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# **Final Report**

**Grant/Contract Title:** 

# CHEMISTRY AND PHYSICS OF ANALYTE IDENTIFICATION IN INTEGRATEED NANOSENSORS

Grant/Contract Number: FA9550-08-1-0395

Date: 8/01/08 to 11/30/08

PI: Professor Ivan K. Schuller



# **Final Report for AFOSR Supplement:**

This supplement was dedicated to the development and modeling of phthalocyanine based chemical sensors. We used Organic Molecular Beam Epitaxy (OMBE) to prepare phthalocyanine based sensors. We lithographically patterned special electrode configurations and mounted them on a universal commercial carrier chip thus facilitating manufacturability in actual field testable devices closer to reality. Two types of metallo-phthalocyanine (M-Pc) based sensors were prepared; Co-MPc films 12 monolayer thick and 3 different kinds of 12 monolayer M-Pcs on the same chip: Co-MPc, Cu-MPc and H2-Pc. These were then tested against a large number of analytes using the UCSD quantitative dosing system. Linear Discriminant analysis of the relative responses of the different MPc films allowed identification of analytes independent of concentration. The devices were also modeled using density functional theoretical methods to determine the binding strength of 12 electron donating analytes to the metal center in the MPc. This allows for a rational sensors design. We are actively seeking the commercial development of these sensors for military and civilian uses.

# **Researcher Effort:**

<ul> <li>Ivan K. Schuller</li> <li>William Trogler</li> </ul>	(PI) (PI)	1 summer month (Aug) <sup>1</sup> / <sub>2</sub> summer month (Aug & Sept)
- Evgueni Chagarov	(Researcher)	<sup>1</sup> / <sub>2</sub> month (Sep & Oct) 1 month (Nov)
- James Royer - David Martin	(Grad Student) (Grad Student)	<sup>1</sup> / <sub>4</sub> month (Oct & Nov) 1 month (Nov)

# Publications: None

# Presentations: None

# FINAL REPORT for "STATISTICAL AND VARIATIONAL METHODS FOR PROBLEMS IN VISUAL CONTROL"

### AFOSR/F49550-05-1-0059

Allen R. Tannenbaum School of Electrical and Computer Engineering Georgia Institute of Technology Atlanta, GA 30332-0250

# **1** Introduction

Our research program was concerned with the synergy between the variational partial differential equation and the statistical approaches to problems in visual control. Moreover, we have given a completely stochastic interpretation of curvature driven flows for tracking.

Vision is a key sensor modality in both the natural and man-made domains. The prevalence of biological vision in even very simple organisms, indicates its utility in man-made machines. More practically, cameras are in general rather simple, reliable passive sensing devices which are quite inexpensive per bit of data. Furthermore, vision can offer information at a high rate with high resolution with a wide field of view and accuracy capturing multi-spectral information. Finally cameras can be used in a more active manner. Namely, one can include motorized lenses mounted on mobile platforms which can actively explore the surroundings and suitably adapt their sensing capabilities.

For some time now, the role of control theory in vision has been recognized. In particular, the branches of control that deal with system uncertainty, namely adaptive and robust, have been proposed as essential tools in coming to grips with the problems of both biological and machine vision. These problems all become manifest when one attempts to use a visual sensor in an uncertain environment, and to feed back in some manner the information. These issues were a key thrust in our proposed research program.

Specifically, we have considered the following problems:

- (i) Dynamic Geodesic Active Contours for Tracking: Visual tracking using active contours is usually accomplished in a static framework. The active contour tracks the object of interest in a given frame of an image sequence, and then a subsequent prediction step ensures good initial placement for the next frame. This approach is unnatural; the curve evolution gets decoupled from the actual dynamics of the objects to be tracked. True dynamic approaches exist, all being marker particle based, and thus prone to the shortcomings of such particle-based implementations. In particular, topological changes are not handled naturally in this framework. The now "classical" level set approach is tailored for codimension one evolutions. However, dynamic curve evolution is at least of codimension two. We have proposed a natural, efficient approach for dynamic curve evolution which removes the artificial separation of segmentation and prediction, while retaining all the desirable properties of level set formulations. This is based on a new energy minimization functional which for the first time puts dynamics into the geodesic active contour framework.
- (ii) Knowledge-Based Tracking: One of the key themes of our work has been the combination of geometric partial differential equation methods with global statistics for tracking and controlled active vision. We have developed a way of combining statistical and anisotropic diffusion methods is via a process we call knowledge-based segmentation which seems to give

some reasonable results for several key applications. Since noise is in general non-additive, anisotropic diffusion and related techniques directly applied to the image do not produce satisfactory results. Moreover, these techniques do not introduce prior information about the number of objects present in the scene when directly applied in the image space. In our approach, we combine Bayes' rule with either anisotropic or isotropic diffusion, introducing *a priori* knowledge into the segmentation process and solving the non-additivity problem of the noise. We also extend this approach to the segmentation of video data, incorporating basic learning capabilities to the knowledge.

