ShapeWorks
Particle-based Shape Correspondence and Visualization Software

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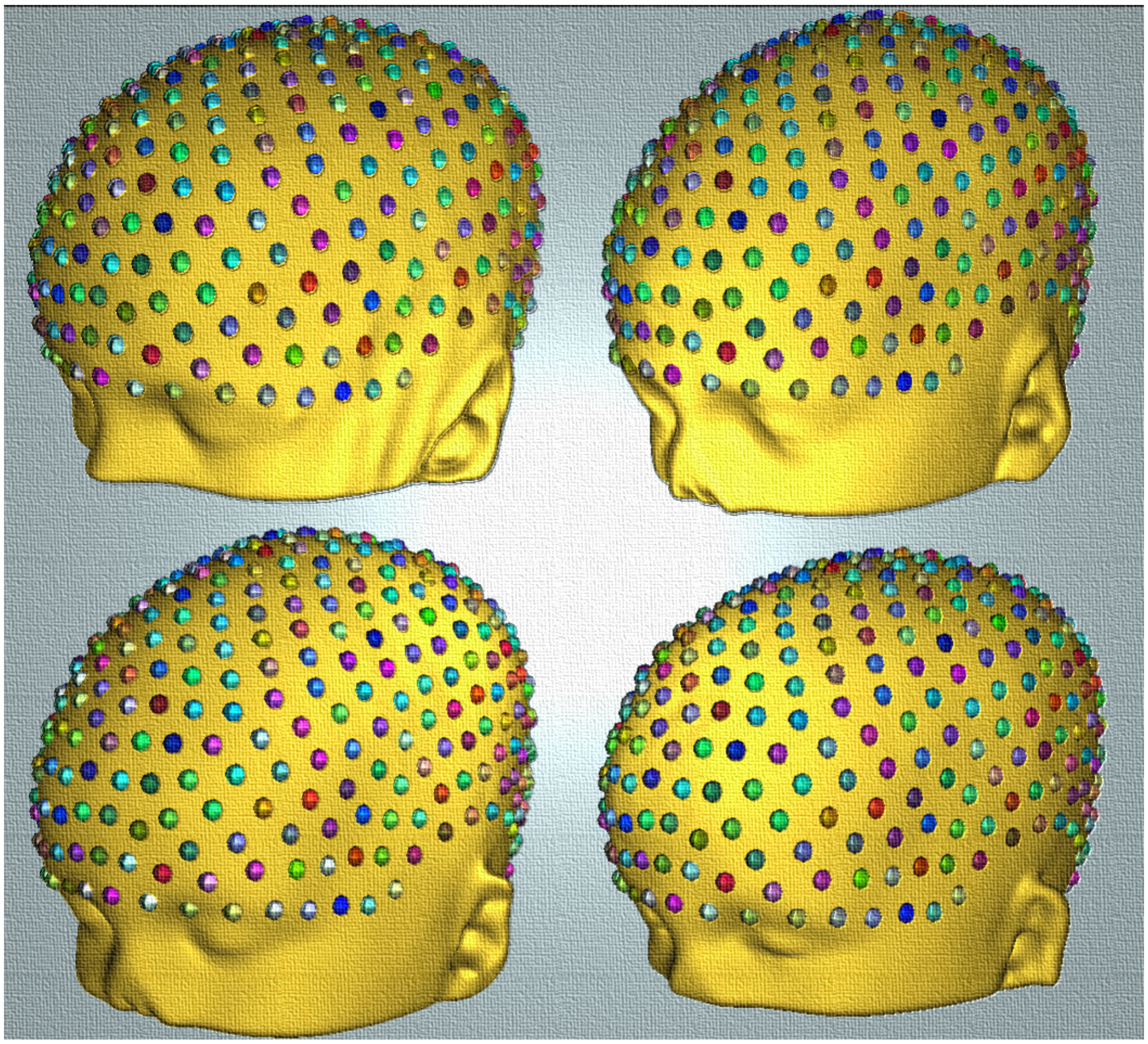

Contents

1 License

2 Introduction

This software is an open source distribution of the algorithm for constructing *correspondence-based* statistical models of sets of similar shapes described by Cates, et al. in [2, 4]. Several relevant extensions to the basic algorithm, as well as their application to clinical and scientific studies, are also published in [5, 3, 5, 8]. This document is intended to provide necessary background information for understanding and using the ShapeWorks software, including a basic tutorial and reference. This section gives a technical overview of correspondence shape models and the correspondence optimization algorithm that is used in the ShapeWorks software. For a more detailed explanation of the ShapeWorks optimization algorithm, please refer to Cates, et al. [4].

2.1 Correspondence Models

Correspondence point models represent shape by sampling each shape surface in a consistently ordered fashion so as to define homologous surface points across the population of shapes. These homologous surface points are called *correspondences*. Once chosen, the 3D positions of all m correspondences on a shape sample can be encoded as a $3m$ shape vector, which is the point-based representation of that shape. The ordering of the particles on each shape implies a correspondence among shapes, and the distribution of all of the shape samples in this $3m$-dimensional vector space (*shape space*) gives rise to the statistical analysis. The problem of how to choose the correspondence positions, and thus the shape-space distribution of the sample population, is a model selection problem. Model selection problems in statistics are typically resolved by choosing the simplest model that explains the observed data (see, e.g. [7]). Consistent with this idea, the ShapeWorks correspondence optimization algorithm seeks a compact distribution for its correspondences in the shape space (for model simplicity), while simultaneously seeking good surface samplings in order to accurately represent the data. Figure 1 illustrates these basic concepts for a population of hand shapes.

