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GRID-FREE MONTE CARLO FOR PDES WITH SPATIALLY VARYING COEFFICIENTS

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The symbols * and † indicate equal contribution.



Geometric & material complexity in science & engineering



building information model

microCT scan







Photorealistic rendering of complex geometry & materials



geometry + materials

rendered output





Physical analysis of complex geometry & materials



Heat radiating from infinitely many blackbodies in a heterogenous medium About 600 million effective vertices from visible viewpoint



Challenge with conventional PDE solvers: scalability





input mesh (used by WoS)



FEM mesh (FastTetWild)

FEM mesh (FastTetWild + AMR)

Challenge with conventional PDE solvers: scalability







Challenge with conventional PDE solvers: scalability



Boundary Element Method (BEM) and Meshless Finite Element (MFEM)



Boundary Element Method (BEM) and Meshless Finite Element (MFEM)



BEM: No support for spatially-varying coefficients



Boundary Element Method (BEM) and Meshless Finite Element (MFEM)



MFEM: Careful node placement & connectivity





Boundary Element Method (BEM) and Meshless Finite Element (MFEM)



MFEM: Careful node placement & connectivity



Monte Carlo Geometry Processing [SIGGRAPH 2020]



ACM Trans, Graph., Vol. 39, No. 4, Article 123, Publication date: July 2020

Monte Carlo Geometry Processing:

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Fig. 1. Real-world geometry has not only rich surface detail (left) but also intricate internal structure (center). On such domains, FEM-based geometric algorithms struggle to mesh, setup, and solve PDEs-in this case taking more than 14 hours and 30GB of memory just for a basic Poisson equation. Our Monte Carlo solver uses about 1GB of memory and takes less than a minute to provide a preview (center right) that can then be progressively refined (far right). [Boundary mesh of Fijian strumigenys FJ13 used courtesy of the Economo Lab at OIST.]

This paper explores how core problems in PDE-based geometry processing can be efficiently and reliably solved via grid-free Monte Carlo methods. Modern geometric algorithms often need to solve Poisson-like equations on geometrically intricate domains. Conventional methods most often mesh the domain, which is both challenging and expensive for geometry with fine details or imperfections (holes, self-intersections, etc.). In contrast, gridfree Monte Carlo methods avoid mesh generation entirely, and instead just evaluate closest point queries. They hence do not discretize space, time, nor even function spaces, and provide the exact solution (in expectation) even on extremely challenging models. More broadly, they share many benefits with Monte Carlo methods from photorealistic rendering: excellent scaling, trivial parallel implementation, view-dependent evaluation, and the ability to work with any kind of geometry (including implicit or procedural descriptions). We develop a complete "black box" solver that encompasses integration, variance reduction, and visualization, and explore how it can be used for various geometry processing tasks. In particular, we consider several fundamental linear elliptic PDEs with constant coefficients on solid regions of \mathbb{R}^n . Overall we find that Monte Carlo methods significantly broaden the horizons of geometry processing, since they easily handle problems of size and complexity that are essentially hopeless for conventional methods. CCS Concepts: • Computing methodologies → Shape analysis.

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A Grid-Free Approach to PDE-Based Methods on Volumetric Domains

ACM Reference Format:

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1 INTRODUCTION

The complexity of geometric models has increased dramatically in recent years, but is still far from matching the complexity found in nature-consider, for instance, detailed microstructures that give rise to physical or biological behavior (Fig. 1). PDE-based methods provide powerful tools for processing and analyzing such data, but have not yet reached a point where algorithms "just work": even basic tasks still entail careful preprocessing or parameter tuning, and robust algorithms can exhibit poor scaling in time or memory. Monte Carlo methods provide new opportunities for geometry processing, making a sharp break with traditional finite element methods (FEM). In particular, by avoiding the daunting challenge of mesh generation they offer a framework that is highly scalable, parallelizable, and numerically robust, and significantly expands the kind of geometry that can be used in PDE-based algorithms.

