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Inria Saclay Centre at Institut Polytechnique de Paris

IN PARTNERSHIP WITH:

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2024
ACTIVITY REPORT

Project-Team

GEOMERIX

Geometry-driven Numerics

IN COLLABORATION WITH: Laboratoire d'informatique de l'école polytechnique (LIX)

DOMAIN

Perception, Cognition and Interaction

THEME

Interaction and visualization

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Project-Team GEOMERIX

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Keywords

Computer sciences and digital sciences

A3.4.1. – Supervised learning

A3.4.2. – Unsupervised learning

A3.4.4. – Optimization and learning

A3.4.6. – Neural networks

A5.5. – Computer graphics

A5.5.1. – Geometrical modeling

A5.5.4. – Animation

A6.1.4. – Multiscale modeling

A6.1.5. – Multiphysics modeling

A6.2.5. – Numerical Linear Algebra

A6.2.6. – Optimization

A6.2.8. – Computational geometry and meshes

A6.5.1. – Solid mechanics

A6.5.2. – Fluid mechanics

A8.3. – Geometry, Topology

A8.7. – Graph theory

A8.12. – Optimal transport

A9.2. – Machine learning

Other research topics and application domains

B9.2.2. – Cinema, Television

B9.2.3. – Video games

B9.5.1. – Computer science

B9.5.2. – Mathematics

B9.5.3. – Physics

B9.5.5. – Mechanics

B9.5.6. – Data science

1 Team members, visitors, external collaborators

Research Scientists

- Steve Oudot [Team leader, INRIA, Senior Researcher]
- Jiong Chen [INRIA, Researcher, from Oct 2024]
- Jiong Chen [INRIA, Starting Research Position, until Sep 2024]
- Mathieu Desbrun [INRIA, Senior Researcher]
- Pooran Memari [CNRS, from Jun 2024]

Faculty Member

- Maksims Ovsjanikovs [LIX, from Jul 2024]

Post-Doctoral Fellows

- Maysam Behmanesh [ECOLE POLY PALAISEAU, from Apr 2024]
- Anouar Abdeldjaoued Ferfache [INRIA, Post-Doctoral Fellow, until Aug 2024]
- Mark Gillespie [INRIA, Post-Doctoral Fellow, from Sep 2024]
- Roman Klokov [ECOLE POLY PALAISEAU, from Feb 2024 until Oct 2024]
- Vincent Mallet [FX CONSEIL, from Feb 2024]
- Emery Pierson [LIX]

PhD Students

- Souhaib Attaiki [LIX, until Mar 2024]
- Nasim Bagheri Shouraki [IP PARIS, from Oct 2024]
- Theo Braune [ECOLE POLY PALAISEAU]
- Diego Gomez [ECOLE POLY PALAISEAU, until Sep 2024]
- Souhail Hadgi [ECOLE POLY PALAISEAU]
- Jingyi Li [IP PARIS]
- Robin Magnet [LIX, from Feb 2024 until May 2024]
- Leopold Maillard [DASSAULT SYSTEMES]
- Julie Mordacq [Ministère des Armées]
- Tim Scheller [ECOLE POLY PALAISEAU]

Interns and Apprentices

- Adrien Lanne [INRIA, Intern, from May 2024 until Oct 2024]
- Garance Perrot [ECOLE POLY PALAISEAU, Intern, until Mar 2024]
- Aristotelis Siozopoulos [ECOLE POLY PALAISEAU, Intern, from Jul 2024]

Administrative Assistant

- Michael Barbosa [INRIA]

Visiting Scientists

- Diana Marin [UNIV VIENNE, until Apr 2024]
- Matteo Pegoraro [UNIV AALBORG, until Feb 2024]
- Shreyas Samaga [Purdue University]

2 Overall objectives

Historical context. Geometry has been a unifying formalism for science: predictive models of the world around us have often been derived using geometric notions which formalize observable symmetries and experimental invariants. Tools such as differential geometry and tensor calculus quickly became invaluable in describing the complexity of natural phenomena and mechanical systems through concise equations, condensing local and global properties into simple relations between measurable quantities. Today, geometry (be it Euclidean or not) is at the core of many current physical theories: general relativity, electromagnetism (E&M), gauge theory, quantum mechanics, as well as solid and fluid mechanics, all have strong underlying structures that are best described and elucidated through geometric notions like differential forms, curvatures, vector bundles, connections, and covariant derivative. Geometry also creeps up in unexpected fields such as number theory and functional analysis, offering new insights and even breakthroughs, e.g., the use of algebraic geometry to address Fermat's last theorem.

Geometry in Digital Sciences. In sharp contrast, the role of geometry was mostly ignored at the inception of computer science. Yet, it has now become clear that digital sciences are imbued with an overwhelming amount of fundamentally geometric and topological concepts. Some are rather obvious, when dealing with the modeling of Euclidean shapes in computer graphics or the analysis of images in computer vision for instance; some are more subtle, such as the "manifold hypothesis" underlying a number of supervised or unsupervised learning techniques; and some are only nascent, such as the fields of Information Geometry (basically, the geometry used to understand probability distributions), Geometric Statistics (new statistical methodology for non-Euclidean entities), and Topological Data Analysis (where algebraic topology is used as a tool to enhance data analysis pipelines). In fact, even the discretization of physical theories needed to offer fast numerical simulation has brought geometry back to the forefront after it was understood that the loss of numerical fidelity in standard numerical methods is due to a fundamental failure to preserve geometric or topological structures of the underlying continuous models: partial differential equations (PDEs) modeling our physical world are typically encoding invariants and structures that are independent of the choice of coordinates used to express the equations and the tensors involved in them; but invariance to the choice of basis is often lost during discretization, as numerical approximations will in general not capture, let alone preserve, the key geometric structures that exist in the continuous case. Seeing these numerical issues through the lens of geometry is thus not just of academic interest: failure to maintain geometric invariants has serious consequences for the accuracy and stability of solutions.

Rationale. Given the unusual reach of geometry and its rich literature, there is an opportunity to assemble a team of experts in geometry and its vernacular, to help broadly impact digital science and technology. We thus propose the creation of a **new project-team whose core scientific mission is to use geometry as a bedrock for the development of numerical tools and algorithms**: we wish to exploit the properties of infinite-dimensional and finite-dimensional spaces that are related with distance, shape, size, and relative position, and bringing them to bear on *computational discretizations and algorithms for analysis, processing, and simulation.* Adhering to geometric structures and invariants as a guiding principle for computations is a rich source of both theoretical and practical challenges, allowing to combine concepts and results from different areas of geometry broadly construed to produce new computational tools with solid mathematical foundations. While our team will be very focused in terms of the mathematical foundations and tools upon which it builds, it will also be very broad in terms of applications given the pervasiveness of geometry in sciences and technology. This makes for an unusual, yet powerful scientific setup that will facilitate interdisciplinary projects through the common use of geometric foundations and their specialized terminology. It will also allow us to contribute sporadically to pure and computational mathematics when appropriate in order to push our scientific mission forward.