(iii) Stochastic Methods for Curvature Driven Flows: Many PDE's in image processing and computer vision are based on curvature driven flows from interfacial physics. Such curvature flows have been extensively considered from a deterministic point of view. They have been shown to be useful for a number of applications including crystal growth, flame propagation, and computer vision. In recent work, we have described a random particle system, evolving on the discretized unit circle, whose profile converges toward the Gauss-Minkowsky transformation of solutions of curvature driven flows. Our computational research program employs this methodology as a new way of evolving curves and surfaces for a powerful alternative to level set methods. It is a cornerstone in our computational program of combining PDE's and statistics in imaging.

### 2 Summary of Work

In this section, we outline some key concepts from dynamic contour tracking, and knowledge-based segmentation methods upon which our new research program is based.

#### 2.1 Dynamic Contour Tracking

Typical level set tracking techniques only make use of static models of active contours. In this section based upon our previous work in [18], we review how dynamics may be put quite naturally into this geometric framework giving us a novel model of dynamic active contours.

#### 2.1.1 Parametrized Dynamic Curves

We consider the evolution of closed curves of the form  $C : S^1 \times [0, \tau) \mapsto \mathbb{R}^2$  in the plane, where C = C(p, t) and C(0, t) = C(1, t) [6], with t being the time, and  $p \in [0, 1]$  the parametrization of the curve. The classical formulation for dynamic curve evolution is derived by means of minimization of the action integral

$$\mathcal{L} = \int_{t=t_0}^{t_1} L(t, \mathcal{C}, \mathcal{C}_t) dt, \tag{1}$$

where the subscripts denote partial derivatives. The Lagrangian L = T - U is the difference between the kinetic and the potential energy. The potential energy of the curve is given by

$$U = \int_0^1 U_{el} + U_{rig} + U_{pf} dp$$
  
=  $\int_0^1 \frac{1}{2} w_1 \|C_p\|^2 + \frac{1}{2} w_2 \|C_{pp}\|^2 + g(C) dp,$ 

where g is some potential function (with the desired location of the curve forming a potential well);  $U_{el}$ ,  $U_{rig}$ , and  $U_{pf}$  are the elasticity, rigidity and potential field contributions, with their (possibly position-dependent) scalar weights  $w_1$ , and  $w_2$ . A common choice for the potential function is

$$g(x) = \frac{1}{1 + \|G * \nabla I(x)\|^{r}},$$
(2)

where  $x = [x, y]^T$  are the image coordinates, I is the image, r is a positive integer, and G is a Gaussian of variance  $\sigma^2$ . The kinetic energy is

$$T = \int_0^1 \frac{1}{2} \mu \|\mathcal{C}_t\|^2 \, dp,$$
(3)

where  $\mu$  corresponds to mass per unit length. The Lagrangian used is then

$$L = \int_0^1 \frac{1}{2} \mu \|\mathcal{C}_t\|^2 - \frac{1}{2} w_1 \|\mathcal{C}_p\|^2 - \frac{1}{2} w_2 \|\mathcal{C}_{pp}\|^2 - g(\mathcal{C}) \, dp.$$
(4)

Computing the first variation  $\delta \mathcal{L}$  of the action integral (1) and setting it to zero yields the Euler-Lagrange equations for the candidate minimizer in force balance form:

$$\mu \mathcal{C}_{tt} = \frac{\partial}{\partial p} (w_1 \mathcal{C}_p) - \frac{\partial^2}{\partial p^2} (w_2 \mathcal{C}_{pp}) - \nabla g.$$
(5)

This formulation is not intrinsic with respect to the geometry of the curve, since it is dependent upon its parametrization, p.

#### 2.1.2 Geometric Dynamic Curves

Minimizing equation (1) using the Lagrangian

$$L = \int_0^1 \left( \frac{1}{2} \mu \| \mathcal{C}_t \|^2 - g \right) \| \mathcal{C}_p \| \, dp, \tag{6}$$

instead results in

$$\mu \mathcal{C}_{tt} = -\mu (\mathcal{T} \cdot \mathcal{C}_{ts}) \mathcal{C}_t - \mu (\mathcal{C}_t \cdot \mathcal{C}_{ts}) \mathcal{T} - (\frac{1}{2} \mu \| \mathcal{C}_t \|^2 - g) \kappa \mathcal{N} - (\nabla g \cdot \mathcal{N}) \mathcal{N},$$
(7)

which is intrinsic and a natural extension of the geodesic (conformal) active contour approach [10]. Here  $\mathcal{N}$  is the unit inward normal, and  $\mathcal{T} = \frac{\partial \mathcal{C}}{\partial s}$  the unit tangent vector to the curve.  $\kappa = \mathcal{C}_{ss} \cdot \mathcal{N}$  denotes curvature and s is arclength.

