Mathematics and Visualization

Series editors

Hans-Christian Hege David Hoffman Christopher R. Johnson Konrad Polthier Martin Rumpf More information about this series at http://www.springer.com/series/4562

Julien Tierny

Topological Data Analysis for Scientific Visualization



Julien Tierny CNRS, Sorbonne Université, LIP6 Department of Scientific Computing Paris. France

ISSN 1612-3786 ISSN 2197-666X (electronic)
Mathematics and Visualization
ISBN 978-3-319-71506-3 ISBN 978-3-319-71507-0 (eBook)
https://doi.org/10.1007/978-3-319-71507-0

Library of Congress Control Number: 2017960812

Mathematics Subject Classification (2010): 68U01

© Springer International Publishing AG 2017

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Any problem which is non-linear in character, which involves more than one coordinate system or more than one variable, or where structure is initially defined in the large, is likely to require considerations of topology and group theory for its solution.

In the solution of such problems classical analysis will frequently appear as an instrument in the small, integrated over the whole problem with the aid of topology or group theory.

Marston Morse [87]



Preface

This book is adapted from my habilitation thesis manuscript, which reviewed my research work since my Ph.D. thesis defense (2008), as a postdoctoral researcher at the University of Utah (2008–2010) and a permanent CNRS researcher at Telecom ParisTech (2010–2014) and at Sorbonne Universités UPMC (2014-present).

This book presents results obtained in collaboration with several research groups (University of Utah, Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, Universidade de Sao Paulo, New York University, Sorbonne Universités, Clemson University, University of Leeds) as well as students whom I informally or formally advised.

This research has been partially funded by several grants, including a Fulbright fellowship (US Department of State), a Lavoisier fellowship (French Ministry for Foreign Affairs), a Digiteo grant (national funding, "Uncertain Topo-Vis" project 2012-063D, Principal Investigator), an ANR grant (national funding, "CrABEx" project ANR-13-CORD-0013, local investigator), a CIFRE partnership with Renault, a CIFRE partnership with Kitware, a CIFRE partnership with Total, and a BPI grant (national funding, "AVIDO" project, local investigator).

During this period, I taught regularly at the University of Utah (2008–2010), Telecom ParisTech (2011–present), Sorbonne Universités (2011–present), and since 2013 at ENSTA ParisTech and University of Versailles, where I am the head instructor for the scientific visualization course.

This book describes most of the results published over this period (Chap. 3: [118, 125], Chap. 4: [63, 125, 128], Chap. 5: [16, 17, 55, 101], Chap. 6: [21, 56–58, 74, 117, 130]). I refer the interested reader to the following publications [12, 49, 50, 52, 80, 83, 95, 96, 107, 108, 111–113, 119–124, 126, 127, 132, 133] for additional results not described in this document.

The reading of this book only requires a basic background in computer science and algorithms; most of the mathematical notions are introduced in a dedicated chapter (Chap. 2).

Paris, France October 2017

Julien Tierny

Acknowledgements

First, I would like to express my gratitude to the editors of the Springer's series *Mathematics and Visualization*, who gave me the opportunity to publish this book. I am sincerely grateful to Isabelle Bloch, Jean-Daniel Fekete, Pascal Frey, Hans Hagen, Chris Johnson, Bruno Lévy, Philippe Ricoux, and Will Schroeder, who did me the honor of accepting to be part of my habilitation committee. I am especially thankful to the reviewers of the manuscript for accepting this significant task.

Second, I would like to thank all my collaborators over the last 8 years. The results presented in this book would not have been possible without them. Since my Ph.D. defense, I had the opportunity to work with more than 50 coauthors, and I like to think that I learned much from each one of them. More specifically, I would like to thank some of my main collaborators (in alphabetical order), hoping the persons I forgot to mention will forgive me: Timo Bremer, Hamish Carr, Joel Daniels, Julie Delon, Tiago Etiene, Attila Gyulassy, Pavol Klacansky, Josh Levine, Gustavo Nonato, Valerio Pascucci, Joseph Salmon, Giorgio Scorzelli, Claudio Silva, Brian Summa, Jean-Marc Thiery. Along the years, some of these persons became recurrent collaborators with whom I particularly enjoyed working and interacting. Some of them even became close friends (even best men!) and I am sincerely grateful for that. Special thanks go to Valerio Pascucci, who gave me a chance back in 2008 when he hired me as a postdoc, although we had never met before. I have no doubt that my career path would have been very different if we had not worked together. Working with Valerio and his group has been a real pleasure and a source of professional and personal development. I am both glad and proud to be able to say that our collaboration lasted well beyond my stay at the University of Utah and that it still continues today. Along the last 8 years, Valerio has been a careful and inspiring mentor and I am sincerely grateful for that.

