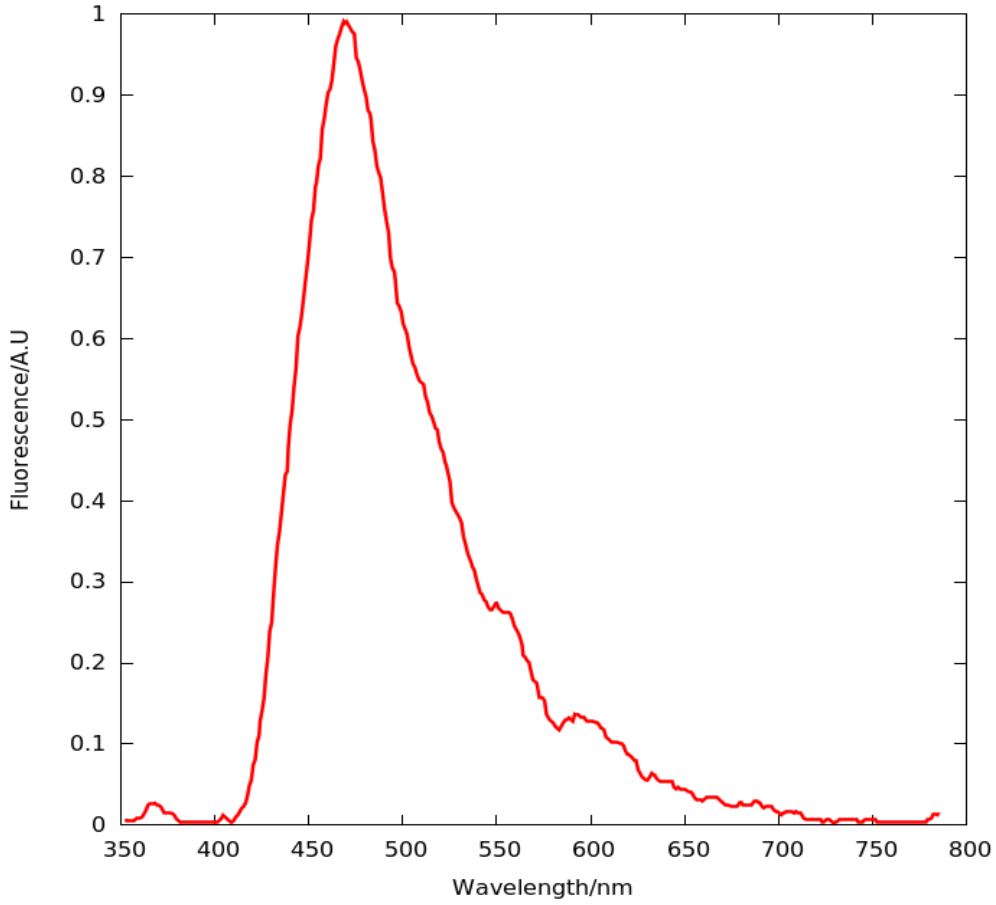


Motivation

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

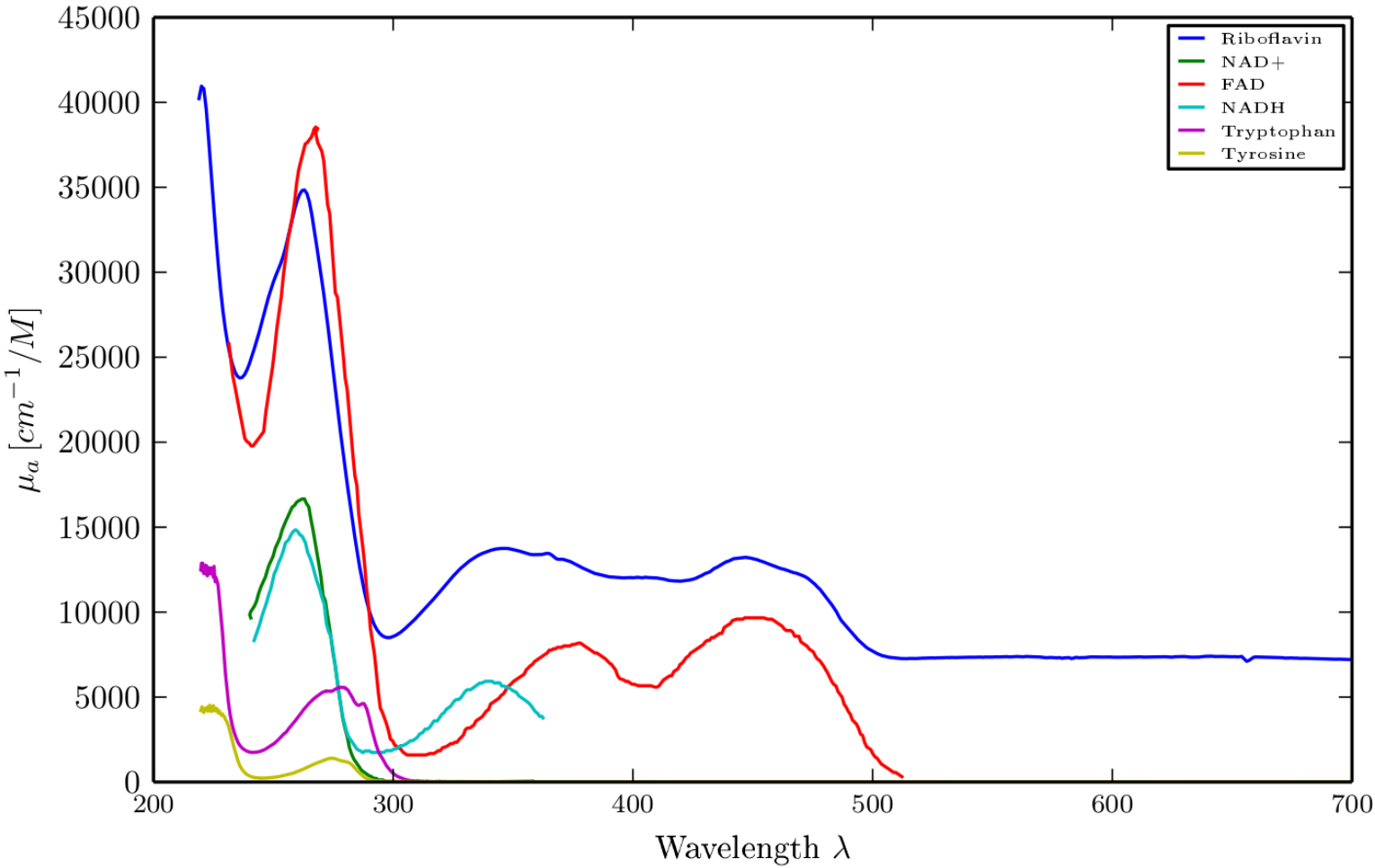
Motivation

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

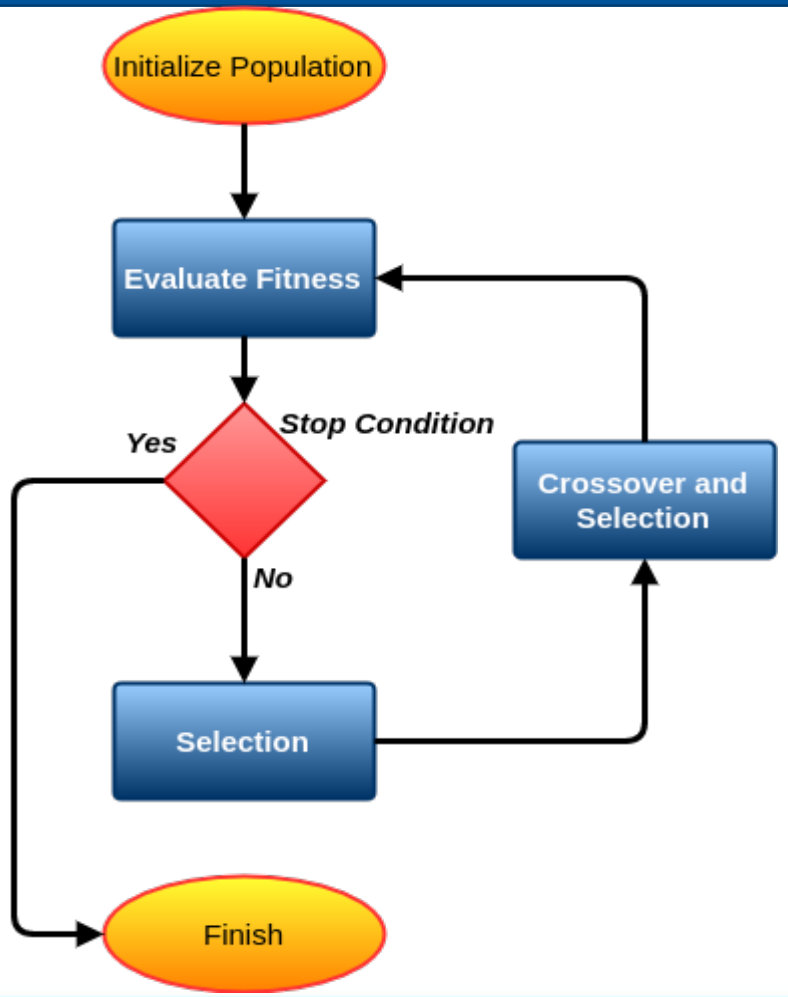


