

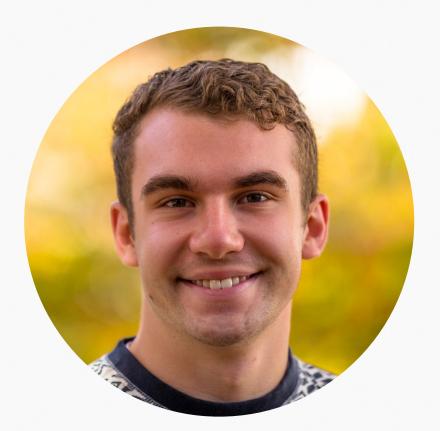
WALKIN' ROBIN: WALK ON STARS WITH ROBIN BOUNDARY CONDITIONS

BAILEY MILLER*, ROHAN SAWHNEY*, KEENAN CRANE[†], IOANNIS GKIOULEKAS[†]

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THE PREMIER CONFERENCE & EXHIBITION ON COMPUTER GRAPHICS & INTERACTIVE TECHNIQUES

team



Bailey Miller CMU PhD



Rohan Sawhney High Fidelity Physics @ Nvidia



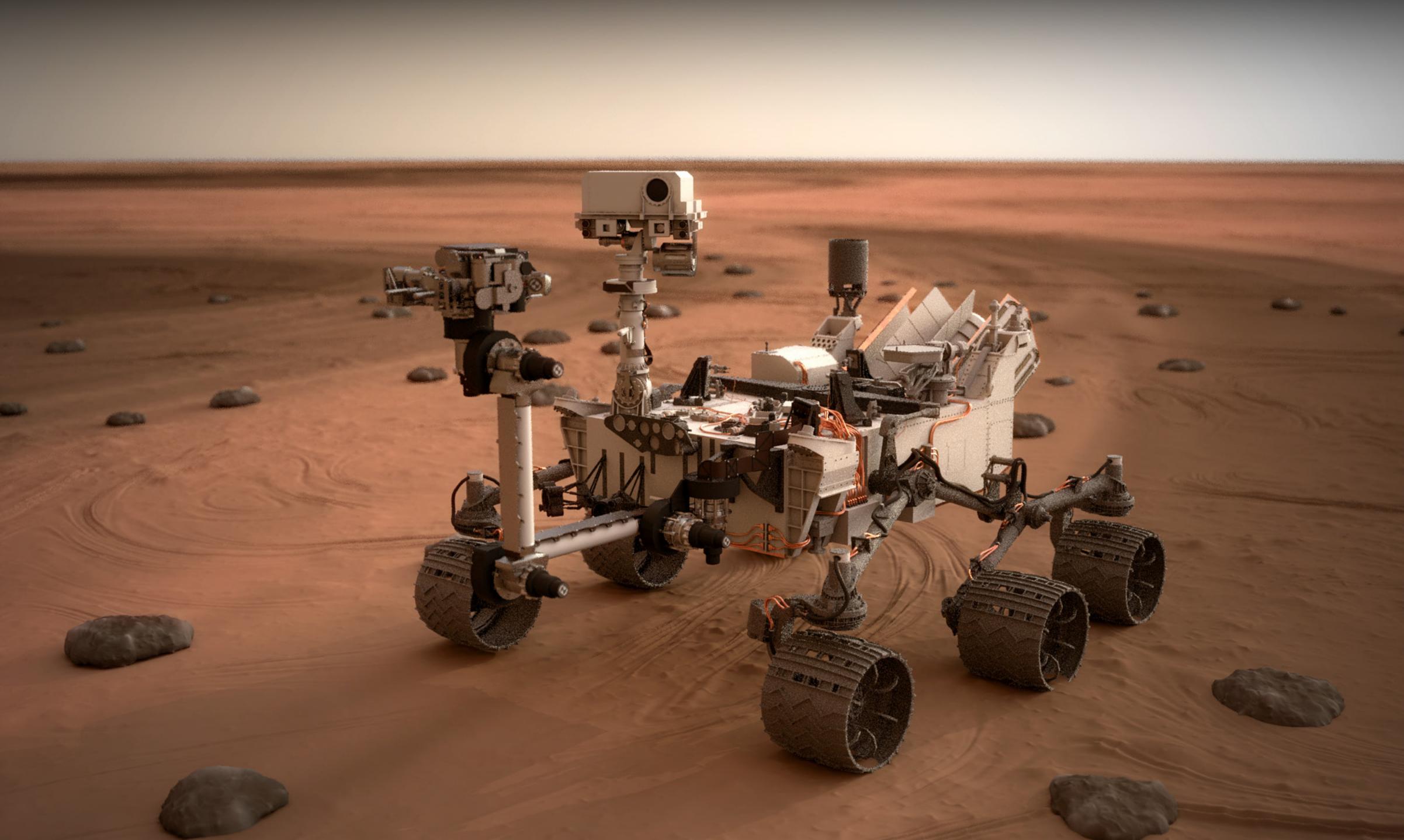






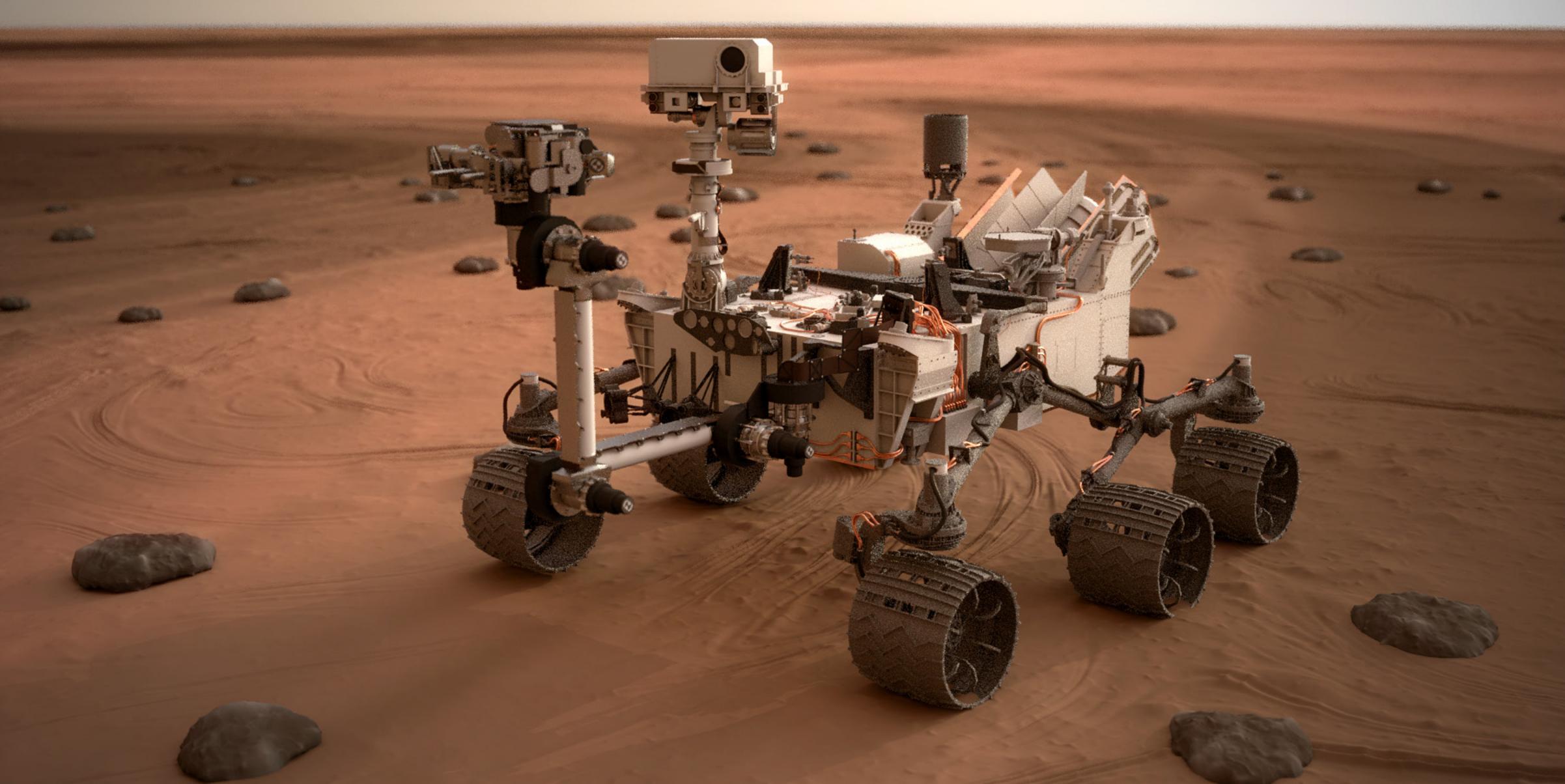
Ioannis Gkioulekas CMU





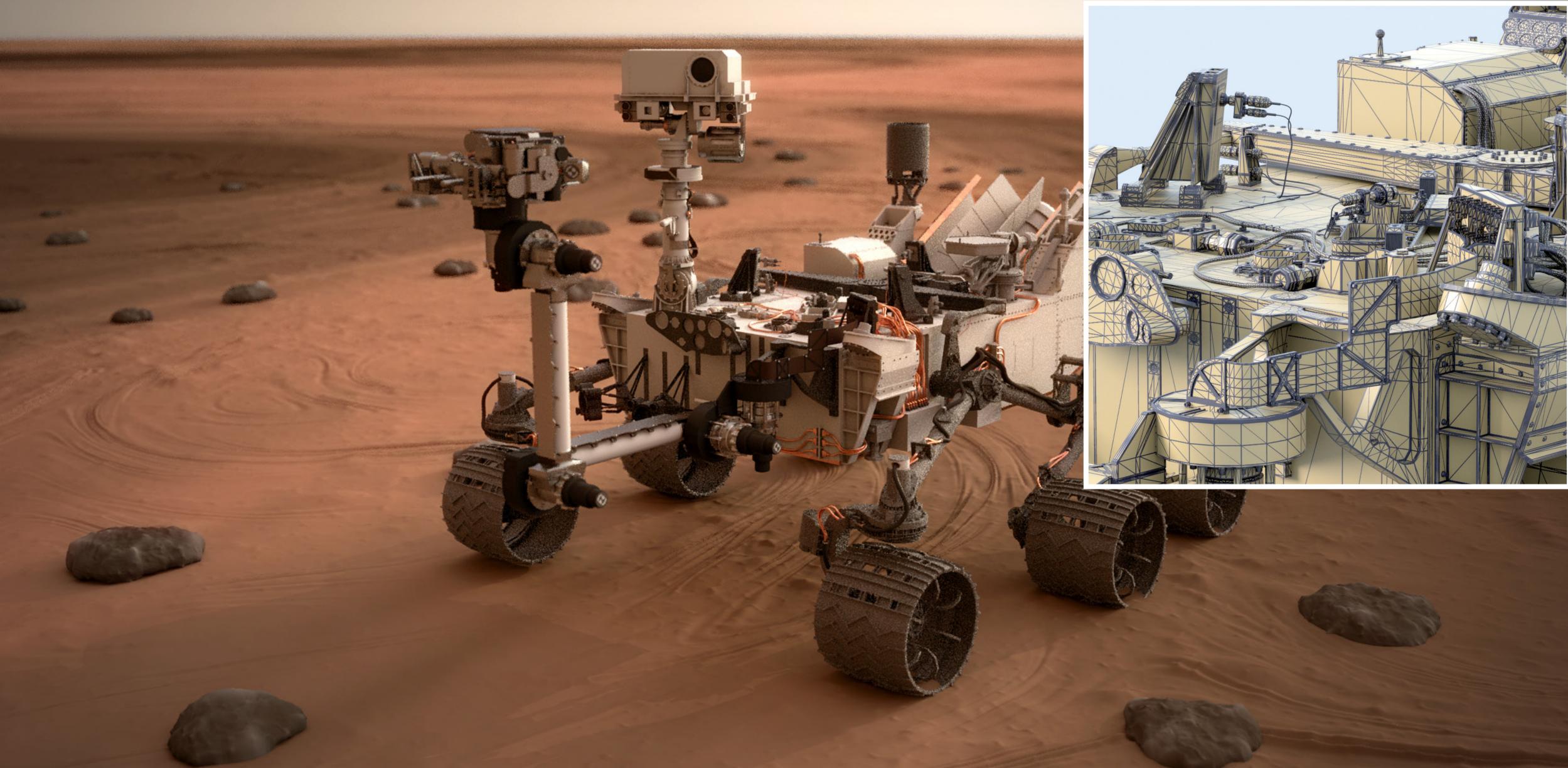


NASA's Curiosity Mars Rover



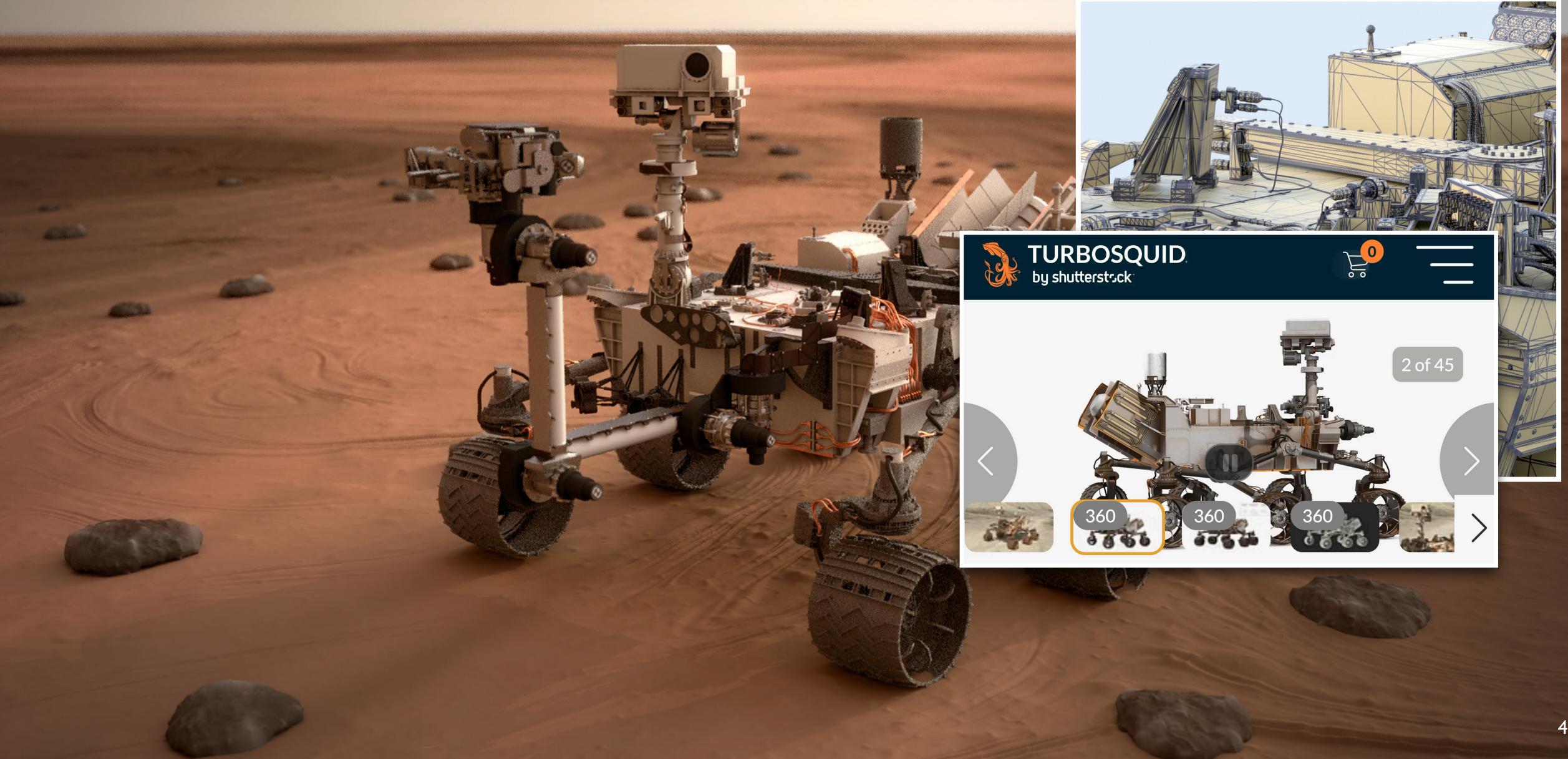


a rendering of NASA's Curiosity Mars Rover



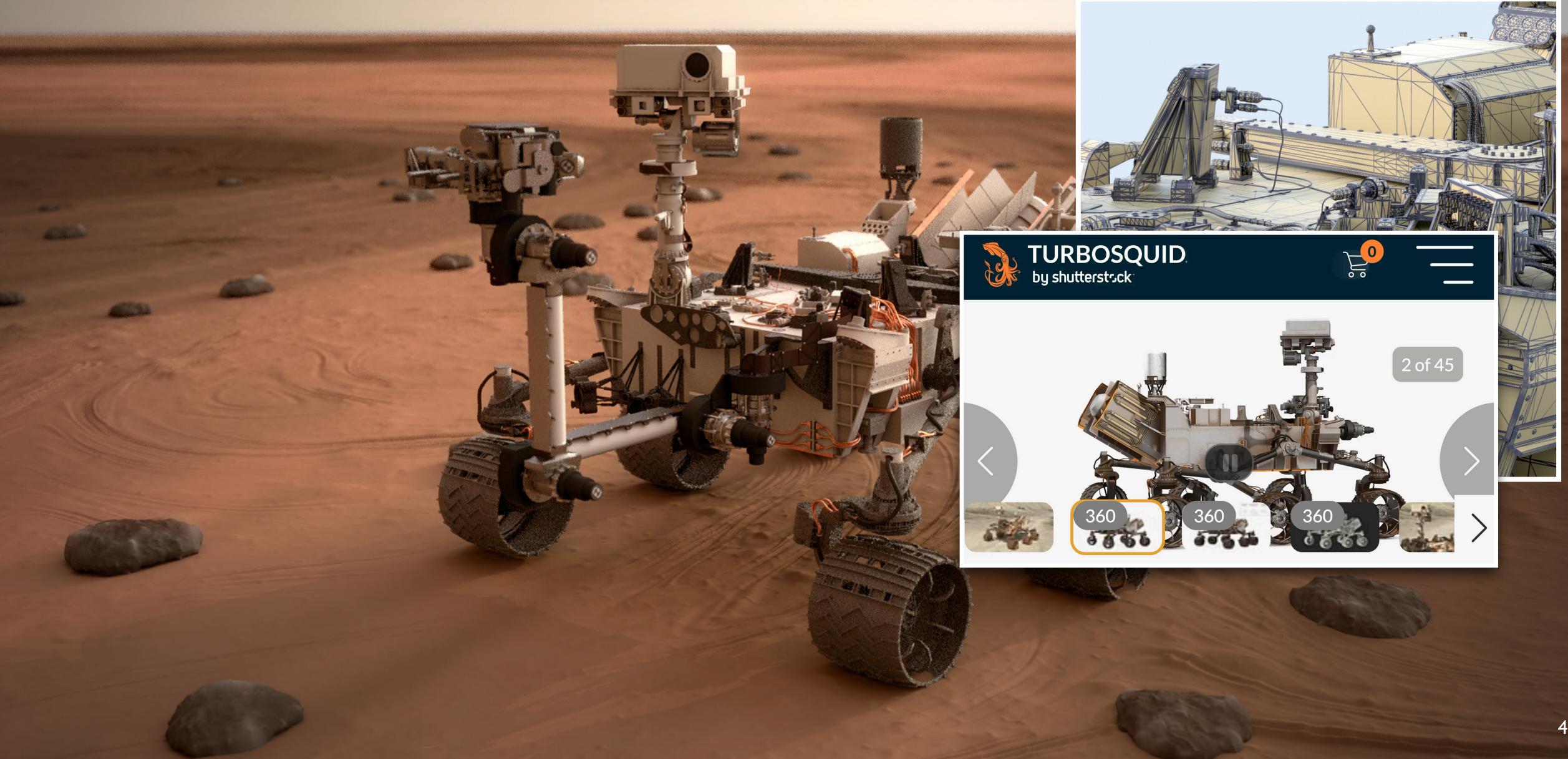








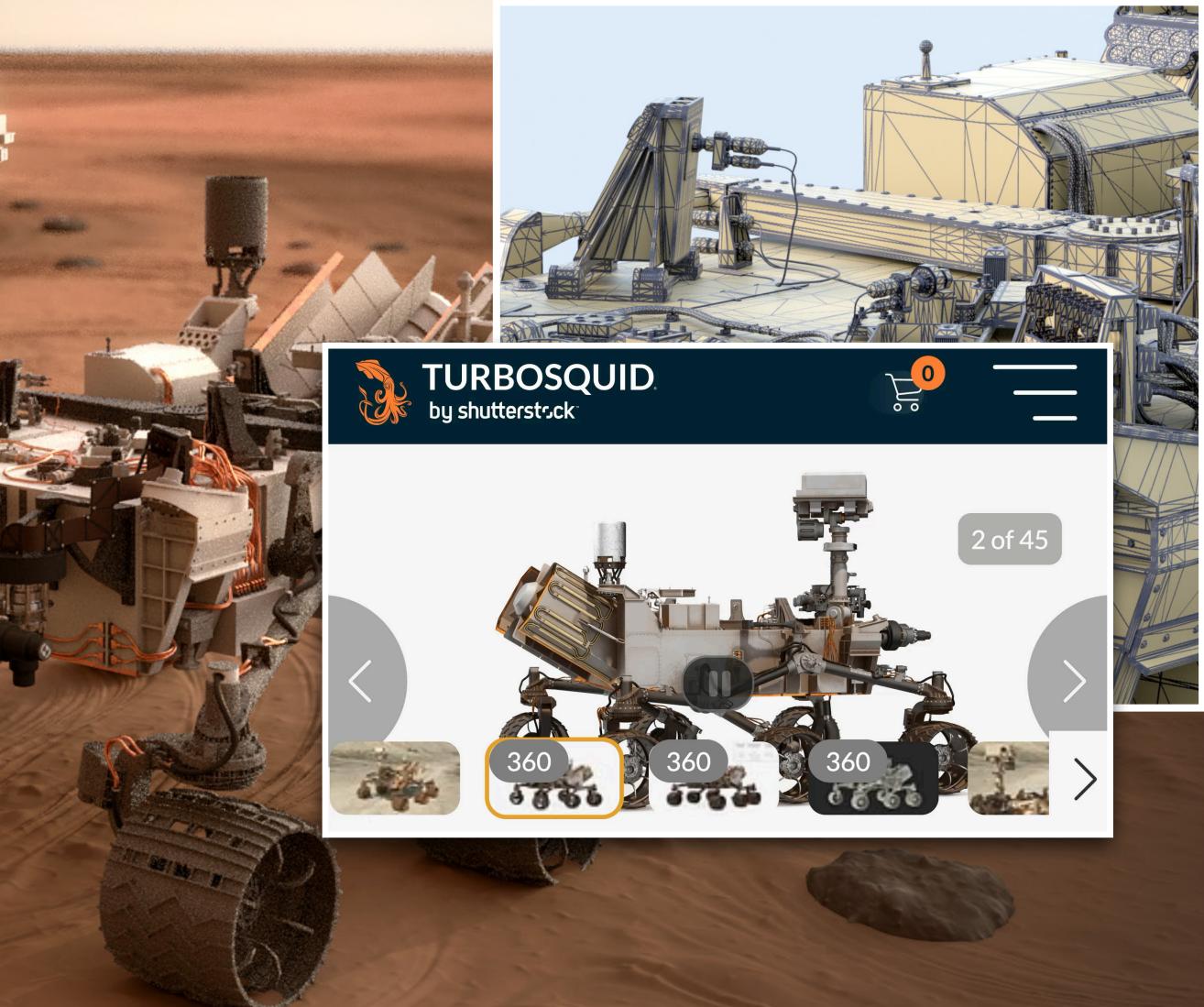








Rendering "just works," and gives immediate feedback, no matter what you throw at it.









Rendering "just works," and gives immediate feedback, no matter what you throw at it.

But what if we need to predict something beyond <u>appearance</u>?

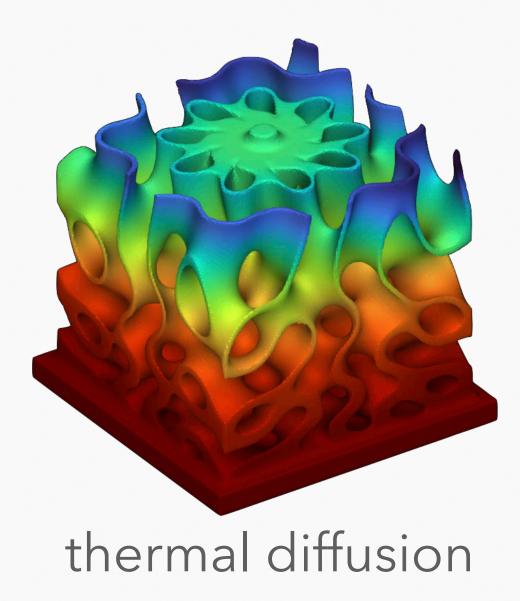


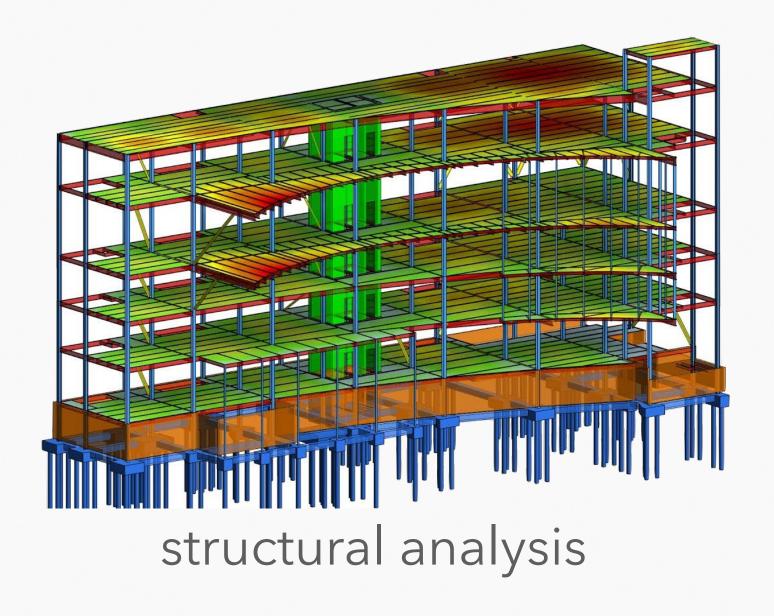






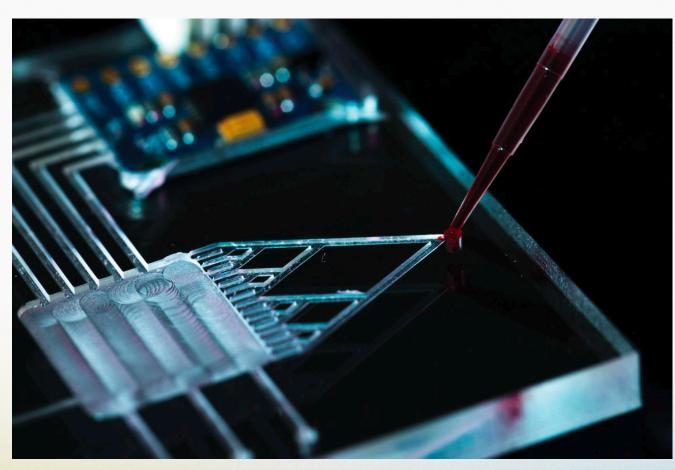
physics beyond light transport







acoustic modeling

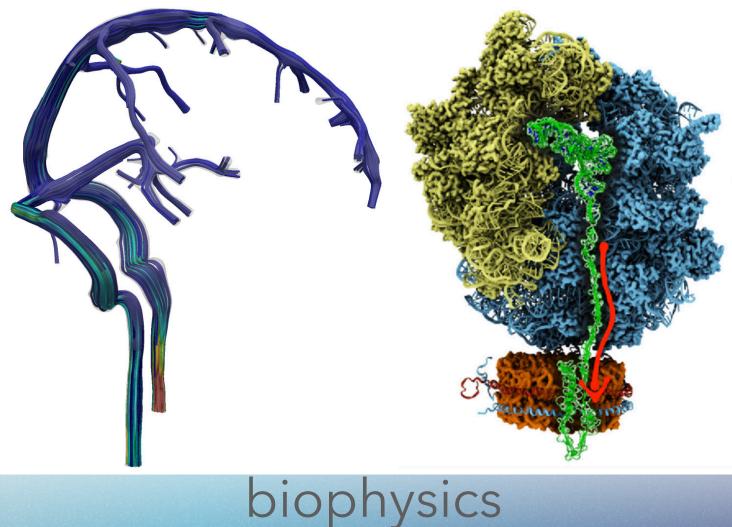






electrostatics

microfluidics





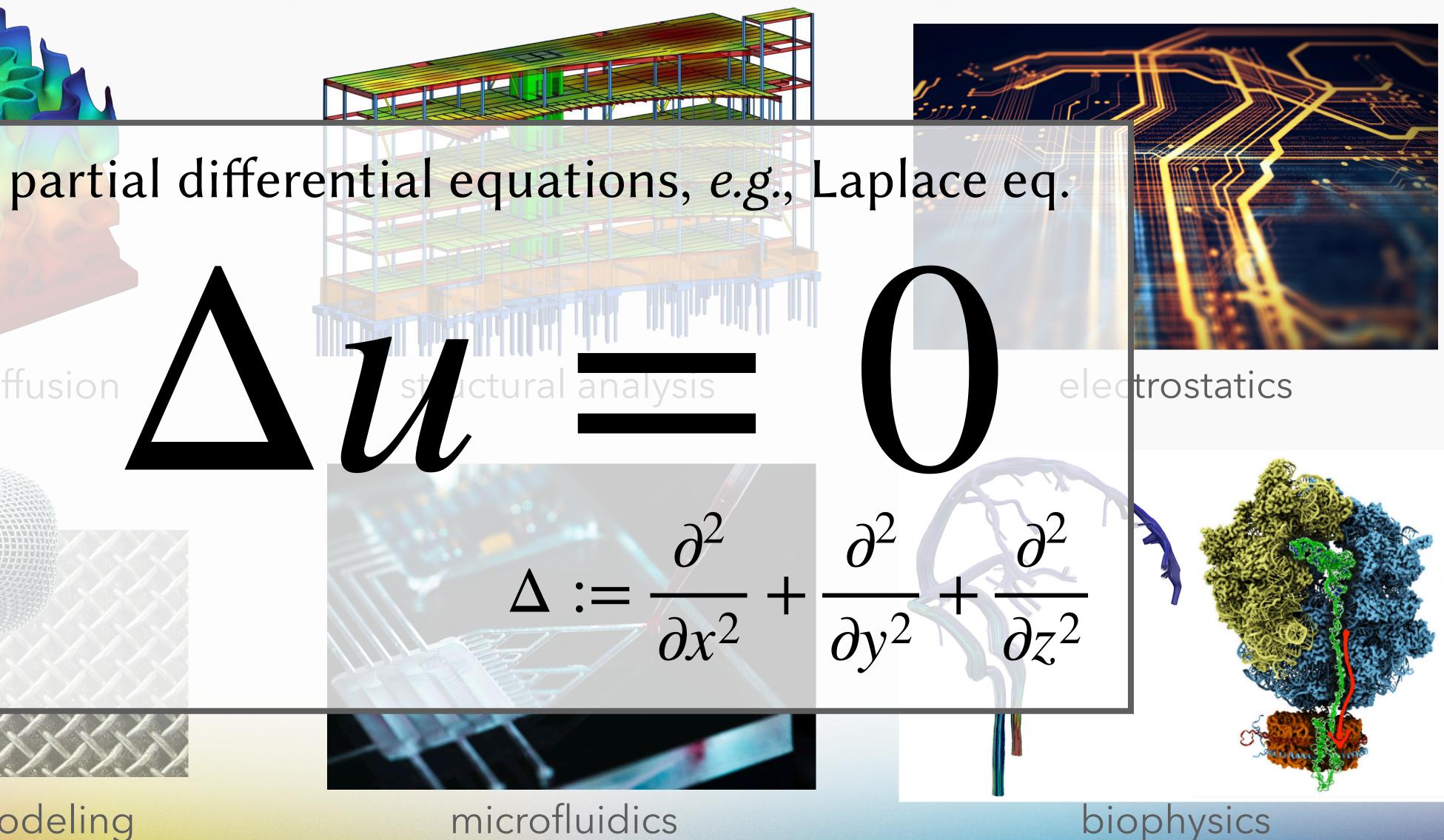


physics beyond light transport

thermal diffusion

acoustic modeling





microfluidics





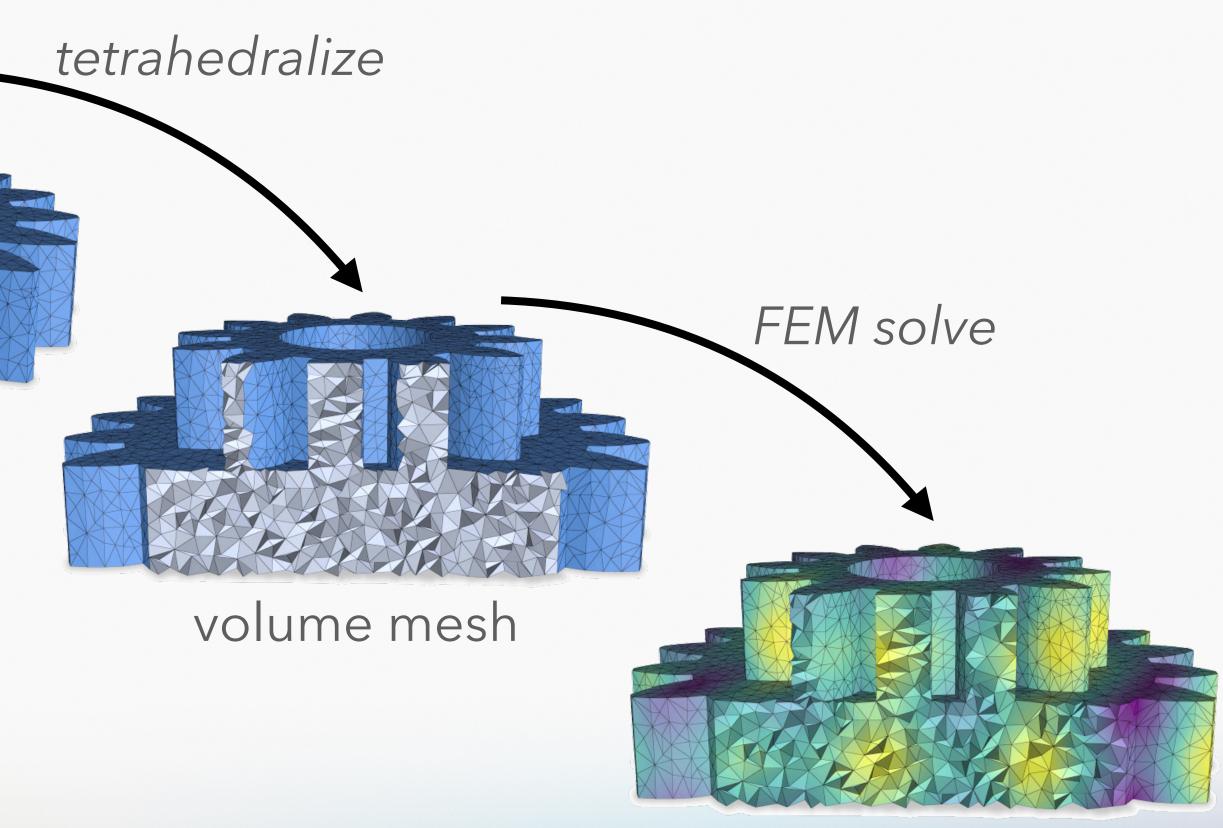
finite element method (FEM) pipeline

input boundary representation

high-quality surface mesh







PDE solution





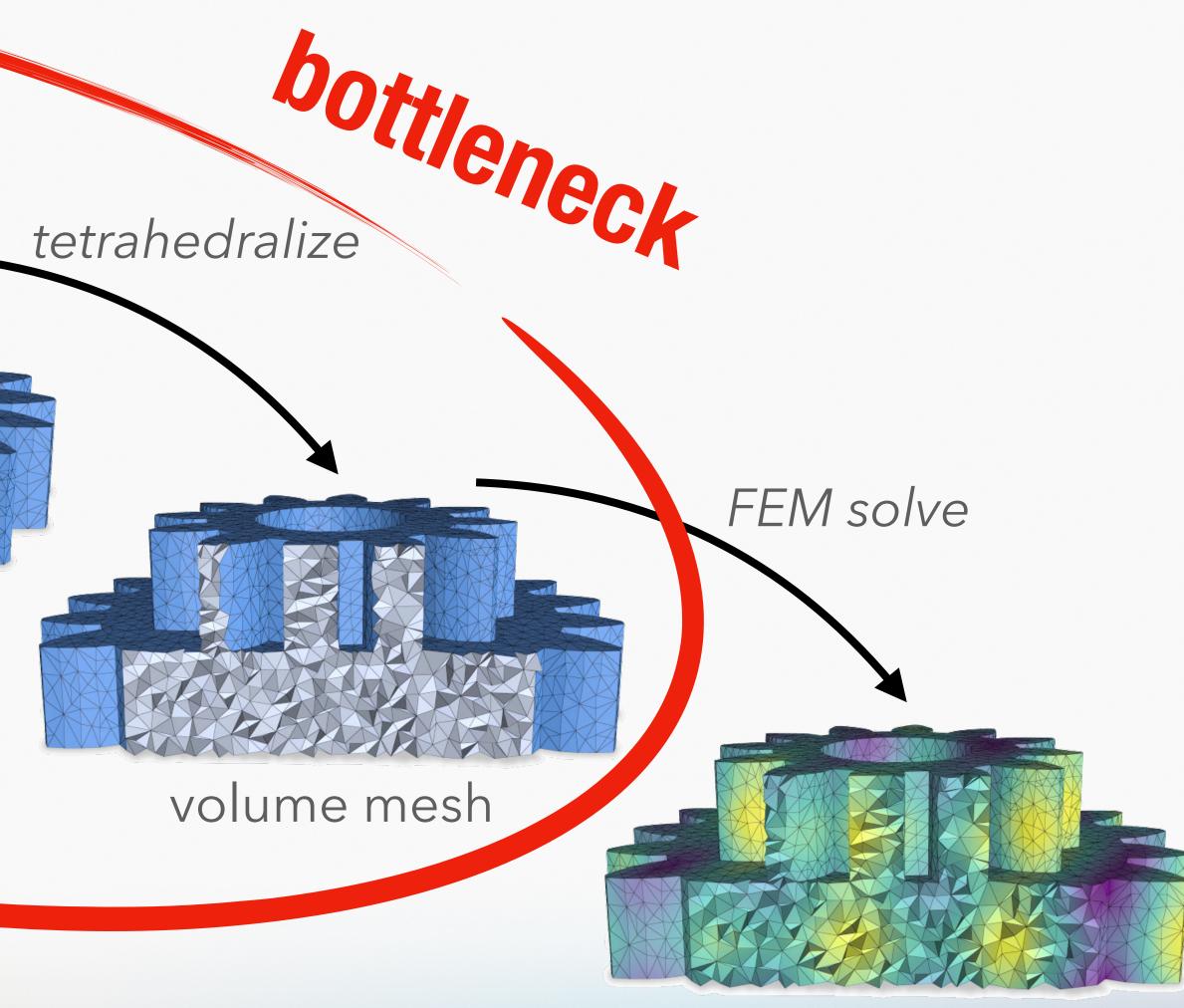
finite element method (FEM) pipeline

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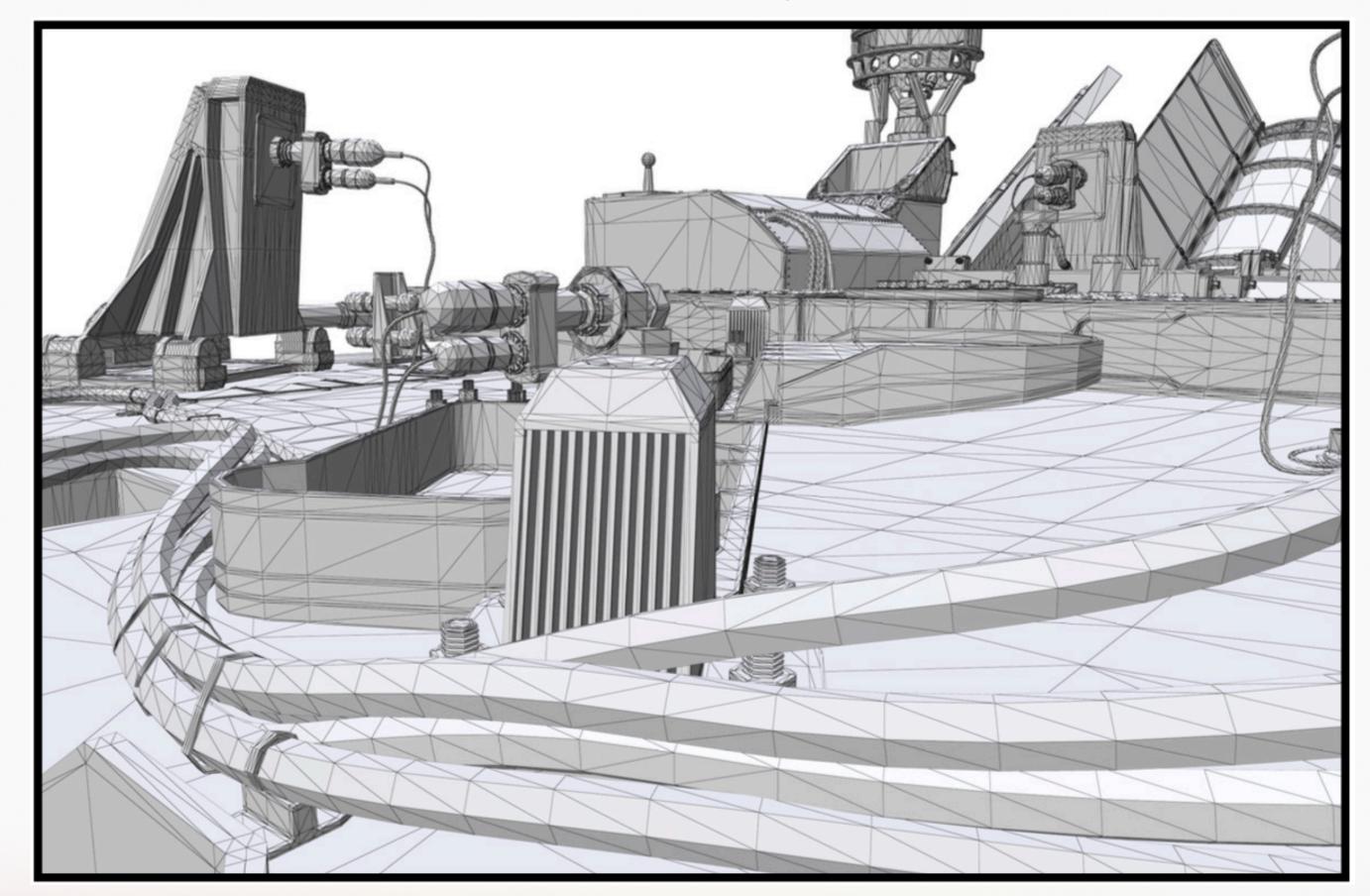
PDE solution