Equation (7) describes a curve evolution that is only influenced by inertia terms and information on the curve itself. To increase robustness, region-based terms could be included in the formulation.

#### Normal Geometric Dynamic Curve Evolution

To be able to interpret the behavior of the curve evolution equation (7) it is instructive to derive the corresponding evolution equations for the tangential and normal velocity components of the curve.

We can write

$$C_t = \alpha(p, t)\mathcal{T} + \beta(p, t)\mathcal{N}, \tag{8}$$

where the parametrization p is independent of time and travels with its particle, and  $\alpha$  and  $\beta$  correspond to the tangential and the normal speed functions respectively. By substituting equation (8) into equation (7), we obtain the two coupled partial differential equations:

$$\alpha_t = -(\alpha^2)_s + 2\kappa\alpha\beta,$$

$$\beta_t = -(\alpha\beta)_s + \left[ (\frac{1}{2}\beta^2 - \frac{3}{2}\alpha^2) + \frac{1}{\mu}g \right] \kappa - \frac{1}{\mu}\nabla g \cdot \mathcal{N}.$$
(9)

Clearly,  $-(\alpha^2)_s$  and  $-(\alpha\beta)_s$  are the transport terms for the tangential and the normal velocity along the contour, and  $g\kappa - \nabla g \cdot \mathcal{N}$  is the well known geodesic active contour image influence term [10]. Note, that in contrast to the static geodesic active contour, this term does not directly influence the curve's position, but the curve's normal velocity. It resembles a force. Finally, the terms  $2\kappa\alpha\beta$  and  $(\frac{1}{2}\beta^2 - \frac{3}{2}\alpha^2)\kappa$  incorporate the dynamic elasticity effects of the curve. If we envision a rotating circle we can interpret the term  $(\frac{1}{2}\beta^2 - \frac{3}{2}\alpha^2)\kappa$  as a rubberband (i.e., if we rotate the circle faster it will try to expand, but at the same time it will try to contract due to its then increasing normal velocity; oscillations can occur). If we restrict the movement of the curve to its normal direction (i.c., if we set  $\alpha = 0$ ) we obtain

$$\beta_t = \frac{1}{2}\beta^2 \kappa + \frac{1}{\mu}g\kappa - \frac{1}{\mu}\nabla g \cdot \mathcal{N}.$$
(10)

This is a much simpler evolution equation. In our case it is identical to the full evolution equation (9) if the initial tangential velocity is zero. The image term g only influences the normal velocity evolution  $\beta$ . It does not create any additional tangential velocity.

If there is an initial tangential velocity, and/or if the image influence g contributes to the normal velocity  $\beta$  and to the tangential velocity  $\alpha$ , the normal evolution equation will not necessarily be equivalent to the full evolution equation (9). We can always parameterize a curve such that the tangential velocity term vanishes. Specifically, if we consider a reparametrization

$$\mathcal{C}(q,t) = \mathcal{C}(\phi(q,t),t), \tag{11}$$

where  $\phi : \mathbb{R} \times [0, T) \mapsto \mathbb{R}, p = \phi(q, t), \phi_q > 0$ , then

$$\frac{\partial \overline{\mathcal{C}}}{\partial t} = \frac{\partial \mathcal{C}}{\partial t} + \frac{\partial \mathcal{C}}{\partial p} \frac{\partial \phi}{\partial t}.$$
(12)

The time evolution for  $\overline{C}$  can then be decomposed into

$$\overline{\mathcal{C}}_t = \overline{\alpha}\mathcal{T} + \overline{\beta}\mathcal{N} = (\alpha(\phi(q,t),t) + \|\mathcal{C}_p(\phi(q,t),t)\|\phi_t)\mathcal{T} + \overline{\beta}\mathcal{N},$$
(13)

where

$$\overline{\alpha} = \alpha(\phi(q,t),t) + \|\mathcal{C}_p(\phi(q,t),t)\|\phi_t, \\ \overline{\beta} = \beta(\phi(q,t),t).$$

