TINSTAAFL — theorem

Optical Technologies.

there's no such thing as a free lunch

SAYING

said to emphasize that you cannot get something for nothing:

[http://dictionary.cambridge.org]

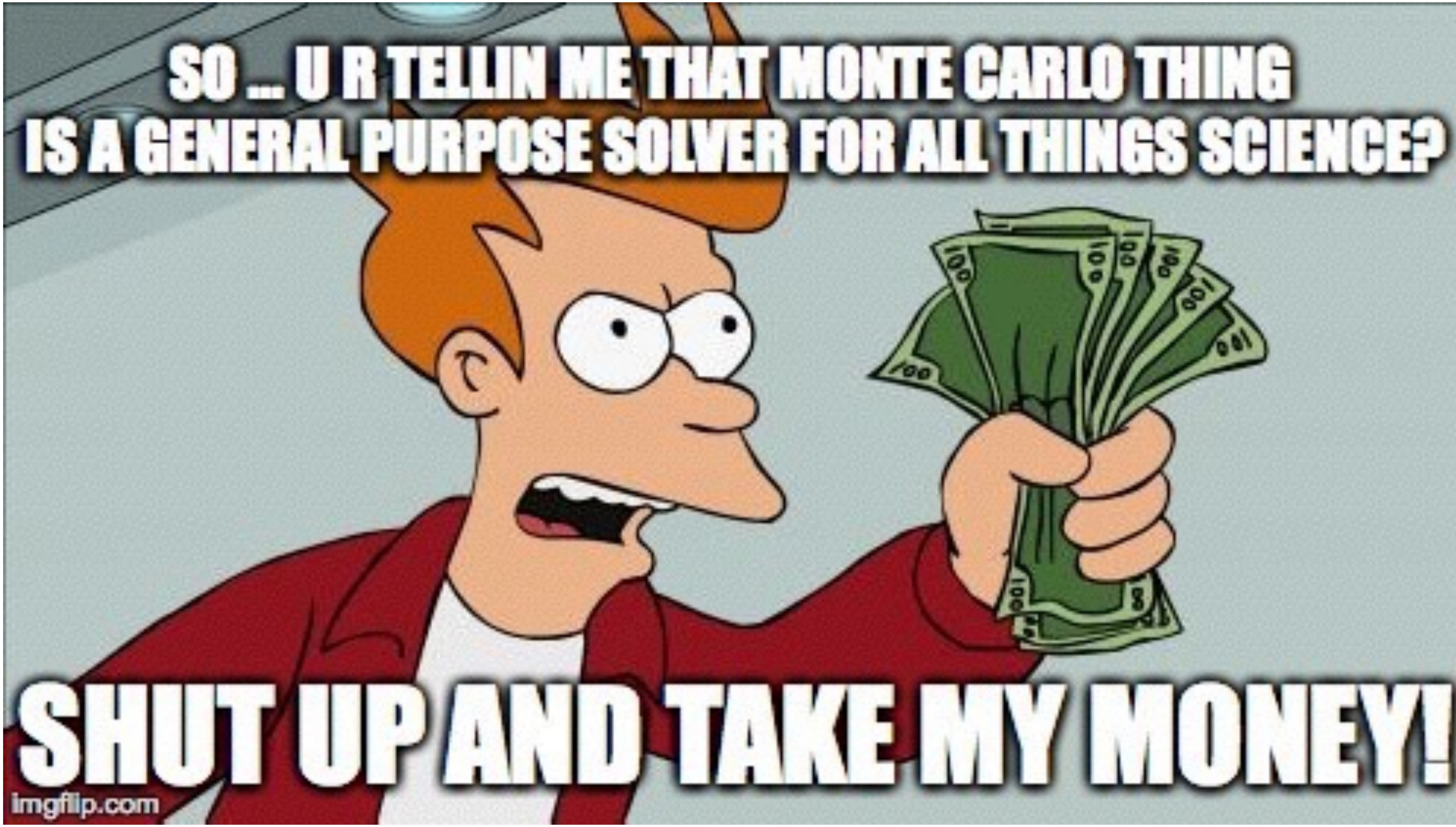
… in order to be graded after the full lecture,
you must visit the exercises!