Next, I would like to thank all of the colleagues I had the chance to interact with at the University of Utah, Telecom ParisTech, and Sorbonne Universités UPMC, in particular my students, who are a daily source of motivation.

Finally, I would like to thank my friends, my family, my wife, and my daughter for their constant love and support.

Contents

1	Intr	troduction					
2	Background						
	2.1	Data I	Representation	3			
		2.1.1	Domain Representation	3			
		2.1.2	Range Representation	11			
	2.2	Topole	ogical Abstractions	14			
		2.2.1		15			
		2.2.2	Notions of Persistent Homology	18			
		2.2.3	Reeb Graph	21			
		2.2.4	Morse-Smale Complex	25			
	2.3	Algor	ithms and Applications	27			
		2.3.1	Persistent Homology	27			
		2.3.2	Reeb Graph	28			
		2.3.3	Morse-Smale Complex	30			
3	Abs	bstraction					
	3.1	Efficie	ent Topological Simplification of Scalar Fields	35			
		3.1.1	Preliminaries	37			
		3.1.2	Algorithm	41			
		3.1.3	Results and Discussion	46			
	3.2			52			
		3.2.1	Preliminaries	53			
		3.2.2	Algorithm	57			
		3.2.3	Results and Discussion	62			
4	Inte	Interaction					
	4.1	Topole	ogical Simplification of Isosurfaces	67			
	4.2						
		4.2.1		71			
		4.2.2	Reeh Graph Editing	79			

xiv Contents

5	Analysis					
	5.1	Exploration of Turbulent Combustion Simulations				
		5.1.1	Applicative Problem	91		
		5.1.2	Algorithm	93		
		5.1.3	Results	96		
	5.2	itative Analysis of Molecular Interactions	101			
		5.2.1	Applicative Problem	101		
		5.2.2	Algorithm	105		
		5.2.3	Results	113		
6	Perspectives					
	6.1	Emerging Constraints		120		
		6.1.1	Hardware Constraints	120		
		6.1.2	Software Constraints	123		
		6.1.3	Exploration Constraints	125		
	6.2	6.2 Emerging Data Types		126		
		6.2.1	Multivariate Data	126		
		6.2.2	Uncertain Data	132		
7	Conclusion					
Re	eferer	ices		141		
Index						

Notations

\mathbb{X}	Topological space
\mathbb{Z}	Boundary of a topological space
\mathbb{M}	Manifold
\mathbb{R}^d	Euclidean space of dimension d
σ, τ	<i>d</i> -simplex, face of a <i>d</i> -simplex
v, e, t, T	Vertex, edge, triangle, and tetrahedron
$Lk(\sigma)$, $St(\sigma)$	Link and star of a simplex
$Lk_d(\sigma)$, $St_d(\sigma)$	d-simplices of the link and the star of a simplex
K	Simplicial complex
T	Triangulation Triangulation
M	Piecewise linear manifold
eta_i	<i>i</i> -th Betti number
χ	Euler characteristic
$lpha_i$	<i>i</i> th barycentric coordinates of a point p relatively to a simplex σ
$f: \mathscr{T} \to \mathbb{R}$	Piecewise linear scalar field
∇f	Gradient of a PL scalar field f
$Lk^{-}(\sigma), Lk^{+}(\sigma)$	Lower and upper link of σ relatively to f
o(v)	Memory position offset of the vertex v
$\mathscr{L}^{-}(i), \mathscr{L}^{+}(i)$	Sub- and sur-level set of the isovalue i relatively to f
$\mathscr{D}(f)$	Persistence diagram of f
$\mathscr{C}(f)$	Persistence curve of <i>f</i>
$\mathscr{R}(f)$	Reeb graph of f
• /	
$l(\mathcal{R}(f))$	Number of loops of $\mathcal{R}(f)$
$\mathcal{T}(f)$	Contour tree of f
$\mathcal{J}(f), \mathcal{S}(f)$	Join and split trees of f
$\mathscr{MS}(f)$	Morse-Smale complex of f