Photorealistic rendering experienced an analogous development around the 1990s: finite element radiosity [Goral et al. 1984] gave way to Monte Carlo integration of the light transport equation [Kajiya 1986], for reasons that are nicely summarized by Wann Jensen [2001, Chapter 1]. Although this shift was motivated in part by a desire for more complex illumination, it has also made it possible to work with scenes of extreme geometric complexity-modern renderers handle trillions of effective polygons [Georgiev et al. 2018] and, in stark contrast to FEM, yield high-quality results even for

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f estimators for PDEs commonly used ng algorithms (Sec. 2), ng derivatives and standard differential

ategies for PDE and derivative estima-

ions that circumvent common meshing nges (Sec. 5.1),

ues for scalar- and vector-valued data ance performance (Sec. 5.2), and enting core geometry processing algonte Carlo framework (Sec. 6).

ects to a large body of work on Monte 2006; Pharr et al. 2016]. From the PDE rence is that the differential equation is first order in space, whereas the PDEs nd order, diffusive terms that demand ues. There are of course many parallels m a mathematical, computational, and which we explore throughout the paper.

r some of the most fundamental PDEs general, there are two complementary on potential theory, is to express the egral equation (akin to the rendering nd apply Monte Carlo integration. The lculus, is to express the solution in terms use Monte Carlo to simulate random llustrated by the WoS algorithm for the which is our starting point for all other ential theory viewpoint is often simpler alculus provides sophisticated tools to rocesses to the integral formulation of arily consider the former in this paper, latter where necessary.

gion $A \subset \mathbb{R}^n$, we use ∂A to denote its volume, and $\mathcal{U}(A) = 1/|A|$ to denote sity function on A. Throughout we use in of interest, and B(x) to denote a ball d around a point x. For a point $x \in \Omega$, sest point on $\partial \Omega$. Finally, we use Δ to inite Laplace operator on \mathbb{R}^n , and $X \cdot Y$ product of vectors $X, Y \in \mathbb{R}^n$.

ion. To keep exposition self-contained acts about Monte Carlo integration; see 13] for a more thorough introduction. egral can be estimated by sampling the sen points. More precisely, let f be an main Ω. Then the integral

 $\int f(x) dx$





Fig. 3. The walk on spheres algorithm repeatedly jumps to a random point on the largest sphere centered at the current point x_i , until it gets within ε of the boundary. Since the largest sphere can be determined from a simple closest point query, no spatial discretization is needed.

is equal to the expected value of the Monte Carlo estimator

$$F_N := |\Omega| \frac{1}{N} \sum_{i=1}^{N} f(X_i), \quad X_i \sim U(\Omega)$$
 (1)

where N is any positive integer, and $X_i \sim U(\Omega)$ indicates that X_i are independent random samples drawn from the uniform distribution on Ω . The error of F_N is characterized by its *variance*: its expected (squared) deviation from the true value I.

Importance Sampling. More generally, let p be any probability distribution on Ω that is nonzero on the support of f. Then the integral of f is equal to the expected value of the estimator

$$\frac{1}{N} \sum_{i=1}^{N} \frac{f(X_i)}{p(X_i)}, \quad X_i \sim p.$$
(2)

Typically, p is chosen to reduce the variance of the estimate by focusing on "important" features in the integrand [Pharr et al. 2016, Section 13.10]. For simplicity, our initial discussion considers only the basic Monte Carlo estimator (Eqn. 1); importance sampling strategies are discussed in Sec. 4.2.

2.1.3 PDE Estimation. The solution to a linear elliptic PDE can be expressed as a linear combination of contributions from the boundary term and the source term. Estimation of these two terms is well-illustrated via the Laplace equation (Sec. 2.2) and Poisson equation (Sec. 2.3), resp. One can then build on these estimators to solve other common equations such as the screened Poisson (Sec. 2.4) and biharmonic equations (Sec. 2.5).

2.2 Laplace Equation

Laplace equations are commonly used to interpolate given boundary data $g: \partial \Omega \rightarrow \mathbb{R}$ (encoding, *e.g.*, color or deformation) over the interior of the domain. The solution u satisfies the PDE

$$\begin{array}{ll} \Delta u = 0 & \mathrm{on} \ \Omega, \\ u = g & \mathrm{on} \ \partial \Omega. \end{array} \tag{3}$$

These so-called harmonic functions have two important characterizations, which are illustrated in Fig. 4:

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Contribution: Bridge between PDEs & Volume Rendering



Partial Differential Equations







Spatial heterogeneity is everywhere!



