Applications of the Voronoi Implicit Interface Method for Shape Optimization Problems Involving Interconnected Regions

Danielle C. Maddix[1,2], Robert I. Saye[2], James A. Sethian[2]

1. Institute of Computational and Mathematical Engineering, Stanford University
2. Lawrence Berkeley National Laboratory

Introduction

- Find an optimal domain decomposition or grouping of clustered particles
- To optimize the geometry of various regions or shapes, mathematically, we must find a shape that minimizes a cost or energy functional, while satisfying a specified constraint set
- Given a set of points in $\mathbb{R}^m$ with associated weights and a set of regions, the goal is to cluster these particles within the phases, subject to certain constraints
- There are various formulations of these problems with different constraint sets and features, such as each region having equal sum of the associated weights of the particles or equal area
- Shape optimization problem with various complicated multiple interconnected interfaces
- We extend the Voronoi Implicit Interface Method (VIIM), which appropriately handles topological changes, by creating a multi-region system, which is evolved using appropriate constraint satisfying speed functions
- Given n fixed randomly scattered particles, $p_j \in \mathbb{R}^m$, with corresponding weights, $w_j \in \mathbb{R}$, the domain, Ω, must be partitioned into N given sub-regions, Ω_i, such that the sums of the weights of the particles are equal in each sub-region.
- Mathematically speaking, this requirement can be expressed as follows:

$$\sum_{\substack{1\le j\le n\\ p_j\in\Omega_i}} w_j = C \quad \forall i,$$

where $\bigcup_i \Omega_i = \Omega$ for some arbitrary constant, C.

Background: Level Set Method and VIIM

- VIIM extends the Level Set Method to track the evolution of the boundaries between multiple regions in any dimension.
- In the level set method, the interface, Γ, separating two phases, is represented by the zero level set, $\{x \in \mathbb{R}^m \mid \phi(x) = 0\}$, of a signed distance function, $\phi(x)$, such that $\phi(x)$ is the initial signed distance to Γ, negative inside a phase and positive outside of it.
- The interface, Γ, is evolved in its normal direction through an initial value partial differential equation, known as the level set equation:

$$\phi_t + F|\nabla\phi| = 0,$$

where F is a speed function arising from a velocity field.
- VIIM uses an unsigned distance function, $\phi(x)$, an indicator function $\chi(x)$, to evolve a multiphase system, through a specified speed function, F
- Solves level set equation using finite difference stencil on a Cartesian grid
- Motion of the interface in this multiphase system is determined by the two nearby ϵ-level sets of $\phi(x)$, for $\epsilon > 0$, surrounding the zero level set.

Speed Function

- VIIM is used along with the following speed function, F on the various different initial interfaces and configurations of particles.
- F is composed of the following three terms:

1. Constraint term
   - The constraint term is used to enforce an equal weight sum of weighted particles in each region.
   - Phase based speed function, that is, it is constant for all the grid points within a phase.
   - Sum up the weights of the particles in each phase and subtract from it the average weight sum:

$$F_{\Omega_i} = \sum_{\substack{1\le j\le n\\ p_j\in\Omega_i}} w_j - \frac{1}{N}\sum_{j=1}^{n} w_j \qquad (1)$$

   - Designed to enlarge phases whose weight sum is less than the average weight sum and to shrink phases whose weight sum is greater than the average weight sum.
2. Forcing term to keep the solution away from the particles

$$F_{\Omega_{ij}} = \max_{p_i\in\Omega_i}\|x-p_i\| - \max_{p_j\in\Omega_j}\|x-p_j\| = F_{\max} \qquad (2)$$

   - Derived from gradient descent on the following energy:

$$E = \sum_{i=1}^{N}\int_{\Omega_i}\|x-p_i\|,$$

   where p_i is the farthest particle in phase Ω_i from point x.
   - For each of these two closest phases to a given gridpoint, we find the furthest particle from the closest point on the interface, x, calculate the distances and then take their difference.
   - This results in a desired solution that wants to be further away from clusters of particles and be attracted to the void regions.
3. Curvature term

$$\kappa = \nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right), \qquad (3)$$

   - Used to find an optimal solution with minimal surface area.