meshing complex geometry is difficult + slow

input boundary mesh



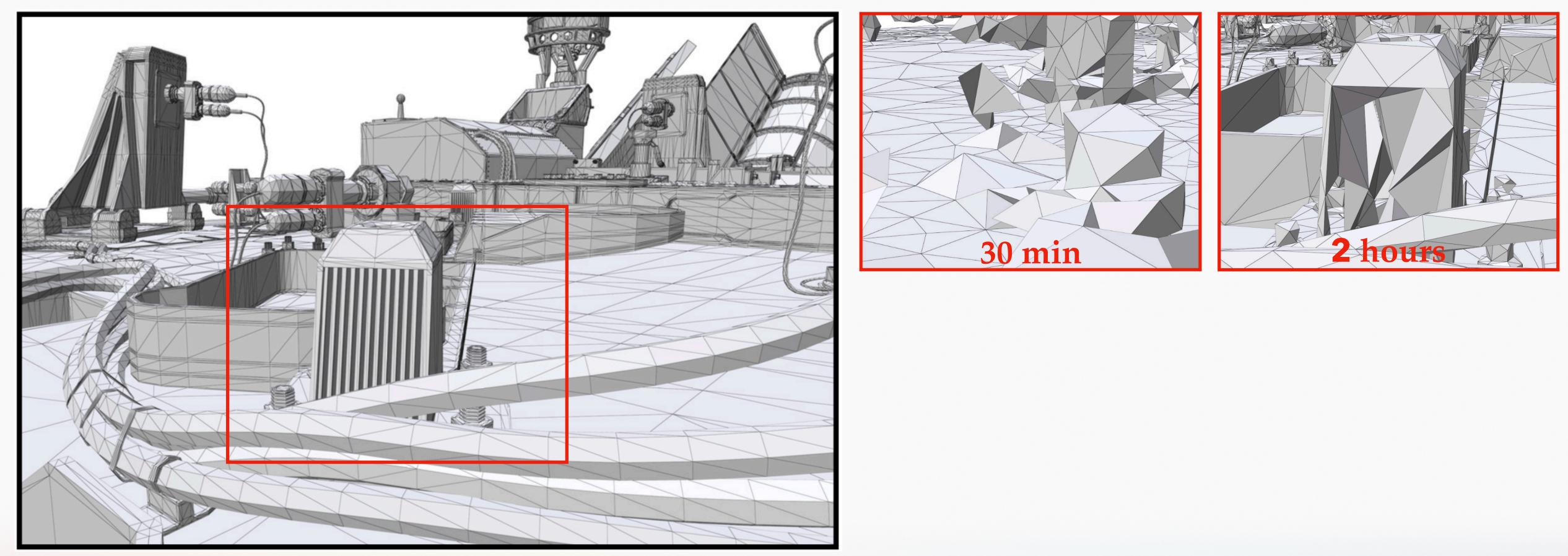




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meshing complex geometry is difficult + slow

input boundary mesh





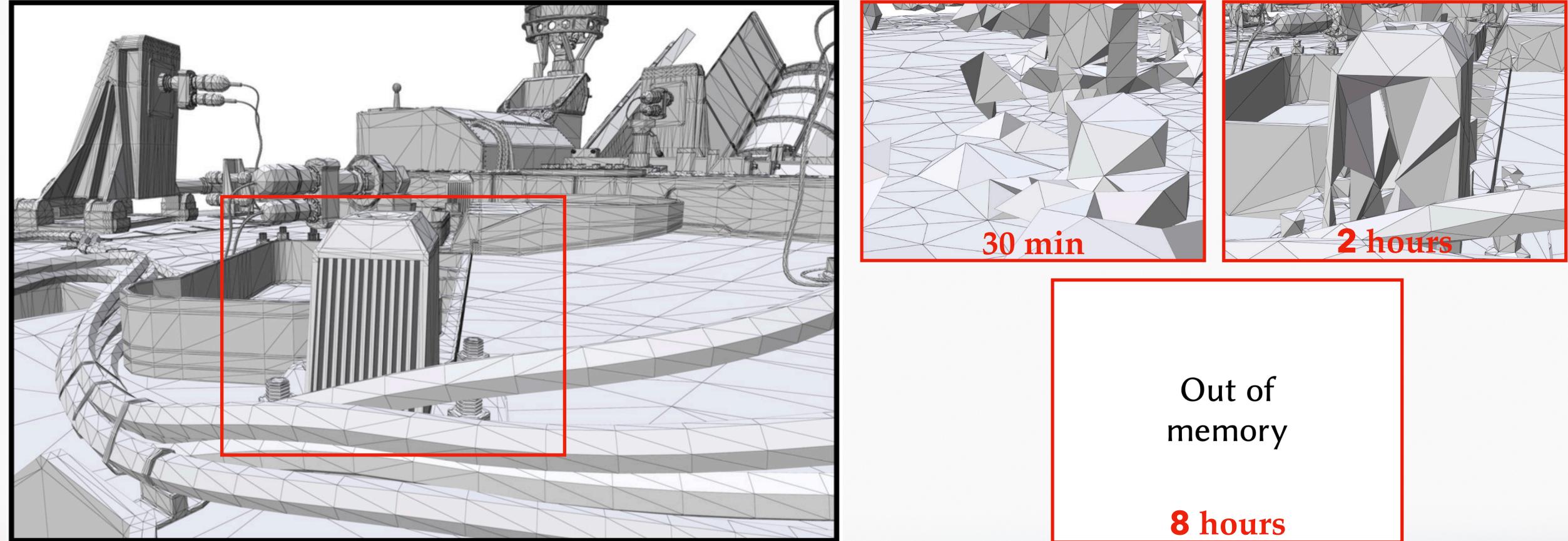
boundary of tetrahedral mesh





meshing complex geometry is difficult + slow

input boundary mesh





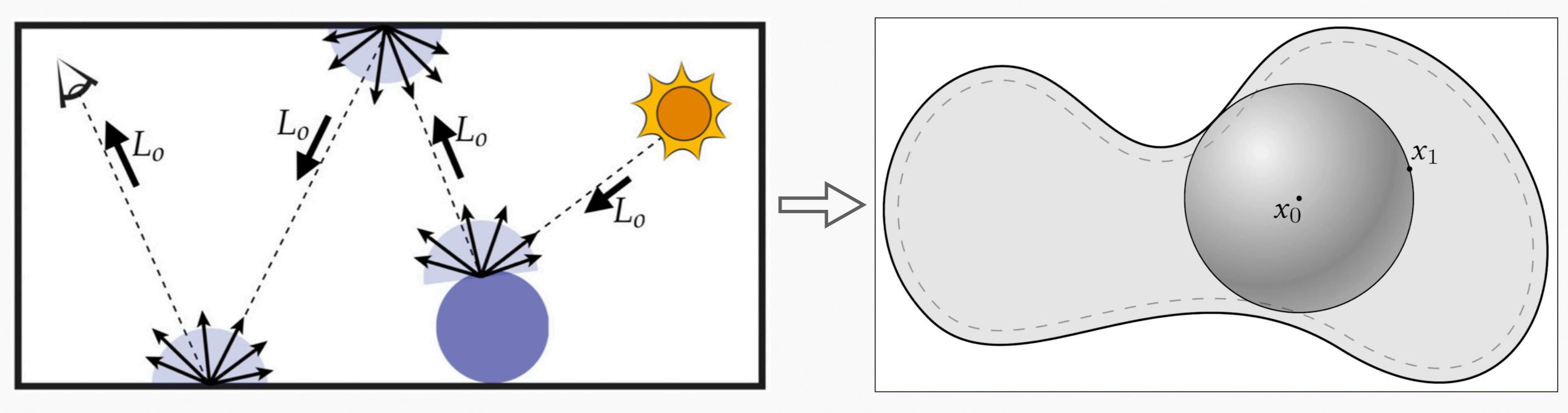
boundary of tetrahedral mesh





grid-free PDE solvers

recursive random walks for solving the Laplace equation $\Delta u = 0$



ray tracing



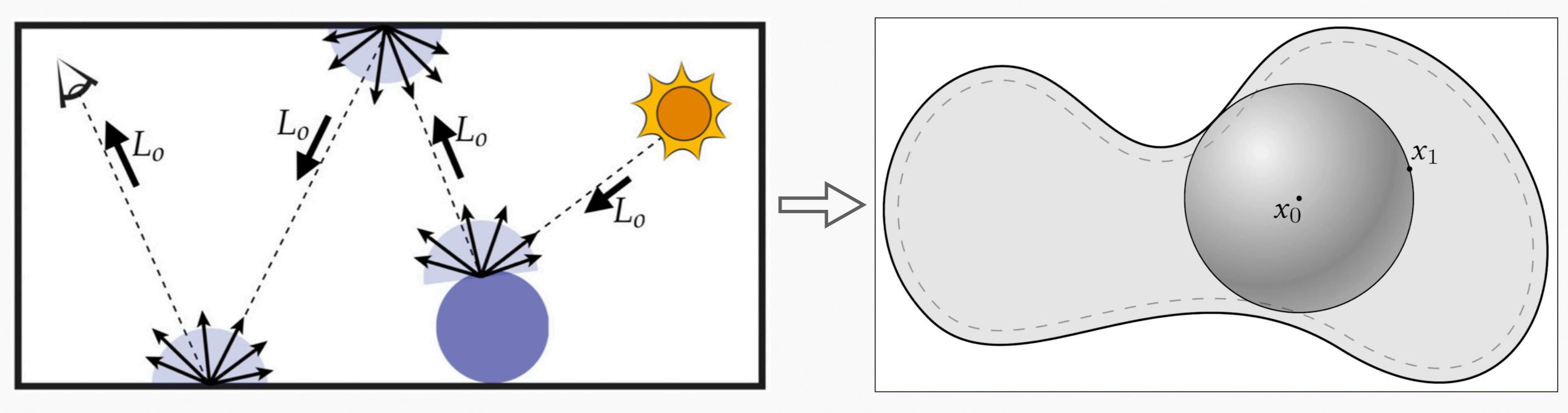
walk on spheres [Muller 1956, Sawhney and Crane 2020]



8

grid-free PDE solvers

recursive random walks for solving the Laplace equation $\Delta u = 0$



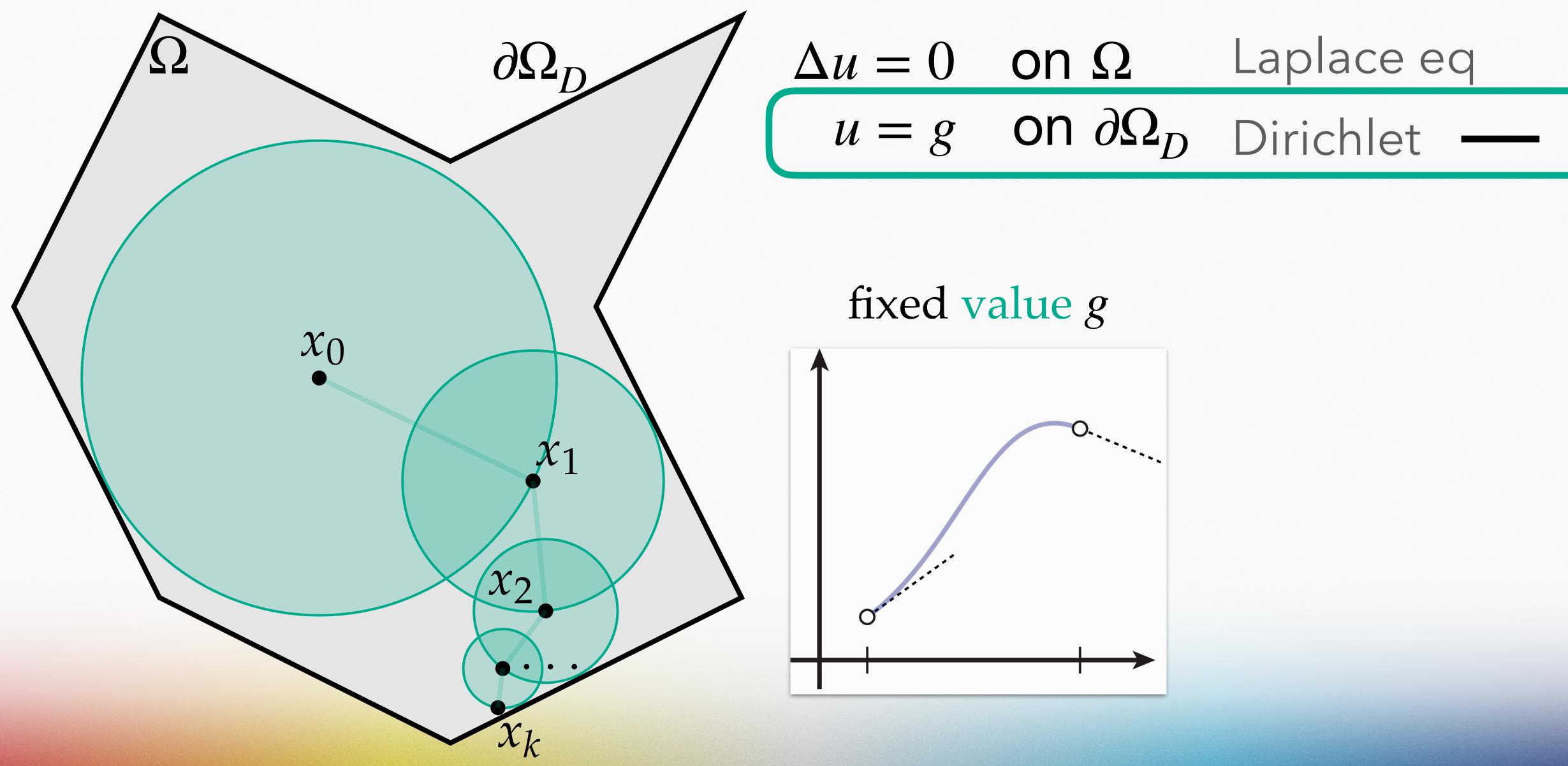
ray tracing



walk on spheres [Muller 1956, Sawhney and Crane 2020]



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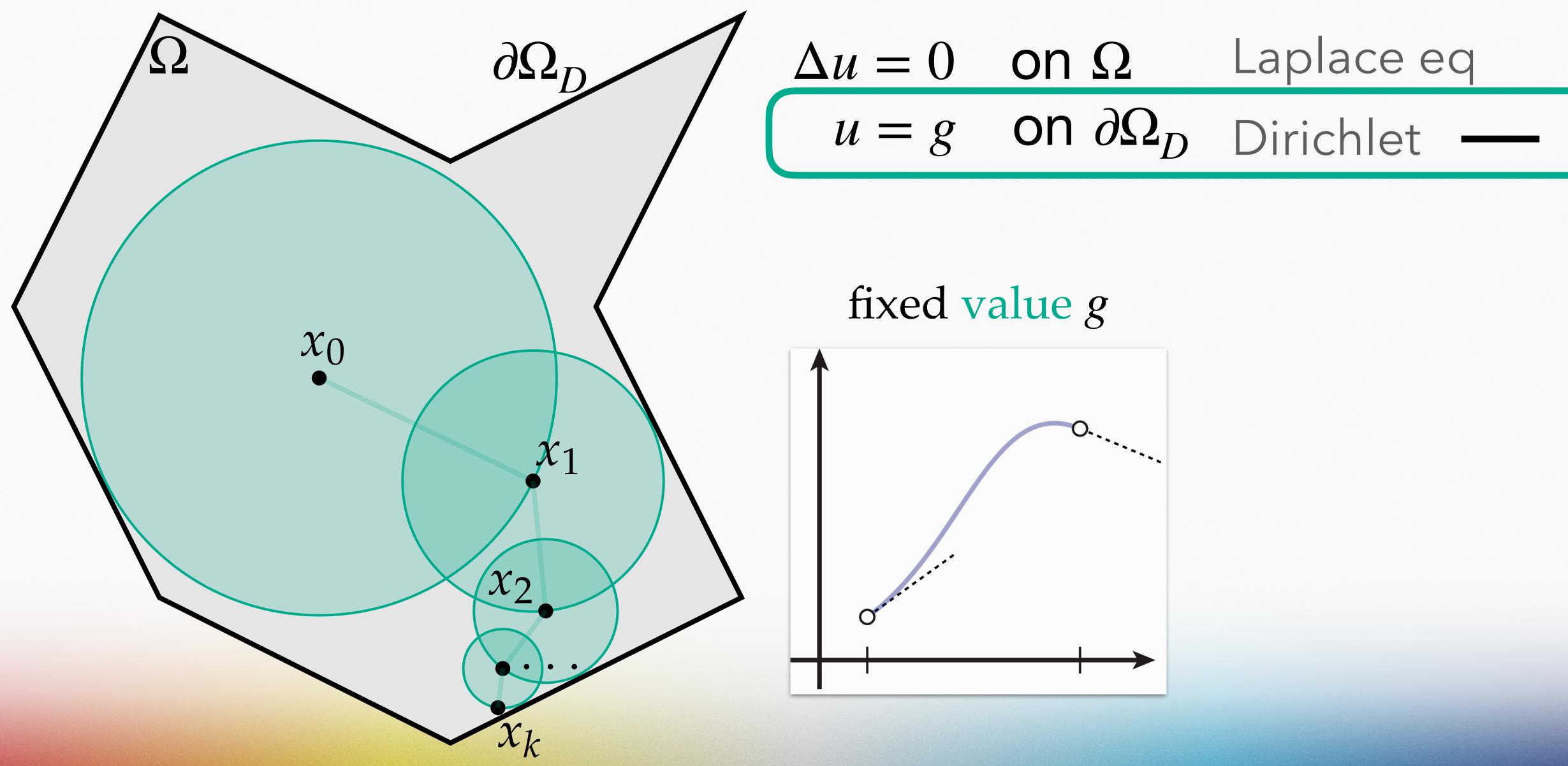












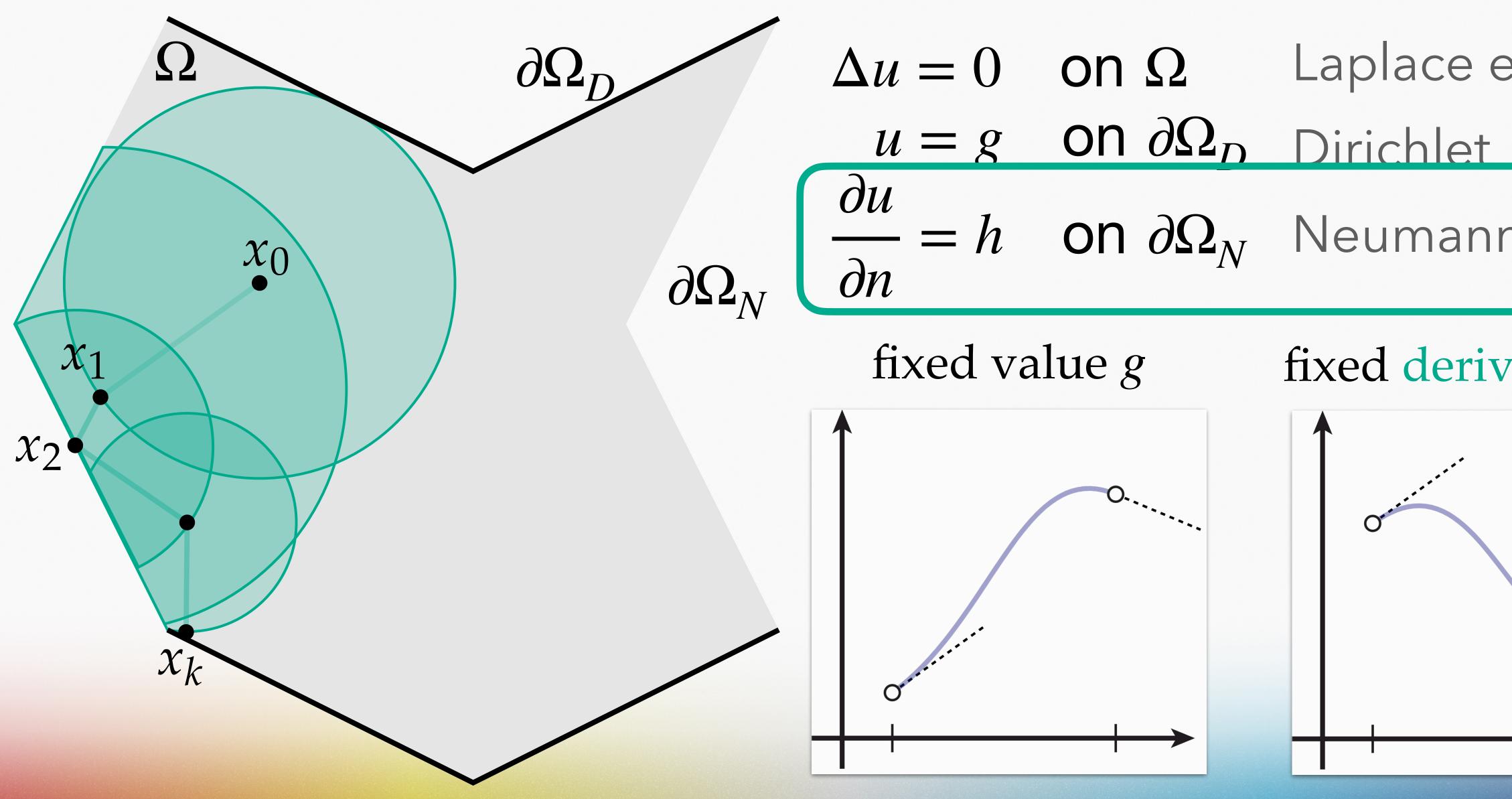








walk on stars [Sawhney et al. 2023]



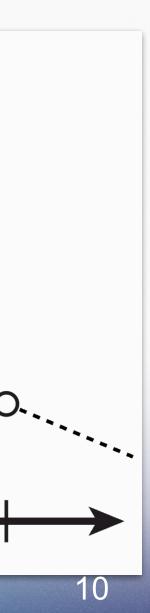




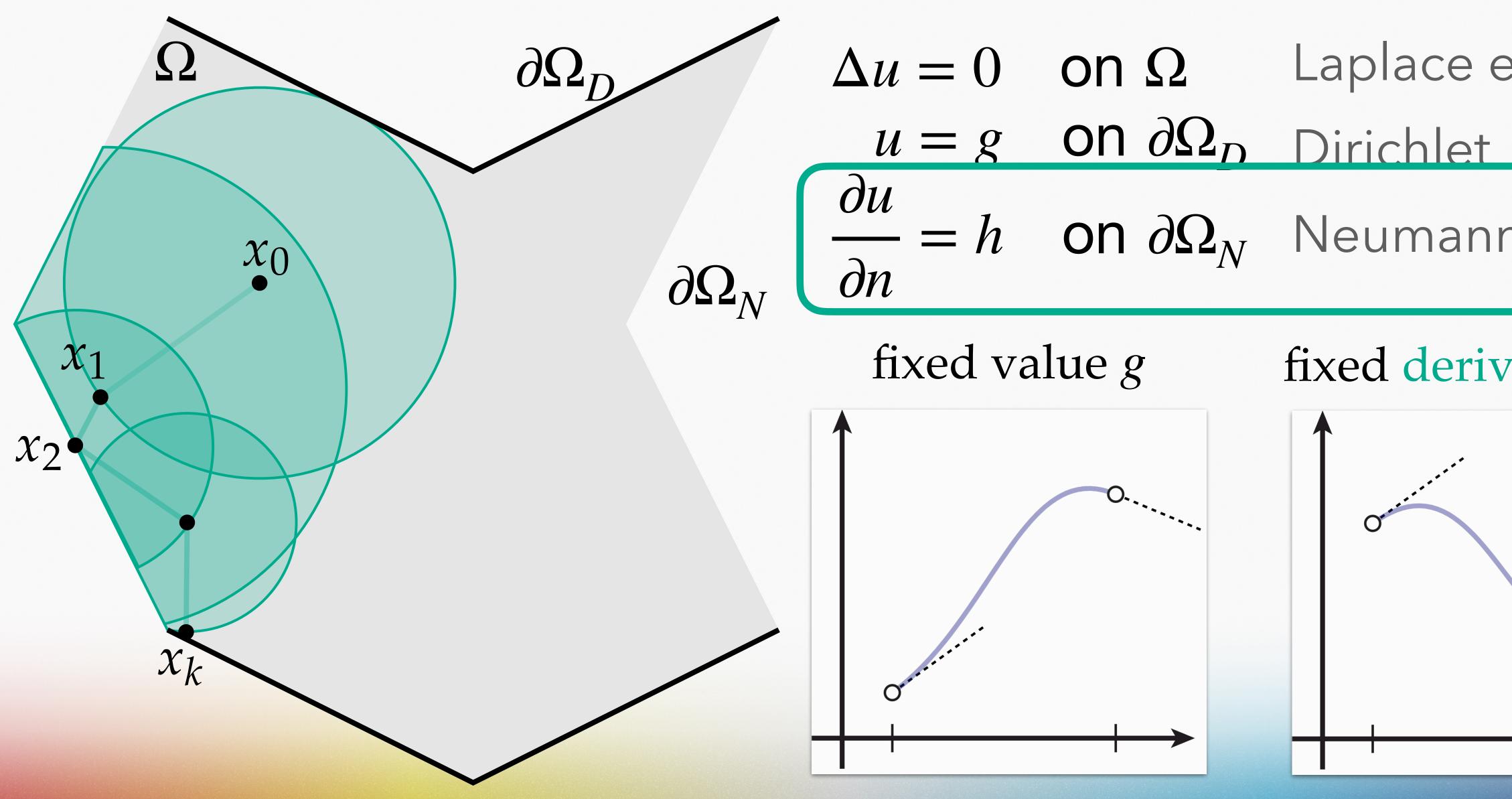
$\Delta u = 0 \quad \text{on } \Omega \quad \text{Laplace eq}$ $u = g \quad \text{on } \partial \Omega_D \quad \text{Dirichlet} \quad -- \frac{\partial u}{\partial n} = h \quad \text{on } \partial \Omega_N \quad \text{Neumann} = \mathbf{n}$







walk on stars [Sawhney et al. 2023]



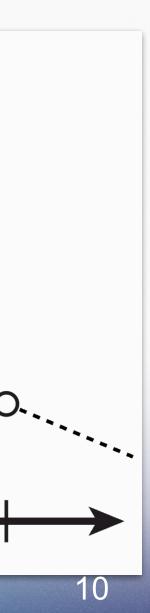




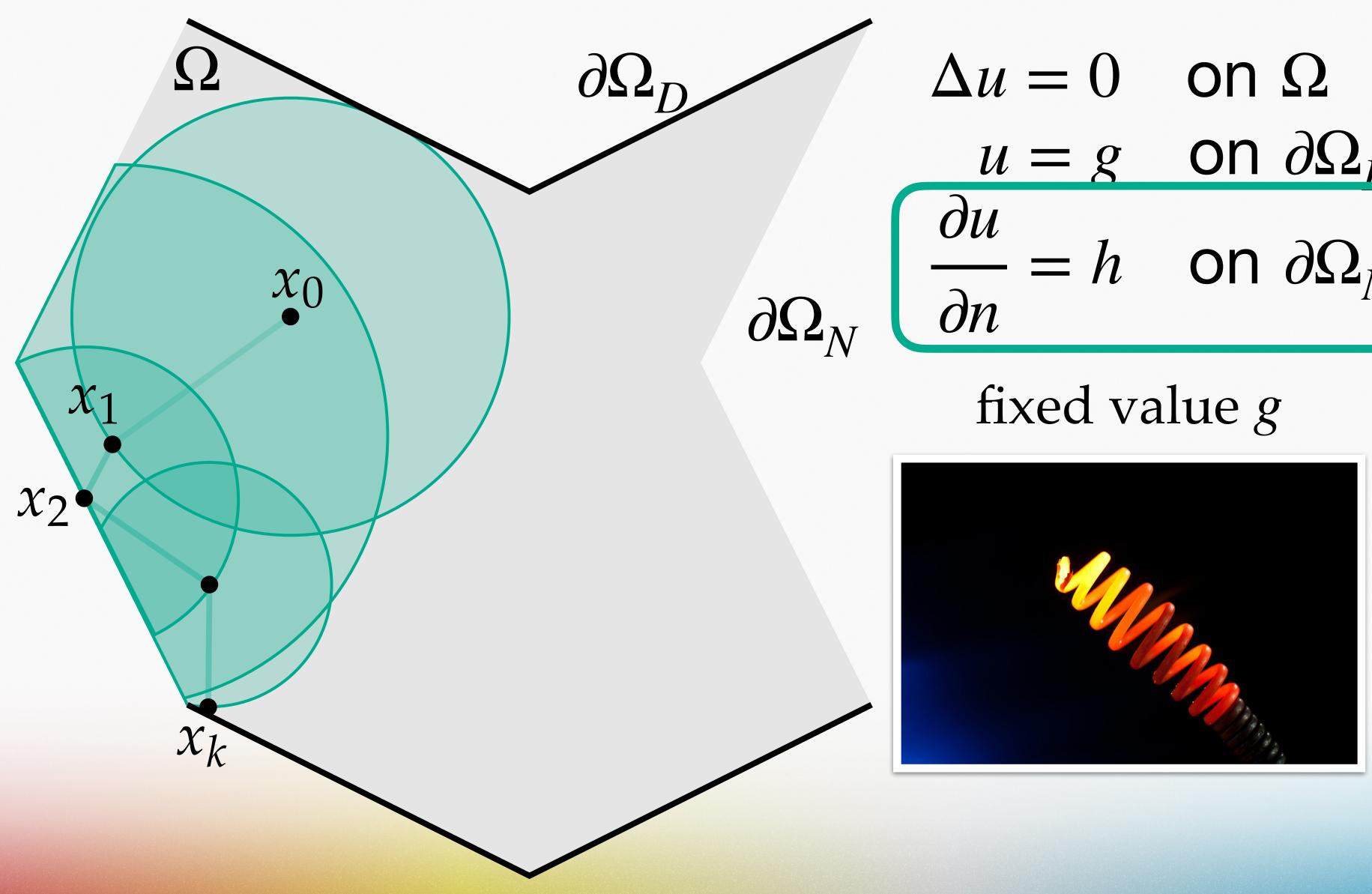
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walk on stars [Sawhney et al. 2023]







$\Delta u = 0$ on Ω Laplace eq u = g on $\partial \Omega_D$ Dirichlet — $\frac{\partial u}{\partial n} = h \quad \text{on } \partial \Omega_N \quad \text{Neumann} = \mathbf{n}$

fixed derivative h







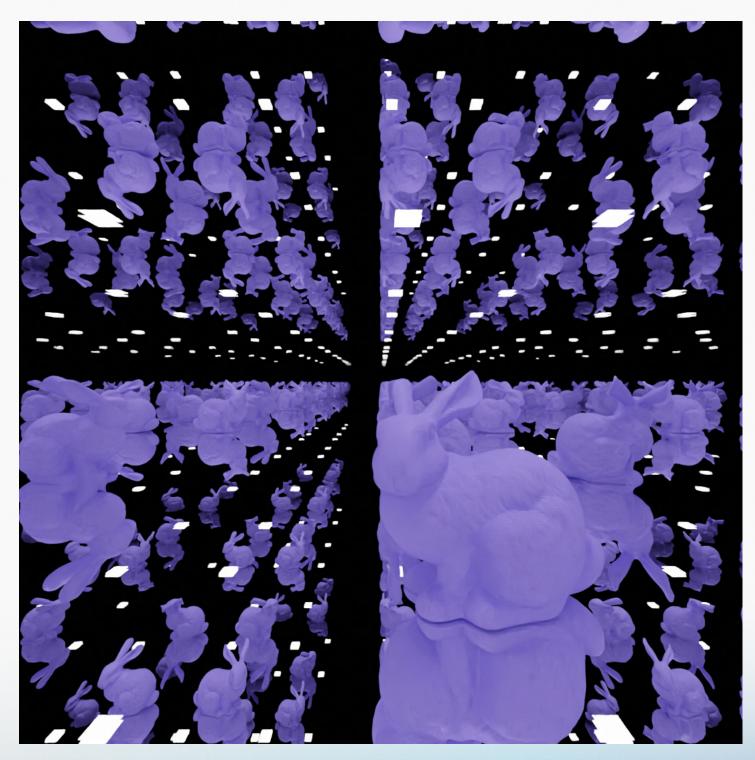


importance of materials in rendering

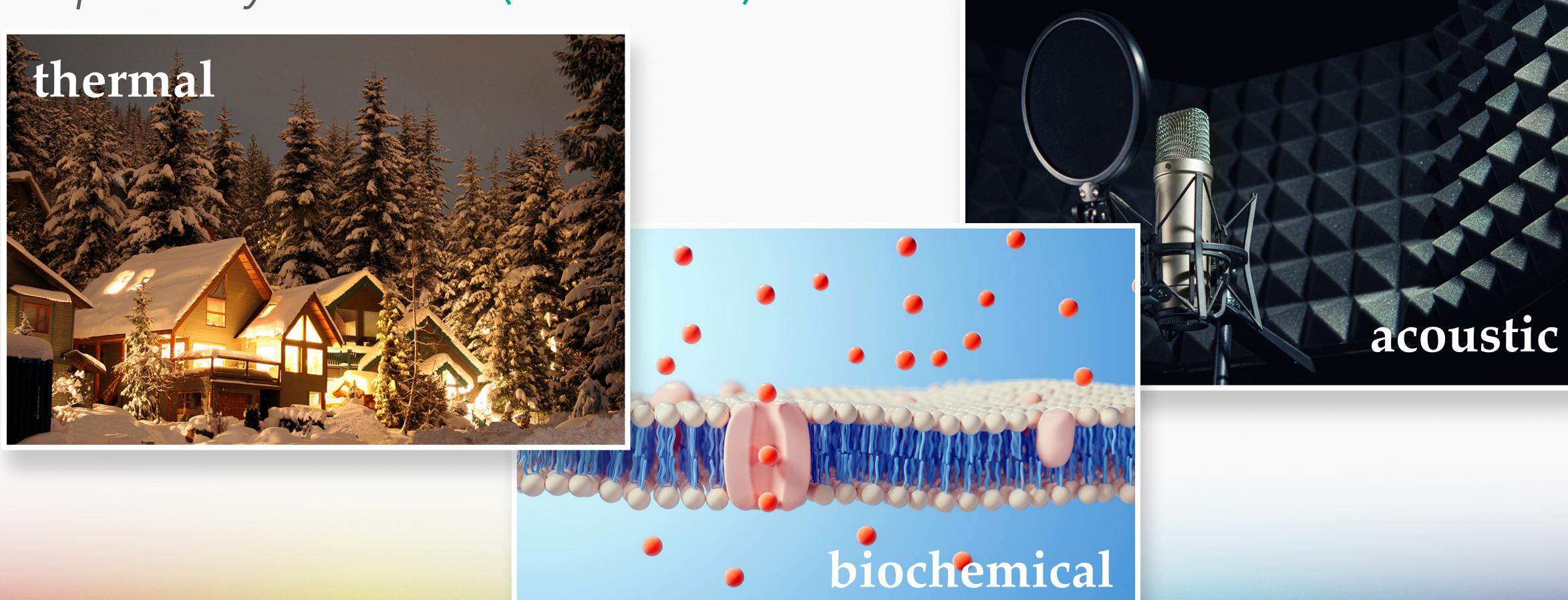
why are idealized materials not enough? "Robin" "Neumann" *partially* reflective walls perfectly reflective walls







real physical materials neither *perfectly* absorptive (Dirichlet) nor perfectly reflective (Neumann)





