THE FASCINATION OF GREEN'S FUNCTIONS AND THEIR APPLICATIONS IN COMPUTER GRAPHICS

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CORE TASKS OF COMPUTER GRAPHICS





CORE TASKS OF COMPUTER GRAPHICS





FAMILY OF PDES





Cauchy-Navier equation $\mu \Delta \boldsymbol{u} + \frac{\mu}{(1-2\nu)} \nabla (\nabla \cdot \boldsymbol{u}) + \boldsymbol{b} = 0.$



Maxwell equation $\nabla \cdot B = 0,$ $B = \mu_0 (H + M),$ $\nabla \times H = J_f + \frac{\partial D}{\partial t},$



Schrödinger equation $i\hbar\dot{\psi}=-\tfrac{\hbar^2}{2}\Delta\psi+p\psi$



Navier-Stokes equation $\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \mathbf{f}$ $\nabla \cdot \mathbf{u} = \mathbf{0},$



Helmholtz equation

$$\nabla^2 p + k^2 p = 0,$$



d'Alembert equation $\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) u(\mathbf{x}, t) = 0,$



Boltzmann transport equation $\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f = \Omega(f - f^{\text{eq}}) + F \cdot \nabla_{\boldsymbol{v}} f,$

APPLICATIONS IN COMPUTER GRAPHICS





FIND NUMERICAL SOLUTIONS

- Classical discretization schemes
 - Finite element method
 - Finite difference method
 - Finite volume method
- Safe choices if you know little about your problems
 - Linear or nonlinear PDEs
 - Spatially varying or constant coefficients
- Challenges
 - Accuracy issues
 - Numerical locking, numerical dissipation, etc.
 - High-quality volumetric meshes are often hard and costly to obtain
 - The problem size increases quickly in the complexity of geometry



Fine simulation

Using a 2x coarse mesh



REVISIT ANALYTICAL METHODS

Green's function – analytical solution to homogenous & "boundless" PDEs w.r.t. a singular impulse

Given a linear and homogeneous PDE

 $\mathcal{L}u(x) = f(x)$

- A Green's function *G*(*x*,*s*) is defined as
 - $\mathcal{L}G(x,s) = \delta(x-s)$
- Solution expressed via convolution

$$u(x) = \int G(x,s)f(s) \,\mathrm{d}s$$

No equation solves, cheap to evaluate!





GREEN'S FUNCTIONS



Differential operator L	Green's function G	Example of application	
∂_t^{n+1}	$\frac{t^n}{n!}\Theta(t)$		
$\partial_t + \gamma$	$\Theta(t)e^{-\gamma t}$		
$(\partial_t+\gamma)^2$	$\Theta(t)te^{-\gamma t}$	DDODI	EM II Operatore 9 CEa
$\partial_t^2 + 2\gamma \partial_t + \omega_0^2$ where $\gamma < \omega_0$	$\Theta(t)e^{-\gamma t}\;rac{\sin(\omega t)}{\omega}\;\;$ with $\;\omega=\sqrt{\omega_0^2-\gamma^2}\;$	1D underdamped harmonic Oscillator	EM I: Operators & GFS
$\partial_t^2 + 2\gamma \partial_t + \omega_0^2$ where $\gamma > \omega_0$	$\Theta(t)e^{-\gamma t}\;rac{\sinh(\omega t)}{\omega}\;\; ext{with}\;\;\omega=\sqrt{\gamma^2-\omega_0^2}$	1D overdar need harmare isot	ropic: they behave the
$\partial_t^2 + 2\gamma \partial_t + \omega_0^2$ where $\gamma = \omega_0$	$\Theta(t)e^{-\gamma t}t$	1D critically damped harmonic oscillator	a in all directions
2D Laplace operator $ abla^2_{2\mathrm{D}}=\partial^2_x+\partial^2_y$	$rac{1}{2\pi}\ln ho$ with $ ho=\sqrt{x^2+y^2}$	2D Poisson equation	ie in all directions.
3D Laplace operator $ abla^2_{ m 3D}=\partial^2_x+\partial^2_y+\partial^2_z$	$r = \frac{-1}{4\pi r}$ with $r = \sqrt{x^2 + y^2 + z^2}$	Poisson equation	
Helmholtz operator $ abla_{ m 3D}^2+k^2$	$rac{-e^{-ikr}}{4\pi r}=i\sqrt{rac{k}{32\pi r}}H^{(2)}_{1/2}(kr)\!=irac{k}{4\pi}h^{(2)}_0(kr)$	stationary 3D Schrödinger equation for free particle	
$ abla^2-k^2$ in n dimensions	$-(2\pi)^{-n/2}igg(rac{k}{r}igg)^{n/2-1}K_{n/2-1}(kr)$	Yukawa potential, Feynman propagator	
$\partial_t^2 - c^2 \partial_x^2$	$\frac{1}{2c}\Theta(t- x/c)$	1D wave equation	
$\partial_t^2 - c^2 abla_{2\mathrm{D}}^2$	$rac{1}{2\pi c\sqrt{c^2t^2- ho^2}}\Theta(t- ho/c)$	2D wave equation PROBLI	EM II: GFs are singular
D'Alembert operator $\Box = rac{1}{c^2}\partial_t^2 - abla_{3\mathrm{D}}^2$	$rac{\delta(t-rac{r}{c})}{4\pi r}$	3D wave equation	at the impulse
$\partial_t - k \partial_x^2$	$\Theta(t) \Big(rac{1}{4\pi k t} \Big)^{1/2} e^{-x^2/4kt}$	1D diffusion	at the impulse.
$\partial_t - k abla_{ m 2D}^2$	$\Theta(t)\left(rac{1}{4\pi kt} ight)e^{- ho^2/4kt}$	2D diffusion	
$\partial_t - k abla_{ m 3D}^2$	$\Theta(t) igg(rac{1}{4\pi kt} igg)^{3/2} e^{-r^2/4kt}$	3D diffusion	X/A
$\frac{1}{c^2}\partial_t^2 - \partial_x^2 + \mu^2$	$\frac{1}{2} \left[(1 - \sin \mu ct) \left(\delta(ct - x) + \delta(ct + x) \right) + \mu \Theta(ct - x) J_0(\mu u) \right] \text{ with } u = \sqrt{c^2 t^2 - x^2}$	1D Klein-Gerdon equation	A THE
$rac{1}{c^2}\partial_t^2 - abla_{2\mathrm{D}}^2 + \mu^2$	$\frac{1}{4\pi}\left[(1+\cos(\mu ct))\frac{\delta(ct-\rho)}{\rho}+\mu^2\Theta(ct-\rho)\sin(\mu u)\right] \ \text{with} \ u=\sqrt{c^2t^2-\rho^2}$	2D Klein–Gordon equation PRO	BLEM III: Boundary
$\Box + \mu^2$	$\frac{1}{4\pi} \left[\frac{\delta\left(t - \frac{r}{c}\right)}{r} + \mu c \Theta(ct - r) \frac{J_1\left(\mu u\right)}{u} \right] \text{with} u = \sqrt{c^2 t^2 - r^2}$	3D Klein-Gardon e Conditio	ns are not considered.
$\partial_t^2+2\gamma\partial_t-c^2\partial_x^2$	$\frac{1}{2}e^{-\gamma t}\left[\delta(ct-x)+\delta(ct+x)+\Theta(ct- x)\left(\frac{\gamma}{c}I_0\left(\frac{\gamma u}{c}\right)+\frac{\gamma t}{u}I_1\left(\frac{\gamma u}{c}\right)\right)\right] \text{with} u=\sqrt{c^2t^2-x^2}$	telegrapher's equation	Contraction of the second
$\partial_t^2 + 2\gamma \partial_t - c^2 abla_{2\mathrm{D}}^2$	$\left \frac{e^{-\gamma t}}{4\pi} \left[(1 + e^{-\gamma t} + 3\gamma t) \frac{\delta(ct - \rho)}{\rho} + \Theta(ct - \rho) \left(\frac{\gamma \sinh\left(\frac{\gamma u}{c}\right)}{cu} + \frac{3\gamma t \cosh\left(\frac{\gamma u}{c}\right)}{u^2} - \frac{3ct \sinh\left(\frac{\gamma u}{c}\right)}{u^3} \right) \right] \text{ with } u = \sqrt{c^2 t^2 - \rho^2} \left[\frac{1}{2} \left(\frac{1}{2} + \frac{1}{2} + \frac{1}{2} \right) \frac{\delta(ct - \rho)}{cu} + \frac{1}{2} \left(\frac{1}{2} + \frac{1}{2} + \frac{1}{2} \right) \frac{\delta(ct - \rho)}{cu} \right]$	2D relativistic heat conduction	x> S
$\partial_t^2 + 2\gamma \partial_t - c^2 abla_{3\mathrm{D}}^2$	$\left \frac{e^{-\gamma t}}{20\pi}\left[\left(8-3e^{-\gamma t}+2\gamma t+4\gamma^2 t^2\right)\frac{\delta(ct-r)}{r^2}+\frac{\gamma^2}{c}\Theta(ct-r)\left(\frac{1}{cu}I_1\left(\frac{\gamma u}{c}\right)+\frac{4t}{u^2}I_2\left(\frac{\gamma u}{c}\right)\right)\right] \text{ with } u=\sqrt{c^2t^2-r^2}$	3D relativistic heat conduction	