Positioning. We see GeomeriX as first and foremost Inria Saclay's graphics team, but with wider objectives afforded by the broad relevance of geometry. It is worth noting that graphics has evolved to the point where it often intersects with applied mathematics, machine learning, vision, and computational science in some of its efforts, and GeomeriX intends to continue this trend.

Objectives. Our project-team's overall scientific objective is to contribute, through a geometric perspective, both foundational and practical methods for geometric data processing. In particular, we seek the development of predictive computational tools by drawing from the many facets of geometry and topology: whether it be *discrete geometry, basic differential geometry or exterior calculus, symplectic geometry, persistent homology or sheaf theory, optimal transport, Riemannian or conformal geometry*, these topics of geometry inform and guide both our discretizations and algorithmic designs towards computing. Note that we do not plan to merely adapt and exploit geometric concepts and understanding for numerical purposes, as our focus on digital data may even result in contributions to these mathematical fields, extending the current body of knowledge. While we intentionally leave the range of our mathematical foundations open so as not to restrict our potential team-wide explorations, **we concentrate our research on four concrete themes, which we believe can be most significantly impacted by a geometric approach to developing new numerical tools**:

① **Euclidean shape processing**: from computer graphics to geometry processing and vision, the analysis and manipulation of low-dimensional shapes (2D and 3D) is an important endeavor with applications covering a wide range of areas from entertainment and classical computer-aided design, to reverse engineering and biomedical engineering. Our project-team intends to lead efforts in this competitive field, with key contributions in shape matching, geometric analysis, and discrete calculus on meshes.

② **Simulation**: traditional finite-element treatments of various physical models have had tremendous success. Recently, a number of geometric integrators have upended the field, either through structure-preserving integration which offers improved statistical predictability by respecting the geometric properties of the exact flow of the differential equations, or through novel discretizations of the state space. We intend to continue introducing novel integration methods for increasingly complex multiphysics systems, as well as exploiting the use of learning methods to accelerate simulation.

③ **Dynamical systems**: we intend to leverage the geometric nature of dynamical systems to investigate and promote high-dimensional data analysis for dynamics: the study of dynamical systems from a limited number of observations of the state of a given system (for example, time series or a sparse set of trajectories) offers a unique opportunity to develop scalable computational tools to detect or characterize unusual features and coherent structures. Meanwhile, the study of dynamical systems from a combinatorial point of view opens up the possibility of characterizing their invariant sets and assessing their stability.

④ **Data science**: finally, we are intent on exploring the underlying role of geometry in machine learning and statistical analysis. This role has been put forward in the recent years, with the emergence of approaches such as geometric deep learning or topological data analysis, whose aim is to leverage the underlying geometry or topology of the data to enhance the performance, robustness, or explainability of the methods used for their analysis. We will pursue investigations toward this goal, concentrating our efforts on topics related to explainable feature design, geometric feature learning, geometry-driven learning, and geometry for categorical and mixed data types.

Evidently, our research efforts may at times lie across multiple of these themes given our multidisciplinary objectives, and it is our hope that we will all eventually participate in the four themes.

3 Research program

Below we introduce the details of our four research themes, in four separate subsections. In each subsection, we first present the scientific focus and research objectives of the corresponding theme, then we detail the research topics we intend to address and how we plan to leverage topology and geometry for each one of them. For each theme, we list the most likely contributors, and organize the various subtopics within each theme from short to long-term goals, based on our current expectations and focus.

3.1 Geometry for Euclidean shape processing

Euclidean space is the default setting of classical geometry in two or three dimensions. Shapes in 3D space are of particular interest as they represent the typical objects we interact with. **Geometry processing** is an area of research focusing on these low-dimensional shapes in Euclidean space, with the goal to design algorithms, data structures, as well as analysis tools for their digital acquisition, reconstruction, analysis, manipulation, synthesis, classification, transmission, and animation. Digital shapes are typically discretized through either point clouds, triangle meshes, or polygonal meshes for surfaces, and through tetrahedron or polytopal meshes for volumes. Analyzing and manipulating these digital representations already involve fundamental difficulties in terms of efficiency, scalability, and robustness to arbitrary sampling, for which computational geometry and computer graphics have generated a number of key algorithms. Simple surface meshes in 3D also offer a simple context in which to define discrete notions of basic topological properties (quantities preserved through arbitrary stretching, such as Euler characteristic, genus, Betti numbers, etc) and relevant geometric properties (normal, curvatures, covariant derivatives, parallel transport, etc). Yet the digital counterpart of the low-dimensional case of Euclidean geometry is far from being settled or complete: it remains obviously relevant in a number of scientific fields on which we plan to focus. A few research directions of particular interest are described below.

Operator-based methods for shape analysis We plan to develop novel approaches for representing and manipulating geometric concepts as *linear functional operators*. Specifically we will focus on tools for shape matching, design and analysis of differential quantities such as vector fields or cross fields, shape deformation and shape comparison, where functional approaches have recently been shown to provide a natural and discretization-agnostic representation [122, 55, 56, 132]. This "functional" point of view is classical in many scientific areas, including **dynamical systems** (where the pullback with respect to a map is closely related to the Koopman or composition operator, allowing the study ergodicity or mixing property of non-linear maps through the spectral properties of a linear operator), **differential geometry** (where vector fields are often defined by their action on real-valued functions) and **representation theory** among others. However, it has only recently been adopted in geometry processing with tremendous and constantly growing potential in both axiomatic or even learning-based approaches [110, 100, 83]. We will continue developing efficient and robust algorithms by considering shapes as functional spaces and by representing various geometric operations as linear operators acting on appropriate real-valued functions. In addition to the efficiency and robustness of methods obtained by considering this linear operator point of view of geometry processing and dynamical systems, another very significant advantage of these techniques is that they allow to express many different geometric operations in a common language. This means, for example, that it makes it easy to define the pushforward of a vector field with respect to a map by simply considering a composition of appropriate discrete operators. Despite the significant recent success of tools within this area, especially related to the functional map framework [123], there does not exist a unified coherent theoretical framework in which different geometric concepts can be represented and manipulated via their functional equivalents. Our main long-term goal therefore would be to establish a novel field within geometry processing by creating both a computational framework and a coherent theoretical formalism in which *all* of the different basic geometric operations can be expressed, and thus in which different concepts can "communicate" with one another. We believe that such a formalism and associated computational tools, already quite well developed, will not only greatly extend the scope of applicability of many existing geometry processing pipelines, but will also help expand this language to novel concepts, and ultimately help pave the way towards representation-agnostic geometric data manipulation.

