

# **Interactive GPU-based Visualization of Large Dynamic Particle Data**

# Synthesis Lectures on Visualization

## Editors

**Niklas Elmqvist**, *University of Maryland*

**David S. Ebert**, *Purdue University*

Synthesis Lectures on Visualization publishes 50- to 100-page publications on topics pertaining to scientific visualization, information visualization, and visual analytics. Potential topics include, but are not limited to: scientific, information, and medical visualization; visual analytics, applications of visualization and analysis; mathematical foundations of visualization and analytics; interaction, cognition, and perception related to visualization and analytics; data integration, analysis, and visualization; new applications of visualization and analysis; knowledge discovery management and representation; systems, and evaluation; distributed and collaborative visualization and analysis.

## Interactive GPU-based Visualization of Large Dynamic Particle Data

Martin Falk, Sebastian Grottel, Michael Krone, and Guido Reina

2016

## Semantic Interaction for Visual Analytics: Inferring Analytical Reasoning for Model Steering

Alexander Endert

2016

## Design of Visualizations for Human-Information Interaction: A Pattern-Based Framework

Kamran Sedig and Paul Parsons

2016

## Image-Based Visualization: Interactive Multidimensional Data Exploration

Christophe Hurter

2015

## Interaction for Visualization

Christian Tominski

2015

## Data Representations, Transformations, and Statistics for Visual Reasoning

Ross Maciejewski

2011

# A Guide to Visual Multi-Level Interface Design From Synthesis of Empirical Study Evidence

Heidi Lam and Tamara Munzner  
2010

© Springer Nature Switzerland AG 2022

Reprint of original edition © Morgan & Claypool 2017

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means—electronic, mechanical, photocopy, recording, or any other except for brief quotations in printed reviews, without the prior permission of the publisher.

Interactive GPU-based Visualization of Large Dynamic Particle Data

Martin Falk, Sebastian Grottel, Michael Krone, and Guido Reina

ISBN: 978-3-031-01476-5      paperback

ISBN: 978-3-031-02604-1      ebook

DOI 10.1007/S00731ED1V01Y201608VIS008

A Publication in the Springer series

*SYNTHESIS LECTURES ON VISUALIZATION*

Lecture #8

Series Editors: Niklas Elmqvist, *Yahoo! Labs*

David S. Ebert, *Purdue University*

Series ISSN

Print 2159-516X    Electronic 2159-5178

# Interactive GPU-based Visualization of Large Dynamic Particle Data

Martin Falk

Linköping University, Sweden

Sebastian Grottel

Technische Universität Dresden, Germany

Michael Krone

University of Stuttgart, Germany

Guido Reina

University of Stuttgart, Germany

*SYNTHESIS LECTURES ON VISUALIZATION #8*

## ABSTRACT

Prevalent types of data in scientific visualization are volumetric data, vector field data, and particle-based data. Particle data typically originates from measurements and simulations in various fields, such as life sciences or physics. The particles are often visualized directly, that is, by simple representants like spheres. Interactive rendering facilitates the exploration and visual analysis of the data. With increasing data set sizes in terms of particle numbers, interactive high-quality visualization is a challenging task. This is especially true for dynamic data or abstract representations that are based on the raw particle data.

This book covers direct particle visualization using simple glyphs as well as abstractions that are application-driven such as clustering and aggregation. It targets visualization researchers and developers who are interested in visualization techniques for large, dynamic particle-based data. Its explanations focus on GPU-accelerated algorithms for high-performance rendering and data processing that run in real-time on modern desktop hardware. Consequently, the implementation of said algorithms and the required data structures to make use of the capabilities of modern graphics APIs are discussed in detail. Furthermore, it covers GPU-accelerated methods for the generation of application-dependent abstract representations. This includes various representations commonly used in application areas such as structural biology, systems biology, thermodynamics, and astrophysics.

## KEYWORDS

particles, visualization, GPU, molecules, rendering, visual analysis, object/image space methods, glyph rendering, atomistic visualization

# Contents

	<b>Acknowledgments</b> .....	<b>ix</b>
	<b>Figure Credits</b> .....	<b>xi</b>
<b>1</b>	<b>Introduction</b> .....	<b>1</b>
1.1	Scope of this Lecture .....	1
1.1.1	Base-line Rendering .....	4
1.1.2	Higher-level Structure .....	5
1.2	Related Topics Beyond the Scope .....	5
<b>2</b>	<b>History</b> .....	<b>7</b>
<b>3</b>	<b>GPU-based Glyph Ray Casting</b> .....	<b>11</b>
3.1	Fragment-based Ray Casting .....	12
3.2	Silhouette Approximation .....	16
3.2.1	Bounding Boxes .....	17
3.2.2	Spheres .....	20
3.3	Geometry Generation .....	22
3.3.1	Bounding Box .....	22
3.3.2	Quad Primitive .....	23
3.3.3	Point Primitive .....	24
3.3.4	GPU-side Generated Quad Primitive .....	25
<b>4</b>	<b>Acceleration Strategies</b> .....	<b>29</b>
4.1	Optimized Data Upload .....	30
4.1.1	Vertex Arrays .....	30
4.1.2	Vertex Buffer Objects .....	32
4.1.3	Shader Storage Buffer Objects .....	35
4.2	Support Geometry Generation .....	40
4.3	Particle Culling Techniques .....	42
4.3.1	Occlusion Queries for Gridded Data .....	42
4.3.2	Manual Early-Z Test .....	46

