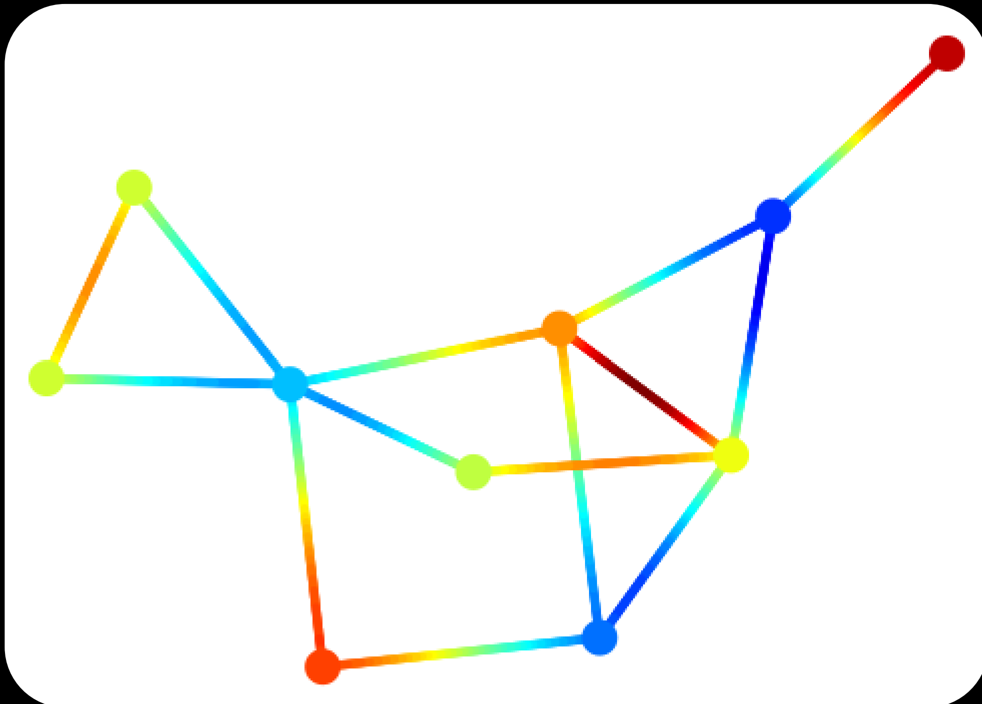
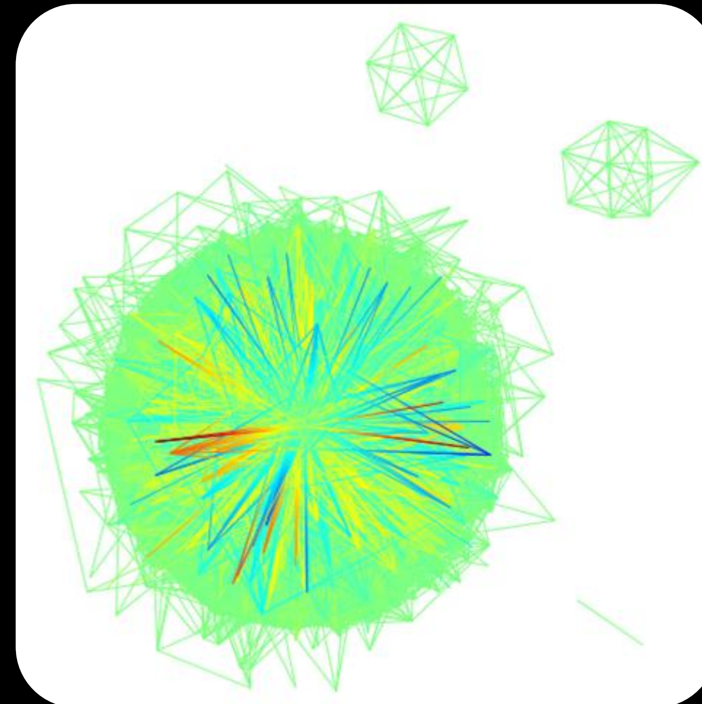




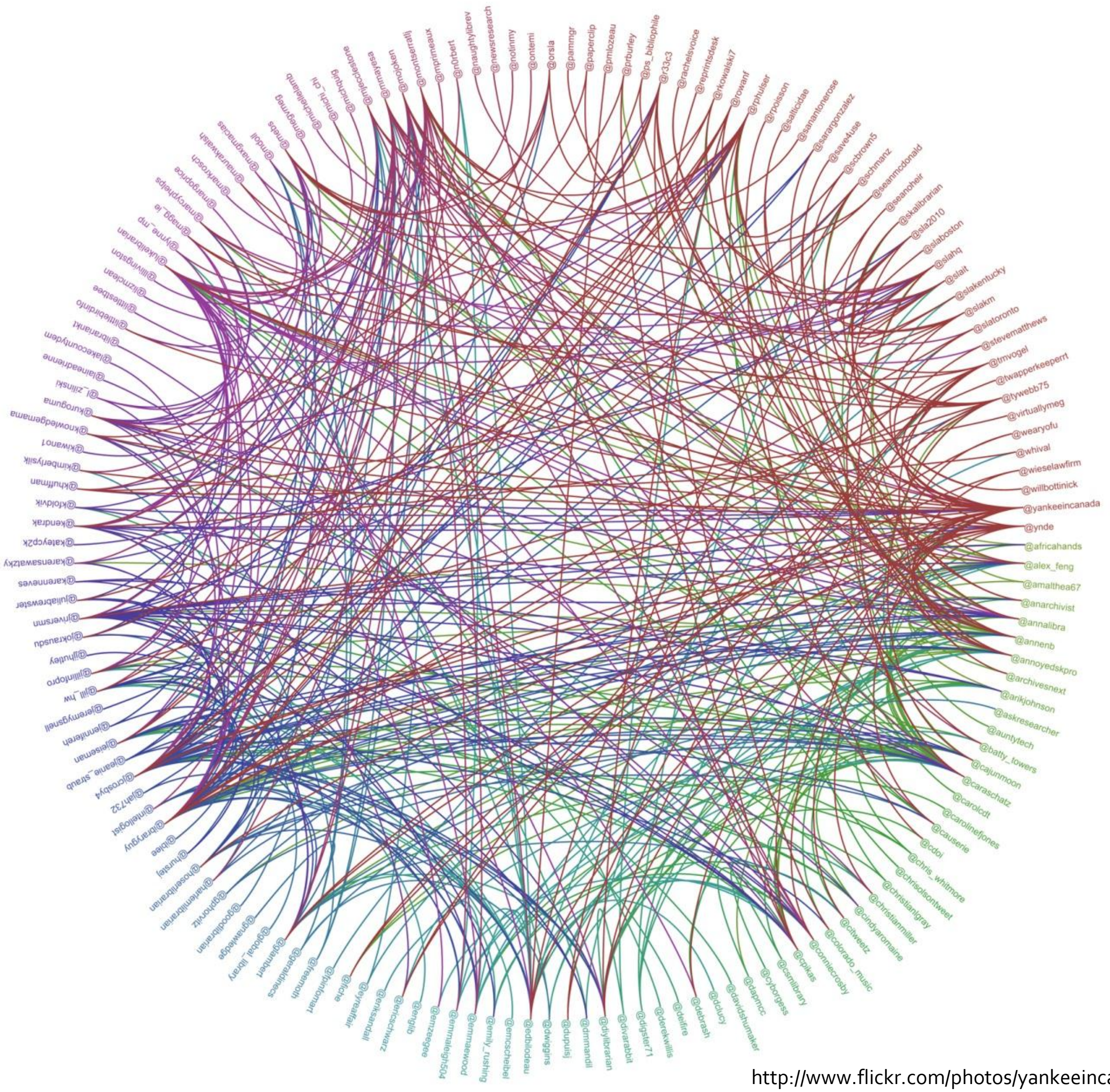
PDE Approaches to Graph Analysis

Justin Solomon

Geometric Computing Group

Stanford University

Understanding Graph Structure



http://www.flickr.com/photos/yankeeincanada/4188088640/sizes/o/in/photostream/

Understanding Graph Structure

Attractive but not informative.

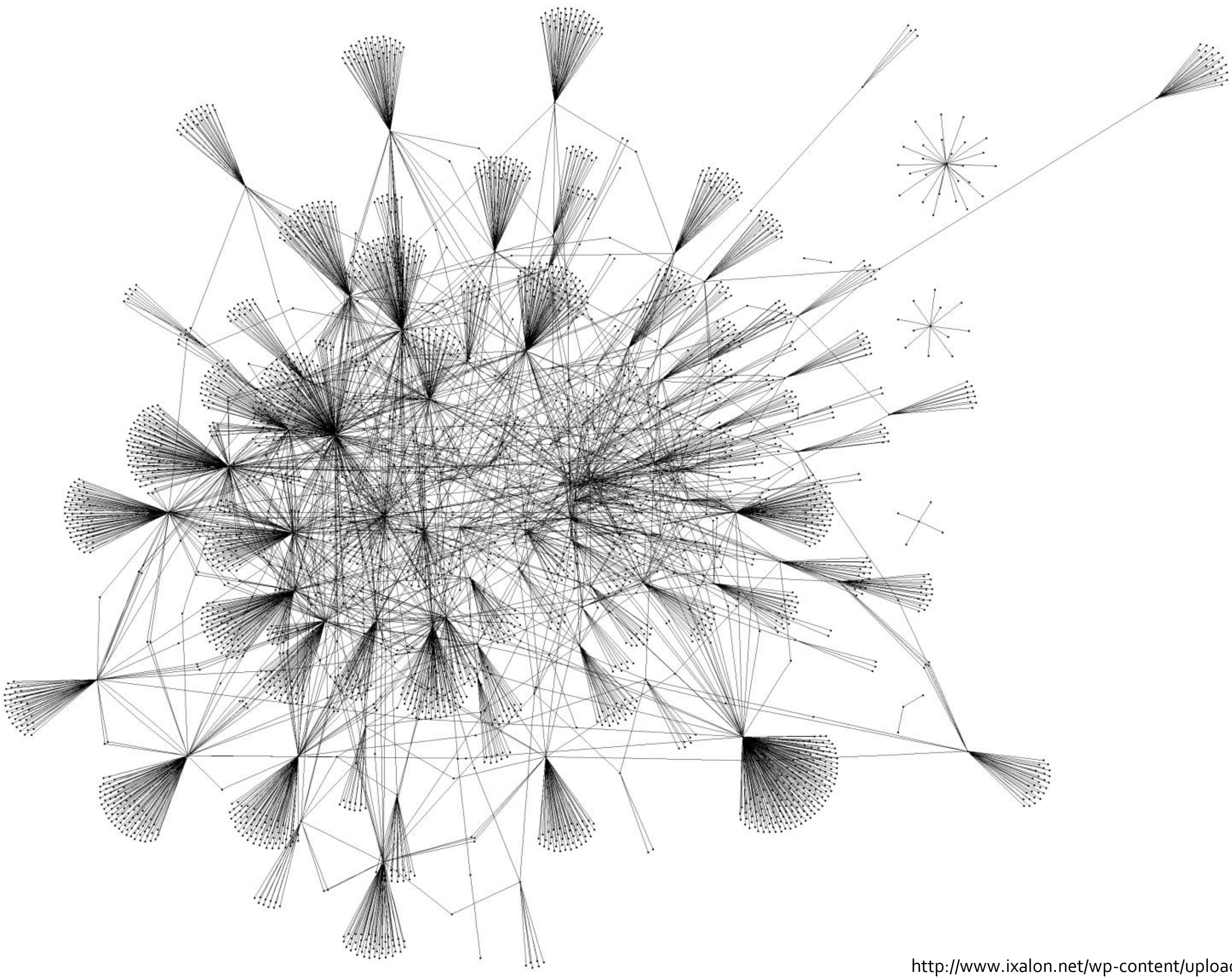
http://www.flickr.com/photos/yankeeincanada/4188088640/sizes/o/in/photostream/

Topology [**t*uh*-pol**-*uh*-jee]: The study and characterization of a domain’s connectivity.

Multiscale Analysis

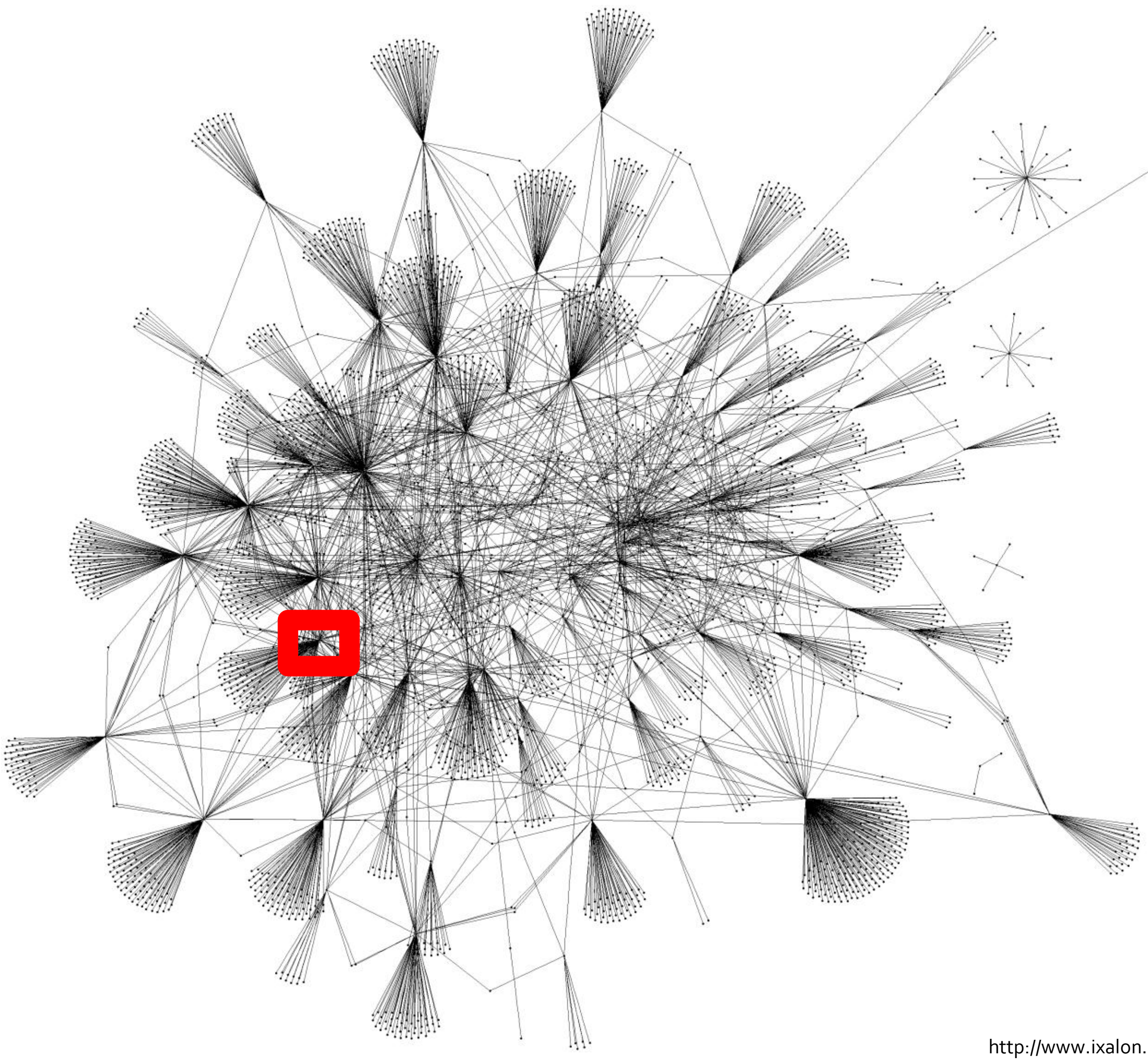
Node’s role changes depending on neighborhood