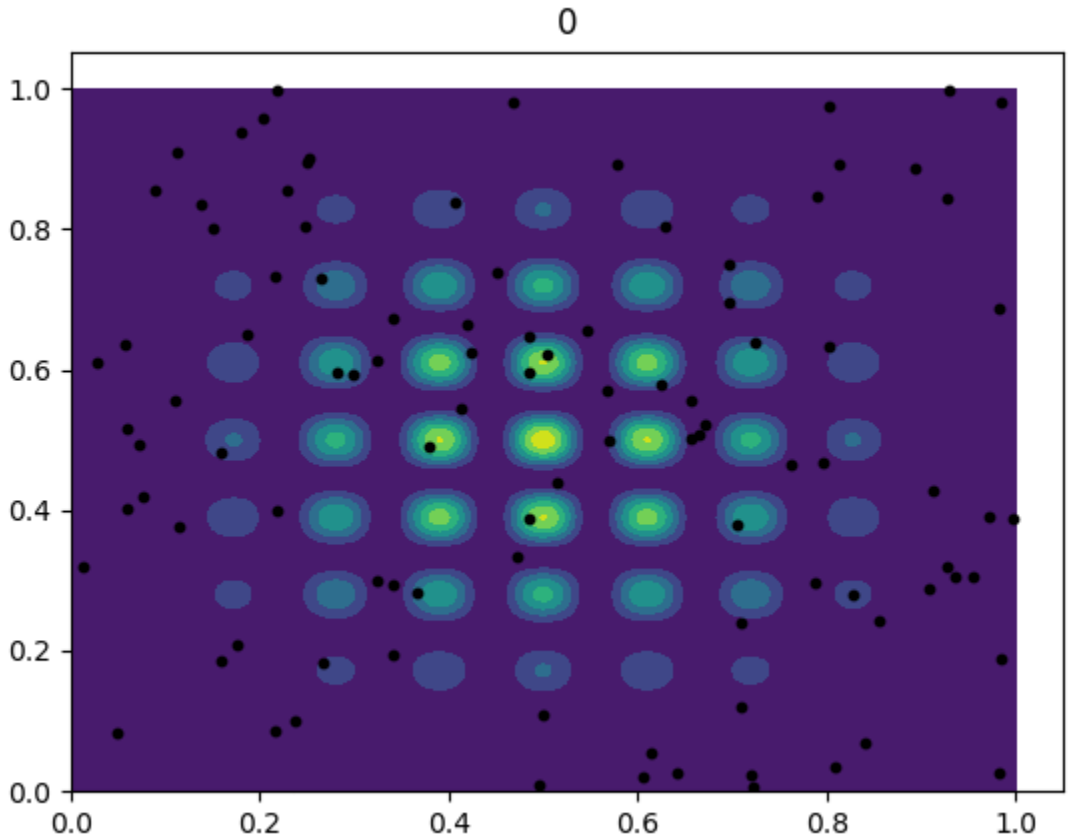
Autofluorescence

- No literature values of concentration of fluorophores



Genetic Algorithms





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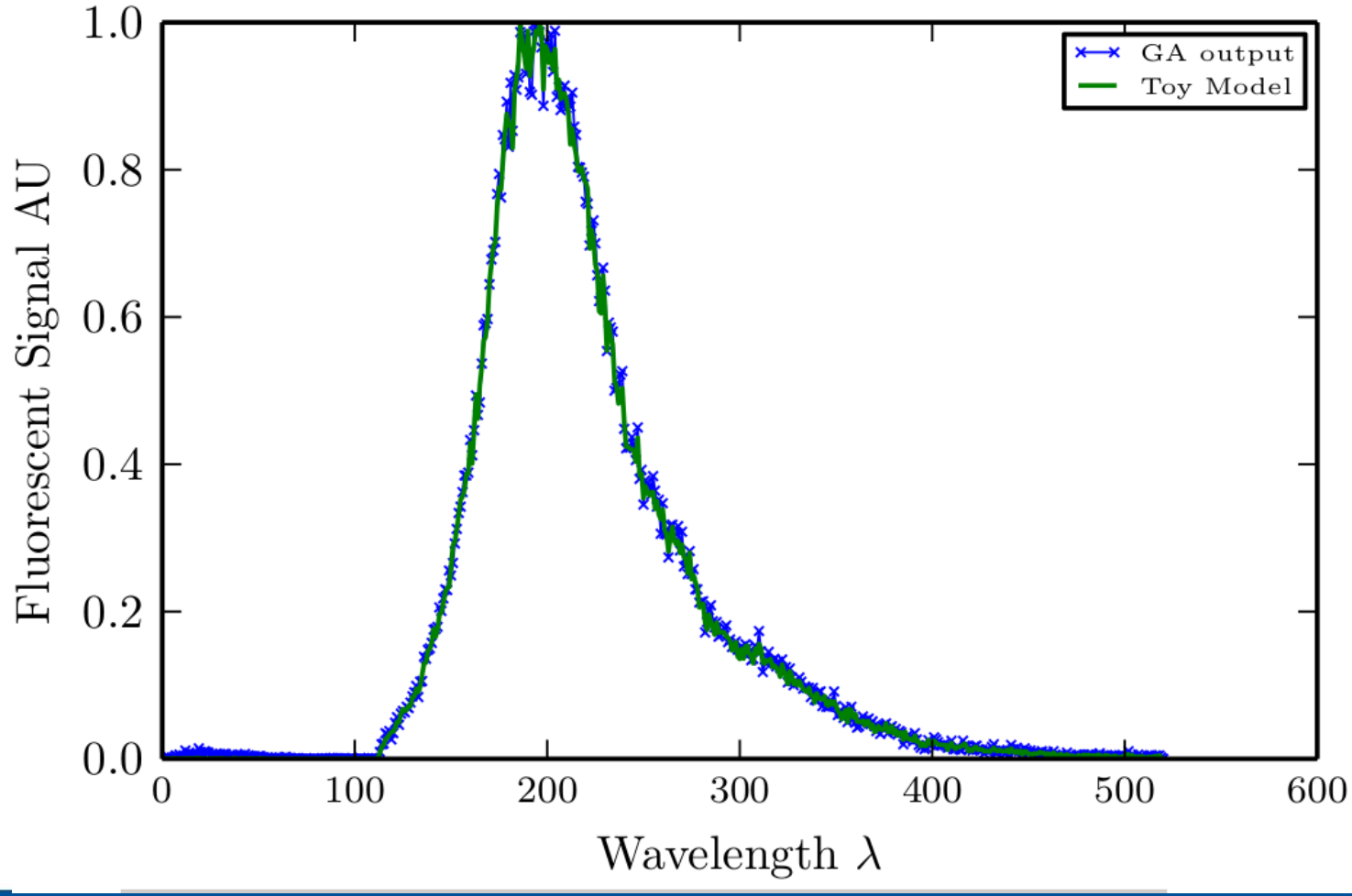
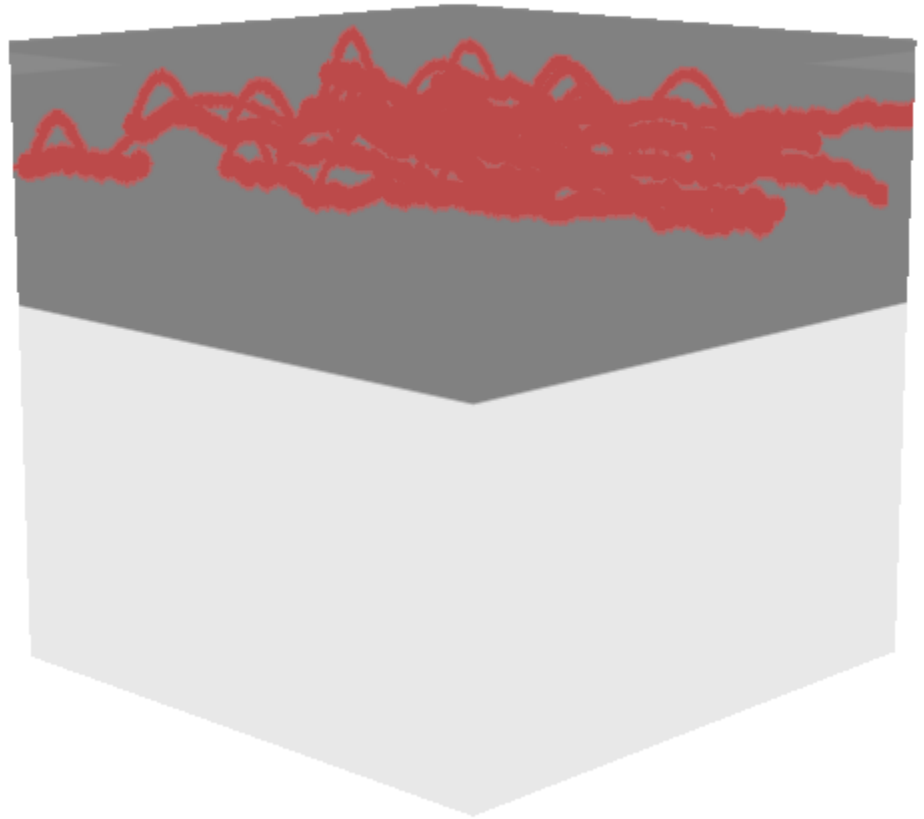
Genetic Algorithm