Problem hand-out date: 2017-06-28

Solution hand-in date: 2017-07-12

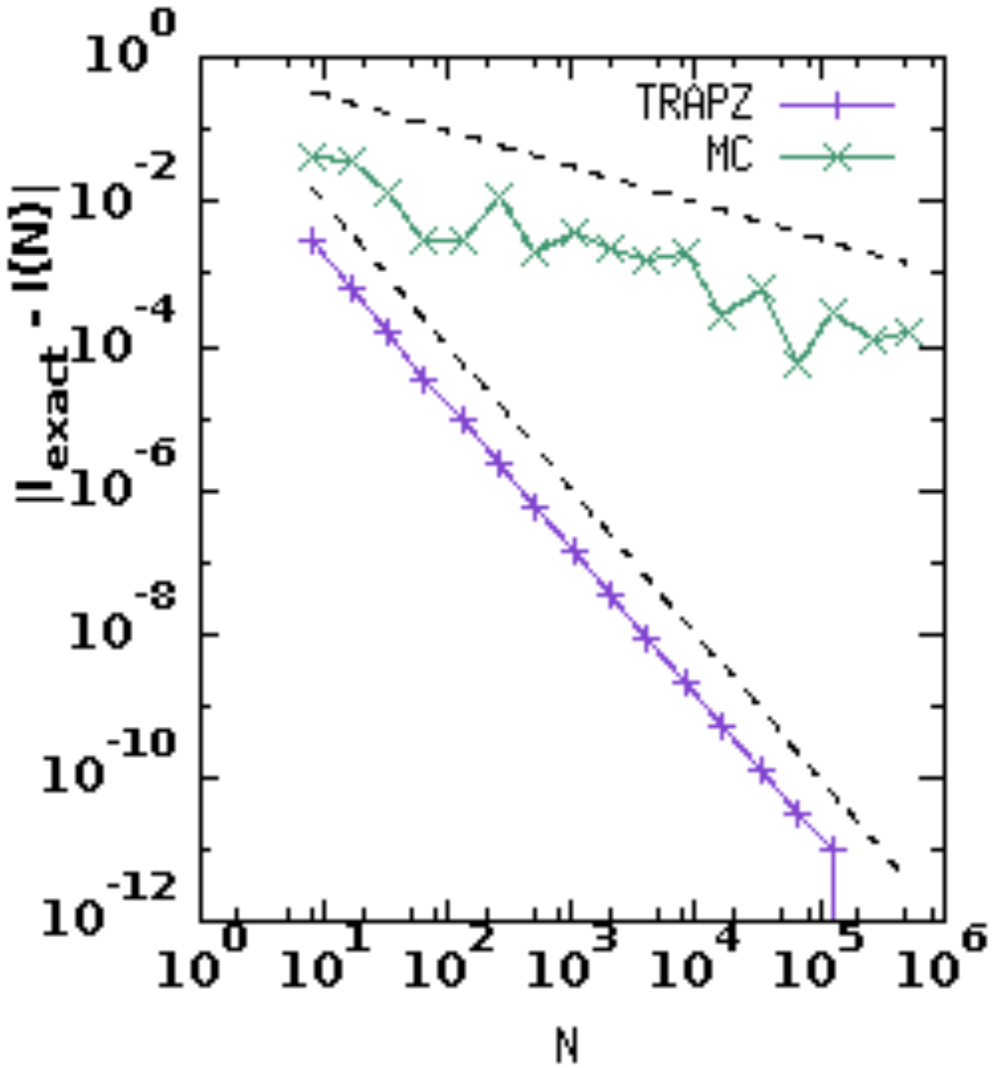
2 students per problem OK!

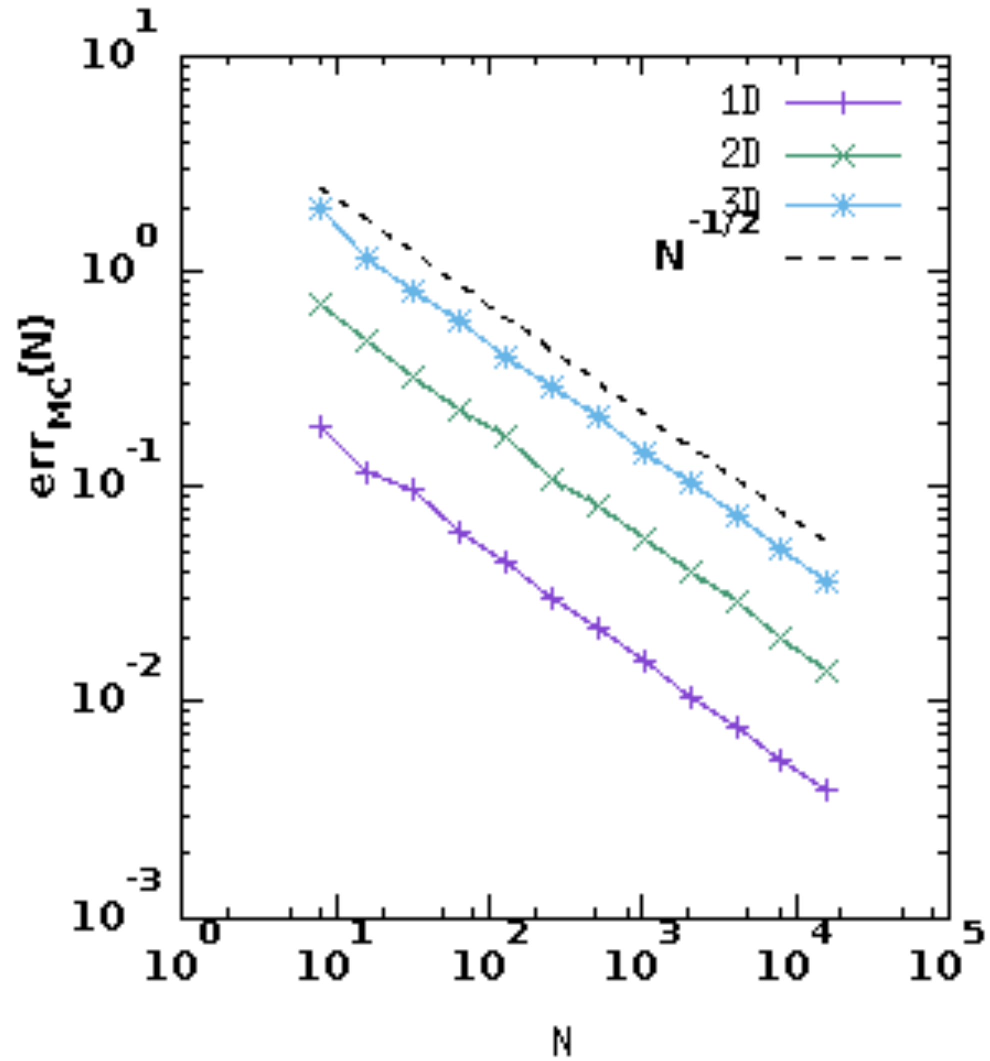
report-volume: 10 pages!