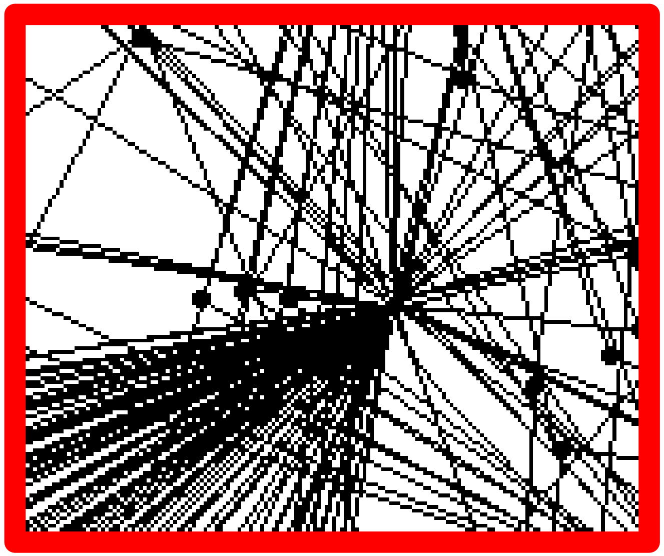
Multiscale Analysis



http://www.ixalon.net/wp-content/uploads/2009/02/lbp_user_hearts_subsample_2877nodes.png

Multiscale Analysis

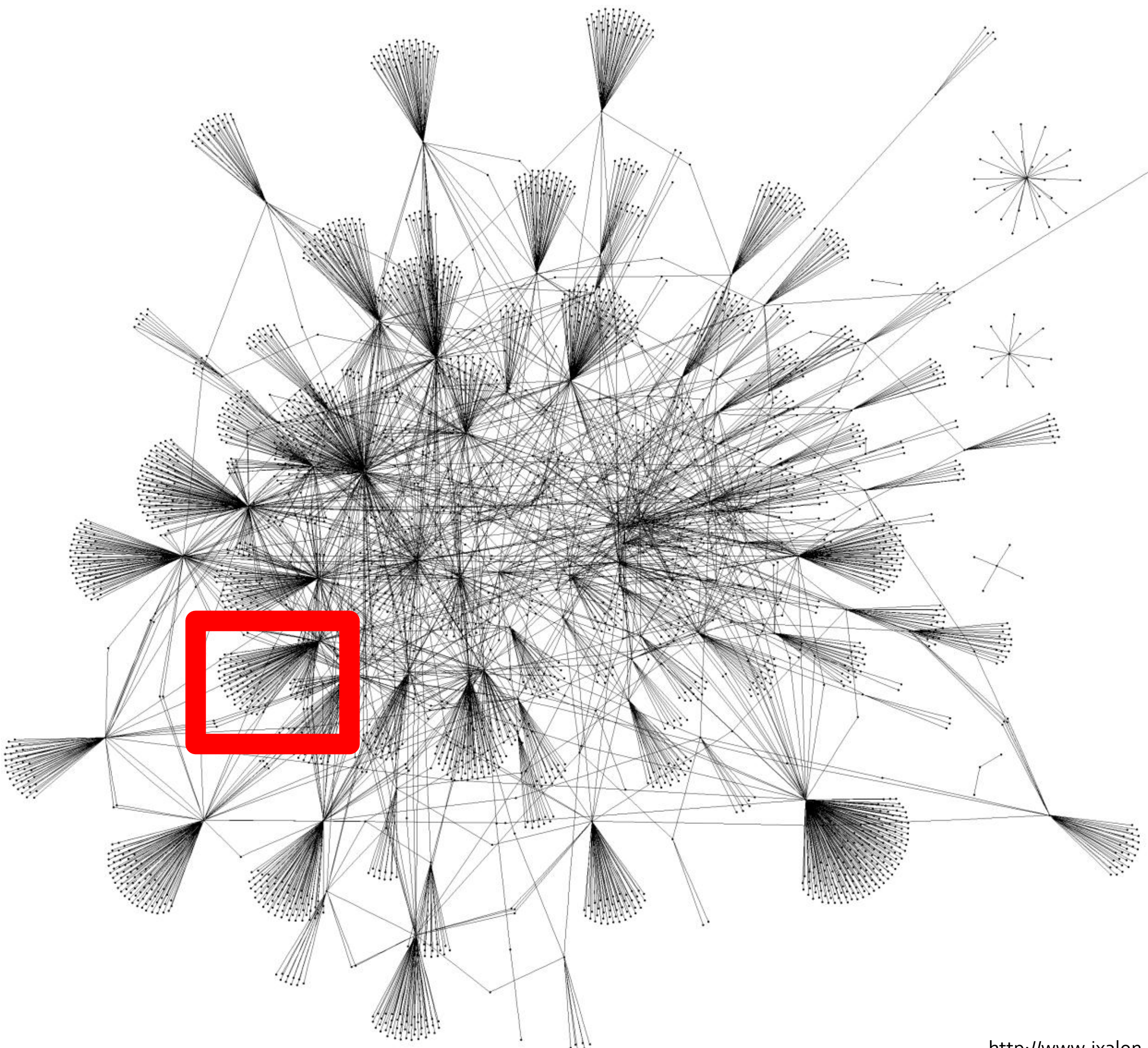


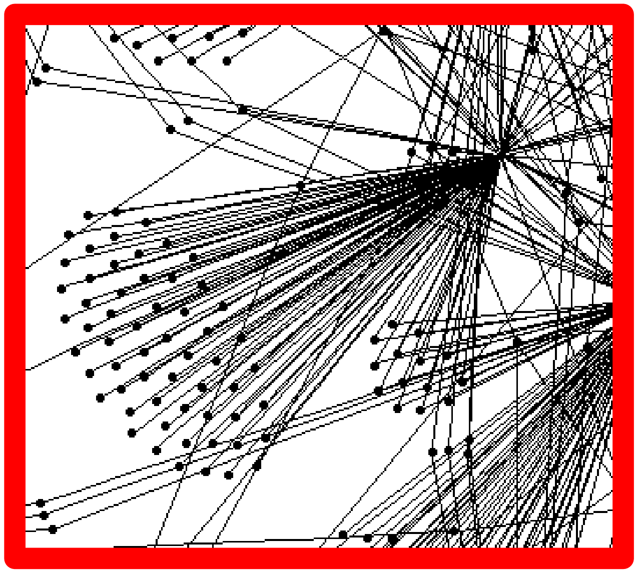


“The Individual”

http://www.ixalon.net/wp-content/uploads/2009/02/lbp_user_hearts_subsample_2877nodes.png

Multiscale Analysis

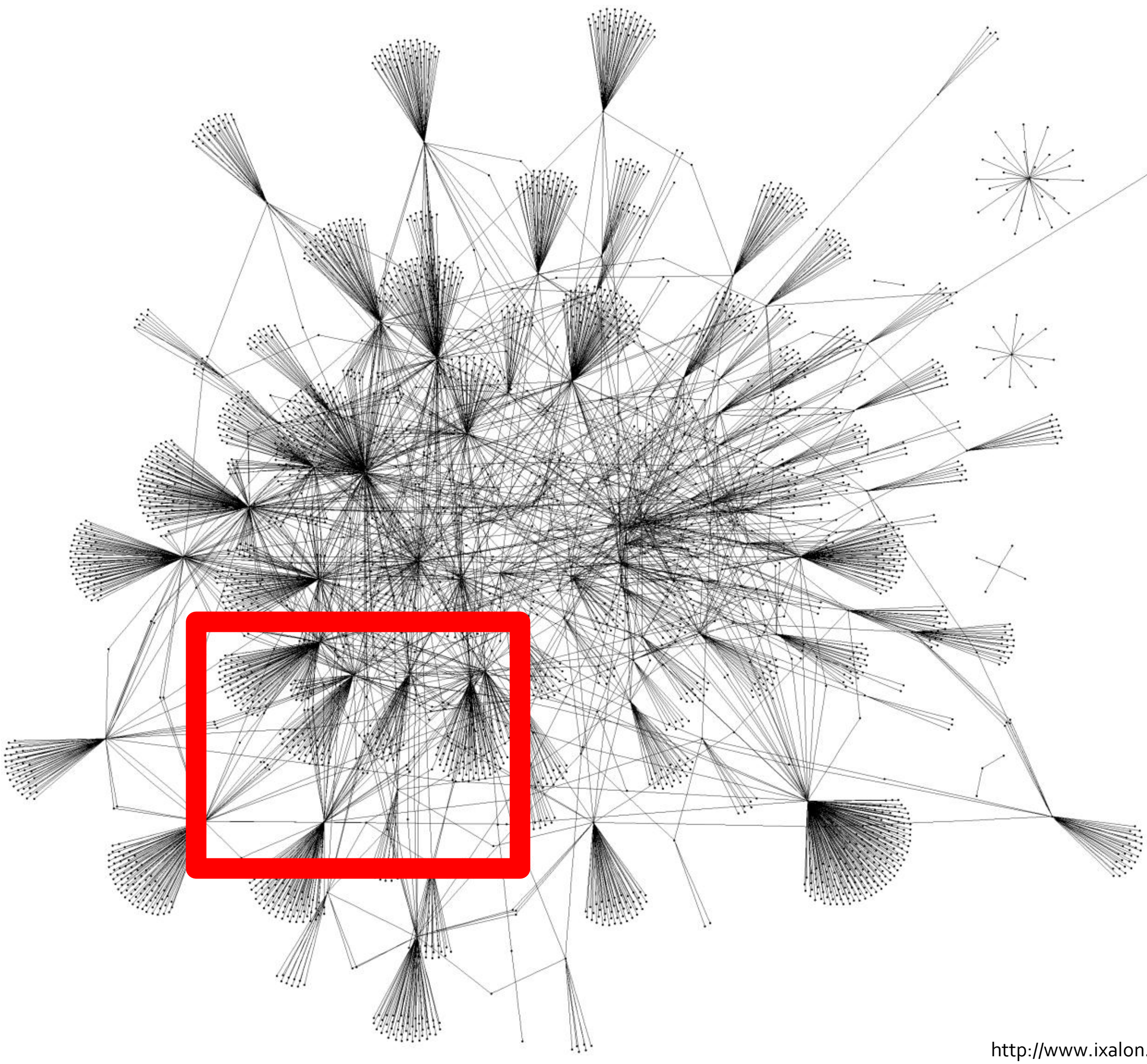




“The Hub”

http://www.ixalon.net/wp-content/uploads/2009/02/lbp_user_hearts_subsample_2877nodes.png

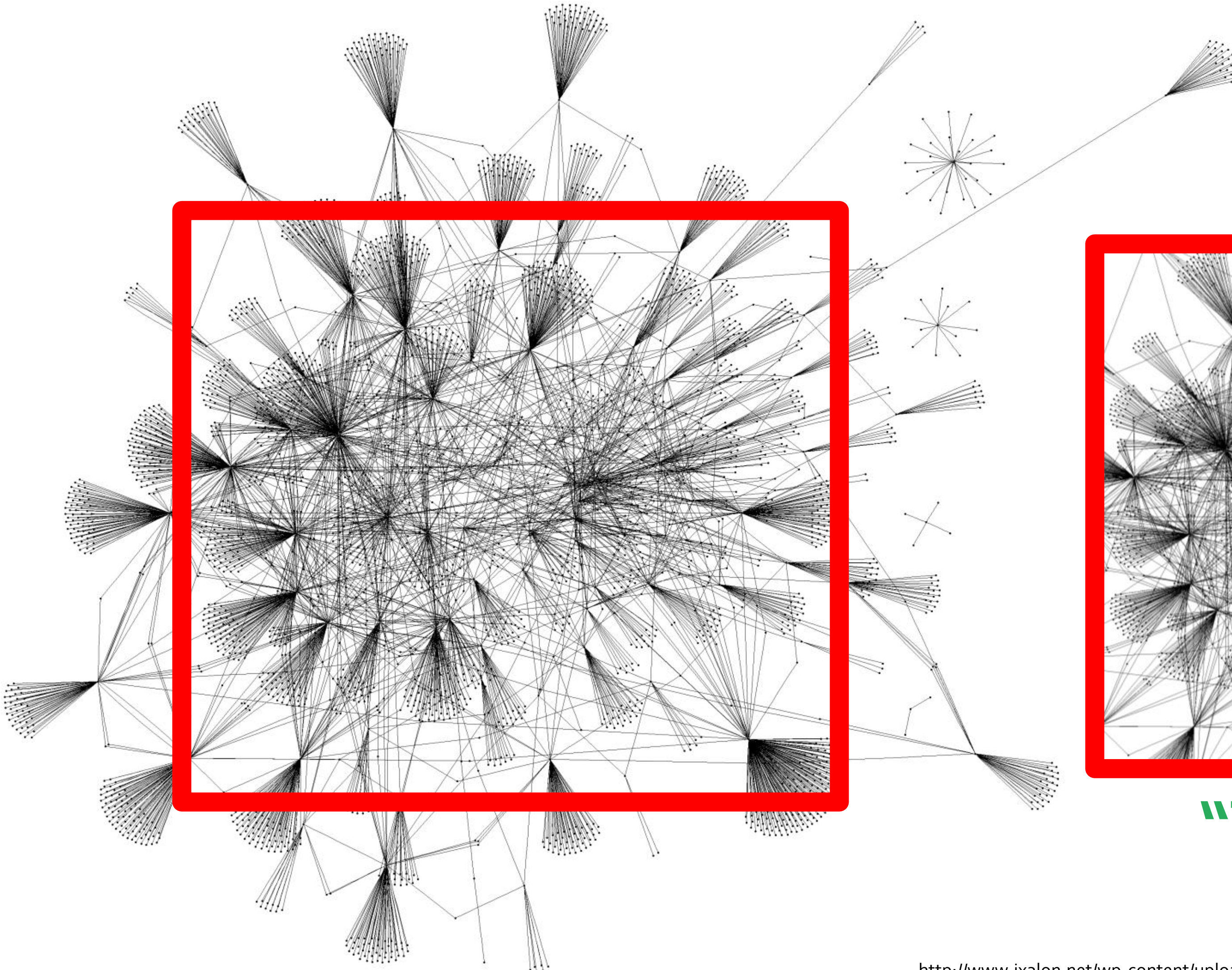
Multiscale Analysis

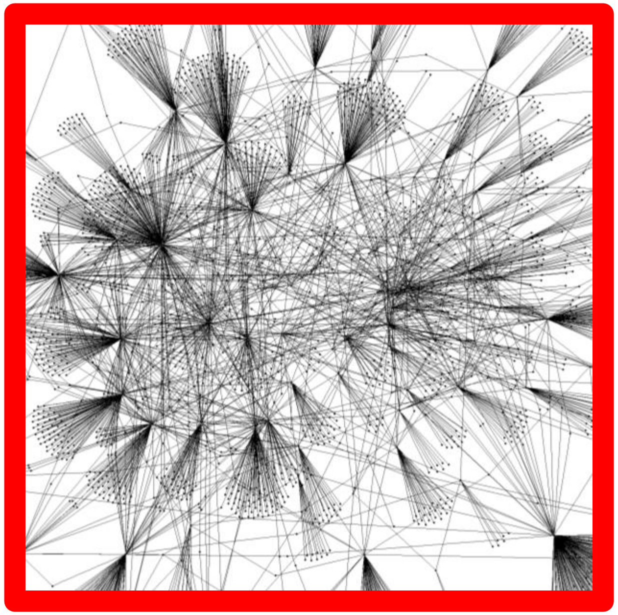


"The Hierarchy"

http://www.ixalon.net/wp-content/uploads/2009/02/lbp_user_hearts_subsample_2877nodes.png

Multiscale Analysis





"The Blob"

http://www.ixalon.net/wp-content/uploads/2009/02/lbp_user_hearts_subsample_2877nodes.png