Rich material properties e.g., wall with thermal insulation, sound proofing et.c



Spatial heterogeneity is everywhere!



thermal performance



geological modeling





acoustic performance



electrical capacitance



biological modeling



Shortcoming of conventional PDE solvers

Spatial discretization: expensive and error-prone



finite difference



finite element



Defective geometry, e.g., self-intersections, non-manifold elements



14 hrs / 30 GB RAM to generate FEM mesh



Shortcoming of conventional PDE solvers

Spatial discretization: destroys geometric features



boundary mesh (input)



34 minutes / 6.1 GB RAM to generate FEM mesh (missing blood vessels)

Sh

Sp

of conventional PDE solvers

tion: causes aliasing in the PDE inputs and solution









Monte Carlo Rendering

Does not require high quality meshing & solving global systems





Ray intersection query



Monte Carlo Rendering

Photorealistic image generation of participating and granular media



Does not require high quality meshing & solving global systems



Does not require high quality meshing & solving global systems



Does not require high quality meshing & solving global systems





Closest point query





Multi-material physical simulation in graphics



Han et al, "A Hybrid Material Point Method for Frictional Contact with Diverse Materials" (2019) Zhu et al, "Codimensional Non-Newtonian Fluids" (2015)

Multi-material physical simulation in graphics



Han et al, "A Hybrid Material Point Method for Frictional Contact with Diverse Materials" (2019) Zhu et al, "Codimensional Non-Newtonian Fluids" (2015)

Goal: extend to broader class of problems \implies PDEs with variable coefficients







BACKGROUND

A tale of three equations...



differential equations

 $\Delta u = f \text{ on } \Omega$ $u = g \text{ on } \partial \Omega$

stochastic equations

 $u(x) = \mathbb{E}\left[\int_0^\tau f(W_t) \, dt + g(W_\tau) \, \middle| \, W_0 = x\right]$



$\nabla \cdot (\alpha \nabla u) + \vec{\omega} \cdot \nabla u - \sigma u = -f \text{ on } \Omega$

solution





Laplace equation





$$\Delta u = 0$$
$$\Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$



Poisson equation



source term f(x)

 $\Delta u = f$

variable diffusion Poisson equation

coeff. $\alpha(x)$

 $\nabla \cdot (\alpha \nabla u) = f$

stationary advection-diffusion equation

transport $\vec{\omega}(x)$

 $\Delta u + \vec{\omega} \cdot \nabla u = f$

screened Poisson equation

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absorption coeff. $\sigma(x)$

 $\Delta u - \sigma u = f$

 $\Delta u = f$

 $\Delta u = 0$

Integral for Laplace equation

Integral for Laplace equation





Integral for Laplace equation





Integral for Laplace equation







Integral for screened Poisson equation (constant absorption)

screened Poisson – PDE

diffusion absorption source term

$$\Delta u - \sigma u =$$

screened Poisson – IE



$\Delta u - \sigma u = -f$ on Ω solution u = g on $\partial \Omega$

+
$$\int_{\partial B(c)}^{\text{solution}} \frac{u(z)P^{\sigma}(x,z)}{P^{oisson}} dz$$





Integral for screened Poisson equation (constant absorption)

screened Poisson – PDE

$$\Delta u - \sigma u =$$

screened Poisson – IE





A tale of three equations...



differential equations

 $\Delta u = f \text{ on } \Omega$ $u = g \text{ on } \partial \Omega$

stochastic equations

 $u(x) = \mathbb{E}\left[\int_0^\tau f(W_t) dt + g(W_\tau) \middle| W_0 = x\right]$



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Ordinary differential equation (ODE)



Deterministic Motion

$dX_t = \vec{\omega}(X_t) \, dt$

• trajectory (X_t) • drift direction $(\vec{\omega})$



Ordinary differential equation (ODE)