Caution, don't get too hyped! … and don't overgeneralize!

Recap — E1.2: Pros and cons of MC integration





Con: In $1\mathrm{D}$, deterministic trapezoidal rule is much better! $\epsilon_{\mathrm{T}} \sim N^{-2/d}$

Pro: In either dimension the error of the MC method decreases as $\epsilon_{\mathrm{MC}} \sim N^{-1/2}$

Advantage over deterministic integration schemes already for moderate dimension d: MC sampling outperforms simple trapezoidal rule for $d > 4$

Lecture focus on tissue optics: outline

Optical Technologies.

Computational tissue optics

Light transport in turbid media (Optical absorption)

Monte Carlo (MC) method

Pseudo random numbers (PRNs)

Top-down approach:

- to understand light transport in general turbid media you need to *master the MC method*
- ~~to master MC method you need to *sample PRNs*~~
- ~~to sample PRNs you need to actually *code*~~

Bottom-up approach:

- ~~Lecture 1: *PRN generation / quality control*~~
- ~~Lecture 2: *MC sampling strategies*~~
- Lecture 3: *MC simulation in turbid media*
- ~~Exercise 1: *extensive Python code examples*~~

Optical Technologies.

Lecture 3

Light transport in turbid media

Outline

- Recap — L1, L2, E1
- Recap — E1.2: Pros and cons of MC integration

Lecture 3: Light transport in turbid media

3.1 - The radiative transfer equation (TE)

3.2 - MC modeling of photon propagation

3.3 - Validation testing

3.1 The radiative transfer equation (TE)

Optical Technologies.

A probably biased history of developments:

- early heuristic approach to describe light propagation in turbid media

THE

ASTROPHYSICAL JOURNAL

AN INTERNATIONAL REVIEW OF SPECTROSCOPY AND ASTRONOMICAL PHYSICS

VOLUME XXI JANUARY 1905 NUMBER 1

RADIATION THROUGH A FOGGY ATMOSPHERE

By ARTHUR SCHUSTER

[Schuster, Astrophys. J., 21 (1905) 1]

- Monte Carlo approach to handle multiple scattering in cosmic nebulae

MULTIPLE SCATTERING IN REFLECTION NEBULAE.
I. A MONTE CARLO APPROACH

ADOLF N. WITT

Ritter Astrophysical Research Center, The University of Toledo; and
Laboratory for Atmospheric and Space Physics, University of Colorado

Received 1977 January 24; accepted 1977 March 14

[Witt, Astrophys. J. Supplement Series, 33 (1977) 1]

… details practical numerical method for computing radiative transfer

3.1 The radiative transfer equation (TE)

Optical Technologies.

- multiple (isotropic) scattering and absorption of laser radiation in tissue

THERMAL EFFECTS OF LASER RADIATION IN BIOLOGICAL TISSUE

LARIMORE CUMMINS
Dominican Santa Cruz Hospital, Santa Cruz, California 95065

MICHAEL NAUENBERG
Institute for Theoretical Physics, University of California, Santa Barbara, California 92106

[Cummins, Nauenberg, Biophys. J., 42 (1983) 99]

… naive but instructive approach! A good read!

- Monte Carlo model for light propagation in tissue (isotropic scattering, homogeneous medium, no interfaces and tissue boundaries)

A Monte Carlo model for the absorption and flux distributions of light in tissue

B. C. Wilson

Department of Physics, Ontario Cancer Treatment and Research Foundation, 711 Concession Street, Hamilton, Ontario, Canada L8V 1C3

G. Adam

Department of Radiobiology, Nuclear Research Centre, Negev, Beersheva, Israel

[Wilson, Adam, Med. Phys., 10 (1983) 824]

… radiative transfer studies in photo radiation therapy

3.1 The radiative transfer equation (TE)

Optical Technologies.