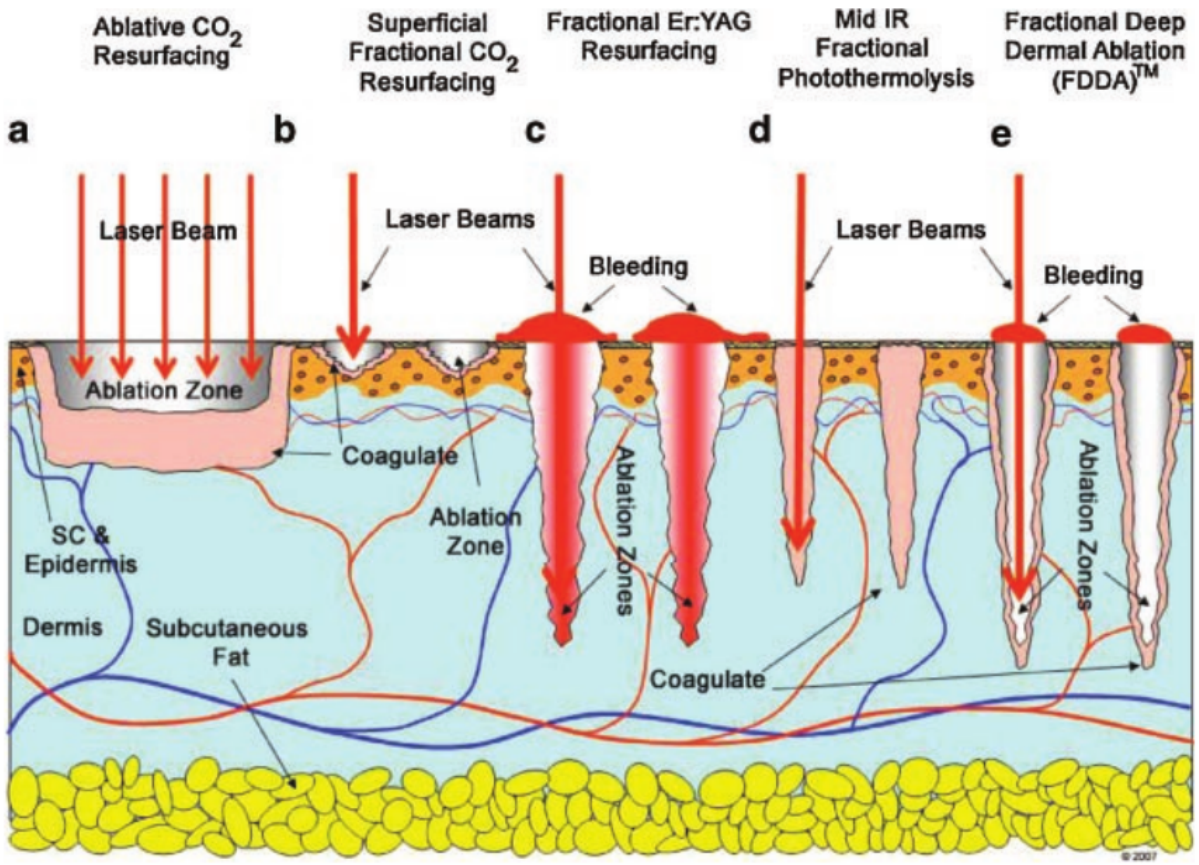


Laser Doppler flowmetry

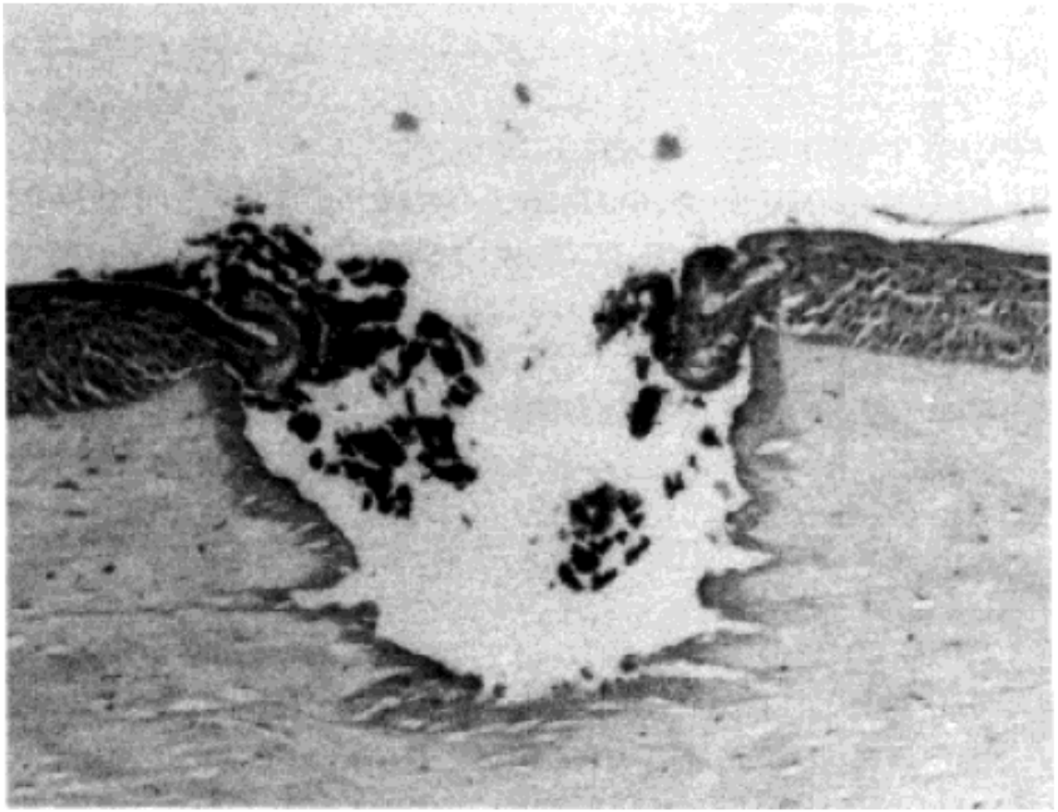


Laser Doppler flowmetry

Tissue Ablation



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



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

Tissue Ablation