If we choose  $\phi$  as

$$\phi(q,t)_t = -\frac{\alpha(\phi(q,t),t)}{\|\mathcal{C}_p(\phi(q,t),t)\|},$$
(14)

we obtain

$$\overline{\mathcal{C}}_t = \overline{\beta}\mathcal{N},\tag{15}$$

which is a curve evolution equation without a tangential component. For all times, t, the curve  $\overline{C}$  will move along its normal direction. However, the tangential velocity is still present in the update equation for  $\overline{\beta}$ . After some algebraic manipulations, we arrive at

$$\mu(\beta_p \phi_t + \beta_t) = \left(\frac{1}{2}\mu\beta^2 + g\right)\kappa - (\nabla g \cdot \mathcal{N})\mathcal{N},\tag{16}$$

which depends on the time derivative of the reparametrization function  $\phi$ , which in turn depends on the tangential component  $\alpha$ . The left hand side of Equation (16) represents a transport term along the curve, the speed of which depends on the time derivative of the reparametrization function  $\phi$ .

### 2.1.3 Level Set Formulation

There are different ways to implement the derived curve evolution equations; see for example [15]. We distinguish full and partial level set implementations. In the full case, curves evolve in a space consistent with the dimensionality of the problem. Geometric dynamic curve evolution would thus be performed in  $\mathbb{R}^4$  in the simplest case. Normal geometric dynamic curve evolution would be at least a problem in  $\mathbb{R}^3$ . If *n* is the dimensionality of the problem the curve will be implicitly described by the intersection of n-1 hypersurfaces or the zero level set of an *n*-dimensional vector distance function. Full level set approaches of this form are computationally expensive, since it is not obvious how to devise a methodology comparable to a narrow band scheme.

A partial level set approach uses a level set formulation for the propagation of an implicit description of the curve itself (thus allowing for topological changes), but explicitly propagates the velocity information associated with every point on the contour by means of possibly multiple transport equations. It trades-off computational efficiency (a narrow band implementation is possible in this case) for object separation: tracked objects that collide will be merged.

In what follows we will restrict ourselves to a partial level set implementation of the normal geometric dynamic curve evolution. See [17] for a detailed discussion of the full level set method in this context.

#### Partial Level Set Approach for the Normal Geometric Curve Evolution

The curve C is represented as the zero level set of the function

$$\Psi(\boldsymbol{x}(t), t) : \mathbb{R}^2 \times \mathbb{R}^+ \mapsto \mathbb{R}, \tag{17}$$

where  $x(t) = (x(t), y(t))^T$  is a point in the image plane. We assume  $\Psi > 0$  outside the curve C and  $\Psi < 0$  inside the curve C. Since the evolution of the curve's shape is independent of the tangential velocity we can write the level set evolution equation for an arbitrary velocity  $x_t$  as

$$\Psi_t + \|\nabla\Psi\| \mathcal{N} \cdot \boldsymbol{x}_t = 0. \tag{18}$$

In our case  $\boldsymbol{x}_t = \beta \mathcal{N}$ , where

$$\mathcal{N} = -\frac{\nabla\Psi}{\|\nabla\Psi\|}.\tag{19}$$

Equation (18) then becomes

$$\Psi_t - \beta \|\nabla \Psi\| = 0, \tag{20}$$

where  $\beta$  is given by equation (10). Using the relation

$$\kappa = \nabla \cdot \left(\frac{\nabla \Psi}{\|\nabla \Psi\|}\right). \tag{21}$$

we obtain

$$\beta_t = \left(\frac{1}{2}\beta^2 + \frac{1}{\mu}g\right)\kappa + \frac{1}{\mu}\nabla g \cdot \frac{\nabla\Psi}{\|\nabla\Psi\|}.$$
(22)

We need to propagate the normal velocity  $\beta$  along with the zero level set of  $\Psi$ . This could be accomplished by the transport equation

$$\beta_t = \beta \frac{\nabla \Psi}{\|\nabla \Psi\|} \cdot \nabla \beta, \tag{23}$$

which is not natural, since equations (22) and (23) are both first order evolution equations for  $\beta$ . Instead of using equation (23) we can:

(a) Neglect equation (23), but compute extension velocities at every time step. Since the extensions are normal to the contours, normal propagation of the level set function will guarantee a constant velocity value along the propagation direction (up to numerical errors). Specifically  $\nabla \beta \perp \nabla \Psi$  in this case and thus

$$\nabla \Psi \cdot \nabla \beta = 0. \tag{24}$$

(b) Incorporate equation (23) into equation (22).