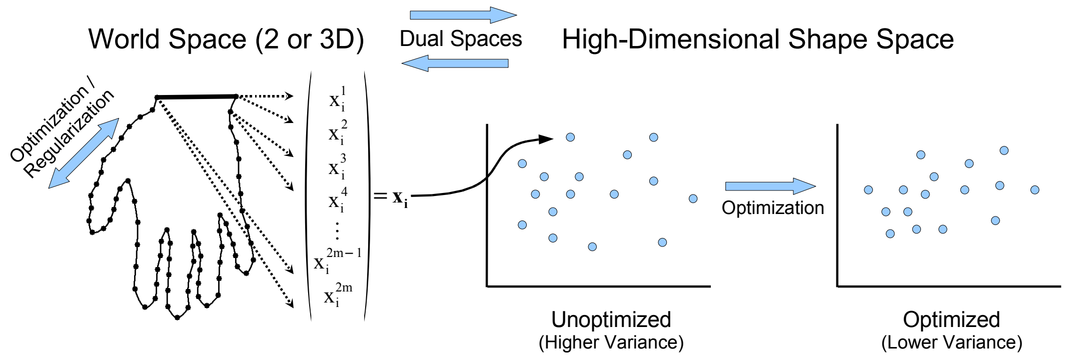

Figure 1: An illustration of the basic concepts the ShapeWorks point-based correspondence optimization.

The figure shows the mapping of all the surface point samples from a single shape to a single point in the higher-dimensional shape space, and the relative compactness of the distribution of all samples in that shape space after optimization.

2.2 The ShapeWorks Correspondence Optimization

The ShapeWorks optimization works by modeling the correspondence positions as sets of dynamic *particles* that are constrained to lie on the set of sample shape surfaces. The positions of the correspondences are optimized by gradient descent on an energy function that balances the negative *entropy* of the distribution of particles on each shape surface with the positive entropy of the distribution of the shape samples shape space. More specifically, and with reference to Figure 1, we consider $\mathbf{x}_k \in \Re^{3m}$ as an instance of a random variable $\mathbf{Z}$ and minimize the energy function

$$Q = H(\mathbf{Z}) - \alpha \sum_k H(\mathbf{x}_k), \tag{1}$$

where H is an estimation of differential entropy. Minimizing the first term in Q produces a compact distribution of samples in shape space, while the second term seeks uniform surface samplings for accurate shape representation. This latter term can also be modified to adaptively over-sample in response to local surface features such as curvature. The free parameter α balances the tradeoff between model compactness and accurate shape representation. Since correspondence points in this formulation are not tied to a specific parameterization, the method operates directly on volumetric data and extends easily to arbitrary shapes, even non-manifold surfaces.

2.3 The ShapeWorks Shape Modeling Pipeline

This software distribution consists of several applications that together make up a full processing pipeline for correspondence computation and visualization. The stages of the pipeline are as follows,

$$\textsf{Preprocessing} \Rightarrow \textsf{Alignment} \Rightarrow \textsf{Initialization} \Rightarrow \textsf{Optimization} \Rightarrow \textsf{Visualization\&Analysis}$$

This section gives an overview of the steps involved in the pipeline. For an example of using the ShapeWorks software to perform each of these steps, see the Tutorial in Section 4.

Preprocessing Any set of implicitly defined surfaces, such as a set of binary segmentations, is appropriate as input to this pipeline. By default, the software will assume a *closed* surface, but can also handle open boundaries (specified by cutting planes) and non-manifold surfaces consisting of multiple closed surfaces. A binary mask, such as the output of an image segmentation process, for example, contains an implicit shape surface at the interface of the labeled pixels and the background. Binary masks contain aliasing artifacts, however, that should first be removed. Typically we follow an antialiasing step with a very slight Gaussian blurring to remove the high-frequency artifacts that can occur as a result of numerical approximations.

Alignment A collection of shape segmentations must often be aligned in a common coordinate frame for modeling and analysis. The ShapeWorks software does not provide full support for this stage of the pipeline, since every new dataset may require a different process of alignment. Some basic alignment tools that are included with ShapeWorks are the ability to align the segmentations with respect to their centers of mass and the orientation of their first principal eigenvectors. For some classes of data, this method is effective as a rough alignment and is followed, *during the optimization process*, by iterative Procrustes alignments based on the correspondence point positions [6]. For more information on this procedure, see Sections 4 and 5.

The ShapeWorks software distinguishes between two separate coordinate frames: a *local* coordinate frame for each shape sample, and a *common* coordinate frame in which all shape samples are coregistered. For applications in which the input data is completely registered, these two coordinate frames are the same. Where there is a distinction, the ShapeWorks software will maintain and output appropriate transformations to the common coordinate frame for each shape sample, as well as separate correspondence files for each coordinate frame.

