Spatial/Angular Contributon Maps for Improved Adaptive Monte Carlo Algorithms

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Introduction

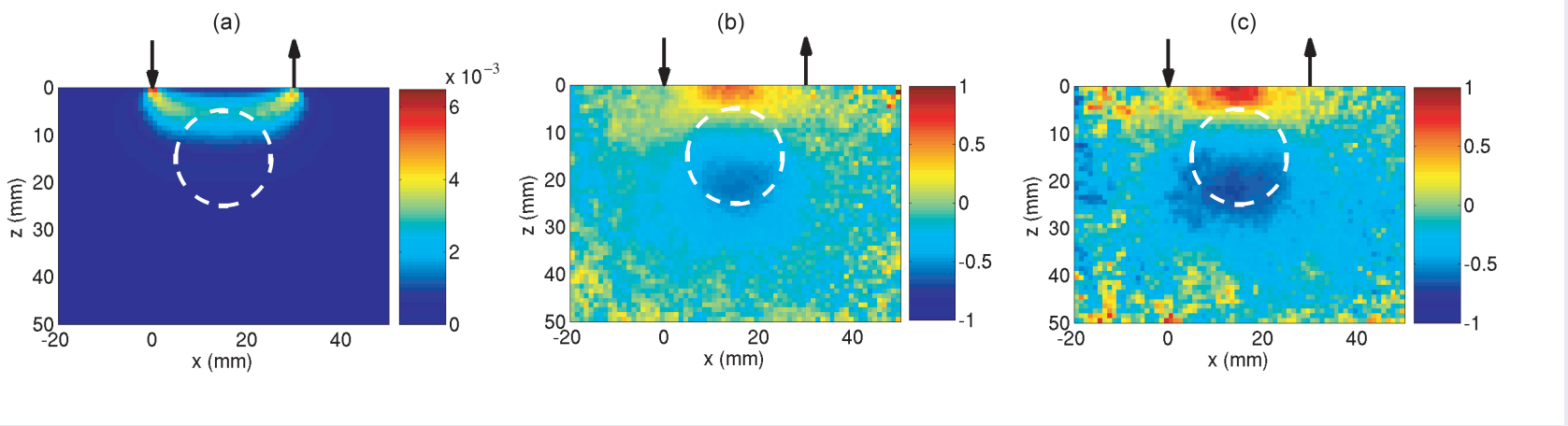
Motivation

To provide improved computational models to simulate and design biomedical diagnostic, imaging and therapeutic techniques using light, a Virtual Tissue Simulator (http://www.virtualphotonics.org) is being developed that:

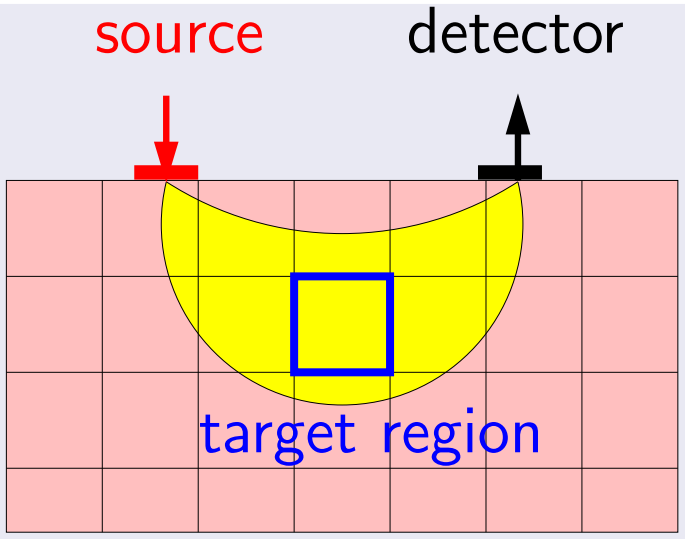
- Simulates tissue models that are biologically faithful.
- Implements fast, accurate Monte Carlo solutions of radiative transport.

Challenge: Tissue is highly turbid media with very forward directed scattering.

Breast Probe Study



Modeling Biological Tissue Problems



Problem Description

- The tissue is segmented into a spatial/angular decomposition or mesh, with each element representing a tissue type with averaged optical properties.
- Probe/tissue geometry identifies a problem with three components: 1) source, 2) detector, and 3) target region.
- Q: How coarse/fine must the tissue definition be in various regions to ensure accuracy in estimates of the detected signal?

This question is answered using a contributon map.