ENFORCING BOUNDARY CONDITIONS



- Boundary element method (BEM)
 - Turn volumetric differential equations to boundary integral equations
 (BIE)
 - Solve unknown boundary data based on given boundary conditions
 - Diffuse out the boundary data to get solutions at arbitrary target points



- No need for volumetric tessellation
 - Meshing a surface is simpler and faster in general
 - Slower growth of the problem size
 - Works for infinite large domains



ENFORCING BOUNDARY CONDITIONS

• Yet, we have to deal with dense linear systems



- Not scalable in time and memory cost
- Often suffer from poor convergence







Solve $\mathcal{L}(u) = 0$ using the method of Green's functions

$$u(x) = \int G(y, x)g(y)dS_y$$

RPESENTATION of the fundamental solutions to general linear operators

S.t.
$$\mathcal{D}(u)|_{\partial\Omega} = u_0$$

SCALABILITY of enforcing boundary conditions for large scale problems





Applications

Boundaryless deformation tool

SIGGRAPH '22



- Mathematical tool
 - Generalized, regularized Green's functions using series expansion
- Tradeoff
 - No equations solves, real-time performance
 - Not aware of any boundaries

Meshless solvers for BIE

SIGGRAPH '24



- Mathematical tool
 - Inverse Cholesky decomposition for accelerating PCG convergence
- Tradeoff
 - Fast, but not real-time due to solving dense systems
 - Boundary conditions are strictly satisfied

OUR ATTEMPTS





- Mathematical tool
 - Generalized Green's functions using series expansion
- Tradeoff
 - No equations solves, real-time performance
 - Not aware of any boundaries

Mathematical tool

- Generalized barycentric coordinates w.r.t. the controlling cage
- Tradeoff
 - Some precomputation, no equations solves, real-time performance
 - Aware of any boundary conditions, but only approximately fulfill them

Meshless solvers for BIE SIGGRAPH '24



- Mathematical tool
 - Inverse Cholesky decomposition for accelerating PCG convergence
- Tradeoff
 - Fast, but not real-time due to solving dense systems
 - Boundary conditions are strictly satisfied



EXTENDED GREEN'S FUNCTIONS A REAL-TIME & CONTROLLABLE TOOL FOR MESH SCULPTING





Extend Green's function to support...



