Project number IST-25582

CGL

Computational Geometric Learning

D3.2: Work Package 3 [Period 2] Report

STREP

Information Society Technologies

Period covered:	November 1, 2010–October 31, 2011
Date of preparation:	October 30, 2012
Date of revision:	
Start date of project:	November 1, 2010
Duration:	3 years
Project coordinator name:	Joachim Giesen (FSU)
Project coordinator organisation:	Friedrich-Schiller-Universität Jena Jena, Germany

In the following we describe the work done within Work Package 3 within the second period. In the description we follow the structure imposed by the tasks for this work package and period. Wherever there is no deviation and all goals have been met, it is *not* mentioned specifically. We start by restating the objectives for Work Package 3 and conclude with a discussion of the milestones for Period 1.

Objectives

Data sets found in Science and Engineering are often large and complex in the sense that they encode subtle correlations between the variables describing the system of interest. One way to apprehend this complexity consists of decomposing the data into appropriate geometric structures, so as to process these individually in order to unravel these complex interactions. This work-package follows this spirit for three application domains.

Work Package 3.1 is concerned with the investigation of specific hyper-surfaces called landscapes, which are height functions parameterized above high-dimensional spaces. Landscapes are central objects in optimization, and in Sciences for modeling macro-molecules and clusters of atoms. In both realms, one generally has a partial knowledge of the landscape through a point cloud sampled on it. While the landscape topology is trivial, learning features such as the significant minima and their basins, together with the connexions between them raises challenging questions. The main goals in Work Package 3.1 will be to develop, in conjunction with Work package 1, novel multi-scale analysis, partitioning and dimensionality reduction techniques for landscapes. Validation-wise, we expect these contributions to provide novel insights for analyzing and exploring landscapes in optimization and biophysics.

Work Package 3.2 investigates configuration spaces (C-spaces, for short), which are fundamental tools for studying a large variety of systems, and in particular moving objects (robots) evolving amidst obstacles, and molecular systems. While tools for accurate representation of low (2,3) dimensional C-spaces exist, current machinery for higher-dimensional C-spaces often offers only rather crude approximation, significantly limiting their applicability. Our major objective in Work Package 3.2 will be to develop methods for accurately and efficiently representing higher-dimensional C-spaces. We will specifically experiment with the newly developed methods on problems in automatic motion planning and molecular motion simulation.

Finally, Work Package 3.3 aims at, in collaboration with cosmologists, improving models and algorithms to analyze the distribution of matter in the universe and its evolution under the action of gravity, in particular in conjunction with the formation of galaxies. Continuing ongoing co-operation with cosmologists in this area, the geometric inference methods developed in Work Package 1 will be applied to detect these global geometric structures by analyzing cosmological data sets.

Tasks

Task 1.b: Dimensionality reduction for landscapes

We ended the first period with the following state of affairs:

> Both goals have been achieved since we now have:
> – an algorithm computing all the transition paths of a sampled landscape;
> – an algorithm performing a multi-scale analysis of the landscape, and also maintaining stable transition paths while simplifying the landscape using topological persistence.

Recall that by sampled landscape we refer to a height function defined over the conformational space of a molecular system. In particular, a molecular dynamics simulation gives direct access to the potential energy of each conformation. Our goal was to exploit the segmentation provided by the stable manifolds of the Morse-Smale (M-S) diagram to design collective coordinates adapted to the number of active degrees of freedom of the system (in a given region of the conformational space).

Thanks to the software setup developed during the first period, we generated molecular dynamics trajectories for polypeptides up to 53 atoms (from alanine dipeptide to penta-alanine). Unfortunately, the persistence diagrams derived from our discrete M-S decomposition were very noisy, and we did not observe a clear signal associated to persistent Betti numbers. This had two consequences:

- We decided to further investigate our discrete M-S algorithm – see our discussion of WP1-Task-2.b.
- We decided to get a better understanding of the free energy properties of macro-molecular systems, with a focus on protein complexes, since a number of cases were recently documented in the binding affinity benchmark. See our discussion of task WP3-Task-1.c.