Discrete metrics and applications. While three-dimensional shapes are often encoded via their Euclidean embedding, numerous research efforts have focused on studying and discretizing their intrinsic metric. Regge calculus [130], an early approach to numerical relativity without coordinates, proposed the use of edge lengths to encode a piecewise-Euclidean metric per simplex, from which the Riemann curvature tensor can be easily computed to derive local areas or curvatures. This early work led to a series of alternative metric representations: tip angles, for instance, are known to encode the intrinsic geometry of a triangle mesh up to a scaling, while local measurements (an angle [131] or a length cross-ratio [113] per edge) later formed the basis of circle patterns [59, 105] as well as conformal representations [137]; the discrete Laplace-Beltrami cotan formula [126] also determines the edge lengths of a triangle mesh (and thus its discrete metric) up to a global scaling [149]. More recently, generalized notions of metrics were proposed; for instance, [97] presented a characterization of an augmented discrete metric resulting from the orthogonal primal-dual structure of weighted triangulations. Common to many of these various metric characterizations is the existence of convex energies which allow to efficiently compute these metrics from various boundary conditions. We intend to investigate the discrete treatment of metric for low-dimensional manifolds as a counterpart to the discretization of antisymmetric tensors (differential forms), which is far less studied — and a discrete theory unifying symmetric and anti-symmetric tensors remains elusive despite recent advances [96]. Moreover, the metric of a surface is known in the continuous realm to induce Hodge stars and a canonical torsion-free Levi-Civita connection (or parallel transport), but this picture is far less clear for discrete manifolds, even if the construction of arbitrary-order discrete Hodge stars and metric connections are well understood by now. A few research directions on generalized metrics seem particularly interesting due to their likelihood of resulting in novel algorithmic and computational frameworks:

- *Metric-dependent meshing:* Given a set of metric-based operators, optimized mesh structures can be designed to offer optimal accuracy akin to Hodge-star mesh optimization for the augmented weighted metric proposed in [119]. Another interesting research question is the existence and construction of intrinsic Delaunay triangulation, the most common discrete shape representation, with respect to a particular metric [60].
- *Metric-aware sampling:* Metric-dependent descriptors such as the pair correlation function are particularly efficient in characterizing statistical properties of point distributions for texture synthesis [84]. Extending this framework to arbitrary non-flat domains through Multi-Dimensional Scaling (MDS) seem particularly promising.
- *Shape characterization:* Highly convoluted embeddings like the cortical surface of the brain and its functional connectivity graph are naturally hyperbolic in nature [65]. However, investigating a link between cortical folding and the volumetric fiber bundle structure from a pure geometric viewpoint through a hyperbolic metric characterization has surprisingly not be done in brain analysis, despite striking visual similarities between brain folding and geometric realizations of the hyperbolic plane (see [142] and Taimiņa's crochet model). We are hoping that this intrinsic metric characterization can be investigated through recent discrete hyperbolic parametrization tools [92], which may also lead to other shape classification techniques in more general contexts.
- *Piecewise-linear maps:* We also wish to study the classification of the deformation of a triangle mesh through its induced metric change in the embedding space. Developing an approach to decompose such a diffeomorphic piecewise-linear map into canonical geometric transformations through either linear algebra or convex minimization could offer new discrete equivalences for conformal, equiareal, and curvature-preserving maps between triangulations, with direct applications to mesh parameterization and more general processing of discrete meshes.
- *Geodesic abstractions:* curve-network representations [95] based on a few geodesics to describe a shape provide a compact encoding of surfaces. While it is increasingly useful for artistic depictions, we also want to study its relevance as a compact compression scheme from which the shape and its metric can be derived with controllable precision.

- *Metric-dependent cage*: Finally, we also want to understand how to define optimized metric-dependent cages for intuitive & expressive deformation and animation of complex shapes [140], and how these cages can be understood as polygonal or polyhedral cells to locally simplify a simplicial complex.

Discrete differential and tensor calculus. When working on low-dimensional spaces, the use of meshes (as opposed to just point clouds) pays dividends as it allows for the development of discrete versions of Exterior Calculus (see DEC [79] or FEEC [53]), where k-dimensional integrals can be directly evaluated in k-cells, and differentiation can formally achieved through the boundary operator: the concept of chains and cochains from algebraic topology forms the basis of a discrete analog of Cartan's exterior calculus of differential forms, providing crucial numerical tools such as a discrete de Rham cohomology and a discrete Helmholtz-Hodge decomposition that precisely mimick their continuous counterparts. Moreover, finite elements of arbitrary order can be associated with these discrete forms through subdivision [94] to provide a powerful Isogeometric Analysis (IGA). Recent developments [111, 93] have offered also a discrete approach to tangent vector fields. While DEC encodes vector fields as 1-forms, processing tangent vectors and, more generally, directional fields sampled at vertices of discrete surfaces requires the development of *discrete (metric) connections* [76, 111] (which can be seen as discrete equivalent to the Christoffel symbols) to handle the non-linearity of non-flat domains. From these connections can be derived the usual continuous notions of covariant derivatives or Killing operator, and these discrete operators demonstrate the same intimate link between geometry and topology as exemplified by the hairy ball theorem (Hopf index theorem). While these operators apply equally well on discrete three-manifolds, much remains to do: properly defining the notion of curvature matrix-valued 2-form or torsion vector-valued 2-form in 3D and checking that these definitions provide consistent Bianchi identities (i.e., there exists an exterior covariant derivative satisfying fundamental geometric and topological properties) is an exciting research direction. Not only will it allow to deal with the line singularities in hexahedral meshing *robustly*, but it will also provide a Bochner Laplacian (also called the vector Laplacian) in 3D devoid of the type of spurious modes that discrete Laplacians over flat domains can introduce if one does not enforce a proper discrete deRham complex. Such a tensor calculus for three-manifolds may allow us to explore possible applications in the context of general relativity in the longer term. Finally, the design of simplicial or cell meshes that guarantee accurate computations while approximating a given domain well remains an important endeavor for practical applications.