Correspondence Initialization Typically, we initialize the ShapeWorks optimization with a single particle that finds the nearest zero of the implicit surface, and then splits under optimization (producing a new, nearby particle) at regular intervals until a specific number of particles are produced and reach a steady state. This initialization procedure is supported with the ShapeWorks software. We have found this procedure to be generally applicable to classes of closed shapes with reasonably smooth surfaces. For more complicated shapes, it may be necessary to specify initial particle positions for the optimization using other means. Initial particle positions may be computed offline and supplied to ShapeWorks as a text file input (see Section 3.2).

Correspondence Optimization The ShapeWorks optimization proceeds as described in Section 2.2, starting with an initial set of particle positions and a set of implicit surfaces (e.g. distance transforms). Several types of optimization procedures are supported: adaptive gradient descent, Jacobi updates, and Gauss-Seidel updates. By default, adaptive gradient descent with Gauss-Seidel updates is used. Important parameters to consider for the optimization are the regularization on the covariance matrix for the shape-space entropy estimation, and the parameter α from Equation 1 which controls the trade-off between the uniformity of the surface sampling and the compactness of the optimized model. Also consider whether iterative Procrustes alignment is necessary and whether or not to remove Procrustes *scale* from the correspondence model.

Visualization and Analysis Statistical analysis of point-based shape models is difficult because point-wise statistical tests require multiple-comparisons corrections that significantly reduce statistical power [3]. Analysis in the full shape space, however, is problematic due to the high number of dimensions and the difficulty of obtaining sufficient samples. A common solution is to employ dimensionality reduction reduction by choosing a subspace in which to project the data for traditional multivariate analysis (see, e.g. [3, 1]).

This software does *not* include specific code for statistical analysis of the correspondences. It does, however, provide principal component analysis (PCA), which can be used for dimensionality reduction prior to subsequent statistical analysis, and visualization of orthogonal modes of variation in the model (see, e.g. [3, 1]. ShapeWorks also includes methods for computing and visualizing the Euclidean mean shapes and the median shapes of populations. Typically, we use a separate statistical package, such as *R* (the R Foundation, `www.r-project.org`), for analysis of the PCA loadings of the correspondence positions. For more ideas regarding visualization and statistical analysis of correspondence models, see the various publications listed in the bibliography section of this document.

3 The ShapeWorks Software

This section provides an overview of how to build and use the ShapeWorks software. The tutorial in this section illustrates a full shape analysis pipeline, starting with binary volume segmentations, and including preprocessing and visualization of correspondences. For more detailed software usage information, see Section 5.

3.1 Overview of the Executables

ShapeWorksGroom This is a command-line preprocessing tool for image volumes. Its primary purpose is to convert binary, volumetric image segmentations (label masks) into distance transforms that are suitable for input to the ShapeWorksRun and ShapeWorksShop applications. Filtering operations are implemented using ITK (The Insight Toolkit), and are applied in batch processing mode. Some of the filtering operations that ShapeWorksGroom supports are antialiasing, automatic cropping, hole-filling, smoothing, and distance transforms.

ShapeWorksRun This is the command-line correspondence optimization tool, and the heart of the ShapeWorks shape analysis pipeline. The minimum required input to this application is a set of distance transforms that are the surface representations of the population of shapes (see Sec. 2.3). Intial particle positions and affine registration information can also be supplied as inputs. ShapeWorksRun can be used to initialize a set of particle positions using the particle-splitting described Sec. 2.3 .

ShapeWorksView This tool can be used to visualize optimized correspondence positions, along with surface reconstructions based on the correspondences. It also computes a principal component analysis (PCA) of the correspondences, and allows you to visualize the variation in each of the modes of the PCA. The mean shapes and the median shapes can be reconstructed, and ShapeWorksView allows you to assign group labels to your samples, in order to visualize the differences in mean shape between the groups.

ShapeWorksShop This is a GUI-based version of ShapeWorksRun that has some additional functionality and optimization parameters exposed. It provides a real-time visualization of the optimation process on the set of shape surfaces. This tool is very useful, for example, for initializing a set of particles prior to the full optimization and for testing parameter settings.

3.2 File Formats

Image volumes Inputs to ShapeWorksGroom, ShapeWorksRun, and ShapeWorksShop are image volumes. ShapeWorks can read and write any image file format supported by the Insight Toolkit. Image inputs to ShapeWorksRun and ShapeWorksShop must be surfaces embedded in image volumes. Shape surfaces must be represented implicitly as the zero level set of a distance transform.

Point files Correspondence point positions are stored in text files. These files contain no header, and are simply a list of the point positions written as follows

```
x1 y1 z1
x2 y2 z2
⋮
xN yN zN ,
```

where `x y z` are floating point numbers and `N` is the number of correspondence points. Two point files are maintained for each shape. The first has file extension `.lpts`, and is the correspondence positions in that shape's *local* coordinate space. The second file has extension `.wpts`, and is the correspondence positions in the *common* (world) coordinate space. The `.lpts` files can be used to initialize particles on shape surfaces for optimization, while the `.wpts` files should be used for any statistical analysis.

Parameter files ShapeWorks software parameters are specified in text files. The syntax for these parameter files is described in Section 5.1.