Potentially Interesting Function

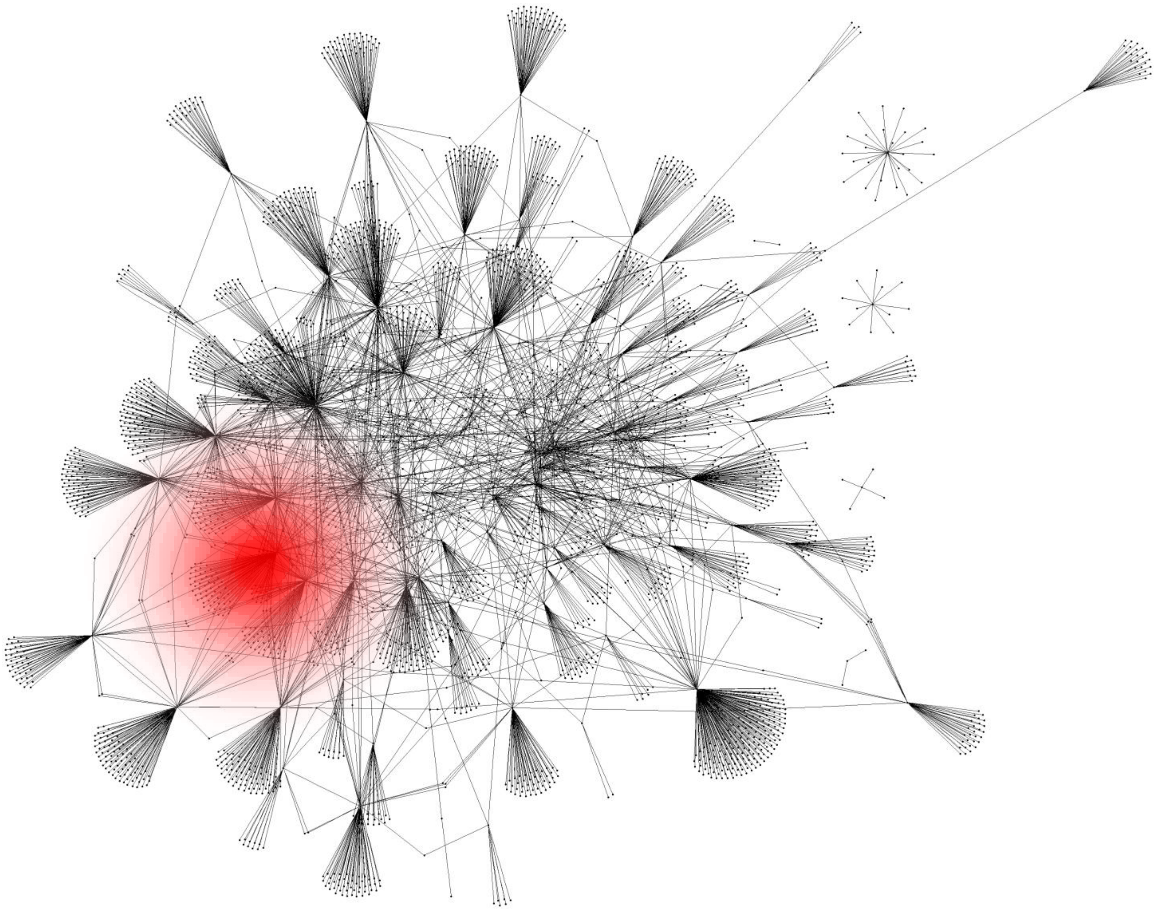
$$\boxed{\text{Topology}(t)}$$

Potentially Interesting Function

$$\boxed{\mathrm{Topology}(t)}$$

Composed of discrete events.

Alternative Viewpoint

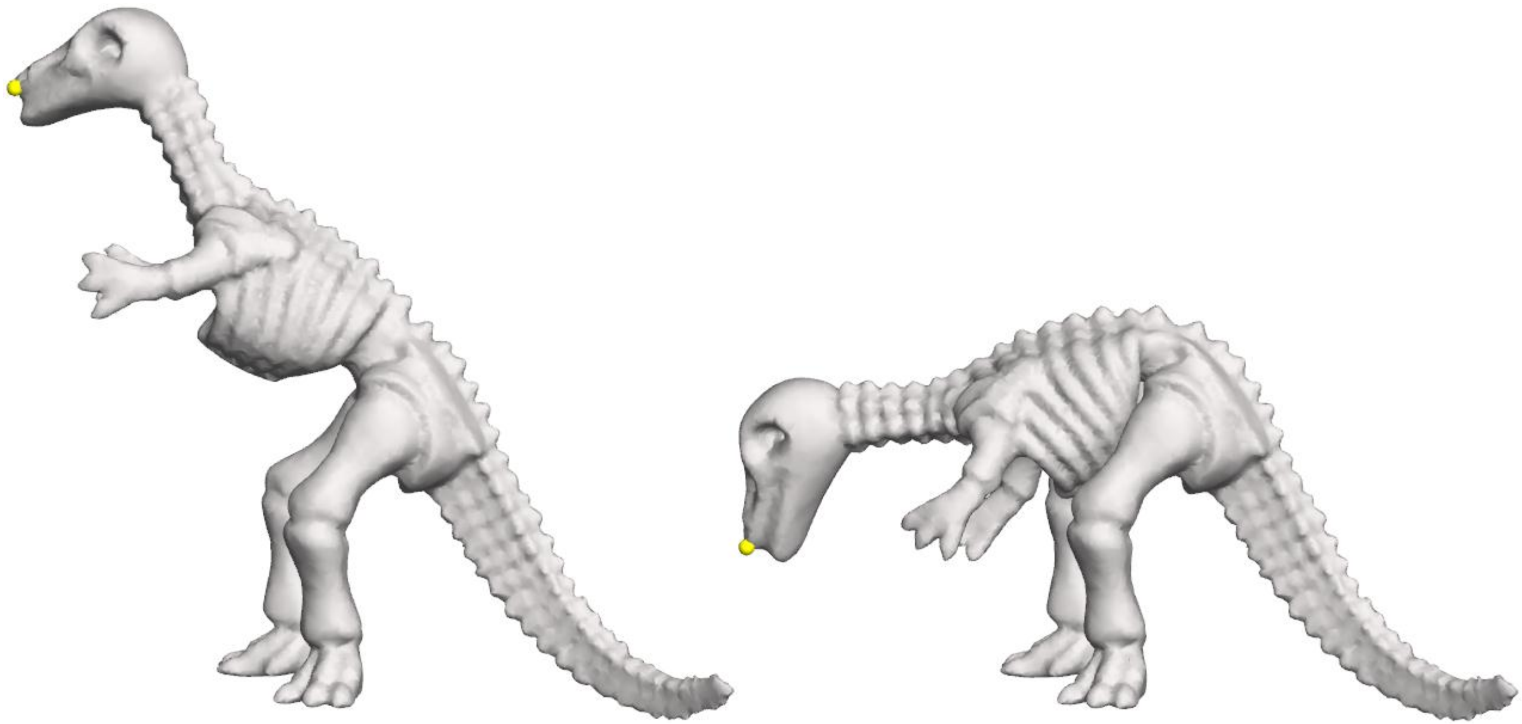


Gaussian weighting

Goal

Topological analysis with continuous dependence on scale.

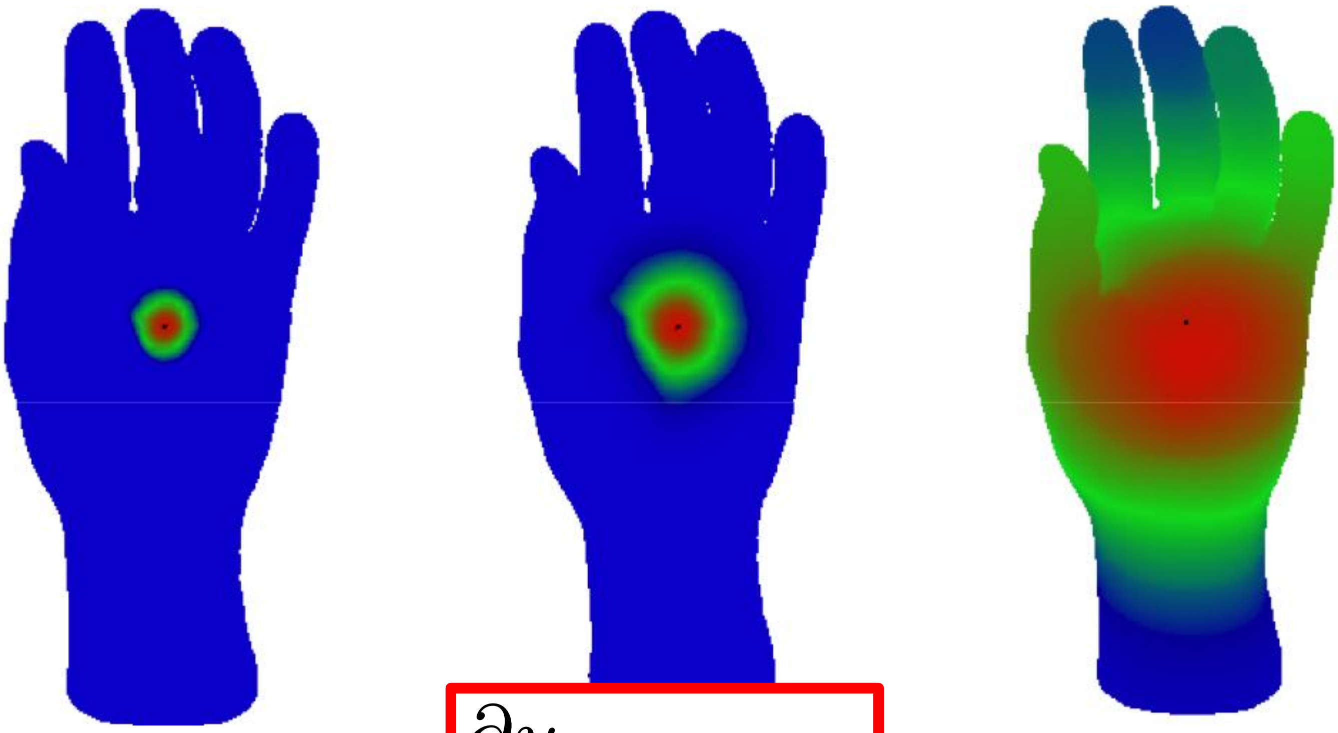
Success Story: Descriptor-Based Matching



igl.ethz.ch/projects/ARAP/

Success Story:

Descriptor-Based Matching

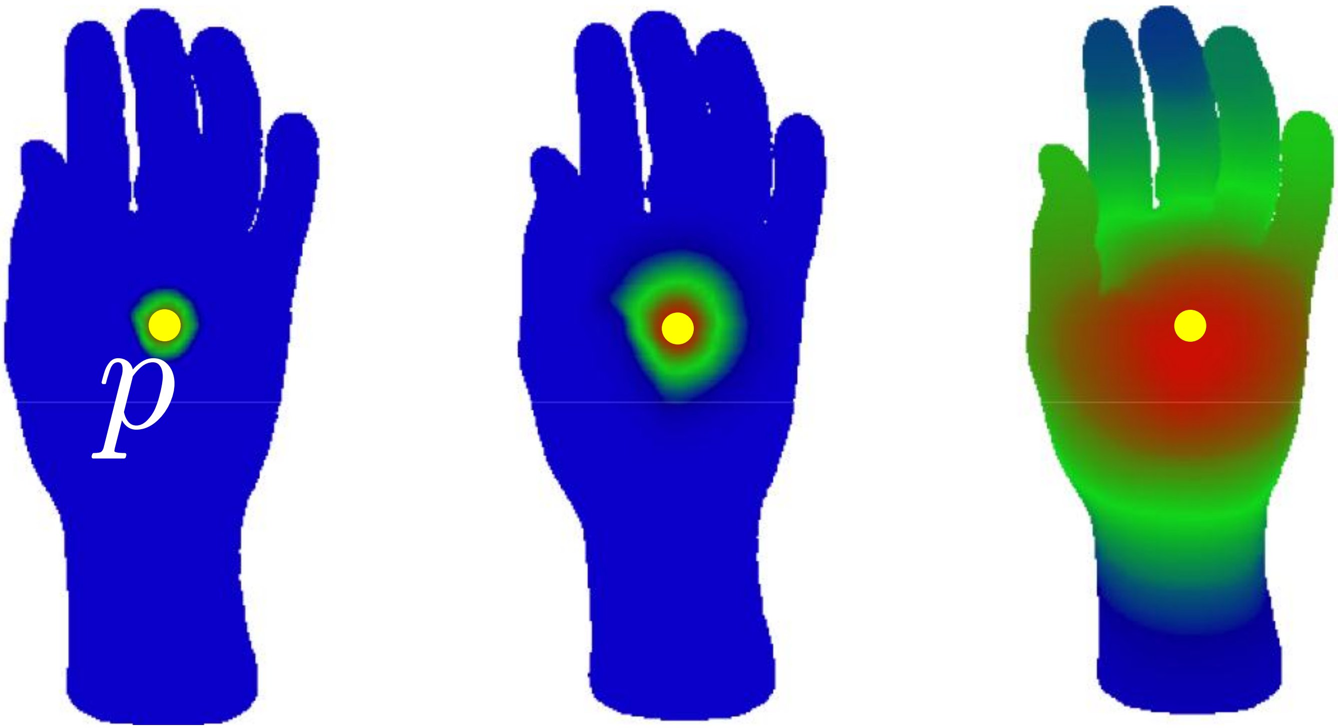


$$\frac{\partial u}{\partial t} = -\Delta u$$

http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf

Heat equation

Success Story: Descriptor-Based Matching



$$HKS_p(t) = \text{Heat left at time } t$$

http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf

Heat Kernel Signature

Problem

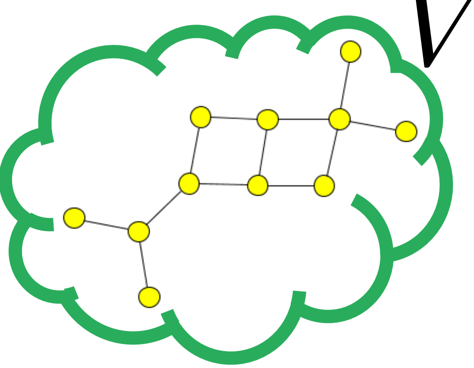
$$G = (V, E)$$

$$V = \{v_1, v_2, v_3, \dots, v_n\}$$
$$E \subseteq V \times V$$

Graphs are topological objects

Problem

$$G = (V, E)$$



$$V = \{v_1, v_2, v_3, \ldots, v_n\}$$

$$E \subseteq V \times V$$

http://graphml.graphdrawing.org/primer/simple.png

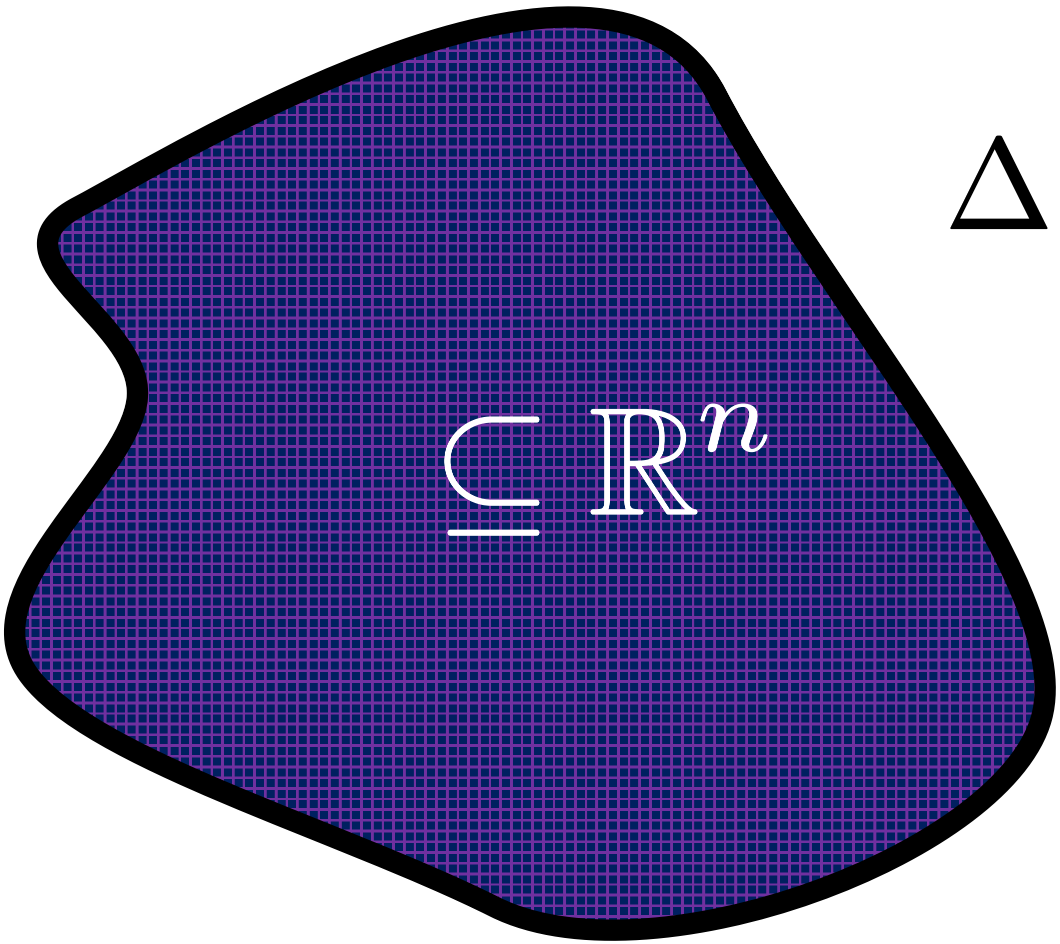
Graphs are topological objects

<question>

How do you model **flows and waves** on graphs?