Task 1.c: Validations in biophysics and optimization

A macro-molecular system has two energy landscapes, namely the potential energy landscape and the free energy landscape: the former is solely based on the internal energy of the system, while the latter also incorporates entropic properties. The so-called stable basins of the free energy landscape are of prime interest, since they precisely define the stable states of the system, and the difference ΔG of free energy between two such states is precisely the quantity which allows one to understand the thermodynamics of folding and docking. Phrased differently, the key (open) question consists of predicting the free energy change when the system moves from one state to another one.

For two proteins forming a complex, the dissociation free energy is known to be related to the binding affinity by $\Delta G = -RT \ln K_d$ with K_d the dissociation constant. In March 2011, a dataset known as the Protein-Protein Interaction Affinity Database was published

http://bmm.cancerresearchuk.org/ bmmadmin/Affinity/

This database of 144 protein complexes has two unique features: first, high resolution crystal structures of both the isolated partners and the complex have been solved; second, dissociation free energies have been measured experimentally.

To understand the importance of this dataset, given two proteins A and B known to form the complex AB, consider the problem of predicting the free energy change of the system undergoing a transition from $A + B$ to AB. The affinity benchmark allows comparing any predicted ΔG against the measured ΔG. Even more, one can assess the performances of the predictor as a function of the flexibility of the partners A and B, since the crystal structures of A and B and AB are known. (Recall that this is key, since a free energy change has an entropic component.)

We undertook this task, and made the following contributions in a paper entitled *Characterizing the morphology of protein binding patches*, which just appeared in Proteins [3] (one of the reference journals in structural biology):

- We developed descriptors characterizing the flexibility of the partners upon docking. Our method is the first one assessing the topological flexibility of the partners, a notion which we introduced to go beyond the stringent geometric flexibility assessment based on least RMSD (root mean square deviations).

- We correlated our descriptors against the experimental ΔG: our correlations are the best ones known to date.

- We assessed the performances of our descriptors as a function of the flexibility of the partners. Not surprisingly, the more rigid the partners upon docking, the better the descriptors at predicting ΔG. The classification of complexes into hardness classes, namely easy, intermediate and hard, for ΔG predictions is of high added value: we shall use it to choose test-cases to test the collective coordinates to be developed upon the full validation of our M-S construction.

Task 2.a/b: Certified approximation and hybrid representation of configuration spaces

The major goal for the second year of the project was to further substantiate our approach, which we presented in the first year of the project [14], of hybridizing exact methods from computational geometry together with the sampling-based techniques which are in prevalent use in robotics, and at the same time consider still higher-dimensional configuration space.

Indeed we continued our work on the general and modular algorithmic framework for path planning of robots, which we call *Motion Planning via Manifold Sample* or MMS for short. The key results for this topic in the second year are:

- A proof of probabilistic completeness of the approach, namely a proof of the convergence of the method to the desired solution if one exists. (In the first year of the project we showed probabilistic completeness for a certain instance only and restricted to three-dimensional C-Space.)

- Characterization of strategies to extend the scheme to higher dimensions. In particular we devised and implemented a *recursive* application of the scheme.

- We introduced the notion of *the dimensionality of narrow passages*, which we use to explain the good performance of our method in certain scenarios over the prevailing alternative practical methods.

These results were presented at the 10th Workshop on Algorithmic Foundations of Robotics [13].

The other central contribution in the area of high-dimensional configuration spaces, is the introduction and study of the problem k-color robot motion planning, a simple and natural extension of the multi-robot problem, where the robots are partitioned into k groups (colors) such that within each group the robots are interchangeable.

These results were presented at the 10th Workshop on Algorithmic Foundations of Robotics (WAFR) [16], and invited to a special issue of the International Journal of Robotics Research dedicated to the workshop.

