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Fast Superposition Algorithm Using Spectral Kernel Decomposition for Photon Beam Dose Calculation In Heterogeneous Media

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ABSTRACT

Purpose:
Convolution/superposition is a widely-used method for radiotherapy dose calculation, in which energy deposited at the first interaction point (TERMA) is convolved with a scatter kernel to obtain the dose. To account for tissue heterogeneities, the kernel can be scaled radially by the path-averaged relative electron density between the source and calculation points. However, this scaling renders the kernel spatially-dependent, precluding fast Fourier transform (FFT)-based acceleration. Several algorithms have been developed to circumvent this increased computational cost, including collapsed cone convolution (CCC). Here, an alternative approach is presented that decomposes the heterogeneous dose kernel into a linear combination of spatially invariant basis kernels, restoring FFT-based acceleration.

Methods:
The analytical kernel is adopted from CCC, i.e., a sum of exponentials with inverse-square decay. A quadrature grid is defined in kernel space using N_r Gauss-Laguerre radial nodes, L Gauss-Legendre polar nodes, and $2L$ uniformly-spaced azimuthal nodes. Each node corresponds to a fixed displacement in TERMA (source) space, allowing the kernel to be factored into a coefficient array in source space and a spatially-invariant Laguerre × Legendre basis kernel. The coefficient field includes the heterogeneity scaling factor, evaluated for each node-defined displacement in source space. The final dose is then computed as the weighted sum over all nodes of FFT-based convolutions, with asymptotic complexity $\mathcal{O}(N_r L^2 N^3 \log(N))$.

Results:
The algorithm was tested for a 6 MV, 10×10cm^2 beam incident on a mediastinum-like water-and-cork phantom. Dose distributions computed with $N_r = 4-12$ and $L = 4-12$ converged quickly to agreement with the GEANT4 Monte Carlo estimate, with gamma passing rates consistently exceeding 95% at 3%/2mm tolerance and 10% threshold for $N_r \geq 5$ and $L \geq 10$.

Conclusion:
Spectral kernel decomposition represents a new framework for fast kernel-based dose calculation in heterogeneous media, enabling FFT-based evaluation without restricting heterogeneity dependence to a finite number of directions. Next steps will include further algorithmic optimization and comparison with existing algorithms such as CCC.

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INTRODUCTION

- The distribution of radiation dose deposition in tissue from an incoming photon beam can be decomposed into a primary energy fluence distribution (TERMA) convolved with a scatter kernel. Formally:

$$D(\boldsymbol{r}) = \frac{1}{\rho(\boldsymbol{r})} \iiint T(\boldsymbol{r_0})\rho(\boldsymbol{r_0}) \cdot K(\boldsymbol{r} - \boldsymbol{r_0})\, \mathrm{d}^3\boldsymbol{r_0}$$

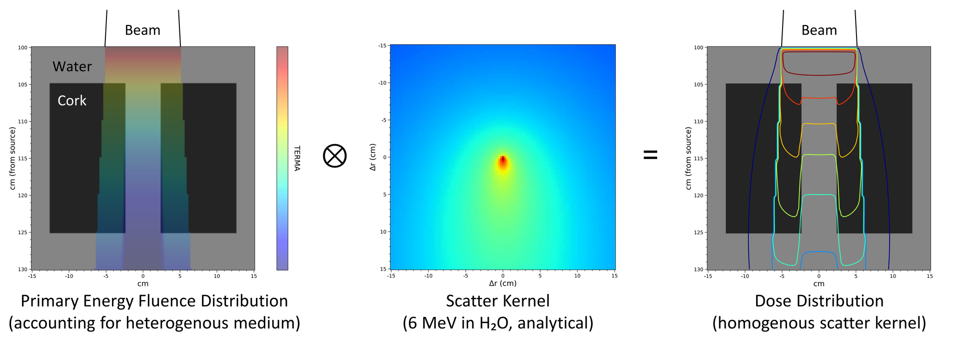

Figure 1: Convolution-based dose computation.