Spatial/Angular Contributon Maps for Improved Adaptive Monte Carlo Algorithms

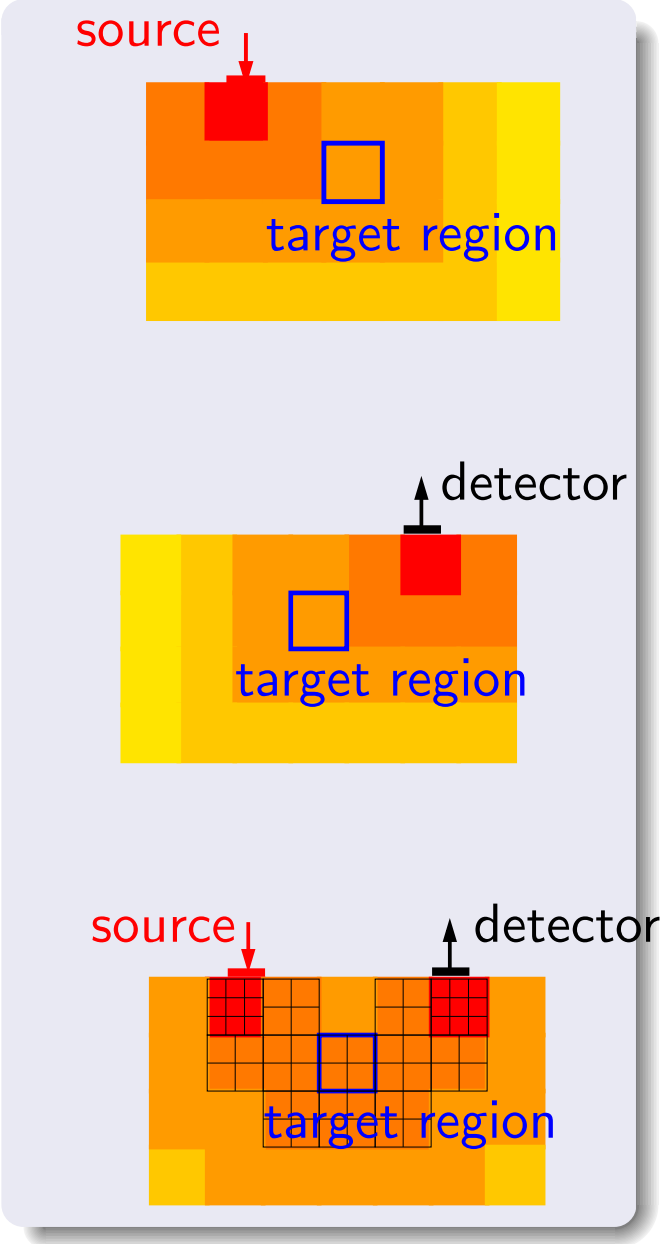
Outline

- Solution Overview (Part I and II)
- Radiative Transport Equation
- Sequential Correlated Sampling
- Part I: Averaged Sequential Correlated Sampling
- Part II: Contributon Maps
  - Adjoint Radiative Transport Equation
  - Contributon Equation
- Application: Automated Tissue Remeshing
- Summary and future work

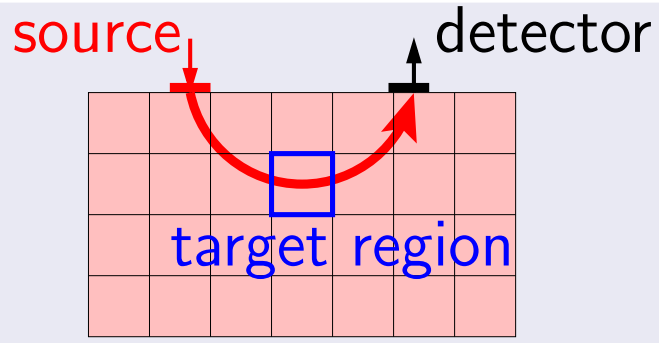
Solution Overview

General Steps

- Part I: Using a very crude spatial/angular mesh, Averaged Sequential Correlated Sampling (ASCS) is used to obtain piecewise constant averages of the spatial/angular flux throughout the tissue.
- Part II: The adjoint ASCS solution is then obtained using same mesh.
- Part II: Using the forward/adjoint estimates of the averaged flux, a contributon map is formed and identifies those regions/angles needing more refinement.
- This refined mesh is used to improve estimates of the detected signal.