V. Madan, ukdermatologist.co.uk

Modelling Tissue Ablation

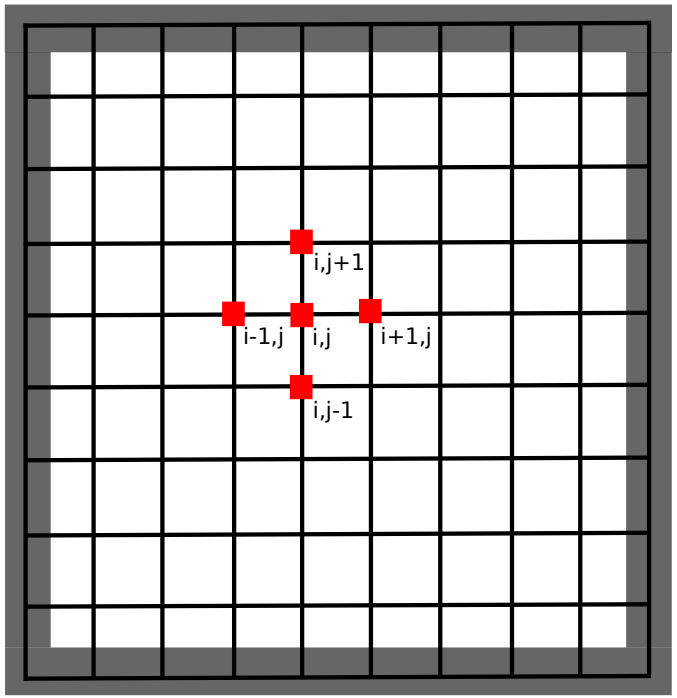
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + S$$

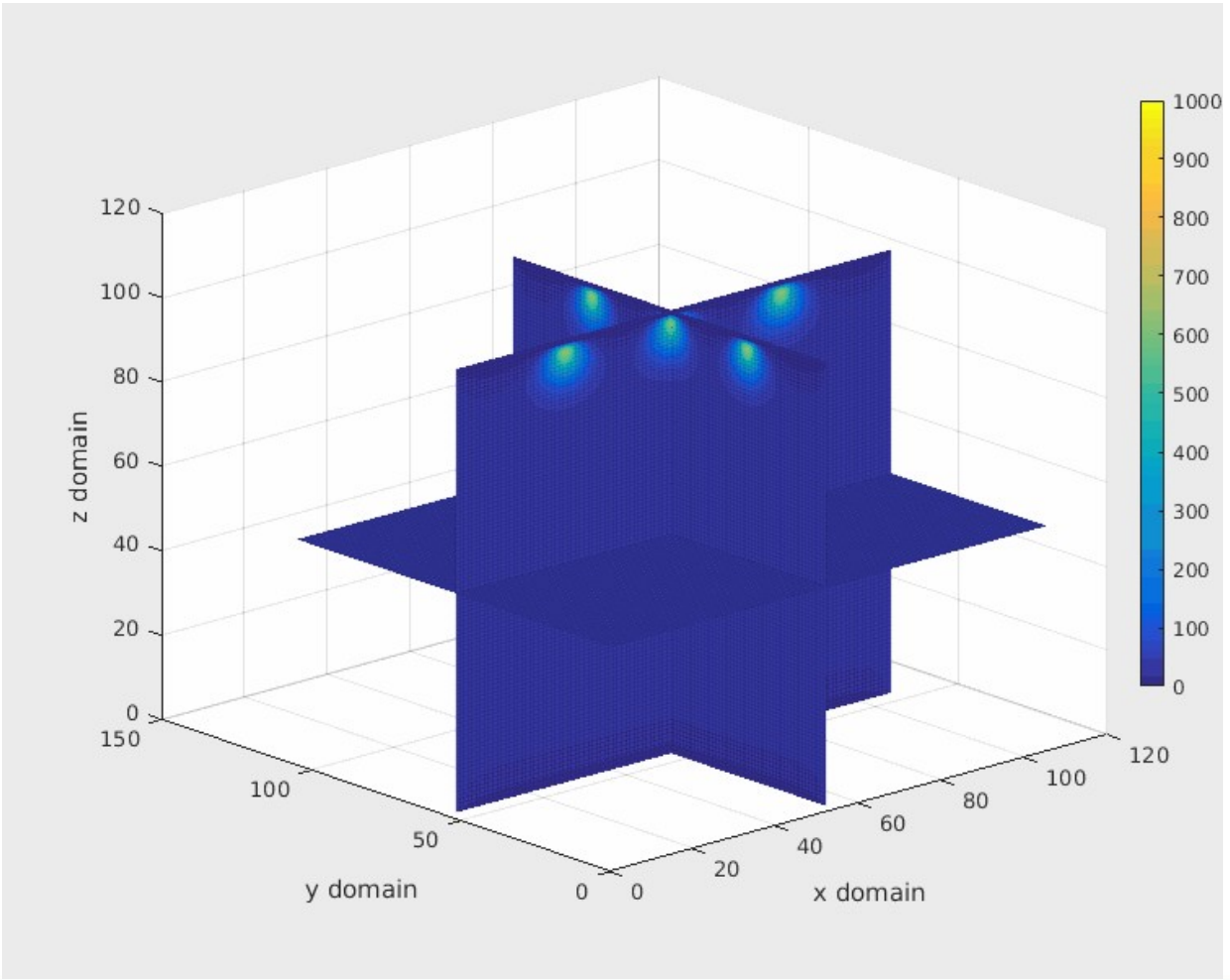
$$S = -hA(T_\infty - T) - \sigma \varepsilon A(T_\infty^4 - T^4) + \dot{q}$$