3.2 Geometry for simulation

Mathematical models of the evolution in time of mechanical systems generally involve systems of differential equations. Simulating a physical system consists in figuring out how to move the system forward in time from a set of initial conditions, allowing the computation of an actual trajectory through classical methods such as fourth-order Runge-Kutta or Newmark schemes. However, a geometric — instead of a traditional numerical-analytic — approach to the problem of time integration is particularly pertinent [98]: the very essence of a mechanical system is indeed characterized by its symmetries and invariants (e.g., momenta), thus preserving these geometric notions into the discrete computational setting is of paramount importance if one wants discrete time integration to properly capture the underlying continuous motion. Considering mechanics from a variational point of view goes back to Euler, Lagrange and Hamilton [86], and Poincaré famously stated that geometry and physics are "indissociable". The variational principle most important for continuous mechanics is due to Hamilton, and is often called **Hamilton's principle** or the *least action principle*: it states that a dynamical system always finds an optimal course from one position to another. One consequence is that we can recast the traditional way of thinking about an object accelerating in response to applied forces, into a geometric viewpoint: the path followed by the object between two space-time positions has optimal geometric properties, analogous to the notion of geodesics on curved surfaces. This point of view is equivalent to Newton's laws in the context of classical mechanics, but is broad enough to encompass physical models ranging to E&M and quantum mechanics [116]. While the idea of discretizing variational formulations of mechanics is standard for elliptic problems using Galerkin Finite Element methods for instance, only recently did it get used to derive variational time-stepping algorithms for mechanical systems [115]. These variational integrators have been shown to be remarkably versatile, powerful, and general for simulations of physical phenomena when compared to traditional numerical time stepping methods: the symplectic character of variational integrators guarantees good statistical predictability through accurate preservation of the geometric properties of the exact flow of the differential equations. We endeavor to continue contributing to this particular application of geometry and extend it further, as we foresee a number of interesting scientific developments and industrial applications.

State-space discretization of statistical physics. Kinetic equations are used to describe a variety of phenomena in various scientific fields, ranging from rarefied gas dynamics and plasma physics to biology and socio-economics, and appear naturally when one considers a statistical description of a large particle system evolving in time. In incompressible fluid simulation, kinetic solvers based on the lattice Boltzmann method (LBM) have generated growing interest due to their use of the Boltzmann transport equation and to its unusual *state-space discretization* based on a computationally-efficient lattice [135]: compared to macroscopic solvers directly integrating Navier-Stokes equations, LBM totally bypasses the difficult issue of discretizing advection to high order, and absence of global pressure solves makes for extremely efficient parallel implementations, which are now surpassing alternative discretizations [108]. However, the numerical treatment of the *collision operator* of the Boltmann equation has not reached maturity; most surprising is the *complete absence of geometric approaches to deal with Boltzmann equations.* One should be able to *formulate a variational approach to LBM* based on Hamilton's principle to derive a systematic integrator with guaranteed accuracy and structure-preserving properties. Moreover, while dealing with isothermal and incompressible flows is a good starting point, the kinetic standpoint of fluid dynamics is not theoretically restricted to this case: far more complex physical systems, from compressible flow (with shocks), to thermal conductivity, to even acoustics for example, can be handled; but far less is known on how to handle these more involved cases computationally, because no systematic numerical approach to handle Boltzmann equations is known. Success in our geometric approach to LBM should offer a much better handle to deal with these difficult cases: between new Hermite regularization tools [61, 75] and the recent introduction of variational integrators for non-equilibrium thermodynamical systems mentioned above should provide the necessary theoretical foundations to establish a geometric solver for this generalized case.

Learning-aided simulation. Computational physics is experiencing a tectonic shift as data-driven approaches are quickly becoming mainstream. While we do not adhere to the idea being floated that numerical integration could be simply "learned" to improve current solvers, the fact is that many machine learning tools may have profound influence in practical applications using simulation. Long standing problems such as the design of perfectly matched layers (PML, an artificial absorbing layer for transport equations used to reduce the domain of simulation without suffering from reflected waves [73]) or flux limiters in high resolution schemes [144] (to avoid the spurious oscillations (wiggles) that would otherwise occur due to shocks or sharp changes) could be found through training, and applied at very low numerical cost. We are curious to see if geometry can help design better architectures or approaches for this type of learning-aided simulation, by helping with better loss functions (with soft constraints) or better architectures (to enforce hard constraints) that account for the importance of structure preservation. Learning the highly non-linear and chaotic dynamics of fluids is also an interesting direction: we believe that one can infer predictive high-frequency details of a turbulent flow from a low-resolution simulation as it is an attractive alternative to non-linear turbulence modeling, extending the computationally-expensive Reynolds-Averaged Navier-Stokes (RANS [51]), Large-Eddy Simulation (LES [103]), or Detached-Eddy Simulation (DES [136]) models used in CFD. Many other learning efforts in the domain of simulation are being explored, in particular towards the goal of allowing real-time design of shapes that satisfy some physical properties, such as lowest drag for improved aerodynamics or highest stiffness for a light cantilever.

Geometric integration of physical systems and multiphysics. Although the use of geometric integrators for differential equations in computational physics has recently brought off many numerical improvements, the large body of knowledge in differential geometric mechanics remains vastly under-utilized in discrete mechanics. Many mechanical systems require geometric objects such as diffeomorphisms, vector fields, or (principal) connections for which no structure-preserving discretization exists. Hydrodynamics, for instance, has well established and rich differential geometric foundations, but rare are the numerical methods that take advantage of this rich body of knowledge as yet. Yet, satisfying a form of "particle relabeling" symmetry [116] on a discrete level could directly enforce Kelvin's circulation theorem, a momentum preservation as important as angular momentum preservation for rigid bodies. Relativity is another example, albeit much more involved, where structure-preserving numerics would strongly impact the scientific community: having discretizations automatically enforcing Bianchi's identities would not only simplify the numerical procedures involved in gravitational theory (as spectral accuracy would no longer be required to avoid spurious modes), but could in fact result in conservation of energy and angular momentum. Moreover, multiphysics (coupled mechanical systems involving more than one simultaneously occurring physical field) can be consistently described through constrained variational principles: a simple, yet already interesting example is the case of the equations of motion for the garden hose, where rod dynamics coupled with fluid motion was only fully modeled (along with its nonlinear solutions of traveling-wave type) a few years back [128] through such a geometric treatment. Now that a variational formulation of nonequilibrium thermodynamics extending Hamilton's principle to include irreversible processes has been proposed [90], we are particularly interested in advancing further the arsenal of computational methods for physical simulation.

3.3 Geometry for dynamical systems

Dynamical systems – whether physical, biological, chemical, or social – are ubiquitous in nature, and their study deals with the concept of change, rate of change, rate of rate of change, etc. Dynamical systems are often better elucidated and modeled through *topology and geometry*. Whether we consider a continuous-time dynamical system (flow) or discrete-time dynamical system (map), the geometric theory of dynamical systems studies phase portraits: on the state-space manifold (a geometric model for the set of all possible states of the system), the global behavior of the dynamical system is determined by a *cellular structure of basins enclosed by separatrices*, each basin being dominated by a different specific behavior or fate. A system's trajectories on the state-space manifold determine velocity vectors by differentiation; conversely, velocity vectors determine trajectories by integration. Bifurcations can also be understood as geometric models for the controlled change of one system into another, while the rate of divergence of trajectories in phase space measures a system's stability. Given this overwhelming relevance of geometry in dynamical systems, we intend to dedicate some of our activities to develop geometry-based computational tools to study time series and dynamical systems: while classic dynamical systems theory has established solid foundations to study structures in steady and time-periodic flows and maps, new tools are needed to analyze the complexity of time series or aperiodic large-scale flows from sampled trajectories, and to automatically generate a simplified skeleton of the overall dynamics of a system from input data. We discuss a few directions we are interested in further impacting next.