Deterministic Motion

$dX_t = \vec{\omega}(X_t) \, dt$

• trajectory (X_t) • drift direction $(\vec{\omega})$







$dX_t = dW_t$









$dX_t = dW_t$







BROWNIAN MOTION WITH DRIFT

$dX_t = \vec{\omega}(X_t) \, dt + dW_t$

• trajectory (X_t) • drift direction $(\vec{\omega})$





BROWNIAN MOTION WITH DRIFT

$dX_t = \vec{\omega}(X_t) \, dt + dW_t$

• trajectory (X_t) • drift direction $(\vec{\omega})$





BROWNIAN MOTION WITH VARIABLE SCALE

$dX_t = \sqrt{\alpha(X_t)} \, dW_t$







BROWNIAN MOTION WITH VARIABLE SCALE

$dX_t = \sqrt{\alpha(X_t)} \, dW_t$







BROWNIAN MOTION IN ABSORBING MEDIUM

$dX_t = dW_t$







BROWNIAN MOTION IN ABSORBING MEDIUM

$dX_t = dW_t$





Feynman-Kac formula



$$\frac{\operatorname{random}_{\text{walk}}}{f(X_t) dt + e^{-\int_0^\tau \sigma(X_t)dt} g(X_t)}$$

$$\frac{f(X_t) dt + e^{-\int_0^\tau \sigma(X_t)dt} g(X_t) dt}{\operatorname{boundary}_{\text{values}}}$$

$$\frac{\operatorname{boundary}_{\text{values}}}{\operatorname{boundary}_{\text{values}}}$$

$$\frac{\operatorname{boundary}_{\text{values}}}{\operatorname{boundary}_{\text{values}}}$$

velocity

diffusion rate

















$u(x) = \mathbb{E}[u(W_{\tau})]$







$u(x) = \mathbb{E}[u(W_{\tau})]$







$u(x) = \mathbb{E}[u(W_{\tau})]$

$= \frac{1}{|\partial B(x)|} \int_{\partial B(x)} u(y) \, dy$









$u(x) = \mathbb{E}[u(W_{\tau})]$

$= \frac{1}{|\partial B(x)|} \int_{\partial B(x)} u(y) \, dy$

WoS simulates Brownian motion efficiently!







Feynman-Kac formula



$$\frac{\operatorname{random}_{\text{walk}}}{f(X_t) dt + e^{-\int_0^\tau \sigma(X_t)dt} g(X_t)}$$

$$\frac{f(X_t) dt + e^{-\int_0^\tau \sigma(X_t)dt} g(X_t) dt}{\operatorname{boundary}_{\text{values}}}$$

$$\frac{\operatorname{boundary}_{\text{values}}}{\operatorname{boundary}_{\text{values}}}$$

$$\frac{\operatorname{boundary}_{\text{values}}}{\operatorname{boundary}_{\text{values}}}$$

velocity

diffusion rate









Next: recursive integral equation for variable coefficients

variablecoefficient PDE

constant coefficient recursive PDE







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WoS for PDEs with source terms

E.g., $\Delta u = f(x)$; sample the **spatially-varying source** f inside each ball











Variable coefficient $\nabla \nabla u = \sigma u = -f$



Variable coefficient $\nabla \nabla \cdot (\alpha \nabla u) + \overrightarrow{\omega} \cdot \nabla u - \sigma u = -f$



Girsanov & delta tracking transformations



Variable coefficient

Constant coefficient

(No approximation!)

 $\nabla \cdot (\alpha \nabla u) + \overrightarrow{\omega} \cdot \nabla u - \sigma u = -f$

Girsanov & delta tracking transformations

 $\Delta u - \bar{\sigma} \ u = f(x, \alpha, \overline{\omega}, \sigma, u)$ constant



Variable coefficient

 ∇

Constant coefficient

(No approximation!)

$$\cdot (\alpha \nabla u) + \overrightarrow{\omega} \cdot \nabla u - \sigma \ u = -f$$

Girsanov & delta tracki transformations
$$\Delta u - \overline{\sigma} \ u = f(x, \alpha, \overrightarrow{\omega}, \sigma, u) \leftarrow \text{recu}$$

king ursive



Variable coefficient

Constant coefficient

(No approximation!)