Radiative Transport Equation



RTE: Integro-differential Form

- Radiative Transport Equation (RTE):

$$\nabla \cdot \mathbf{\Omega}\, \Psi(\mathbf{r}, \mathbf{\Omega}) \quad + \quad \mu_t(\mathbf{r}) \Psi(\mathbf{r}, \mathbf{\Omega}) = \mu_s(\mathbf{r}) \int_{4\pi} f(\mathbf{\Omega}' \to \mathbf{\Omega}) \Psi(\mathbf{r}, \mathbf{\Omega}')\, d\mathbf{\Omega}' + Q(\mathbf{r}, \mathbf{\Omega}) \qquad (1)$$

  $\Psi(\mathbf{r}, \mathbf{\Omega})$=flux (radiance), $\mu_t = \mu_s + \mu_a$=total attenuation,
  μ_a=absorption coefficient, μ_s=scattering coefficient,
  $f(\mathbf{\Omega}' \to \mathbf{\Omega})$ = scattering phase function, Q=source.

- Detected light (eg. Reflectance/Transmittance) of interest

$$R = \int Q^* \Psi$$

  where Q^*= detector (adjoint source) function.

Integral Form of RTE: Foundation of MC Simulation

RTE: Integral Form

- Integral form of Radiative Transport Equation:

$$\Phi(\mathbf{r}, \mathbf{\Omega}) = K\Phi(\mathbf{r}, \mathbf{\Omega}) + S(\mathbf{r}, \mathbf{\Omega}) \tag{2}$$

  $\Phi(\mathbf{r}, \mathbf{\Omega})$=collision density,
  $K[\cdot] = \int K[\cdot]$=transport kernel, S=density of first collisions.

- Φ and Ψ are related: $\Phi = \mu_t \Psi$
- Neumann series solution

$$\Phi = S(I + K + K^2 + K^3 \cdots) \tag{3}$$

- Detected light (eg. Reflectance/Transmittance) of interest

$$R = \int S^* \Phi$$

  where S^*= detector (adjoint source) function.

Lead up to Part I: Sequential Correlated Sampling (SCS)

SCS Idea

- Subtract approximate solution $\tilde{\Phi}$ from integral RTE:

$$\begin{aligned} \Phi - \tilde{\Phi} &= K\Phi + S - \tilde{\Phi} && (4) \\ &= K\Phi - K\tilde{\Phi} + K\tilde{\Phi} + S - \tilde{\Phi} && (5) \\ &= K[\Phi - \tilde{\Phi}] + (K\tilde{\Phi} + S - \tilde{\Phi}) && (6) \end{aligned}$$

- Initiate random walks using "reduced source"

$$\begin{aligned} S^{n+1}(\mathbf{r}, \mathbf{\Omega}) &= K\tilde{\Phi}^n(\mathbf{r}, \mathbf{\Omega}) + S^n(\mathbf{r}, \mathbf{\Omega}) - \tilde{\Phi}^n(\mathbf{r}, \mathbf{\Omega}) && (7) \\ S^0(\mathbf{r}, \mathbf{\Omega}) &= S(\mathbf{r}, \mathbf{\Omega}) && (8) \end{aligned}$$

- Solution $\Phi = \Phi^0 + \Phi^1 + \cdots$ is used to provide detected light $R = \int S^* \Phi$.

Part I: Averaged Sequential Correlated Sampling (ASCS)

Can we estimate R using only averaged values of $\bar{\Phi}$ throughout phase space Γ and save a lot of time?

Yes!

- Decompose Γ into space, angle bins $\delta_i \times \Delta_j$
- Average values of Φ are determined for each space-angle bin

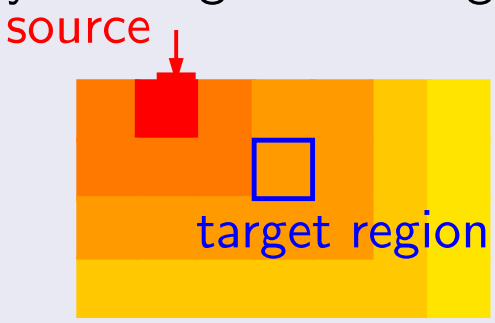
$$\bar{\Phi}_{ij} = \frac{1}{|\delta_i||\Delta_j|} \int_{\Delta_j} \int_{\delta_i} \Phi(\mathbf{r}, \mathbf{\Omega}) d\mathbf{r} d\mathbf{\Omega} \tag{9}$$

- $\bar{\Phi}^0_{ij}$ determined using conventional MC
- New "reduced source"

$$\bar{S}^{n+1}_{ij} = K\bar{\Phi}^n_{ij} + \bar{S}^n_{ij} - \bar{\Phi}^n_{ij} \tag{10}$$

Part I: ASCS continued

- This ASCS geometrically converges to histogram solution of Φ[a]



- But! Accuracy of solution obtained limited by selected mesh.