- The scatter kernel, $K(\boldsymbol{r_0} - \boldsymbol{r})$, for water can be calculated using Monte Carlo simulations. Alternatively, the scatter kernel can be modeled analytically with high accuracy [1] in the following form:

$$K(\Delta r, \theta) = \frac{A_\theta e^{-a_\theta \cdot \Delta r} + B_\theta e^{-b_\theta \cdot \Delta r}}{\Delta r^2},$$

where the first term represents energy deposited by direct electrons from the primary interaction and the second term represents energy deposited by secondary radiation.

- In homogeneous media, the scatter kernel is shift-invariant and fast Fourier transform (FFT) methods may be used to compute the convolution in $\mathcal{O}(N^3 \log(N))$ time, with N^3 the number of voxels in the computational domain.

But real anatomy is not homogeneous…

- Scattered photons and electrons travel further in low-density regions, so the effect of medium heterogeneity is to 'stretch' the kernel in the direction of lower relative electron density η.
- In heterogeneous media, the analytical kernel may be modified as follows:

$$K(\boldsymbol{r} - \boldsymbol{r_0}) = \eta(\boldsymbol{r}) \cdot c^2(\boldsymbol{r_0}, \boldsymbol{r}) \cdot K_{\mathrm{H_2O}}\big(c(\boldsymbol{r_0}, \boldsymbol{r}) \cdot (\boldsymbol{r} - \boldsymbol{r_0})\big)$$
$$= \eta(\boldsymbol{r}) \cdot \frac{A_\theta e^{-a_\theta \cdot c \cdot \Delta r} + B_\theta e^{-b_\theta \cdot c \cdot \Delta r}}{\Delta r^2},$$

where:

$$c(\boldsymbol{r_0}, \boldsymbol{r}) = \int_0^1 \eta\big(\boldsymbol{r_0} + t(\boldsymbol{r} - \boldsymbol{r_0})\big)\mathrm{d}t = \int_0^1 \eta(\boldsymbol{r_0} + t\Delta\boldsymbol{r})\mathrm{d}t$$

- The dose is thus:

$$D(\boldsymbol{r}) = \frac{\eta(\boldsymbol{r})}{\rho(\boldsymbol{r})} \iiint [T(\boldsymbol{r_0}) \cdot \rho(\boldsymbol{r_0})] \cdot \left[c^2(\boldsymbol{r_0}, \boldsymbol{r}) \cdot K_{\mathrm{H_2O}}\big(c(\boldsymbol{r_0}, \boldsymbol{r}) \cdot (\boldsymbol{r} - \boldsymbol{r_0})\big)\right] \mathrm{d}^3\boldsymbol{r_0}$$

and the kernel is no longer shift-invariant.

- Directly computing dose via this superposition formula would be an $\mathcal{O}(N^7)$ operation, which is intractable.
- Here, we derive a new computational method for fast, accurate superposition-based dose calculation using spectral kernel decomposition (SKD) to restore fast Fourier transform (FFT)-based acceleration in heterogeneous media.

METHODS

- If we presume that the inhomogeneous analytical kernel could be well-represented by a discretized orthogonal expansion with spatially-invariant basis functions $f_i(\Delta\boldsymbol{r})$ with coefficients $K(\boldsymbol{r_0}, \Delta\boldsymbol{r_i})$ and weights w_i, i.e.:

$$K(\boldsymbol{r_0}, \Delta\boldsymbol{r}) \approx \frac{\eta(\boldsymbol{r})}{\Delta r^2} \cdot \sum_i w_i \cdot K(\boldsymbol{r_0}, \Delta\boldsymbol{r_i}) \cdot f_i(\Delta\boldsymbol{r}),$$

then the dose could be written as a sum over expansion terms of FFT convolutions:

$$D(\boldsymbol{r}) = \frac{\eta(\boldsymbol{r})}{\rho(\boldsymbol{r})} \iiint \left[T(\boldsymbol{r_0}) \cdot \rho(\boldsymbol{r_0}) \cdot \sum_i w_i \cdot K(\boldsymbol{r_0}, \Delta\boldsymbol{r_i}) \cdot f_i(\Delta\boldsymbol{r})/\Delta r^2\right] \mathrm{d}^3\boldsymbol{r_0}$$
$$= \frac{\eta(\boldsymbol{r})}{\rho(\boldsymbol{r})} \cdot \sum_i w_i \iiint [T(\boldsymbol{r_0}) \cdot \rho(\boldsymbol{r_0}) \cdot K(\boldsymbol{r_0}, \Delta\boldsymbol{r_i})] \cdot \left[\frac{f_i(\Delta\boldsymbol{r})}{\Delta r^2}\right] \mathrm{d}^3\boldsymbol{r_0}$$
$$= \frac{\eta(\boldsymbol{r})}{\rho(\boldsymbol{r})} \cdot \mathcal{F}^{-1}\left[\sum_i w_i \cdot \mathcal{F}[T(\boldsymbol{r_0}) \cdot \rho(\boldsymbol{r_0}) \cdot K(\boldsymbol{r_0}, \Delta\boldsymbol{r_i})] \cdot \mathcal{F}\left[\frac{f_i(\Delta\boldsymbol{r})}{\Delta r^2}\right]\right],$$

with $\Delta\boldsymbol{r_i}$ representing the vector coordinates of orthogonal quadrature nodes in kernel space.

- The quadrature grid is defined in spherical coordinates, with N_r Gauss-Laguerre radial nodes, L Gauss-Legendre polar nodes, and $2L$ uniformly-spaced azimuthal nodes. The angular expansion is thus:

$$K(\Delta r, \theta, \varphi) \approx \sum_q^L \sum_p^{2L} w_q \cdot w_p \cdot S_{q,p}(\Delta\boldsymbol{r}) \cdot K(\Delta r, \theta_q, \varphi_p),$$

with the angular basis kernels $S_{q,p}(\Delta\boldsymbol{r})$ efficiently calculated using the addition theorem for spherical harmonics, while the radial expansion acts only on the exponential terms, e.g., for the first term:

$$e^{-a_\theta \cdot c(\boldsymbol{r_0}, \Delta\boldsymbol{r}) \cdot \Delta r} \approx \sum_j^{N_r} \frac{e^{a_\theta \cdot \Delta r_j} w_j}{a_\theta} \cdot R_{j,a}(\Delta\boldsymbol{r}, \Delta\boldsymbol{r_j}) \cdot e^{-a_\theta \cdot c(\boldsymbol{r_0}, \Delta\boldsymbol{r_j}) \cdot \Delta r_j},$$

where the radial basis kernels $R_j(\Delta\boldsymbol{r}, \Delta\boldsymbol{r_j})$ are efficiently calculated using the Laguerre addition theorem.

- The radial expansion requires computation of the inhomogeneity scale factor as a function of $\boldsymbol{r_0}$ for a given node $\Delta\boldsymbol{r_j}$:

$$c(\boldsymbol{r_0}, \Delta\boldsymbol{r_j}) = \int_0^1 \eta(\boldsymbol{r_0} + t\Delta\boldsymbol{r_j})\mathrm{d}t,$$

which is now, for each kernel-displacement node $\Delta\boldsymbol{r_j}$, purely dependent on $\boldsymbol{r_0}$ (Figure 2).