3.3 Building the Software

Dependencies The ShapeWorks software depends on several open-source, freely-available software toolkits. To build the full set of tools, including the graphical interfaces, you will need the following packages.

CMake is used to configure the build, and is available from `http://www.cmake.org`. The SCMoguls build is compatible with CMake 2.6. Earlier versions of CMake may not be supported.

The Insight Toolkit (ITK) is required for all ShapeWorks applications. ITK is available from `http://www.itk.org`. Make sure to use ITK version 2.8.1 or higher. For compatibility with ShapeWorks, build ITK using CMake and compile in *Release* mode.

The VisualizationToolkit (VTK) is required only for ShapeWorksView and ShapeWorksShop. VTK is available from `http://www.itk.org`. ShapeWorks has been tested with VTK version 5.0 and higher. For compatibility with ShapeWorks, build VTK using CMake and compile in *Release* mode.

Fast Light Toolkit (FTLK) is required for ShapeWorksView and ShapeWorksShop. FLTK is available from `http://www.fltk.org`. The most recent stable release of FLTK version 1.1.x is recommended. For compatibility with ShapeWorks, build FLTK using CMake and compile in *Release* mode.

Supported Platforms The ShapeWorks software is ANSI C++ code and has been built successfully on Windows 32-bit, Linux 32-bit, and Linux 64-bit platforms. Any platform for which ITK, VTK, and FLTK are supported should, in theory, also support the ShapeWorks software.

Binary Distributions Binary distributions of the ShapeWorks software for Windows 32-bit platforms are also available for download. Binaries for other platforms (e.g. Macintosh and Windows 64-bit) may be released in the future. Unless you intend to do development with the ShapeWorks source code, it is highly recommended that you use a binary distribution, if one is available for your system.

Support Questions regarding the ShapeWorks software can be addressed to the ShapeWorks mailing list at `shapeworks-users@gforge.sci.utah.edu`. You can sign up for this mailing list by visiting `https://gforge.sci.utah.edu/mailman/listinfo/shapeworks-users`.
You can visit the ShapeWorks discussion forums, and browse news and development information at the ShapeWorks GForge page
`https://gforge.sci.utah.edu/gf/project/shapeworks/`.

Build Instructions ShapeWorks uses the CMake build system to configure the build and generate makefiles or Microsoft Project files. Once configured, ShapeWorks can be built with your platform's native compiler (gcc, Microsoft C++, etc). The following configure instructions are the same for every platform. For more information on using CMake, please refer to www.cmake.org.

1. Unzip or untar the source code distribution.
2. Create a separate build directory for your ShapeWorks build files and exectuables. If your source code is in `/home/username/ShapeWorks`, for example, you might choose to create a directory `/home/username/ShapeWorks_build`. On linux/unix platforms, you will need a build for each compilation configuration, e.g. you might have two build directories: `/home/username/ShapeWorks_release` and `/home/username/ShapeWorks_debug`. Note that you will also need corresponding *Debug* and *Release* builds for ITK, VTK, and FLTK.

3. Start the CMake GUI, or run `ccmake` if building from a terminal shell.
4. Enter the `ShapeWorks/code` directory as your source code directory and your newly-created directory as the build directory.
5. In the CMake GUI, choose “Configure”. CMake will attempt to find your ITK build. If not found, you will need to specify the *build* directory for ITK.
6. In the CMake GUI, you will have the option to choose to build the ShapeWorksView and ShapeWorksShop applications. If selected, CMake will attempt to automatically configure FLTK and VTK. If these builds are not found, you will need to specify their locations.
7. Specify the `CMAKE_INSTALL_PREFIX`. This is the directory in which the executables will be installed.
8. On Linux/Unix systems, specify *Release* mode for your build. If you also want a developmental build, you will need to configure a separate build directory for a *Debug* mode. On Windows platforms, you may choose either Debug or Release at compile time.
9. Once ITK, VTK, and FLTK are properly configured, click “Generate” to create the makefiles.
10. Build the *INSTALL* target in the CMake-generated makefiles using your native compiler.

! Important: Make sure to build using *Release* mode for best results. Because ShapeWorks and ITK both rely heavily on compile-time optimizations, if built using a *Debug* configuration, SCIRunMoguls code may run up to ten times slower!

4 Tutorial: Torus Example

This tutorial will illustrate how to use the ShapeWorksRun software to optimize correspondences on image segmentations (i.e., binary volumes), which are a common format in many shape studies that rely on 3D imaging to extract anatomy. In this example, we will compute a statistical model of 20 synthetically generated tori. The tori are parameterized by small radii r and a large radii R, each randomly sampled from a Gaussian distribution. The resulting shape model will therefore show two orthogonal modes, with the variance in each of these modes corresponding to that of the sampled distributions for r and R. This tutorial proceeds step-by-step through the full analysis pipeline described in Section 2.3. An example of 7 synthetically generated misaligned ”mickey” datasets is also provided to illustrate how iterative closest point (ICP) registration can be used to improve the alignment in ShapeWorksGroom (ShapeWorks/example directory).

4.1 The Torus Data

The example set of torus shapes is provided in the `ShapeWorks/examples` directory. Navigate to this directory and unzip the `TorusExample.tgz/.zip` data file. You should now have a new directory, `ShapeWorks/examples/TorusExample`, which contains 20 synthetically generated tori, The tori are represented as binary volumes, i.e. as image segmentations. Pixels inside each torus have value 1, and pixels outside have value 0.