Time series. Geometric methods play an important part in the study of time series. Of particular interest are time-delay embeddings, which are generically able to capture the underlying state space and dynamics from which the time series data have been acquired, by the Takens embedding theorem [139]. Such embeddings transform discrete time series into point clouds in Euclidean space, so that the underlying geometry of the point cloud reflects the geometry of the phase space the data originate from. By doing so, questions related to the seasonality or anomalous behavior of the time series are naturally reformulated into questions about the geometry or topology of their embeddings [125]. Beside this approach, other more direct methods apply geometric or topological tools in the original physical or frequency domain, which, despite its simplicity, has proven to be relevant in various contexts [78, 82]. A common thread to all these developments is their restriction to numerical time series, including (but not restricted to) data for which geometry plays an obvious role—e.g. inertial or gyroscopic sensor data. With potential medical applications in mind, one of our main long-term goals will be to adapt and extend these approaches to handle *categorical data*, in connection to the item *Geometry for categorical and mixed data types* in the *Geometry for data science* theme. We also plan to find principled methods to tuning the various parameters involved in the techniques, e.g. the window size in time-delay embeddings: we will seek to optimize or learn these parameters automatically, in connection to the item *Geometry-driven learning* in the *Geometry for data science* theme. We will also seek to make these parameters adaptive, e.g. using time-varying window sizes in time-delay embeddings of irregular time series, in order to obtain more accurate data representations and improved learning performance.

Coherent structures. Another interesting area in need of new numerical methods concerns coherent structures, i.e., persisting features of a flow over long periods that tend to favor or inhibit material transport between distinct flow regions. While there is no universally agreed-upon definition for coherent structures (there exist ergodicity-based [64], observer-based [117], and probabilistic [88] approaches to their definition), most variants and associated computational methods assume a fine knowledge of the Eulerian velocity field in space and time to deduce a good approximation of the flow. However, flows are often known only as a set of sparse particle trajectories in time (an example is the trajectory of buoys in the ocean). Such a sparse sampling of the dynamical system does not lend itself well to a geometric analysis of transport, so topological methods have recently been proposed to extract structures from a sparse set of trajectories by measuring their entanglement [141, 52, 148] based on the theory of *braid groups*, a classical area of topology. Coherent regions can then be defined as containing particles that possibly mix with other particles within the region itself but do not mix with particles outside the region; the set of trajectories arising from the particles within a coherent region forms a *coherent bundle*. Even if the use of braid groups offers sound foundations and numerical tools for the definition of coherent structures in 2D, there has been only limited efforts in developing practical and scalable computational tools for the efficient analysis of flow structures in 3D, offering a clear opportunity for us to try new geometric insights.

Invariant sets. Much of the theory of dynamical systems revolves around the existence and structure of invariant sets, which by definition are subsets of the state space that are invariant under the action of the dynamics. Invariant sets come in many different forms (stationary solutions, periodic orbits, connecting orbits, chaotic invariant sets, etc), and their structure can be very complicated and can undergo drastic changes under perturbations of the system, thus making their study difficult. This is all the more true in practical applications, where the systems are only known through space and/or time discretizations. *Conley index theory* [74] overcomes these issues by restricting the focus to invariant sets that admit an isolating neighborhood, and by introducing a topological invariant—the Conley index—that characterizes whether such isolated invariant sets are attracting, repelling, or saddle-like. It is defined as the homotopy type of a pair of compact subsets of the neighborhood, and it is proven to be independent of the choice of neighborhood—thus characterizing the invariant set itself. We are interested in the study of invariant sets in the discrete space and continuous time setting, where the space is typically described by a simplicial complex and the dynamics by a combinatorial vector (or multivector) field. Building upon Forman's seminal work in combinatorial dynamical systems [85], recent advances [57, 109] have shown that isolated invariant sets and their Conley indices can be properly defined even in this setting, and that they can be related to the dynamics of some upper semicontinuous acyclic multivalued map defined on the geometric realization of the simplicial complex; in simpler terms, not only can Conley index theory be adapted to the combinatorial setting, but it also connects to its classical analog in the underlying space. Two important questions for applications arise from this line of work: (1) how to compute the invariant sets and their Conley indices (including choosing relevant isolating neighboroods) efficiently? (2) how do they behave under perturbations of the input vector field or simplicial complex? These questions have just started to be addressed [80, 81], mostly through the lens of single-parameter topological persistence theory, developed in the context of topological data analysis. We intend to push this direction further, notably using multi-parameter persistence theory to cope with some of the key difficulties such as the choice of isolating neighborhoods.

3.4 Geometry for data science

The last decade has seen the advent of machine learning (ML), and in particular deep learning (DL), in a large variety of fields, including some directly connected to geometry. For instance, DL-based approaches have become increasingly popular in geometry processing [129] due to their ability to outperform state-of-the-art, domain-specific methods by leveraging the ever-increasing amounts of available labeled data. On the downside, DL approaches suffer from a general lack of explainability. Moreover, their performances can be disappointing on small data due to their large numbers of parameters; this is especially true with end-to-end learning pipelines, which tend to require humongous amounts of training data to learn the right data representation. Finally, DL is by essence tied to Euclidean data representations, and as such it requires intermediate transforms in order to be applicable to non-Euclidean data types such as graphs or probability measures. Because of these limitations, we are seeing a rise of geometric and topological methods for data science in general, and for ML and DL in particular, whose aim is to help address the aforementioned challenges as well as others. For instance, geometric deep learning [62] tries to generalize deep neural models to non-Euclidean domains. This includes for instance using information geometry to apply deep neural models in probability spaces. Topological data analysis (TDA) [121] is another popular approach to enhance ML and DL methods. It contributes to data science in at least three different ways: first, by providing data mining tools that can help users uncover hidden structures in data; second, by providing generic descriptors for geometric data that can be turned into features for ML and DL with provable stability properties; third, by integrating itself deeply into existing ML methods or DL architectures to enhance their performances or to analyze their behavior [70, 112]. Other contributions of geometry to data science at large include: the use of Forman's Ricci curvature and its corresponding Ricci flow in networks, to understand the networks' properties and growth [145]; the application of the Hodge-Hemholtz decomposition to statistical ranking problems with sparse response data, with theoretical connections to both PageRank and LASSO [102]; the use of Reeb graphs or Morse-Smale complexes in statistical inference [72] as well as in data visualization [143]. These important developments reinforce our argument that geometry and topology have their role to play in the elaboration of the next-generation data analysis tools. We plan to focus on a few research directions related to these developments, which are of particular interest in our view.