- simulation of light transport in multi-layered tissue

MCML — Monte Carlo modeling of light transport in multi-layered tissues

Lihong Wang*[a], Steven L. Jacques[a], Liqiong Zheng[b]

[a] *Laser Biology Research Laboratory, Box 17, University of Texas M.D. Anderson Cancer Center, 1515 Holcombe Boulevard, Houston, TX 77030, USA*

[b] *Department of Computer Science, University of Houston, Houston, TX 77204-3475, USA*

[Wang et al., Comp. Meth. and Progs. in Biomed. 47 (1995) 47]

- pedagogical introduction

MONTE CARLO MODELING OF LIGHT TRANSPORT IN TISSUES

Steven L. Jacques and Lihong Wang

[Jacques & Wang in Optical-Thermal Response of Laser-Irradiated Tissue, 1995, Springer]

3.1 The radiative transfer equation (TE)

- simulation of light transport in 3D voxelized tissue

TING LI, HUI GONG, and QINGMING LUO, *J. Innov. Opt. Health Sci.* **03**, 91 (2010).
DOI: http://dx.doi.org/10.1142/S1793545810000927

MCVM: MONTE CARLO MODELING OF PHOTON MIGRATION IN VOXELIZED MEDIA

[Li *et al.*, J. Innov. Opt. Health Sci., 3 (2010) 91]

- GPU optimized Monte Carlo code

Next-generation acceleration and code optimization for light transport in turbid media using GPUs

Erik Alerstam,[1,5,*] William Chun Yip Lo,[2,5] Tianyi David Han,[4] Jonathan Rose,[4] Stefan Andersson-Engels,[1] and Lothar Lilge[2,3]

[Alerstam *et al.*, Biomed. Opt. Express, 1 (2010) 658]

3.1 The radiative transfer equation (TE)

Optical Technologies.

How to describe transfer of light energy in tissue:

- analytical solution via Maxwell's equations
  …not feasible due to inhomogeneity of biological tissue
- feasible alternative: numerical transport theory
  … broad technical basis to solve problems in different fields

Light propagation model (steady state domain):

- transfer of laser energy in (isotropic) tissue based on photon transport

$$\vec{s}\cdot\vec{\nabla} I(\vec{r},\vec{s}) = -(\mu_a+\mu_s)I(\vec{r},\vec{s}) + \mu_s \int_{4\pi} p(\vec{s},\vec{s}')I(\vec{r},\vec{s})\ \mathrm{d}\Omega$$

$I(\vec{r},\vec{s}) =$ Intensity traveling from $\vec{r}$ in direction of $\vec{s}$

scattering anisotropy: $g = \int_{4\pi} p(\vec{s},\vec{s}')(\vec{s}\cdot\vec{s}')\ \mathrm{d}\Omega$

$p(\vec{r},\vec{s}) =$ phase function

$\mu_a =$ absorption coefficient

$\mu_s =$ scattering coefficient

[Cheong, Prahl, Welch, *Optical Properties of Biological Tissue*, J. Quant. El. 26 (1990) 2166]

- transport equation (TE) = gold standard in tissue optics

3.1 The radiative transfer equation (TE)

Optical Technologies.

3.1.1 Limiting case 1: unscattered transmission

- simple solution for TE for $\mu_s \ll \mu_a$

$$\vec{s}\cdot\vec{\nabla} I(\vec{r},\vec{s}) \approx -\mu_a I(\vec{r},\vec{s})$$

- choosing, e.g., $\vec{s}=\vec{e}_z$, and setting $I(\vec{r},\vec{e}_z)=I_z(\vec{r})$ thus yields

$$\boxed{I_z(\vec{r}) = I_0(\vec{r})\exp\{-\mu_a z\}} \qquad \text{(Beer's law)}$$

3.1.2 Limiting case 2: diffusion approximation

- simplified solution for TE for $\mu_a \ll \mu_s$
- based on expansion of intensity in spherical harmonics
- yields approximate solution in terms of diffusion equation

$$\{\nabla^2 - 3\mu_a[\mu_a + (1-g)\mu_s]\}\,\Phi(\vec{r}) = -Q_0(\vec{r})$$

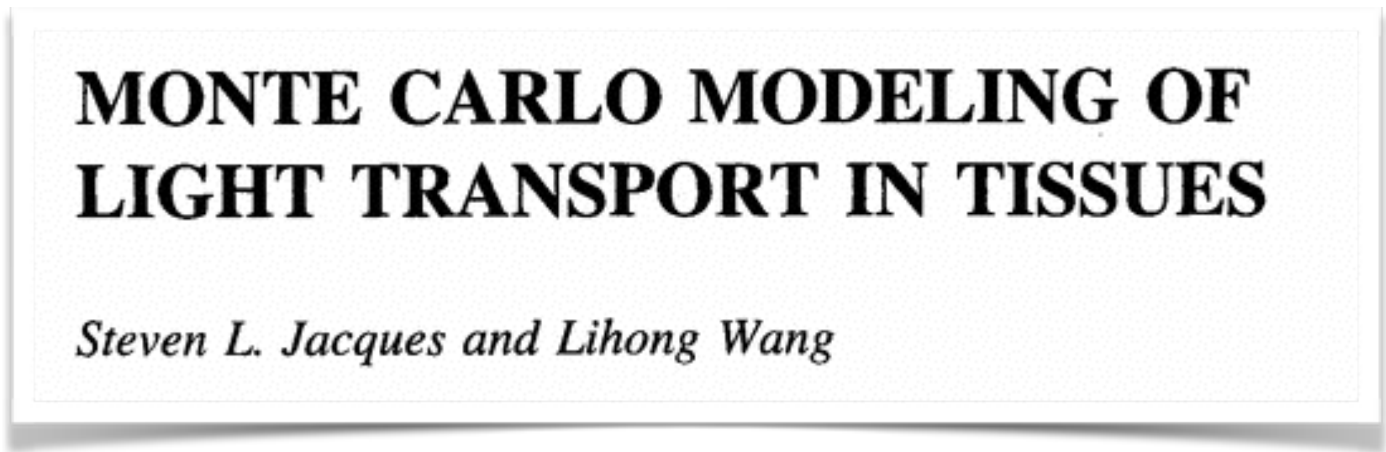
fluence rate: $\Phi(\vec{r}) = \int_{4\pi} I(\vec{r},\vec{s})\ \mathrm{d}\Omega$ $\qquad$ $Q_0(\vec{r}) =$ source function

scaling behavior of fluence rate: $\boxed{\Phi(\vec{r}) \sim \exp\{-\mu_{\rm eff}|\vec{r}|\}}$