</question>

The Laplacian



$$\Delta = -\sum_i \frac{\partial^2}{\partial x_i^2}$$

Key Properties

- **Linear**

$$\Delta(c_1 u + c_2 v) = c_1 \Delta u + c_2 \Delta v$$

- **Compact and bounded**

$$\|\Delta u\| \cdot \quad M\|u\| \ \forall u$$

- **Self-adjoint**

$$\langle \Delta u, v\rangle = \langle u, \Delta v\rangle$$

- **Categorizes extrema**

$$x \in \quad \text{local minimum} \implies [\Delta u](x) \cdot \quad 0$$

Key Properties

- **Linear**

$$\Delta(c_1 u + c_2 v) = c_1 \Delta u + c_2 \Delta v$$

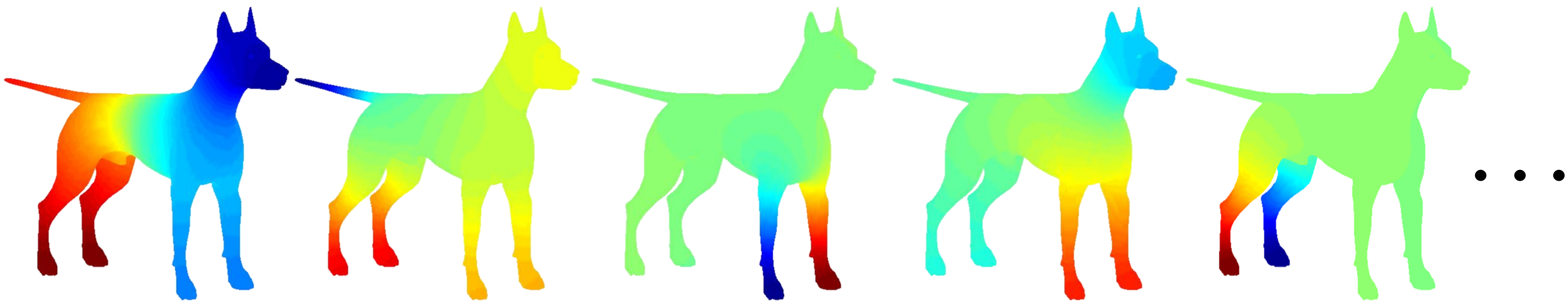
[redacted]

Sufficient for many model equations.

- **Categorizes extrema**

$$x \in \quad \text{local minimum} \quad \Longrightarrow [\Delta u](x) \cdot \quad 0$$

Laplacian Eigenfunctions



$\Delta\phi_1 = \lambda_1\phi_1$ $\Delta\phi_2 = \lambda_2\phi_2$ $\Delta\phi_3 = \lambda_3\phi_3$ $\Delta\phi_4 = \lambda_4\phi_4$ $\Delta\phi_5 = \lambda_5\phi_5$

$(\Delta\phi_0 = 0)$

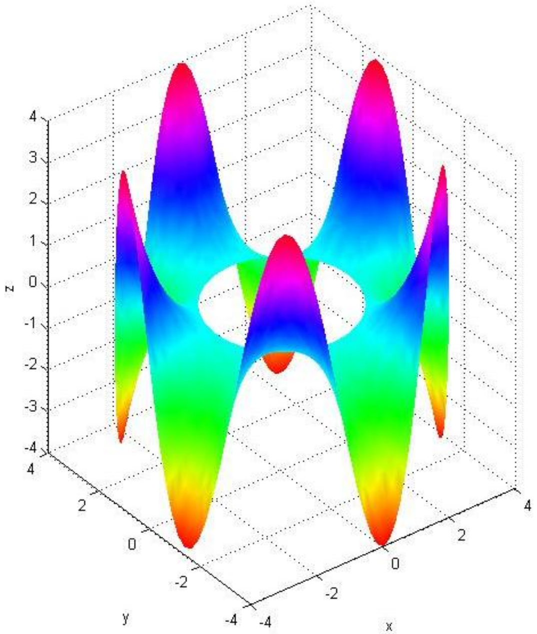
Prescribe boundary conditions on $S \subseteq \Omega$.

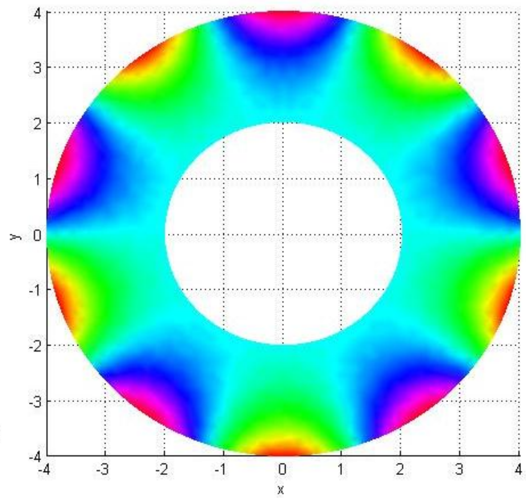
Analogous to Fourier basis

Model PDEs

$$\Delta u = 0$$

$$\Delta u = f$$





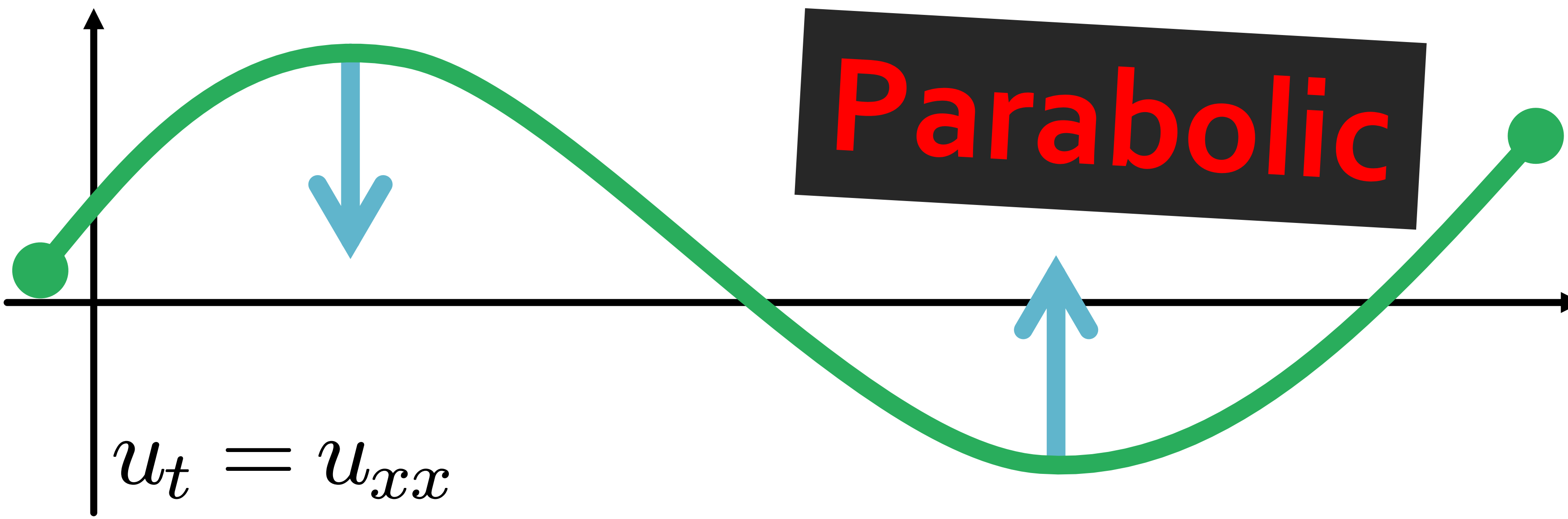
Elliptic

http://upload.wikimedia.org/wikipedia/commons/8/85/Laplace%27s_equation_on_an_annulus.jpg

Poisson and Laplace equations

Model PDEs

$$u_t = -\Delta u$$



Heat equation

Model PDEs

$$u_{tt} = -\Delta u$$

Hyperbolic

http://www.youtube.com/watch?v=l_yxwgh7Nbc&feature=related

Wave equation

Eigenfunction Solutions

Heat equation

$$u = \sum_i a_i e^{-\lambda_i t} \phi_i$$

Wave equation

$$u = \sum_{\lambda_i = 0} (a_i + b_i t)\phi_i + \sum_{\lambda_i \neq 0} a_i \cos(\sqrt{\lambda_i} t + b_i)\phi_i$$

Generic Strategy

1. Define the domain Ω.
2. Define the Laplacian Δ.
3. See what happens.

Three Approaches

WAVE EQUATIONS FOR GRAPHS AND THE EDGE-BASED LAPLACIAN

JOEL FRIEDMAN AND JEAN-PIERRE TILLICH

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graph theory

Discrete Green's Functions

Fan Chung[1]

University of California, San Diego, La Jolla, California 92093-0112

and

S.-T. Yau

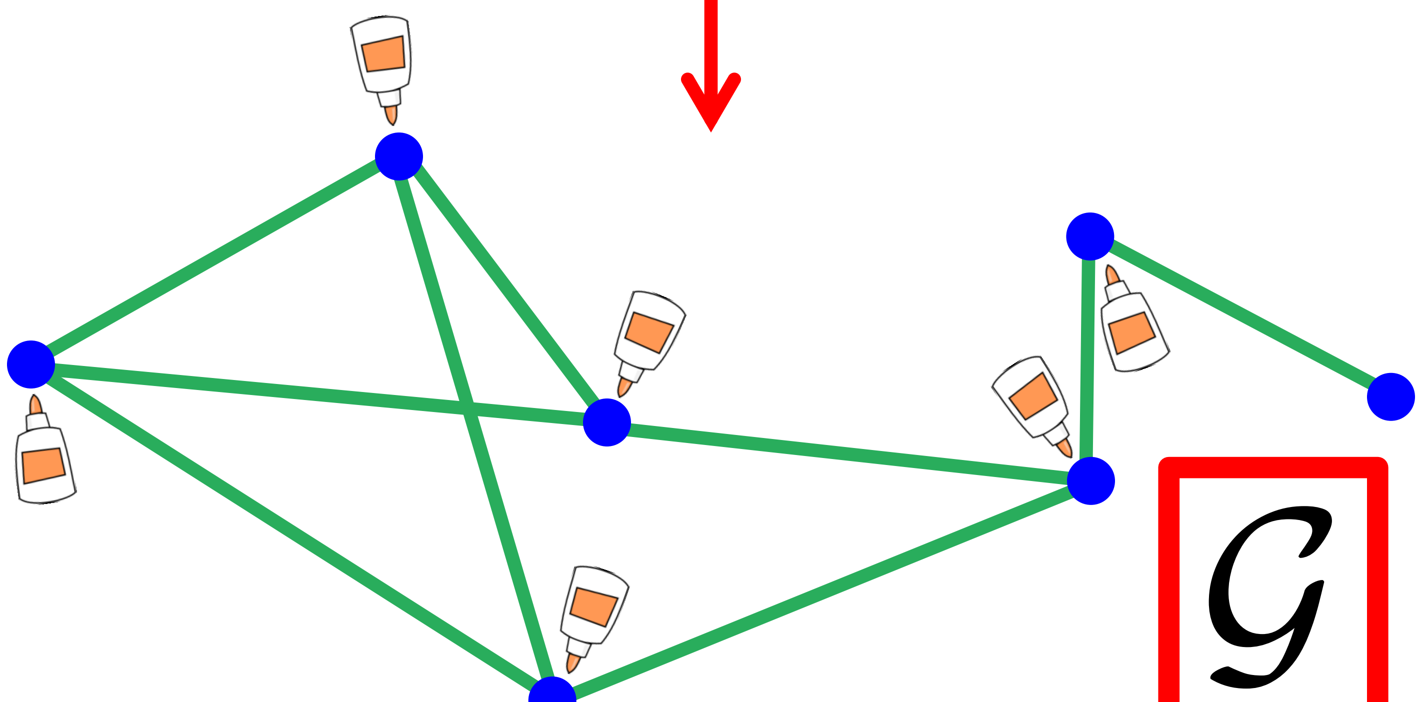
Diffusion and Elastic Equations on Networks