We produced several additional results:

- We continued the work on developing an optimal local approximation of surface patches, and in particular patches of negative curvature (as described in the part of WP1). This approach will be used in order to obtain a triangulation of the contact surfaces in the configuration space of a planar robot. Once this approximation will be established, we will benchmark the two approaches for solving the motion planing problem; namely either use the MMS approach, or first discretize the problem and use standard arrangement of polylines computations. To that end, we started the work on adding a feature to the CGAL library which will support the computation of unbounded polylines. This feature is needed for the benchmarking process.

- In preparation for studying high-dimensional *motion spaces*, which arise in assembly planning, and where each point represents one plausible path for a set of three-dimensional parts, we devised and implemented an output-sensitive algorithm for detecting all the lines that pass through quadruples of segments from a give set of segments or polytopes (where the segments are polytope edges).

  Presented at the European Symposium on Algorithm (ESA) 2012 [8].

- In the first year of the project we presented (CGL-TR-05) preliminary results and the basic idea on how to generate a three-dimensional surface mesh based on a conservative voxelization of the swept volume using CGAL's Delaunay refinement. In the second year we extended the work (CGL-TR-44) to also present and compare two different approaches to parallelize voxel generation, a multi-core version as well as a GPU based solution using CUDA. Moreover, we devised an improved memory management scheme which allows handling of industrial data sets on the required precision as it is shown in our experiments. We anticipate that the approach can also be extended to compute approximations of three-dimensional Minkowski sums of polyhedral objects.

  Presented at the IEEE International Conference on Robotics and Automation (ICRA) 2012 [17].

- We have studied a fundamental issue in geometric data structures that are based on randomized incremental construction, namely the issue of structure depth vs. maximal query length. In the case of point location in planar maps we have shown a huge gap between the two quantities. In addition to being interesting from a theoretical point of view, we show in the paper that such results have practical implications.

  Presented at the European Symposium on Algorithm (ESA) 2012 [10].

- Using an explicit parameterization of the contact surfaces in the configuration space of a planar robot we compiled a visualization of instances of such spaces. The video, which was presented in SoCG 2012, visualizes the formation of the contact surfaces, and the correspondence between motions of the robot in the plan and motions of the configuration point in the configuration space. In addition, it visualizes motions of the robot such it maintains a contact with an obstacle.

  Video presented at the Symposium on Computatioanl Geometry (SoCG) 2012 [2].

Outlook. One of our goals in the third year of the project is to devise compact representations of high-dimensional configuration spaces. A step in this direction is our recent work on "Roadmap sparsification by edge contraction", where we adapt a method for surface simplification from computer graphics to the case of motion-planning roadmaps. Preliminary results show promise [15]. We also intend to investigate alternative ways to explore high-dimensional configuration spaces, aiming for more focused search techniques (for example, for answering a single planning query rather than trying to map the entire C-Space).

Task 2.c: Validations in robotics

The new results for the MMS framework described above have been tested on a system with six degrees of freedom—coordinating the motion of two arbitrary polygons, each translating and rotating in the plane. The results show considerable speed up over the standard tools for the problem [13].

For the new k-color motion planning algorithm, KPUMP, we carried out a variety of experiments in settings of varying difficulties and for different values and k, comparing with standard tools. Again KPUMP exhibits much better behavior [16].

In the experiments using our recent roadmap sparsification technique, we show that we can sometime compress more than 98% of the edges and vertices of the roadmap at the cost of degradation of average shortest path length by at most 2%. We also show that our method is more effective than a spanner-based algorithm, which has been proposed for that goal. See [15] for details.

We mention two more systems, devised as part of a robot-algorithm course, which we have been delivering[1] (i) A physical system of iCreate robots that coordinates the motion of two robots while a third robot moves around in an unpredictable manner and serves as a moving obstacle. (ii) A simulation system that extends the MMS framework to the case where two robots compete to reach many goals.