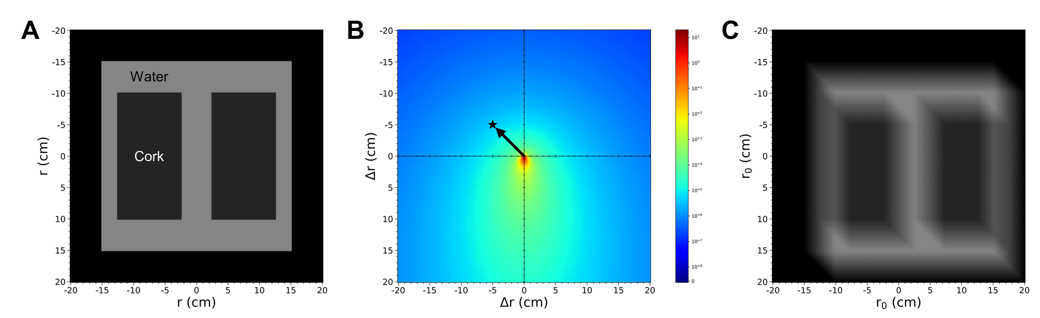

Figure 2: (**A**): Mediastinum-like phantom consisting of water and cork used for testing. (**B**): 6MV dose kernel cross-section with a sample SKD node and vector. (**C**) Heterogeneity scaling factor field $c(\boldsymbol{r_0}, \Delta\boldsymbol{r}_{q,p,j})$ for the sample node shown in (B).

- The direction of $\Delta\boldsymbol{r_i}$ is the same for all j in a given (q, p). Thus, if the algorithm is structured such that the outer loop is over angular nodes, then $c(\boldsymbol{r_0}, \Delta\boldsymbol{r}_{q,p,j})$ can be calculated with an $\mathcal{O}(N^3)$ operation for each radial node.
- The FFTs dominate the asymptotic complexity of SKD, which is therefore $\mathcal{O}(N_r L^2 N^3 \log(N))$.

RESULTS

- The SKD algorithm was evaluated with $N_r = 4-12$ and $L = 4-12$ for two geometries with a 6 MV 10×10 cm^2 beam at 100 cm SSD:
  a) A mediastinum-like phantom composed of water and cork.
  b) A simplified four-material extended cardiac-torso (XCAT) phantom consisting of adipose, muscle, bone, and lung.
- Using an NVIDIA RTX 3070 GPU, the current Python implementation achieves a speed of up to ~50 nodes/sec for the evaluated 121×121×121-voxel grids.

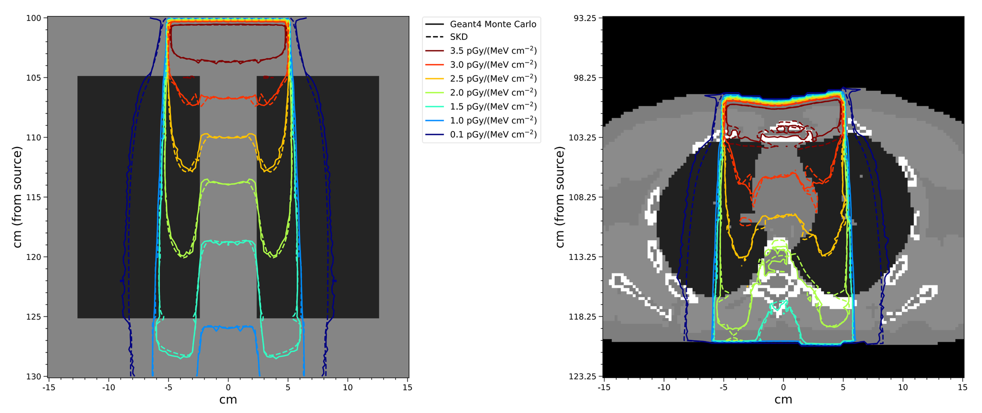

Figure 3: SKD-computed dose distribution using N_r =8 and $L = 6$ (576 total nodes; dashed isodose curves) versus the GEANT4 Monte Carlo-computed dose (solid isodose curves) for the water and cork mediastinum phantom (left) and the simplified XCAT phantom (right).