By

Soon-Yeong CHUNG*, Yun-Sung CHUNG** and Jong-Ho KIM***

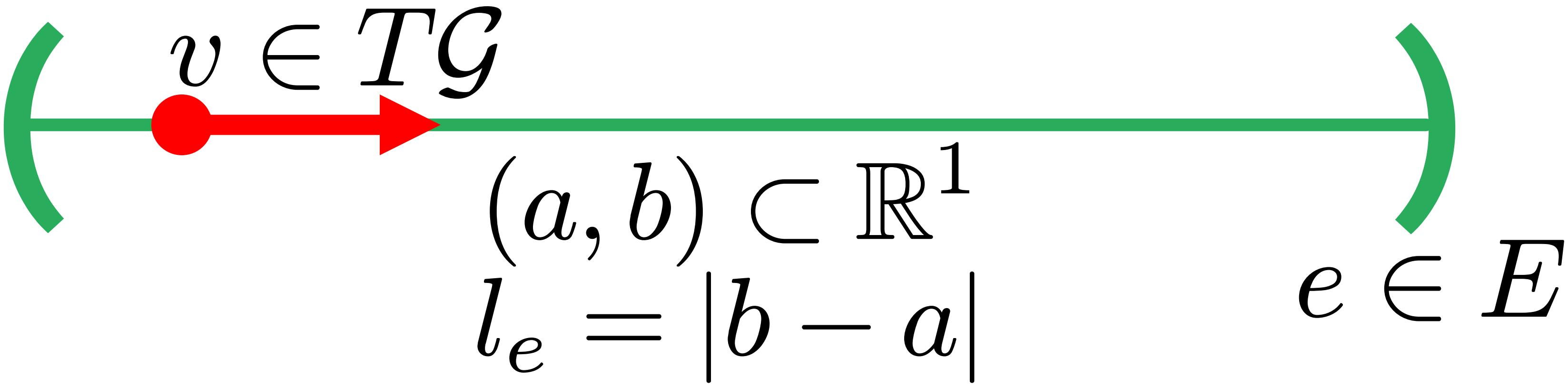
Geometric Realization

$$G = (V, E)$$



$$\mathcal{G}$$

Edge Interior



Allowable operations:

$$\nabla f \qquad \nabla_{\text{calc}} \cdot X$$

Admits differential structure

Two Measures

Discrete **vertex** measure

$$\mathcal{V}$$

Lebesgue **edge** measure

$$\mathcal{E}$$

Integrating Factors

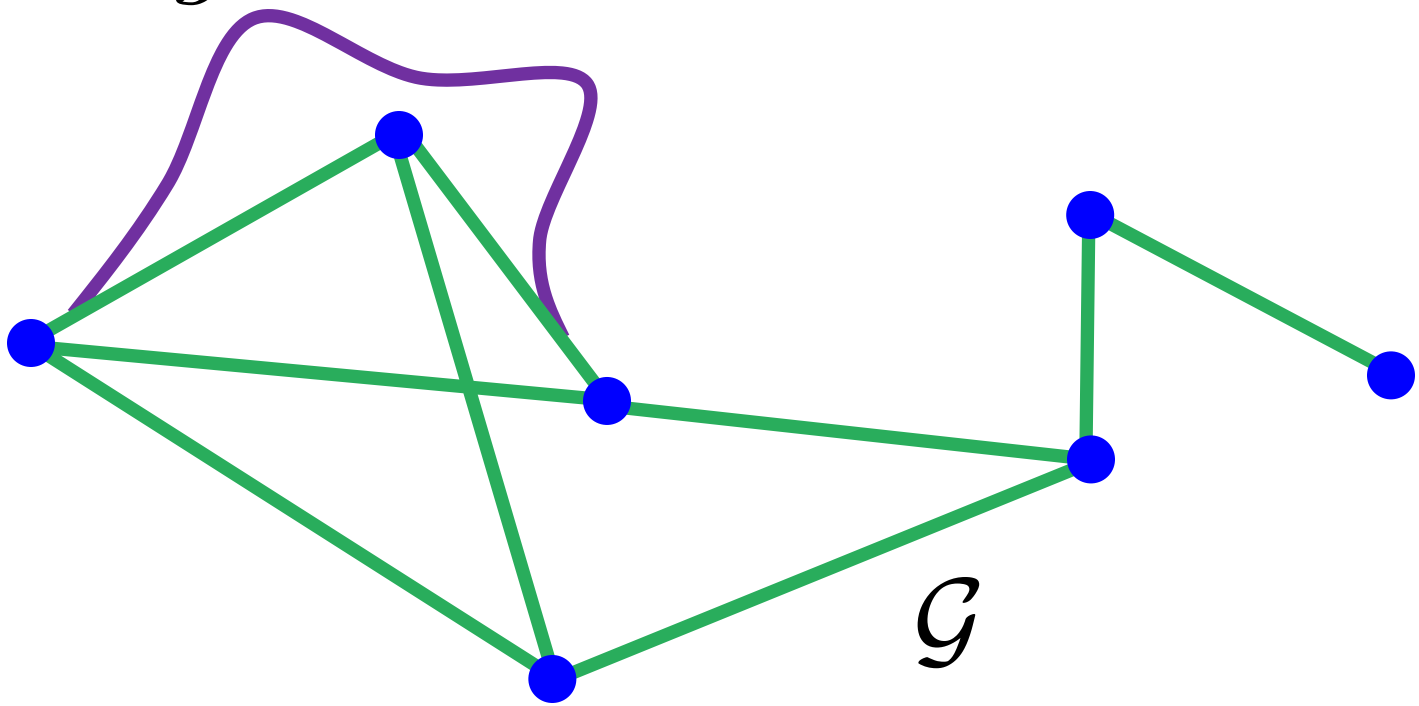
$$d\Gamma = \alpha \; d\mathcal{V} + \beta \; d\mathcal{E}$$

$$\int_{\mathcal{G}} f \; d\Gamma = \int_{\mathcal{G}} f\alpha \; d\mathcal{V} + \int_{\mathcal{G}} f\beta \; d\mathcal{E}$$

Integration by Parts

$$\mathcal{D}_X(g) \equiv -\int_{\mathcal{G}\backslash V} X \cdot \nabla g \; d\mathcal{E} = \int_{\mathcal{G}} [(\nabla_{calc} \cdot X) g \; d\mathcal{E} - (\tilde{n} \cdot X) g \; d\mathcal{V}]$$

$$g : \mathcal{G} \to \mathbb{R}$$



Integration by Parts

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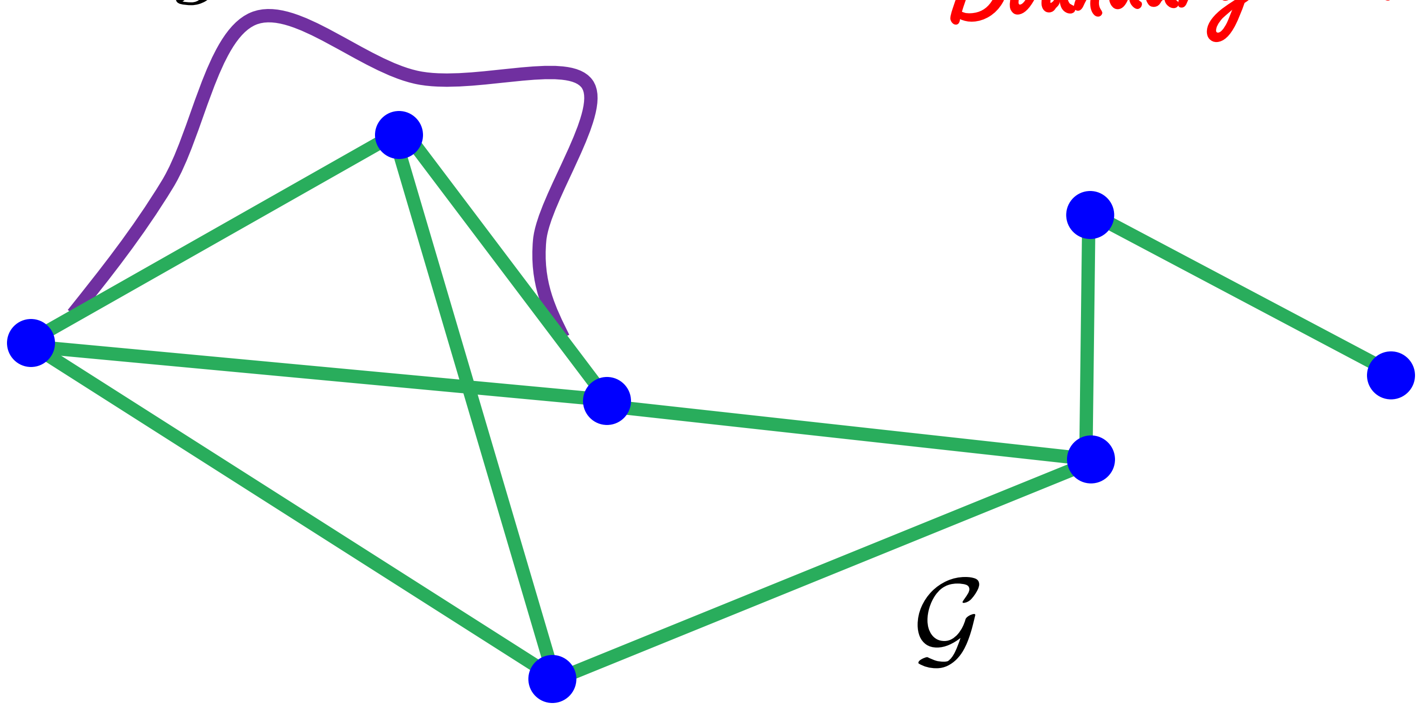
Boundary conditions!

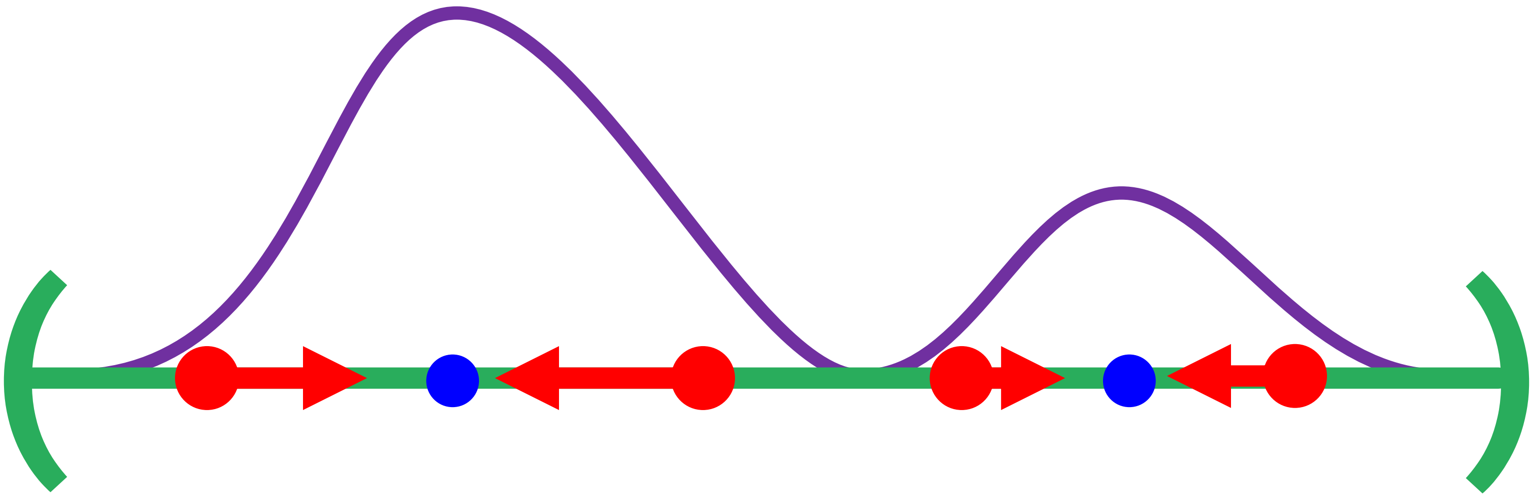
$$g : \mathcal{G} \rightarrow \mathbb{R}$$



Divergence Factor

$$dD_X \equiv (\nabla_{calc} \cdot X)\ d\mathcal{E} - (\tilde{n} \cdot X)\ d\mathcal{V}$$

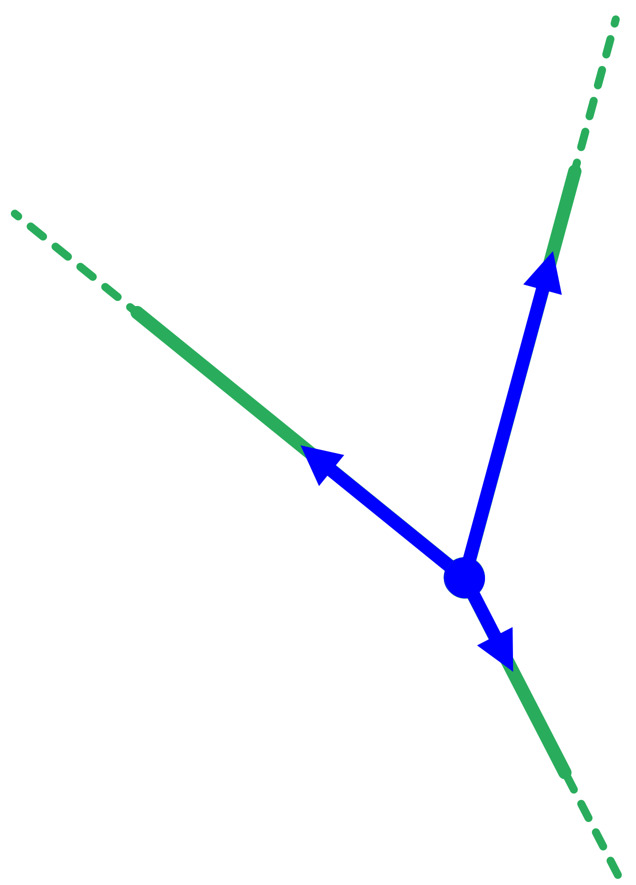
Divergence in edge interior



Divergence Factor

$$d\mathcal{D}_X \equiv (\nabla_{calc} \cdot X)\, d\mathcal{E} - (\tilde{n} \cdot X)\, d\mathcal{V}$$

Divergence at vertices



Divergence Factor

$$d\mathcal{L}_f \equiv -d\mathcal{D}_{\nabla f}$$

Divergence Factor

$$d\mathcal{L}_f \equiv -d\mathcal{D}_{\nabla f}$$

$$\Delta f = -\nabla \cdot (\nabla f)$$

Divergence Factor

$$d\mathcal{L}_f \equiv -d\mathcal{D}_{\nabla f}$$

$$d\mathcal{L}_f = \Delta_E \, d\mathcal{E} + \Delta_V \, d\mathcal{V}$$

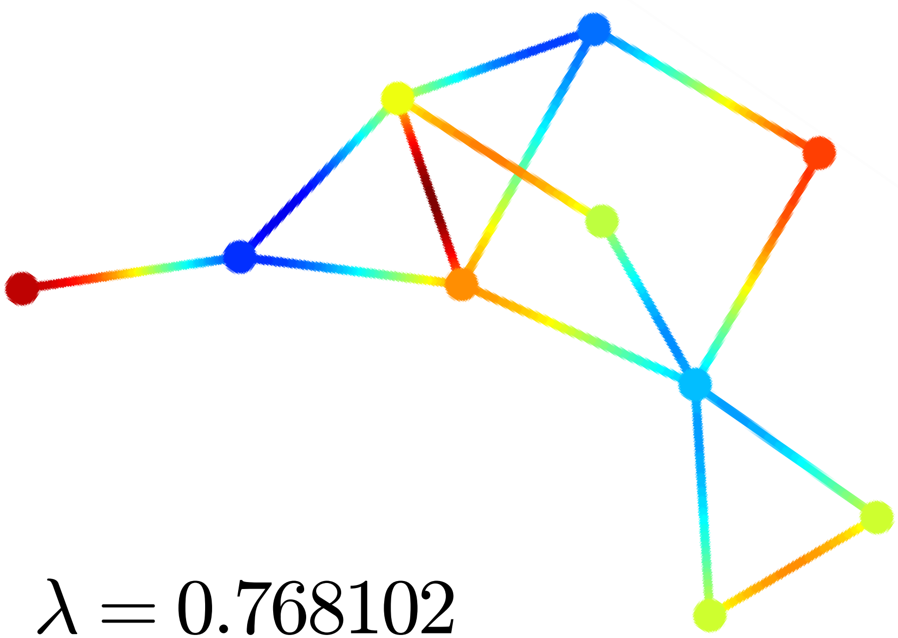
$$\Delta_E f = -\nabla_{calc} \cdot \nabla f$$