$\Rightarrow$ Intelligent mesh refinement determined using Contributon Map.

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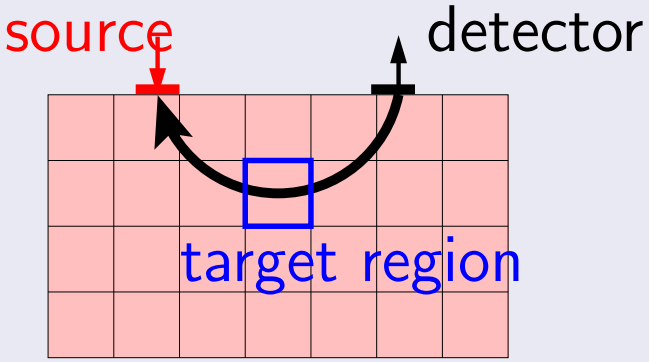
[a] R. Kong and J. Spanier. "Geometric convergence of second generation adaptive Monte Carlo algorithms for general transport problems based on correlated sampling." *Intl. J. Pure & Appl. Math.*, 59(4):435–455, 2010.

Part II Contributon Maps: Adjoint Radiative Transport Equation



Adjoint RTE: Intro-differential Form

- Adjoint RTE equation:

$$-\nabla \cdot \mathbf{\Omega}\Psi^*(\mathbf{r},\mathbf{\Omega}) \quad + \quad \mu_t(\mathbf{r})\Psi^*(\mathbf{r},\mathbf{\Omega}) = \mu_s(\mathbf{r}) \int_{4\pi} f(\mathbf{\Omega} \rightarrow \mathbf{\Omega}')\Psi^*(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}' + Q^*(\mathbf{r},\mathbf{\Omega}) \quad (11)$$

- Detected light (eg. Reflectance*/Transmittance*) can also be measured (by reciprocity)

$$R^* = \int Q\Psi^*$$

where Q= source function.

Contributon Equation

Multiply (1) by Ψ^* and (11) by Ψ and subtract $\rightarrow$ a new transport equation

$$\begin{aligned}\nabla \cdot \mathbf{\Omega}\Psi\Psi^* &= \Psi^*(\mathbf{r},\mathbf{\Omega})\mu_s(\mathbf{r})\int_{4\pi} p(\mathbf{\Omega}' \rightarrow \mathbf{\Omega})\Psi(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}' \\ &\quad -\Psi(\mathbf{r},\mathbf{\Omega})\mu_s(\mathbf{r})\int_{4\pi} p(\mathbf{\Omega} \rightarrow \mathbf{\Omega}')\Psi^*(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}' + Q\Psi^* - Q^*\Psi\end{aligned}$$

Introduce a new dependent variable: C=contributon function

$$C(\mathbf{r},\mathbf{\Omega}) = \Psi(\mathbf{r},\mathbf{\Omega})\Psi^*(\mathbf{r},\mathbf{\Omega})$$

$$\begin{aligned}\nabla \cdot \Omega C(\mathbf{r},\mathbf{\Omega}) + \Sigma_s(\mathbf{r},\mathbf{\Omega})C(\mathbf{r},\mathbf{\Omega}) &= \Psi^*\int_{4\pi}\Sigma(\mathbf{r},\mathbf{\Omega}' \rightarrow \mathbf{\Omega})C(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}' \\ &\quad + Q\Psi^* - Q^*\Psi \qquad (12)\end{aligned}$$

where $\Sigma_s(\mathbf{r},\mathbf{\Omega}) = \int_{4\pi}\Sigma(\mathbf{r},\mathbf{\Omega}' \rightarrow \mathbf{\Omega})d\mathbf{\Omega}'$

and $\Sigma(\mathbf{r},\mathbf{\Omega}' \rightarrow \mathbf{\Omega}) = \mu_s(\mathbf{r})p(\mathbf{r},\mathbf{\Omega}' \rightarrow \mathbf{\Omega})\frac{\Psi^*(\mathbf{r},\mathbf{\Omega}')}{\Psi^*(\mathbf{r},\mathbf{\Omega})}$