3.2 MC modeling of photon propagation

- pedagocial introduction:

  [Jacques & Wang in Optical-Thermal Response of Laser-Irradiated Tissue, 1995, Springer]



MONTE CARLO MODELING OF LIGHT TRANSPORT IN TISSUES

Steven L. Jacques and Lihong Wang

- stochastic simulation of photon random walk in medium
- flexible approach based on simple propagation rules
- absorption and scattering properties need to be know *a priori*

$$p(\vec{r}, \vec{s}) = \text{phase function}$$

$$\mu_a = \text{absorption coefficient}$$

$$\mu_s = \text{scattering coefficient}$$

Here: photon transport in infinite homogeneous medium

3.2 MC modeling of photon propagation

3.2.1 Photon packet propagation

- Variance reduction technique:

Implicit photon capture

  - Idea: propagate photon *packet*
  - Motivation: conserve CPU time by reducing number of photons needed to reach desired accuracy in MC simulation

[Kahn & Harris in MC Method, National Bureau of Standards, 1951]

Code Listing 1: photon packet attributes

```python
class PhotonPacket(object):
    """random walker in 3D space"""
    def __init__(self, sSamp, wSamp, x0=(0,0,0), w0=(0,0,1) ):
        """instance of 3D random walker class

        Args:
            x0 (3-tuple, floats) starting point of walk (default: x0=(0,0,0))
            w0 (3-tuple, floats) ini directional cosines (default: w0=(0,0,1))
            wSamp (function) directional cosine sampler
            sSamp (function) stepsize sampler

        Attrib:
            x (3-tuple, float) current walker position
            w (3-tuple, float) current directional cosines
            nSteps (int) number of steps taken
            E (float) current photon packet weight
            dE (float) last weight decrement
        """
```

3.2 MC modeling of photon propagation

Optical Technologies.

- variable stepsize method
  - probability density function (pdf) for stepsize s

$$p(s) = (\mu_a + \mu_s)\exp\{-(\mu_a + \mu_s)s\}$$

  - cumulative distribution function (cdf)

$$F(u) = 1 - \exp\{-(\mu_a + \mu_s)u\} \quad \rightarrow \quad u = -\frac{\ln(1 - F(u))}{(\mu_a + \mu_s)}$$

easy to compute *iid* random variates via inversion method

- implementing photon packet propagation

Code Listing 2: combine translation and re-orientation

```
    def propagate(self):
        """perform single propagation step

        Implements single propagation step for 3D photon migration by
        computing new stepsize, followed by translation and computing new
        directions for the next step
```

3.2 MC modeling of photon propagation

3.2.2 Scattering events

- photon packet is split into two parts:
  - part 1: absorbed portion of the wave packet

    Weight decrease following Beer-Lambert law

$$E_{i+1} = E_i \frac{\mu_s}{(\mu_a + \mu_s)}$$

Code Listing 3: absorption of photon energy

```
          Proc. SPIE IS, 5 (19
"""
dE = (1.-a)*self.E
self.dE = dE
self.E -= dE
```

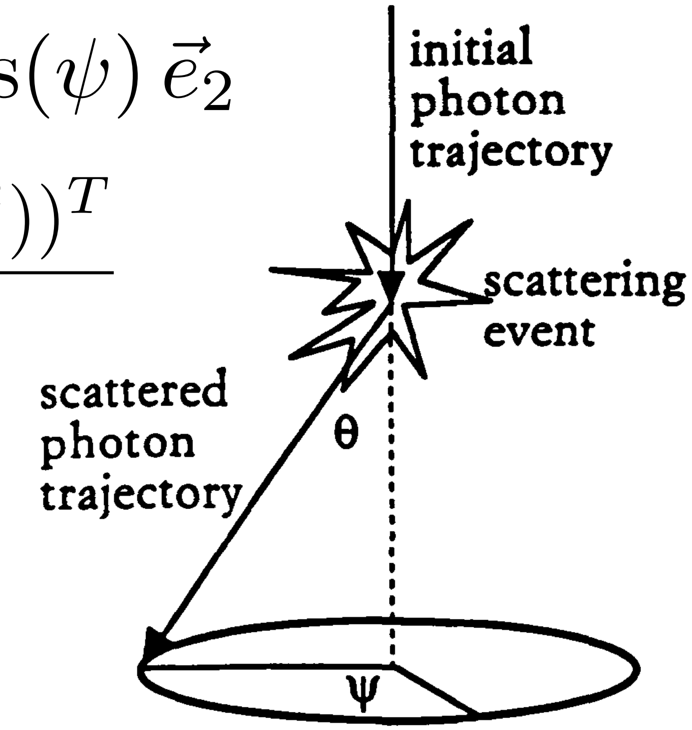
  - keep weight decrement for later measurement
  - subdivide computational domain into finite volumes called „bins“
  - accumulate absorbed weight within corresponding bin