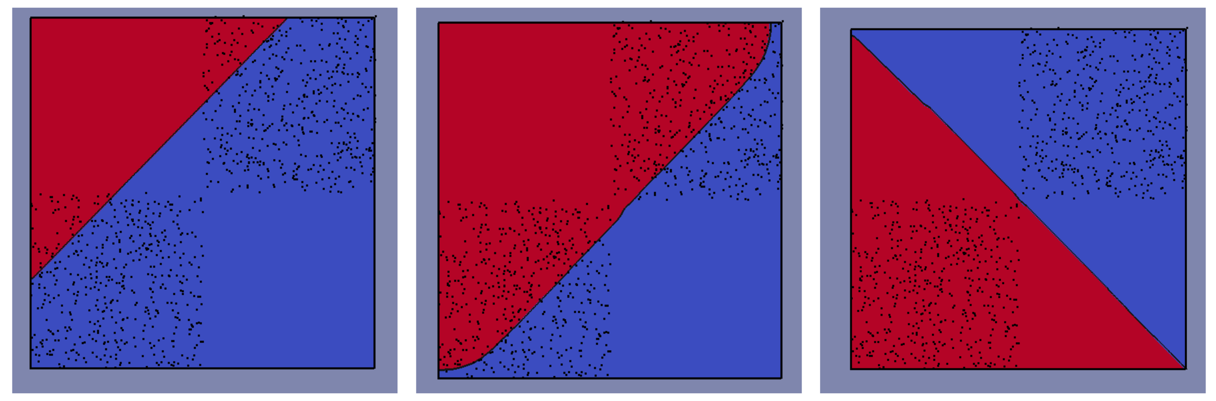
Numerical Methods

- F_{constr} constant within a phase and calculated at each domain gridpoint.
- $F_{\max}$ is evaluated in an initial band around the interface in the Voronoi reconstruction, where we find the closest point on the interface to the given gridpoint, as well as the two closest phases.
- $F_{\max}$ is extended, using the Fast Marching Method by solving the Eikonal Equation

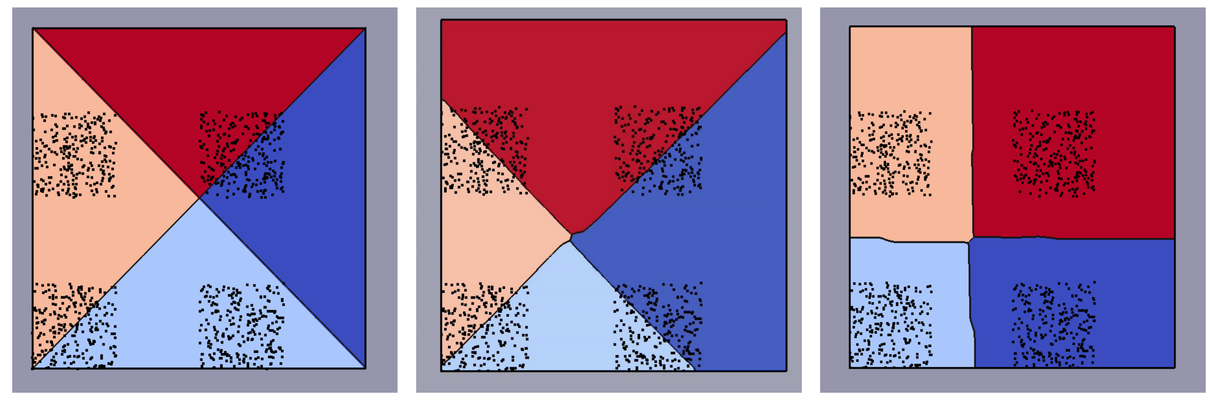
$$|\nabla\phi| = 1,$$

outside this initial band, using a finite difference upwind scheme
- Efficient k-d tree data structure for conducting the farthest neighbor searches for k-dimensional points
- The curvature term is calculated using central differences
- At each gridpoint, we take a linear combination of these speed functions: $F = F_{constr} + C_1F_{\max} + C_2\kappa$, where $C_1, C_2 < 1$.
- The interface is evolved in time by using Forward Euler to solve the level set equation, where the time step $\Delta t \le \frac{h}{\max|F|}$ satisfies the CFL condition, where h is the size of a grid cell
- Repeat the procedure of evolving ϕ and reconstructing every four timesteps until an equilibrium solution has been reached.
- MPI Parallel Implementation: Data is synchronized using ghost layers of appropriate sizes and a Domain class is utilized.
- Boundary conditions: zero Neumann $\frac{\partial\phi}{\partial\mathbf{n}} = 0$
- Connected components identifying and labeling algorithm. The area of each component is calculated and only the one with the largest area remains. The others vanish under curvature flow.