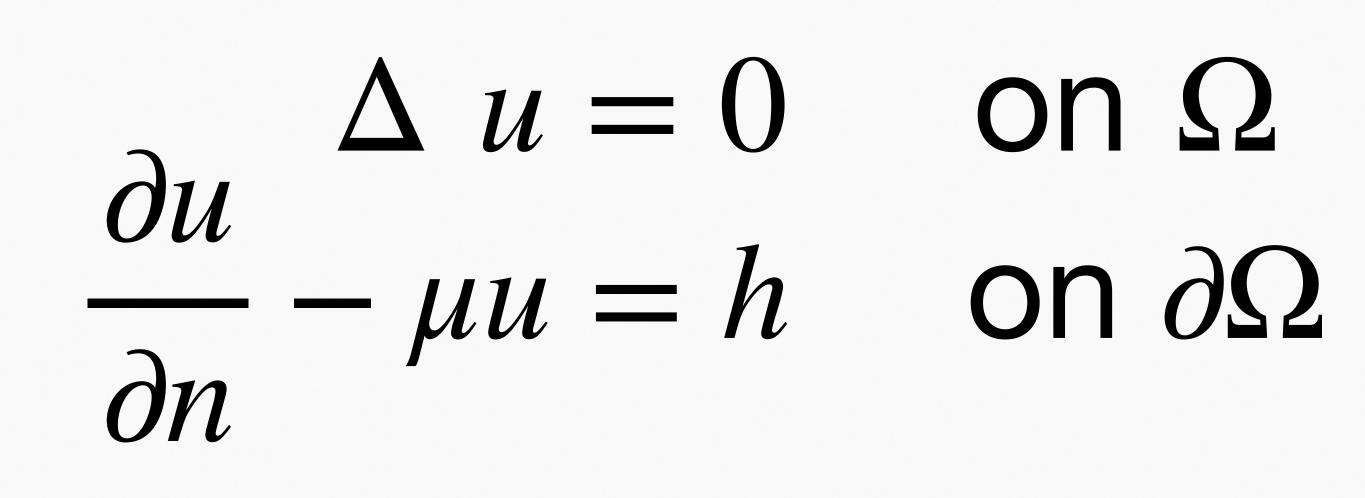








- real physical materials neither *perfectly absorbing* (Dirichlet) nor perfectly reflecting (Neumann)
- more realistic behavior modeled by Robin boundary conditions



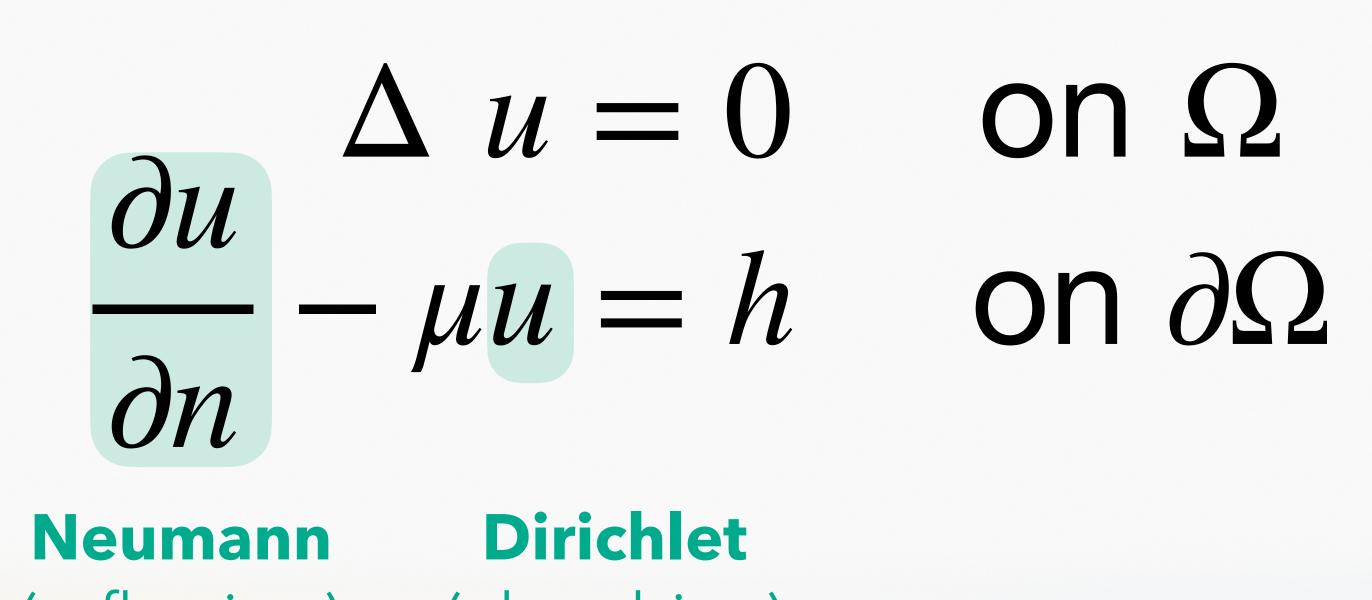








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- more realistic behavior modeled by Robin boundary conditions



(reflective) (absorbing)

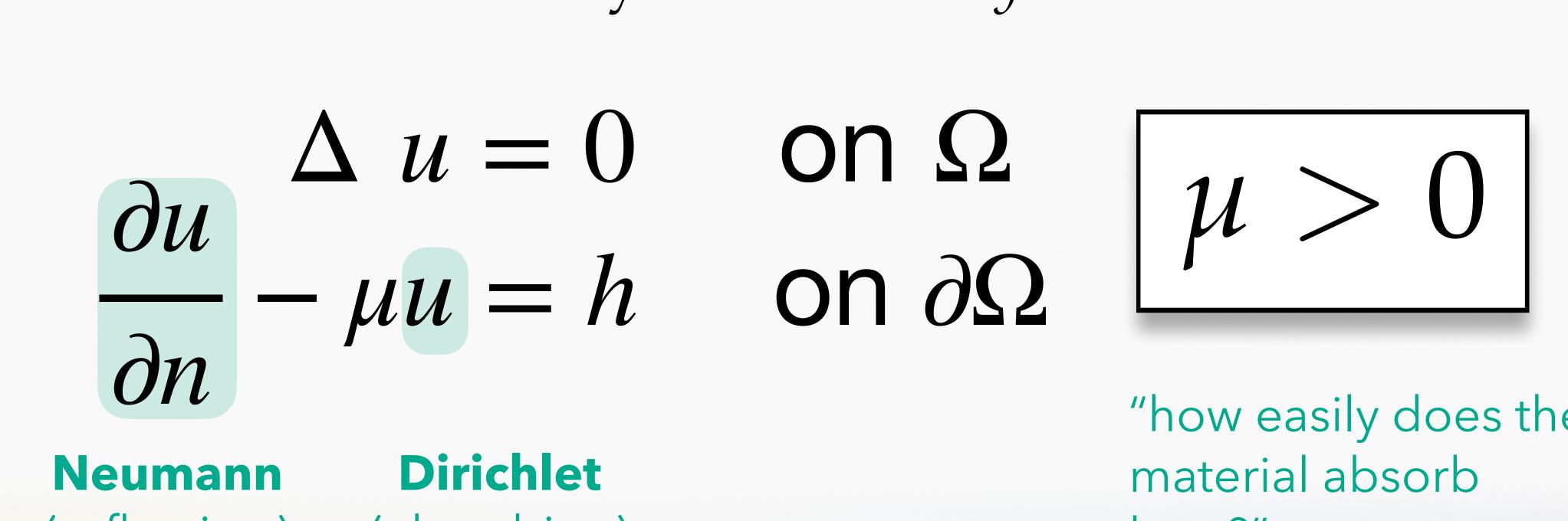








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- more realistic behavior modeled by Robin boundary conditions



(reflective) (absorbing)



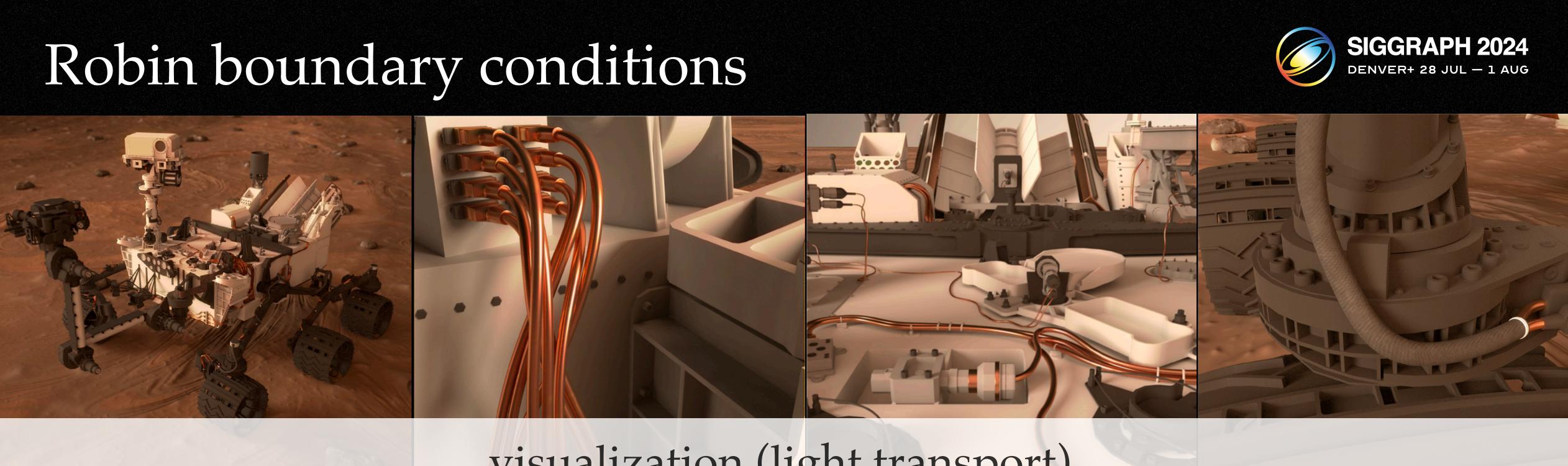


"how easily does the material absorb heat?"



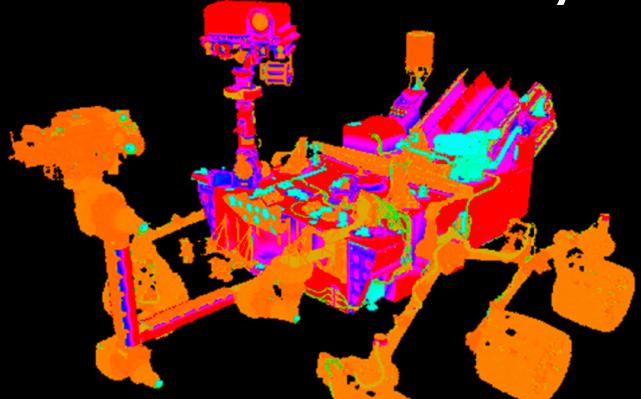


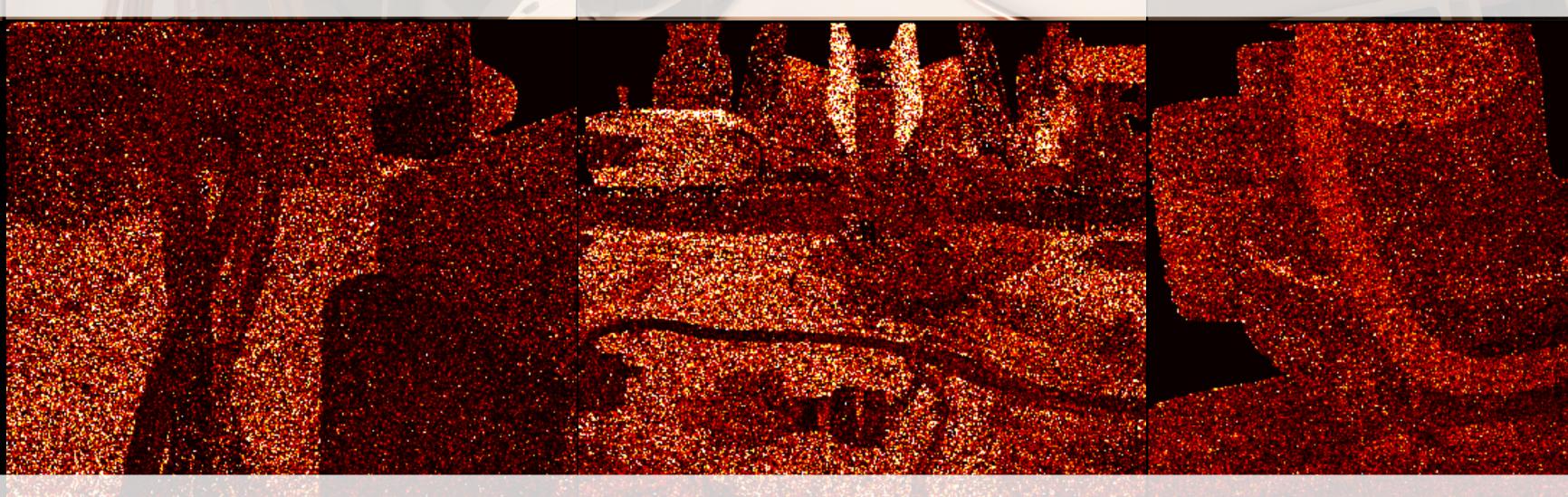




visualization (light transport)

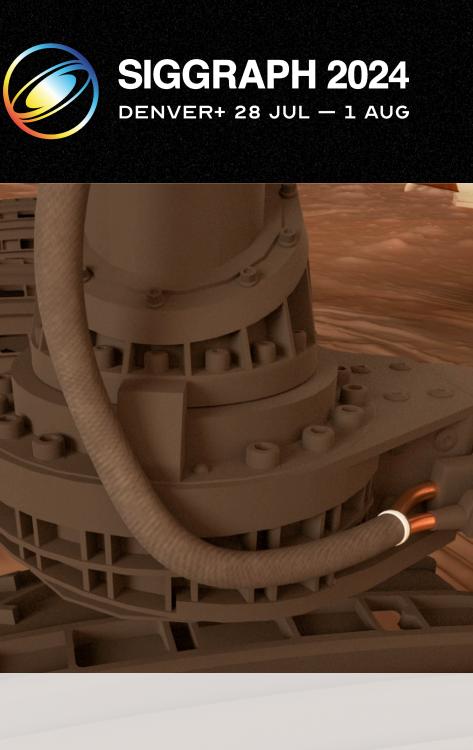
Robin coefficients μ

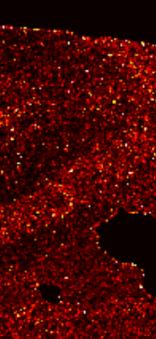




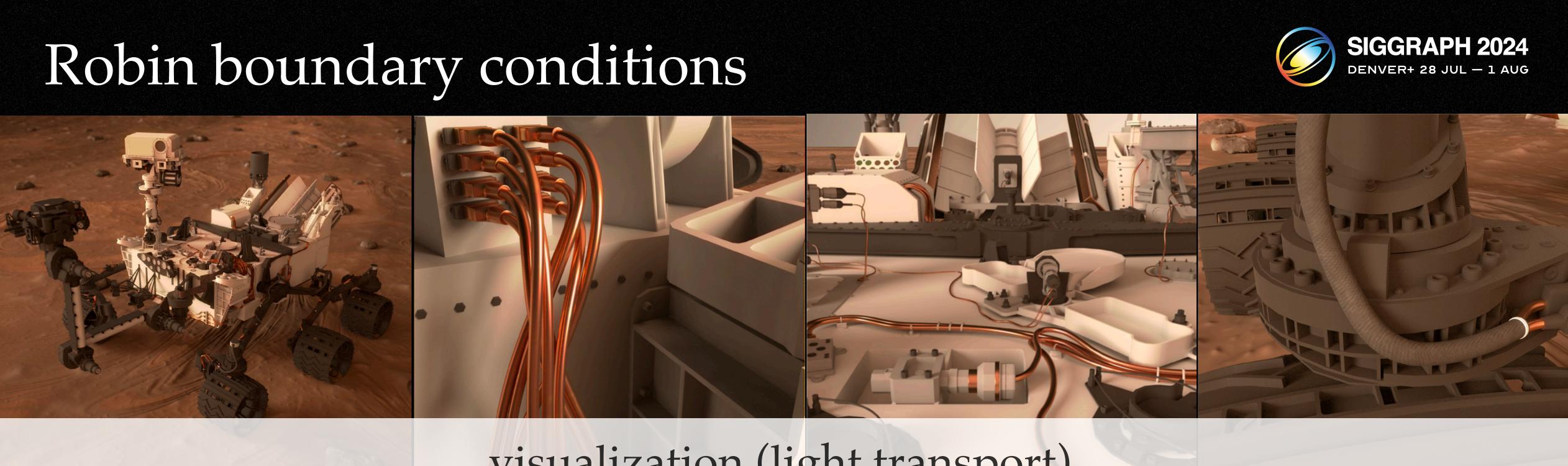
simulation (thermal conduction)





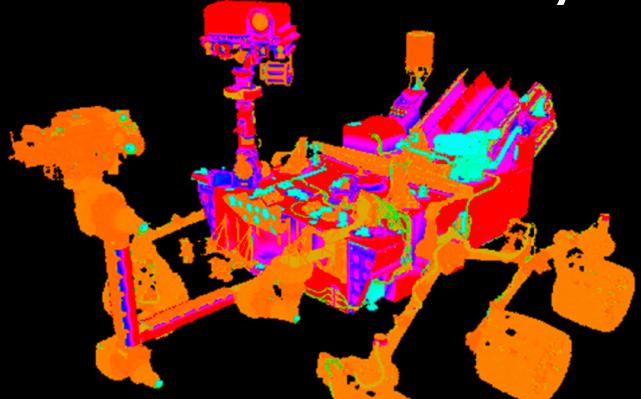


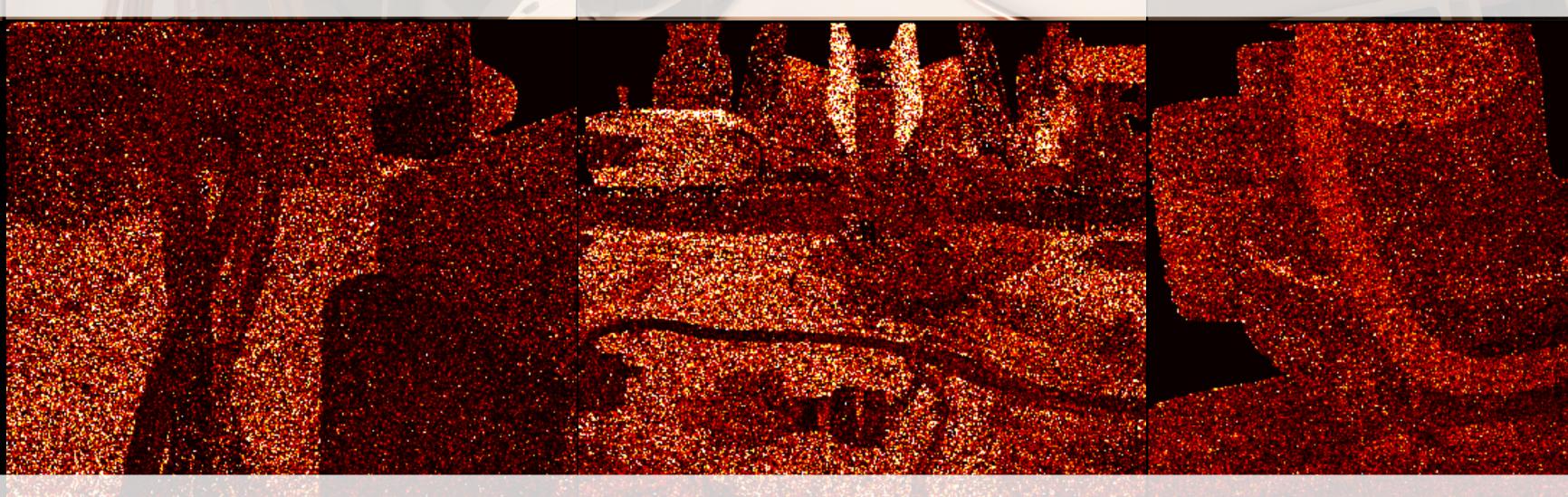




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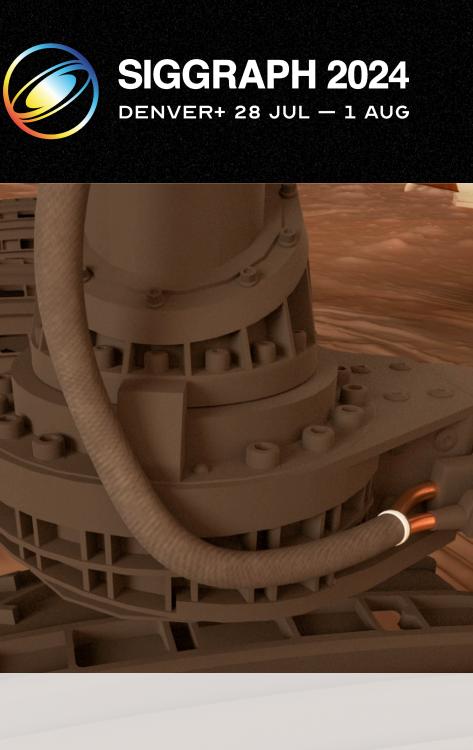
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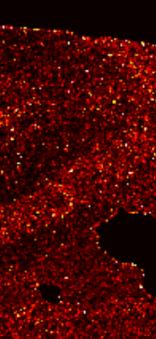




simulation (thermal conduction)









generalizing walk on stars

[Sawhney et al. 2023]

 $\mathbf{x} = \mathbf{x}\mathbf{0}$

return g(x)

until Dirichlet boundary reached:

 $S = find_largest_star_shape(x)$ x = sample_point_on_boundary(S)

 $\partial\Omega_N$ x_0 $\partial \Omega_D$

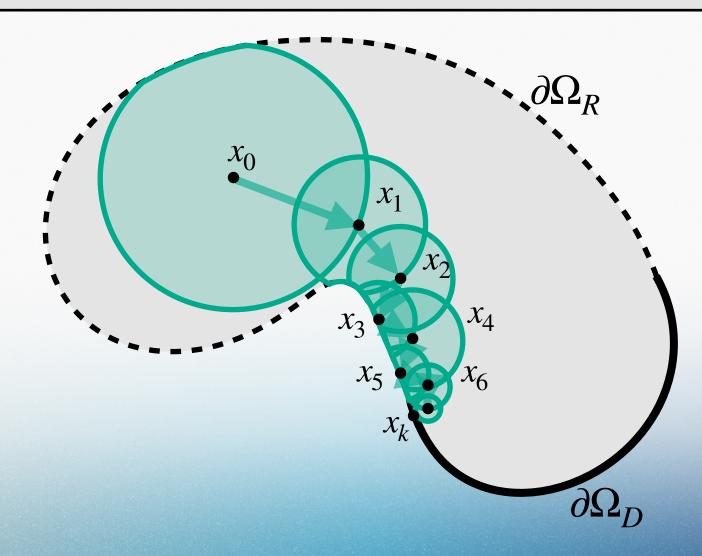


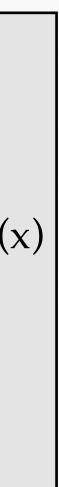
ours

with Robin boundary conditions r = 1; x = x0**until** Dirichlet boundary reached:

> S = find_reflectance_bounded_star_shape(x) x = sample_point_on_boundary(S) r *= reflectance(S, x)

return r * g(x)







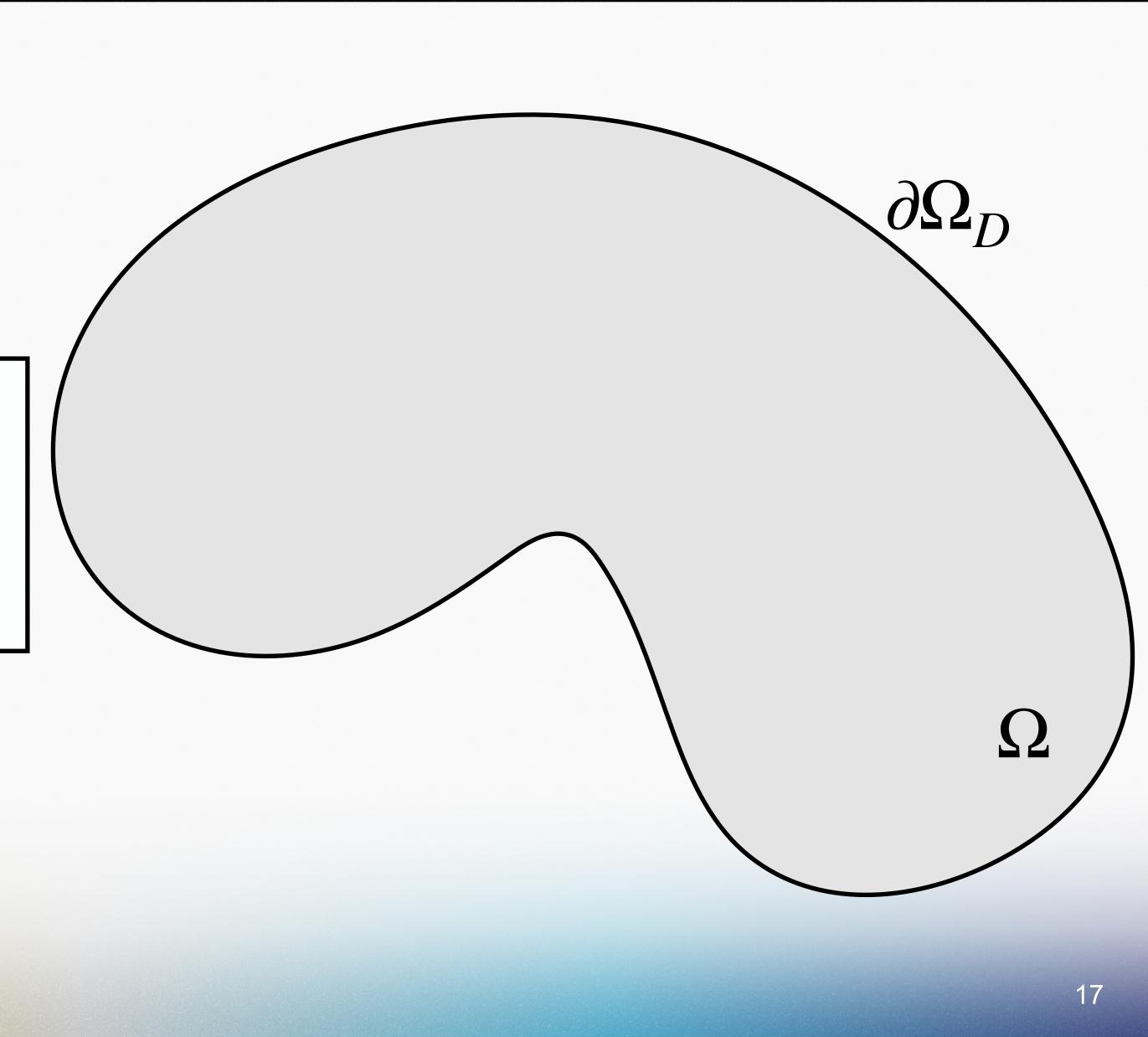


WALK ON SPHERES TO WALK ON STARS

Dirichlet problem

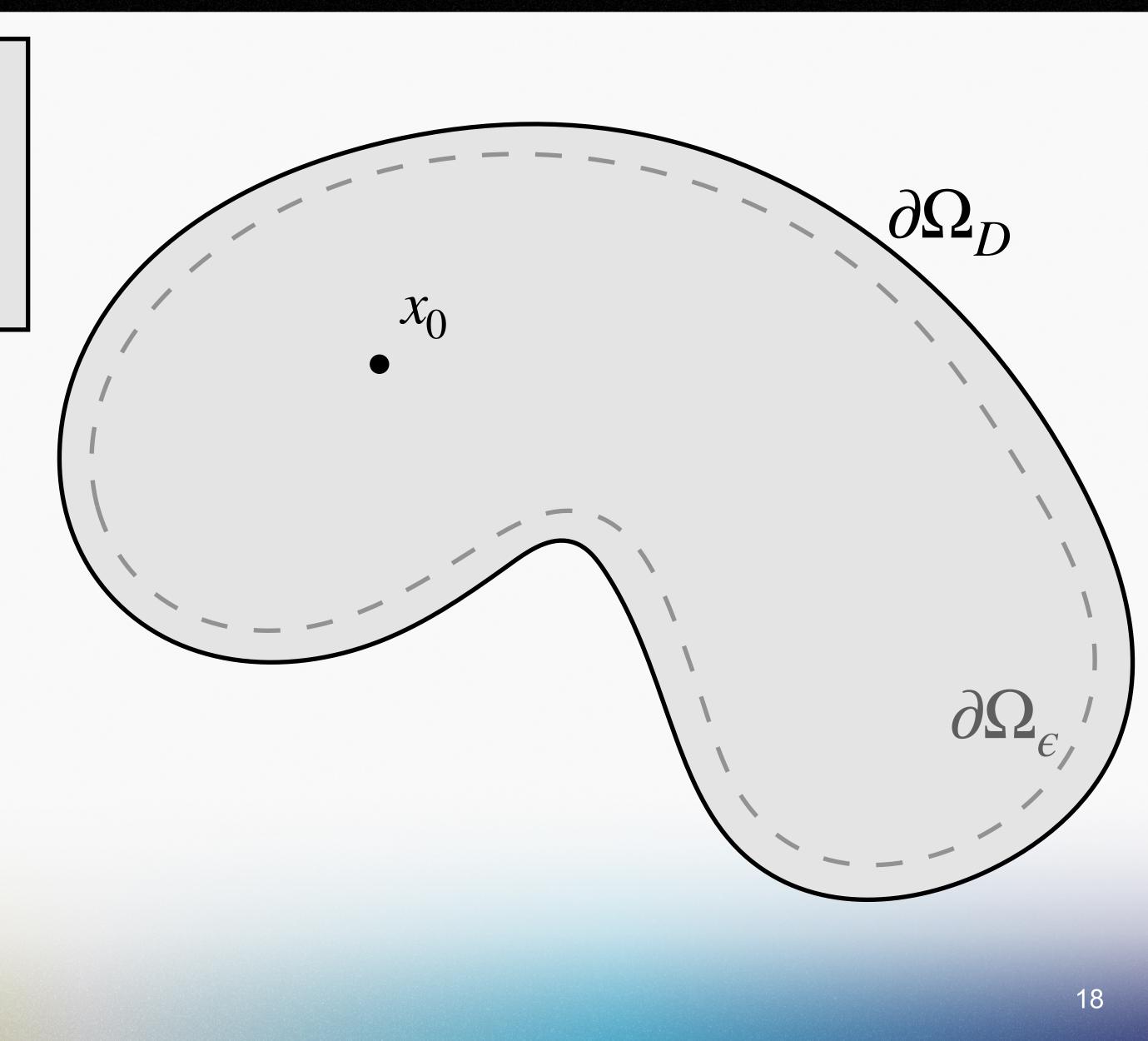
$\Delta u = 0 \quad \text{on } \Omega$ $u = g \quad \text{on } \partial \Omega_D \quad _$





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

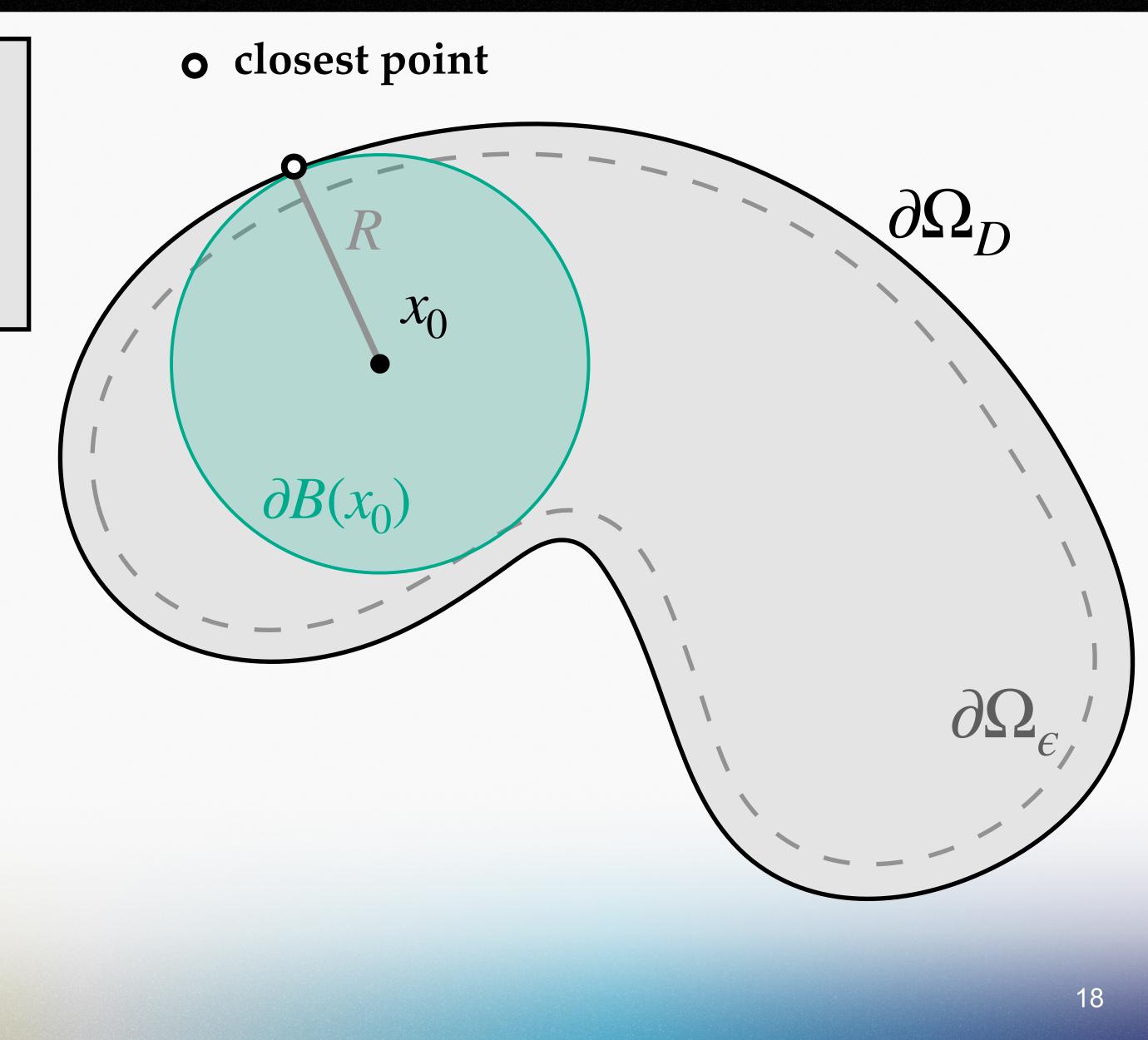






mean value integral
$$u(x) = \frac{1}{|\partial B(x)|} \int_{\partial B(x)} u(y) \, dy$$







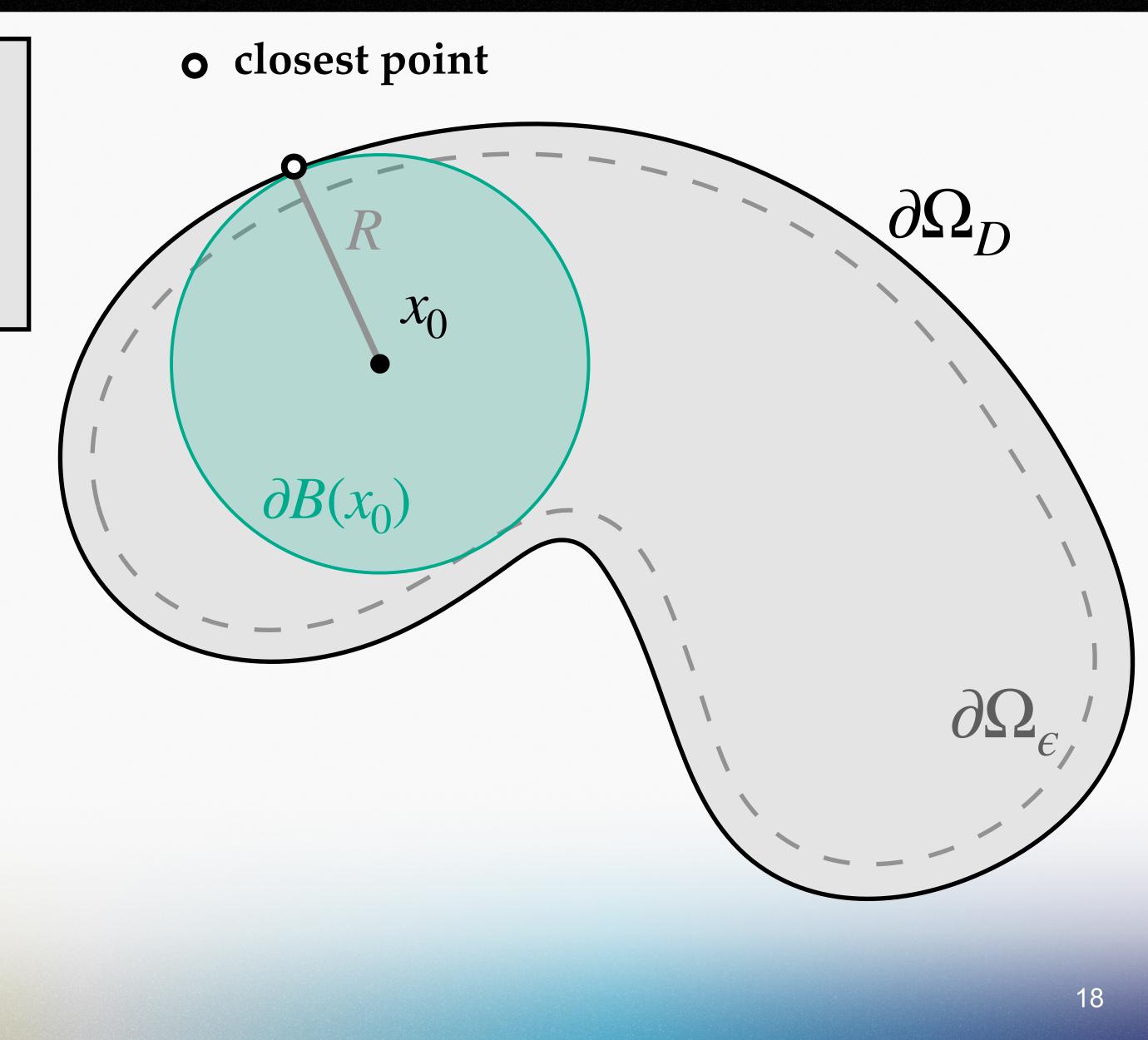
mean value integral
$$u(x) = \frac{1}{|\partial B(x)|} \int_{\partial B(x)} u(y) \, dy$$

Monte Carlo estimator

$$\widehat{u}(x) = \begin{cases} g(\overline{x}), & x \in \partial \Omega_{\epsilon} \\ \widehat{u}(y), & \text{otherwise} \end{cases}$$

uniform distribution on sphere $y \sim U[\partial B(x)]$







walk on spheres [Muller 1956, Sawhney and Crane 2020]

