# Phase-field based structural topology optimization using unstructured polygonal meshes



#### Arun L. Gain Glaucio H. Paulino Department of Civil and Environmental Engineering University of Illinois at Urbana-Champaign





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#### **Introduction & Motivation**

Topology optimization refers to optimum distribution of material in a given design space under certain specified boundary conditions so as to meet certain prescribed performance objective.

**Implicit function methods:** Topology represented in terms of implicit functions and evolved over time using certain PDEs.



#### **Introduction & Motivation**

• Implicit function method such as level-set function, although attractive, require periodic reinitializations, for example, to maintain signed distance characteristics for numerical convergence.



- Reinitializations often performed heuristically.
- Phase field function does not have to be signed distance function so no need of any reinitialization.

#### **Motivation for using polygonal elements**

- For simplicity, uniform grids are often used for topology optimization. Over-constrained geometrical features of structured grids can bias the orientation of the members, leading to mesh dependent, sub-optimal designs.
- Traditional density based topology optimization on Cartesian meshes suffer from numerical anomalies such as checkerboard patterns and one-node connections.



Talischi C., Paulino G. H., Pereira A., and Menezes I. F. M. (2010) Polygonal finite elements for topology optimization: A unifying paradigm. International Journal for Numerical Methods in Engineering, 82: 671-698

#### **Motivation for using polygonal elements**

• Explore general and curved domains rather than the traditional Cartesian domains (box-type) that have been extensively used for topology optimization.



Talischi C., Paulino G. H., Pereira A., and Menezes I. F. M. (2012) PolyMesher: A general-purpose mesh generator for polygonal elements written in Matlab. *Structural and Multidisciplinary Optimization*, 45(3): 309-328

#### **Presentation Outline**

- 1. Introduction & Motivation
- 2. Polygonal finite element method
- 3. Phase-field method for topology optimization
- 4. Centroidal Voronoi Tessellation (CVT) based finite volume method to solve the Allen-Cahn equation
- 5. Implementation flow chart
- 6. Numerical examples
- 7. Future research directions

## Following objective functions will be considered for topology optimization using phase-field method:

$$\inf_{\phi} \overline{J}(\phi) = J_i(\phi) + \lambda P(\phi) \qquad \text{for } i = 1,2$$

where,

$$J_{i}(\phi) = \begin{cases} \int_{D} \boldsymbol{f} \cdot \boldsymbol{u} dD + \int_{\partial D_{N}} \boldsymbol{g} \cdot \boldsymbol{u} ds \\ -\boldsymbol{u}_{out}(\phi) \end{cases}$$

Compliance minimization

Compliant mechanism

$$P(\phi) = \int_{D} \phi \, dD$$

Volume constraint

#### Brief review of polygonal finite elements used in this work

**Polygonal finite elements:** Finite element space of polygonal elements is constructed using natural neighbor scheme based non-Sibson interpolants (Laplace interpolants)



$$N_{i}(\mathbf{x}) = \frac{\alpha_{i}(\mathbf{x})}{\sum_{Q} \alpha_{j}(\mathbf{x})}, \qquad \alpha_{i}(\mathbf{x}) = \frac{s_{i}(\mathbf{x})}{h_{i}(\mathbf{x})}, \qquad \mathbf{x} \in \Re^{2}$$
  
where,  $Q = \{q_{1}, q_{2}, \dots, q_{n}\}$ 

**Conforming shape functions:** 

$$0 \le N_i(\mathbf{x}) \le 1$$
,  $N_i(\mathbf{x}_j) = \delta_{ij}$ ,  $\sum_{p} N_i(\mathbf{x}) = 1$   
 $\sum_{p} \mathbf{x}_i N_i(\mathbf{x}) = \mathbf{x}$ 

Belikov VV, Ivanov VD, Kontorovich VK, Korytnik SA, Semenov AY (1997) The non-Sibsonian interpolation: a new method of interpolation of the values of a function on an arbitrary set of points. *Computational Mathematics and Mathematical Physics* 37(1): 9-15