To accomplish the latter we change our Lagrangian, and extend it over a range of level sets. For each time t, and  $0 \le r \le 1$  let

$$\mathcal{C}^{(r)}(t) := \{ (x, y) \in \mathbb{R}^2 : \Psi(x, y, t) = r \}.$$
(25)

Using the Lagrangian

$$L = \int_0^1 \int_{\mathcal{C}} \left(\frac{1}{2}\mu\beta^2 - g\right) \, ds \, dr,\tag{26}$$

we obtain the action integral

$$\mathcal{L} = \int_{t} \int_{0}^{1} \int_{\mathcal{C}} \left( \frac{1}{2} \mu \beta^{2} - g \right) \, ds \, dr \, dt, \tag{27}$$

which is

$$\mathcal{L} = \int_0^1 \int_0^T \int_{\mathcal{C}} (\frac{1}{2}\mu\beta^2 - g) \, ds \, dt \, dr$$
  
$$= \int_0^T \left( \int_0^1 \int_{\mathcal{C}} (\frac{1}{2}\mu\beta^2 - g) \, d\mathcal{H}^1 \lfloor_{\mathcal{C}} \, dr \right) dt$$
  
$$= \int_0^T \int_{\Omega} (\frac{1}{2}\mu\beta^2 - g) \|\nabla\Psi\| \, dx \, dy \, dt, \qquad (28)$$

where  $\mathcal{H}^1$  is the one-dimensional Hausdorff measure and we applied the coarea formula. This casts the minimization problem into minimization over an interval of level sets in a fixed coordinate frame (x and y are time independent coordinates in the image plane). Using equation (20) we can express  $\beta$ as

$$\beta = \frac{\Psi_t}{\|\nabla\Psi\|}.\tag{29}$$

Substituting (29) into equation (28) yields

$$\mathcal{L} = \int_0^T \int_\Omega \left( \mu \frac{\Psi_t^2}{2 \|\nabla \Psi\|} - g \|\nabla \Psi\| \right) dx \, dy \, dt := S[\Psi], \tag{30}$$

which is the new  $\Psi$ -dependent action integral to be minimized. Then,  $\delta S = 0$  if and only if

$$\frac{\partial}{\partial t} \left( \frac{\Psi_t}{\|\nabla\Psi\|} \right) = \nabla \cdot \left( \left( \frac{g}{\mu} + \frac{\Psi_t^2}{\|\nabla\Psi\|^2} \right) \frac{\nabla\Psi}{\|\nabla\Psi\|} \right).$$
(31)

The curve evolution is thus governed by the system:

$$\beta_t = \nabla \cdot \left( \frac{\nabla \Psi}{\|\nabla \Psi\|} \left( \frac{g}{\mu} + \frac{1}{2} \beta^2 \right) \right), \qquad (32)$$
$$\Psi_t = \beta \|\nabla \Psi\|.$$

Expanding equation (32) yields

$$\beta_t = \left(\frac{1}{2}\beta^2 + \frac{1}{\mu}g\right)\kappa + \frac{1}{\mu}\nabla g \cdot \frac{\nabla\Psi}{\|\nabla\Psi\|} + \beta\nabla\beta \cdot \frac{\nabla\Psi}{\|\nabla\Psi\|},\tag{33}$$

which, as desired, combines the velocity update equation (22) with the velocity propagation equation (23). Naturally, this equation reduces to the result obtained from our original minimization problem (see equation (22)) if extension velocities are used to the evolution of all level sets to the evolution of the zero level set. Note, that the system of equations (32) constitutes a hyperbolic conservation law for the velocity v. The propagation of the level set function  $\Psi$  is described (as usual) by an equation of Hamilton-Jacobi type.

#### 2.2 Statistics and Curvature Driven Flows: Knowledge-Based Segmentation

We summarize here some of our results on the synergy of geometric partial differential equation and statistical methods based on *knowledge-based segmentation*. We combine Bayes' rule with either anisotropic or isotropic diffusion, introducing *a priori* knowledge into the segmentation process and solving the non-additivity problem of the noise. We also extend this approach to the segmentation of video data, incorporating basic learning capabilities to the knowledge.

This has a number of applications including SAR imagery [7] and missile tracking [9, 23]. In particular, in the case of tracking missiles for the airborne laser (ABL) program, we are interested in tracking the location of the nose of the missile. Thus we only need to separate the relevant portion of the missile from the background. Because of the noisy nature of the images due to atmospheric effects simpler thresholding techniques (e.g., histogramming the pixel distributions and trying to separate the peaks) do not work very well for the missile videos. On the other hand, we have found that the knowledge-based approach of [9, 23] gave excellent results in comparison to weighted centroid techniques especially when combined with geometric active contours.