Integral

 $\int_{B(x)} f(y, \alpha, \overrightarrow{\omega}, \sigma,$

 ∇



Transformation 1: Girsanov

Re-express Feynman Kac in terms of Brownian motion $u(x) = \mathbb{E}\left[\int_0^\tau e^{-\int_0^t \sigma(W_s) \, ds} f(W_t) \, dt + e^{-\int_0^\tau \sigma(W_t) \, dt} g(W_\tau)\right]$





Transformation 1: Girsanov

Re-express Feynman Kac in terms of Brownian motion $u(x) = \mathbb{E} \left[\int_{0}^{\tau} e^{-\int_{0}^{t} \sigma(W_{s}) \, ds} f(W_{t}) \, dt + e^{-\int_{0}^{\tau} \sigma(W_{t}) \, dt} g(W_{\tau}) \right]$

 $dX_t = \overrightarrow{\omega}(X_t) dt + \sqrt{\alpha(X_t)} dW_t$





 $dX_t = dW_t$



Volume Rendering Equation (VRE)

VRE describes the radiance in heterogeneous absorbing & scattering media

$$L(w, \vec{\omega}) = \int_0^d e^{-\int_0^t \sigma(x_s) \, ds} f(s)$$

 $(x_t, \overrightarrow{\omega}) dt + e^{-\int_0^d \sigma(x_t) dt} g(x_d, \overrightarrow{\omega})$

 $x_t, \dot{\omega})$



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Structural connection between VRE & Feynman-Kac



$$L(w,\vec{\omega}) = \int_0^d e^{-\int_0^t \sigma(x_s) \, ds} f(x_t,\vec{\omega}) \, dt + e^{-\int_0^d \sigma(x_t) \, dt} g(x_d,\vec{\omega}) \qquad u(x) = \mathbb{E}\left[\int_0^\tau e^{-\int_0^t \sigma(W_s) \, ds} f(W_t) \, dt + e^{-\int_0^\tau \sigma(W_t) \, dt} g(x_d,\vec{\omega})\right]$$

VRE describes the radiance in heterogeneous absorbing & scattering media

Feynman-Kac for 2nd order variable coefficient PDEs





Transformation 2: Delta tracking

Variable coefficient u(x) =

Constant coefficient

u(x)

(No approximation!)

$$\mathbb{E}\left[\int_{0}^{\tau} e^{-\int_{0}^{t} \sigma(W_{s}) ds} f(W_{t}) dt + e^{-\int_{0}^{\tau} \sigma(W_{t}) dt} g(t)\right]$$
$$= \mathbb{E}\left[\int_{0}^{\tau} e^{-\bar{\sigma}t} f(W_{t}, \sigma, u) dt + e^{-\bar{\sigma}\tau} g(W_{\tau})\right]$$





Transformation 2: Delta tracking

Constant coefficient

(No approximation!)

Variable coefficient $u(x) = \mathbb{E} \left[\int_{0}^{\tau} e^{-\int_{0}^{t} \sigma(W_{s}) ds} f(W_{t}) dt + e^{-\int_{0}^{\tau} \sigma(W_{t}) dt} g(W_{\tau}) \right]$ $u(x) = \mathbb{E}\left[\int_{0}^{\tau} e^{-\bar{\sigma}t} f(W_{t}, \sigma, u) dt + e^{-\bar{\sigma}\tau} g(W_{\tau})\right]$




Transformation 2: Delta tracking

Constant coefficient

(No approximation!)

Variable coefficient $u(x) = \mathbb{E} \left[\int_{0}^{\tau} e^{-\int_{0}^{t} \sigma(W_{s}) ds} f(W_{t}) dt + e^{-\int_{0}^{\tau} \sigma(W_{t}) dt} g(W_{\tau}) \right]$ $u(x) = \mathbb{E}\left[\int_{0}^{\tau} e^{-\bar{\sigma}t} f(W_{t}, \sigma, u) dt + e^{-\bar{\sigma}\tau} g(W_{\tau})\right]$ constant





Transformation 2: Delta tracking

(No approximation!)