#### **Review of the phase-field method employed**

Evolution equation: Allen-Cahn equation

 $\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi - f'(\phi), \qquad \frac{\partial \phi}{\partial n} = 0 \text{ on } \partial D$ where, f(0) = 0,  $f(1) = \eta \frac{\overline{J}'(\phi_{t1})}{\|\overline{J}'(\phi_{t1})\|}$ , f'(0) = f'(1) = 0  $\sqrt{\frac{\overline{J}'(\phi_{t1})}{\|\overline{J}'(\phi_{t1})\|}}$  $\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi + \phi (1 - \phi) \left| \phi - \frac{1}{2} - 30\eta \frac{\overline{J}'(\phi_{t1})}{\|\overline{J}'(\phi_{t1})\|} \phi (1 - \phi) \right|$  $\Omega_0(\phi = 0)$  $\boldsymbol{C}^{*}(\boldsymbol{\phi}) = \begin{cases} \boldsymbol{C} & \boldsymbol{x} \in \Omega_{1}, \\ \boldsymbol{\phi}^{p} \boldsymbol{C} & \boldsymbol{x} \in \boldsymbol{\xi}, \\ k_{\min} \boldsymbol{C} & \boldsymbol{x} \in \Omega_{0}. \end{cases}$ **Effective elasticity tensor:** 

Takezawa A., Nishiwaki S., and Kitamura M. (2010) Shape and topology optimization based on the phase field method and sensitivity analysis. *Journal of Computational Physics*, 229: 2697-2718

### Centroidal Voronoi Tessellation (CVT) based finite volume method is used to solve the Allen-Cahn equation

**Allen-Cahn equation:** 

$$\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi - f'(\phi)$$



**Integral form:** 

$$\int_{t,D_p} \frac{\partial \phi}{\partial t} dt dD = \int_{t,D_p} \kappa \nabla^2 \phi dt dD - \int_{t,D_p} f'(\phi) dt dD$$

$$\int_{t,D_p} \frac{\partial \phi}{\partial t} dt dD = \int_{t,\Gamma_p} \kappa \nabla \phi \cdot \boldsymbol{n} dt d\Gamma - \int_{t,D_p} f'(\phi) dt dD$$

Vasconcellos J. F. V. and Maliska C. R. (2004) A finite-volume method based on voronoi discretization for fluid flow problems. Numerical Heat Transfer, Part B, 45: 319-342

### Centroidal Voronoi Tessellation (CVT) based finite volume method is used to solve the Allen-Cahn equation

Integral form: 
$$\int_{t,D_p} \frac{\partial \phi}{\partial t} dt dD = \int_{t,\Gamma_p} \kappa \nabla \phi \cdot \mathbf{n} dt d\Gamma - \int_{t,D_p} f'(\phi) dt dD$$

Simplifying each term:

•

• 
$$\int_{t,D_p} \frac{\partial \phi}{\partial t} dt dD = \int_{D_p} \left( \phi^{n+1} - \phi^n \right) dD \approx \left( \phi_p^{n+1} - \phi_p^n \right) V_p$$



$$\int_{t,\Gamma_{p}} \kappa \nabla \phi \cdot \boldsymbol{n} \, dt \, d\Gamma \approx \int_{t} \sum_{p} \left[ \kappa \nabla \phi^{n} \cdot \boldsymbol{n} \, S \right]_{i} dt = \left( \sum_{p} \left[ \left( \kappa \frac{\partial \phi^{n}}{\partial \boldsymbol{n}} \right)_{p,p_{i}} S_{i} \right] \right) \Delta t = P_{3}$$
$$\left( \frac{\partial \phi^{n}}{\partial \boldsymbol{n}} \right)_{p,p_{i}} = \frac{\phi_{p_{i}}^{n} - \phi_{p}^{n}}{H_{i}}$$

• 
$$\int_{t,D_p} f'(\phi) dt dD \approx V_p \Delta t f'(\phi_p^n) = V_p \Delta t \begin{cases} \phi_p^{n+1} \left(1 - \phi_p^n\right) r\left(\phi_p^n\right) & \text{for } r\left(\phi_p^n\right) \le 0 \\ \phi_p^n \left(1 - \phi_p^{n+1}\right) r\left(\phi_p^n\right) & \text{for } r\left(\phi_p^n\right) > 0 \end{cases}$$