Deep learning for large-scale 3D geometric data analysis. We first propose to develop efficient algorithms and mathematical tools for analyzing large geometric data collections using Deep Learning techniques. This includes 3D shapes represented as triangle or quad meshes, volumetric data, point clouds possibly embedded in high-dimensions, and graphs representing geometric (e.g. proximity) data. Our project is motivated by the fact that large annotated collections of geometric models have recently become available [69, 147], and that machine learning algorithms applied to such collections have shown promising initial results, both for data analysis as well as synthesis. We believe that these results can be significantly extended by building on recent advances in geometry processing, optimization and learning. Our ultimate goal is to design novel deep learning techniques capable both of handling geometric data directly and of combining and integrating different data sources into a unified analysis pipeline. A key challenge in this project is the fact that geometric data can come in a myriad different representations, such as point clouds and meshes among others, with variable sampling and discretization. Furthermore, geometric shapes can undergo both rigid and non-rigid deformations. Unfortunately, most existing deep learning approaches focus only on a particular type of representations and deformation classes (e.g., considering purely extrinsic or purely intrinsic methods). Instead we propose to place special focus on designing learning techniques capable of handing *diverse* multimodal data sources undergoing arbitrary deformations, in a coherent theoretical and practical framework. Moreover we propose to develop novel powerful *interactive* tools for analysis and annotation, to help harness user input, and also provide better mechanisms for exploration of variability in the data [132, 124].

Explainable geometric and topological features for data. Another of our goals is to design geometric and topological features that can capture richer content from the data, while maintaining the robustness and stability properties that the existing features enjoy. If we can make our features rich enough so that they characterize the input data (or their underlying geometric structures, assuming such structures exist) completely, then we will be able to leverage them in the context of explainable AI, to compute pre-images with guarantees on the corresponding interpretations. In cases where our features cannot completely describe the data, we will study the geometry of the fibers of the feature extraction step, in order to quantify the discrepancy that may appear between different interpretations of the same feature. We envision two complementary approaches for this:

- The first approach relies on feature aggregation. In the context of TDA for instance, one may consider using multiple filtrations (or filter functions on a fixed simplicial complex), computing their corresponding topological descriptors, then aggregating these descriptors together to form a feature vector.
- The second approach relies on more elaborate geometric and topological tools to design the features. The idea is to encode the joint effect of multiple geometric and topological constructions on the data, in a more integrated way than just by aggregating the corresponding features. By encoding more complex effects, we hope to extract a richer content using smaller constructions.

Research on the first approach in TDA started with [77, 91], who proved that, in the special case where the data are sampled from some subanalytic compact sets in Euclidean space $\mathbb{R}^n$, the compact sets themselves are fully described by the aggregated features obtained by orthogonal projections onto lines. This follows from a more fundamental result on the invertibility of the Radon transforms of constructible functions [134], to which the above aggregated features belong. This initial result has sparked a thriving new direction of research, exploring larger and larger classes of compact sets [101, 114, 120]. Many important questions arise from this line of work, some of which have been partially addressed, including: what kind of stability or robustness properties do these aggregated features enjoy? Can the size of the collection of filter functions used be reduced, to become finite and (more importantly) independent of the compact set under consideration? Can the aggregated features be computed efficiently? Can non-Euclidean compact sets, such as manifolds or length spaces, be considered as well, with similar guarantees?

The second approach is related to the development of *multi-parameter persistence* [66], which is undeniably the most widely open and long-standing research topic in TDA today. The core challenge is to define computationally tractable algebraic invariants that can capture as much of the joint structure of multiple topological constructions as possible. The notorious difficulty of this question comes from the fact that the algebraic objects underlying multi-parameter topological constructions are significantly more complicated than the ones underlying single-parameter constructions. The question also connects to notoriously hard problems in other areas of pure mathematics, such as the classification of isomorphism classes of indecomposable poset representations in quiver representation theory for instance. It can benefit from these connections, as mathematical tools that have been developed for those problems can be imported into the TDA literature—several promising such imports have been made in the recent past, including from representation theory [58] and from sheaf theory [104]. In turn, mathematical and algorithmic advances made in multi-parameter persistence may benefit these other areas of mathematics as well. This is clearly a high-risk and long-term research topic, but if successful, it may eventually have an enormous impact on TDA and related areas.

Geometric feature learning. Geometry and topology have played a key role in the design of feature extraction pipelines for certain types of data. The numerous existing geometric features for geometry processing (shape contexts [87], differential and integral invariants [127], heat or wave kernel signatures [54, 138], etc.) are a sign of the importance of this topic for the computer graphics community. Meanwhile, the TDA community has developed generic feature extraction pipelines, based on combinatorial constructions and their algebraic invariants, which have proven to be useful in a variety of application domains [121]. All these approaches are, however, handcrafted, with hyperparameters being tuned via manual, grid, or random search. Our goal is to make these approaches transition from a paradigm of feature engineering to that of feature learning, in order to set up end-to-end learning pipelines for improved performances and adaptability. Two complementary directions are considered:

- designing piecewise-smooth variants of the existing pipelines, with a fine control over the underlying stratification. This will make it possible to apply variational optimization methods, typically stochastic (sub-)gradient descent, and to optimize the gradient sampling steps for improved convergence rates.
- designing novel pipelines based on a combination of geometric/topological tools and deep learning, in order to get the best out of both worlds.

Research in the first direction is still in its infancy. Promising theoretical advances were made recently, towards understanding the piecewise differentiability of the basic *topological persistence* operator in full generality [107], as well as towards optimizing its parameters using classical stochastic gradient descent [67]. Can the knowledge gained in these studies about the underlying stratification of the operator be leveraged to optimize the gradient sampling step and thus improve the convergence rates? Can these results be extended to more advanced pipelines, such as the one for Mapper or for zigzags and multi-parameter persistence?

The idea behind the second direction is to integrate topological or geometric layers into neural network architectures such as auto-encoders or GANs for feature extraction — the challenge being to determine how to do it in the appropriate way, so that we can make the most of this combination. This question connects to the research topic *Geometry-driven learning* described further down in this section.