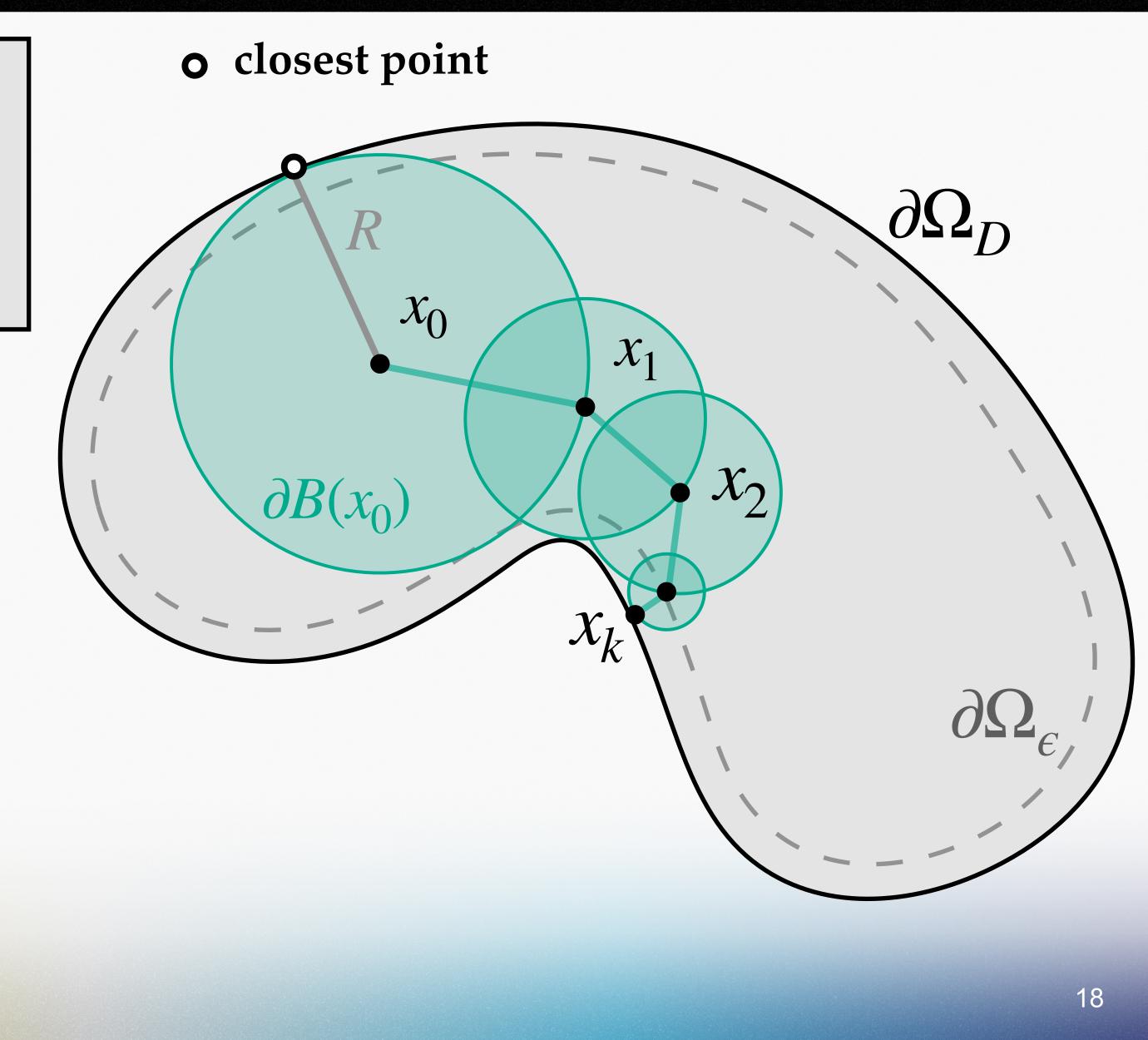
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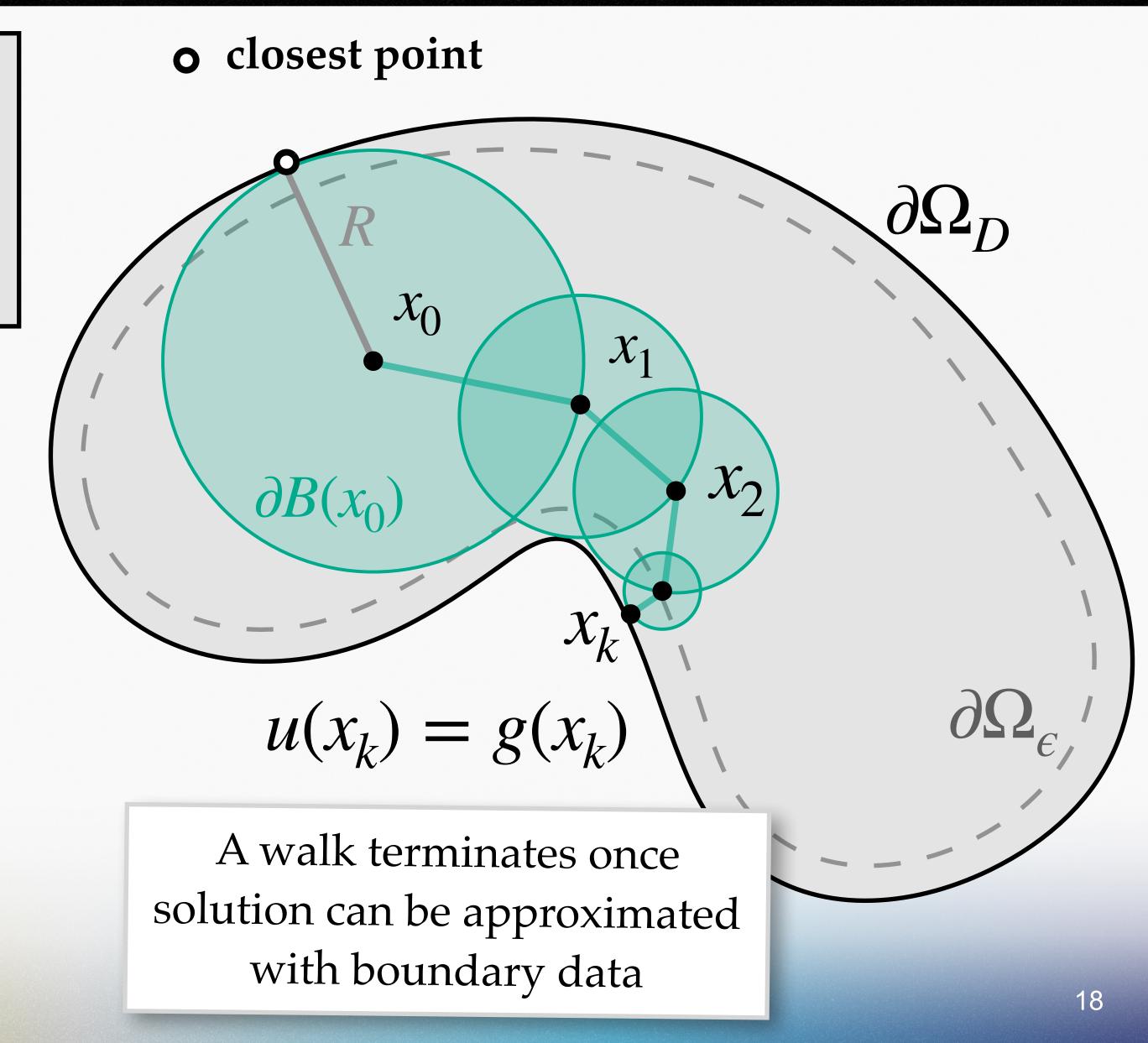
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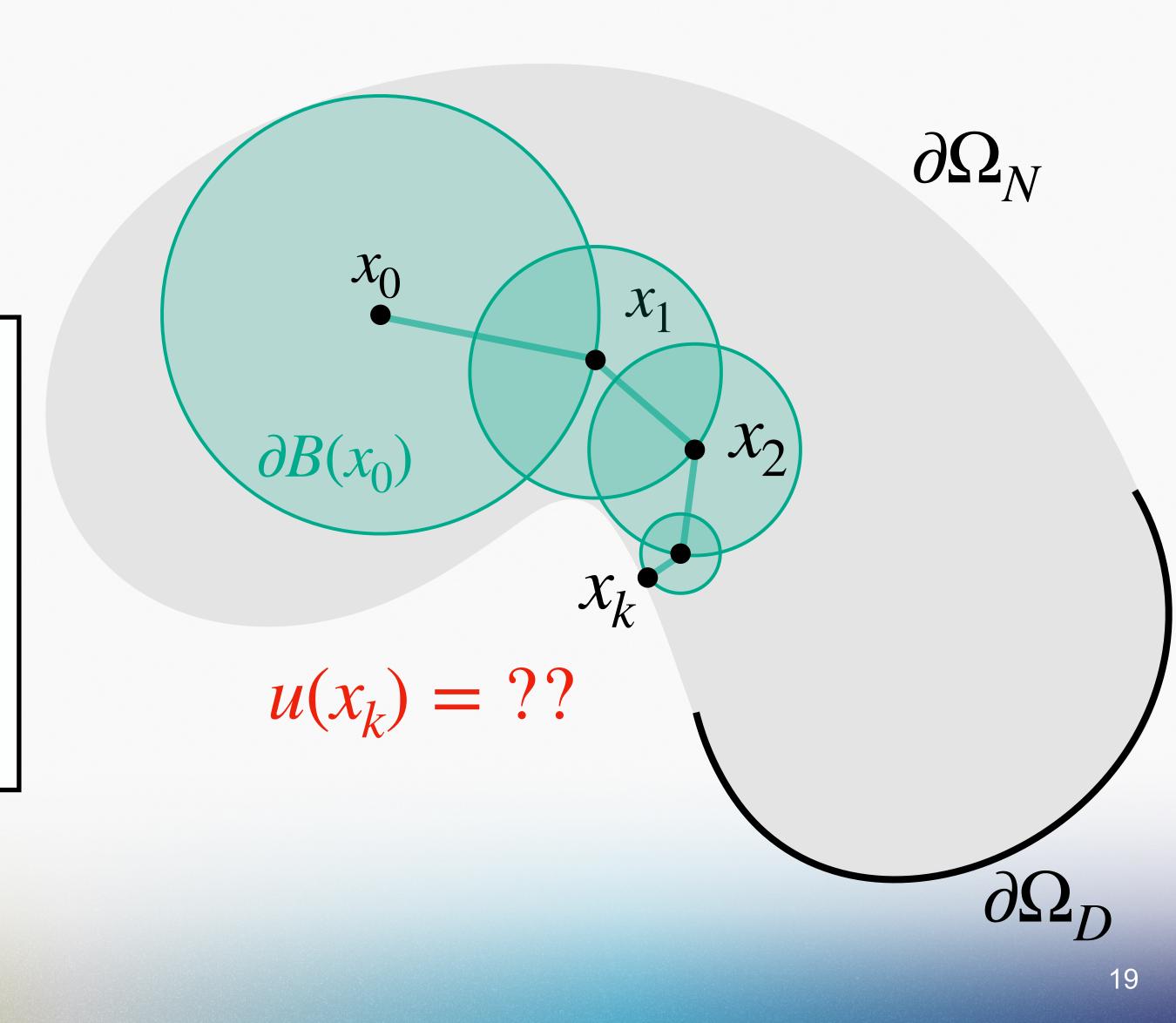




Neumann problem

$$\Delta u = 0 \quad \text{on } \Omega$$
$$u = g \quad \text{on } \partial \Omega_D \quad --$$
$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial \Omega_N \quad --$$



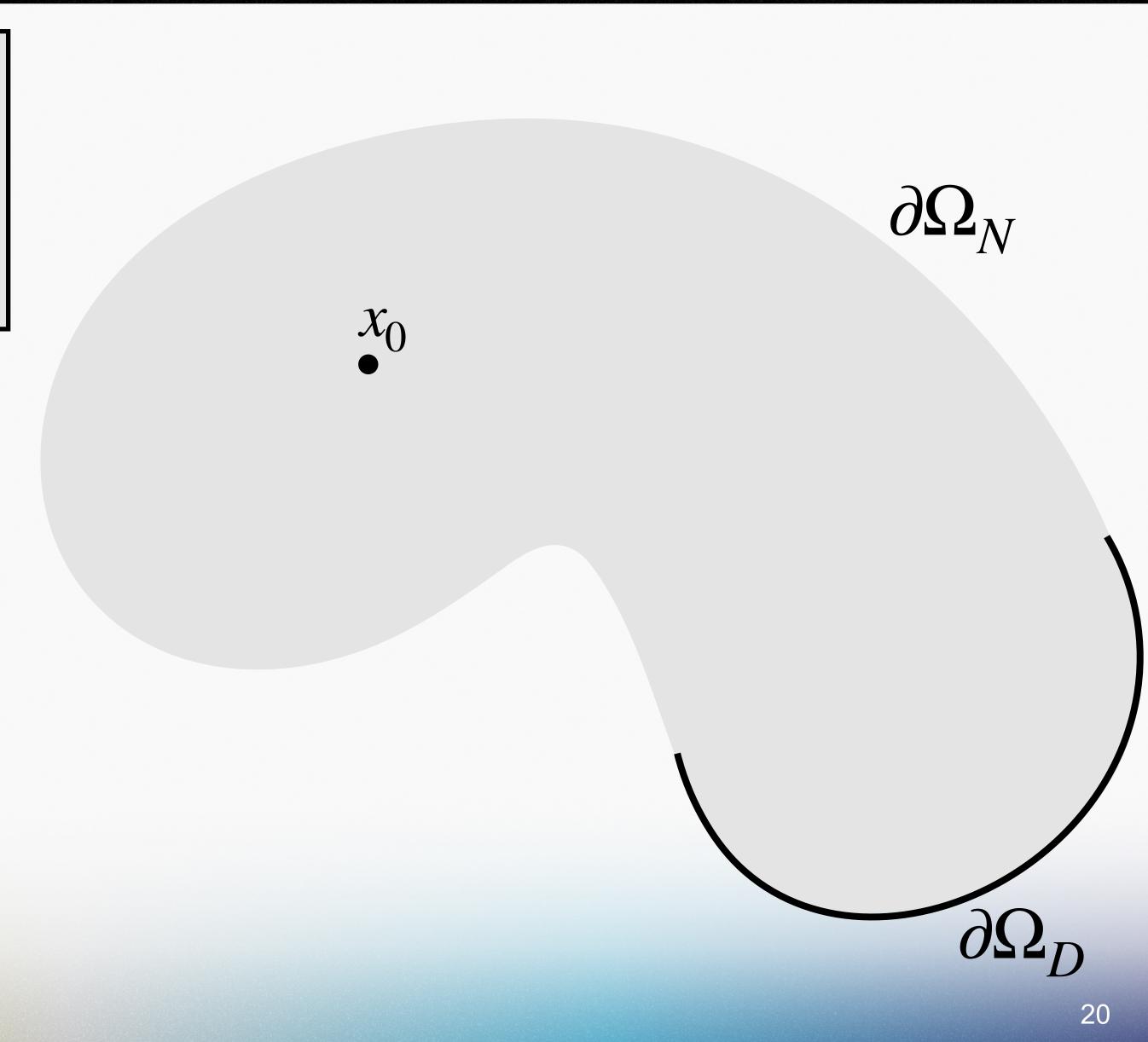


generalized mean value integral $u(x) = \int_{\partial St} P^B(x, y) u(y) \, dy$

Monte Carlo estimator

$$\widehat{u}(x) = \begin{cases} g(\overline{x}), & x \in \partial \Omega_{\epsilon} \\ \widehat{u}(y), & \text{otherwise} \end{cases}$$



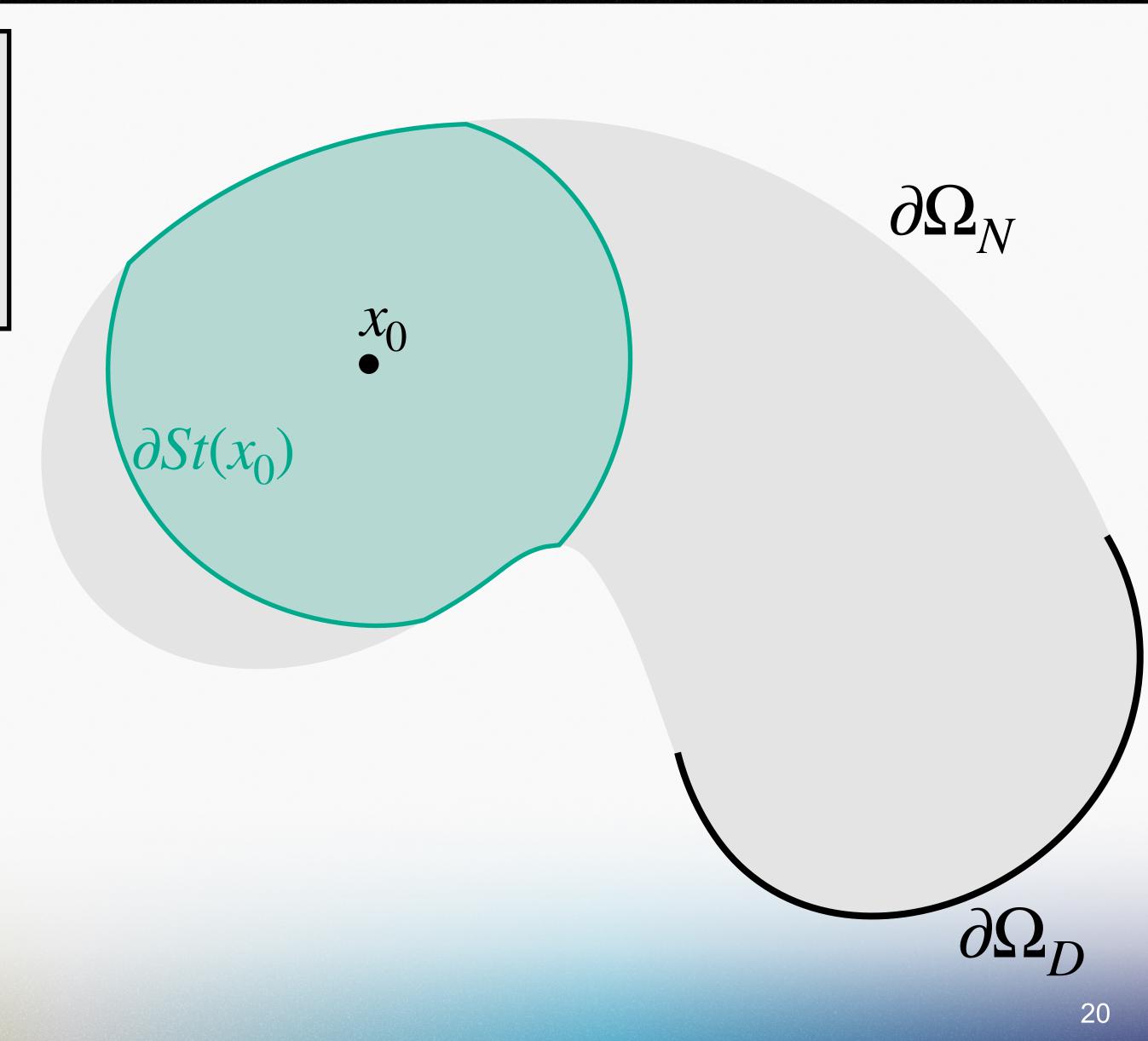


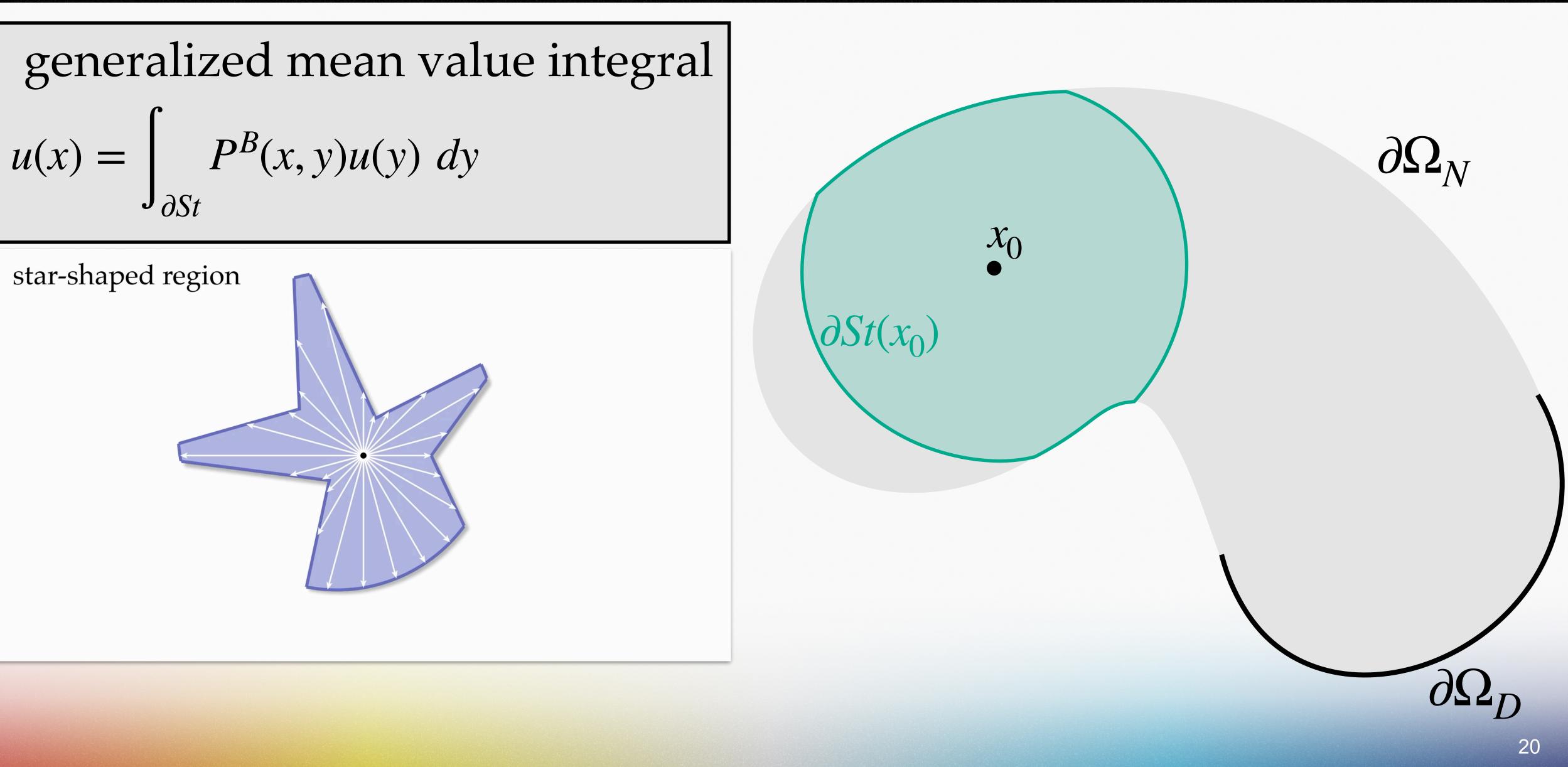
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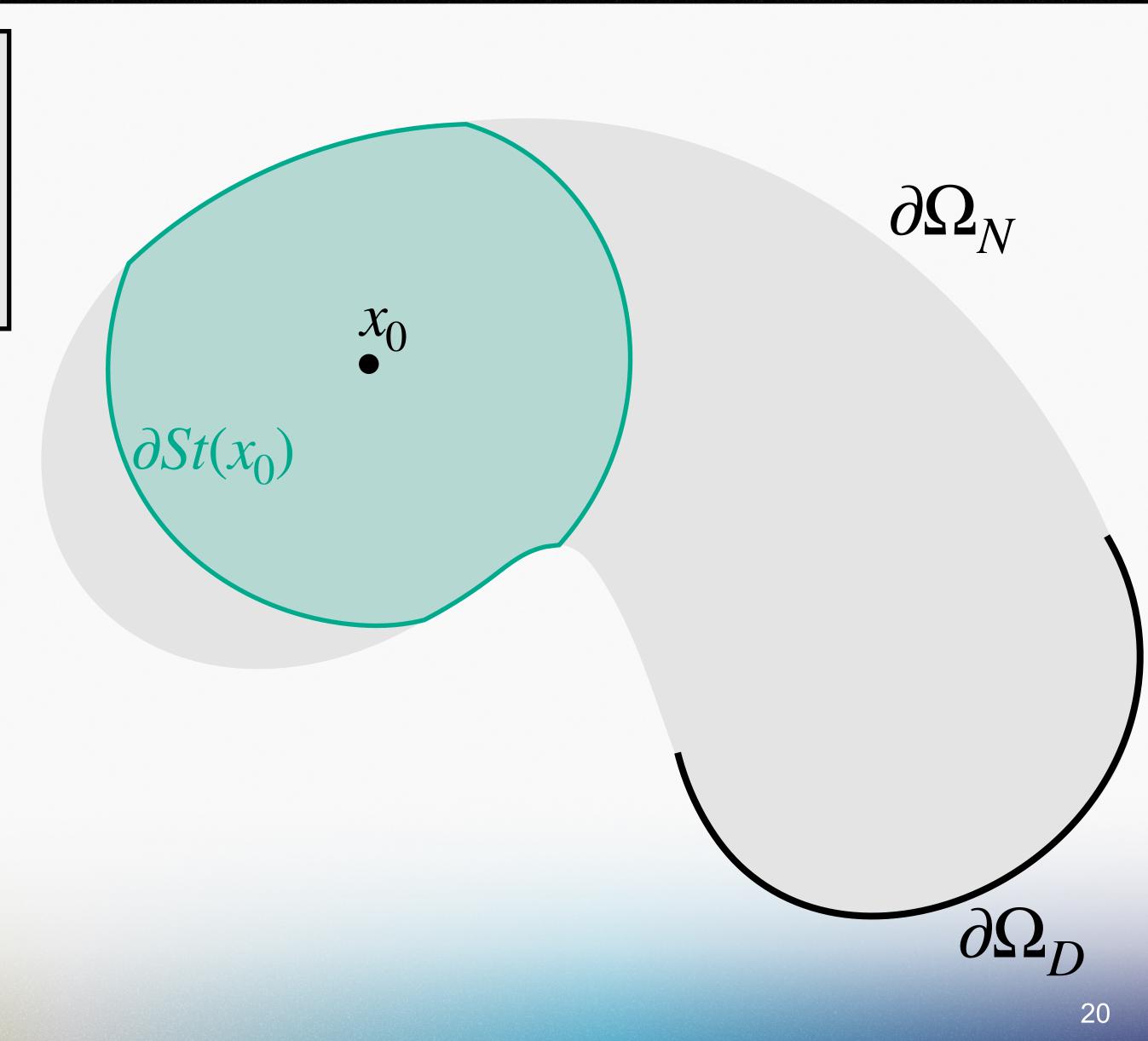


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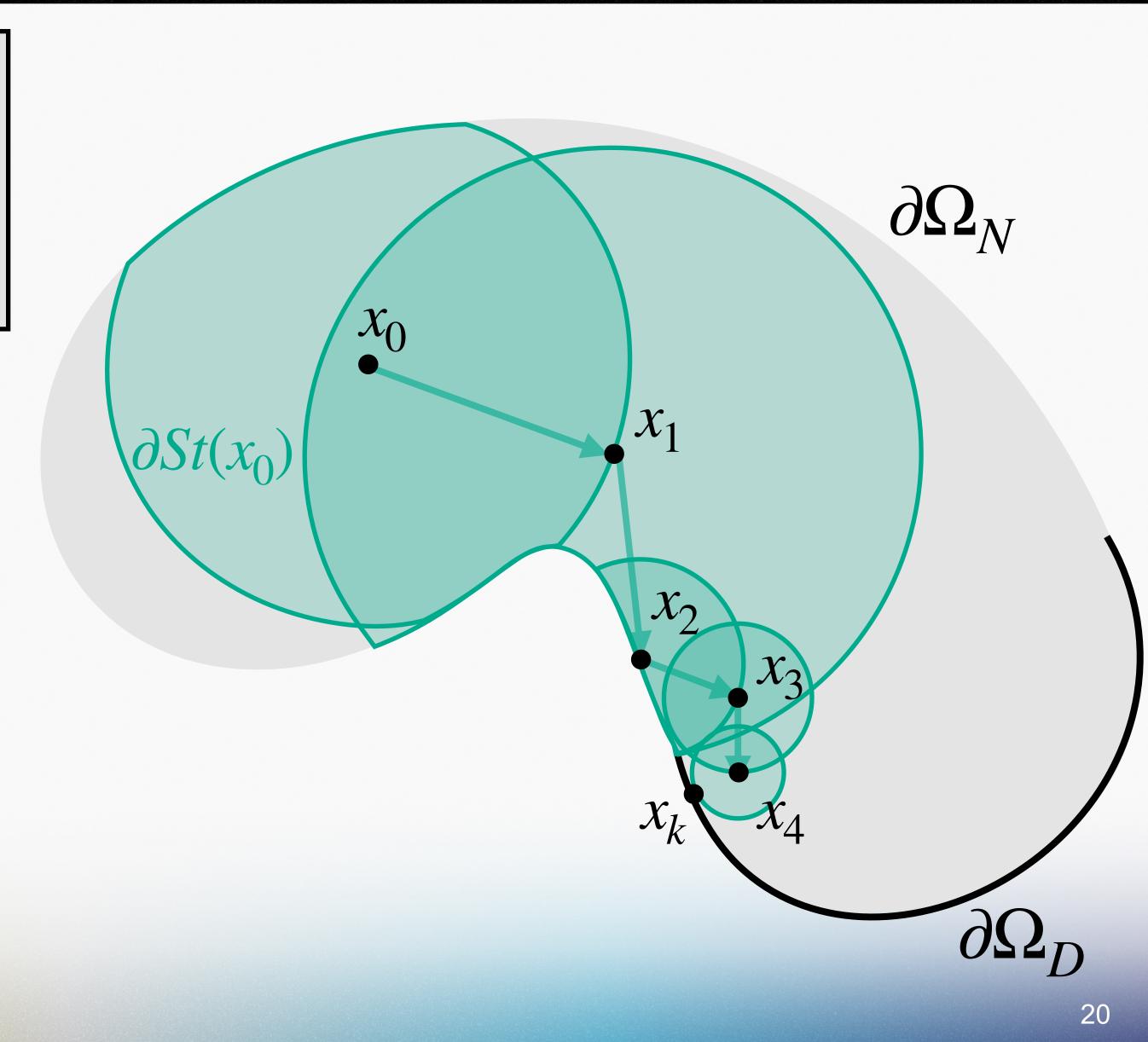
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uniform direction sample $y \sim |P(x, y)|$





generalized mean value integral $u(x) = \int_{\partial St} P^B(x, y) u(y) \, dy$

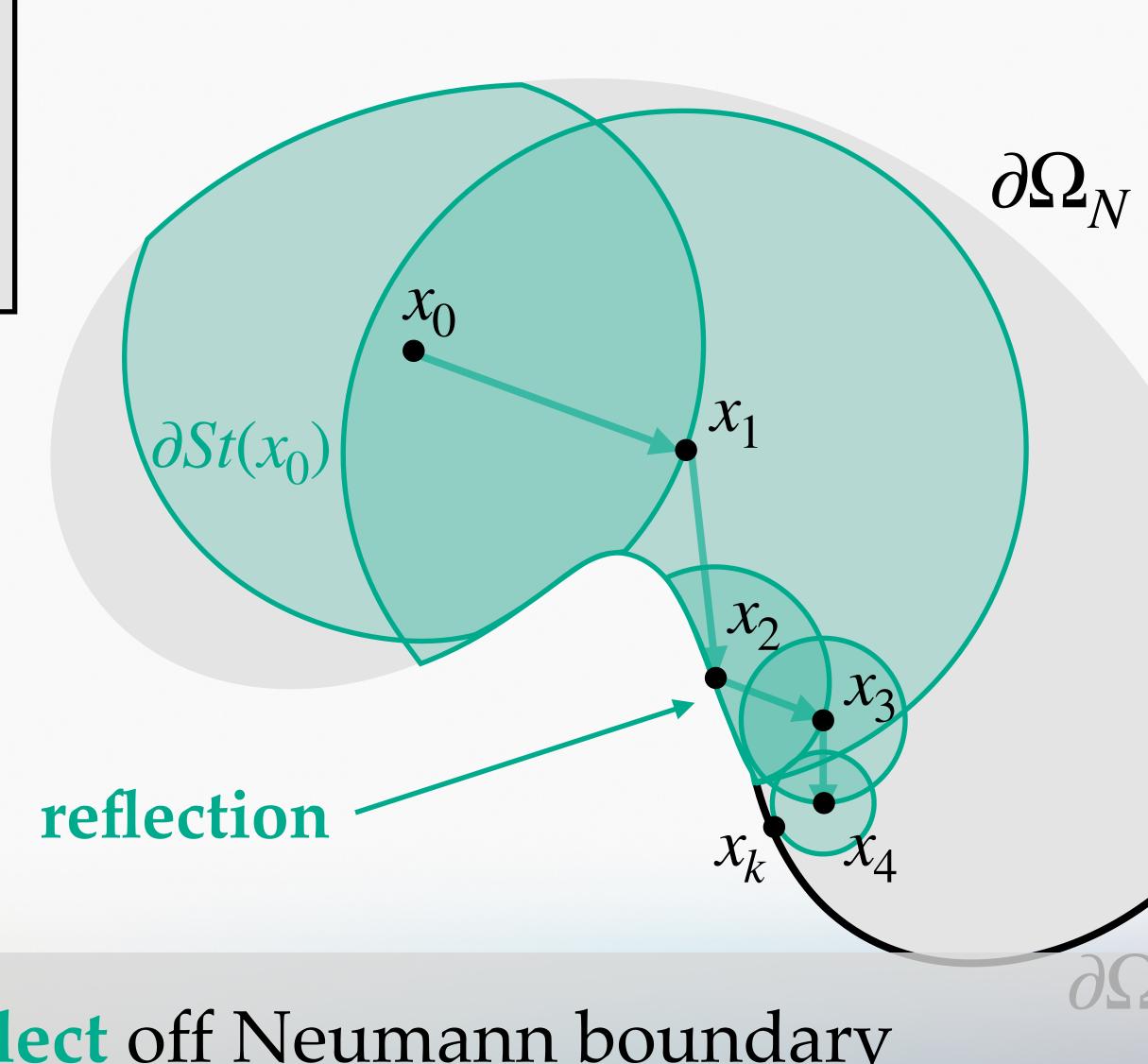
Monte Carlo estimator

$$\widehat{u}(x) = \begin{cases} g(\overline{x}), & x \in \partial \Omega_{\epsilon} \\ \widehat{u}(y), & \text{otherwise} \end{cases}$$

uniform direction sample $y \sim |P(x, y)|$

key difference: walk can now reflect off Neumann boundary







2

20

avoiding multiple intersections

generalized mean value integral $u(x) = \int_{\partial A} P^B(x, y) u(y) \, dy$

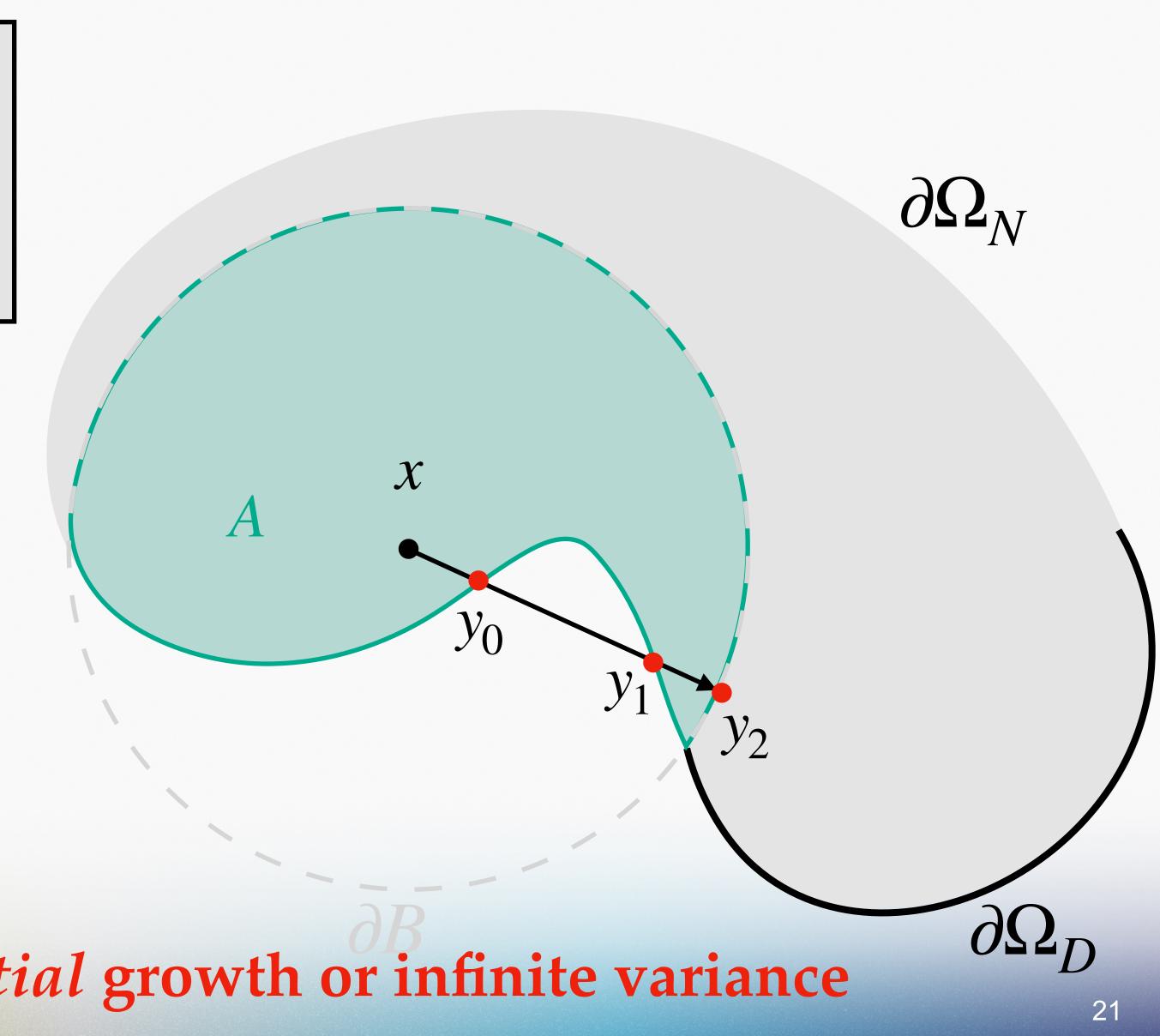
Monte Carlo estimator

$$\widehat{u}(x) = \sum_{i=1}^{n} \frac{P(x, y_i)}{|P(x, y_i)|} \widehat{u}(y_i)$$

uniform direction sample $y \sim |P(x, y)|$

multiple intersections \implies *exponential* growth or infinite variance





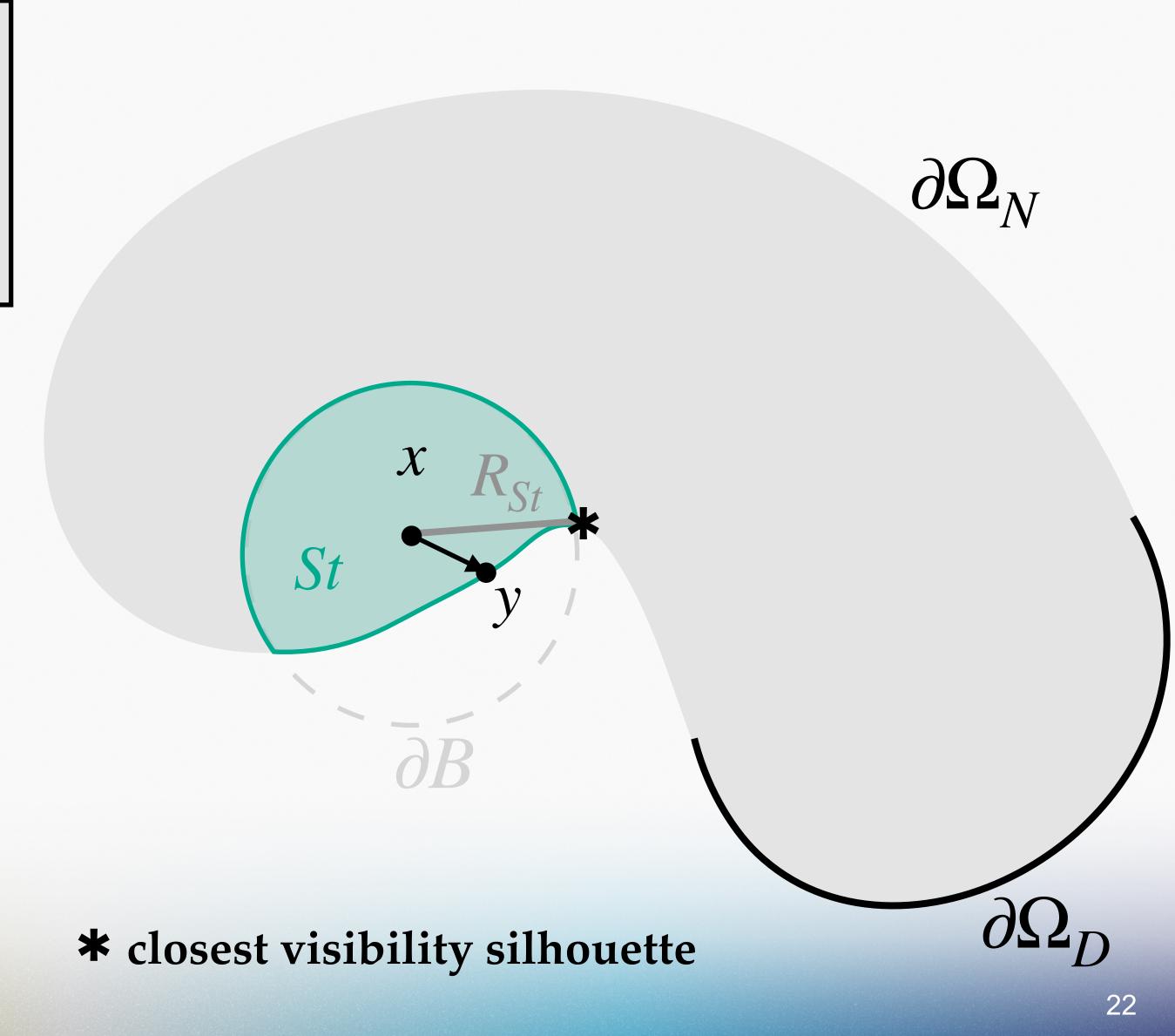


generalized mean value integral $u(x) = \int_{\partial S^t} P^B(x, y) u(y) \, dy$