#### 2.2.1 Basic Set-up

Our set-up begins with the assumption that the image is composed of n classes of objects. For sequences of images, this value n is assumed constant. For the missile problem [23], we assume two classes, corresponding to the missile and the background. Thus in this setting we will see that we have a form of *adaptive thresholding*. This is the case we will describe here. The technique however is general and can be applied to any number of classes. (In [7] for SAR data, the number of classes was three.) The goal of our segmentation is to determine to which class each pixel in each image belongs. Our basic model assumes that the value of each pixel in a given class can be thought of as a random variable with a known distribution, and that these variables are independent across pixels (this just simplifies the exposition, but any distribution can be used). Thus, for example for the case of normal distributions the likelihood of a particular pixel *i* having a certain value *v* given that it is in class  $c \in \{\text{missile}, \text{background}\}$  is:

$$\Pr(V_i = v | C_i = c) = \frac{1}{\sqrt{2\pi\sigma_c}} \exp\left(-\frac{1}{2} \frac{(v - \mu_c)^2}{\sigma_c^2}\right),$$
(34)

where *i* is an index ranging over all pixels in the image,  $V_i$  is the value of the pixel, and  $C_i$  is its class. As usual,  $\mu_c$  and  $\sigma_c$  denote the mean and standard deviation of class *c*. In practice, these parameters are estimated from a set of sample images or learned from past frames for video data.

Next, we assume that there is some known prior probability that a particular pixel will belong to a cortain class. For single-image data sets, we assume a homogeneous prior, i.e., that  $Pr(C_i = c)$  is the same over all spatial indices *i*. It is, however, possible to incorporate *a priori* knowledge about the image here, for example if it were known that the missile is more likely to be near the center of the image than near the edge. For sequences of images, we have used a learned prior, as described below.

Given a set of intensity distributions  $Pr(V_i = v | C_i = c)$  and priors  $Pr(C_i = c)$ , we can apply Bayes' Rule from elementary probability theory to calculate the posterior probability that a given pixel belongs to a particular class, given its intensity:

$$\Pr(C_i = c | V_i = v) = \frac{\Pr(V_i = v | C_i = c) \Pr(C_i = c)}{\sum_{\gamma} \Pr(V_i = v | C_i = \gamma) \Pr(C_i = \gamma)}.$$
(35)

Our approach is to calculate the posteriors  $P_i^c := \Pr(C_i = c | V_i = v)$  using the given distributions and (35) above, and then to apply either isotropic or anisotropic smoothing to each  $P^c$  (note that the denominator is just a normalization constant that can be "ignored"). Specifically, we have chosen to smooth by evolving  $P^c$  according to a discretized version of the partial differential equation

$$\frac{\partial P^c}{\partial t} = ((P_y^c)^2 P_{xx}^c - 2P_x^c P_y^c P_{xy}^c + (P_x^c)^2 P_{yy}^c)^{1/3}.$$
(36)

This equation defines the affine geometric heat flow, under which the level sets of  $P^c$  undergo affine curve shortening. This particular diffusion equation was chosen because of its affine invariance, because it preserves edges well, and because of its numerical stability and ease of computation. The goal of this process is to diffuse information from one pixel to the other, making then a region-based (adaptive) decision and not just a local pixel-wise one.

The segmentation is then obtained using the maximum a posteriori probability estimate after anisotropic smoothing. That is,

$$C_i^* = \frac{\arg \max}{c \in \{\text{missile, background}\}} \operatorname{Pr}^*(C_i = c | V_i = v)$$
(37)

where  $\Pr^*(C_i = c | V_i = v)$  is the smoothed posterior probability.

#### 2.2.2 Application to Visual Tracking

When segmenting sequences of images, we have extended the model so that information from one frame is used in the segmentation of the next, and in this way have introduced a kind of learning into the method. There are a number of ways in which this can be done. By far the most effective way we have found is to modify our assumption of homogeneous priors. In particular, we have used the smoothed posteriors  $P^c$  from one frame as priors  $\Pr(C_i = c)$  in the segmentation of the next frame. Thus this scheme fits into a Bayesian tracking framework. We have also tested relaxing our assumption that the pixel intensities are distributed according to fixed normal distributions. We estimated the distribution parameters of the normal distributions from frame to frame by calculating new sample means and variances based on the segmentation of earlier images. Finally, we completely removed the assumption that the intensities are normally distributed. This was done by calculating the sample distribution of intensities within each class as images were segmented, and then using this distribution as  $\Pr(V_i = v | C_i = c)$  in (34) when segmenting succeeding frames.

This type of approach combined with active contours was found to be extremely effective for ABL missile tracking [23]. For other scenarios, it is possible to introduce multi-scale texture models for the likelihood of the background. Another possible extension would be to consider that n, the number of classes in the image, is not given and needs to be estimated as well. This can be done for example via expectation maximization (EM) type algorithms. Note though that since the scheme here described is extremely fast, especially for video data where the number of smoothing steps is dramatically reduced, a brute-force search for n in a given range might be good enough for a number of applications.