4.2 Preprocessing with ShapeWorksGroom

As discussed in Section 2.3, the first step is to convert the binary volume into a distance transform suitable for use with ShapeWorksRun. We will do this using ShapeWorksGroom to perform a set of filtering operations. The first preprocessing step is to crop all of the image volumes to the same size, and shift the center of each volume to the center-of-mass of the segmentations. This establishes a common coordinate frame, an initial, rough translational alignment, and a common image volume size. This latter consideration is highly recommended when using ShapeWorksRun. Note that if the shapes embedded in your own image volumes are already in alignment, then these operations are not

```
// torus.preprocess1.params
// Preprocessing parameters 1 for Torus example
(background 0.0) // Value of background pixels in the image
(foreground 1.0) // Value of foreground pixels in the image
(pad 10)         // Number of background pixels to pad the edges of
                 // the cropped volume

(verbose 1)      // Output progress information

(inputs          // Set of input files to process
"torus.00.mha"  "torus.01.mha"  "torus.02.mha"  "torus.03.mha"
"torus.04.mha"  "torus.05.mha"  "torus.06.mha"  "torus.07.mha"
"torus.08.mha"  "torus.09.mha"  "torus.10.mha"  "torus.11.mha"
"torus.12.mha"  "torus.13.mha"  "torus.14.mha"  "torus.15.mha"
"torus.16.mha"  "torus.17.mha"  "torus.18.mha"  "torus.19.mha"
)

(outputs            // Output filenames to use
"torusDT.00.mha"  "torusDT.01.mha"  "torusDT.02.mha"  "torusDT.03.mha"
"torusDT.04.mha"  "torusDT.05.mha"  "torusDT.06.mha"  "torusDT.07.mha"
"torusDT.08.mha"  "torusDT.09.mha"  "torusDT.10.mha"  "torusDT.11.mha"
"torusDT.12.mha"  "torusDT.13.mha"  "torusDT.14.mha"  "torusDT.15.mha"
"torusDT.16.mha"  "torusDT.17.mha"  "torusDT.18.mha"  "torusDT.19.mha"
)
```

Figure 2: Parameter file for the first stage of torus preprocessing with ShapeWorksGroom: foreground isolation, hole-filling, and automatic volume cropping.

needed. (In the case of the torus data, this step is also not necessary, but is illustrated here because it may be generally useful for real-world data.) Before cropping, we will also perform morphological operations to isolate the foreground and fill any existing holes in the segmentations.

From the example directory, type the following command. Note that you may need to also specify a path to the executables if they are not already in your system path. This preprocessing step should take less than 5 minutes to run, depending on the speed of your computer. The parameter file for this step is shown in Figure 2, and contains all of the required parameters for each stage of processing.

```
ShapeWorksGroom torus.preprocess1.params isolate hole_fill center auto_crop
```

The second preprocessing step antialiases the binary surface, and then computes a distance transform from that surface using the fastmarching method. Finally, we blur the distance transform slightly to get rid of high-frequency artifacts. Type the following command. This step should also take less than 5 minutes to complete. The parameter file for this step is given in Figure 3. Type the following command.

```
ShapeWorksGroom torus.preprocess2.params antialias fastmarching blur
```

At this stage, you should have a set of implicit surface volumes labeled `torusDT.00.mha, torusDT.01.mha, ..., torusDT.19.mha`. These new files are suitable inputs to the correspondence optimization.

4.3 Optimizing Correspondence with ShapeWorksRun

The next step is to initialize and optimize the particle system. In this example, we will use relatively few points, just 256 particles per torus. Correspondences are initialized on the shape surfaces using the splitting strategy described

```
// torus.preprocess2.params
// Preprocessing parameters 2 for Torus example

(background 0.0) // Value of background pixels in image
(foreground 1.0) // Value of foreground pixels in image
(antialias_iterations 20) // Number of anti-aliasing iterations
(blur_sigma 2.0) // Size of Gaussian blurring kernel for smoothing
(fastmarching_isovalue 0.0)  // Pixel value associated with shape surfaces

(inputs                         // Name of input files
"torusDT.00.mha" "torusDT.01.mha" "torusDT.02.mha" "torusDT.03.mha"
"torusDT.04.mha" "torusDT.05.mha" "torusDT.06.mha" "torusDT.07.mha"
"torusDT.08.mha" "torusDT.09.mha" "torusDT.10.mha" "torusDT.11.mha"
"torusDT.12.mha" "torusDT.13.mha" "torusDT.14.mha" "torusDT.15.mha"
"torusDT.16.mha" "torusDT.17.mha" "torusDT.18.mha" "torusDT.19.mha"
)

(outputs                        // Name of output files
"torusDT.00.mha" "torusDT.01.mha" "torusDT.02.mha" "torusDT.03.mha"
"torusDT.04.mha" "torusDT.05.mha" "torusDT.06.mha" "torusDT.07.mha"
"torusDT.08.mha" "torusDT.09.mha" "torusDT.10.mha" "torusDT.11.mha"
"torusDT.12.mha" "torusDT.13.mha" "torusDT.14.mha" "torusDT.15.mha"
"torusDT.16.mha" "torusDT.17.mha" "torusDT.18.mha" "torusDT.19.mha"
)
```