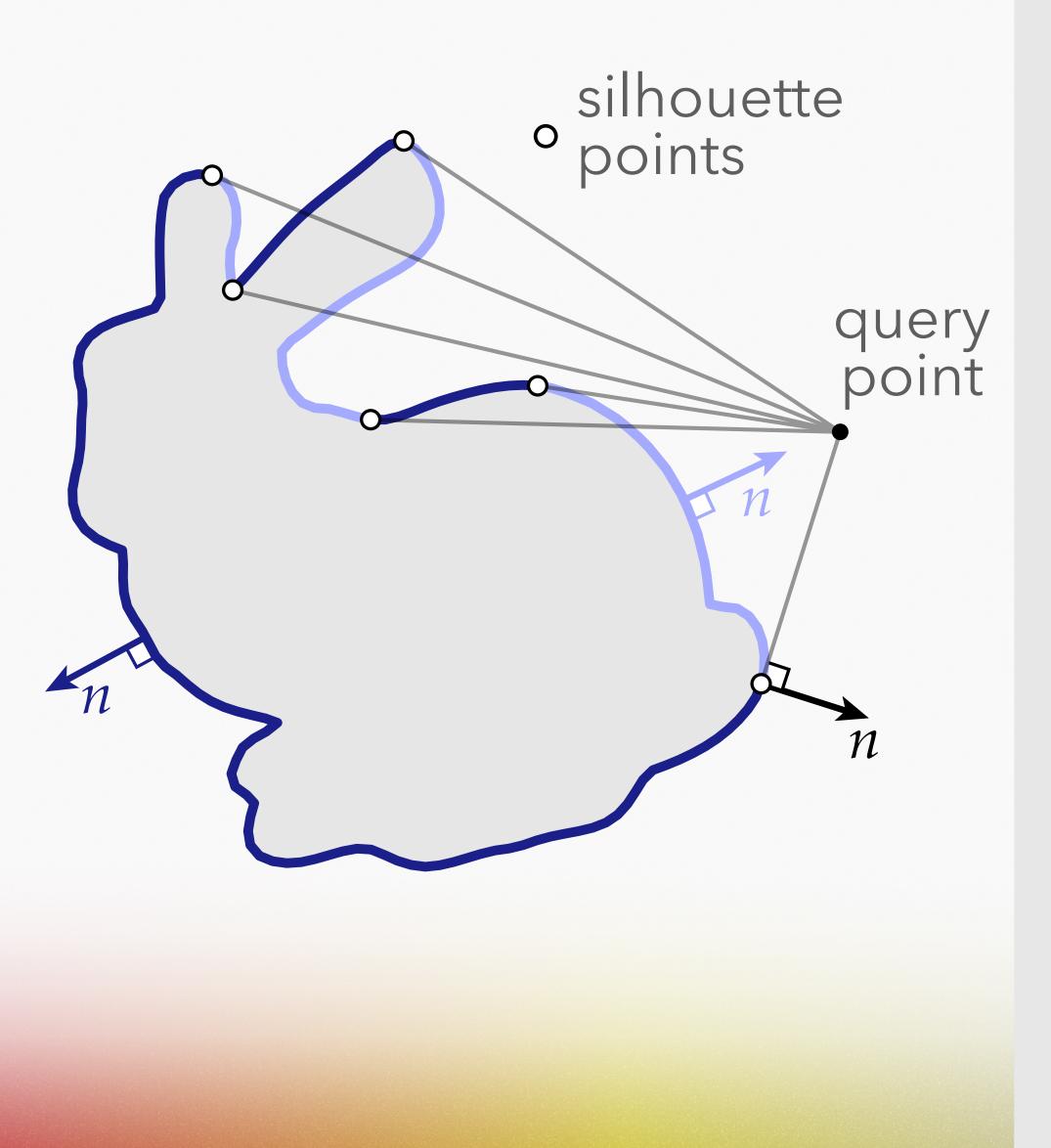
Monte Carlo estimator $\widehat{u}(x) = \widehat{u}(y)$

uniform direction sample $y \sim |P(x, y)|$





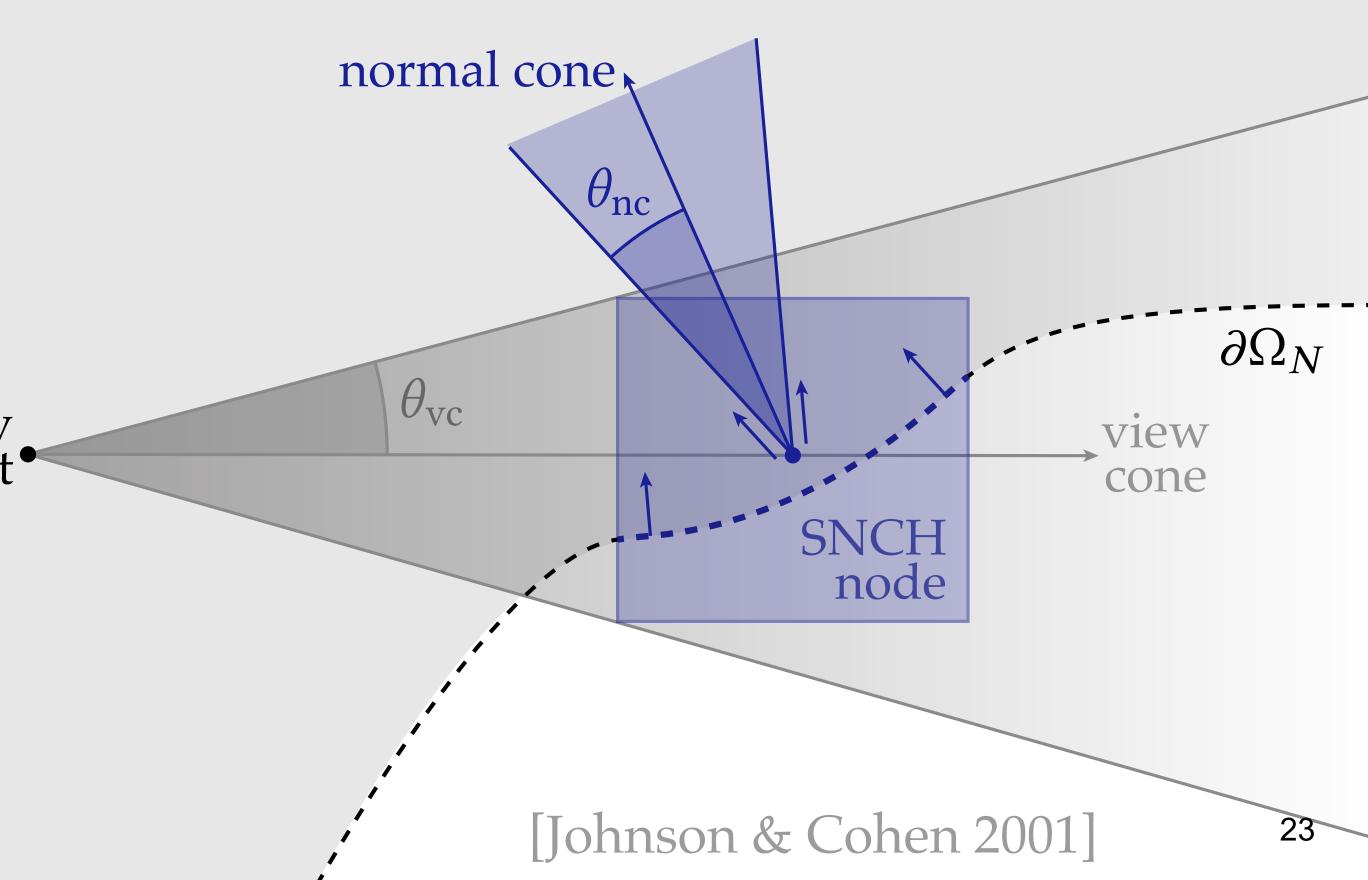
closest silhouette points



query point•



normal cone hierarchy

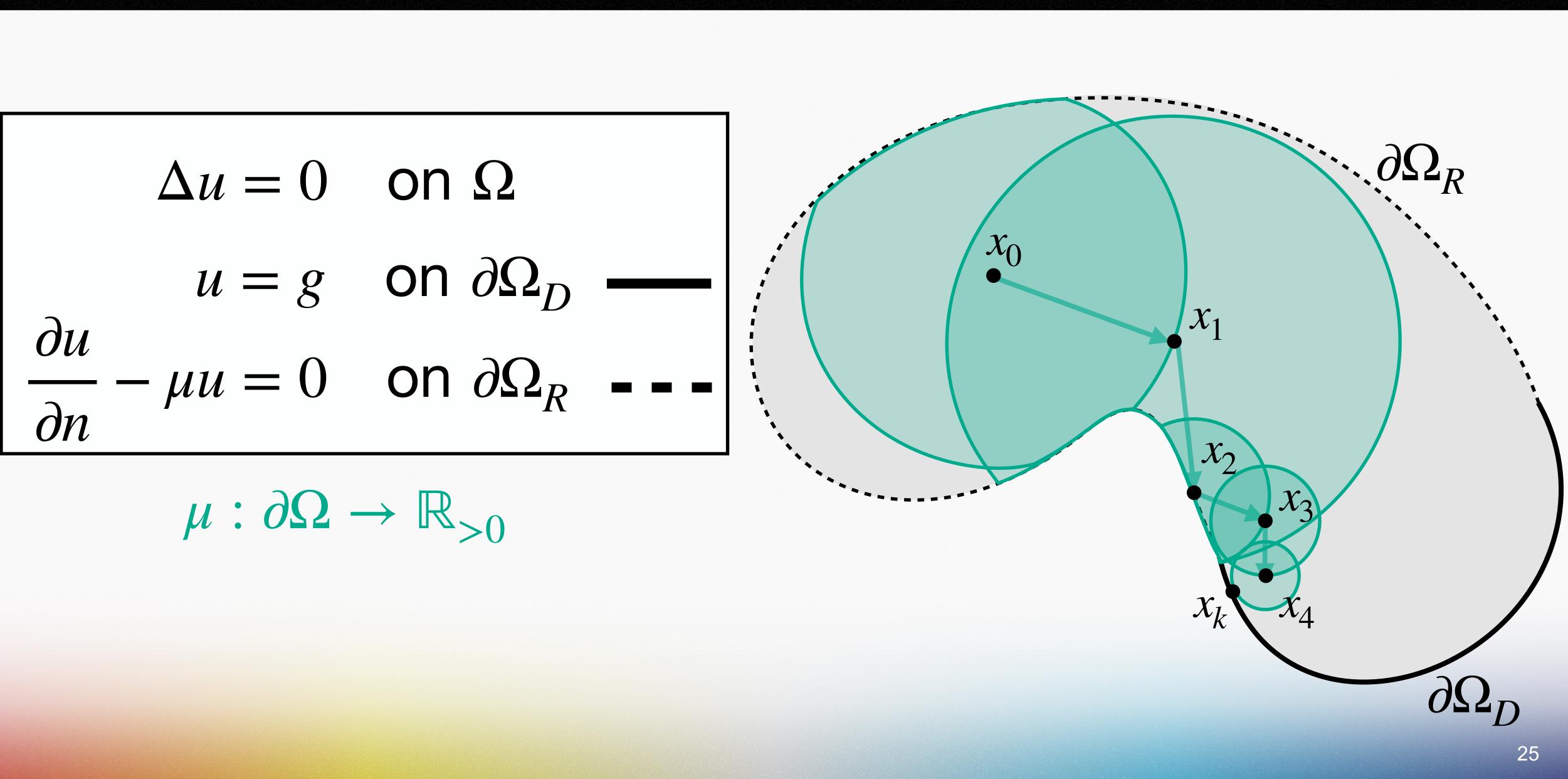






GENERALIZING WALK ON STARS

Robin problem





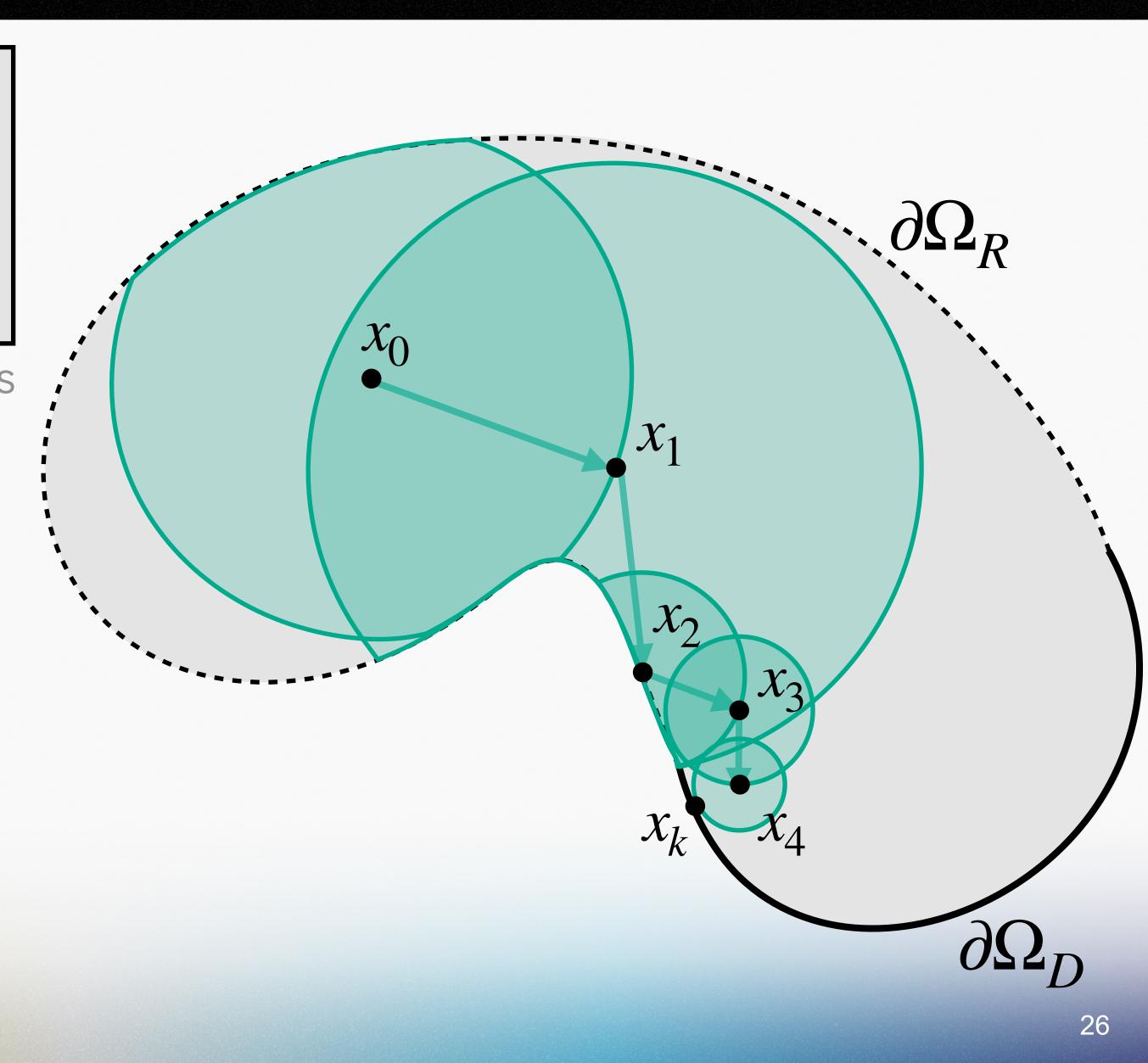
generalized boundary integral $u(x) = \int_{\partial St} \rho_{\mu}(x, y) P^{B}(x, y) u(y) \, dy$

no change from walk on stars

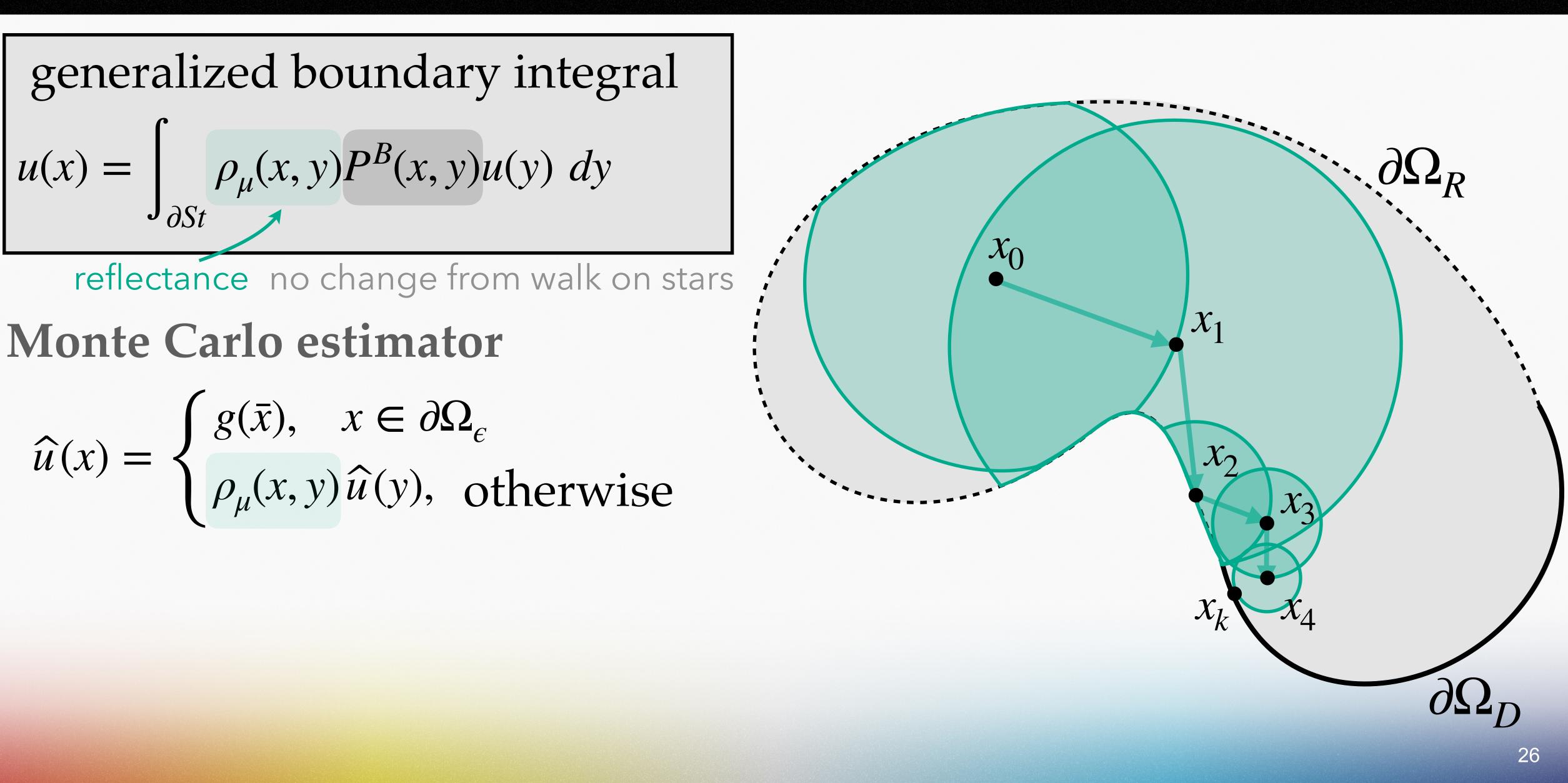
Monte Carlo estimator

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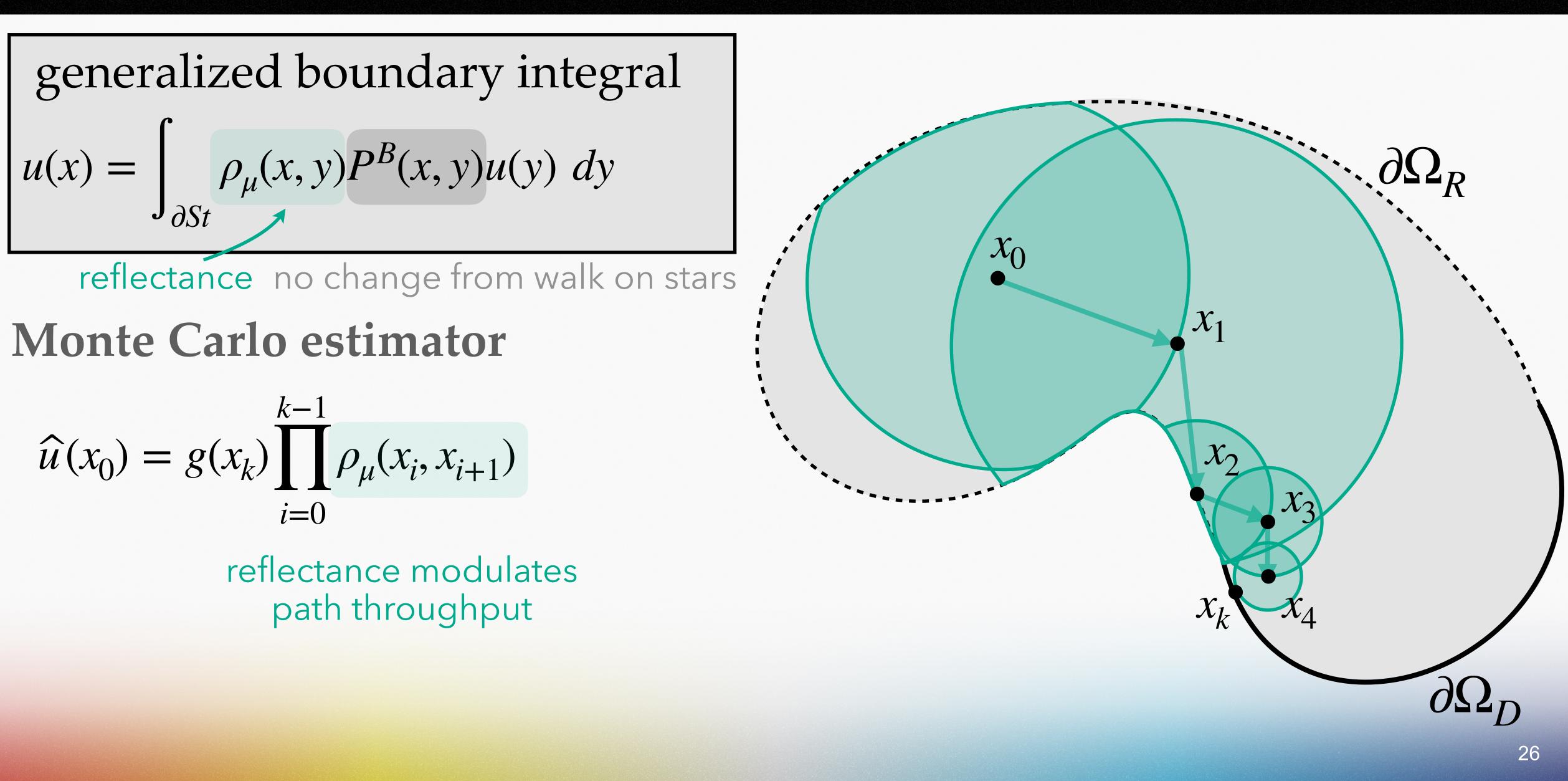








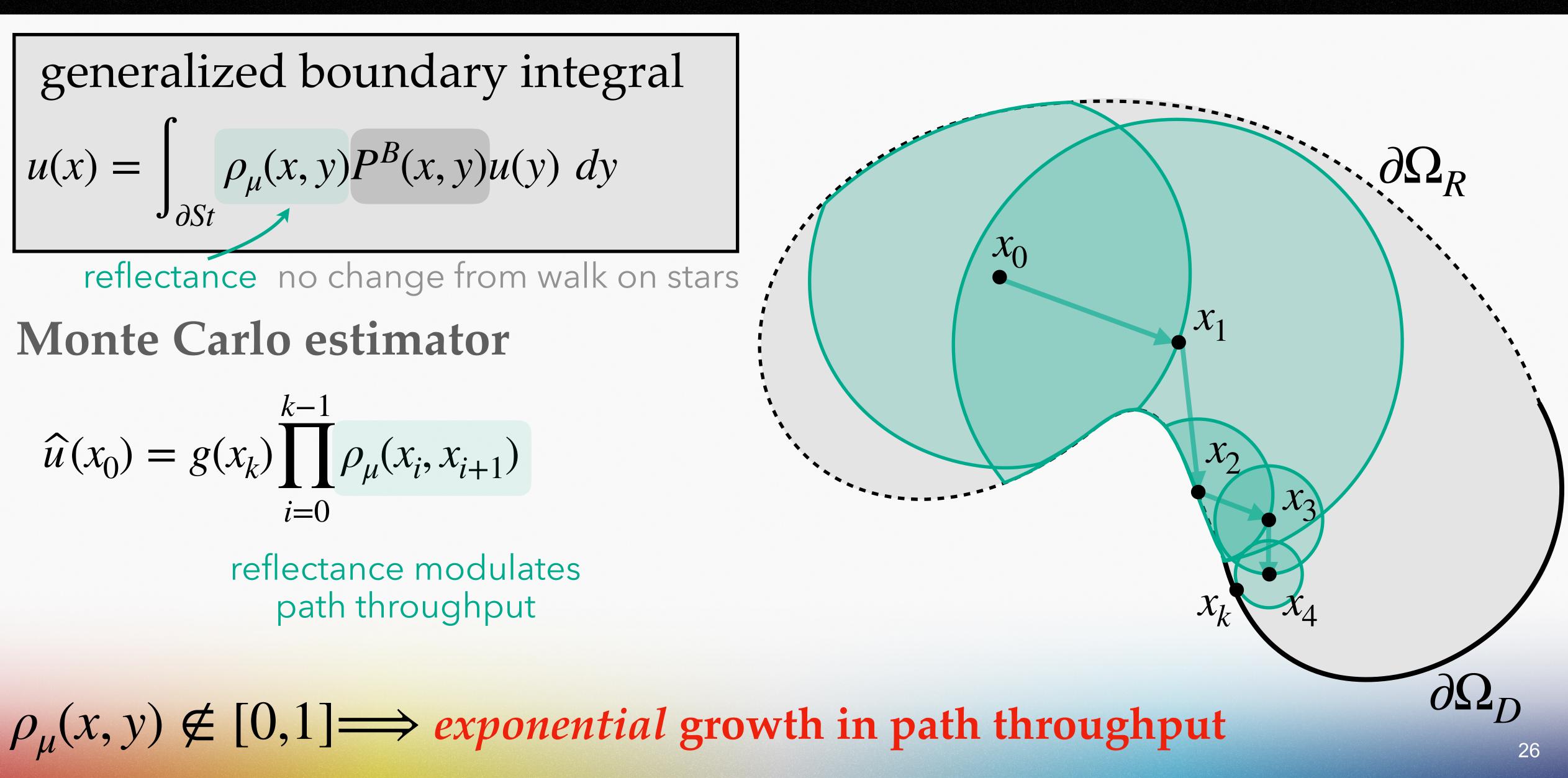




$$\hat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$







$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$





Neumann $\mu = 0$

***** closest visibility silhouette

intuition: interpolate between WoSt and WoS





Robin

Dirichlet $\mu = \infty$

$\rho_u(x, y) \notin [0, 1]$

• closest point on boundary



Neumann $\mu = 0$

***** closest visibility silhouette

intuition: interpolate between WoSt and WoS

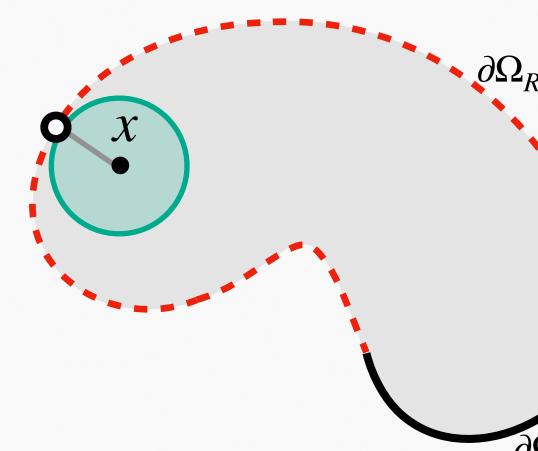




Robin

Dirichlet $\mu = \infty$

Walk on Spheres

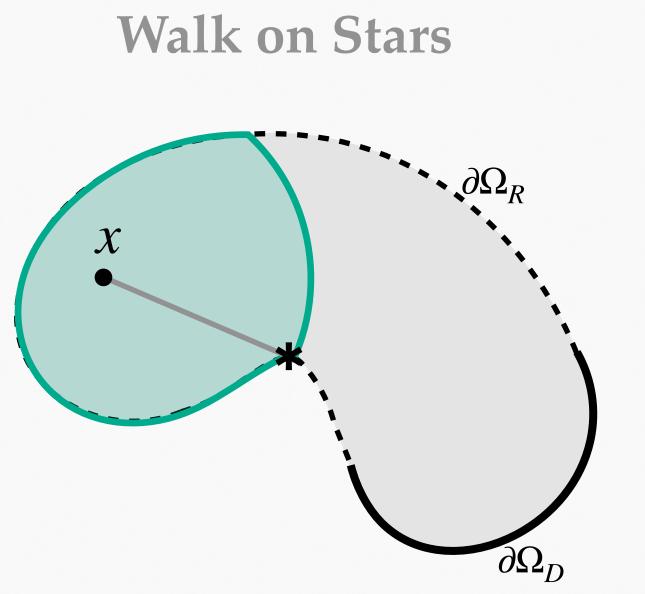


$\rho_{\mu}(x,y) \notin [0,1]$

O closest point on boundary



Neumann
$$\mu = 0$$



***** closest visibility silhouette

intuition: interpolate between WoSt and WoS

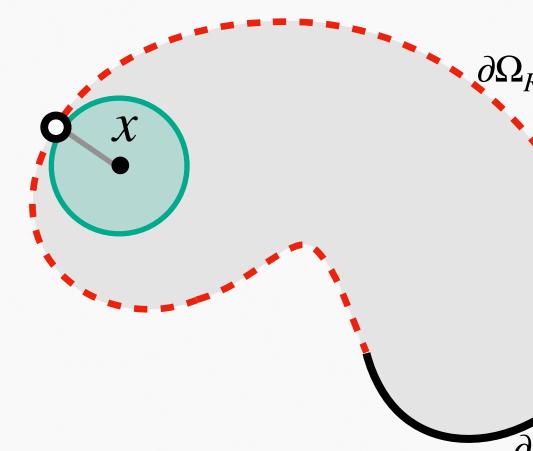




Robin

Dirichlet $\mu = \infty$

Walk on Spheres

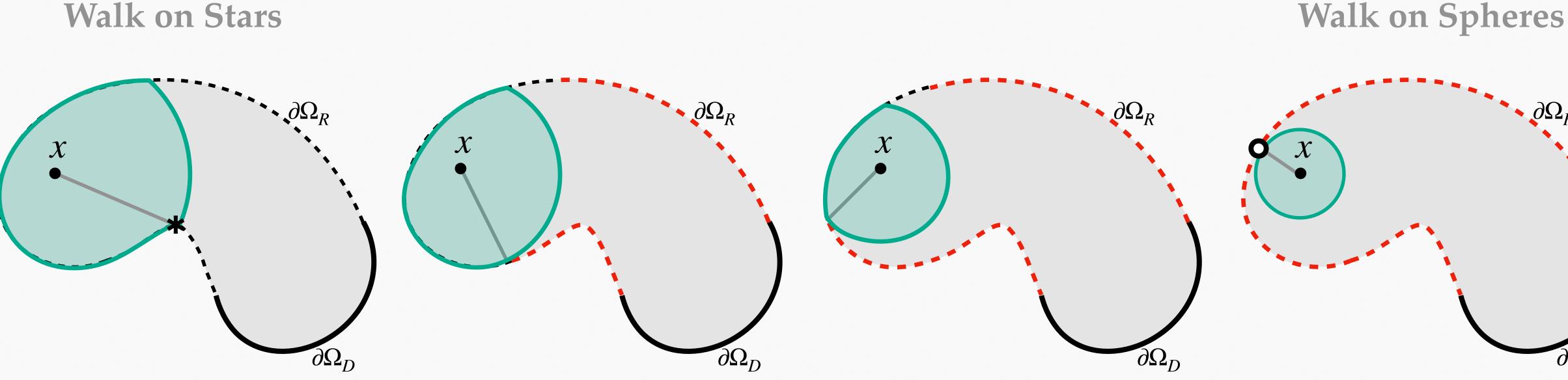


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Neumann
$$\mu = 0$$



***** closest visibility silhouette

intuition: interpolate between WoSt and WoS





Robin

Dirichlet $\mu = \infty$

 $\rho_u(x,y) \notin [0,1]$

O closest point on boundary

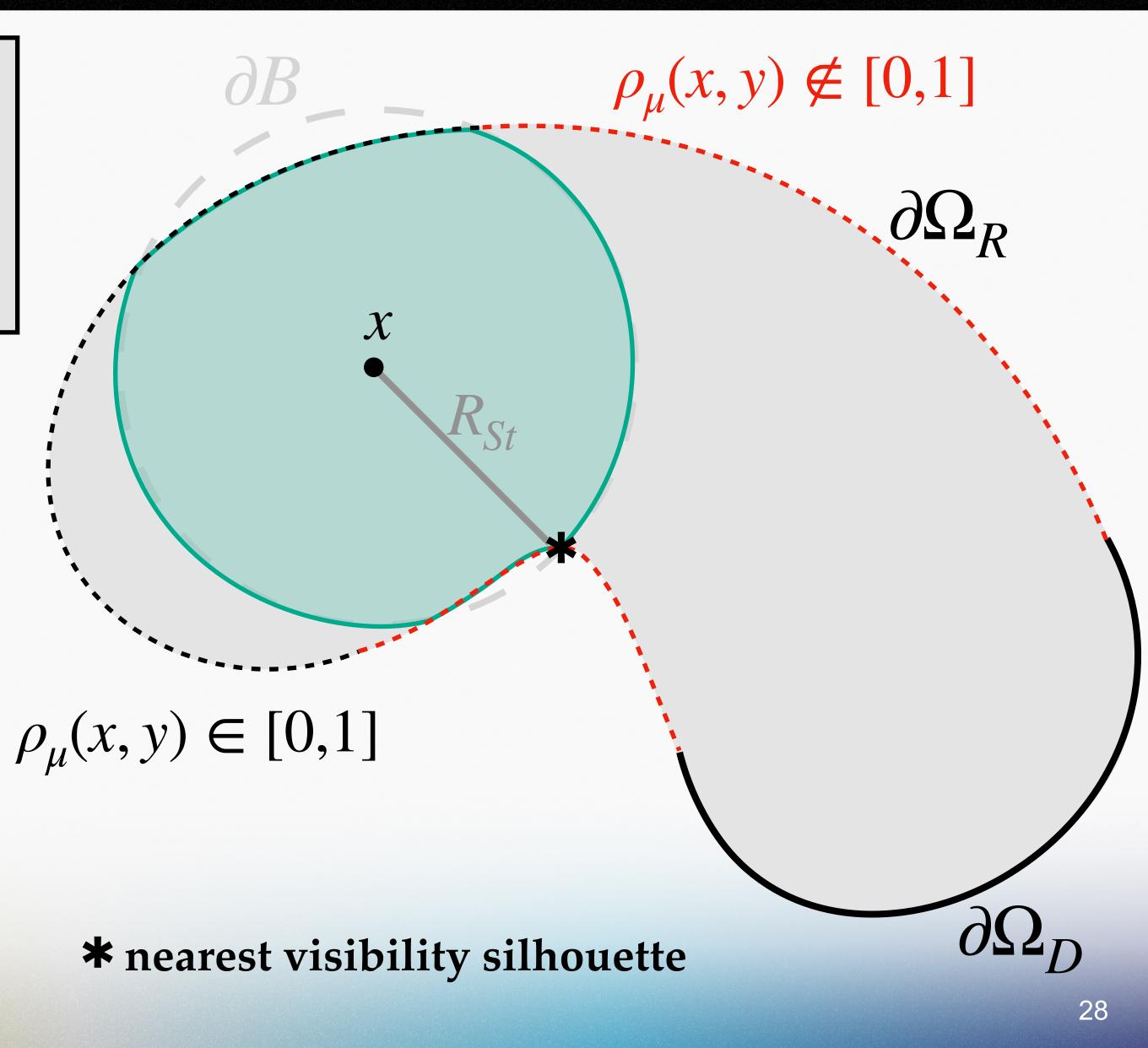


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Monte Carlo estimator

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$



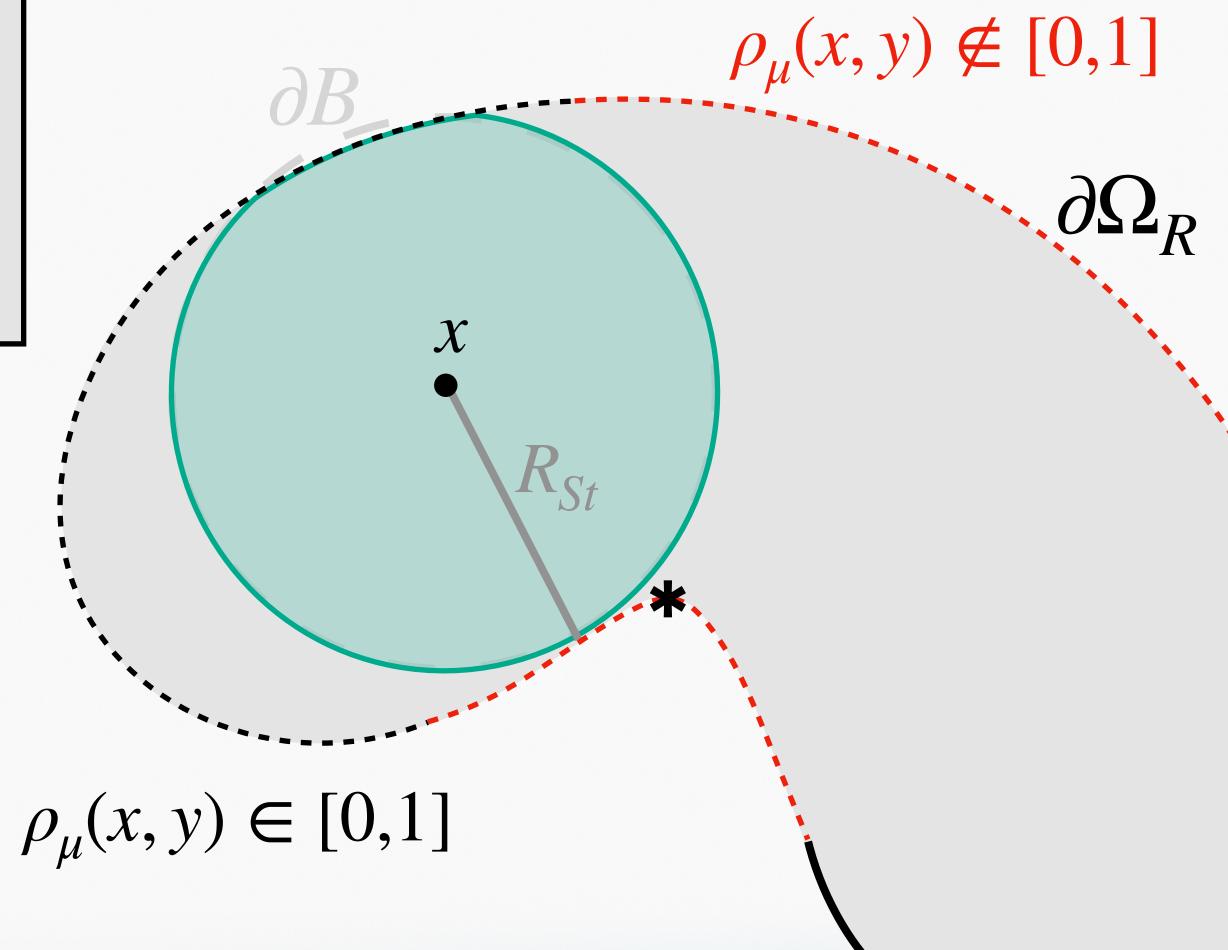


generalized boundary integral $u(x) = \int_{\partial St} \rho_{\mu}(x, y) P^{B}(x, y) u(y) \, dy$