3.2 MC modeling of photon propagation

- part II: scattered portion of the wave packet

$$\vec{\omega}_i = \cos(\theta)\,\vec{\omega}_{i-1} + \sin(\theta)\cos(\psi)\,\vec{e}_1 + \sin(\theta)\cos(\psi)\,\vec{e}_2$$

$$\vec{e}_1 = \frac{(-\omega_y, \omega_x, 0)^T}{\sqrt{1-w_z^2}} \qquad \vec{e}_2 = \frac{(\omega_x\omega_z, \omega_y\omega_z, -(1-\omega_z^2))^T}{\sqrt{1-w_z^2}}$$



(see lecture 2 - 2.2.3.2)

[Jacques, S. L. and Wang, L., in *Optical-Thermal Response of Laser-Irradiated Tissue*, Plenum Press, (1995)]

Code Listing 4: update for directional cosines

```
if abs(wz) < 0.99999:
    fac = 1./np.sqrt(1.- wz*wz)
    wxp = wx*cosT - fac*(wy*sinTcosP - wx*wz*sinTsinP)
    wyp = wy*cosT + fac*(wx*sinTcosP + wy*wz*sinTsinP)
    wzp = wz*cosT - sinTsinP*np.sqrt(1-wz*wz)
else:
    wxp = sinTcosP
    wyp = sinTsinP
    wzp = cosT*wz
```

Optical Technologies.

3.2.3 Photon termination

Problem:

- photon packet weight decreases but never reaches zero
- propagating a packet with small weight is not efficient

Remedy:

roulette strategy to terminate photons below weight threshold

- photon propagates further with probability p_m and weight $E/p_m > E$
- photon is terminated with probability $(1 - p_m)$

conserves CPU time, yields unbiased removal of photons and ensures energy conservation

Code Listing 5: roulette strategy for photon termination

```
def _roulette(pm):
    if random.random() < pm:
        self.E /= pm
        myState = True
    else:
        myState = False
    return myState
```

3.2 MC modeling of photon propagation

3.2.4 Interaction with tissue — monitoring observables

- symmetry of the problem often helps to choose a proper binning
- here: subdivide volume into spherical shells to compute fluence rate

Code Listing 6: Fluence rate

```
class FluenceRate(object):
    """class defining data structure for measurement of fluence rate
    """
    def __init__(self,nBins,nP):
        """initialize an instance of fluence rate data structure

        Args:
            nBins (int) number of bins for data accumulation
            nP (int) number of photons for normalization

        Attrib:
            shellWidth (float) shell width in microns (default: 50 mu)
            h (array) bins for energy accumulation
        """
        self.nBins      = nBins
        self.nPhotons   = nP
        self.shellWidth = 50
        self.h          = [0. for i in range(nBins)]
```

3.2 MC modeling of photon propagation

3.2.5 Irradiation source profiles

Optical Technologies.

Simulation using isotropic point source:

```python
class PhotonPacket(object):
    """random walker in 3D space"""
    def __init__(self, sSamp, wSamp, x0=(0,0,0), w0=(0,0,1) ):
```

Code Listing 7: default initialization for isotropic point source

Yields Greens function as response of the medium

- obtain fluence rate for arbitrary irradiation profile by convolution

$$\Phi(r,z) = \int_0^\infty \int_0^{2\pi} G(r',z)\ S(\sqrt{r'^2 + r^2 - 2rr'\cos(\theta)})\ d\theta\ r'dr'$$

- ex1: irradiation source function for Gaussian beam profile:

$$S(r) = S_0 \exp\{-2(r/R_0)^2\}$$

- ex2: irradiation source function for flat-top beam profile:

$$S(r) = S_0 \Theta(r - R_0)$$

Optical Technologies.

- convolution for special „easy“ responses:

[Wang et al., Comp. Meth. and Progs. in Biomed. 54 (1997) 141]

CONV—convolution for responses to a finite diameter photon beam incident on multi-layered tissues

Lihong Wang [a,*], Steven L. Jacques [b], Liqiong Zheng [c]

- convolution for general „difficult“ responses:

[O. Melchert, M. Wollweber, B. Roth , arXiv (2016)]

An efficient procedure for custom beam-profile convolution in polar coordinates: testing, benchmarking and application in tissue optics

O. Melchert, M. Wollweber and B. Roth

3.2 MC modeling of photon propagation

3.2.6 Performing a simulation

- proper main routine: →
- „good“ programming style:
  - separate declaration and initialization of variables
  - no silly documentation
  - keep everything clean

```python
import random
from randomVariateGenerator import *
from fluenceRate import FluenceRate
from photonPacket3D import PhotonPacket


def main():
    nP = int(sys.argv[1])            # number of independent photons
    mua = float(sys.argv[2])         # absorption coefficient
    mus = float(sys.argv[3])         # scattering coefficient
    g = float(sys.argv[4])           # scattering anisotropy
    nBins = 100                      # number of bins for measurement

    mut = mua + mus                  # total attenuation coeff.
    a   = mus/mut                    # single particle albedo

    lenSamp = ExpoVariate(mut)       # step length sampler
    dirSamp = HenyeyGreenstein(g)    # directional cosinge sampler
    Phi = FluenceRate(nBins,nP)      # fluence rate data structure

    while(nP):
        random.seed(nP)
        myPhoton = PhotonPacket(lenSamp.generate, dirSamp.generate)
        while(myPhoton.exists()):
            myPhoton.propagate()
            myPhoton.absorb(a)
            Phi.measure(myPhoton.x, myPhoton.dE)
        nP -= 1

    Phi.dump()


main()
```