Geometry-driven learning. Most of the contributions of geometry and topology to machine learning until recently have been to the design of pre-processing steps (e.g. feature extraction) to enhance the performances of the learning pipeline. There is now a thriving effort of the community toward integrating geometric and/or topological computations deeper into the core of the pipeline. This includes for instance: *ToMATo* [70], which integrates a TDA-based feedback loop into density based algorithms to improve their stability and robustness; *topological regularizers* [71, 99], which add topology-based regularization terms to the loss in supervised statistical learning; *topological layers* [68, 89, 106], which are meant to be incorporated into neural networks. Meanwhile, geometry and topology have been used to analyze the behavior of neural networks [133, 63]. This exciting line of work is just emerging, and our intent is to push this direction further, in particular to address the following important questions:

- How can we generalize the use of topological layers in neural networks? This question is connected to the differentiability of the TDA pipeline, addressed in the research topic *Geometric feature learning*. Inded, generalizing the current (nascent) framework for differential calculus and optimization with the TDA pipeline will be key to designing both generic and effective topological layers. Another more practical aspect of the question is to evaluate the contribution of topological layers as initial or intermediate layers, depending on the neural network architecture that they are combined with and on the data they are applied to.
- The same question arises for topological regularizers, with similar theoretical and practical challenges.
- The development of richer families of geometric and topological descriptors, undertaken in the item *Richer geometric and topological features for data*, will eventually lead to the question of generalizing the current differentiable framework to these new descriptors, in order to make them as widely applicable as the current descriptors, and also to the practical question of determining how to best combine them with existing loss functions, regularizers, or neural network architectures.
- The aforementioned contributions and research directions concern mostly supervised learning. Can we contribute as well to unsupervised learning problems, including clustering (as ToMATo does already for density-based clustering), dimensionality reduction, or unsupervised feature

learning? This question connects also to the research topic *Geometric feature learning* described previously. One direction we may explore is the design of geometric or topological layers to be inserted in unsupervised neural network architectures such as auto-encoders or GANs.

- Finally, as TDA is concerned primarily with topology, an obvious (yet still wide open) question to ask is whether it can contribute to the current effort towards generating neural network architectures automatically.

Geometry for categorical and mixed data types. Categorical data types are notoriously hard to deal with in the context of ML and AI. Indeed, most of the existing ML toolbox has been designed specifically to work with numerical variables, usually sitting in some vector or metric space. By contrast, spaces of categorical data do not naturally come equipped with a linear structure nor a metric. More importantly, these spaces are discrete by nature, so choices of metrics or (dis-)similarity measures can be scarce, with limited effects on the learning efficiency. To make things worse, categorical variables are often mixed with numerical variables, and choosing a proper weighting for them is a challenge in its own right. Meanwhile, categorical variables play an important part in many applications: for instance, in precision medicine, where the monitoring of patients relies on collected longitudinal data that include not only numerical variables such as temperature or blood pressure, but also categorical variables such as illness antecedents or symptoms lists. Thus, handling categorical and mixed data types represents an important challenge today. Unfortunately, with very few exceptions [146], it has been mostly overlooked so far in the development of topological methods for ML and AI, so our goal will be to help fix this situation. The standard approach for handling categorical variables is to define a proper vector representation, then to apply—either off-the-shelf or with minor adaptations—an analysis method designed for numerical variables to the new data representation. A prototypical instance of this approach is Multiple Correspondance Analysis for dimensionality reduction [50], which applies classical PCA to the one-hot encoding matrix of the input data. A variant of the approach replaces the vector representation by a suitable metric or (dis-)similarity measure on the initial categorical variables or on some transformed version of those. For instance, in clustering, one can define a metric on the input data, e.g. Jaccard or Hamming distance, then apply a hierarchical bottom-up clustering algorithm such as single-linkage to the resulting distance matrix. This variant seems quite appropriate for geometric or topological methods, since the latter typically work with metric or (dis-)similarity spaces. The challenge is to determine with which metrics or (dis-)similarity measures, and on which data types, geometric or topological methods will be provably better.

A more refined version of the approach learns the new data representation instead of engineering it, which is particularly relevant when end-to-end learning pipelines are sought for. The methods are usually taylored to a specific data type, for instance word2vec [118] computes word embeddings for text data using a two-layer neural network. Our developments in the research topic *Geometry-driven learning* will make it possible to combine TDA layers with such networks, and thus to benefit from the most recent advances on representation learning for these data types. The challenge will be to understand when and how to make the most of this combination.

4 Application domains

Our work aims at a wide range of applications covering 3D shape analysis and processing, simulation, and data science in general. While we typically focus on contributions that are of a fundamental, mathematical and algorithmic nature, we seek collaborations with academics and industrial from applied fields, who can use our tools on practical and concrete problems. Here are a few examples of collaborations:

- In the context of 3D geometry processing, we collaborate with Dassault Systèmes for a) the PhD of Lucas Brifault on the design of novel geometric representations for shapes through measure theory and b) the PhD of Mariem Mezghanni on the design of physical simulation layers for 3D modeling.

- In the context of personalized medicine, we collaborate with statisticians and medical doctors to incorporate our geometric and topological features into learning pipelines to design better dynamic treatment regimens (AEx PreMediT).
- In a collaboration with the French Ministry of Defense, we seek to develop tools to analyze multimodal time series data in order to predict the appearance of G-LOCs among fighter jet pilots in training or in operation (PhD of Julie Mordacq).

Beside these few illustrative examples, GeomeriX also maintains regular collaborations with Sanofi, EDF, Danone R&D, Immersion Tools, as well as with several key players in the world-wide tech industry, including Ansys, Adobe Research, Disney/Pixar, NVidia.

5 Highlights of the year

5.1 Thematic programs organization

- Mathieu Desbrun, in collaboration with Jacques-Olivier Lachaud (Université de Savoie Mont-Blanc), organized the *Year of Geometry* under the auspices of CNRS' GdR Informatique Fondamentale et ses Mathématique. Two workshops (one on AI for Geometry, one on Geometry in Industry), two Young Researchers in Geometry meetings, and a 5-day capstone conference at CIRM in Luminy were organized for this year-long effort.

5.2 Awards

- Jiong Chen and Mathieu Desbrun received a Best Paper award at the ACM SIGGRAPH 2024 conference in Denver, CO, the premier conference in graphics, for their paper on preconditioning of boundary integral equations [20].

5.3 Distinctions

- Steve Oudot was an Invited Speaker at the 9th European Congress of Mathematics (ECM), a quadriennal event that, together with the International Congress of Mathematicians, constitute the two main events of the mathematics community — see details here.

5.4 HdR

- Pooran Memari defended her Habilitation à diriger des recherches at Institut Polytechnique de Paris on September 5, 2024. Title: "Points, Patterns, and Shapes Towards Accessible Geometric Modeling." The corresponding HdR Jury was composed of:
  - David Coeurjolly, Directeur de recherche au CNRS, Université de Lyon (Examiner)
  - Stefanie Hahmann, Professor at Université de Grenoble - Ensimag (Examiner)
  - Leif Kobbelt, Professor of Computer Science, RWTH Aachen University (Reviewer)
  - Sylvain Lefebvre, Directeur de recherche, Inria Nancy (Reviewer)
  - Daniele Panozzo, Associate Professor of Computer Science, New York University (Reviewer)

6 New software, platforms, open data

Although software production and maintenance is not a priority for our team, code is systematically used to develop proof-of-concept implementations, both for reproducibility and to facilitate technology transfer. We adopt an opportunistic approach to code development depending on the project being carried out and the will of the main developers of the software: while many projects limit their involvement in code sharing to a minimum just in order to prove the usefulness and reliability of their contributions, others have large applicability and therefore deserve more time and effort to be devoted in order to provide full-fledged software packages. In particular, our research sometimes yields new packages in well-established libraries such as Cgal in computational geometry or Gudhi in topological data analysis, to which we contribute either directly or indirectly.