Anisotropy

Arbitrary regularization

Isotropic strain-stress relationship

ELASTICITY EQUATION

$$\boldsymbol{\sigma} = 2\boldsymbol{\mu}\boldsymbol{\varepsilon} + \lambda \mathrm{tr}(\boldsymbol{\varepsilon})\mathbf{I}$$

• Linear anisotropic strain-stress relationship

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$$

• Equation of elasticity

$$C_{ijkl}\frac{\partial^2 u_k}{\partial x_l \partial x_j} + f_i = 0,$$





GREEN'S FUNCTION OF ELASTICITY





GENERAL REGULARIZED GREEN'S FUNCTION

we use Fourier transform •

$$\widehat{G}_{km}(\boldsymbol{\xi}) = (C_{ijkl}\xi_l\xi_j)^{-1}\delta_{im}\widehat{g}_{\varepsilon}(\boldsymbol{\xi}).$$

symmetry

To derive **GF** from $C_{ijkl} \frac{\partial^2 G_{km}}{\partial x_l \partial x_j} + \delta_{im} g_{\varepsilon}(\mathbf{x}) = 0$,

and its inverse Fourier transform •

$$\mathbf{G}(\mathbf{x}) = \frac{1}{8\pi^3} \int_{\mathbb{R}^3} \widehat{\mathbf{G}}(\boldsymbol{\xi}) \exp(\mathbf{i} \mathbf{x} \cdot \boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi},$$

Thus, given a load function $f(x) = g_{\varepsilon} (x - x')h$ •

$$\mathbf{u}(\mathbf{x}) = \operatorname{Re}[\mathbf{G}(\mathbf{x} - \mathbf{x'})] \mathbf{h},$$

$$f(\xi) = \widehat{g}_{\varepsilon}(|\xi|) = \frac{(2\pi)^{\frac{3}{2}}}{\sqrt{|\xi|}} \int_{0}^{\infty} J_{\frac{1}{2}}(|\mathbf{x}||\xi|)g_{\varepsilon}(|\mathbf{x}|)|\mathbf{x}|^{\frac{3}{2}}$$
How to evaluate this integral?

Spatial Frequency
domain
$$f(x) = \int_{\infty}^{\infty} f(x) e^{i\xi x} dx$$

 $a \cdot f(x) \longrightarrow a \cdot \hat{f}(\xi)$
 $\frac{d^n f(x)}{dx^n} \longrightarrow (i\xi)^n \hat{f}(\xi)$

$$\widehat{g}_{\varepsilon}(\boldsymbol{\xi}) = \widehat{g}_{\varepsilon}(|\boldsymbol{\xi}|) = \frac{(2\pi)^{\frac{3}{2}}}{\sqrt{|\boldsymbol{\xi}|}} \int_{0}^{\infty} J_{\frac{1}{2}}(|\mathbf{x}||\boldsymbol{\xi}|)g_{\varepsilon}(|\mathbf{x}|)|\mathbf{x}|^{\frac{3}{2}} d|\mathbf{x}|,$$

SPHERICAL HARMONIC EXPANSION

- For arbitrary material C_{ijkl} , $\mathbf{G}(\mathbf{x})$ has no analytical expressions in general
- Plane-wave expansion, or Rayleigh expansion

 ∞

l=0 m=-l

• Recall: $\widehat{G}_{km}(\xi) = (C_{ijkl}\xi_l\xi_j)^{-1}\delta_{im}\widehat{g}_{\varepsilon}(\xi).$

$$\mathbf{G}(\mathbf{x}) = \frac{1}{8\pi^3} \int_{\mathbb{R}^3} \widehat{\mathbf{G}}(\boldsymbol{\xi}) \exp(\mathbf{i} \mathbf{x} \cdot \boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi},$$

 $\exp(\mathbf{i}\,\mathbf{x}\cdot\boldsymbol{\xi}) = 4\pi \sum \sum \mathbf{i}^l j_l(|\mathbf{x}||\boldsymbol{\xi}|) Y_l^m(\widetilde{\mathbf{x}}) \overline{Y}_l^m(\widetilde{\boldsymbol{\xi}}),$





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Recall: $\widehat{G}_{km}(\boldsymbol{\xi}) = (C_{ijkl}\xi_l\xi_j)^{-1}\delta_{im}\widehat{g}_{\varepsilon}(\boldsymbol{\xi}).$

•

$$G(\mathbf{x}) = \frac{1}{2\pi^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l Y_l^m(\widetilde{\mathbf{x}}) \int_0^{\infty} \widehat{g}_{\varepsilon}(|\boldsymbol{\xi}|) j_l(|\mathbf{x}||\boldsymbol{\xi}|) \, \mathrm{d}|\boldsymbol{\xi}| \cdot \int_{\mathbb{S}^2} (C_{ikjl} \widetilde{\xi}_k \widetilde{\xi}_l)^{-1} \overline{Y}_l^m(\widetilde{\boldsymbol{\xi}}) \, \mathrm{d}\mathbb{S}(\widetilde{\boldsymbol{\xi}}),$$

 $\exp(\mathbf{i}\mathbf{x}\cdot\boldsymbol{\xi}) = 4\pi \sum \sum \mathbf{i}^l j_l(|\mathbf{x}||\boldsymbol{\xi}|) Y_l^m(\widetilde{\mathbf{x}}) \overline{Y}_l^m(\widetilde{\boldsymbol{\xi}}),$





GREEN'S FUNCTION IN SERIES



• Expressed in spherical coordinates, G(x) is decomposed as





ISOTROPIC CASE — KELVINLETS [DE GOES & JAMES 2017]



- For isotropic material, $C_{ijkl} \Rightarrow \mu, \lambda$
- G(x) are only non-zero at degree 0 and 2.