Task 3.a: Validations in cosmology

We have made substantial progress on three aspects of our program to develop innovative new instruments for the dissection of the Cosmic Web into filaments and walls. Two of these are integral part of the CGL project, one is directly related.

The work has been presented at a range of scientific meetings. Two of these international meetings were organized by van de Weygaert. With prof. E. Saar (Tartu Observatory, Estonia) he organized a Large Scale Structure session at the 13th Marcel Grossmann Conference, where a substantial amount of work mentioned in this section of the report was presented. The conference took place in the week of July 1-7, 2012. With dr. F. Kitaura (Leibniz Inst. Astrophysics, Potsdam), a workshop on the Structure and Dynamics of the Cosmic Web was organized in Potsdam from October 14-20, 2012.

Tessellations and the Dynamics of the Cosmic Web. The first aspect on which a substantial amount of work was finished over 2012 concerned the dynamics of cosmic structure formation and the study of caustics in the six-dimensional phase-space of an evolving cosmic mass distribution. The project revolves around the PhD project of J. Hidding, supervised by R. van de Weygaert and G. Vegter. Hidding has finished two papers on using computational geometry for solving the Burger's equation for a given random field of potential perturbations. It was demonstrated that it is equivalent to determining the weighted Delaunay tessellation defined by the peaks in the (primordial) velocity potential field, i.e., in the Lagrangian space. This follows directly from evaluating the analytical solution to Burger's equation and the notion that this follows directly after determining the convex hull of the velocity potential plus a time changing quadratic term.

Hidding managed to connect this directly to the structure that emanates in Eulerian space, that is evolved structure observed in the cosmic mass distribution. Interestingly, this structure is traced by the dual of the primordial Delaunay tessellation, the Voronoi tessellation. In other words, it was shown that following a Lagrangian formalism for the gravitational evolution of the cosmic matter

[1] http://acg.cs.tau.ac.il/courses/workshop/spring-2012/high-quality-motion-planning-for-robots

distribution leads to a profound and intricate connection between Lagrangian and Eulerian space in the form of the geometric duality between Delaunay and Voronoi tessellations. By identifying the morphology of the local structure in Eulerian space on the basis of the triangles/tetrahedra in Lagrangian space, we obtain a highly informative map of the location of filaments, walls, voids and clumps. Given the computational efficiency of the calculation, the resulting formalism enables us to systematically study the changing outline and morphology of the Cosmic Web as a function of the underlying cosmology, as well as its time evolution.

Hidding turned his findings into a video publication which was accepted for the SOCG2012 conference in Chapel Hill. The publication went along with a short paper on astroph. The video can be found on youtube,

http://www.youtube.com/watch?v=ujnM6tG-S8E

Following these results, Hidding, van de Weygaert and Vegter have started a close collaboration with prof. S. Shandarin, currently on sabbatical leave at the Univ. Groningen, on the issue of the phase space evolution of the weblike patterns in the cosmic mass distribution and the identification of caustics. Again, this turns around the innovative new application of geometric tools. Following a tessellation of Lagrangian space, i.e. of the primordial mass distribution, the evolution of the matter distribution can be accurately followed by assessing the deformation of the Lagrangian tessellation. Shandarin and two other groups have discovered that this evaluation leads to an accurate tracing of caustics in a discretely sampled mass distribution. Currently, Hidding is working on using this geometric formalism to classify the full range of 3-D caustics. In turn, this ties in to the identification of structures on the basis of Morse theory.