Figure 3: Parameter file for the second stage of torus preprocessing with ShapeWorksGroom: antialiasing, distance transform computation, and slight blurring.

in Section 2.3, and optimized using Gauss-Seidel adaptive gradient descent on the minimum-entropy algorithm from Section 2.2. We will save the progress of the optimization every 20 iterations by setting the checkpointing option. A full parameter file for this step is shown in Figure 4. The command to start the optimization is as follows.

```
ShapeWorksRun torus.correspondence.params
```

During the optimization, ShapeWorksRun outputs the variance associated with each of the orthogonal modes of variation in the data, obtained via principal component analysis (PCA). As the optimization proceeds, notice how almost all of the variation in the model is shifted into the top two modes of variation (modes 18 and 19). These two modes represent our two real parameters of the model, big R and little r. The initialization and optimization process will take between 5 to 10 minutes, depending on the speed of your computer. In practice, you will need to modify the regularization parameter and the number of iterations for your data. In general, real data will require more particles per shape and more iterations for a better model fit. Also consider setting the `adaptivity_strength` parameter to introduce oversampling in regions of higher curvature. The `relative_weighting` parameter, which sets α from Equation 1, may also be of interest. By default, α is set to 1.

4.4 Visualization and Analysis with ShapeWorksView

We will now use the ShapeWorksView application to view the output of the correspondence optimization. Note that you can also view the intermediate results of the optimization after each checkpointing save. First, start the ShapeWorksView application using the supplied parameter file, as given in Figure 5. Note that this parameter file load the `*.wpts` files, which are the correspondences in the common (world) coordinate space. To start the ShapeWorksView application, type the following command.

```
ShapeWorksView torus.analyze.params
```

Once the applications starts, you will see the mean correspondence positions for the ensemble of tori, and a surface reconstruction of the mean. Let's start by adjusting the reconstruction parameters for a better visualization. From the "Options" menu, choose "Reconstruction", and set the "Neighborhood size" to 7, and the "Spacing" to 4.5. This will give a slightly improved surface reconstruction.

Next we will view the correspondence points for each of the torus samples. In the "View" menu, select "Samples". You can now scroll through each of the samples and see its correspondences and surface reconstruction. Correspondence positions are indicated by the spherical glyphs, which are colored consistently from one sample to the next to indicate correspondence. Glyph parameters can be changed under the "Options" menu. Notice that each sample is assigned a Group ID. For this example, we have not indicated groups, so these IDs are not valid. For group comparison, however, we could specify group IDs in the parameter file, and then view the group means and group medians separately.

Finally, we can look at the variation in the PCA modes of our model. In the "View" menu, choose "PCA Modes". Select Mode 1, the PCA mode with the largest amount of variation, and move the slider next to the mode selection box right and left. You will see that this mode correspondends to little r for the torus. The units to the left of the slider are units of standard deviation in that mode. Now select Mode 2. By moving the slider, you will see that this mode corresponds to big R. The remaining modes can be considered noise, and show increasingly less variation. Running the optimization further for this set of data will decrease the variation in those remaining modes.

5 Command Reference

5.1 Parameter Files

Parameter files for each of the ShapeWorks applications are text files consisting of a list of parameters, enclosed in parentheses, and separated by white space or a new line.. Each parameter has an associated list of values. Parameter values can be integer (`<int>`), floating-point (<float¿), or string (<string¿), and are also separated by white space or

```
// torus.correspondence.params
// Parameters for the correspondence point optimization with ShapeWorksRun
// (or ShapeWorksShop)
(inputs  // List of files containing the set of shape surfaces (distance transforms)
"torusDT.00.mha" "torusDT.01.mha" "torusDT.02.mha" "torusDT.03.mha"
"torusDT.04.mha" "torusDT.05.mha" "torusDT.06.mha" "torusDT.07.mha"
"torusDT.08.mha" "torusDT.09.mha" "torusDT.10.mha" "torusDT.11.mha"
"torusDT.12.mha" "torusDT.13.mha" "torusDT.14.mha" "torusDT.15.mha"
"torusDT.16.mha" "torusDT.17.mha" "torusDT.18.mha" "torusDT.19.mha"
)

// OPTIONALLY we could specify a set of point files to initialize
// the optimization like this:
// (point_files torusDT.00.lpts torusDT.01.lpts ... torusDT.19.lpts)

(number_of_particles 256) // If point files are not specified, then
                          // the application will initialize particles
                          // by splitting until each shape has this
                          // total number of particles.

(iterations_per_split 200) // Iterations between splitting during
                          // initialization phase.

(starting_regularization 10.0) // Starting regularization for the
                               // entropy-based correspondence
                               // optimization.

(ending_regularization 0.1) // Final regularization for the entropy-
                            // based correspondence.

(optimization_iterations 200) // Number of iterations for the entropy-
                              // based correspondence.

(checkpointing_interval 20) // Number of iterations between checkpoints
                            // (iterations at which results are saved)

(output_points_prefix "torus") // Prefix for the output files.
```