 $q_{\varepsilon}(r) = 15\varepsilon^4/(8\pi)(r^2 + \varepsilon^2)^{-\frac{1}{2}}$ $q_{\varepsilon}(r) = \delta(r)$ $G_{11}(r,\theta,\varphi) = \frac{r^2 \sin^2(\theta)(\lambda+\mu)\cos^2(\varphi) + r^2(\lambda+3\mu) + \varepsilon^2(2\lambda+5\mu)}{8\pi\mu(\lambda+2\mu)\left(r^2+\varepsilon^2\right)^{3/2}},$ $G_{11}(r,\theta,\varphi) = \frac{\sin^2(\theta)(\lambda+\mu)\cos^2(\varphi) + \lambda + 3\mu}{8\pi\mu r(\lambda+2\mu)},$ $G_{12}(r,\theta,\varphi) = G_{21}(r,\theta,\varphi) = \frac{\sin^2(\theta)(\lambda+\mu)\sin(\varphi)\cos(\varphi)}{8\pi\mu r(\lambda+2\mu)},$ $G_{12}(r,\theta,\varphi) = G_{21}(r,\theta,\varphi) = \frac{r^2 \sin^2(\theta)(\lambda+\mu)\sin(\varphi)\cos(\varphi)}{8\pi\mu(\lambda+2\mu)\left(r^2+\varepsilon^2\right)^{3/2}},$ $G_{13}(r,\theta,\varphi) = G_{31}(r,\theta,\varphi) = \frac{r^2 \sin(\theta) \cos(\theta) (\lambda+\mu) \cos(\varphi)}{8\pi\mu(\lambda+2\mu) (r^2+\varepsilon^2)^{3/2}},$ $G_{13}(r,\theta,\varphi) = G_{31}(r,\theta,\varphi) = \frac{\sin(\theta)\cos(\theta)(\lambda+\mu)\cos(\varphi)}{8\pi\mu r(\lambda+2\mu)},$ $G_{22}(r,\theta,\varphi) = \frac{\sin^2(\theta)(\lambda+\mu)\sin^2(\varphi) + \lambda + 3\mu}{8\pi\mu r(\lambda+2\mu)},$ $G_{22}(r,\theta,\varphi) = \frac{r^2 \sin^2(\theta)(\lambda+\mu) \sin^2(\varphi) + r^2(\lambda+3\mu) + \varepsilon^2(2\lambda+5\mu)}{8\pi\mu(\lambda+2\mu) \left(r^2 + \varepsilon^2\right)^{3/2}},$ $G_{23}(r,\theta,\varphi) = G_{32}(r,\theta,\varphi) = \frac{\sin(\theta)\cos(\theta)(\lambda+\mu)\sin(\varphi)}{\cos(\theta)(\lambda+\mu)\sin(\varphi)}$ $G_{23}(r,\theta,\varphi) = G_{32}(r,\theta,\varphi) = \frac{r^2 \sin(\theta) \cos(\theta) (\lambda+\mu) \sin(\varphi)}{8\pi\mu(\lambda+2\mu) (r^2+\varepsilon^2)^{3/2}},$ $8\pi\mu r(\lambda+2\mu)$ $G_{33}(r,\theta,\varphi) = \frac{\lambda c \mathbf{t}^{2}(\theta) + \mu \cos^{2}(\theta) + \lambda}{8\pi\mu r(\lambda + 2\mu)} \quad \text{Equivalent to}$ $G_{33}(r,\theta,\varphi) = \frac{r^2 \cos^2(\theta)(\lambda + \frac{1}{4})r^2(\lambda + 3\mu) + \varepsilon^2(2\lambda + 5\mu)}{8\pi\mu(\lambda - 2\mu)(r^2 + \varepsilon^2)^{3/2}}.$ Kelvinlet $\boldsymbol{u}(\boldsymbol{r}) = \left[\frac{(a-b)}{r}\boldsymbol{I} + \frac{b}{r^3}\boldsymbol{r}\boldsymbol{r}^t\right]\boldsymbol{f}$ $\boldsymbol{u}_{\varepsilon}(\boldsymbol{r}) = \left[\frac{(a-b)}{r_{c}}\boldsymbol{I} + \frac{b}{r^{3}}\boldsymbol{r}\boldsymbol{r}^{t} + \frac{a}{2}\frac{\varepsilon^{2}}{r^{3}}\boldsymbol{I}\right]\boldsymbol{f}$

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• Then given an affine load $F(x) = \delta(x - x')H$

$$\mathbf{u}(\mathbf{x}) = \operatorname{Re}\left[\nabla \mathbf{G}(\mathbf{x} - \mathbf{x'})\right] : \mathbf{H},$$



IMPLEMENTATION

Offline computations

- $\mathbf{P}_{l}^{m}(\mathbf{C}) = \int_{\mathbb{S}^{2}} (C_{ikjl} \widetilde{\xi}_{k} \widetilde{\xi}_{l})^{-1} \overline{Y}_{l}^{m}(\widetilde{\xi}) \, \mathrm{d}\mathbb{S}(\widetilde{\xi})$
- and $\mathcal{P}_{l,p}^{m}(\mathbf{C}) = \int_{\mathbb{S}^{2}} (C_{ikjl} \widetilde{\xi}_{k} \widetilde{\xi}_{l})^{-1} \overline{Y}_{l}^{m}(\widetilde{\xi}) \widetilde{\xi}_{p} \, \mathrm{d}\mathbb{S}(\widetilde{\xi}).$
- No analytical expressions in general
- Can be precomputed using Lebedev quadrature



Online computations

• $\mathbf{G}_{l}(\mathbf{x}) \equiv 0$ for $l = 1,3,5 \dots$

l = 1

1=2





- $\operatorname{Re}[\mathbf{G}_l^{-m}(\mathbf{x})] \equiv \operatorname{Re}[\mathbf{G}_l^m(\mathbf{x})]$
- $\operatorname{Re}[\nabla \mathbf{G}_l^{-m}(\mathbf{x})] \equiv \operatorname{Re}[\nabla \mathbf{G}_l^m(\mathbf{x})]$





ANISOTROPY CONTROL



PARTICULAR TYPES OF MATERIAL

 e.g., orthotropic material with 3 Young's moduli, 3 shear moduli and 3 Poisson ratios



GENERAL CASES

 Homogenize bi-materials on a regular grid [Kharevych et al. 2008]



 C_{ijkl} in Voigt notation

ANISOTROPY CONTROL





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DEFORMATION PROPAGATION CONTROL



Ínia IIX

DEFORMATION PROPAGATION CONTROL

• Limitations:

- $g_{\epsilon}(r)$ is neither intuitive nor flexible
- the integral $R_l(r)$ (or $\mathcal{R}_l(r)$) is hard to evaluate given $g_{\epsilon}(r)$
 - may not even exist!