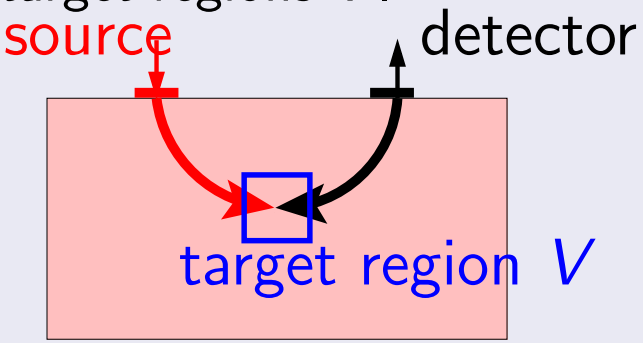
Contributon Equation

Concepts

- Contributon transport equation defines an information density function that describes the lossless flow of "contributons" from the source through the tissue to the detector[b]
- If BCs are dual, no loss of information density at the boundaries
- Instead of solving directly, we estimate

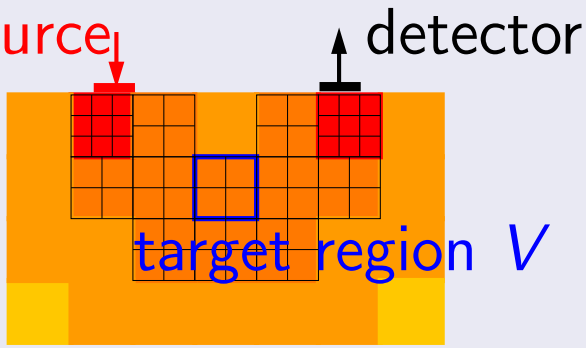
$$\int C(\mathbf{r}, \mathbf{\Omega}) = \int \Psi(\mathbf{r}, \mathbf{\Omega}) \Psi^*(\mathbf{r}, \mathbf{\Omega}) \tag{13}$$

by matching Ψ and Ψ^* solutions, both spatially and angularly, over the volume of selected target regions V.



[b]Williams, M.L., "The concept of spatial channel theory applied to reactor shielding analysis." *Nucl. Sci. Eng.*, 62, 92-104, 1977.

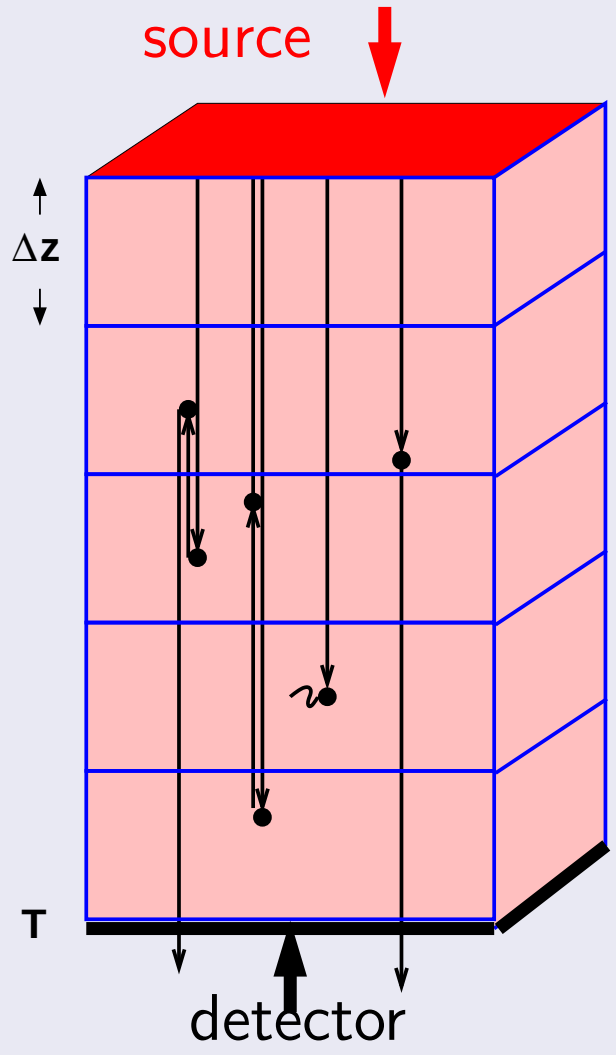
Contributon Map Algorithm



- The relative magnitude of $\int C$ dictates how each region should be subdivided until each region has roughly equal information content.
- Algorithm goal: Uniformize $\int C$ over remeshed phase space.
- The ASCS algorithm is repeated using the new remeshing.
- Previous results have illustrated the benefit in using **spatial** or scalar contributon map in 1D model problems[c]
- Our current goal is to analyze how **angular** contributon map can improve results and to move into higher dimensional systems.

[c] R. Kong, M. Ambrose, and J. Spanier. "Efficient, automated Monte Carlo methods for radiation transport." *J. Comp. Physics*, 227(22):9463–9476, 2008.