This knowledge-based approach has a very strong connection to Markov random field (MRF) techniques. Indeed, the prior smoothing of the posterior probabilities gives the MAP solution to a discrete MRF with a non-interacting, analog discontinuity field. The combination of a discontinuity field with a discrete MRF can have some important consequences since it allows the disabling of clique potentials across discontinuities. This is in contrast to the isotropic (linear) smoothing of the posterior probabilities, which corresponds to computing the MAP solution of a single discrete MRF using continuous relaxation labeling. Thus we see that the random field, anisotropic diffusion, and curvature driven flow approaches to segmentation and tracking are intimately related.

#### 2.3 Interacting Particle Systems and Approximate Flows

In typical methods such as those described above for knowledgc-based segmentation for combining statistics with PDE's, the underlying PDE model remains deterministic and is implemented as such, for example using level sets. We have developed a very different class of algorithms in which the PDE is eliminated and the evolution takes place using a random process. We should note that this methodology first proposed for curvature driven flows in [2, 3] is mathematically well founded, and may be justified using the theory of hydrodynamical limits.

The new class of algorithms is very much connected to scale in physical systems. The typical way of modelling a physical system is on a macroscopic scale, that is via a continuous partial differential equation. Level set computational methods fall into this category of algorithms. Here we are looking at a microscopic approach: collections of discrete particles undergoing random walks. What we are doing then is replacing the PDE by an underlying microscopic interacting particle system.

The theory of interacting particle systems goes back at least to [22] who studied new types of random walk models with interactions among the particles. There are many examples including exclusions processes, branch processes, and contact processes. There are several advantages to this type of methodology including:

- 1. PDE's and continuous analysis become unnecessary.
- 2. No discretizations are necessary. The interacting particle system is already constructed on a discrete fixed lattice.
- 3. Increased robustness to noise, and ability to include processes into the given system.

In summary, this framework gives a completely stochastic way of modelling the key flows used in controlled active vision will all the possible benefits just described.

#### 2.3.1 Basic Definitions of a Particle System

In the theory of interactive particle systems, particles are distributed on a d-dimensional discrete integer lattice. The nodes of the lattice represent sites where particles reside. The state of the lattice is the distribution of particles over the sites. This state can evolve over time due to events such as births and deaths of particles, as well as jumps of particles to neighboring sites. The probability of an event happening at a particular site can be influenced by the number of particles at neighboring sites, therefore adding interaction between particles. If the rate of events at a site is only influenced by the number of particles at that site, then the process is called a *zero range process*. For our purposes, we are interested in zero range processes where particles only interact with particles sitting on the same site.

#### 2.3.2 Geometric Interpretation of a Particle System

In our AFOSR sponsored research, we were able to construct an interacting particle system that evolves microscopically on a 1D lattice according to the macroscopic behavior of the mean curvature flow PDE. This is a fundamental result that links the microscopic scale (particles evolving independently of particles at neighboring sites) to the macroscopic scale (curve evolving according to a macroscopic PDE).

Before we detail our particle system, we explain its geometric interpretation. This interpretation is fundamental for the use of particle systems as a tool for stochastic curve evolution. What we want to do is to be able to represent the particle system graphically as a curve. As the particle system evolves, the corresponding curve is updated, resulting in a stochastic curve evolution.

Our particle system is a 1D line of sites with connected ends, that we call a discrete torus where each site is a point space evenly on the unit circle. Therefore each site is parameterized by an angle. Each site contains a certain positive number of particles, denoted with the positive function  $m(\theta)$  where  $\theta$  parameterizes each site. In order to map our particle system to a curve, we can connect segments oriented according to the angle of each site and scaled by the number of particles at that site.

#### 2.3.3 Birth and Death Zero Range Particle Systems

We first set-up some notation.Let

$$\mathcal{C}(p,t): S^1 \times [0,T] \to \mathbf{R}^2$$

be a family of embedded curves where p parametrizes the curve and t the family. Then we consider curvature-driven flows of the form

$$\frac{\partial \mathcal{C}}{\partial t} = \hat{V}(\kappa(p,t))\mathcal{N},\tag{38}$$

where  $\kappa$  denotes the curvature and  $\mathcal{N}$  the inward unit normal. Using the standard angle parametrization  $\theta$ , we interpret  $m(\theta, t) := 1/\kappa(\theta, t)$  as a density, and compute it evolution to be:

$$\frac{\partial m(\theta, t)}{\partial t} = -\frac{\partial^2 V(m(\theta, t))}{\partial t^2} - V(m(\theta, t)),$$

$$V(x) := \hat{V}(1/x).$$
(39)

Note that V(x) = 1/x corresponds to the Euclidean curve shortening flow. In Equation (39), the first term on the right hand side is called the *diffusion term* and the second term the *reaction term*.