Code Listing 8: complete main routine

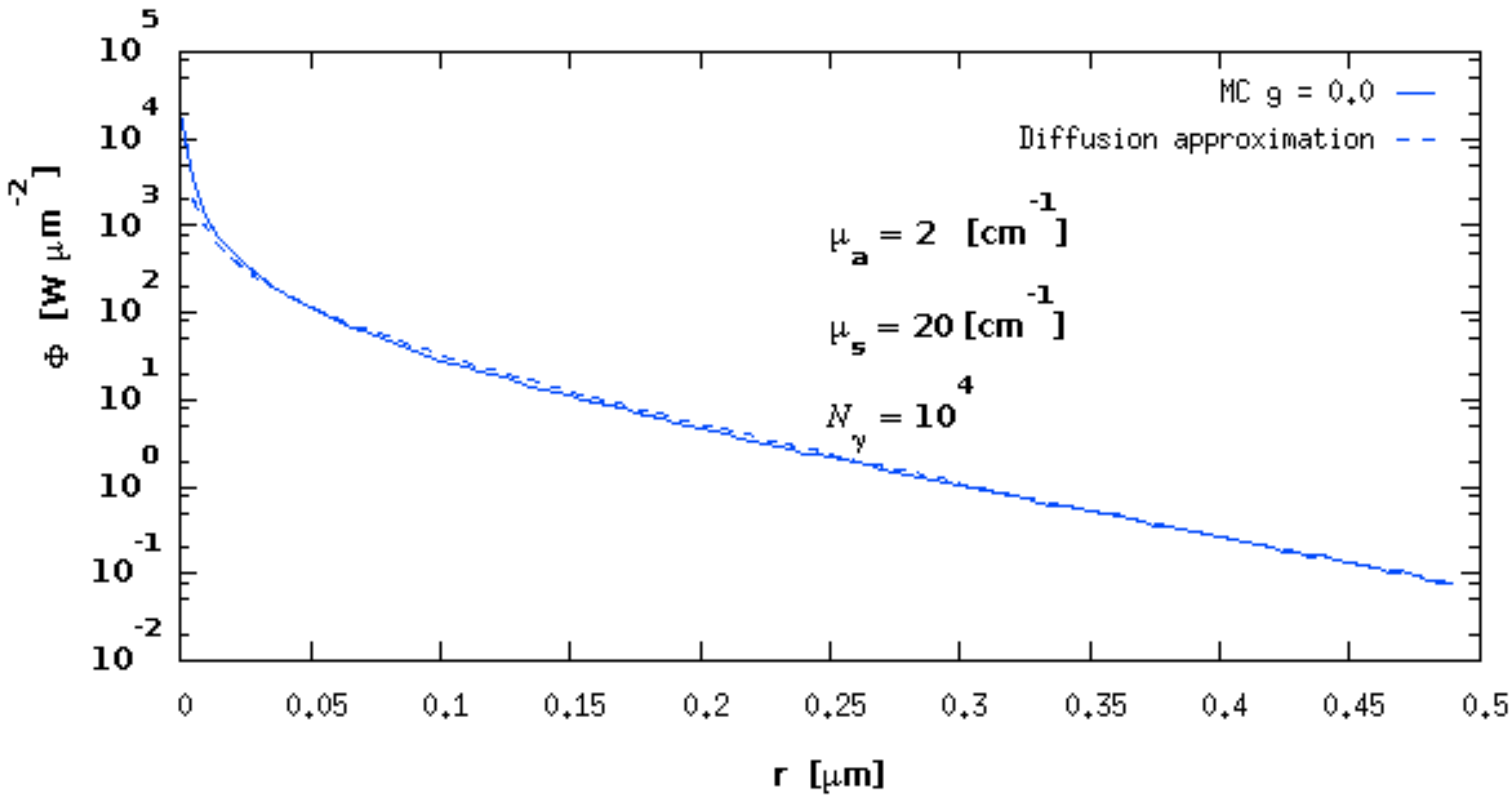
- general hints:
  - write lots of tests
  - refactor if needed
  - use debugger / memchecker
  - profile and optimize for running time

3.3 Validation testing

3.3.1 Comparison to diffusion approximation

- prediction in diffusion approximation:

$$\Phi(\vec{r}) = \frac{1}{4\pi r D} \exp\left\{ -\sqrt{\frac{\mu_a}{D}} |\vec{r}| \right\} \quad \text{diffusion coefficient: } D = \frac{1}{3[\mu_a + (1-g)\mu_s]}$$



3.3 Validation testing

3.3.2 Semi-analytic solution for anisotropic scattering

- analytic expression for infinite-space steady state point source fluence … cool … usually analytic solutions only possible for isotropic scattering