Convective Radiative Laser heat source

Modelling Tissue Ablation

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

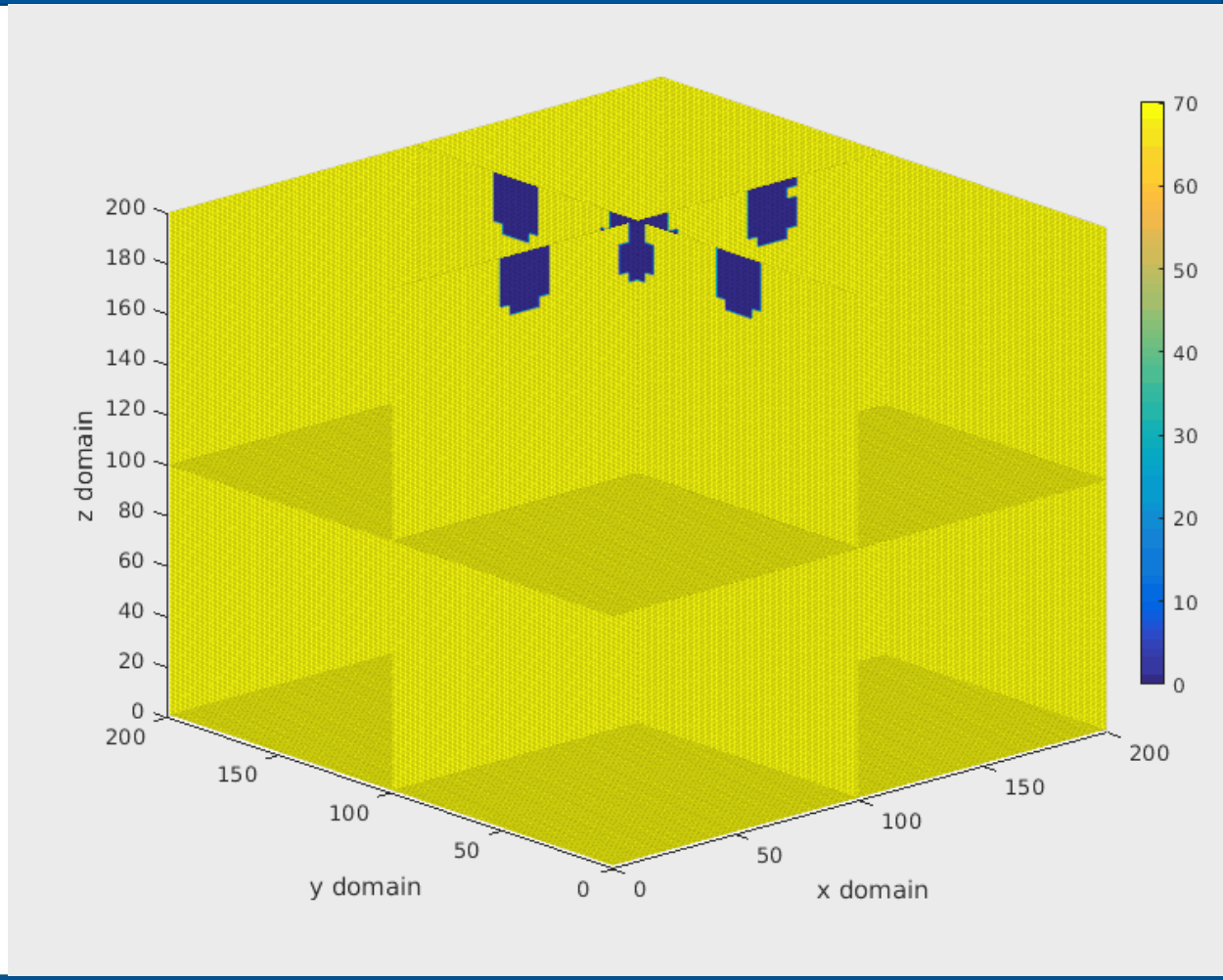




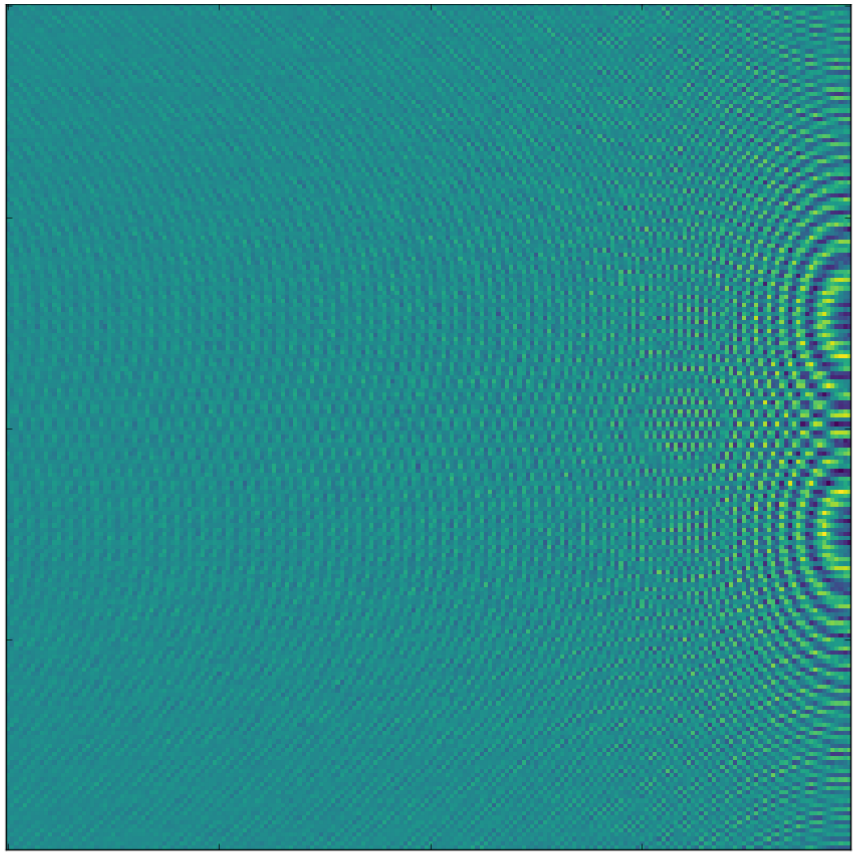
Modelling Tissue Ablation

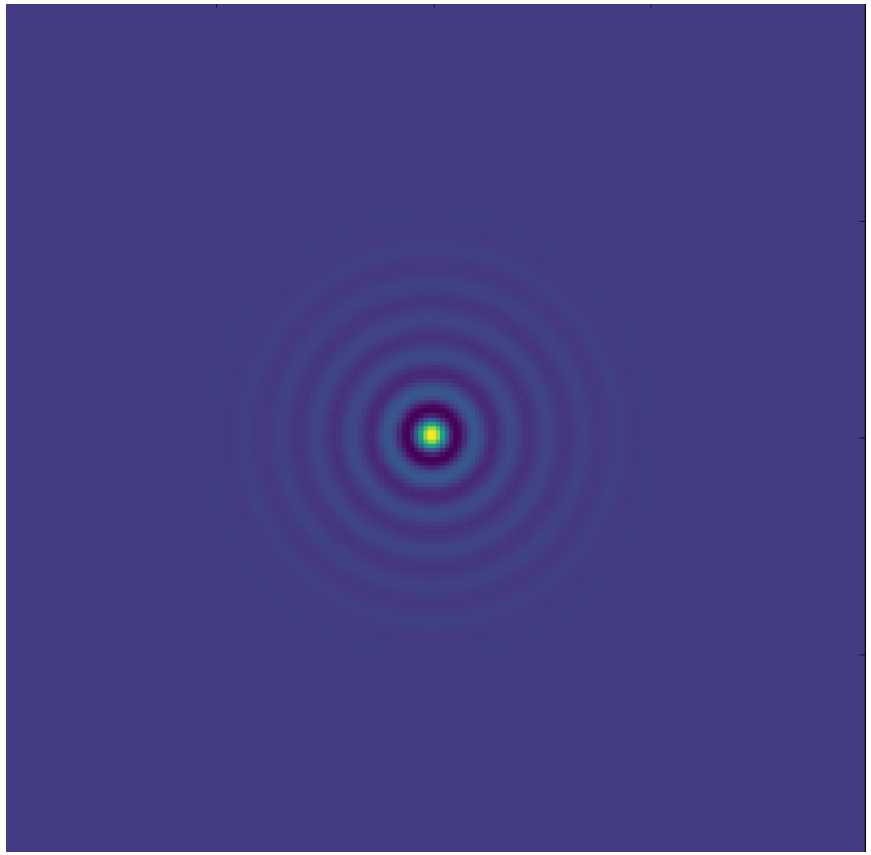
$$\Omega(t) = \int_{t_0}^{t_f} Ae^{(-\frac{\Delta E}{RT})dT}$$