Model Problem Analysis

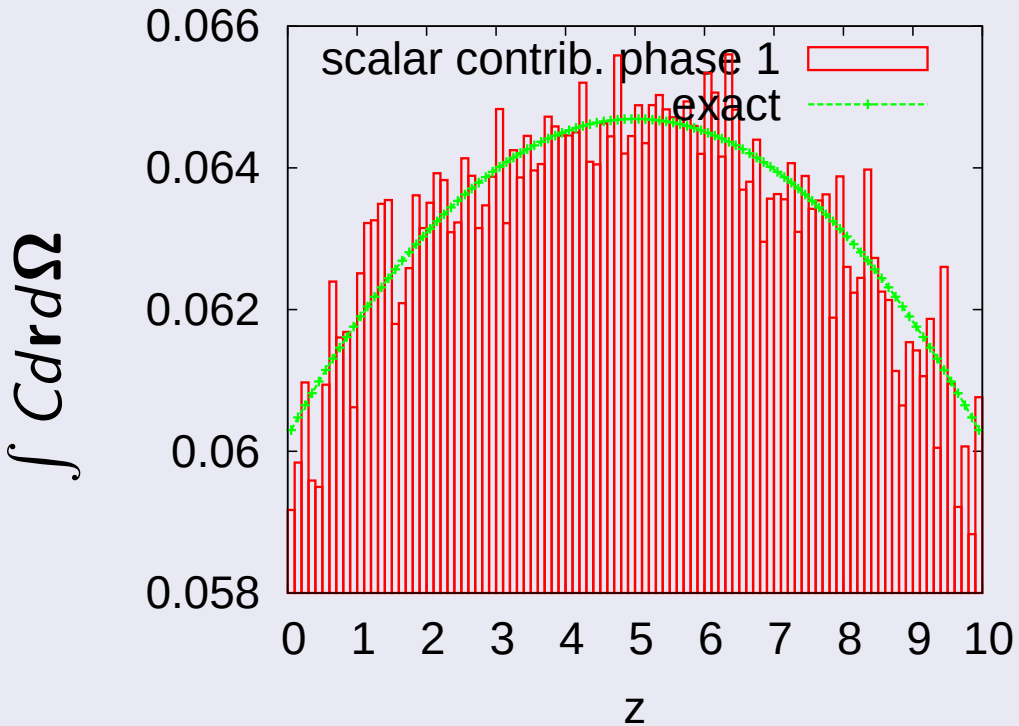


- The method is applied to a 3D model problem with tissue-like optical properties: μ_a=0.01/mm, μ_s=0.99/mm, $g = 0.9$, $T = 10$mfps.
- Only bidirectional scattering allowed (analytic solution available).
- Initial mesh 1: 100 uniform spatial bins, 2 angular hemispheres, 30rws/interval/direction

Spatial Refinement

Scalar contributon:

$$\int_{V_i}\int_{4\pi} C(\mathbf{r},\mathbf{\Omega})d\mathbf{r}d\mathbf{\Omega} = \int_{\mathbf{r}_i}[\Psi(\mathbf{\Omega})\Psi^*(\mathbf{\Omega}) + \Psi(-\mathbf{\Omega})\Psi^*(-\mathbf{\Omega})]d\mathbf{r}$$
$$\approx [\bar{\Psi}_i(\mathbf{\Omega})\bar{\Psi}_i^*(\mathbf{\Omega}) + \bar{\Psi}_i(-\mathbf{\Omega})\bar{\Psi}_i^*(-\mathbf{\Omega})]\Delta\mathbf{r}_i$$



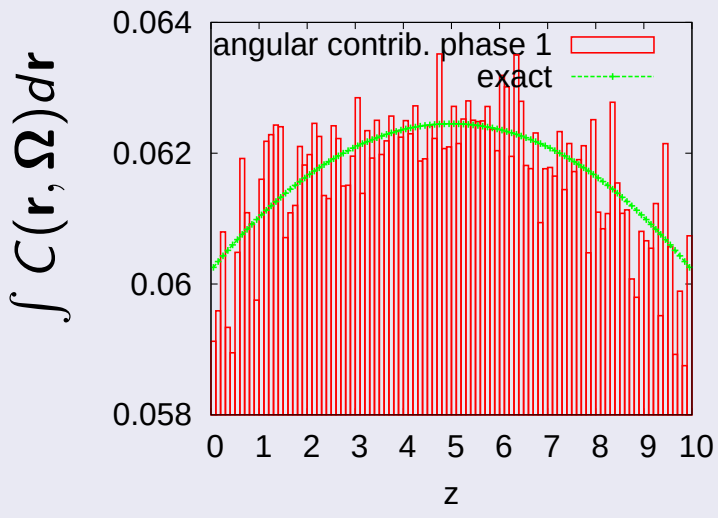
Small variation in scalar contributon designates no spatial subdivision.