Delta tracking variant of WoS



WoS delta tracking

delta tracking method in volume rendering [Woodcock et al., 1965, Raab et al. 2008]



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WoS next-flight





WoS next-flight

Next-flight algorithm in volume rendering [Cramer 1978]





WoS next-flight

Fewer distance queries higher correlation compared to delta tracking WoS

Next-flight algorithm in volume rendering [Cramer 1978]





WoS next-flight

Fewer distance queries higher correlation compared to delta tracking WoS Similar variance & run-time characteristics as volume rendering counterparts

Next-flight algorithm in volume rendering [Cramer 1978]



Weight window [Hoogenboom and Légrády 2005]

Uses splitting and Russian roulette to reduce noise





Implementation & Results

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PDE inputs

$\nabla \cdot (\alpha \nabla u) + \vec{\omega} \cdot \nabla u - \sigma u = -f \text{ on } \Omega$

solution





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Acceleration of closest point queries

Accelerate closest point queries using BVH





input mesh w/ F (Thingi10k #996816) 1 hour 2

mesh w/ FASTTETWILD 1 hour 25 minutes







Acceleration of closest point queries

Accelerate closest point queries using BVH





input mesh w/ F (Thingi10k #996816) 1 hour 2

Unlike bad meshes, BVHs do not impact correctness/accuracy of PDE solution!



Interactive editing







No model cleanup, reduction or homogenization!



End-to-end cost of conventional PDE solvers



Finite Element Method (FEM) Pipeline

PDE solution



End-to-end cost of conventional PDE solvers





Conventional PDE solvers can be brittle

Poor mesh quality completely throws off FEM solution





Source: Sharp and Crane, A Laplacian for Nonmanifold Triangle Meshes

FEM solution

Reference solution



The **boundary element method (BEM)** does not require volumetric meshing







BEM does not support problems with source terms or variable coefficients

The **boundary element method (BEM)** does not require volumetric meshing







Meshless FEM solvers also do not require a volume mesh



Meshless FEM solvers also do not require a volume mesh

• Require dense sampling of the domain







Meshless FEM solvers also do not require a volume mesh

• Require dense sampling of the domain

 Require solving large linear systems



(~25k vertices after reordering)

(~25k nodes after reordering)





Meshless FEM is unreliable

 10^{3}









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Meshless FEM is unreliable

vers have unpredictable convergence under refinement Meshless FEM (RBF-FD w. polynomial augmentation)



Tested on 10



dataset







Tested on **10k models** from the Thingi10k dataset

2×10^{-2}

walks n



Stopping tolerance ϵ

Introduces minimal bias and has little impact on performance





Stopping tolerance ϵ

Introduces minimal bias and has little impact on performance







Discretized random walks

Explicit time stepping of diffusion process: $X_{k+1} = X_k + \vec{\omega}(X_k) h + \sqrt{\alpha(X_k)} (W_{k+1} - W_k)$





Discretized random walks

Explicit time stepping of diffusion process: $X_{k+1} = X_k + \vec{\omega}(X_k) h + \sqrt{\alpha(X_k)} (W_{k+1} - W_k)$



Discretized walks can leave the domain, biasing estimates





Discretized random walks

Explicit time stepping of diffusion process: $X_{k+1} = X_k + \vec{\omega}(X_k) h + \sqrt{\alpha(X_k)} (W_{k+1} - W_k)$







Discretized walks can leave the domain, biasing estimates





No spatial aliasing

Monte Carlo decouples boundary conditions/coefficients from geometry





No spatial aliasing

Monte Carlo decouples boundary conditions/coefficients from geometry





No spatial aliasing

Monte Carlo decouples boundary conditions/coefficients from geometry





Physical analysis of complex geometry & materials

No homogenization of PDE coefficients!







Example application: variable coefficient diffusion curves

Additional control over sharp details







Example application: diffusion curves on surfaces

Use variable coeffs on flat domains to model constant coeffs on curved domains






Example application: subsurface scattering

Easy to mix volumetric path tracing (VPT) and walk on spheres (WoS)



Hybrid strategy : VPT near boundary, WoS deeper inside volume



Limitations & Future Work



High variance due to large spatial variation

diffusion coefficient

delta tracking (250 walks/point)









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High variance due to large spatial variation

diffusion



Future: local coefficient bounds, low-variance VRE estimators, adaptive weight window





Future: support for important features

Neumann & Robin boundary conditions

Anisotropic diffusion coefficients

Non-linear PDEs

High performance distance queries

Differentiable implementation



The promise of grid-free Monte Carlo



ISCRETIZATION-FREE	
	eliminate major bottleneck
	accelerate design cycle
	improve reliability/robustness
	avoid approximation error
al)	focus computation only where it's needed

. . .







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The symbols * and † indicate equal contribution.





I don't know...