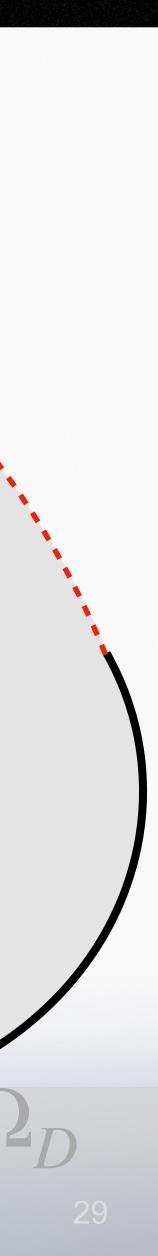
Monte Carlo estimator

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$



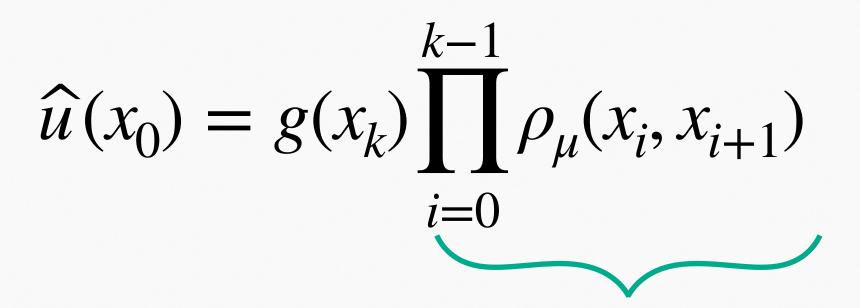


key idea: shrink star-shaped domain to ensure $\rho_u(x, y) \in [0,1]$



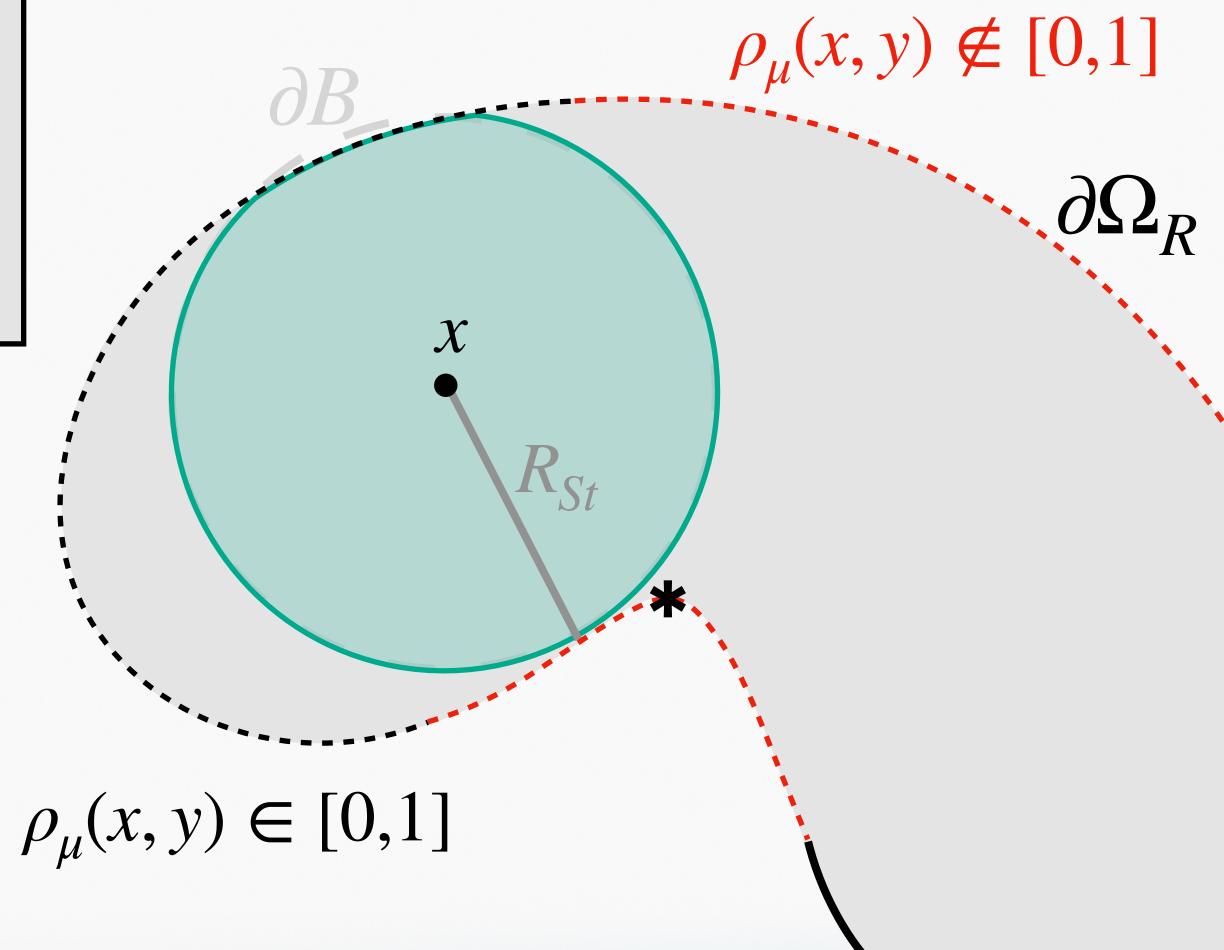
generalized boundary integral $u(x) = \int_{\partial S_t} \rho_{\mu}(x, y) P^B(x, y) u(y) \, dy$

Monte Carlo estimator

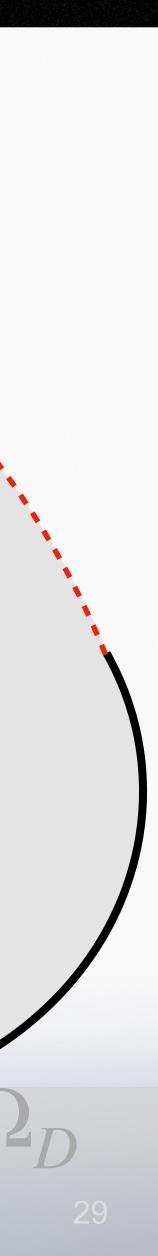


reflectance product bound to [0,1]



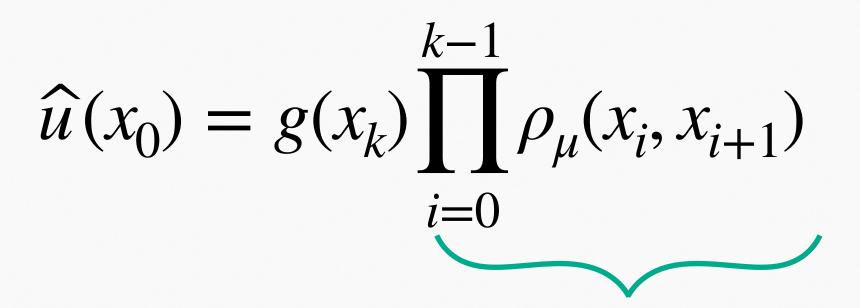


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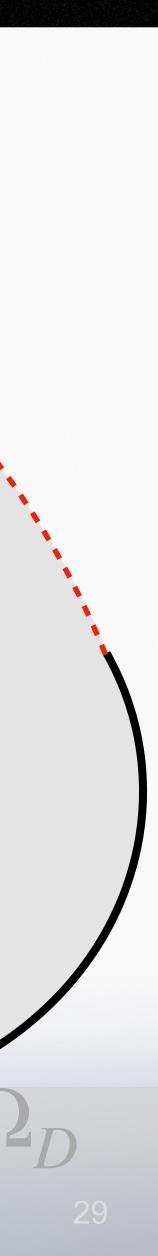


reflectance product bound to [0,1]



same mapping A. Using the corresponding integral operator C_{α}^{St} (29) **F***R* proof of estimator convergence based on operator-theoretic analysis provided in appendix $\int_{\partial \mathrm{St}(x,R)} |\rho_{\mu}(x,y)| dy \int_{\partial \mathrm{St}(x,R)} |P^{\mathrm{B}}(x,y)| dy =$ $\rho_{\mu}(x, y)$

key idea: shrink star-shaped domain to ensure $\rho_{\mu}(x, y) \in [0, 1]$



walk on stars with probabilistic termination

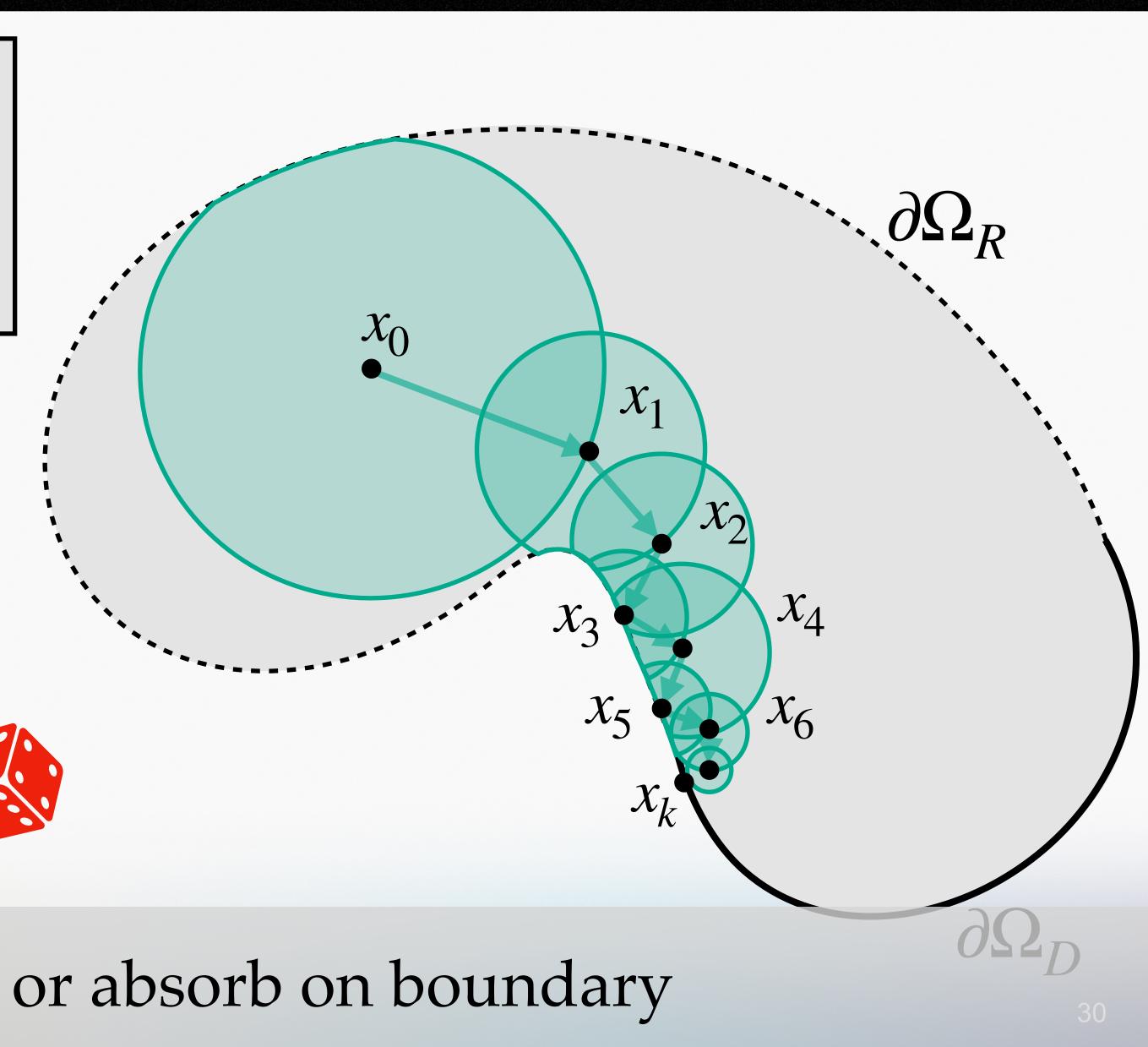
generalized boundary integral $u(x) = \int_{\partial St} \rho_{\mu}(x, y) P^{B}(x, y) u(y) \, dy$

Monte Carlo estimator

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$
apply Russian roulette to terminate walks with low throughput

key idea: probabilistically reflect or absorb on boundary







walk on stars with probabilistic termination

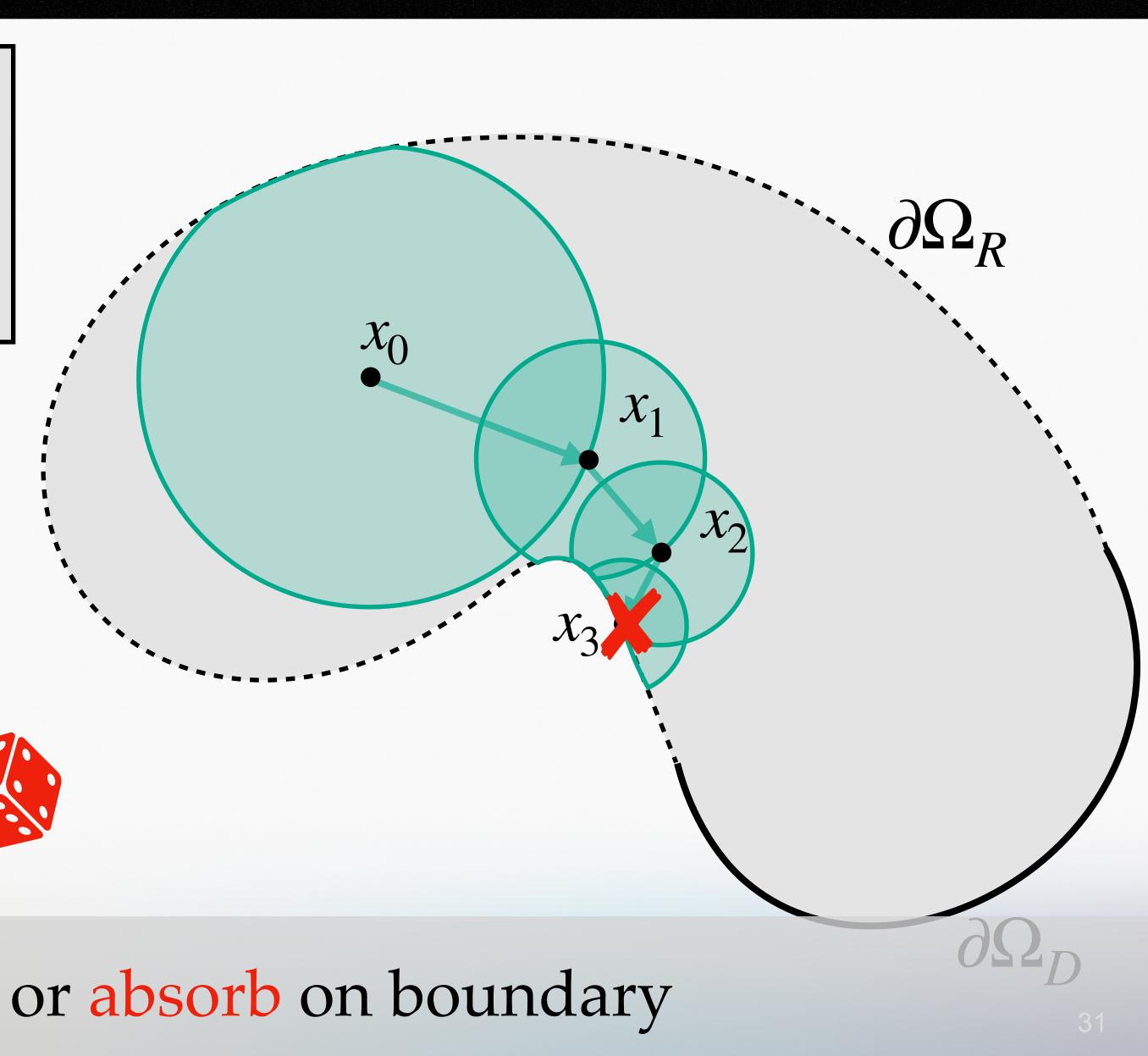
generalized boundary integral $u(x) = \int_{\partial St} \rho_{\mu}(x, y) P^{B}(x, y) u(y) \, dy$

Monte Carlo estimator

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$
apply Russian roulette to terminate walks with low throughput

key idea: probabilistically reflect or absorb on boundary











only minor changes to original walk on stars method:









only minor changes to original walk on stars method:

modulate contributions by reflectance

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$
apply Russian roulette to terminate walks with low throughput









only minor changes to original walk on stars method:

modulate contributions by reflectance

probabilistically terminate paths at each boundary hit

$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$
apply Russian roulette
to terminate walks
with low throughput













only minor changes to original walk on stars method:

modulate contributions by reflectance

probabilistically terminate paths at each boundary hit

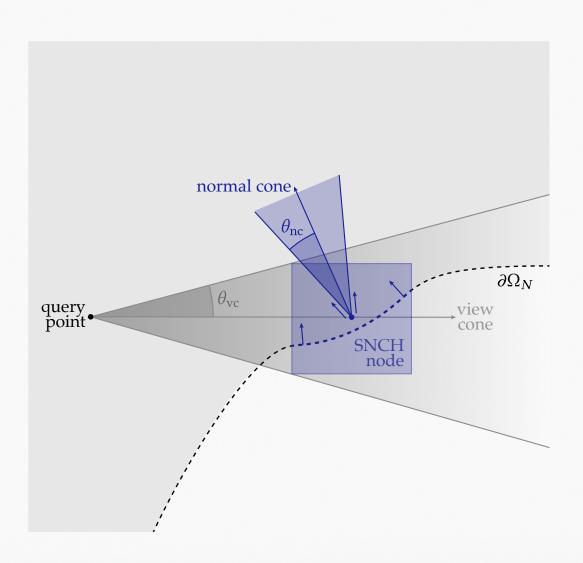
$$\widehat{u}(x_0) = g(x_k) \prod_{i=0}^{k-1} \rho_{\mu}(x_i, x_{i+1})$$
apply Russian roulette
to terminate walks
with low throughput







update SNCH to query reflectance bounds

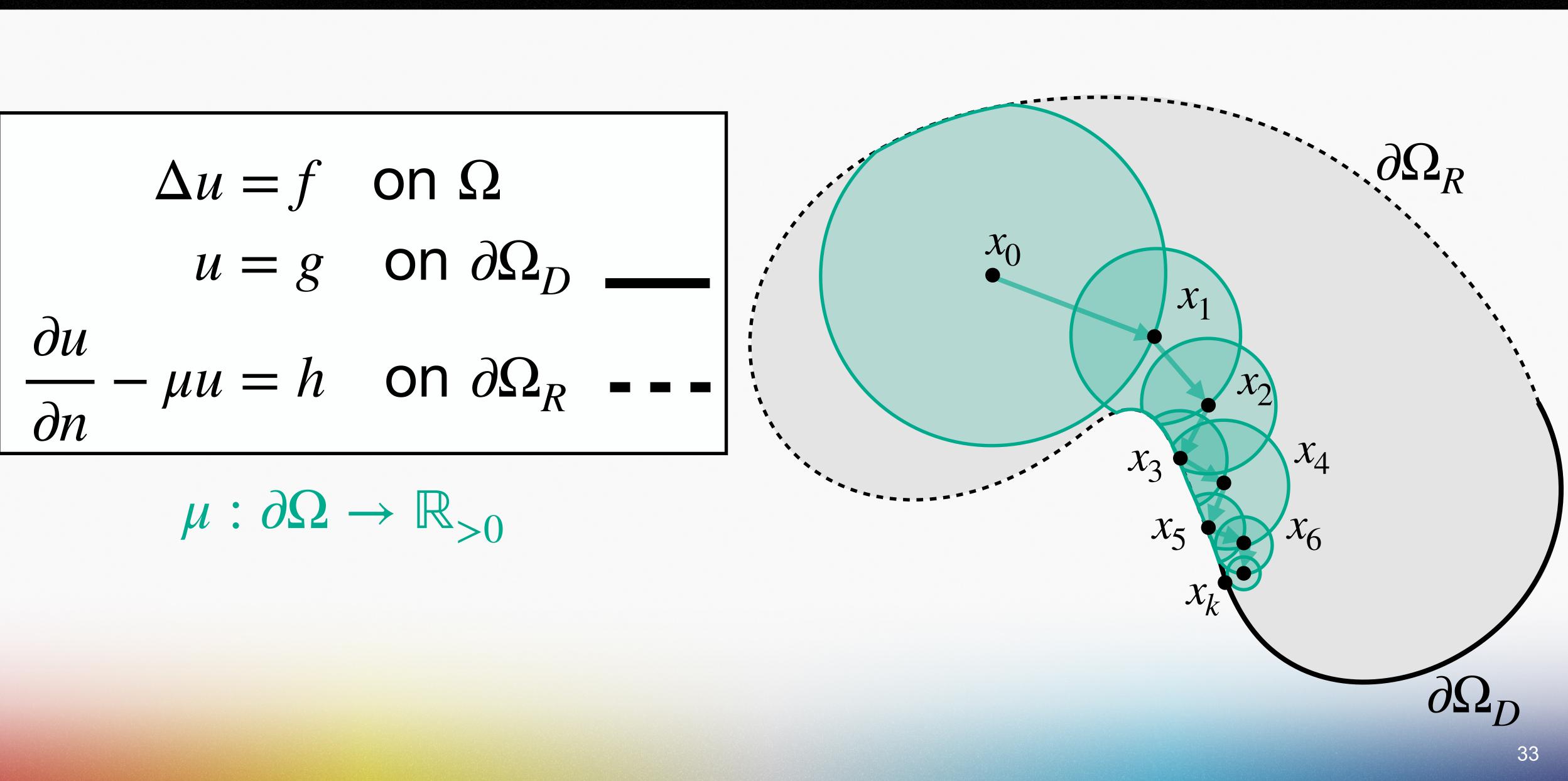






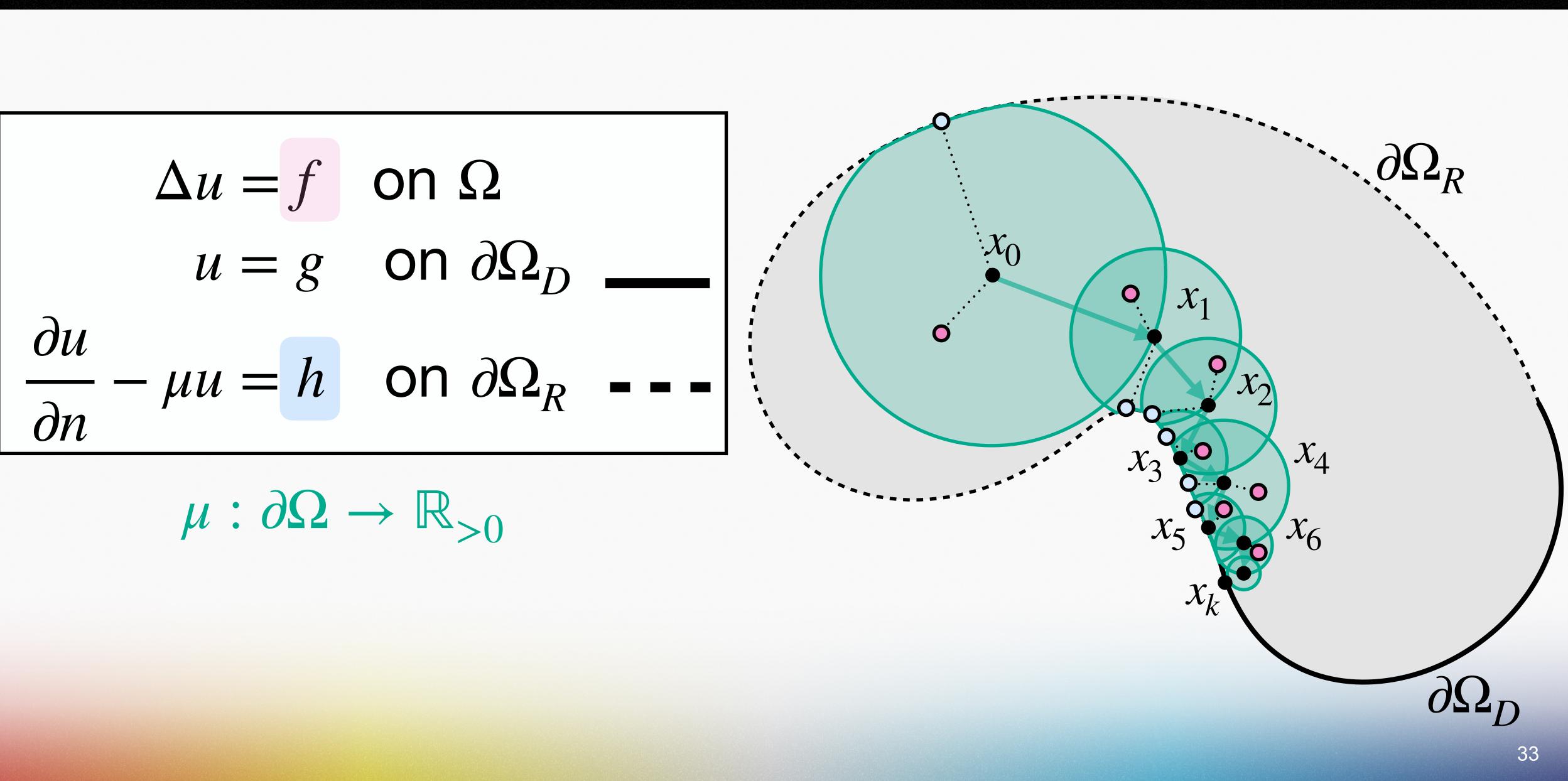


Poisson equation and non-zero Robin condition 🖉 SIGGRAPH 2024





Poisson equation and non-zero Robin condition

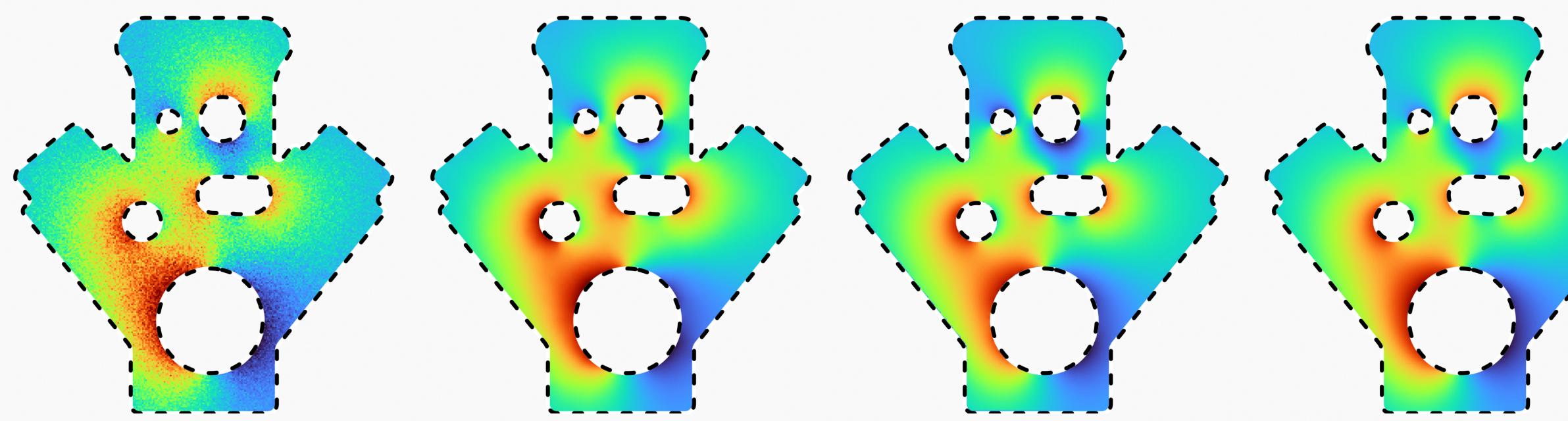




variance reduction

WoSt

reverse WoSt [Qi et al. 2022]



min value max value



boundary value caching

[Miller et al. 2023]

reference

Robin boundary condition

key idea: can directly apply existing variance reduction techniques









EVALUATION

walk on boundary vs walk on stars

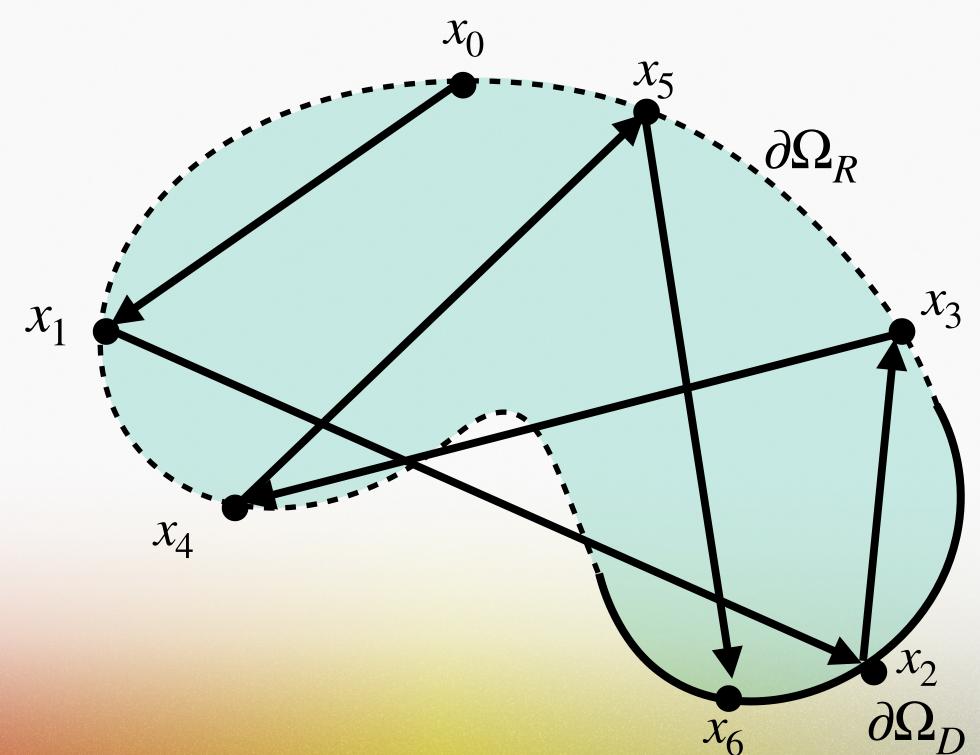
walk on boundary

[Sabelfeld and Simonov 2013, Sugimoto et al. 2023]

branching paths (multiple intersections)

unbounded path throughput

ray trace on entire domain





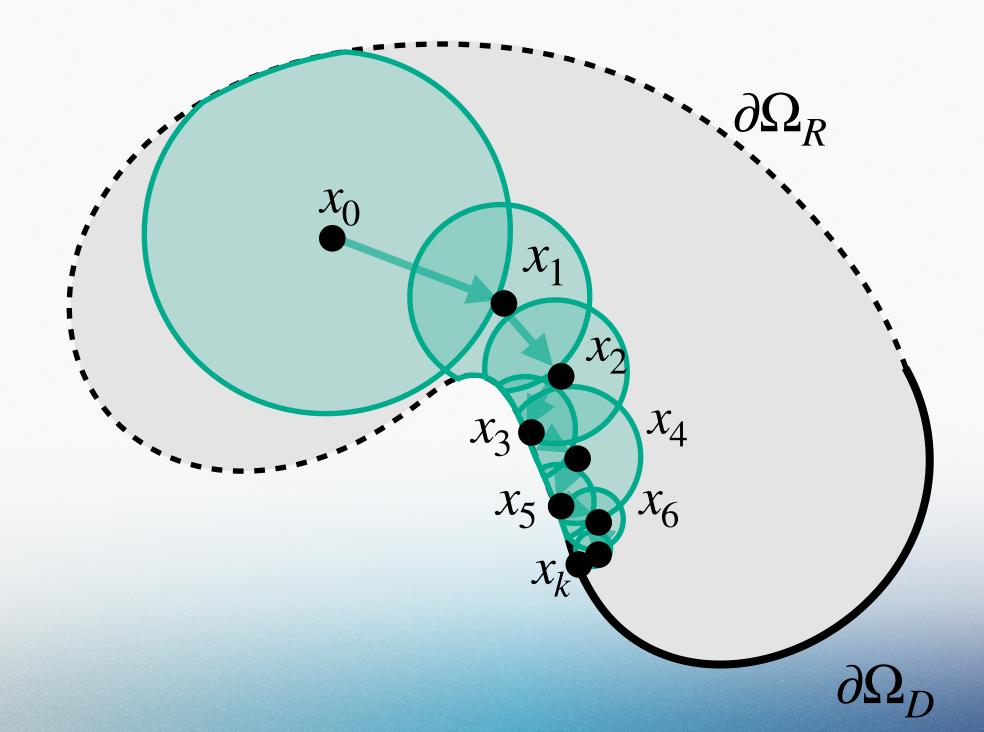
walk on stars

[Sawhney et al. 2023, ours]

no branching (single-intersections)

bounded path throughput [0,1]