## Centroidal Voronoi Tessellation (CVT) based finite volume method is used to solve the Allen-Cahn equation

Semi-implicit updating scheme:

$$\phi_p^{n+1} = \begin{cases} \frac{V_p \phi_p^n + P_3}{V_p \left(1 - \left(1 - \phi_p^n\right) r\left(\phi_p^n\right) \Delta t\right)}, & \text{for } r\left(\phi_p^n\right) \leq 0\\ \frac{V_p \phi_p^n \left(1 + r\left(\phi_p^n\right) \Delta t\right) + P_3}{V_p \left(1 + \phi_p^n r\left(\phi_p^n\right) \Delta t\right)}, & \text{for } r\left(\phi_p^n\right) > 0 \end{cases}$$

where,

$$r(\phi_{p}^{n}) = \phi_{p}^{n} - \frac{1}{2} - 30\eta \frac{\overline{J}'(\phi_{t1})}{\|\overline{J}'(\phi_{t1})\|} \phi_{p}^{n}(1 - \phi_{p}^{n})$$

#### **Implementation flow chart**



**Cantilever beam problem** 



- **<u>Objective</u>**: Compliance minimization
- **Domain size**: 2x1 with 20,000 polygonal elements
- For each FE iteration, 20 Allen-Cahn equation updates using CVT based FV method
- $\kappa = 2 \times 10^{-5}$ ,  $\eta = 10$ ,  $k_{\min} = 10^{-4}$ ,  $\lambda = 95$

#### **Cantilever beam problem**



Q4 Elements

Initial configuration

Converged topology

#### Cantilever beam problem with <u>different initial guesses</u>







Initial configuration

Converged topology

Bridge problem – Study the influence of diffusion coefficient,  $\kappa$ 



- **<u>Objective</u>**: Compliance minimization
- **Domain size:** 2x1.2 with 15,360 polygonal elements
- For each FE iteration, 20 Allen-Cahn equation updates using CVT based FV method
- $\kappa = 2 \times 10^{-5}$ ,  $10 \times 10^{-5}$

Bridge problem – Study the influence of diffusion coefficient,  $\kappa$ 





 $\kappa = 2 \times 10^{-5}$  $\phi \in [0.01, 0.99] = 28.2\%$ 

 $\kappa = 10 \times 10^{-5}$  $\phi \in [0.01, 0.99] = 46.3\%$ 

Bridge problem on semi-circular design domain



- **<u>Objective</u>**: Compliance minimization
- **Domain size:** 11,000 polygonal elements
- For each FE iteration, 20 Allen-Cahn equation updates using CVT based FV method
- $\kappa = 2 \times 10^{-5}$ ,  $\eta = 10$ ,  $k_{\min} = 10^{-4}$ ,  $\lambda = 60$

Bridge problem on semi-circular design domain



Initial configuration



Converged topology

Curved cantilever beam problem



- **<u>Objective</u>**: Compliance minimization
- **Domain size:** 20,000 polygonal elements
- For each FE iteration, 20 Allen-Cahn equation updates using CVT based FV method
- $\kappa = 2 \times 10^{-5}$ ,  $\eta = 10$ ,  $k_{\min} = 10^{-4}$ ,  $\lambda = 250$

Curved cantilever beam problem



**Curved cantilever beam problem** 





Initial configuration

Converged topology

Inverter problem on circular segment design domain



- **Objective:** Compliant mechanism
- **Domain size**: 6,000 polygonal elements
- For each FE iteration, 20 Allen-Cahn equation updates using CVT based FV method

• 
$$\kappa = 10 \times 10^{-5}$$
,  $\eta = 10$ ,  $k_{\min} = 10^{-4}$ 

Curved cantilever beam problem



Initial configuration



Converged topology

#### **Summary and Conclusions**

- Phase-field based topology optimization with polygonal elements offer a general framework for topology optimization on arbitrary domains.
- Meshes based on simplex geometry such as quads/bricks or triangles/tetrahedrons introduce intrinsic bias in standard FEM, but polygonal/polyhedral meshes do not.
- Polygonal/polyhedral meshes based on Voronoi tessellation not only provide greater flexibility in discretizing non-Cartesian design domains but also remove numerical artifacts such as one-node connections and checkerboard pattern in density based methods.

#### We are looking at the following future research directions:

Implementation of phase-field method in three-dimensions using polyhedral meshes





Leonardo et al.



Phase field method using polygonal meshes paves the way for medical engineering applications including craniofacial segmental bone replacement

Sutradhar A, Paulino GH, Miller MJ, Nguyen TH (2010) Topology optimization for designing patient-specific large craniofacial segmental 27 bone replacements. Proceedings of the National Academy of Sciences 107(30): 13222-13227

### **Questions and Comments?**