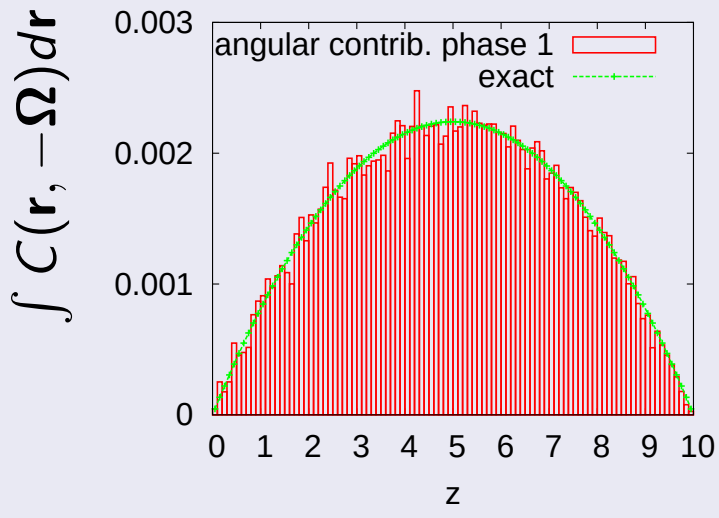
Angular Refinement

Angular contributon:

$$\int_{V_i} C(\mathbf{r}_i, \mathbf{\Omega}) d\mathbf{r} \approx \bar{\Psi}_i(\mathbf{\Omega}) \bar{\Psi}_i^*(\mathbf{\Omega}) \Delta \mathbf{r}_i \quad (14)$$

$$\int_{V_i} C(\mathbf{r}_i, -\mathbf{\Omega}) d\mathbf{r} \approx \bar{\Psi}_i(-\mathbf{\Omega}) \bar{\Psi}_i^*(-\mathbf{\Omega}) \Delta \mathbf{r}_i \quad (15)$$



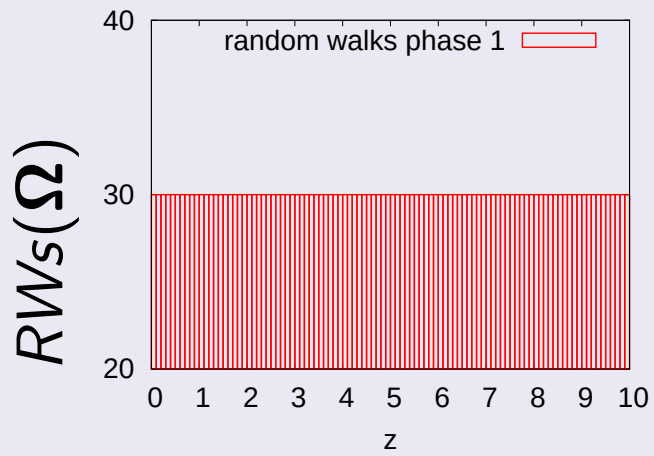


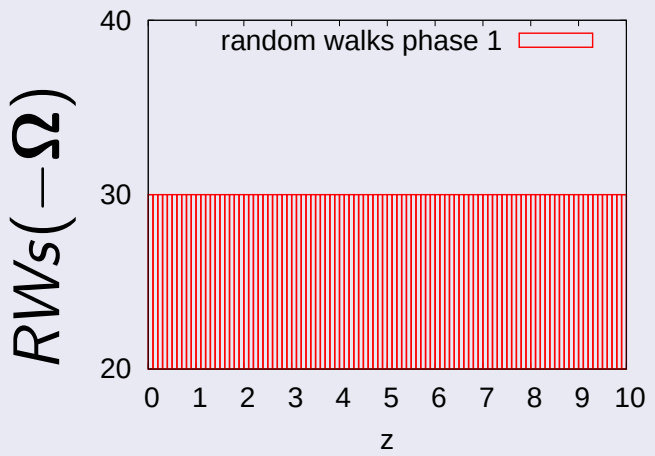
Large variation in angular contributon designates angular subdivision.