• Our approach:

- Edit $R_l(r)$ (or $\mathcal{R}_l(r)$) directly via cubic splines instead of constructing an integrable $g_{\epsilon}(r)$







TRUNCATING SPHERICAL HARMONIC SERIES



EXPLOIT EARLY TRUNCATION





CONSTRAINED DEFORMATION





• Solve a dense linear system

$$\begin{bmatrix} \operatorname{Re}[\mathbf{G}(\mathbf{x}_0 - \mathbf{x}_0)] & \dots & \operatorname{Re}[\mathbf{G}(\mathbf{x}_0 - \mathbf{x}_{k-1})] \\ \vdots & \ddots & \vdots \\ \operatorname{Re}[\mathbf{G}(\mathbf{x}_{k-1} - \mathbf{x}_0)] & \dots & \operatorname{Re}[\mathbf{G}(\mathbf{x}_{k-1} - \mathbf{x}_{k-1})] \end{bmatrix} \begin{bmatrix} \mathbf{h}_0 \\ \vdots \\ \mathbf{h}_{k-1} \end{bmatrix} = \begin{bmatrix} \mathbf{u}_0 \\ \vdots \\ \mathbf{u}_{k-1} \end{bmatrix}$$

• By superposition:

$$\mathbf{u}(\mathbf{x}) = \sum_{i=0}^{k} \mathbf{G}(\mathbf{x} - \mathbf{x}_{i})\mathbf{h}_{i}$$



SPEEDUP ITERATIVE SOLVERS FOR

SPEEDUP ITERATIVE SOLVERS FOR MESHLESS BIES



•



- Methods to build Boundary Integral Equation (BIE) systems [Costabel 1984]
 - Direct approaches: solve for Dirichlet or Neumann boundary conditions
 - based on Green's third identity or its variants
 - Indirect approaches: solve for an unknown density on the boundary
 - E.g., "charges" for potential problems, "forces" for elasticity
- Indirect approach: single layer potential for Dirichlet problems







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 $\int_{\mathcal{M}} G(\boldsymbol{z}, \boldsymbol{y}) \sigma(\boldsymbol{y}) \, \mathrm{d} v_{\boldsymbol{y}} = b(\boldsymbol{z}) \ \forall \boldsymbol{z} \in \mathcal{M}.$

• Evaluation stage: evaluate the "potential" at any target point in space

$$u(\boldsymbol{x}) = \int_{\mathcal{M}} G(\boldsymbol{x}, \boldsymbol{y}) \sigma(\boldsymbol{y}) \, \mathrm{d} v_{\boldsymbol{y}}.$$



RECAP BEM

- Methods to build Boundary Integral Equation (BIE) systems [Costabel 1984]
 - Direct approaches: solve for Dirichlet or Neumann boundary conditions
 - based on Green's third identity or its variants
 - Indirect approaches: solve for an unknown density on the boundary
 - E.g., "charges" for potential problems, "forces" for elasticity
- Indirect approach: single layer potential for Dirichlet problems
 - Solve stage: solve for "charges" that enforce a set of given boundary "potential"

 $\int_{\mathcal{M}} G(\boldsymbol{z}, \boldsymbol{y}) \sigma(\boldsymbol{y}) \, \mathrm{d} v_{\boldsymbol{y}} = b(\boldsymbol{z}) \ \forall \boldsymbol{z} \in \mathcal{M}.$

• Evaluation stage: evaluate the "potential" at any target point in space

$$u(\boldsymbol{x}) = \int_{\mathcal{M}} G(\boldsymbol{x}, \boldsymbol{y}) \sigma(\boldsymbol{y}) \, \mathrm{d} v_{\boldsymbol{y}}.$$

Results in Fredholm integral
 equation of the first kind, more
 Ill-posed than the second kind

- Need efficient preconditioners
- Any symmetric and sparse structures to leverage to get a stable and scalable solver?

source points

boundary points




EXPLOIT SYMMETRY



K s = b

target points

Discretize boundary integral equations (BIE)



EXPLOIT SPARSITY

- Directly applying incomplete Cholesky to factorize K
 [Chen et al. 2021]
 - Accuracy issue: Numerous entries must be dropped out for efficiency
 - Stability issue: Loss of positive definiteness causes breakdowns
- However, boundary integral operators are conceptually close to the inverse of their differential operator
 - Green function is the solution subject to a singular impulse
 - E.g., in elasticity, a BIE matrix acts like the inverse of stiffness, or compliance
- So, the inverse of BIE matrices could be sparse
 - True for many covariance matrices assembled by fast-decaying kernel functions in Gaussian Process
 - Similar for Green's functions as well



 $\underset{\text{Forces}}{\text{Ks} = b}_{\text{Displacements}}$

 $K \approx LL^T$



[Chow and Saad 2014]

INVERSE CHOLESKY PRECONDITIONER



We leverage inverse Cholesky factorization to precondition BIE matrices

$$Ks = b - \frac{K^{-1} \approx L_S L_S^T}{\Rightarrow} s \approx L_S L_S^T b$$

Kaporin's construction for L_S [Kaporin 1994]

$$\boldsymbol{L}_{\mathcal{S}_{j},j} = \frac{\boldsymbol{K}_{\mathcal{S}_{j},\mathcal{S}_{j}}^{-1} \boldsymbol{\mathbb{e}}_{j}}{\sqrt{\boldsymbol{\mathbb{e}}_{j}^{\mathsf{T}} \boldsymbol{K}_{\mathcal{S}_{j},\mathcal{S}_{j}}^{-1} \boldsymbol{\mathbb{e}}_{j}}}, \quad \forall j = 1..B,$$