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



Phase Monte Carlo

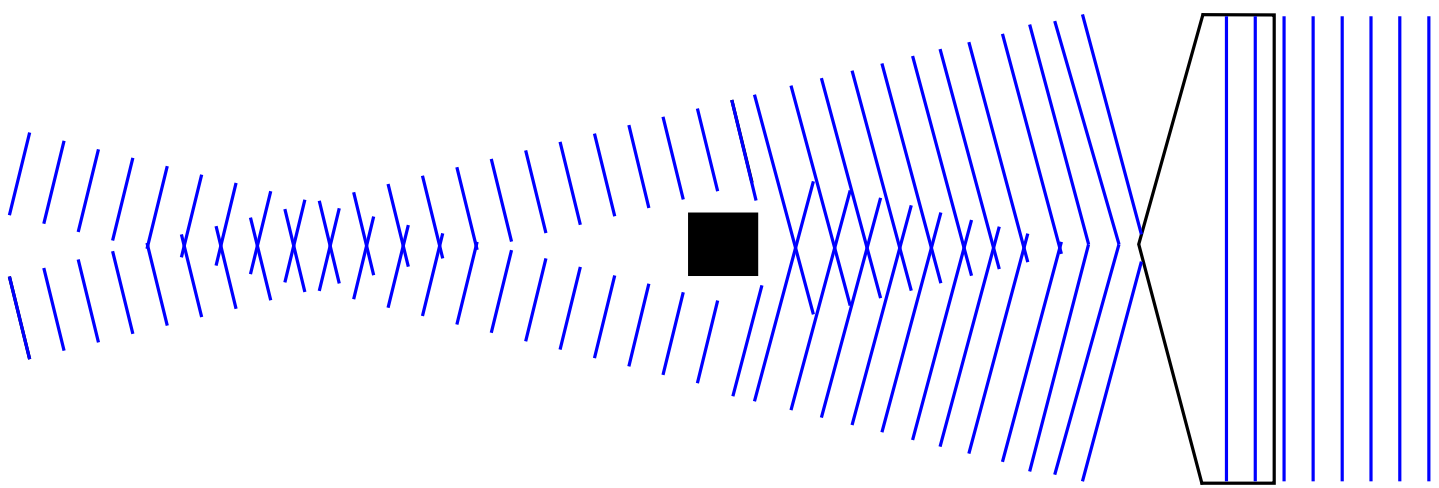


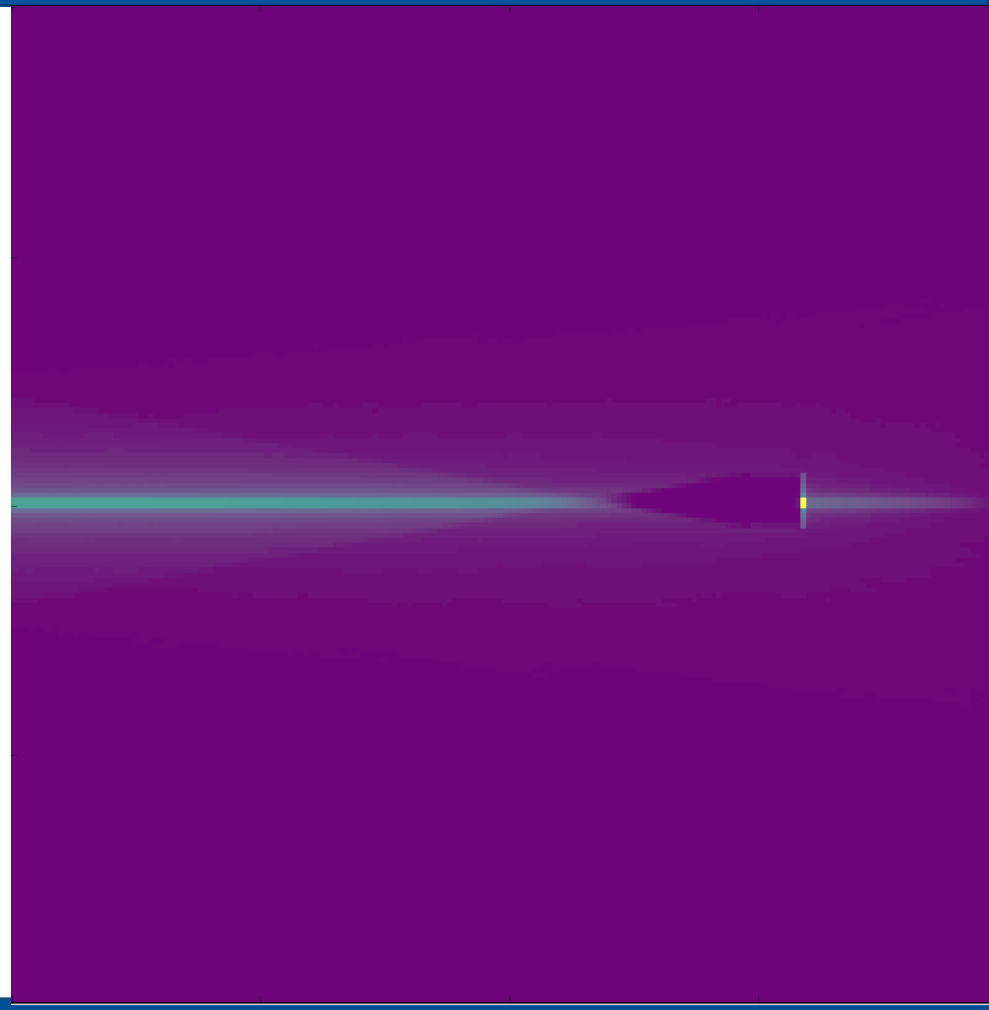


- Track phase of ‘ballistic’ photons
- Recover some of the wave behavior of photons