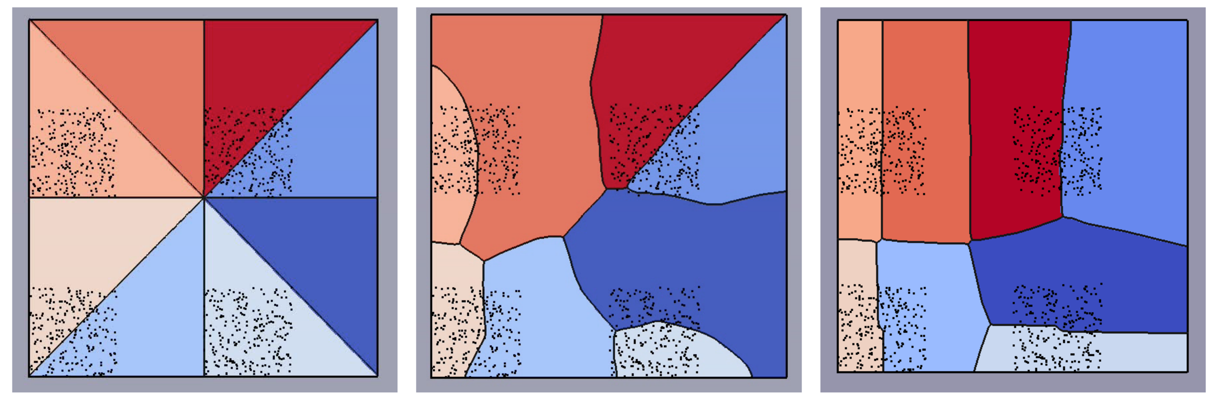
Numerical Experiments



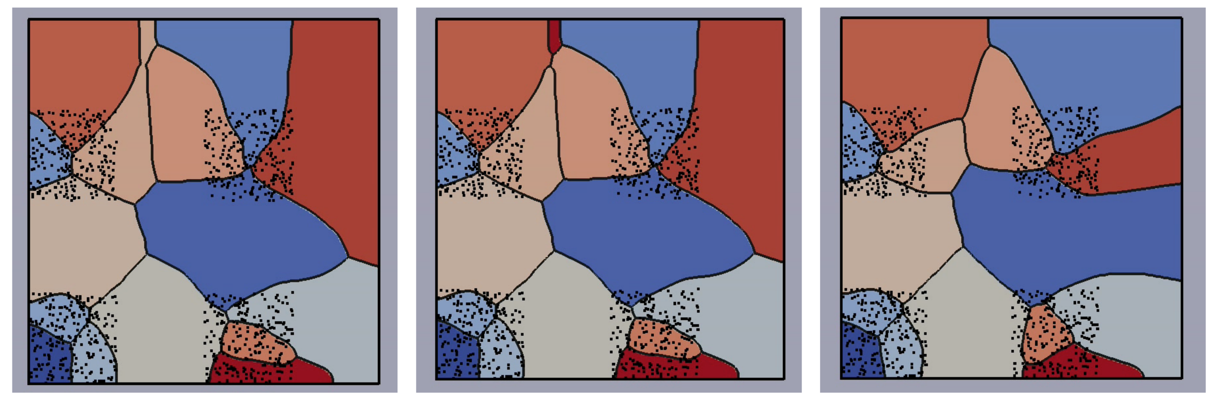
Initial Condition | Midway State | Equilibrium State



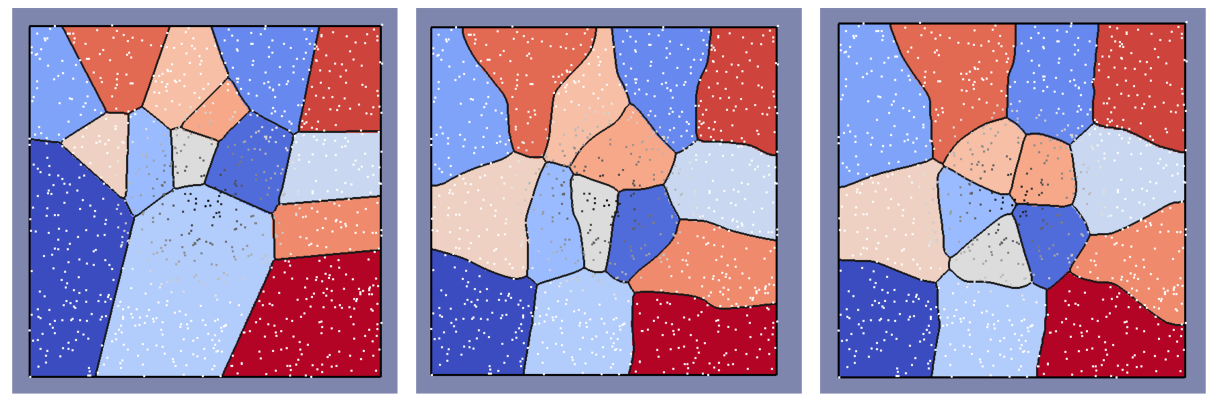
Initial Condition | Midway State | Equilibrium State