Our interest is in constructing stochastic approximations to the solutions of the Equation (38) or equivalently Equation (39). Approximations corresponding to polygonal curves have been discussed in the literature under the name "crystalline motion." Our approach is different and can be thought of as a stochastic crystalline algorithm: we construct a stochastic particle system whose profile defines an atomic measure on  $S^1$ , such that the corresponding curve is a polygon. Applying standard tools from hydrodynamic limits, it is proven in [2] that the (random) evolution of this polygonal curve converges, in the limit of a large number of particles, to curve evolution under the curve shortening flow.

The approximations we use are based on so-called **birth and death zero range particle systems.** To get a flavor of the simplicity of the algorithm, we write down this system down in some detail. Let  $T_N = \mathbb{Z}/N\mathbb{Z}$  denote the discrete torus. Let  $g : \mathbb{N} \to \mathbb{R}_+$  (the *jump rate*, with g(0) = 0),  $b : \mathbb{N} \to \mathbb{R}_+$  (the *birth rate*),  $d : \mathbb{N} \to \mathbb{R}_+$  (the *death rate*, with d(0) = 0) be given, and define the Markov generator on the particle configuration  $E_N = \mathbb{N}^{T_N}$  by

$$(\mathcal{L}^N f)(\eta) = N^2(\mathcal{L}_0 f)(\eta) + (\mathcal{L}_1 f)(\eta), \quad f \in C_b(E_N),$$

where

$$(\mathcal{L}_0 f)(\eta) = \frac{1}{2} \sum_{i \in T_N} g(\eta(i)) \left[ f(\eta^{i,i+1}) + f(\eta^{i,i-1}) - 2f(\eta) \right]$$
$$(\mathcal{L}_1 f)(\eta) =$$
$$\sum_{i \in T_N} \left[ b(\eta(i)) \left[ f(\eta^{i,+}) - f(\eta) \right] + d(\eta(i)) \left[ f(\eta^{i,-}) - f(\eta) \right] \right],$$

and

$$\eta^{i,i\pm 1}(j) = \begin{cases} \eta(j) + 1, & j = i \pm 1, \eta(i) \neq 0, \\ \eta(j) - 1, & j = i, \eta(i) \neq 0, \\ \eta(j), & \text{clse} \end{cases}$$
$$\eta^{i,+}(j) = \begin{cases} \eta(j) + 1, j = i, \\ \eta(j), \text{else} \end{cases}$$
$$\eta^{i,-}(j) = \begin{cases} \eta(j) - 1, j = i, \eta(i) > 0, \\ \eta(j), \text{elsc} \end{cases}.$$

Note that the **zero-range part**  $\mathcal{L}_0$  approximates diffusion term of equation (39) while the **birth-death** part  $\mathcal{L}_1$  approximates the reaction term of (39).

#### 2.3.4 Example: Approximate Euclidean curvature flows

As an example, in this section we give the stochastic approximation of the Euclidean curvature flow. For the general curve shortening case; see [2, 3] for the details. We now present candidates for the functions b, d, g defining the particle systems. Indeed, for curve shortening (V(x) = 1/x in Equation (39) above) one may show that the rates are

$$g(1) = \epsilon^{-2}, \qquad g(k) = \epsilon^{-1} k / (k-1), \ k \ge 2,$$
  

$$b(2) = 2\epsilon^{-2}, \qquad b(k) = 0, \ k \ne 2,$$
  

$$d(1) = \epsilon^{-2}, \qquad d(k) = 0, \ k \ne 1.$$
(40)

This means that as the number of cites N goes to infinity and as  $\epsilon$  goes to zero, the stochastic particle system converges to the solution of curve shortening.

#### 2.3.5 Stochastic Snakes

We have formulated a geometric active contour model stochastically, and derived a complete stochastic snake formulation. In this research program, we plan to derive fully stochastic versions of all the segmentation results described above. For the geometric active contour model case which we considered in this preliminary study, the density function evolves according to

$$m_t = -(m^{-1})_{\theta\theta}\phi - 2(m^{-1})_{\theta}\phi_{\theta} - m^{-1}(\phi_{\theta\theta} + \phi),$$
(41)

where  $\phi$  is the (conformal) stopping term, and subscripts indicate partial derivatives. The corresponding birth-death zero range process is defined exactly as above with the addition of the following for the first-order drift term on the right hand side of (41):

$$N\sum_{i\in T_N}g(\eta(i))(f(\eta^{i,i+1})-f(\eta)).$$

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- 3. Patricio Vela (postdoc; now assistant professor at Georgia Tech)