Homology of the Cosmic Web. A second major component of our program concerns the study of the topology of the Cosmic Web, and the systematic application of the machinery of computational topology towards the analysis of the cosmic mass distribution. P. Pranav, in close collaboration with Edelsbrunner, and together with van de Weygaert and Vegter has been substantially improving and clarifying the application of homology analysis - in terms of Betti number curves and persistence diagrams - of modelled cellular point distributions and of multiscale fractal models. Instead of basing the analysis on alpha shape filtrations, the analysis revolves around the density field filtration. The practical implementation revolves around DTFE density field reconstructions and the identifications of singular points in these. The DTFE density field reconstructions translate the discrete sample point distribution into a piecewise linear density field, with constant field gradient in each Delaunay tetrahedron. The density field values at each sample point are the inverse of the Delaunay star at that point. The persistence and Betti diagrams for a range of different cellular Voronoi clustering models and for a range of different multiscale Soneira-Peebles models have produced new insight into the signature of different morphological characteristics in persistence and Betti diagrams. We are on the verge of completing a major paper on the results, which will be the fundamental paper for introducing homology for cosmological and astronomical data analysis. The intention is to submit the paper before the end of November 2012. In the meantime, we have started work on the use of the developed homology instruments to analyze realistic cosmological simulations of structure formation, in particular to the dark matter and dark halo distribution in standard LCDM cosmological scenarios.

For the application of the homology instruments to real observational astronomical datasets, the crucial questions of noise and selection biases play a key role. We have found that for a meaningful homology analysis, the data need to be preprocessed. We have been working with F. Chazal and D. Cohen-Steiner on the use of Geometric Inference to to cosmological data (work package 1.1). While the principal application is the cleaning of the astronomical data, it also provides new insights into the filamentary network and their connection to clusters of galaxies. In an extended work-visit by Chazal and Cohen-Steiner in January, we have been investigating the effects of the variation in input parameters on the resulting weblike network. We have started to write a publication on the results.

Homology of Gaussian Random Fields. Another integral aspect of the cosmic homology project concerns our investigation of the persistence and Betti diagrams of Gaussian random fields. The primordial cosmic mass distribution has the character of a Gaussian random density and velocity field. These primordial Gaussian fields are the initial conditions of the current cosmic mass distribution, which has emerged from these initial conditions as a result of gravitational growth. J. Feldbrugge en M. van Engelen have been working on an analytical and numerical study of persistence diagrams and Betti numbers in Gaussian fields. Following a study based on Morse theory, they defined a Morse graph by connecting the singularities in a Gaussian field. They managed to derive analytical expressions for the Betti numbers in a 2-D random Gaussian field, and find a fitting function that reproduced the numerically found Betti diagram accurately. Subsequently, they found an integral expression for the persistence diagram of Gaussian fields. Currently, Feldbrugge is trying to evaluate this integral expression via path integrals. The importance of this study stems from the urge to detect possible tiny non-Gaussian deviations in the primordial density field. These would inform us of processes in the very early Universe, as they would be generated at the inflationary epoch at around $t \sim 10^{-34}$ sec after the Big Bang. In a preliminary numerical study they showed the potentially sensitive nature of persistence diagrams to tiny non-Gaussian deviations. This will form a major point of interest in the coming years, as we hope to be able to apply this to the map of the Cosmic Microwave Background temperature fluctuations observed by the Planck satellite. The first results have been published in the MSc thesis of Feldbrugge & van Engelen, "Analysis of Betti Numbers and Persistence Diagrams of 2-Dimensional Gaussian Random Fields" (Univ. Groningen) [7].

Euler Characteristic and Gauss-Bonnet Theorem. The Euler characteristic of the level sets of a Gaussian random field is perhaps the best known topological invariant associated to the field, especially in the Cosmology community. There exists an explicit expression for the Euler characteristic [4], which is based on the Gauss-Bonnet formula which relates the Euler characteristic of a surface to the integral of the Gaussian curvature. It is not immediately obvious whether the Euler characteristic is the only topological invariant that can be determined by a straightforward integral. This has been established by Abrahamov [1], see Gilkey [9] for a modern (and more extensive) treatment. Both the work by Abrahamov and the modern treatment by Gilkey involve a significant amount of analysis and machinery (in the case of Gilkey related to the Heat equation and Atiyah-Singer index theorem). We have provided a new elementary proof of this result in low dimensions (CGL-TR-43).