Figure 4: Parameter file for the correspondence point optimization of the torus data using ShapeWorksRun.

```
// torus.analyze.params
// Parameters for viewing correspondence points using ShapeWorksView
(point_files    // Set of correspondence points in the common coordinate space.
"torus.00.wpts" "torus.01.wpts" "torus.02.wpts" "torus.03.wpts"
"torus.04.wpts" "torus.05.wpts" "torus.06.wpts" "torus.07.wpts"
"torus.08.wpts" "torus.09.wpts" "torus.10.wpts" "torus.11.wpts"
"torus.12.wpts" "torus.13.wpts" "torus.14.wpts" "torus.15.wpts"
"torus.16.wpts" "torus.17.wpts" "torus.18.wpts" "torus.19.wpts"
)
```

Figure 5: Parameter file for visualizing optimized correspondence points on the torus data using ShapeWorksView.

new lines. Strings must be enclosed by quotation marks. An example parameter with an associated list of three values (one integer, one floating point and one string), is as follows

```
(example_parameter 10 10.0 ``ten'') // here is a comment
```

As shown in the previous example, single lines of a parameter file may be commented using C++ comment syntax. Several examples of full parameter files are given in Figures 2–5.

5.2 ShapeWorksGroom

```
ShapeWorksGroom <parameterfile> <options>
```

Example parameter files are given in Figures 2–3. All filtering operations must specify a list of inputs and outputs in the parameter file. The size of the input list must match the size of the output list.

```
(inputs
"torus.00.mha"
"torus.01.mha"
⋮
"torus.19.mha"
)
(outputs
"torus.00.mha"
"torus.01.mha"
⋮
"torus.19.mha"
)
```

The following is a list of valid command-line options that specify filtering operations, followed by any additional parameters that must be present in the parameter file. Filtering operations are applied in the order in which they are specified on the command line.

isolate Find and isolate the largest connected component. The foreground and background intensity values must be specified in the parameter file.

```
(background <float>)
(foreground <float>)
```

hole_fill Fill any holes in the binary segmentation of interest. The background and foreground intensity values must be specified in the parameter file.

```
(background <float>)
(foreground <float>)
```

auto_crop Use this option to find the largest bounding box containing all input shapes, and crop all input volumes accordingly. No additional parameters are required.
Note: Works only with binary volumes.

antialias Antialias the binary input volumes. The number of antialiasing iterations can be set in the parameter file. The output of this operation is an image volume containing a distance transform in a narrow band around the binary surface.

```
(antialias_iterations <int>).
```

fastmarching Levelset-based computation of a distance transform volume from a specified isovalue. The isovalue corresponding to the surface of interest in the input volume must be specified in the parameter file using the syntax

```
(fastmarching_isovalue <float>)
```

Note: If fastmarching is carried out after antialiasing, the isovalue should be set to 0.0

blur Gaussian blurring to remove high-frequency artifacts as described in 2.3. The standard deviation (in voxel-space units) for the blurring kernel can be set in the parameter file using the parameter
`(blur_sigma <float>)`.

icp Iterative closest point 3D rigid registration to align two datasets as described in 2.3. If present, icp should be the last option passed to ShapeWorksGroom. The number of ICP iterations can be set in the parameter file using the parameter
`(icp_iterations <int>)`.

5.3 ShapeWorksRun

```
ShapeWorksRun <parameterfile>}
```

An example parameter file is given in Figure 4. The following is a partial list of valid parameters that will affect the optimization.

The input to the particle system is a set of implicit surfaces (e.g. distance transforms).

```
(inputs
"./ExampleData/preprocessed/torus.00.mha"
"./ExampleData/preprocessed/torus.01.mha"
⋮
'./ExampleData/preprocessed/torus.19.mha"
)
```

`number_of_particles <int>`
Specifies the number of particles to be used to represent each shape in the ensemble. If enough initial point positions are supplied for the optimization, then ShapeWorksRun will not conduct a splitting-based initialization phase. If insufficient particle initializations are supplied (or none at all), then ShapeWorksRun will initialize the model as described in Section 2.3 until this number of particles exists on each shape surface.

`iterations_per_split <int>`
Specifies the number of iterations to run between successive particle splits during an initialization phase. This allows the particle system at a given granularity to converge to a stable state before more particles are added.

`checkpointing_interval <int>`
Specifies the number of iterations between successive saves of the optimized correspondence positions (and transforms) to files. One file per shape is written out using the prefix defined by the prefix parameter. These files can be used to visualize the progress of the optimization process using SCIMOgulsView as described Sec. 4. By default, ShapeWorksRun will perform no checkpointing, so it is advisable to specify this parameter.

`output_points_prefix <string>`
Specifies prefix for the correspondence point output files and transform files. Two files per shape are written, one with points in the *local* coordinate frame (`*.ltps`), and one for points in the *common* (or world) coordinate frame (`*.wpts`). Note that statistical analysis should generally be done in the common coordinate frame. See Section 2.3.

`starting_regularization <float>`

`ending_regularization <float>`

`optimization_iterations <float>`
Specify the range for a constant regularization factor that is added to the covariance matrix of the correspondences during the optimization process. This range, along with the number of optimization iterations, define the rate at which the system converges. The starting regularization decays to the ending regularization over the specified number of iterations.