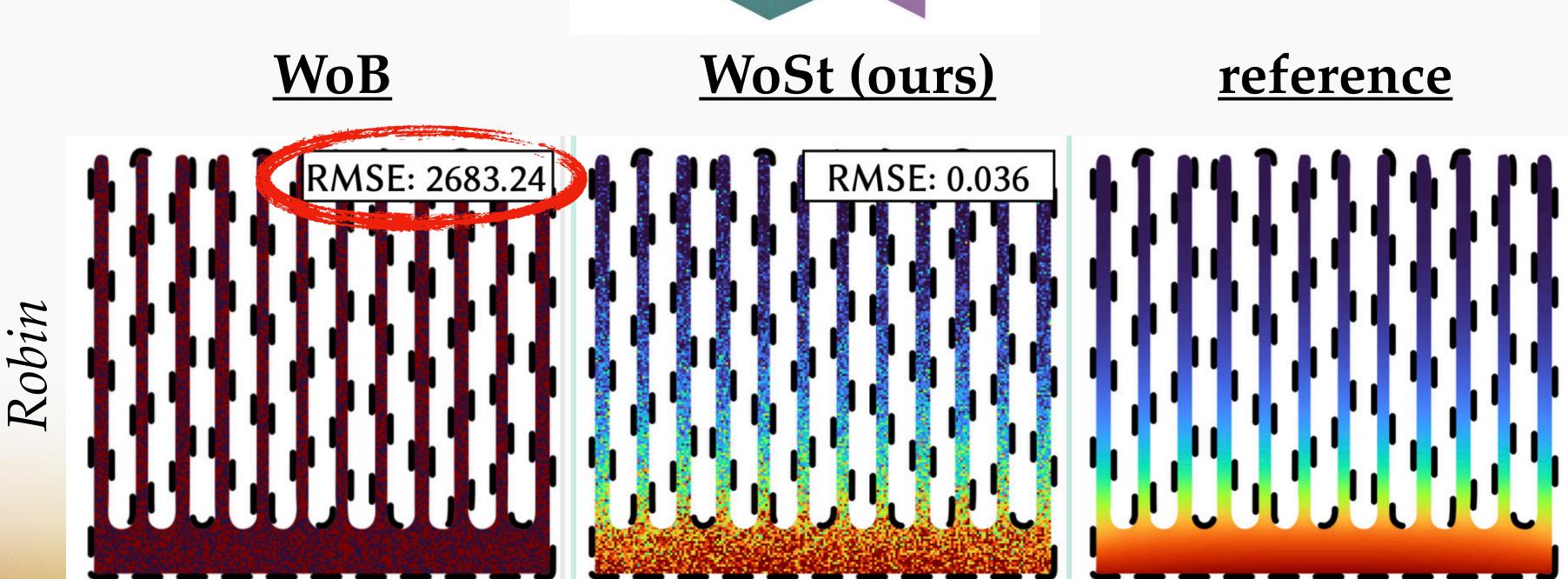
construct star-shaped subomdinas



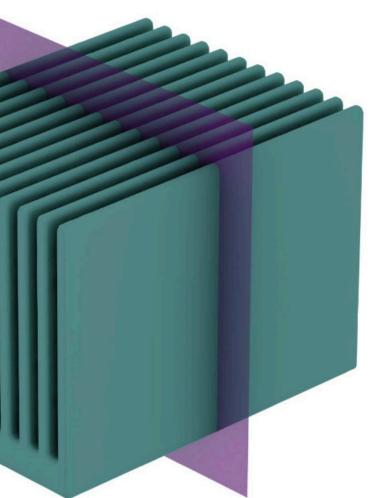




walk on boundary vs walk on stars

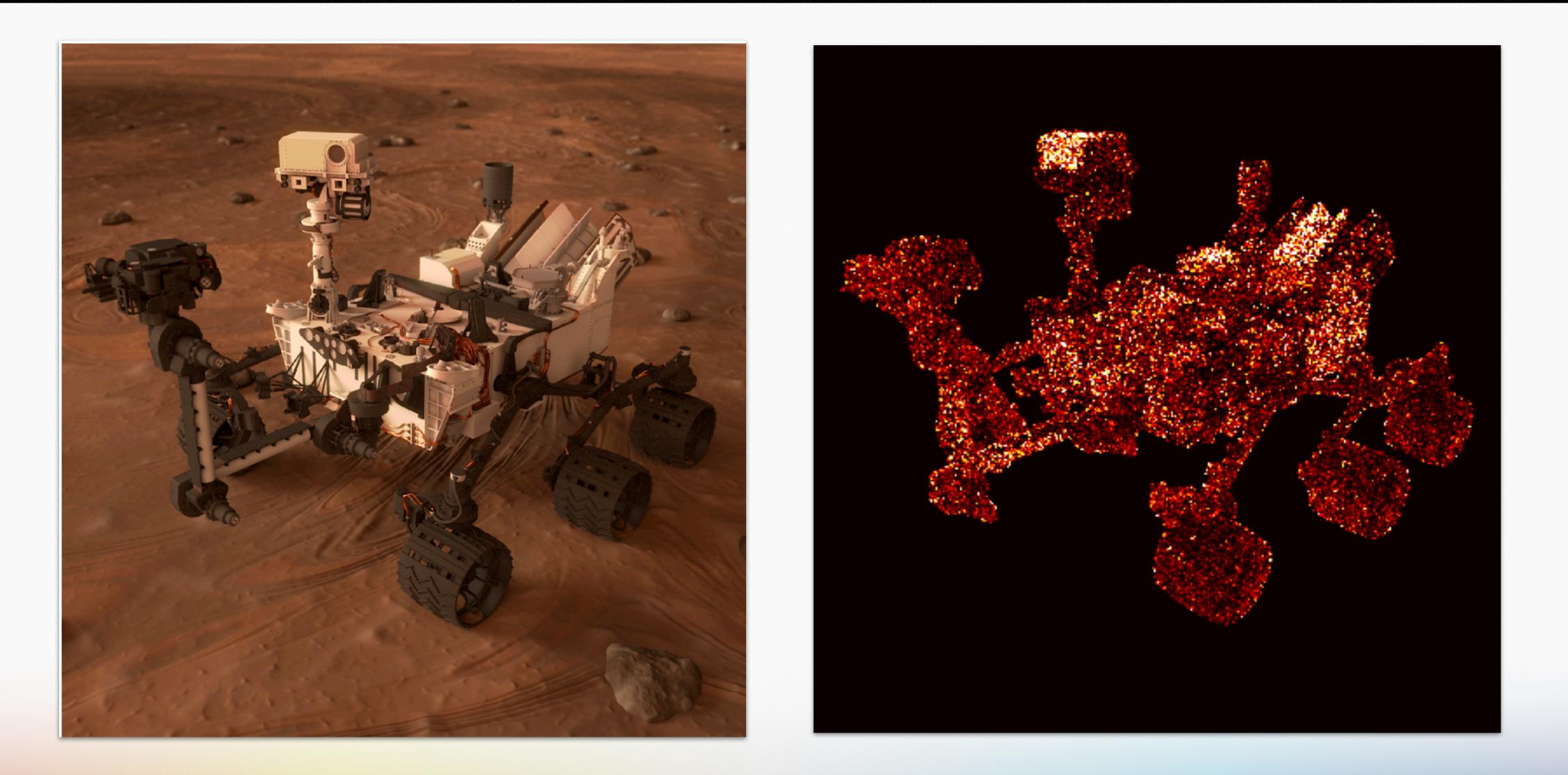








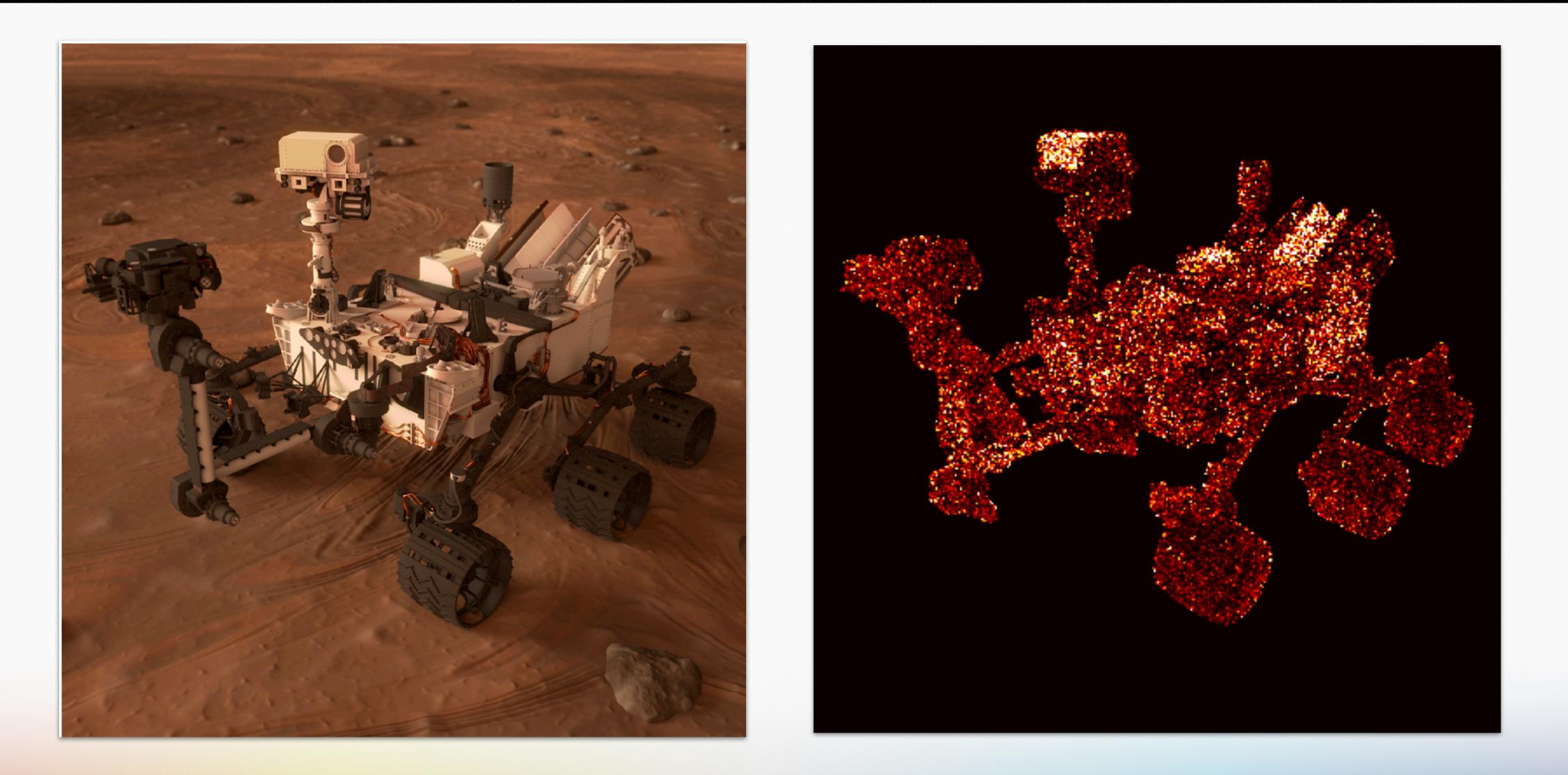








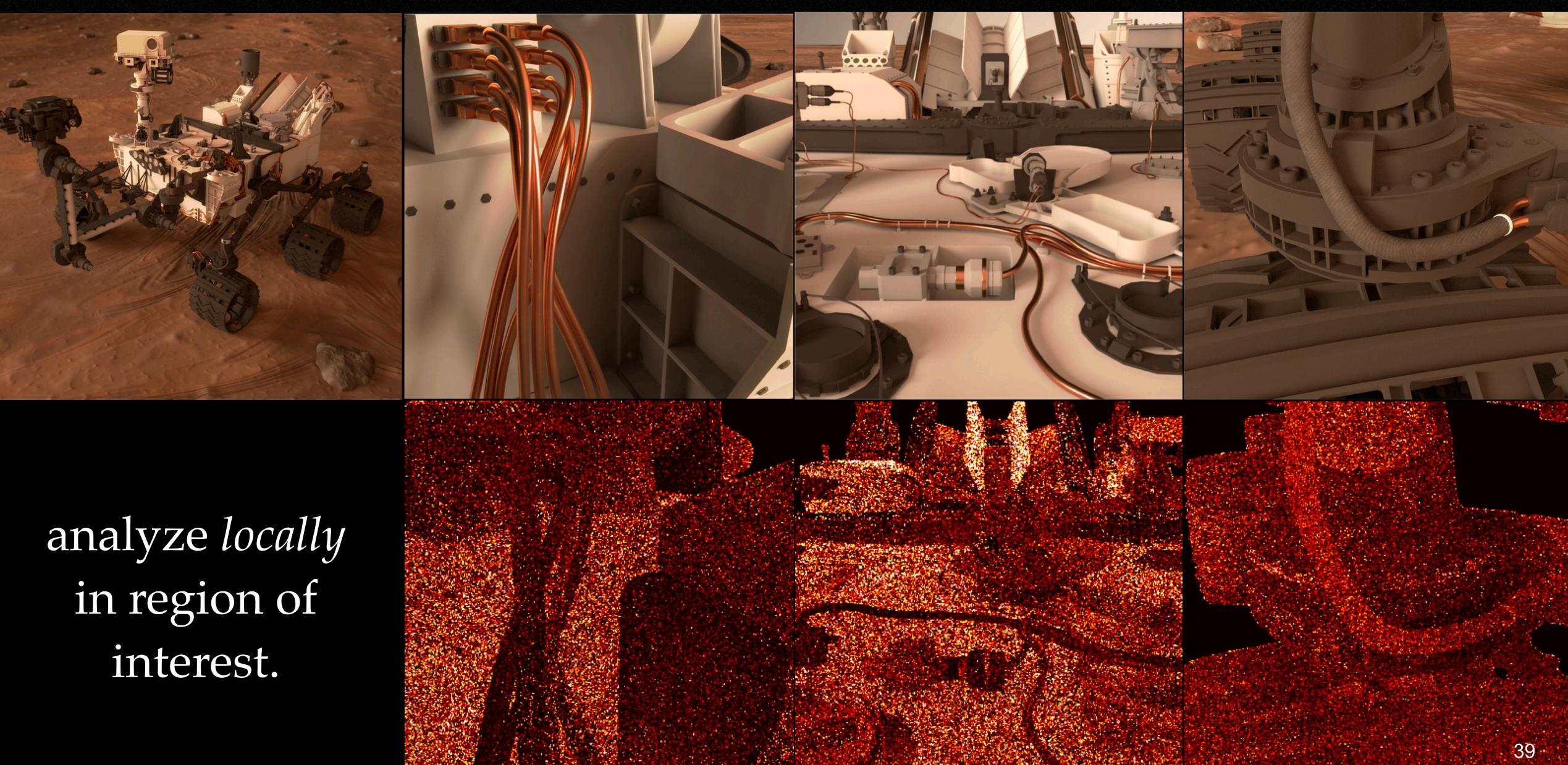








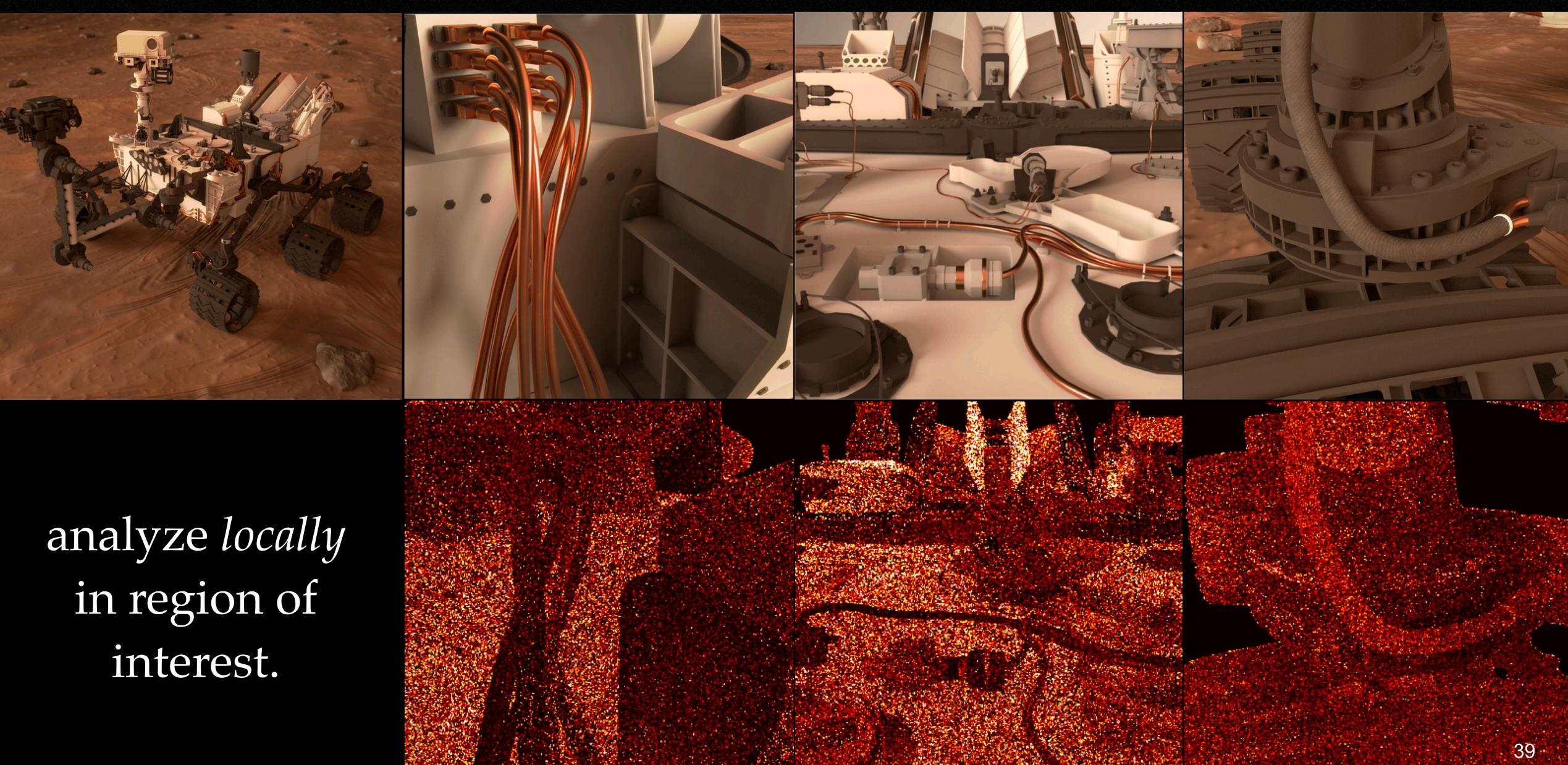








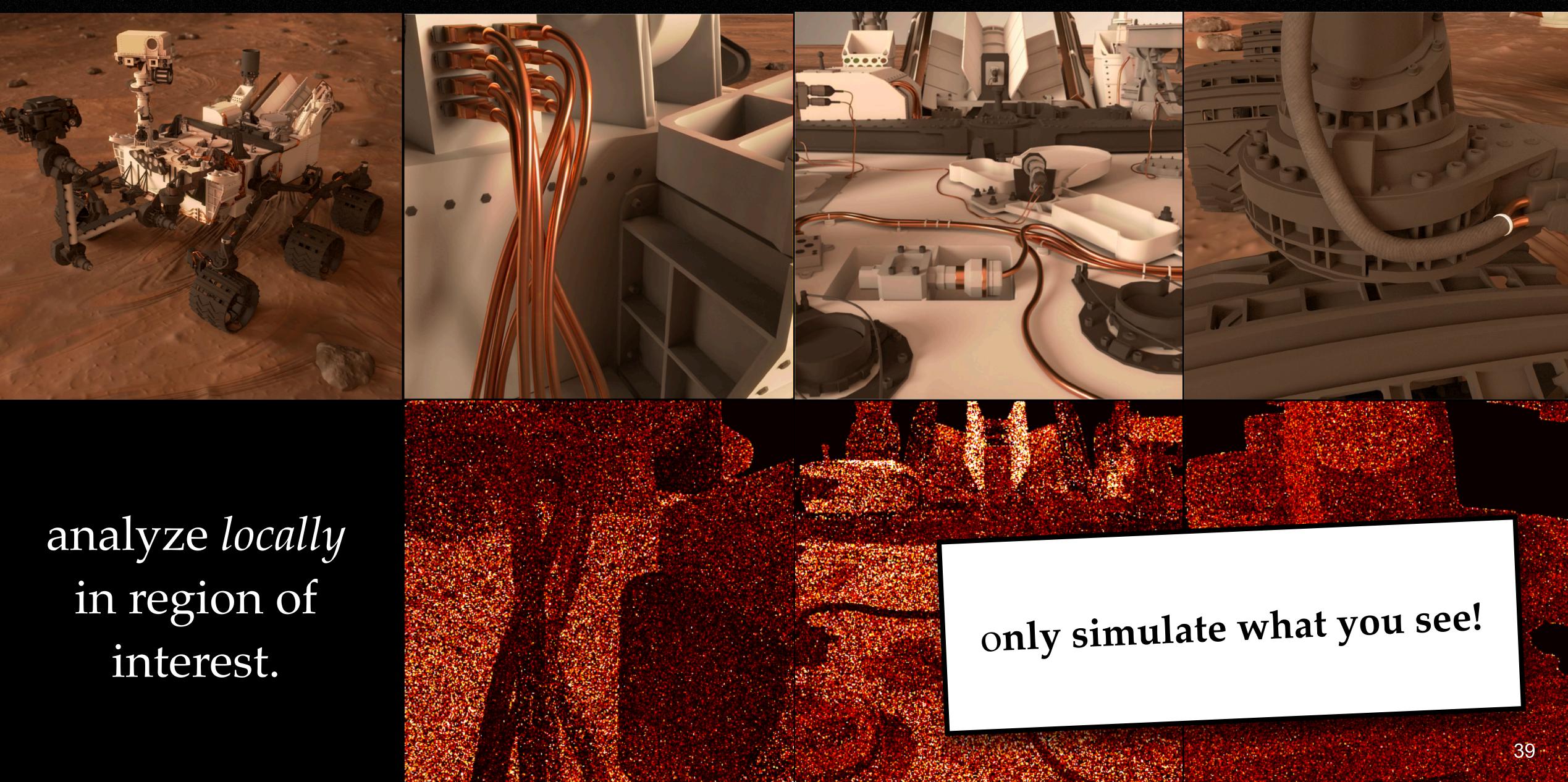
















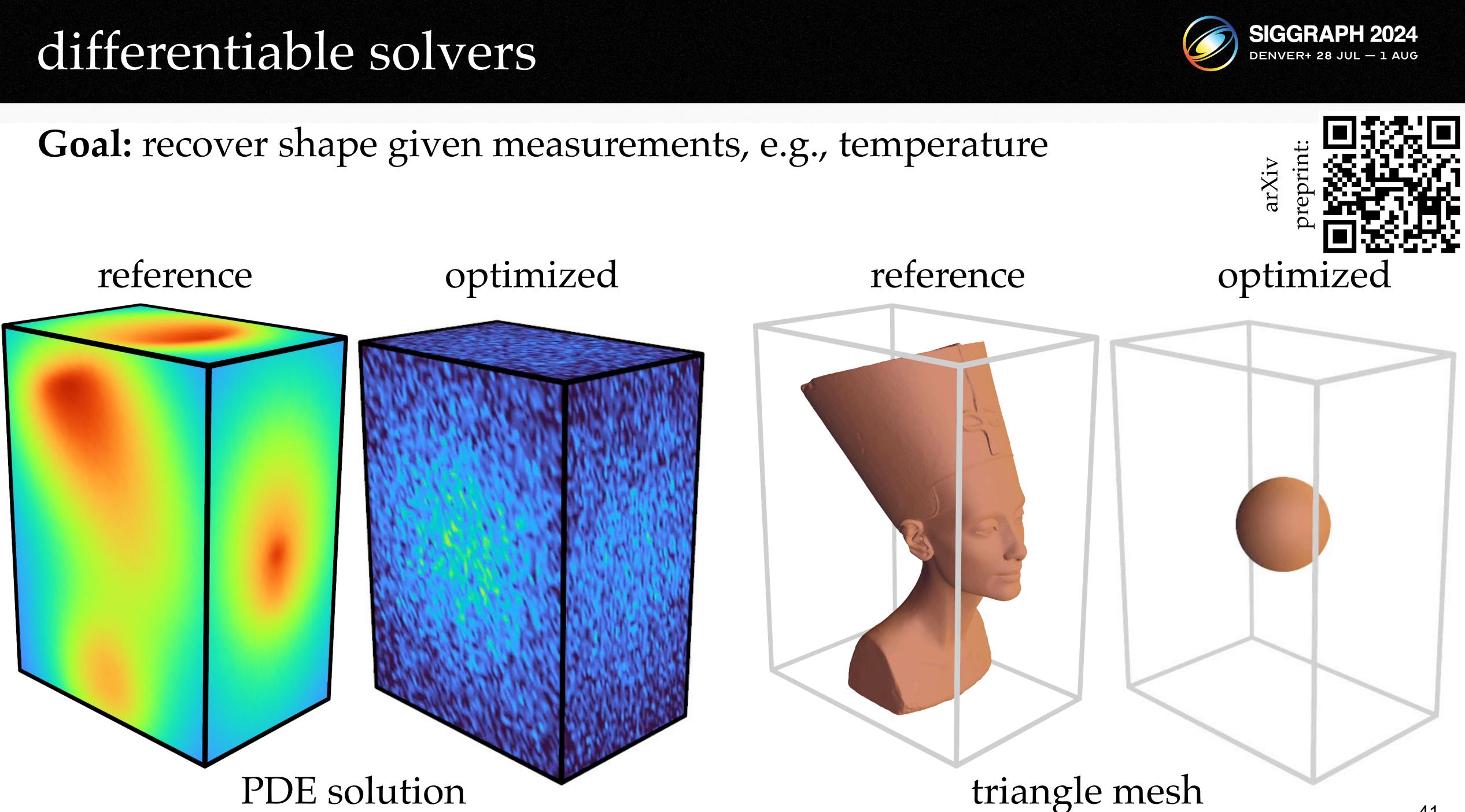






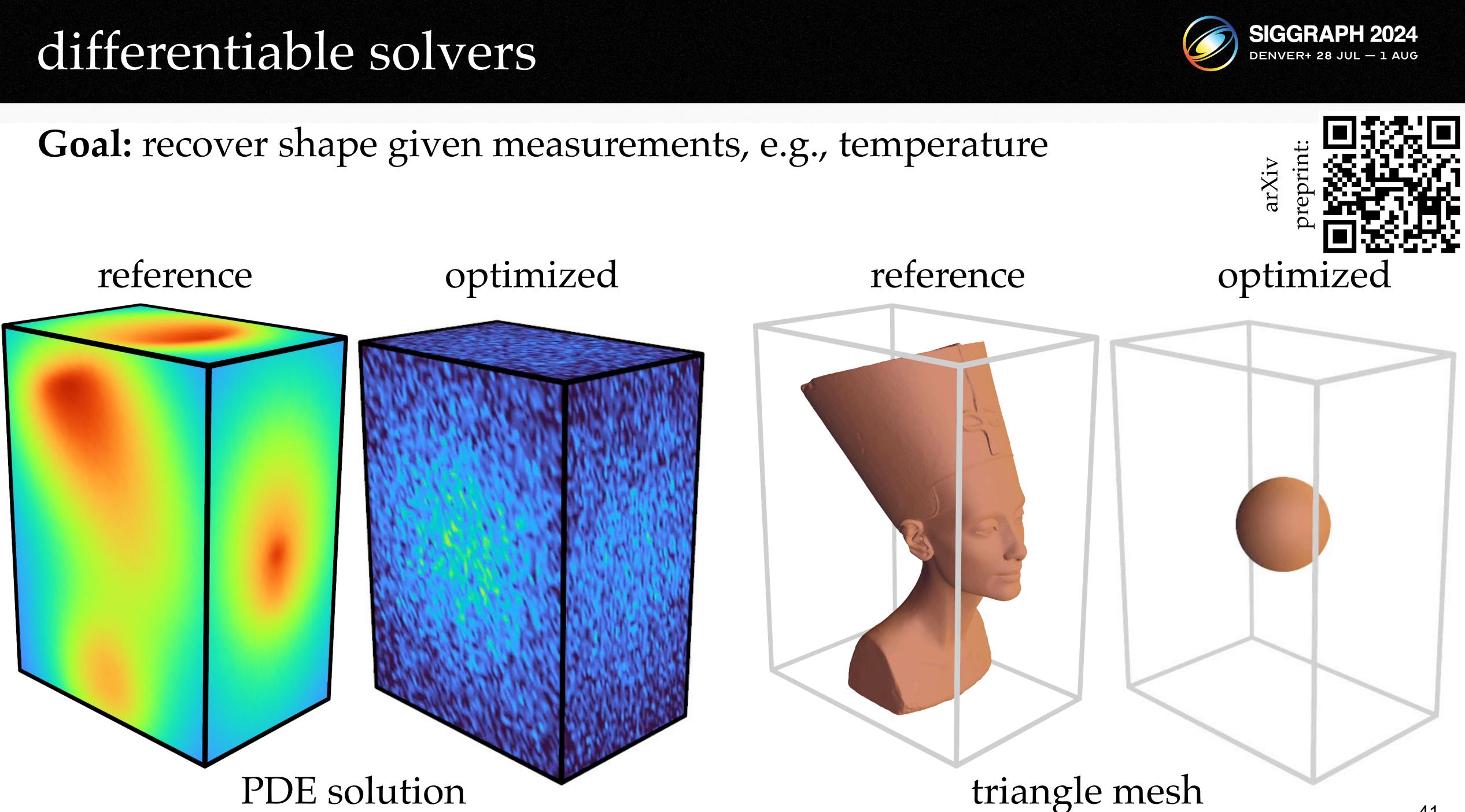
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WHAT'S NEXT?













differentiable solvers

boundary and source terms [Yilmazer et al. 2022]

Solving Inverse PDE Problems using Grid-Free Monte Carlo Estimators

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Modeling physical phenomena like heat transport and diffusion is crucially dependent on the numerical solution of partial differential equations (PDEs). A PDE solver finds the solution given coefficients and a boundary condition, whereas an inverse PDE solver goes the opposite way and reconstructs these inputs from an existing solution. In this article, we investigate techniques for solving inverse PDE problems using a gradient-based methodology.

Conventional PDE solvers based on the finite element method require a domain meshing step that can be fragile and costly. Grid-free Monte Carlo methods instead stochastically sample paths using variations of the walk on spheres algorithm to construct an unbiased estimator of the solution. The uncanny similarity of these methods to physically-based rendering algorithms has been observed by several recent works.

In the area of rendering, recent progress has led to the development of efficient unbiased derivative estimators. They solve an adjoint form of the problem and exploit arithmetic invertibility to compute gradients using a onstant amount of memory and linear time complexity

Could these two lines of work be combined to compute cheap parametric derivatives of a grid-free PDE solver? We investigate this question and present preliminary results.

CCS Concepts: • Mathematics of computing -> Partial differential equations; • Computing methodologies \rightarrow Rendering.

Additional Key Words and Phrases: walk on spheres, Monte Carlo, differentiable simulation, path replay backpropagation

1 INTRODUCTION

Many physical phenomena are naturally described using partial differential equations (PDEs). For example, the heat equation models the spread of thermal energy in a potentially heterogeneous material. Solvers that numerically approximate solutions of such PDEs are in widespread use. We pursue the opposite direction in this article, which is known as an inverse PDE problem: estimating unknown parameters from observations of the solution. This set of unknown parameters could include various PDE coefficients, boundary conditions, and even the shape of the domain.

Such problems arise in diverse scientific and engineering contexts, for example to determine the physical parameters of a thermal conductor from measurements [Cannon 1964]. Electrical impedance tomography [Cheney et al. 1999] seeks to reconstruct the interior of a living organism. Electrodes provide measurements of the electric field, which is influenced by the tissue's conductivity, impedance, and dielectric permittivity.

Our approach entails differentiating the solver and recovering the unknown parameters using gradient descent. However, one issue with conventional PDE solvers based on the finite element method (FEM) is that they require a meshing step that can be fragile

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and computationally costly. An alternative are Monte Carlo PDE solvers based on the walk on spheres (WoS) [Muller 1956]. These grid-free methods sample random paths in the domain to compute unbiased estimates of the solution. Grid-free solvers have recently attracted significant attention in the computer graphics community, partly owing to the remarkable similarities to Monte Carlo rendering methods [Sawhney and Crane 2020] and the algorithmic synergies that this creates [Sawhney et al. 2022; Qi et al. 2022].

A common issue with gradient-based optimization is that the standard approach for reverse-mode differentiation (known as backpropagation) reverses all data dependencies of an underlying computation. When applied to the WoS algorithm, this means that intermediate results of a large number of iterations would need to be stored to enable the subsequent differentiation.

In the field of rendering, recent progress has led to the development of differentiable rendering methods [Gkioulekas et al. 2013; Li et al. 2018; Nimier-David et al. 2019] that estimate parametric derivatives of complete light transport simulations. A similar issue arises here as well: light paths can potentially be very long, particularly in highly-scattering media, which makes naïve reverse-mode differentiation prohibitively memory-intensive. Methods like radiative backpropagation [Nimier-David et al. 2020] and path replay backpropagation [Vicini et al. 2021] cast the differentiation step into an independent simulation of "derivative light" to address this issue. The latter project solves an adjoint version of the underlying equation and furthermore exploits arithmetic invertibility in the computation to differentiate using a constant amount of memory and a runtime cost that is linear in the number of path vertices.

Given these striking similarities, could a similar approach be useful to compute reverse-mode derivatives of grid-free Monte Carlo solvers? We show that this is indeed the case and that this combination yields an unbiased derivative estimator in the same complexity class. The paper presents preliminary results on synthetic inverse problems. We make no claims about the utility of such an approach for solving concrete inverse-PDE problems but find it a promising direction for future work

2 METHOD

2.1 Background

Inverse PDE problems. We seek to solve an inverse PDE problem of the form:

 $\widehat{\boldsymbol{\pi}} = \arg\min\ell(\boldsymbol{u}(\boldsymbol{\pi})),$

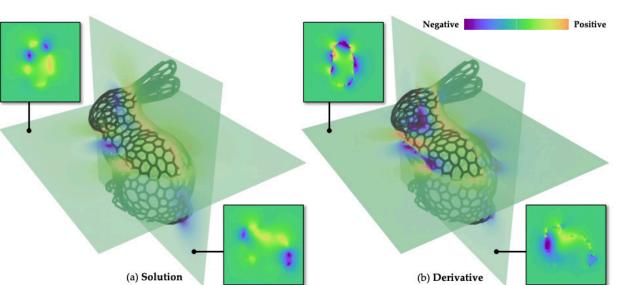
where $u(\pi)$ is the solution of a PDE parameterized by the vector π containing the boundary values, source terms, etc. The function ℓ is a differentiable objective function. In the simplest case, this could be the L_2 difference between the solution of the PDE and a reference solution evaluated at a set of locations spread throughout

ACM Trans. Graph., Vol. 1, No. 1, Article . Publication date: August 2022.

A Differential Monte Carlo Solver For the Poisson Equation

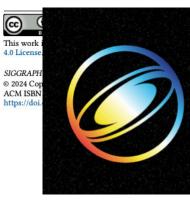
Zihan Yu zihay19@uci.edu University of California, Irvine & NVIDIA USA

> Zhiqian Zhou zhiqiaz8@uci.edu University of California, Irvine USA



ABSTRACT

(PDE) with numerous applications in physics, engineering, and computer graphics. Conventional solutions to the Poisson equation require discretizing the domain or its boundary, which can be very expensive for domains with detailed geometries. To overcome this challenge, a family of grid-free Monte Carlo solutions has recently been developed. By utilizing walk-on-sphere (WoS) processes, these





shape derivatives [Yu et al. 2024, Miller et al. 2024]



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USA

Lifan Wu

Figure 1: We introduce a new grid-free technique to estimate derivatives of solutions to the Poisson equation with respect to arbitrary parameters including domain shapes. This example includes a 3D Laplace problem with Dirichlet boundary conditions on a wired bunny shape. We visualize the solution to this problem in two cross-sectional planes in (a) and the derivative of this solution (with respect to the translation of the bunny) estimated with our method in (b).

The Poisson equation is an important partial differential equation

techniques are capable of efficiently solving the Poisson equation over complex domains. In this paper, we introduce a general technique that differentiates

solutions to the Poisson equation with Dirichlet boundary conditions. Specifically, we devise a new boundary-integral formulation for the derivatives with respect to arbitrary parameters including shapes of the domain. Further, we develop an efficient walk-onspheres technique based on our new formulation-including a new approach to estimate normal derivatives of the solution field. We demonstrate the effectiveness of our technique over baseline meth-

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Differential Walk on Spheres

BAILEY MILLER, Carnegie Mellon University, USA **ROHAN SAWHNEY, NVIDIA, USA** KEENAN CRANE, Carnegie Mellon University, USA IOANNIS GKIOULEKAS, Carnegie Mellon University, USA

to a partial differential equation (PDE) with respect to problem parameters

(such as domain geometry or boundary conditions). Derivatives can be eval-

uated at arbitrary points without performing a global solve, or constructing

a volumetric grid or mesh. The method is hence well-suited to inverse prob-

lems with complex geometry, such as PDE-constrained shape optimization

Like other walk on spheres (WoS) algorithms, our method is trivial to paral-

lelize, and is agnostic to boundary representation (meshes, splines, implicit

surfaces etc.), supporting large topological changes. We focus in particular

on screened Poisson equations, which model diverse problems from scien-

estimate derivatives with respect to all parameters-hence, cost does not

grow significantly with parameter count. In practice, even noisy deriva-

tive estimates exhibit fast, stable convergence for stochastic gradient-based

optimization-as we show via examples from thermal design, shape from

 $\label{eq:ccs} \text{CCS Concepts:} \bullet \textbf{Computing methodologies} \to \textbf{Physical simulation};$

Additional Key Words and Phrases: Walk on spheres, differentiable simulation

diffusion, and computer graphics.

Rendering

tific and geometric computing. As in differentiable rendering, we jointly

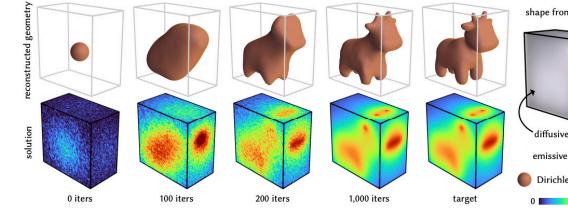


Figure 1. For a given PDE, our differential walk on spheres algorithm makes it possible to differentiate solution values with respect to problem parameters. Here we consider an inverse problem where we recover the shape of an emissive object from its observed diffusion profile on the boundary of a box, via gradient-based optimization. Unlike conventional mesh- or grid-based approaches, we can evaluate derivatives at points of interest without needing to compute a global solution (here, only at the observed points).

We introduce a Monte Carlo method for evaluating derivatives of the solution **Reference** Format:

Bailey Miller, Rohan Sawhney, Keenan Crane, and Ioannis Gkioulekas. 2024. Differential Walk on Spheres. Technical Report 1, 1 (May 2024), 17 pages. https://doi.org/10.1145/nnnnnn.nnnnn

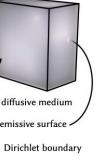
INTRODUCTION

Which shape best explains observed physical behavior? How can one design shapes that maximize (or minimize) a target physical quantity? Such inverse problems are fundamental to numerous challenges in science and engineering. For instance, one might need to assess damage to an airplane wing using indirect thermal measurements [Zalameda and Parker 2014], or infer the shape of a tumor through deep layers of tissue [Arridge 1999]. Likewise, one might seek to design circuit geometry that maximizes dissipation of heat [Zhan et al. 2008], airfoils that generate prescribed lift [Hicks and Henne 1977], or lightweight structures that withstand significant load [Allaire et al. 2014]. To solve such problems, one must be able to efficiently and accurately differentiate solutions to partial differential equations (PDEs) with respect to the shape of the domain, or its boundary conditions [Hadamard 1908; Céa et al. 1973]. However, for problems with complex geometry, even just solving such PDEs



May

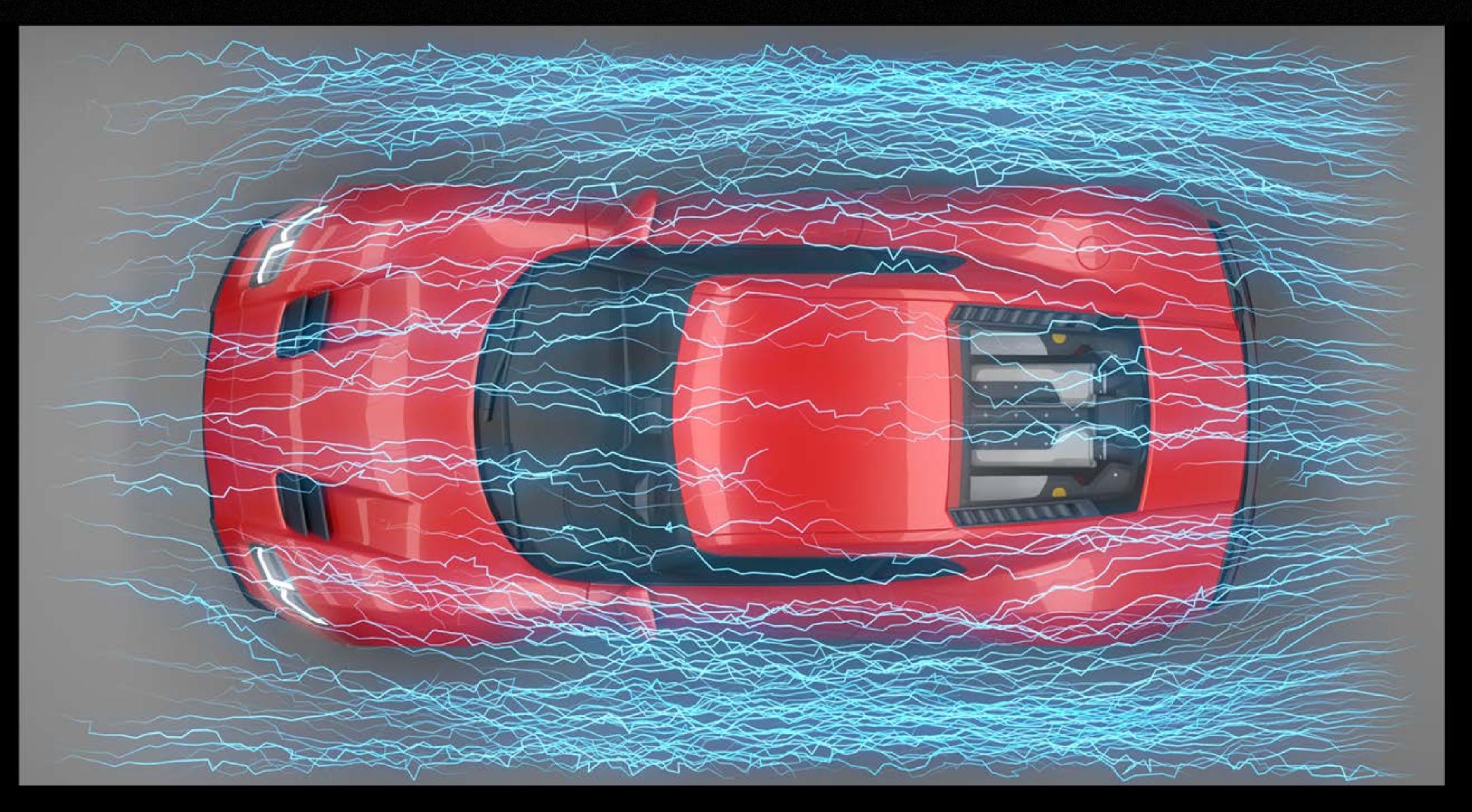








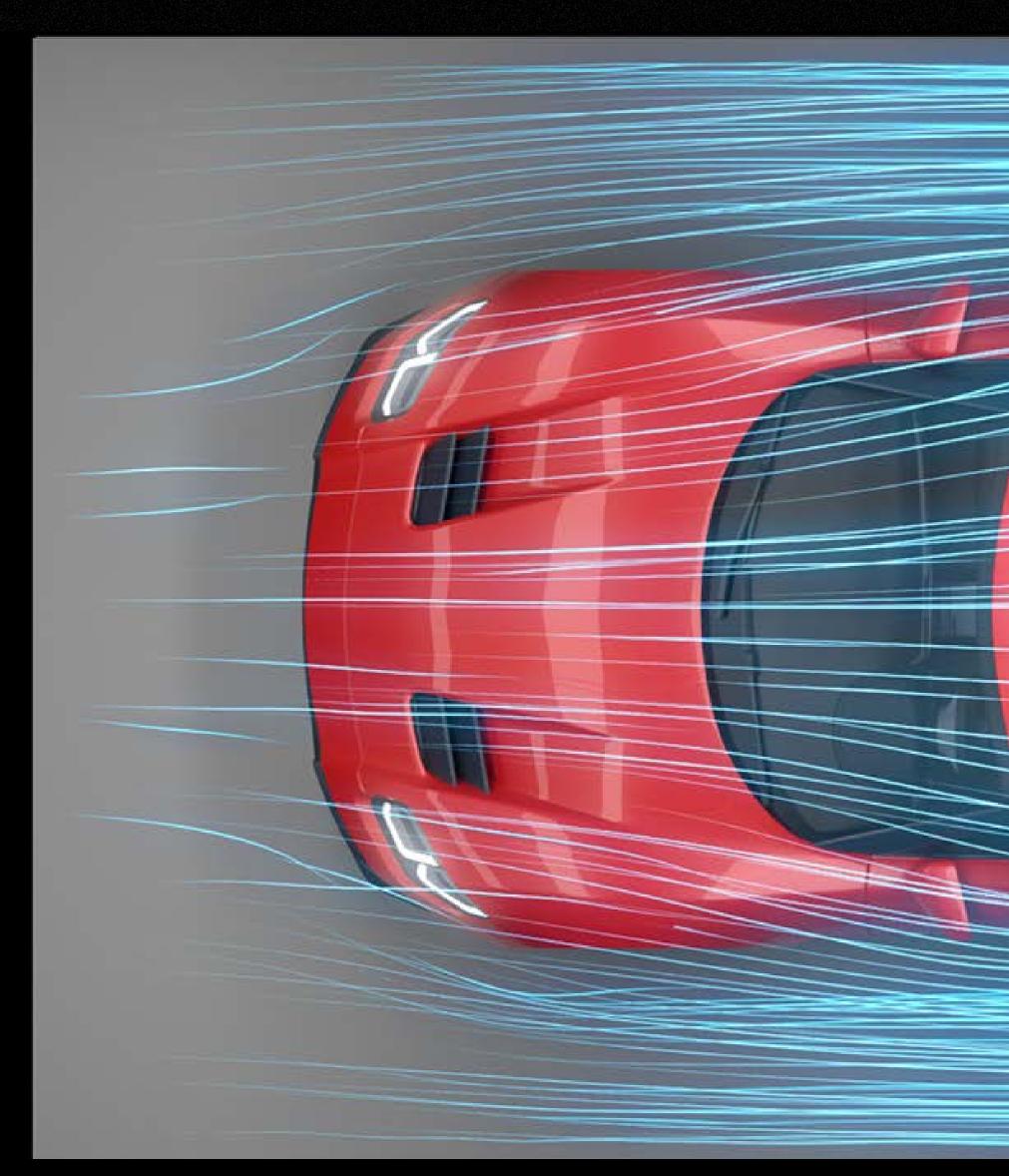
variance reduction, variance reduction, var.