Angular Refinement

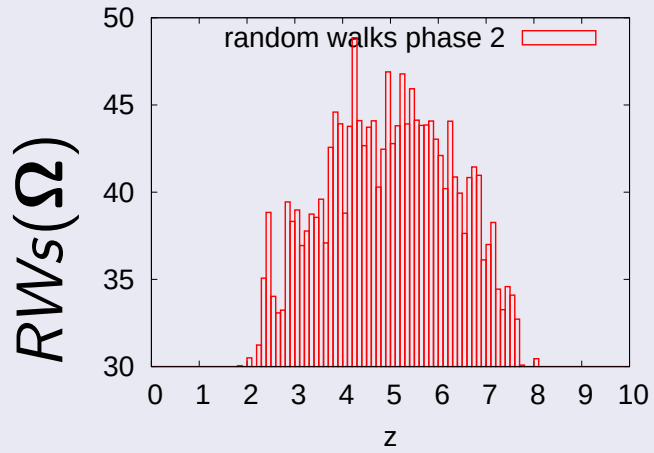
Instead of angular subdivision, modify number of rws in each direction using ratio $[\int C(\mathbf{r}, \mathbf{\Omega})d\mathbf{r} / \int C(\mathbf{r}, -\mathbf{\Omega})d\mathbf{r}]$ angular contributon maps.

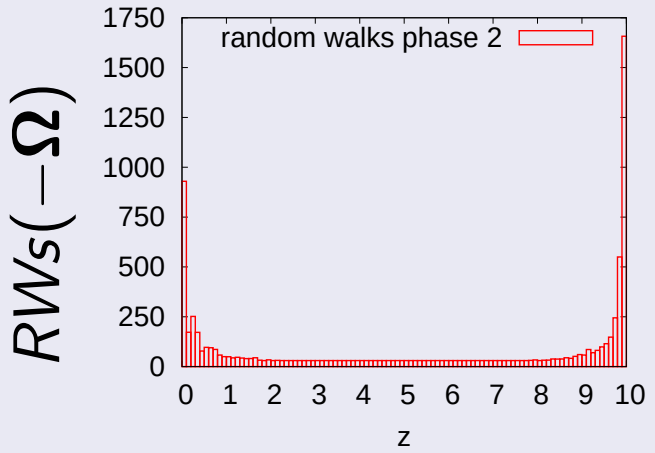
Phase I





Phase II



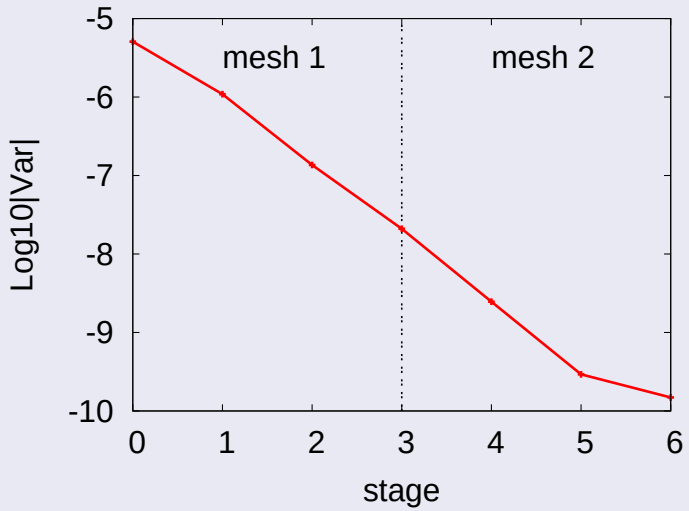


Results

Relative efficiency gains

Method	stages	Estimate	SD	time [sec]	Rel. Eff.
exact	-	0.602096	-	-	∞
CMC	1	0.601018	0.002254	6.50	1
Mesh I	4	0.602136	0.000145	25.93	60
Mesh II	7	0.602127	0.000012	71.13	3120

Variance reduction as a function of stage



Summary/Future Work

Contributon maps:

- describe the flow of radiation from source to detector.
- designate appropriate remeshing, both spatially and angularly, of the tissue for improved efficiency.
- complete application of contributon maps to more complex angular scattering problems and fully heterogeneous problems.

Acknowledgements:

- NIH K25-EB007309.
- NIH P41-RR01192.

Virtual Tissue Simulator – Rationale

Even though Modeling and Computation is an essential element in nearly all applications of Biophotonics. . .

- Biomedical community lacks ready access to advanced computational tools for modeling light interactions with cells and tissues.
- Advanced tools exist but are rarely consolidated and ‘packaged’ for general use.
- As a result, a high barrier remains for the non-expert to develop modeling and simulation tools for data analysis and measurement design.

Virtual Tissue Simulator

http://www.virtualphotonics.org