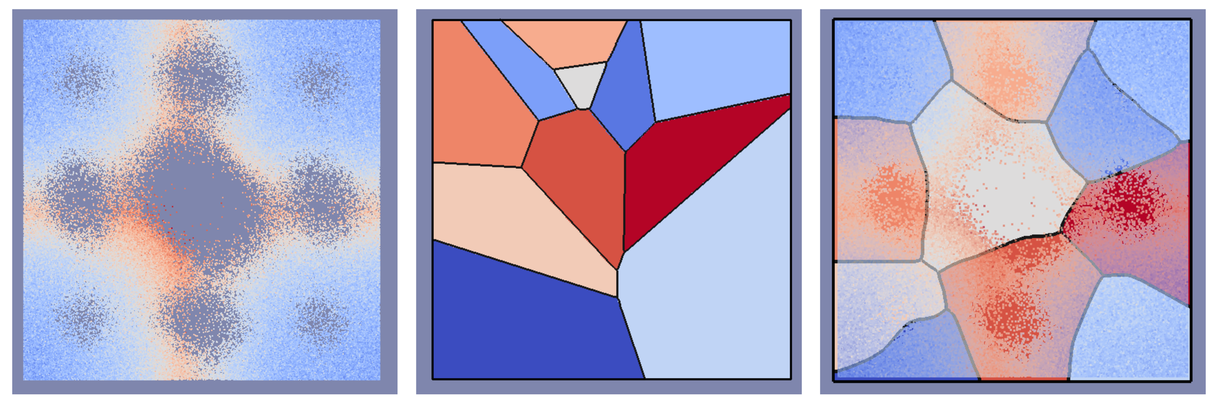
Initial Condition | Midway State | Equilibrium State