$$\Delta_V f = \tilde{n} \cdot \nabla f$$

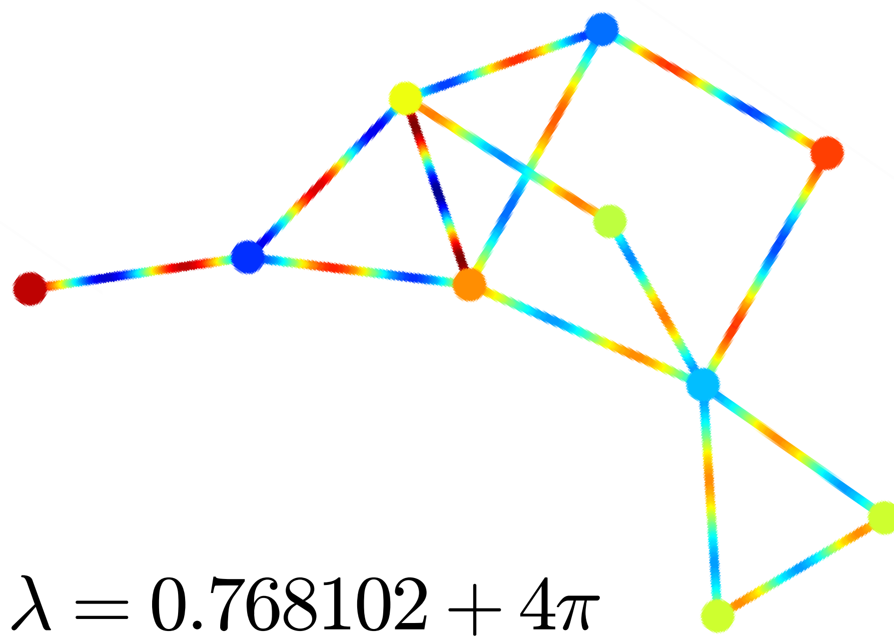
Edge-Based Eigenfunctions

$$\Delta_E f = -\nabla_{calc} \cdot \nabla f = \lambda f$$

$$\Delta_V f = \tilde{n} \cdot \nabla f = 0$$

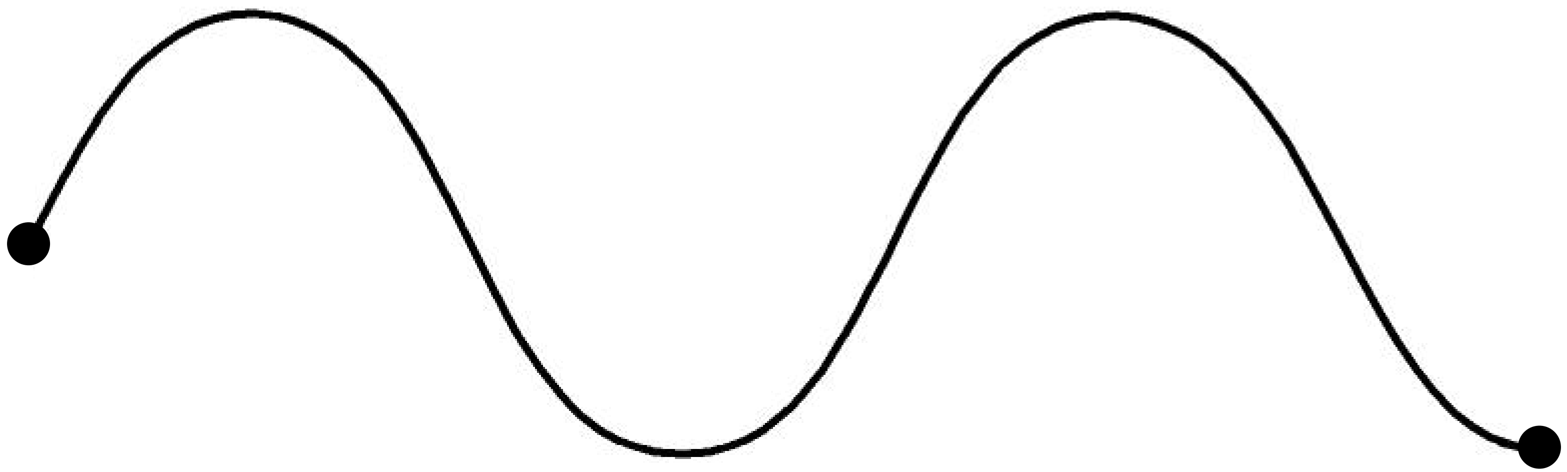


$\lambda = 0.768102$



$\lambda = 0.768102 + 4\pi$

Eigenfunction in Edge Interior



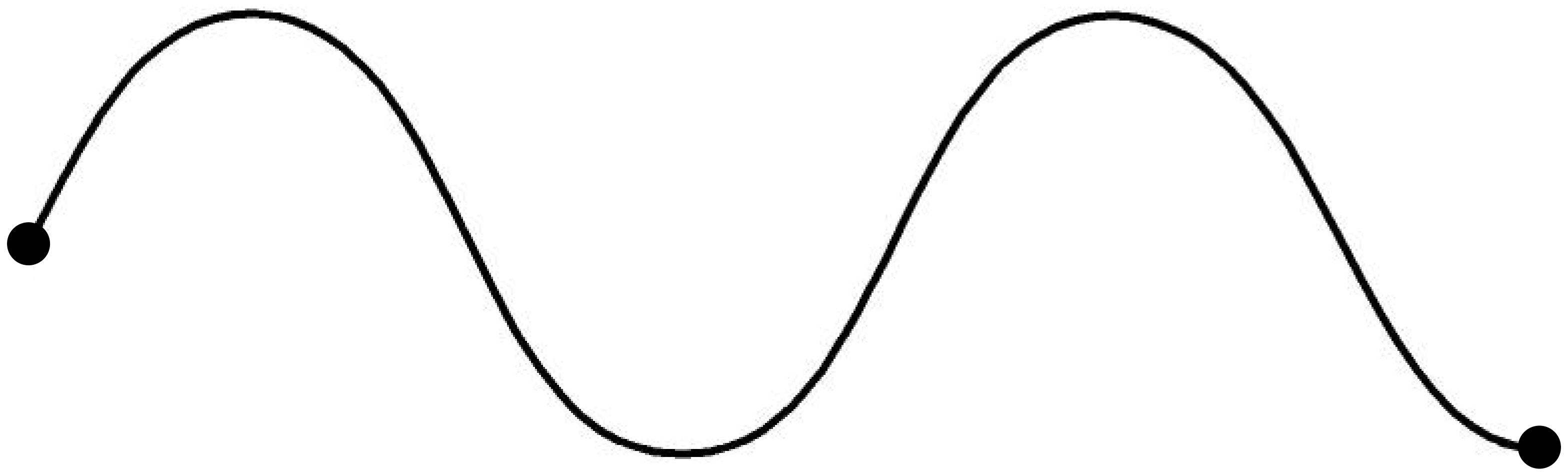
$$f(u) = f_e(0) = A\cos B$$

$$f(v) = f_e(l_e) = A\cos(\omega l_e + B) = A\cos(\omega l_e)\cos(B) - A\sin(\omega l_e)\sin(B)$$

$$f'(0) = -A\omega\sin B = -\omega\frac{f(v) - \cos(\omega l_e)f(u)}{\sin(\omega l_e)}$$

$$0 = \Delta_V f|_u = \sum_{e=(u,v)\in E}\frac{f(v) - \cos(\omega l_e)f(u)}{\sin(\omega l_e)}$$

Eigenfunction in Edge Interior



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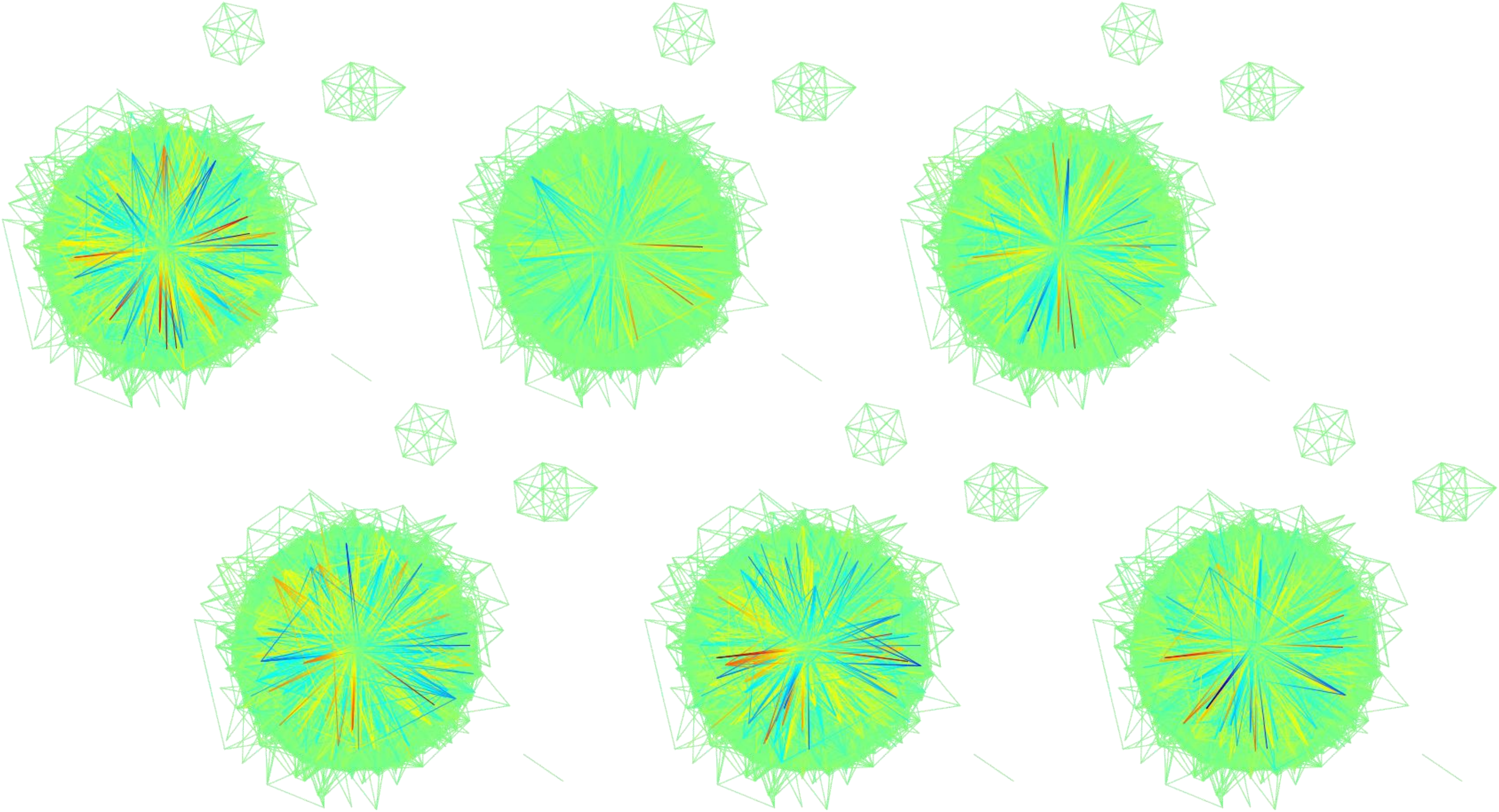
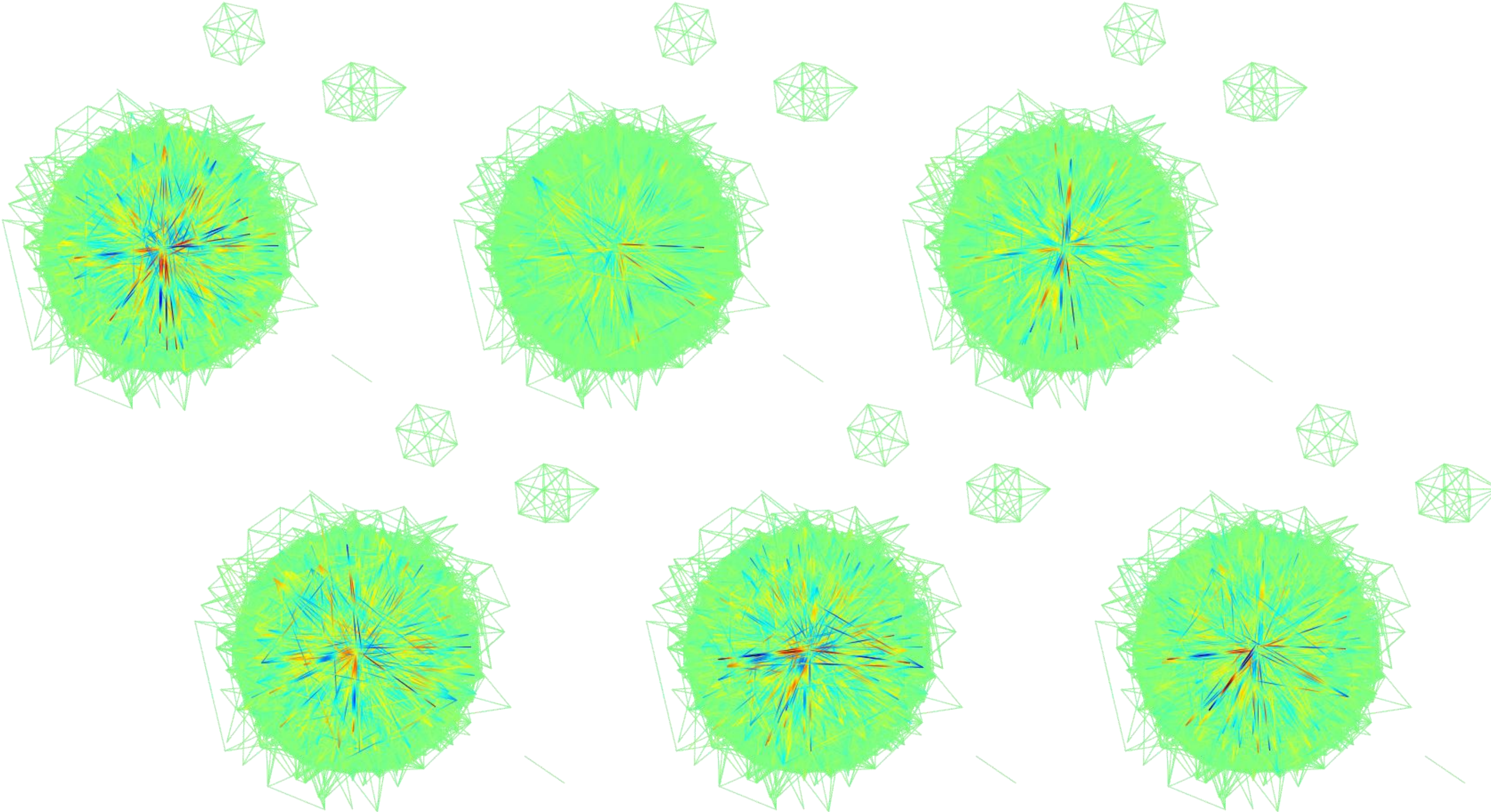
Edge-Based Eigenfunctions



"Marvel Universe Looks Almost Like a Social Network" / Alberich, Miro-Julia, Rossello

Edge-Based Eigenfunctions



“Marvel Universe Looks Almost Like a Social Network” / Alberich, Miro-Julia, Rossello

Geometric Graph Wave Equation

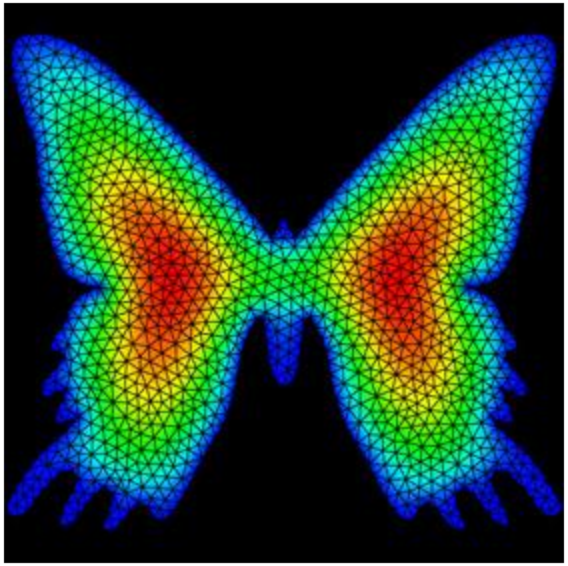
$$(\alpha\ d\mathcal{V} + \beta\ d\mathcal{E})u_{tt} = d\mathcal{D}_{\gamma\nabla u}$$

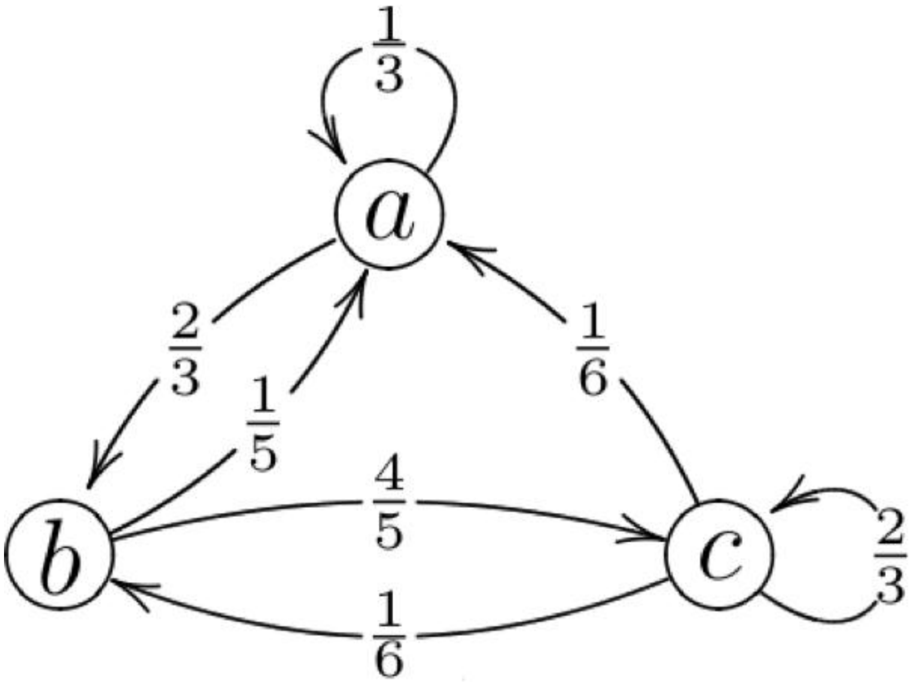
- Encodes boundary conditions
- Preserves energy
- Constant speed of propagation

Geometrization: Conclusion

Mostly theoretical, needs more work for practical applications.