Nexus. In a strongly related but different project we have been developing a multiscale morphological classification scheme for the cosmic web. Following on the basis of the Multiscale Morphology Filter (MMF), Cautun has developed a sophisticated instrument for identifying filaments, walls, cluster clumps and voids in a multiscale density field. The Nexus formalism not only looks at the density field, but also incorporates the log(density) field, the divergence and shear of the velocity field and the tidal gravitational field. The most superior version of the Nexus formalism is based on the log(density) field, and is called Nexus+. The results have been published in MNRAS [6]. The method is being applied to the study of various aspects of the cosmic web, currently in particular involving issues of environmental influences on galaxy formation.

Summary of Principal Results.

- Adhesion model calculations of cosmic web evolution substantially improved by the use of Delaunay and Voronoi tessellations in modeling the convex hull of gravitational potential. On the basis of this a publication in the form of a SOCG movie. Subsequently, geometrical study of phase space and caustic detection [11].
- Wintraecken & Vegter demonstrated that the Euler characteristic is the only topological invariant that can be determined by a straightforwaard integral.
- Completion and publication of multiscale morphology technique, Nexus (Cautun et al. 2012).
- Publication of Watershed Void Finder study of shapes of void population and the feasibility of extracting information on the nature of dark energy [5].
- Substantial progress in understanding of homology results in the context of multiscale weblike point distributions. Key publication [12] on the verge of submission.
- Profound analytical and numerical study of Betti number and persistence diagrams in Gaussian random fields. Accurate fitting function has been derived for Betti number diagrams in 2-D Gaussian random fields. Numerical studies indicates high sensitivity of persistence diagrams to subtle non-Gaussian deviations. Published in MSc thesis, Feldbrugge and van Engelen (2012). Publication for Monthly Notices in Royal Astronomical Society in preparation.

Outlook. In the third year of the project we will concentrate on four aspects. The geometric study of caustics and singularities in evolving gravitational systems will lead to new ways of identifying cosmic structures. It will be largely based on efficient geometric calculations, starting from tesselated initial conditions. Homology analysis will be applied to the outcome of realistic cosmological simulations, and a beginning will be made with the application to observational datasets. Following recent results, we will follow the potential of persistence diagrams to discriminate between cosmological scenarios with different non-Gaussian conditions. The multiscale morphology code of Nexus will prove instrumental for characterizing cosmic environment. We will systematically compare its outcome to other formalisms, in particular the geometric phase-space sheet method of Shandarin, in order to calibrate its physical foundation.

Milestones

MS 13: Stratifying vs. c-coordinates

The third milestone reads as *Stratifying high-dimensional point clouds prior to dimensionality reduction looks promising. Should we not be able to develop practical algorithms, we shall investigate* *c-coordinate designs based on simpler strategies, e.g. mixing normal modes associated to persistent minima of the landscape.*

The work reported in WP3-Task-1.b and WP3-Task-1.c precisely follows this pattern. Because we could not, at this stage, find an interesting signal in the persistence diagrams of our M-S complex, designing c-coordinates from normal modes was not an option. On the other hand, in March 2011, the affinity benchmark got published. We therefore tackled the question of predicting transitions via ΔG predictions based on topological and geometric descriptors of macro-molecules.

But as also explained, we have not given up on c-coordinates (with or without normal modes), since our improved M-S complex needs to be confronted to molecular data.

MS 14: Decide on benchmark for hybrid solutions

The question we are addressing is what should be the dimension of the *workspace* where we will carry out a benchmark for our methods. The dimension of the relevant *configuration space* will be high at any case, and the debate is whether we should carry out the benchmark for polygons or for polytopes. While we do plan to move towards three-dimensional workspaces, we decided to do the benchmark in a planar setting with many robots. The rationale is that we have better experience and machinery to cope with two-dimensional robots. This still leaves us to deal with the high dimensionality of the interesting problems that arise from the high dimension of the configuration space.

MS 15: Assess problem of heterogeneous and partially missing data

See Deliverable 3.3 (Report).

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