[Liemert, Kienle, Phys. Rev. A, 83 (2011) 015804]

- semi-analytic algorithm follows three-step procedure:

(1) Legendre expansion of intensity and phase function in planar-geometry RTE

$$I(x,\tau) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \phi_n(x) P_n(\tau) \qquad p(\tau,\tau') = \sum_{n=0}^{\infty} \frac{2n+1}{2} p_n P_n(\tau) P_n(\tau')$$

$\phi_n(x), p_n =$ Legendre moments

(2) deriving linear set of equations for $\phi_0(k)$ in wavenumber domain and solving for lowest Legendre moment via Carmer's rule

(3) Compute the fluence from plane wave expansion of $\phi_0(x)$ as

$$\Phi(x) \equiv \phi_0(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \phi_0(k) e^{ikx} \, \mathrm{d}k$$

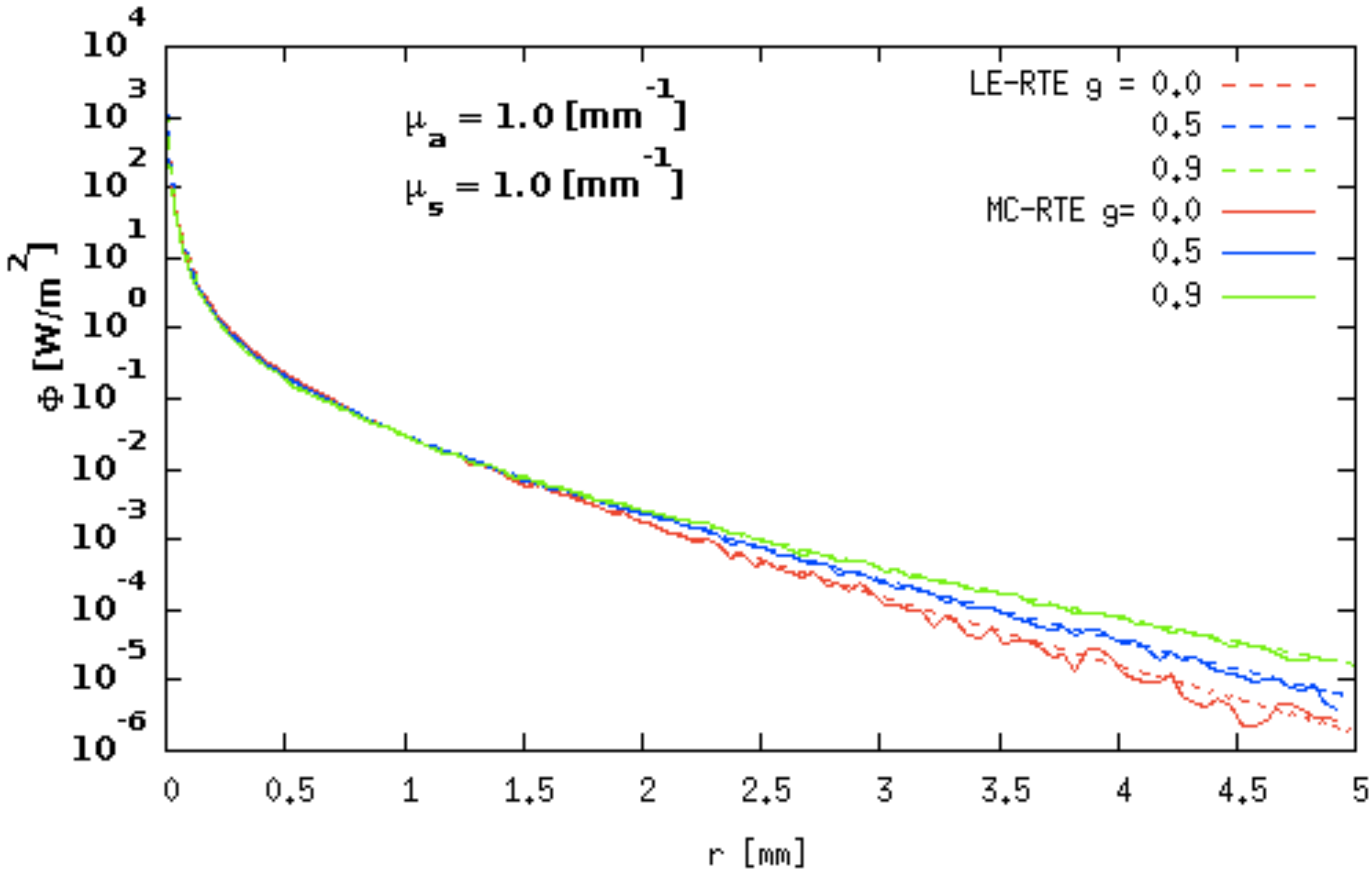
- yields Greens-function response of the medium
- many orders of magnitude faster than MC approach

Basically a one-trick-pony!

… and a great tool for validation testing within the limits of the analytic theory

3.3 Validation testing

- testcase for $\mu_a \approx \mu_s$



Notes on lecture 3:

- *next*: fancy things outside the scope of the limiting cases we used for validation testing

After lecture: example programs available at

https://github.com/omelchert/CompTissueOpt-2017.git