<b>5</b>	<b>Data Structures</b>	<b>49</b>
5.1	Uniform Grids for Molecular Dynamics Data	49
5.1.1	Template-based Instancing	50
5.1.2	Algorithm	51
5.2	Hierarchical Data Structures	58
5.2.1	Implicit Hierarchy	59
5.2.2	Position Coordinate Quantization	61
<b>6</b>	<b>Efficient Nearest Neighbor Search on the GPU</b>	<b>65</b>
<b>7</b>	<b>Improved Visual Quality</b>	<b>71</b>
7.1	Deferred Shading	72
7.2	Ambient Occlusion	74
<b>8</b>	<b>Application-driven Abstractions</b>	<b>83</b>
8.1	Spline Representations	84
8.2	Particle Surfaces	90
8.3	Clustering and Aggregation	95
<b>9</b>	<b>Summary and Outlook</b>	<b>99</b>
	<b>Bibliography</b>	<b>101</b>
	<b>Authors' Biographies</b>	<b>109</b>



# Acknowledgments

This book is the result of more than a decade of active research. We have been supported by many people over the years, but we want to especially thank our common Ph.D. adviser, Professor Dr. Thomas Ertl, for support. We also want to thank our colleagues for their support and fruitful discussions as well as the undergraduate students supporting our work with theirs. Finally, our particular appreciation goes to the funding agencies that made this possible. The respective projects and agencies are, in no particular order:

- Landesstiftung Baden-Württemberg Project 688, “Massiv parallele molekulare Simulation und Visualisierung der Keimbildung in Mischungen für skalenübergreifende Modelle” (2004–2005)
- German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) collaborative research center SFB 716 as subprojects D.3 and D.4 (2007–2018)
- German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) Cluster of Excellence in Simulation Technology (EXC 310/1) (2008–2013)
- Centre Systems Biology in Stuttgart, Germany (2007–2010)
- Excellence Center at Linköping and Lund in Information Technology (ELLIIT) (2013–2015)
- Swedish e-Science Research Centre (SeRC) (2013–present)
- Federal Ministry of Education and Research (BMBF) Project No. 01IS14014, Scalable Data Services And Solutions (ScaDS, 2014–present)
- European Social Fund (ESF) Project No. 100098171, Visual and Interactive Cyber-physical Systems Control and Integration (VICCI, 2012–2014)

Martin Falk, Sebastian Grottel, Michael Krone, and Guido Reina  
September 2016

# Figure Credits

- Figure 1.1** From: S. Grottel, P. Beck, C. Müller, G. Reina, J. Roth, H.-R. Trebin, and T. Ertl. Visualization of Electrostatic Dipoles in Molecular Dynamics of Metal Oxides. *IEEE Transactions on Visualization and Computer Graphics*, 18(12):2061–2068, 2012a. Copyright © 2012 IEEE. Used with permission.
- Figure 1.2** Courtesy of Mathieu Le Muzic.
- Figure 2.3** From: A. Knoll, Y. Hijazi, A. Kensler, M. Schott, C. Hansen, and H. Hagen. Fast Ray Tracing of Arbitrary Implicit Surfaces with Interval and Affine Arithmetic. *Computer Graphics Forum*, 28(1):26–40, 2009. Copyright © 2009 John Wiley & Sons, Inc. Used with permission.
- Figure 3.3** From: S. Grottel, G. Reina, and T. Ertl. Optimized Data Transfer for Time-dependent, GPU-based Glyphs. In *IEEE Pacific Visualization Symposium (PacificVis 2009)*, pages 65–72, 2009a. Copyright © 2009 IEEE. Used with permission.
- Figure 5.7** From: M. Le Muzic, J. Parulek, A. Stavrum, and I. Viola. Illustrative visualization of molecular reactions using omniscient intelligence and passive agents. *Computer Graphics Forum*, 33(3):141–150, 2014. ISSN 1467-8659. Copyright © 2014 John Wiley & Sons, Inc. Used with permission.
- Figure 5.8** Courtesy of Mathieu Le Muzic.
- Figure 5.9** Courtesy of Mathieu Le Muzic.
- Figure 5.10** Based on: M. Hopf and T. Ertl. Hierarchical splatting of scattered data. In *IEEE Visualization 2003*, 2003.
- Figure 5.11** From: M. Hopf and T. Ertl. Hierarchical splatting of scattered data. In *IEEE Visualization 2003*, 2003. Copyright © 2003 IEEE. Used with permission.
- Figure 5.12** From: M. Hopf and T. Ertl. Hierarchical splatting of scattered data. In *IEEE Visualization 2003*, 2003. Copyright © 2003 IEEE. Used with permission.

- Figure 7.4** From: S. Grottel, G. Reina, C. Dachsbacher, and T. Ertl. Coherent Culling and Shading for Large Molecular Dynamics Visualization. *Computer Graphics Forum*, 29(3):953–962, 2010a. Copyright © 2010 John Wiley & Sons, Inc. Used with permission.
- Figure 8.6** From: K. Bidmon, S. Grottel, F. Bös, J. Pleiss, and T. Ertl. Visual Abstractions of Solvent Pathlines near Protein Cavities. *Computer Graphics Forum*, 27(3):935–942, 2008. Copyright © 2008 John Wiley & Sons, Inc. Used with permission.
- Figure 8.7** From: S. Grottel, G. Reina, J. Vrabec, and T. Ertl. Visual Verification and Analysis of Cluster Detection for Molecular Dynamics. *IEEE Transactions on Visualization and Computer Graphics*, 13(6):1624–1631, 2007. ISSN 1077-2626. Copyright © 2007 IEEE. Used with permission.
- Figure 8.8** From: T. Ertl, M. Krone, S. Kesselheim, K. Scharnowski, G. Reina, and C. Holm. Visual Analysis for Space-Time Aggregation of Biomolecular Simulations. *Faraday Discussions*, 169:167–178, 2014. ISSN 1364-5498. Copyright © 2014 Royal Society of Chemistry. Used with permission.