`relative_weighting <float>`
: This is the value of parameter α from Equation 1.

`adaptivity_strength <float>`
: If set to a value greater than zero, this parameter will introduce adaptive oversampling in higher-curvature regions of shapes. Typical parameter settings are from 1.0 to 3.0 and roughly correspond to the relative sampling density desired in the regions of the shape with the highest curvature, versus the regions of the shape surface with the lowest curvature.

`procrustes_interval <int>)`
: If set, ShapeWorks will do a Procrustes registration based on the current correspondence positions at the specified interval. The registration establishes a different *common* coordinate frame for correspondences, but preserves the *local* coordinate frames for each shape sample. See Section 2.3 for more information.

`procrustes_scaling <int>)`
: If set to a value of 1, the Procrustes registration will also normalize with respect to scale. Use this option if you want to analyze shape independently from scale.

5.4 ShapeWorksView

```
ShapeWorksView <parameterfile>
```

ShapeWorksView only requires a list of point files as input. ShapeWorksRun produces point files in both the local and common coordinate frames. Typically, you will want to input the point files from the *common* coordinate frame as inputs to ShapeWorksView (the `*.wpts` files). Point files are specified in the parameter file as follows:

```
(point_files
"./ExampleData/torus.00.wpts"
"./ExampleData/torus.01.wpts"
⋮
"./ExampleData/torus.19.wpts"
)
```

You may optionally also input a set of group IDs for each input file as follows. You must specify one group id per input file. Groups *must* be labeled as either “1” or “2”. Currently, arbitrary group labels are recognized and may cause runtime errors.

```
(group_ids
1
1
⋮
2
2
)
```

ShapeWorksView can also compute a linear regression in shape space with respect to an independent scalar variable. To enable this option, specify the independent variable values in the parameter file as follows. There must be one floating-point value per input file. When regression is indicated, a new menu option will appear under the “View” menu, allowing you to view shape variation along the regression line.

```
(explanatory_variable <float>
<float>
⋮

<float> )
```

5.5 ShapeWorksShop

```
ShapeWorksShop <parameterfile>
```

ShapeWorksShop uses the same basic parameters as ShapeWorksRun. Some options, however, are not controlled through the parameter file, and must be enabled within the ShapeWorksShop interface. ShapeWorksShop is provided in this distribution with limited support, and may be more fully documented in future releases.

5.6 Important Considerations and Known Issues

Image Headers It is important that the image headers for your data contain correct and consistent image information. Pay special attention to the image spacing and origin information, as ShapeWorks software relies heavily on this information.

Setting Parameters The authors highly recommend constructing a downsampled subset of your data to test parameter settings before running full optimizations. Create, for example, five or six test volumes that are no larger then 128^3 pixels, so that a full initialization and optimization can be run in just a few minutes. With a sufficiently small set of data, you can then use the ShapeWorksShop application to initialize particles and test optimization parameters in real time.

Floating-point Numbers in Parameter Files The parser for ShapeWorks parameter files distinguishes between floating-point numbers and integer numbers by the presence or absence of a decimal. For this reason, any parameter that expects a floating-point number must include the decimal (instead of 20, for example, you should enter 20.0).

Aliasing Artifacts The authors highly recommend removing aliasing artifacts in your data, as they can adversly affect the quality of the correspondence optimization.

References

[1] J. Cates, P. Fletcher, M. Styner, H. Hazlett, and R. Whitaker. Particle-based shape analysis of multi-object complexes. In *Proceedings of the 11th International Conference on Medical Image Computing and Computer Assisted Intervention*, page to appear. MICCAI, 2008.

[2] J. Cates, P. Fletcher, and R. Whitaker. Entropy-based particle systems for shape correspondence. In *Mathematical Foundations of Computational Anatomy Workshop*, pages 90–99. MICCAI, 2006.

[3] J. Cates, P. Fletcher, and R. Whitaker. A hypothesis testing framework for high-dimensional shape models. In *Mathematical Foundations of Computational Anatomy Workshop*, pages 170–181. MICCAI, 2008.

[4] J. Cates, P. T. Fletcher, M. Styner, M. Shenton, and R. Whitaker. Shape modeling and analysis with entropy-based particle systems. In *Information Processing in Medical Imaging (IPMI 2007), LNCS 4584*, pages 333–345, 2007.

[5] J. Cates, P. T. Fletcher, Z. Warnock, and R. Whitaker. A shape analysis framework for small animal phenotyping with application to mice with a targeted disruption of hoxd11. In *Proc. 5th IEEE International Symposium on Biomedical Imaging (ISBI '08)*, pages 512–516, 2008.

[6] C. Goodall. Procrustes methods in the statistical analysis of shape. *J. R. Statistical Society B*, 53:285–339, 1991.

[7] M. Hansen and B. Yu. Model selection and the principle of minimum description length. *Journal of the American Statistical Association*, 96(454):746–774, June 2001.

[8] I. Oguz, J. Cates, P. T. Fletcher, Z. Warnock, R. Whitaker, D. Cool, S. Aylward, and M. Styner. Cortical correspondence using entropy-based particle systems and local featrues. In *Proc. 5th IEEE International Symposium on Biomedical Imaging (ISBI '08)*, pages 1637–1640, 2008.