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INVERSE CHOLESKY PRECONDITIONER



We leverage inverse Cholesky factorization to precondition BIE matrices

$$Ks = b - \frac{K^{-1} \approx L_S L_S^T}{r} \rightarrow s \approx L_S L_S^T b$$

Kaporin's construction for L_S [Kaporin 1994]

$$\boldsymbol{L}_{\mathcal{S}_{j},j} = \frac{\boldsymbol{K}_{\mathcal{S}_{j},\mathcal{S}_{j}}^{-1} \boldsymbol{e}_{j}}{\sqrt{\boldsymbol{e}_{j}^{\mathsf{T}} \boldsymbol{K}_{\mathcal{S}_{j},\mathcal{S}_{j}}^{-1} \boldsymbol{e}_{j}}}, \quad \forall j = 1..B,$$

- Properties
 - Massively parallel: each column of L_S is computed independently to others. Good for GPUs!
 - **Memory efficient:** no need to assemble the global BIE matrix.
 - Stable: no breakdowns will occur
 - Variational interpretation(s): minimizing Kaporin's condition number*, KL-divergence, and a constrained quadratic form



REORDERING DOFS

- Fine-to-coarse ordering by farthest point sampling [Chen et al. 2021]

 - $\begin{array}{l} \text{Max-min ordering } i_k = \mathop{\mathrm{argmax}}_{q} \min_{p \in \{0,k-1\}} \operatorname{dist}(\pmb{y}_q,\pmb{y}_{i_p}), \\ \text{Reverse max-min ordering } \pmb{P} \!=\! \{i_{B-1},...,i_1,i_0\} \text{, i.e., fine-to-coarse} \end{array}$
- Intuition
 - Make sampling points space uniformly within each scale
 - The screening effect in kriging [Stein 2002]
 - GP: conditioning a subset of points results in localized correlations





A fine-to-coarse reordering

 $f(A, B, C, D) = f(A)f(B|A)f(C|A, B)f(D|A, B, C) = N(0, \Sigma)$ $f(A, B, C, D) \approx f(A)f(B|A)f(C|A, \mathbf{R})f(D|A, B, \mathbf{K}) = N(0, (LL^{\mathrm{T}})^{-1})$ Too far Too far

CONSTRUCTING SPARSITY PATTERN





Length scale returned in coarse-to-fine ordering

$$\ell_{i_k} = \min_{p \in \{0, k-1\}} \operatorname{dist}(\boldsymbol{y}_{i_k}, \boldsymbol{y}_{i_p})$$

Lower-triangular sparsity patter

$$S := \left\{ (i, j) | i \ge j \text{ and } \operatorname{dist}(x_i, x_j) \le \rho \min(\ell_i, \ell_j) \right\}$$

Again, screening effect: a fine-scale point is unlikely to be correlated to distant points on coarser scales

EFFICIENT IMPLEMENTATION



FOR PRECONDTIONER

Supernode mode to reuse local factorizations as much as possible

Supernodal sparsity pattern



FOR PCG ITERATIONS

• Fast Multipole Method to evaluate matrix-vector products



EXAMPLES OF APPLICATION



LAPLACE'S EQUATIONLINEAR ELASTICITYHELMHOLTZ EQUATION $\Delta u = 0$ $\Delta u + \frac{1}{1-2\nu} \nabla (\nabla \cdot u) = 0,$ $\Delta u + k^2 u = 0,$ $G(\mathbf{x}, \mathbf{y}) = \begin{cases} -\frac{1}{2\pi} \ln(r), & \text{in } 2D \\ \frac{1}{4\pi r}, & \text{in } 3D \end{cases}$ $G(\mathbf{x}, \mathbf{y}) = \begin{cases} \frac{a-b}{r} \ln(1/r)I + \frac{b}{r^2}rr^{\mathsf{T}}, & \text{in } 2D \\ \frac{a-b}{r}I + \frac{b}{r^3}rr^{\mathsf{T}}, & \text{in } 3D \end{cases}$ $G(\mathbf{x}, \mathbf{y}) = \begin{cases} \frac{\dot{a}}{4}H_0^{(1)}(kr), & \text{in } 2D, \\ \frac{a-b}{r}I + \frac{b}{r^3}rr^{\mathsf{T}}, & \text{in } 3D \end{cases}$

The method of fundamental solutions (MFS)



















LINEAR ELASTICITY



 $\rho = 3$

#iter. = 10 t (pcg) = 7.270s t (eval.) = 11.686s Err = 0.003106

t(precomp.) = 0.132s

t(comp.) = 0.644s

sources (box): 14408 # target (car): 199249

Constrained Kelvinlet deformer [de Goes and James 2017]



HELMHOLTZ EQUATION



- Least-squares solves are always needed for Helmholtz equations
 - The BIE/MFS matrices are complex symmetric, but not Hermitian
 - Cholesky factorization does no exist



COMPARISON WITH SVD



Boundary size

В	SVD		Ours					
	t(fac.)	t(slv.)	<i>t</i> (precomp.)	<i>t</i> (comp.)	#iters	t(pcg)	f(total)	Err
1280	4.864	0.003	0.004	0.419	15	0.005	0.427	0.000706
2560	33.757	0.011	0.007	0.715	15	0.013	0.735	0.000679
5120	261.454	0.045	0.013	1.270	15	0.048	1.331	0.004405
7680	911.212	0.156	0.023	3.478	15	0.099	3.600	0.003497
10240	2405.59	0.303	0.032	7.170	15	0.167	7.369	0.003665