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

Phase Monte Carlo





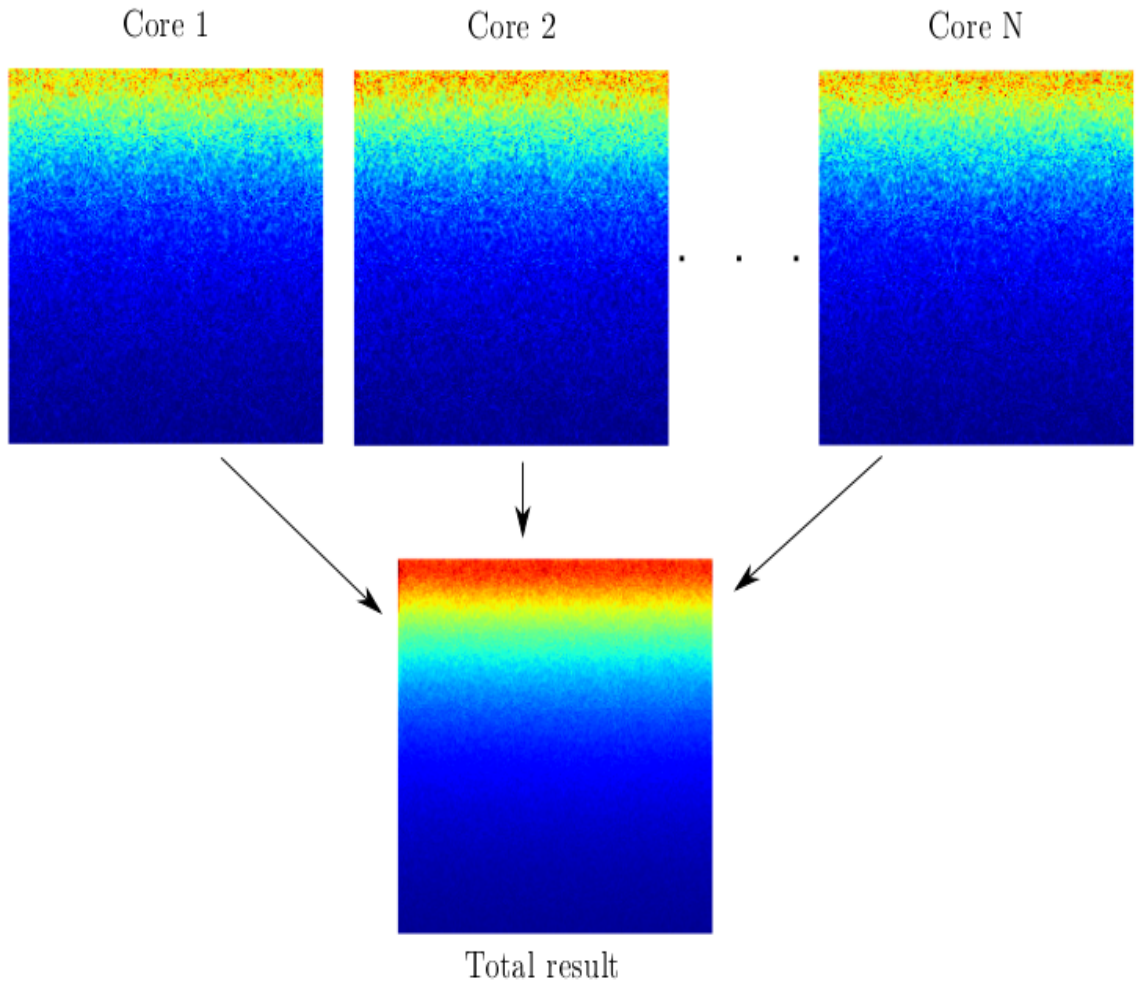
Parallelisation

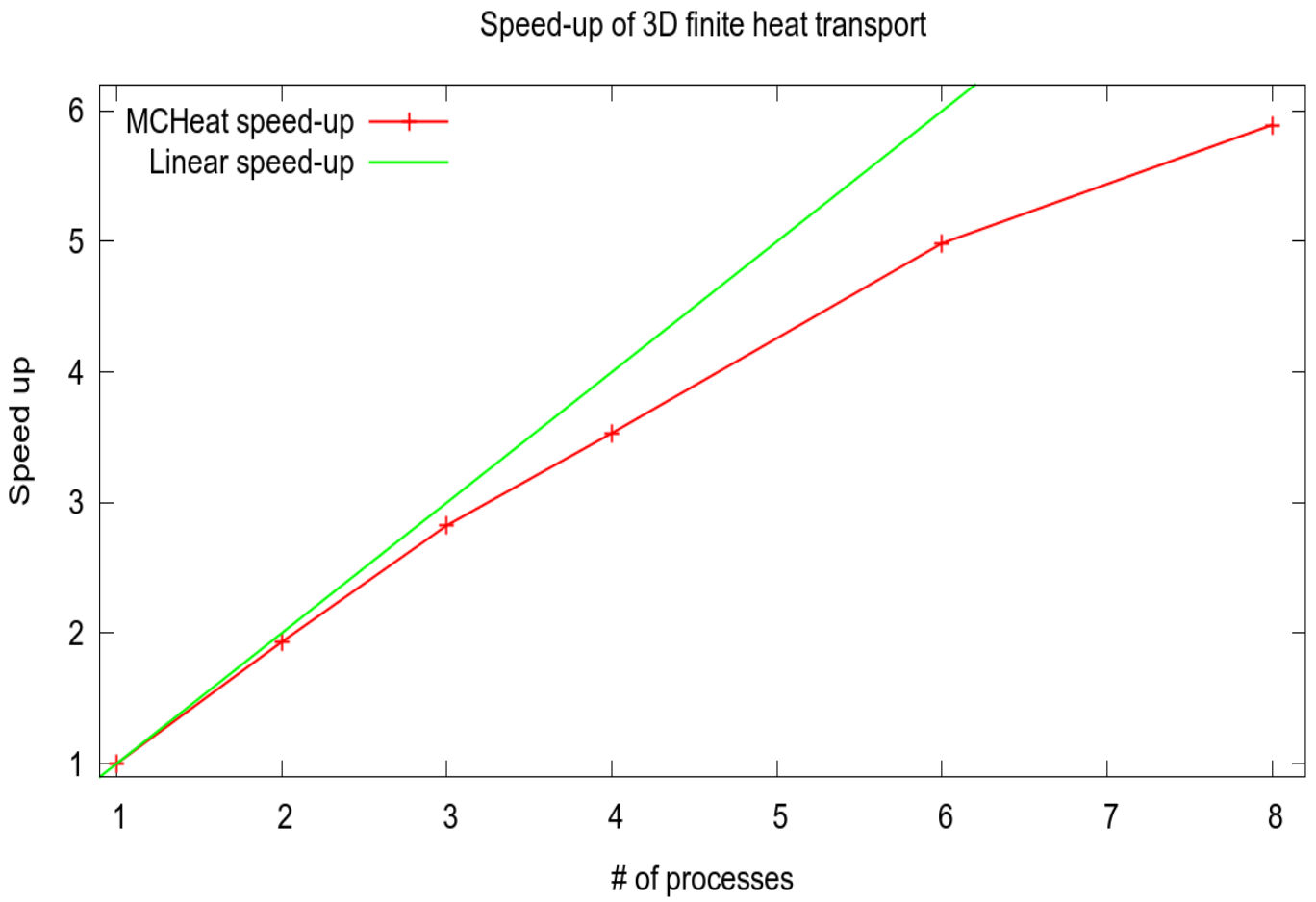
- Monte Carlo is classed as embarrassingly parallel
- Easy (most of the time...) to parallelise a MCRT code

- Various libraries: Openmpi, Intel Mpi, Cray Mpi...
- In various languages: Fortran, C, Python, MATLAB, R...

Openmpi

Parallelisation





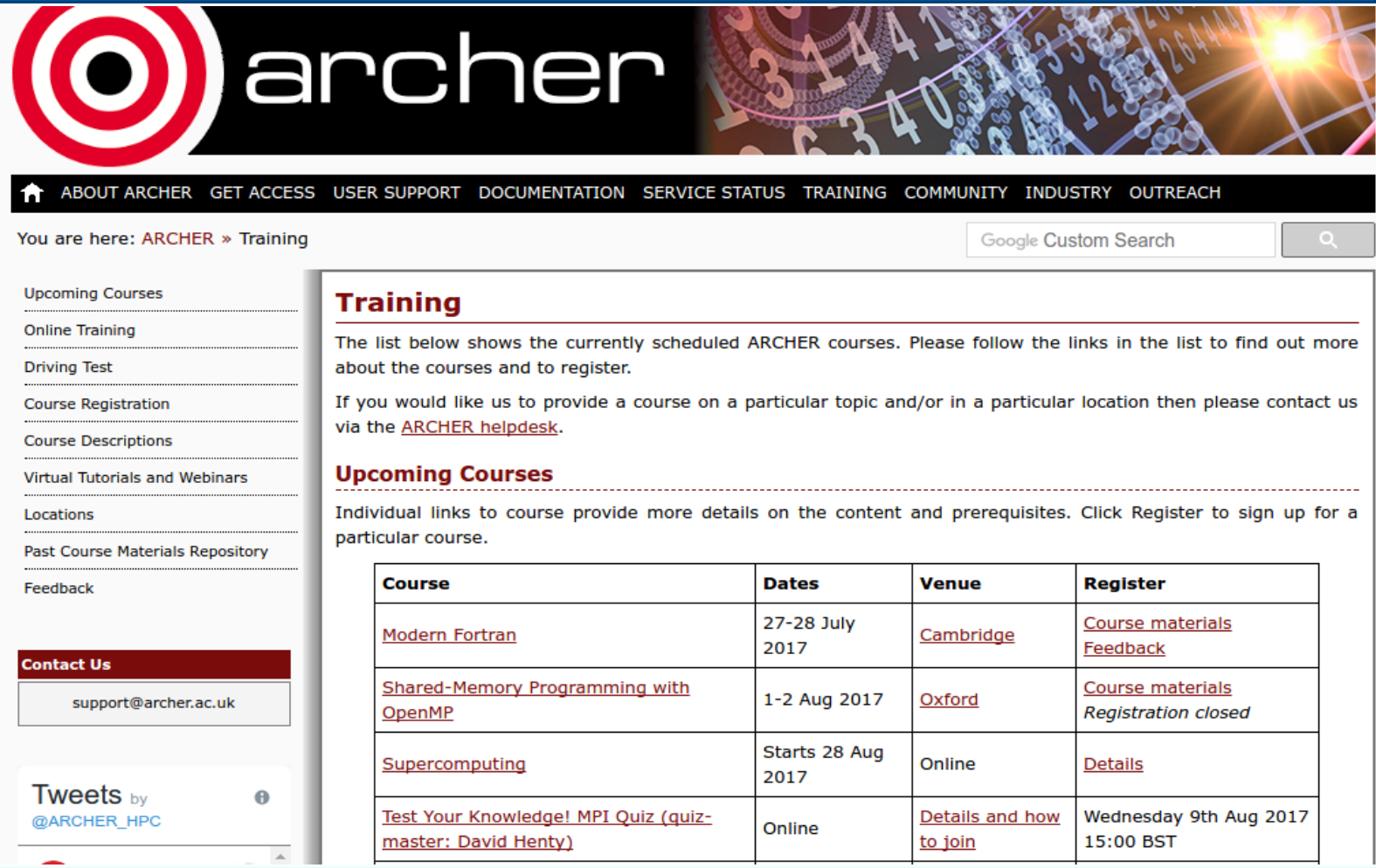
mpi_example.f90

```
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     !initalise 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
33     size_fluence = n * n * n
34
35     !sum all fluence arrays and give result to master process
36     call mpi_reduce(fluence, fluenceGLOBAL, size_fluence, mpi_real, mpi_sum, master, comm, error)
37
38     !finalize mpi
39     call mpi_finalize(error)
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



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…)