Conn. Comp. Forming | Conn. Comp. Shrinking | Equilibrium State



Initial Condition | Midway State | Equilibrium State



Pentane entropies | Initial Condition | Equilibrium State

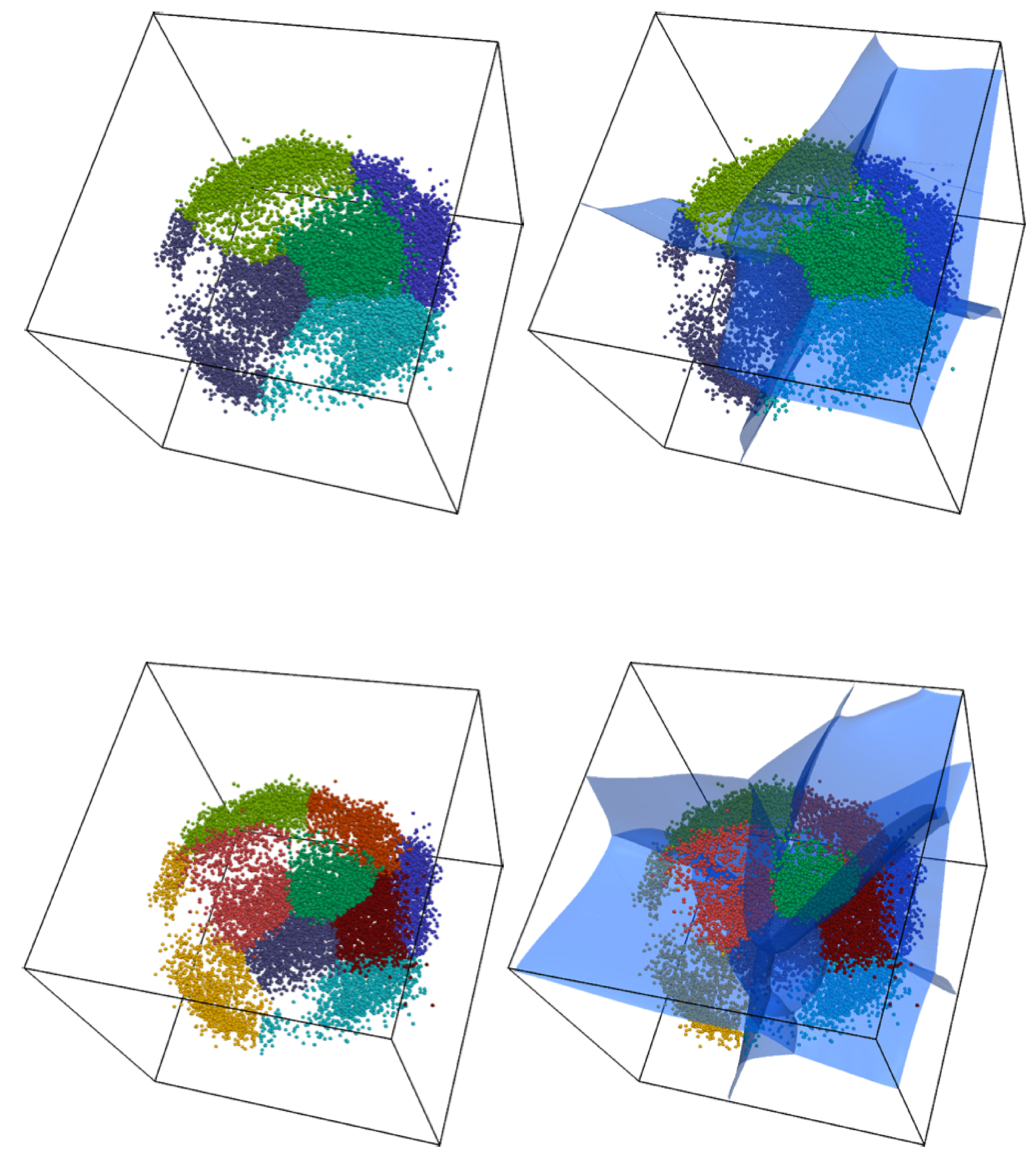
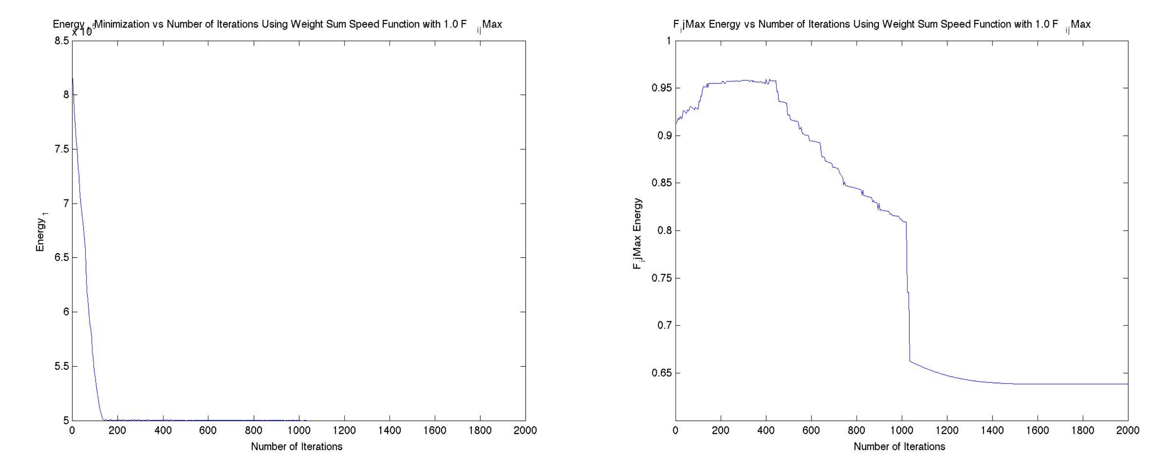


Figure 1: Initial 5 and 9 phase Voronoi tessellations and equilibrium states, respectively for 13,001 3D unequally weighted particles.

Energy Minimizations



$$E_i^{cons} = \sum_{\substack{1\le j\le n\\ p_j\in\Omega_i}} w_j \qquad E_i^{F_{max}} = \int_{\Omega_i}\|x-p_i\|$$

Corresponding minimization of the two-norm of various energies for simple two phase case with two clusters. We see that the energy from the constraint is minimized at the midway state, whereas the energy from F_{max} is minimized once the line rotates and then there is maximum separation from the particles and the interface.

References

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