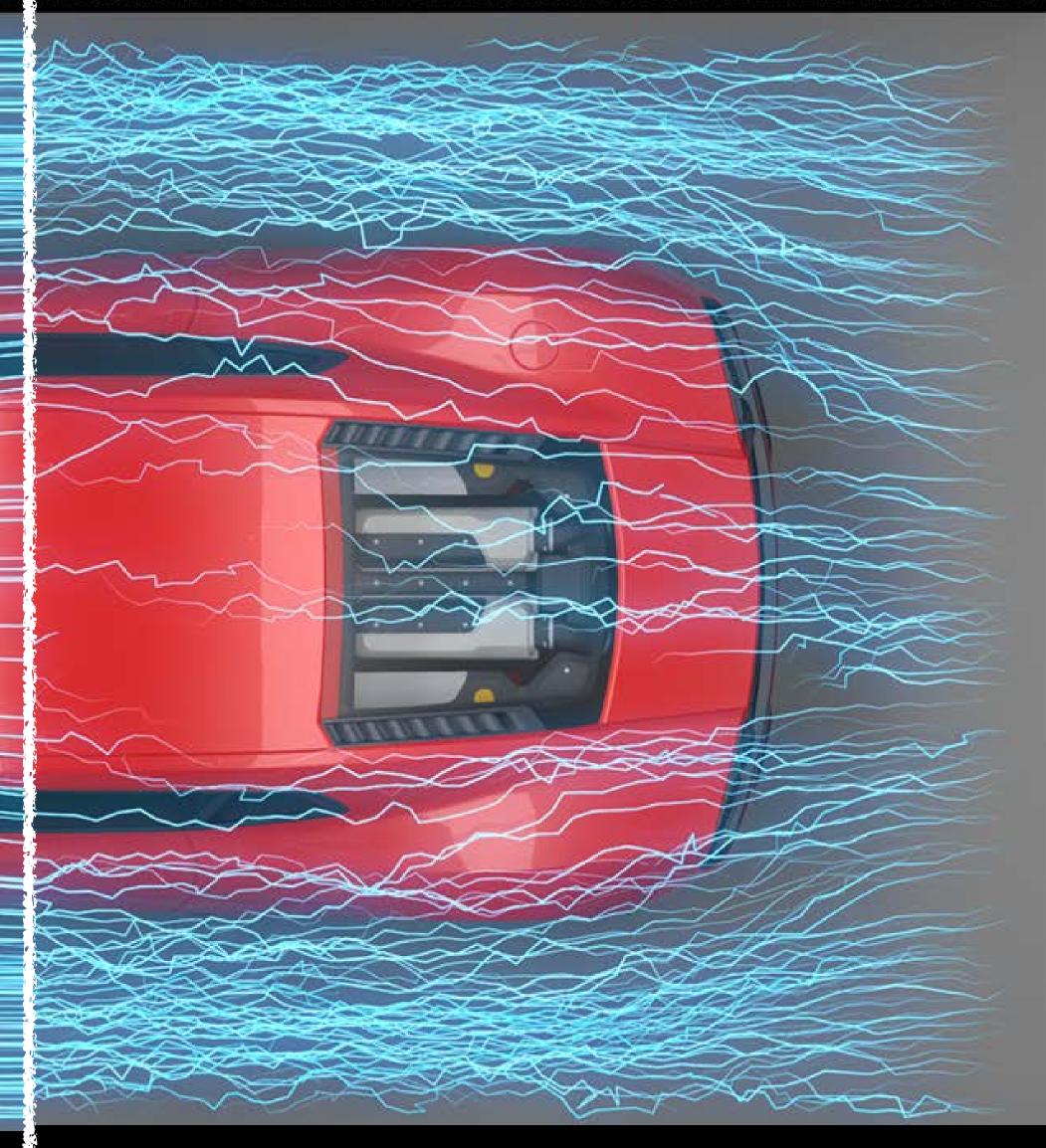
pointwise estimator

variance reduction, variance reduction, var.



boundary value caching [Miller et al. 2023]





pointwise estimator

variance reduction, variance reduction, var.

caching methods

[Miller et al. 2023, Bakbouk and Peers 2023, Li et al. 2023]

Boundary Value Caching for Walk on Spheres

BAILEY MILLER*, Carnegie Mellon University, USA ROHAN SAWHNEY*, Carnegie Mellon University and NVIDIA, USA KEENAN CRANE[†], Carnegie Mellon University, USA IOANNIS GKIOULEKAS[†], Carnegie Mellon University, USA



Pieter Peers

ply performing the first step in a W

ume instead of its boundary leads to reduces Monte Carlo noise over m

overing a volume. We also show th

erty leads to an efficient caching s

formly distributed cache samples.

between evaluation points, we desc

sampling strategy. Furthermore, w

mean value property to improve

when using a low number of cache

by recursively applying the volum

also reduce the variance in the cach

We validate our mean value ca

Neural Caches for Monte Carlo Partial Differential Equation Solver

Guandao Yang*

Zilu Li* Cornell Universit zl327@cornell.ed Christopher De Sa

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Xi Deng Cornell Universit xd93@cornell.edu Steve Marschner Cornell University

srm@cs.cornell.edu

WoS. 2022 Reference

Figure 1: We visualize a slice of the solution to an elliptic PDE within a dragon-shaped boundary. Our hybrid solver can reduce the error of the neural field baseline, while achieving lower variance compared to the Walk-on-Spheres [Sawhney et al. 2022] method when working within the constraints of a limited computing budget ABSTRACT

Zilu Li, Guandao Yang, Xi Deng, Christopher De Sa, Bharath Harihara and Steve Marschner. 2023. Neural Caches for Monte Carlo Partial Di ferential Equation Solver. In SIGGRAPH Asia 2023 Conference Papers (SA Conference Papers '23), December 12-15, 2023, Sydney, NSW, Australia. ACM New York, NY, USA, 10 pages. https://doi.org/10.1145/3610548.361814

1 INTRODUCTION

Solving elliptic PDEs is critical for various computer graphics ap plications, including 3D reconstruction, animation, and physics simulation. Conventional PDE solvers, however, typically involve suming and error-prone discretization of space with finite elements or meshes. Monte Carlo PDE solvers based on the Walk on Spheres (WoS) algorithm [Sawhney and Crane 2020: Sawhney et al 2023, 2022] offer a way to circumvent these issues by estimating so lution values without discretization. These solvers, however, suffer from high variance, making them slow as they require numerou samples to reduce the variance. This prevents their use in many

An alternative to both discretized and Monte Carlo solvers is to are a class of neural networks that take spatial coordinates as inpu and output values of a continuous field [Raissi et al. 2019; Xie et al. be used to optimize a neural field so that it satisfies a given PDE

1. Introduction

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tion estimate at a single evaluation point. However, in many prac-tical cases, the solution over the whole volume or region of in-terest in the volume is desired. Because the solution estimate is PDEs and show that we can redu our contributions are: computed for each evaluation point separately and independently, A hybrid volume and boundary many similar sub-walks are recomputed multiple times. To re-

ilarity to path tracing, many Monte trategies from rendering have been

Ghada Bakbouk

Abstract Walk on Spheres (WoS) is a grid-free Monte Carlo method for numerically estimating solutions for ellip equations (PDE) such as the Laplace and Poisson PDEs. While WoS is efficient for computing a so evaluation point, it becomes less efficient when the solution is required over a whole domain or a computes a solution for each evaluation point separately, possibly recomputing similar sub-walks mult evaluation points. In this paper, we introduce a novel filtering and caching strategy that leverages : property (in contrast to the boundary mean value property that forms the core of WoS). In addition, to sparse cache regimes, we describe a weighted mean as well as a non-uniform samiline method. Final

sparse cache regimes, we describe a weighted mean as well as a non-uniform sampling method. Final reduce the variance within the cache by recursively applying the volume mean value property on the ca

College of William & Mary

duce recomputation, prior work looked at interpolation with Movduce recomputation, prior work looked at interpolation with Movie Carlo noise over uniformly a large number of reverse walks to ensure a sufficiently dense over-lap with each evaluation point. In this paper we present a novel method for reusing forward

In this paper we present a novel method for reusing *forward* walks that is easy to implement in existing WoodS frameworks. At the core of our method is the *volume mean value property*, hence we call our method (volume) mean value caching. The volume mean value property that enables walking on spheres. We show that sim-value property that enables walking on spheres. We show that sim-

sium on Rendering (2023

 $\begin{array}{l} \textbf{CCS Concepts} \\ \bullet \textit{Computing methodologies} \rightarrow \textit{Shape analysis} \end{array}$

Partial differential equations (PDEs) form the basis of many fun-

damental computer graphics problems. The recently introduced Monte Carlo Geometry Processing (MC-GP) framework [SC20]

offers an exciting new strategy for solving PDEs defined over vo

unes without the need to discretize or create a grid. At its core MC-GP builds on the Walk on Spheres (WoS) algorithm for solvin, PDEs. Due to its conceptual similarity to path tracing, many Mont

plied to MC-GP, such as importance sampling [SC20] and re-rse and bidirectional algorithms [OSBJ22].

Monte Carlo techniques are very effective for computing a solu-

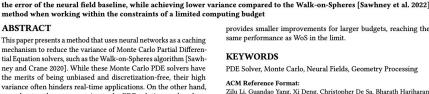
1. Introduction

T. Ritschel and A. Weidlich (Editor

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DOI: 10.2312/sr.20231120

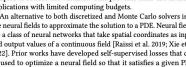




variance often hinders real-time applications. On the other hand, neural networks can approximate the PDE solution, and evaluating these networks at inference time can be very fast. However ons may suffer from convergence difficulties and high bias. Our hybrid system aims to combine these two potentially complementary solutions by training a neural field to imate the PDE solution using superon from a WoS sol This neural field is then used as a cache in the WoS solver to reduce variance during inference. We demonstrate that our neural field training procedure is better than the commonly used self-supervised objectives in the literature. We also show that our hybrid solver exhibits lower variance than WoS with the same computational budget: it is significantly better for small compute budgets and

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applications with limited computing budgets.



2022]. Prior works have developed self-supe

Mean Value Caching for Walk on Spher





sampling methods [Qi et al. 2022]

control variates [Sawhney and Crane 2020, Li et al. 2024]

ium on Rendering 2022 A. Ghosh and L.-Y. Wei

Volume 41 (2022), Number 4

A bidirectional formulation for Walk on Spheres

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Numerically solving partial differential equations (PDEs) is central to many applications in computer graphics and scientific modeling. Conventional methods for solving PDEs often need to discretize the space first, making them less efficient for complegeometry. Unlike conventional methods, the walk on spheres (WoS) algorithm recently introduced to graphics is a grid-free Monte Carlo method that can provide numerical solutions of Poisson equations without discretizing space. We draw analogies between WoS and classical rendering algorithms, and find that the WoS algorithm is conceptually equivalent to forward path tracing. Inspired by similar approaches in light transport, we propose a novel WoS reformulation that operates in the reverse direction, starting at source points and estimating the Green's function at "sensor" points. Implementations of this algorithm show improvement over classical WoS in solving Poisson equation with sparse sources. Our approach opens exciting avenues for future algorithms for PDE estimation which, analogous to light transport, connect WoS walks starting from sensors and source and combine different strategies for robust solution algorithms in all cases

CCS Concepts • Computing methodologies \rightarrow Ray tracing; Modeling and simulation; • Mathematics of computing \rightarrow Stochastic processes

Monte Carlo methods have been very successful in rendering. They provide accurate solution estimates to the rendering equation ij86] in very complex scenes with an often simple im tion compared to mesh based methods such as radiosity [CW93; GTGB84]. While initially Monte Carlo methods were comm slow and of mostly academic interest, they now form the predomi nant rendering methodology in movie production [CJ16; FHF*17] and increasingly in interactive applications such as games.

Catalyzed by the recent introduction of the walk-on-spheres (WoS) algorithm [Mul56] to graphics [SC20; SSJC22], a similar development is now happening for numerical solvers of partial differential equations (PDEs). Analogous to path tracing in rendering, WoS uses random walks to compute point estimates of the solution of harmonic PDEs [Eva10]. These equations are of great importance in many areas of science since they can model natural phere such as heat dissipation, diffusion of electrostatic charges, and distribution of water in soil. Additionally, diffusion equations are often used in rendering and related fields to approximate the behaviour of light in highly scattering media [JMLH01; Sta95].

Analogous to path tracing, existing WoS algorithms start "paths" (i.e. walks) at "sensor points" and end them at "lights" (i.e. boundary points). This works well when the probability of finding source points is high, but produces high variance for sparse sources.

Because of the apparent parallels between the Monte Carlo algorithms used for solving rendering problems and those solving PDEs,

we hope to leverage the decades of rendering research and apply them to PDEs to develop new robust and efficient Monte Carlo PDE solvers. A major step in rendering was the transition from unidirectional "forward" methods like path tracing to "backward' methods such as light tracing, photon mapping [Jen96] and virtual point lights (VPLs) [Kel97]. This precipitated the comprehensive framework of bidirectional rendering methods [Vea97] and, ulti-mately, the wealth of transport methods available today [PJH16]. In this paper, we mirror this development and propose extensions of WoS in both forward and backward directions

The standard "forward" WoS algorithm leverages the mean value theorem to form recursive estimators for the solution. We instead formulate a mean value theorem for the Green's function. This allows us to derive a new class of WoS algorithm that start paths "backwards" from source and boundary points, distributing energy more evenly throughout the domain, before connecting either to sensor points directly, or to short sensor subpath, mimicking a form of "final gather" [Rei92] to reduce structured sampling artifacts

We demonstrate the effectiveness and correctness of our method both by solving the diffusion equation in highly scattering media, and by rendering diffusion curve images [OBW*08]. Much like in light transport, we hope that the development of these algorithms opens the path to comprehensive bidirectional methods in the future for fully robust Monte Carlo solution of PDEs

For simplicity, we limit ourselves to a particular class of ellipti PDEs called the Poisson equation with Dirichlet boundary condi-

Monte Carlo Geometry Processing: A Grid-Free Approach to PDE-Based Methods on Volumetric Domains

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Fig. 1. Real-world geometry has not only rich surfaalgorithms struggle to mesh, setup, and solve PDEs—ir Carlo solver uses about 1GB of memory and takes les Boundary mesh of Fijian strumigenys FJ13 used courtes

This paper explores how core problems in PDE-based g can be efficiently and reliably solved via grid-free Me Modern geometric algorithms often need to solve Poiss eometrically intricate domains. Conventional method the domain, which is both challenging and expensive fine details or imperfections (holes, self-intersections, free Monte Carlo methods avoid mesh gen evaluate closest point queries. They hence do not d nor even function spaces, and provide the exact solu even on extremely challenging models. More broadl benefits with Monte Carlo methods from photorealistic scaling, trivial parallel implementation, view-depender ability to work with any kind of geometry (including in descriptions). We develop a complete "black box" solv integration, variance reduction, and visualization, and sed for various geometry processing tasks. In particula fundamental linear elliptic PDEs with constant coefficie of \mathbb{R}^n . Overall we find that Monte Carlo methods sign orizons of geometry processing, since they easily has and complexity that are essentially hopeless for conve

CCS Concepts: • Computing methodologies \rightarrow Sha Additional Key Words and Phrases: numerical method

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Neural Control Variates with Automatic Integration Guandao Yang

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Qingqing Zhac Stanford Universit Palo Alto, USA cvanzhao@stanford.edu Bharath Hariharan Cornell University Ithaca, USA bharathh@cs.cornell.edu Integral $\int_{a}^{b} \frac{\partial}{\partial x} G_{\theta}(x) dx$ $\frac{\partial}{\partial x}G_{\theta}(x)$ \bullet Computing methodologies \rightarrow Computer graphics; Modeling and simulation; Neural networks. 42

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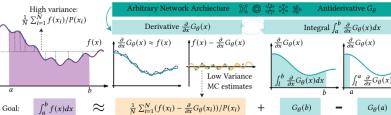


Figure 1: We propose a novel method to use arbitrary neural network architectures as control variates (CV). Instead of usin the network to approximate the integrand, we deploy it to approximate the antiderivative of the integrand. This allows us to construct pairs of networks where one is the analytical integral of the other, tackling a main challenge of neural CV methods ABSTRACT

This paper presents a method to leverage arbitrary neural network rchitecture for control variates. Control variates are crucial in reducing the variance of Monte Carlo integration, but they hinge n finding a function that both correlates with the integrand and has a known analytical integral. Traditional approaches rely on heuristics to choose this function, which might not be expressiv enough to correlate well with the integrand. Recent research alleviates this issue by modeling the integrands with a learnable parametric model, such as a neural network. However, the chalenge remains in creating an expressive parametric model with a known analytical integral. This paper proposes a novel approach to construct learnable para ntrol variates functions from

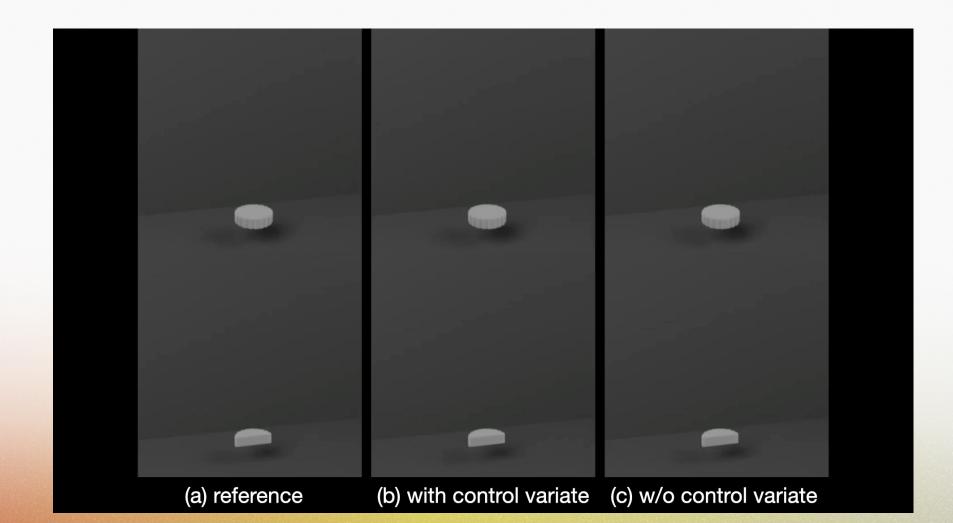
arbitrary neural network architectures. Instead of using a network to approximate the integrand directly, we employ the network to approximate the anti-derivative of the integrand. This allows us to utomatic differentiation to create a function whose integratio can be constructed by the antiderivative network. We apply our method to solve partial differential equations using the Walk-onsphere algorithm [Sawhney and Crane 2020]. Our results indicate that this approach is unbiased using various network architecture and achieves lower variance than other control variate methods.



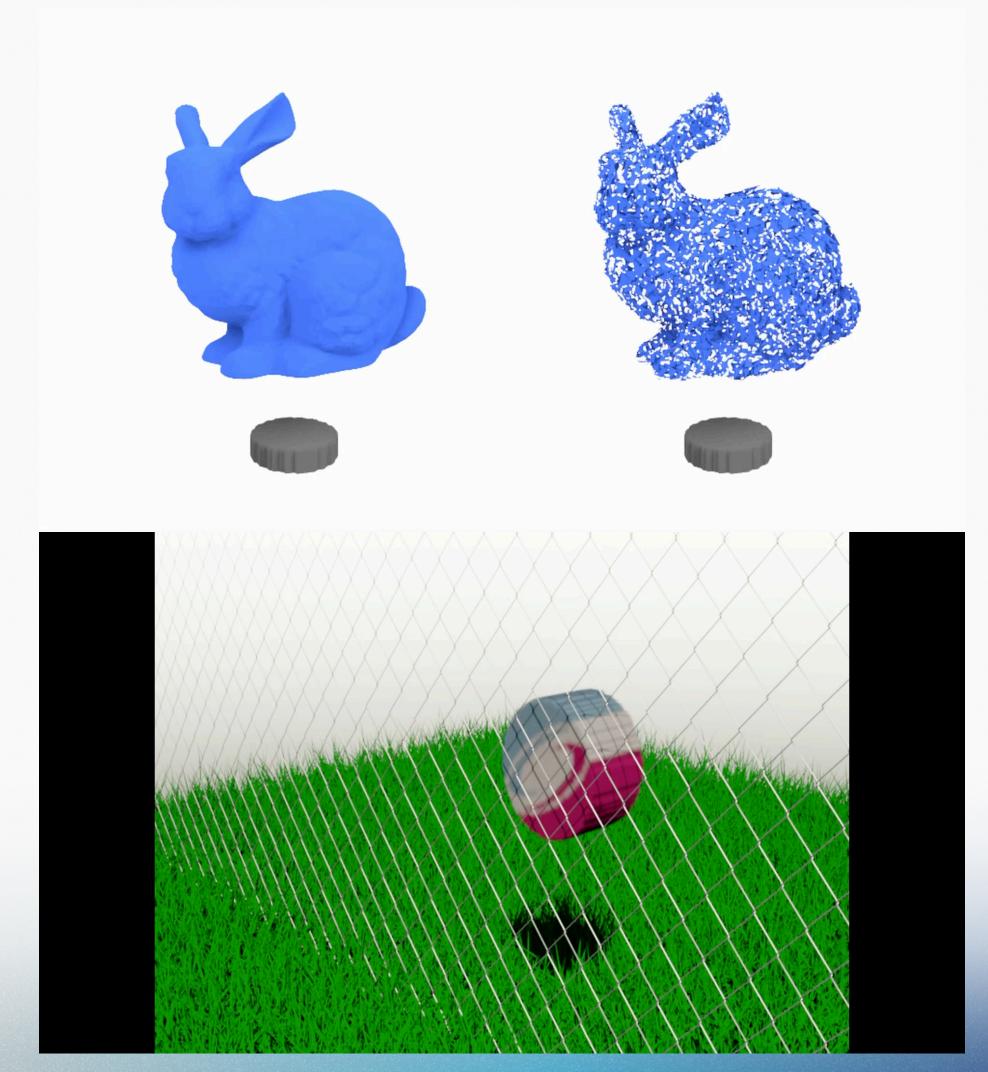
broader range of physics

Rioux-Lavoie et al. 2022, "A Monte Carlo Method for Fluid Simulation"







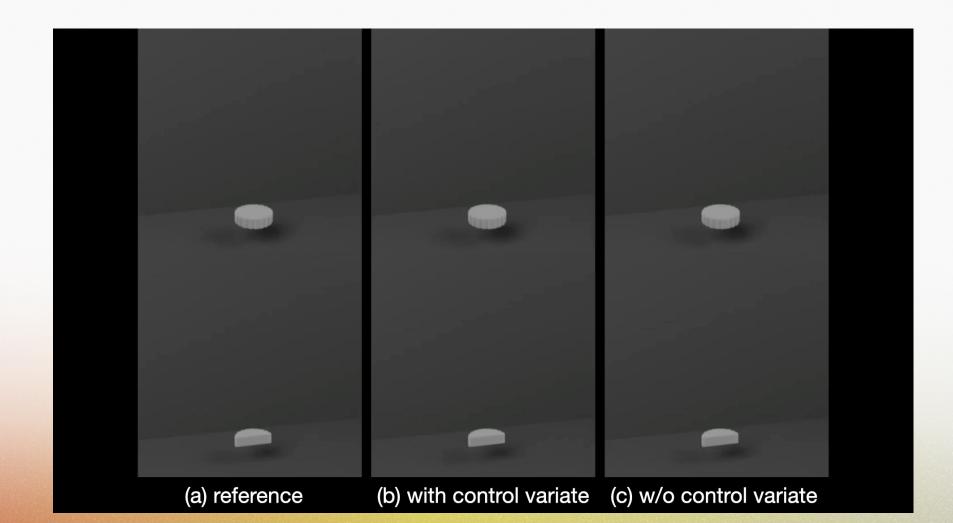




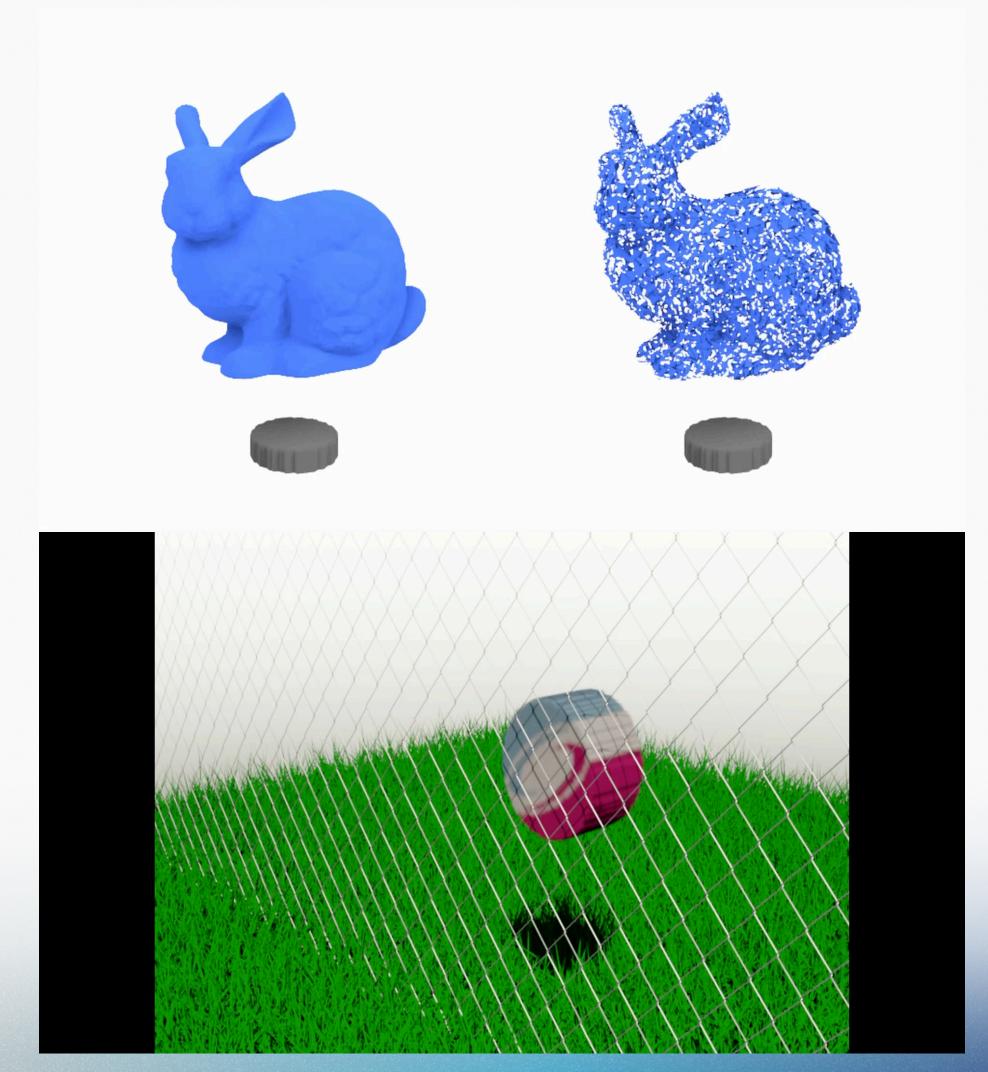
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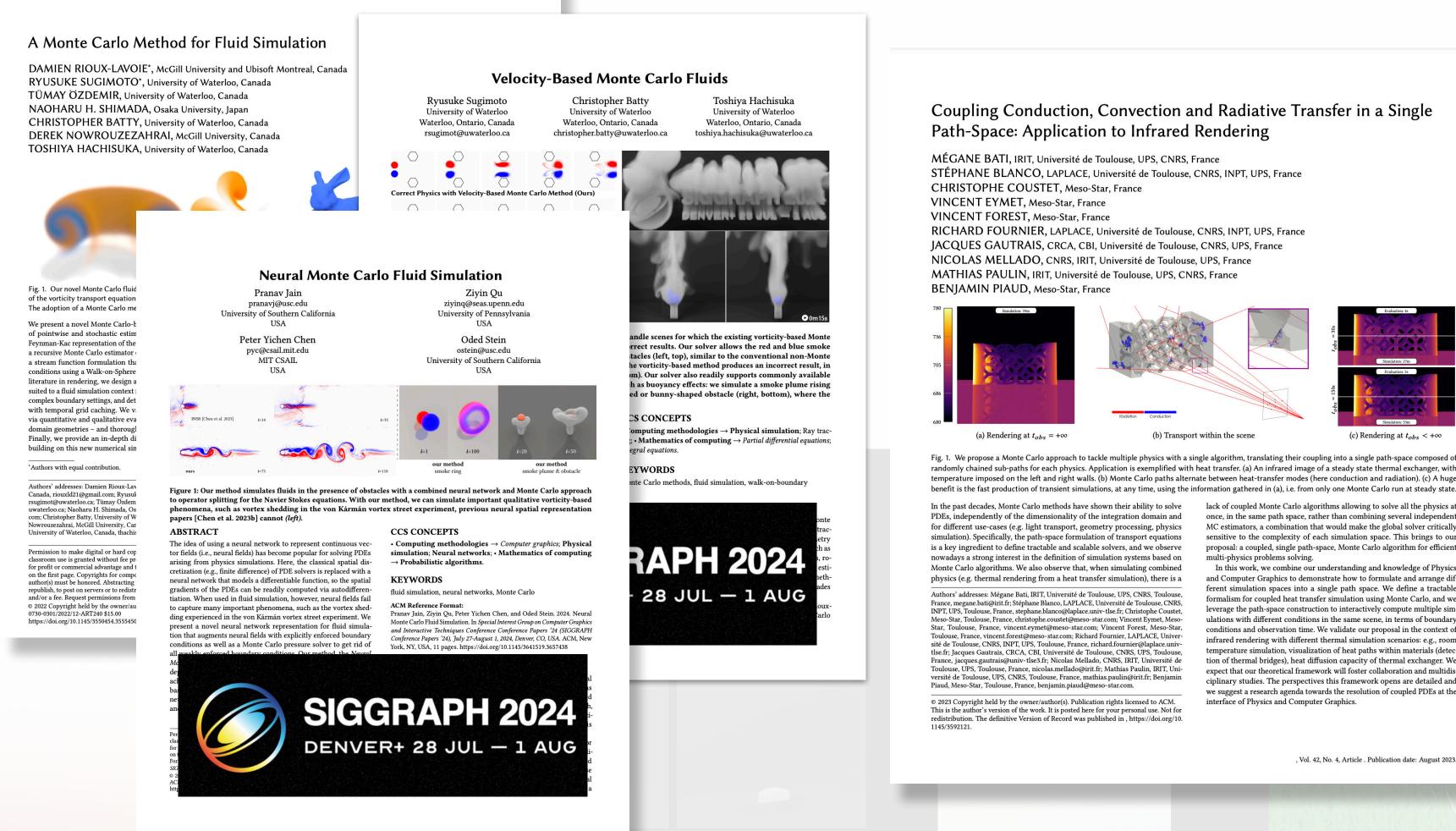




broader range of physics

MC solver as subroutine coupling MC physics solvers [Bati et al. 2023]

[Rioux-Lavoix et al. 2022, Sugimoto et al. 2024, Jain et al. 2024]





new MC physics solvers

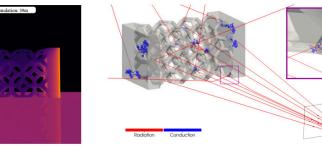
Coupling Conduction, Convection and Radiative Transfer in a Single Path-Space: Application to Infrared Rendering

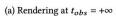
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(b) Transport within the scene

Fig. 1. We propose a Monte Carlo approach to tackle multiple physics with a single algorithm, translating their coupling into a single path-space composed of randomly chained sub-paths for each physics. Application is exemplified with heat transfer. (a) An infrared image of a steady state thermal exchanger, with temperature imposed on the left and right walls. (b) Monte Carlo paths alternate between heat-transfer modes (here conduction and radiation). (c) A huge

In the past decades, Monte Carlo methods have shown their ability to solve PDEs, independently of the dimensionality of the integration domain and for different use-cases (e.g. light transport, geometry processing, physics simulation). Specifically, the path-space formulation of transport equations is a key ingredient to define tractable and scalable solvers, and we observe nowadays a strong interest in the definition of simulation systems based on Monte Carlo algorithms. We also observe that, when simulating combined physics (e.g. thermal rendering from a heat transfer simulation), there is a

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© 2023 Copyright held by the owner/author(s). Publication rights licensed to ACM. This is the author's version of the work. It is posted here for your personal use. Not for redistribution. The definitive Version of Record was published in , https://doi.org/10. lack of coupled Monte Carlo algorithms allowing to solve all the physics at once, in the same path space, rather than combining several independent MC estimators, a combination that would make the global solver critically sensitive to the complexity of each simulation space. This brings to our proposal: a coupled, single path-space, Monte Carlo algorithm for efficient multi-physics problems solving.

In this work, we combine our understanding and knowledge of Physics and Computer Graphics to demonstrate how to formulate and arrange different simulation spaces into a single path space. We define a tractable formalism for coupled heat transfer simulation using Monte Carlo, and we leverage the path-space construction to interactively compute multiple simulations with different conditions in the same scene, in terms of boundary conditions and observation time. We validate our proposal in the context of infrared rendering with different thermal simulation scenarios: e.g., room temperature simulation, visualization of heat paths within materials (detection of thermal bridges), heat diffusion capacity of thermal exchanger. We expect that our theoretical framework will foster collaboration and multidisciplinary studies. The perspectives this framework opens are detailed and we suggest a research agenda towards the resolution of coupled PDEs at the interface of Physics and Computer Graphics.

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(c) Rendering at $t_{obs} < +\infty$

lots to explore here!

wave equations, linear elasticity, Etc.







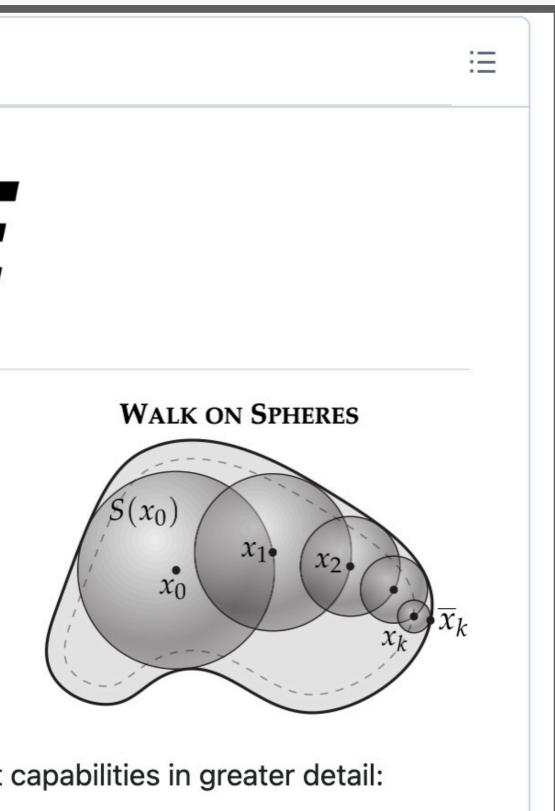
open-source walk on stars solver

MIT license

ZOMBKE

Zombie is a C++ header-only library for solving fundamental partial differential equations (PDEs) like the Poisson equation using the *walk on spheres (WoS)* method and its extensions. Unlike finite element, boundary element, or finite difference methods, WoS does not require a volumetric grid or mesh, nor a high-quality boundary mesh. Instead, it uses random walks and the Monte Carlo method to solve the problem directly on the original boundary representation. It can also provide accurate solution values at a single query point, rather than needing to solve the problem over the entire domain. This talk provides an overview of WoS, while the following papers discuss its present capabilities in greater detail:











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