Discrete Laplacians

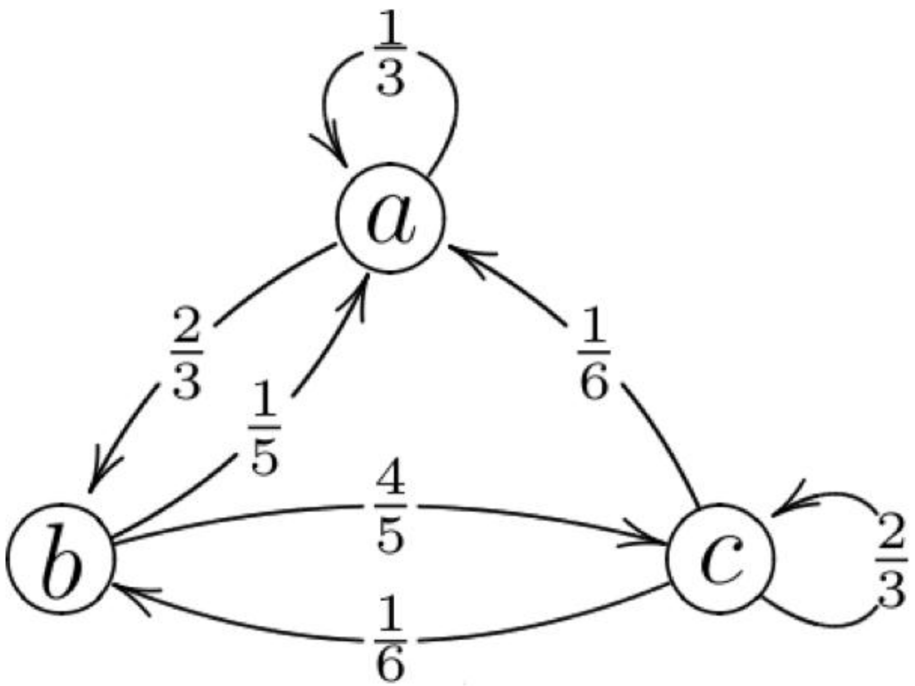




http://www.bugman123.com/Engineering/FEM-triangles.jpg http://www.codinghorror.com/blog/2008/06/markov-and-you.html

Markov Chain Stationary States

$$\Delta(u,v) \equiv [I - P](u,v) = \begin{cases} 1 & \text{if } u = v \\ -P(u,v) & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$



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- **Linear**

  $$\Delta(c_1 u + c_2 v) = c_1 \Delta u + c_2 \Delta v$$

- **Compact and bounded**

  $$\|\Delta u\| \leq M \|u\| \; \forall u$$

- **Self-adjoint**

  $$\langle \Delta u, v \rangle = \langle u, \Delta v \rangle$$

- **Categorizes extrema**

  $$x \in \Omega \text{ local minimum} \implies [\Delta u](x) \leq 0$$

Markov Chain Stationary States

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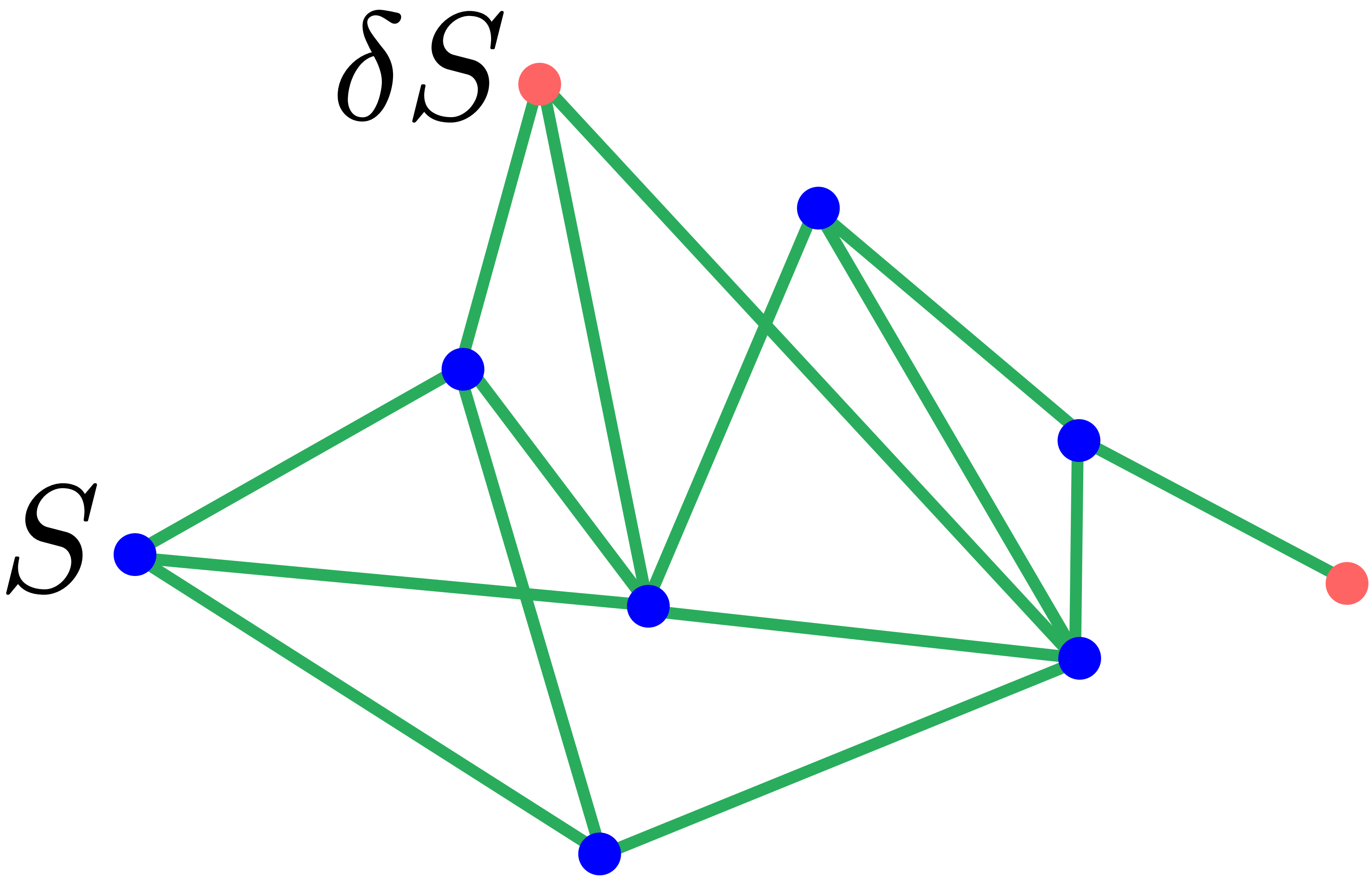
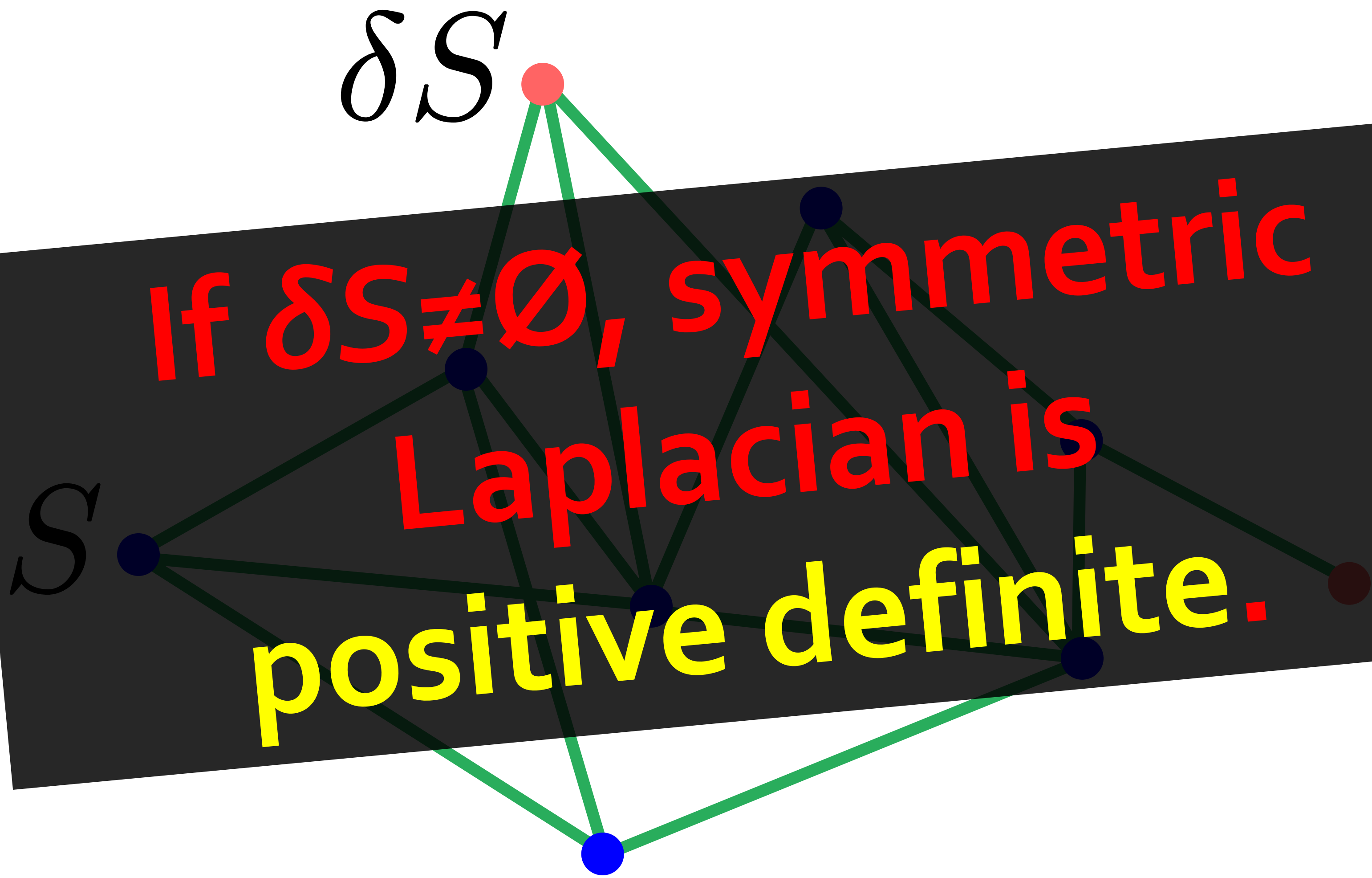
$$\mathscr{L} = T^{1/2} \Delta T^{-1/2}$$

Discrete Setup



Discrete Setup



If δS≠Ø, symmetric Laplacian is positive definite.

Discrete Green's Functions

$$\Delta_S u = f$$

$$\text{“}\Delta_S^{-1}\text{”}$$

$$u = G_S f$$

Closed-Form Laplace Solution

Lemma 7 ([CY00], Theorem 1). *Suppose $\Delta f = 0$ on S with $f(x) = \sigma(x)$ for $x \in \delta S$. Then, f satisfies*

$$f(z) = d_z^{-1/2} \sum_i \frac{1}{\lambda_i} \phi_i(z) \sum_{\substack{x \in S \\ (x,y) \in E \\ y \in \delta S}} d_x^{-1/2} \phi_i(x) \sigma(y)$$

$$\mathscr{L} = T^{1/2} \Delta T^{-1/2}$$

$$\mathscr{L} \phi_i = \lambda_i \phi_i$$

Proof strategy: **Construct solution to symmetric Laplace equation from *f*, expand its projection onto Fourier basis.**

Semi-Discrete PDEs

- **Discrete** along the graph
- **Continuous** in time

$$u_t = -\Delta u$$

$$u_{tt} = -\Delta u$$

Two Dual Viewpoints

$$u_t = -\Delta u$$

Heat equation

$$u_{tt} = -\Delta u$$

Wave equation

PDE standpoint

Two Dual Viewpoints

$$u_t = -\Delta u \qquad u_{tt} = -\Delta u$$

Heat equation | Wave equation

Properties similar to physical phenomena.

PDE standpoint

Two Dual Viewpoints

$$\vec{u}_t = M\vec{u}$$

Linear ordinary differential equation

ODE standpoint

Two Dual Viewpoints

$$\vec{u}_t = M\vec{u}$$

Linear ordinary differential equation

Can solve without convergence arguments and other technicalities.