BEM FROM GAUSSIAN PROCESS VIEWPOINT



- Formulate stochasticity in Computer Graphics
 - Geometry processing, e.g., surface reconstruction [Sellán and Jacobson 2022]
 - Rendering, e.g., light transport [Seyb et al. 2024]
- Boundary value problems from a statistical point of view
 - Investigate the distribution of all possible solutions, not just a single one!
- Gaussian-process based inference v.s. MFS
 - Beyond conditional mean

 $\mu(f(\boldsymbol{x}) \mid \boldsymbol{y}, f(\boldsymbol{y})) = \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{y}) \boldsymbol{K}(\boldsymbol{y}, \boldsymbol{y})^{-1} f(\boldsymbol{y}),$

Conditional variance for uncertainty quantification

$$\sigma_{\boldsymbol{y}_i}^2 = \boldsymbol{K}(\boldsymbol{y}_i, \boldsymbol{y}_i) - \boldsymbol{K}(\boldsymbol{y}_i, \boldsymbol{x}) \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{x})^{-1} \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{y}_i).$$

Tell the probability of the solution falling within a given range



Gaussian Process	MFS		
Kernel function	Green's function		
Observation	Boundary condition		
Conditional mean	Solution		
Prediction	Evaluation		

(a) boundary condition

(c) conditional (b) diffusion result (conditional mean) standard deviation (d) Pr(0.3 < u < 1) (e) Pr(0.6 < u < 1)



Uncertainty quantification of BIE solves



Ours (global) - zero Poisson ratio



SOMIGLIANA COORDINATES CONTROL VOLUMETRIC DEFORMATION USING A CAGE

CAGE DEFORMER

- Cage deformer
 - based on generalized barycentric coordinates
 - many options available now (see our survey [Ströter et al. 2024])
 - 🛛 Boundary-aware, meshfree, extremely fast 🛛 🏹 🗃
 - Purely geometric, no elastic feel or volume control ε,









Mean-value coords [Floater 2003; Ju et al. 2005; Thiery et al. 2018]



Maximum entropy coords [Hormann and Sukumar 2008]

Harmonic coords [Joshi et al. 2007]



Complex coords [Weber et al. 2009]



CAGE DEFORMER

- and daf
 - based on generalized barycentric coordinates
 - many options available now (see our survey [Ströter et al. 2024]) •

 - Purely geometric, no elastic feel or volume control $[\xi,]$



 \boldsymbol{v}_i n_k $\boldsymbol{x} = \sum_{i} \phi_{i}(\boldsymbol{x})\boldsymbol{v}_{i} + \sum_{k} \psi_{k}(\boldsymbol{x})\boldsymbol{n}_{k}$

$$\widetilde{\mathbf{x}}(\mathbf{x}) = \sum_{i} \phi_{i}(\mathbf{x}) \widetilde{\mathbf{v}}_{i} + \sum_{k} \psi_{k}(\mathbf{x}) \left(c_{k} \widetilde{\mathbf{n}}_{k} \right)$$





Maximum entropy coords [Hormann and Sukumar 2008]

Harmonic coords [Joshi et al. 2007]



Complex coords [Weber et al. 2009]

+ Green coordinates [Lipman et al. 2008]







CONTRIBUTIONS

- Inject *elasticity* into cage deformers for fast volumetric deformation
 - Matrix-valued coordinates, extending Green coordinates
 - Derived from linear elasticity and mimicking elastic behaviors
 - Invariant under similarity transformations through corotational formulation
 - Control over volume change and local bulge





FROM GREEN TO SOMIGLIANA



Green coordinates (GC)

PDE: $\Delta \boldsymbol{u} = \boldsymbol{0}$ $G(\mathbf{y}, \mathbf{x}) = \begin{cases} -\frac{1}{4\pi r}, & d = 3, \\ \frac{1}{2\pi} \log(r), & d = 2. \end{cases}$ $\mathbf{u}(\mathbf{x}) = \int_{\partial \Omega} \left[\nabla_{\mathbf{n}} G(\mathbf{y}, \mathbf{x}) \mathbf{u}(\mathbf{y}) - G(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{n}} \mathbf{u}(\mathbf{y}) \right] d\sigma_{\mathbf{y}}$ **Fundamental** solutions: Boundary reformulation: u(x) = x $\{\phi_i(\mathbf{x}), \psi_k(\mathbf{x})\} \in \mathbf{R}$

FROM GREEN TO SOMIGLIANA











THE CONNECTION TO BEM

- When the cage is deformed, i.e., with new specified vertex positions
 - $\widetilde{\mathbf{x}}(\mathbf{x}) = \sum_{i} T_{i}(\mathbf{x})\widetilde{\mathbf{v}}_{i} + \sum_{k} K_{k}(\mathbf{x}) (c_{k}\widetilde{\mathbf{n}}_{k})$ Should be $\partial_{n}\widetilde{\mathbf{x}}$ in BEM
- In BEM, $\partial_n \widetilde{x}|_{\partial\Omega}$ is solved from $\widetilde{x}|_{\partial\Omega}$
 - Dirichlet and Neumann boundary conditions are compatible
- In cage deformation, we "guess" the boundary normal derivatives
 - Efficient for real-time manipulation
 - Parameterize Neumann conditions to support flexible control over the interior deformation
- Price to pay: normal terms are not compatible with cage vertex positions
 - The interior deformation could be not intuitive, e.g., not following the cage tightly







COROTATIONAL FORMULATION

 $T_i(\mathbf{x})$ and $K_k(\mathbf{x})$ are not rotationally invariant

Typical remedy: corotational formulation ٠

 R_i

 $\widetilde{x}(x)$

$$\widetilde{x}(x) = \left(\sum_{i} R_{i}T_{i}(x)R_{i}^{t}\right)^{-1} \left[\sum_{i} R_{i}T_{i}(x)R_{i}^{t}\widetilde{v}_{i} + \sum_{k} R_{k}K_{k}(x)R_{i}(\widetilde{\tau}_{k})\right]$$

$$\widetilde{\tau}_{k} = S_{k}R_{k}n_{k}$$

$$= \left[\frac{2(1-\nu)}{1-2\nu}\eta_{k} + \frac{2\nu(d-1)}{1-2\nu}\lambda_{k}\right]R_{k}n_{k}$$