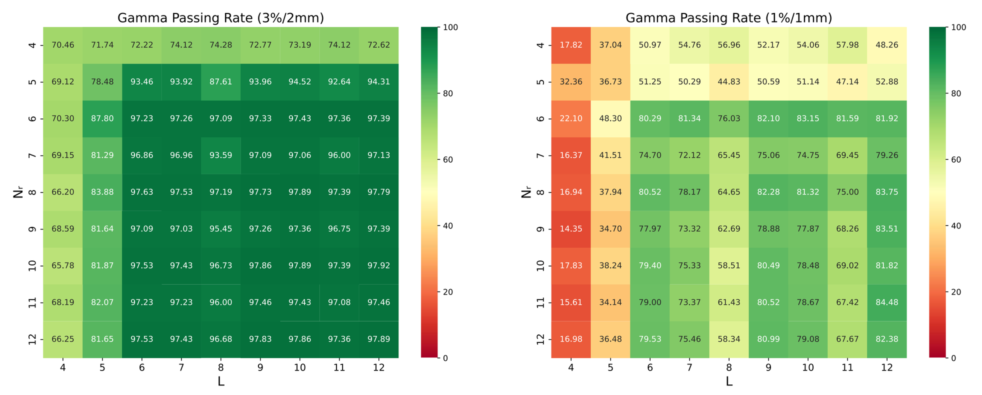

Figure 4: Gamma passing rates for SKD vs the GEANT4 Monte Carlo-computed dose for the water and cork mediastinum phantom at 10% threshold and 3%/2mm tolerance (left) and 1%/1mm tolerance (right) for varying N_r and L.

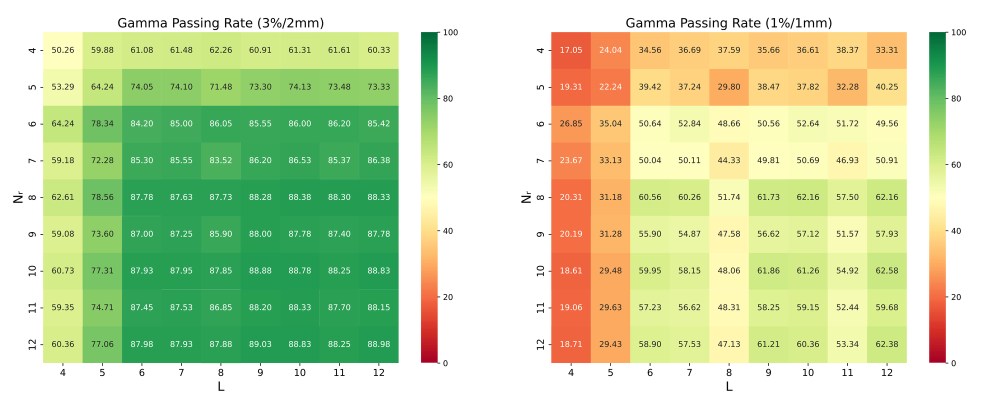

Figure 5: Gamma passing rates for SKD vs the GEANT4 Monte Carlo-computed dose for simplified XCAT phantom at 10% threshold and 3%/2mm tolerance (left) and 1%/1mm tolerance (right) for varying N_r and L.

CONCLUSIONS

- SKD is a new framework for fast kernel-based dose calculation in heterogeneous media, where dose at any point is influenced by all heterogeneity in the computational domain.
- SKD computes dose as a linear combination of independent FFT-based convolutions, making it highly-parallelizable.
- Next steps include algorithmic optimization and comparison with existing algorithms, such as Collapsed Cone Convolution.

REFERENCES

1. Ahnesjö A. Collapsed cone convolution of radiant energy for photon dose calculation in heterogeneous media. Med Phys. 1989 Jul-Aug;16(4):577-92. doi: 10.1118/1.596360.