ODE standpoint

Huygens Property

Lemma 11 ([CCK07], "Huygens Property" Theorem 3.6). *Suppose u satisfies the heat equation $u_t = -\Delta u$ on a graph with $S = V$. Then, for every $t, \delta > 0$ we have*

$$u(x, t + \delta) = \langle K(x, \cdot, \delta), u(\cdot, t) \rangle \tag{54}$$

Huygens Property

Lemma 11 ([CCK07], "Huygens Property" Theorem 3.6). *Suppose u satisfies the heat equation $u_t = -\Delta u$ on a graph with $S = V$. Then, for every $t, \delta > 0$ we have*

$$u(x, t+\delta) = \langle K(x, \cdot, \delta), u(\cdot, t) \rangle \quad (54)$$

Heat kernel

$$u(x,t) = \langle K_S(x,\cdot,t), f(\cdot) \rangle_S$$

$$K_S(u,v,t) = \sum_{i=1}^{|S|} e^{-\lambda_i t} \phi_i(u) \phi_i(v) \sqrt{\frac{d_v}{d_u}}$$

Huygens Property

Lemma 11 ([CCK07], "Huygens Property" Theorem 3.6). *Suppose u satisfies the heat equation $u_t = -\Delta u$ on a graph with $S = V$. Then, for every $t, \delta > 0$ we have*

$$u(x, t+\delta) = \langle K(x, \cdot, \delta), u(\cdot, t) \rangle \tag{54}$$

$$u(x,t) = \frac{1}{\sqrt{d_x}} \sum_i c_i e^{-\lambda_i t} \phi_i(x)$$

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$$\begin{aligned}
u(x, t+\delta) &= \frac{1}{\sqrt{d_x}} \sum_i c_i e^{-\lambda_i (t+\delta)} \phi_i(x) \\
&= \frac{1}{\sqrt{d_x}} \sum_i e^{-\lambda_i \delta} c_i e^{-\lambda_i t} \phi_i(x) \\
&= \frac{1}{\sqrt{d_x}} \sum_i e^{-\lambda_i \delta} \phi_i(x) \left\langle \sqrt{d_y} \phi_i(y), \frac{1}{\sqrt{d_y}} \sum_j c_j e^{-\lambda_j t} \phi_j(y) \right\rangle \\
&= \frac{1}{\sqrt{d_x}} \sum_i e^{-\lambda_i \delta} \phi_i(x) \langle \sqrt{d_y} \phi_i(y), u(\cdot, t) \rangle \\
&= \langle K(x, \cdot, \delta), u(\cdot, t) \rangle
\end{aligned}$$

Huygens Property

Lemma 11 ([CCK07], "Huygens Property" Theorem 3.6). *Suppose u satisfies the heat equation $u_t = -\Delta u$ on a graph with $S = V$. Then, for every $t, \delta > 0$ we have*

$$u(x, t+\delta) = \langle K(x,\cdot,\delta), u(\cdot,t)\rangle \qquad (54)$$

$$u(x,t+\delta) = \frac{1}{\sqrt{d_x}} \sum_i c_i e^{-\lambda_i (t+\delta)} \phi_i(x)$$

$$u(x,t) = \frac{1}{\sqrt{d_x}} \sum_i c_i e^{-\lambda_i t} \phi_i(x)$$

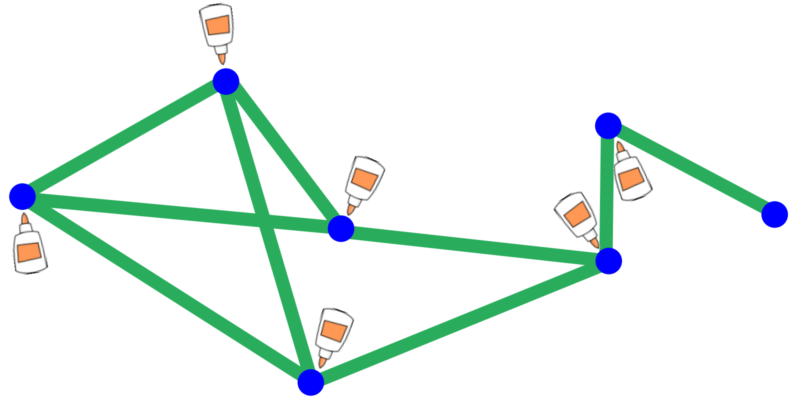
Generic proof strategy doesn't change from continuous case.

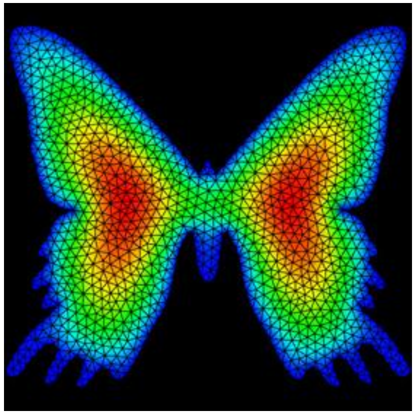
$$= \langle K(x,\cdot,\delta), u(\cdot,t)\rangle$$

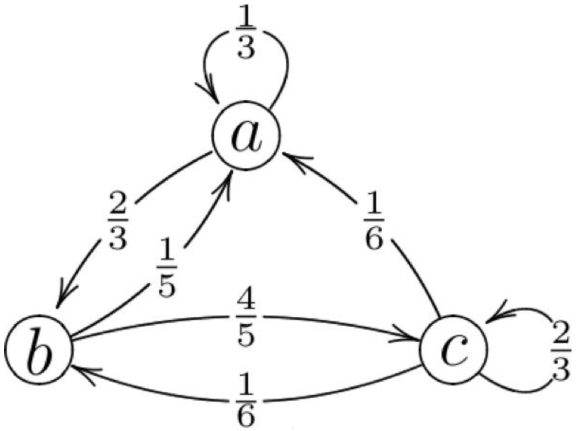
Themes

Ingredients:

1. Domain
2. "Differential" operator



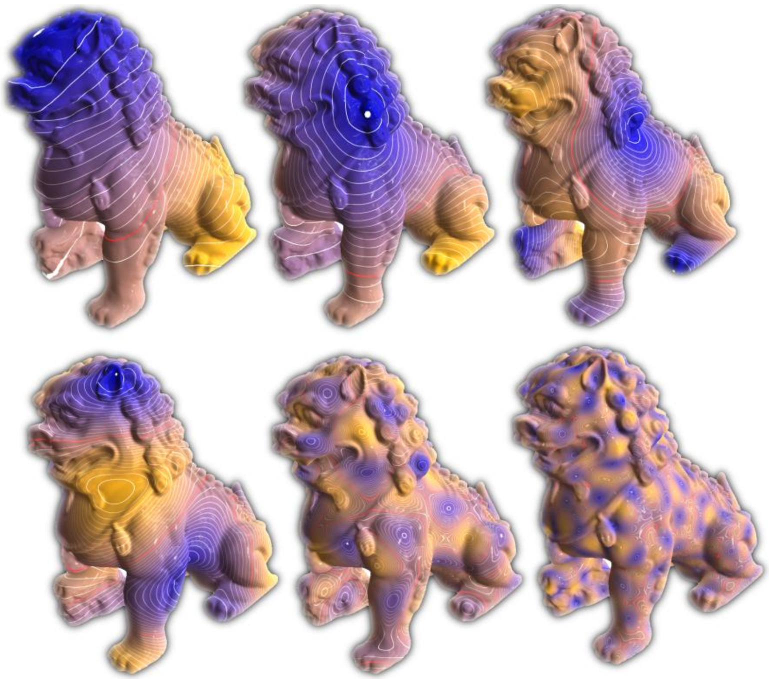


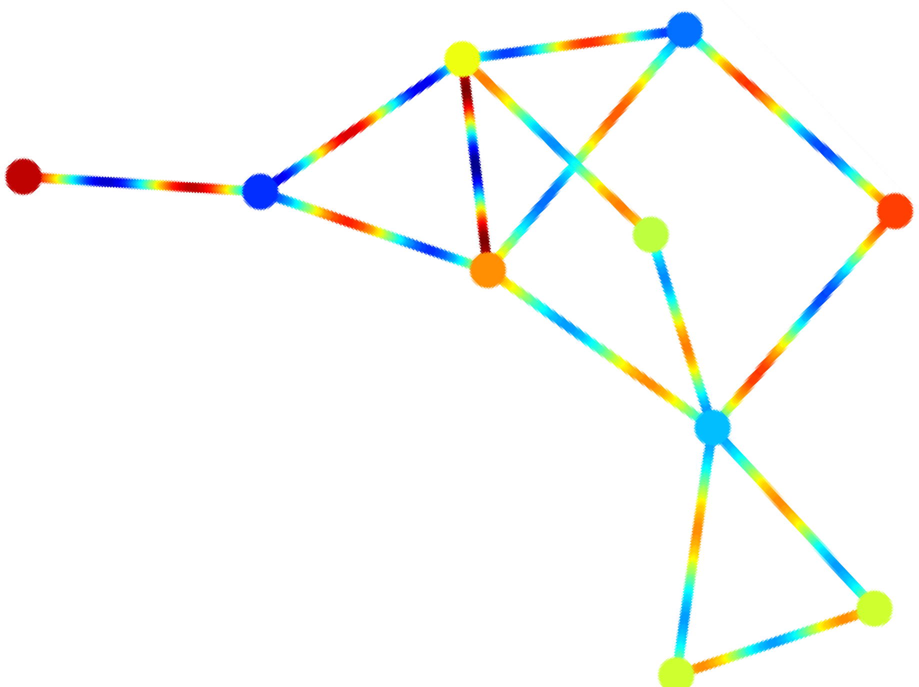


Themes

Hammer:

Eigen-analysis



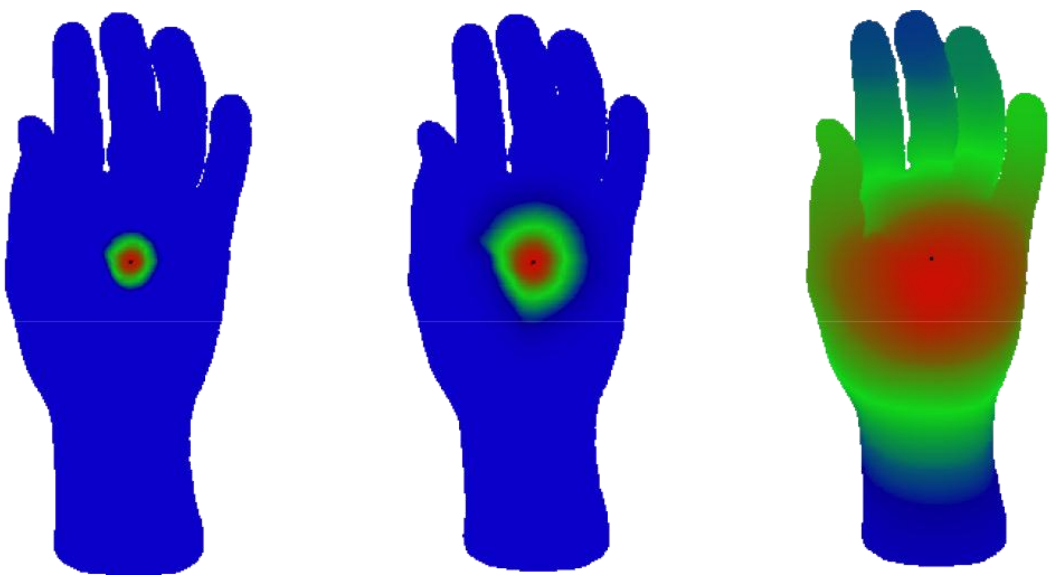


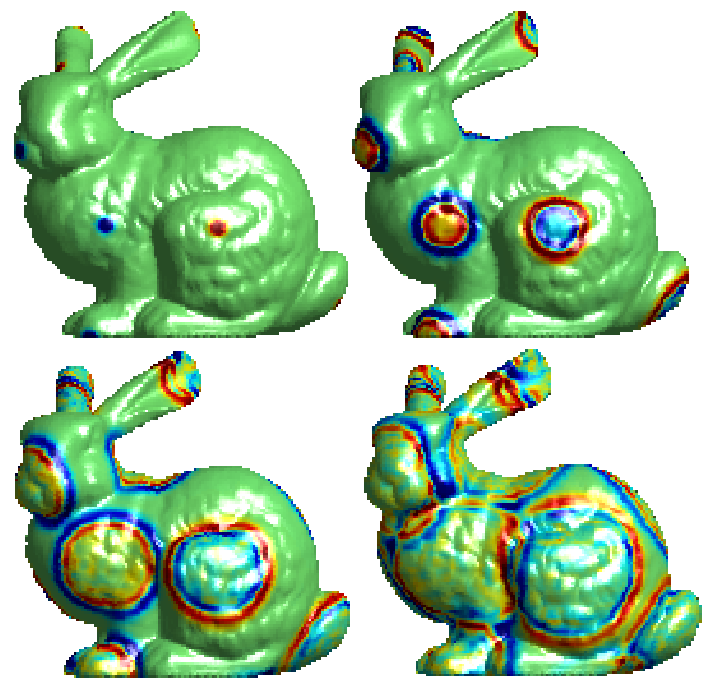
http://alice.loria.fr/publications/papers/2008/ManifoldHarmonics//photo/dragon_mhb.png

Themes

Result:

PDE-like behavior





http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf

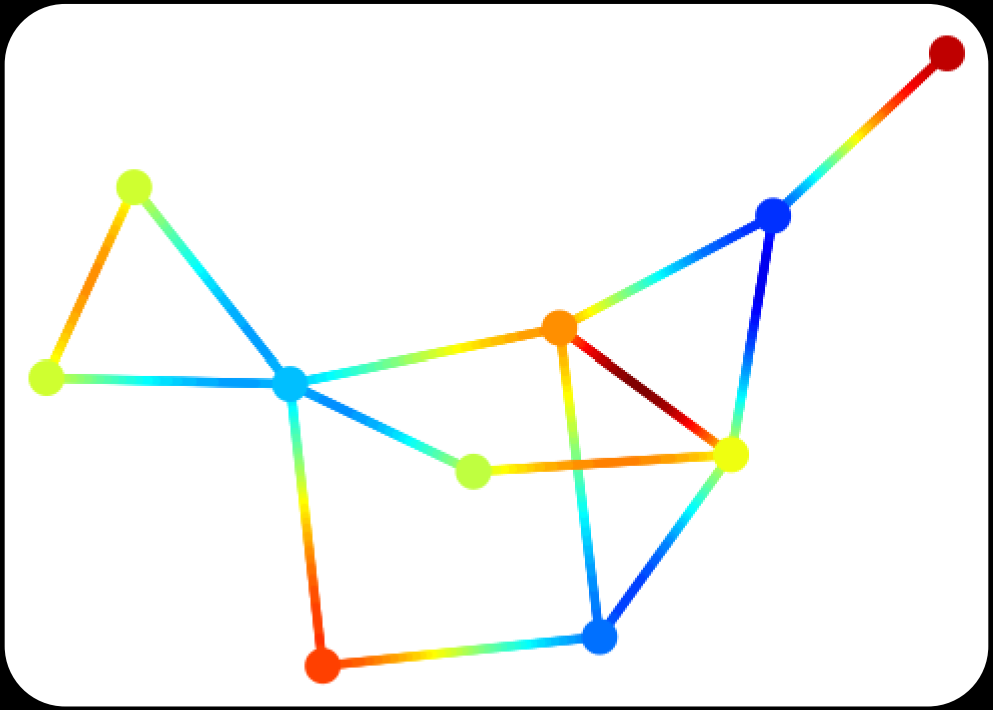
http://www.ceremade.dauphine.fr/~peyre/numerical-tour/tours/meshproc_5_pde/index_06.png

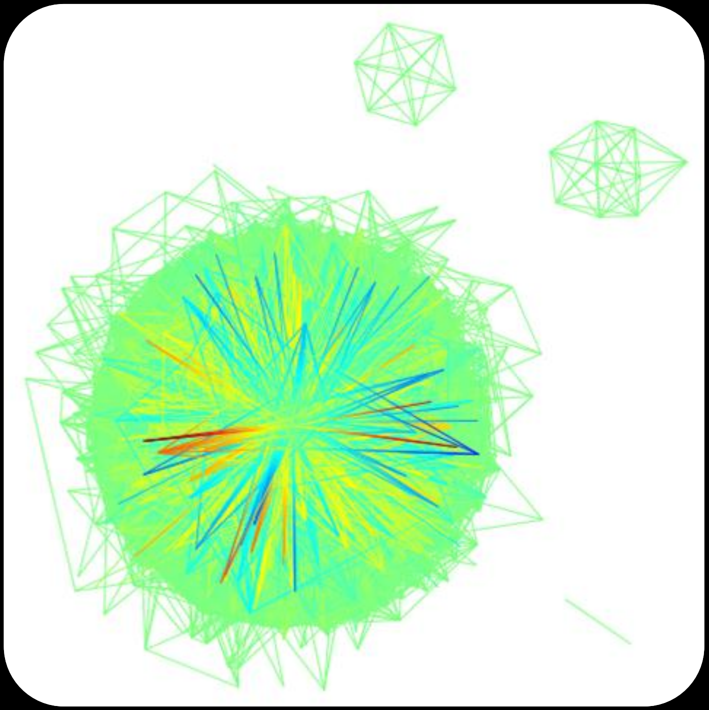
In Other Words…

PDE behavior can be
domain-independent
in a rigorous way.

Next Steps

- Improve practicality of edge-based approach
- Adaptation of geometric methods to graph problems
- Organized advantages/limitations of each representation





PDE Approaches to Graph Analysis

Questions?