Estimate $\{R_k, \lambda_k, \eta_k\}$ for each boundary facet





GLOBAL VS. LOCAL ROTATION & TANGENT STRETCHES







Rest pose







In between

blend global and local R_k , λ_k



Local variant

 R_k and λ_k are decuded on per facet basis



CURVATURE-BASED NORMAL STRETCHES



- Normal stretching factor η_k for each cage facet
 - No information about out-of-plane deformation
 - E.g., account for curvature change for local bulging
 - $\eta_k = \lambda_k \exp(\gamma \beta_k / (2^{d-1}\pi))$
 - Compute on-the-fly
- Our choice of R_j , λ_j , η_j keeps the deformation invariant under similarity transformations

 $\widetilde{\mathbf{x}}(sR\mathbf{x} + \mathbf{t}) = sR\widetilde{\mathbf{x}}(\mathbf{x}) + \mathbf{t}$





IMPLEMENTATION





$$K_k(\mathbf{x}) = \int_{\Delta_k} \mathcal{K}(\mathbf{y}, \mathbf{x}) d\sigma_{\mathbf{y}} = 2|\Delta_k| \int_0^1 d\alpha \int_0^{1-\alpha} d\beta \, \mathcal{K}(\mathbf{y}(\alpha, \beta), \mathbf{x})$$

- #query points: **39k**
- #quadratures per face: 7500
- #cage faces: 184





$$2|\Delta_k|\sum_j w_j\left(\frac{a-b}{r(\alpha_j,\beta_j)}\boldsymbol{I} + \frac{b}{r^3(\alpha_j,\beta_j)}\boldsymbol{r}(\alpha_j,\beta_j)\boldsymbol{r}^t(\alpha_j,\beta_j)\right)$$



 $\{(\alpha_j,\beta_j),w_j\}$

ANALYTICAL EXPRESSIONS OF SOMIGLIANA COORDS.



• Biharmonic coordinates for 3D triangular cages [Thiery et al. 2024]

Biharmonic coordinates

$$f(\eta) = \sum_{i \in \mathcal{V}} \phi_i(\eta) a_i + \sum_{j \in \mathcal{T}} \psi_j(\eta) b_j + \sum_{i \in \mathcal{V}} \bar{\phi}_i(\eta) c_i + \sum_{j \in \mathcal{T}} \bar{\psi}_j(\eta) d_j,$$

Boundary integral formulation of biharmonic functions $\Delta^2 f = 0$

$$\begin{split} f(\eta) &= \int f(\xi) \frac{\partial_1 G_1}{\partial n} (\xi, \eta) d\xi - \int G_1(\xi, \eta) \frac{\partial f}{\partial n} (\xi) d\xi \\ &+ \int \Delta f(\xi) \frac{\partial_1 G_2}{\partial n} (\xi, \eta) d\xi - \int G_2(\xi, \eta) \frac{\partial \Delta f}{\partial n} (\xi) d\xi, \end{split}$$

$$\int_{\xi \in t} \|\xi - \eta\| d\xi = \frac{d_t^3 \omega_t(\eta)}{3}$$

$$+ \sum_{e \in t} \frac{a_e^t}{6} \left((2d_t^2 + D_e^2) \log\left(\frac{l_{e_1} - \zeta_{e_1}}{l_{e_0} - \zeta_{e_0}}\right) - l_{e_1} \zeta_{e_1} + l_{e_0} \zeta_{e_0} \right)$$

Expressing Somigliana coords. with biharmonic coords.

$$K_t(\eta) = \frac{b}{\lambda_2} \underbrace{H_{\eta}(\bar{\psi}_t)(\eta)}_{-\frac{a}{\lambda_1}} \psi_t(\eta) I_3$$

$$T_{t^{i}}^{t}(\eta) = \frac{2bd_{t}}{\lambda_{1}} \underbrace{H_{\eta}\left(\psi_{t}^{i}\right)(\eta)}_{-\frac{a}{\lambda_{1}}} - \frac{a}{\lambda_{1}} \phi_{t^{i}}^{t}(\eta) I_{3} - \frac{a-2b}{\lambda_{1}} \left[n_{t} \underbrace{\nabla_{\eta}^{T}(\psi_{t}^{i})}_{-\frac{a}{\lambda_{1}}} - \underbrace{\nabla_{\eta}(\psi_{t}^{i})}_{-\frac{a}{\lambda_{1}}} n_{t}^{T} \right]$$



VOLUME PRESERVING VS. LOCAL BULGING





2D COMPARISONS





3D COMPARISONS





COMPARISONS









- Extended Green's functions
 - A systematical approach to represent and derive Green's functions for general linear operators
 - Regularization for practical use
- Meshless solver for boundary integral equations
 - Massively parallel preconditioner based on inverse Cholesky factorization
 - Scalable to large scale problems
- Matrix-valued barycentric coordinates for cage deformation
 - Compromise between pointwise deformers and boundary element methods
 - Flexible control over the "fake" Neumann boundary conditions
FUTURE WORKS

- Generalize the idea to ...
 - Asymmetric systems from elliptic PDEs or non-elliptic PDEs without least-squares solves, e.g., wave equations [Schreck et al. 2019]
 - Nonlinear problems, e.g., Gaussian process hydrodynamics [Owhadi 2023]
- The art of preconditioning
 - Dilemma between convergence and cost per iteration
 - Analogue of the uncertainty principle of Fourier transform
- Simulation meets stochasticity
 - Make use of uncertainty quantification for adaptive simulation
 - Develop stochastic representation to account for the uncertainty of a complex dynamical system