6.1 Open Source Code

- Ballmerge Surface Reconstruction CGAL package with Telecom Paris, TU Wien, TU Delft, was released in 2024.
- We have released several packages in github associated with the papers published by Maks Ovsjanikov and Mathieu Desbrun (and their collaborators). All of these packages are freely available and provide open-source implementations for nearly all the published papers.

6.2 New software

6.2.1 MFS-chol

Name: Lightning-fast Method of Fundamental Solutions

Keywords: 3D, Boundary element method

Functional Description: The method of fundamental solutions (MFS) and its associated boundary element method (BEM) are commonly used due to the reduced dimensionality they offer: for three-dimensional linear problems, they only require variables on the domain boundary to solve and evaluate the solution throughout space, making them a valuable tool in a wide variety of applications. However, MFS and BEM have poor computational scalability and huge memory requirements for large-scale problems, limiting their applicability and efficiency in practice. By leveraging connections with Gaussian Processes and exploiting the sparse structure of the inverses of boundary integral matrices, we introduce a variational preconditioner that can be computed via a sparse inverse-Cholesky factorization in a massively parallel manner. We show that applying our preconditioner to the Preconditioned Conjugate Gradient algorithm greatly improves the efficiency of MFS or BEM solves, up to four orders of magnitude in our series of tests.

Release Contributions: N/A

Publication: hal-04589038v1

Contact: Mathieu Desbrun

Participants: Jiong Chen, Mathieu Desbrun

7 New results

We list our new results for each of the four themes that our team is articulated around.

7.1 Geometry for Euclidean shape processing

7.1.1 SING: Stability-Incorporated Neighborhood Graph

Participants: Pooran Memari, Steve Oudot.

In collaboration with Diana Marin, Stefan Ohrhallinger and Michael Wimmer (TU Wien) and Amal Dev Parakkat (Telecom, IP-Paris).

We introduce the Stability-Incorporated Neighborhood Graph (SING) [38], a novel density-aware structure designed to capture the intrinsic geometric properties of a point set. We improve upon the spheres-of-influence graph by incorporating additional features to offer more flexibility and control in encoding proximity information and capturing local density variations. Through persistence analysis on our proximity graph, we propose a new clustering technique and explore additional variants incorporating extra features for the proximity criterion. Alongside the detailed analysis and comparison to evaluate its performance on various datasets, our experiments demonstrate that the proposed method can effectively extract meaningful clusters from diverse datasets with variations in density and correlation. Our application scenarios underscore the advantages of the proposed graph over classical neighborhood graphs, particularly in terms of parameter tuning.

7.1.2 Stochastic Computation of Barycentric Coordinates

Participants: Mathieu Desbrun.

In collaboration with Fernando de Goes (Pixar).

In this work [22], we present a practical and general approach for computing barycentric coordinates through stochastic sampling. Our key insight is a reformulation of the kernel integral defining barycentric coordinates into a weighted least-squares minimization that enables Monte Carlo integration without sacrificing linear precision. Our method can thus compute barycentric coordinates directly at the points of interest, both inside and outside the cage, using just proximity queries to the cage such as closest points and ray intersections. As a result, we can evaluate barycentric coordinates for a large variety of cage representations (from quadrangulated surface meshes to parametric curves) seamlessly, bypassing any volumetric discretization or custom solves. To address the archetypal noise induced by sample-based estimates, we also introduce a denoising scheme tailored to barycentric coordinates. We demonstrate the efficiency and flexibility of our formulation by implementing a stochastic generation of harmonic coordinates, mean-value coordinates, and positive mean-value coordinates.

7.1.3 PoNQ: a Neural QEM-based Mesh Representation

Participants: Mathieu Desbrun, Nissim Maruani, Maks Ovsjanikov.

In collaboration with Pierre Alliez (Inria Sophia).

Although polygon meshes have been a standard rep resentation in geometry processing, their irregular and combinatorial nature hinders their suitability for learning based applications. In this work [39], we introduce a novel learnable mesh representation through a set of local 3D sample Points and their associated Normals and Quadric error metrics (QEM) w.r.t. the underlying shape, which we denote PoNQ. A global mesh is directly derived from PoNQ by efficiently leveraging the knowledge of the local quadric errors. Besides marking the first use of QEM within a neu ral shape representation, our contribution guarantees both topological and geometrical properties by ensuring that a PoNQ mesh does not self-intersect and is always the bound ary of a volume. Notably, our representation does not rely on a regular grid, is supervised directly by the target sur face alone, and also handles open surfaces with boundaries and/or sharp features. We demonstrate the efficacy of PoNQ through a learning-based mesh prediction from SDF grids and show that our method surpasses recent state-of-the-art techniques in terms of both surface and edge-based metrics.

7.1.4 Biharmonic Coordinates and their Derivatives for Triangular 3D Cages

Participants: Jiong Chen.

In collaboration with Jean-Marc Thiery and Élie Michel (Adobe).

This work [32] extends biharmonic coordinates, which were previously derived for 2D shape deformation, into three dimensions. The key contribution is deriving closed-form mathematical expressions for biharmonic coordinates and their derivatives specifically for 3D triangular cages. At the heart of this work is the development of closed-form expressions that calculate how the Euclidean distance integrates over a triangle, along with the derivatives of this integration. The significance of this advancement is twofold: it completes a gap in the theory of generalized barycentric coordinates, and it enables practical applications in 3D shape manipulation. These applications include creating various types of biharmonic deformations, solving shape deformation problems through variational methods, and providing efficient closed-form solutions for the recently developed Somigliana coordinates. This work ultimately bridges a theoretical gap while offering practical tools for 3D shape manipulation and deformation.

7.1.5 A Survey on Cage-based Deformation of 3D Models

Participants: Jiong Chen.

In collaboration with Daniel Ströter, Johannes Sebastian Mueller-Roemer, Sebastian Besler, Andre Stork and Dieter W. Fellner (Technical University of Darmstadt), Jean-Marc Thiery and Tamy Boubekeur (Adobe), Kai Hormann and Qingjun Chang (University of Italian Switzerland).

In this work [30], we review the advancement of 3D cage-based deformation. Cage-based deformation enables users to quickly manipulate 3D geometry by deforming the cage. Due to their utility, cage-based deformation techniques increasingly appear in many geometry modeling applications. For this reason, the computer graphics community has invested a great deal of effort in the past decade and beyond into improving automatic cage generation and cage-based deformation. Recent advances have significantly extended the practical capabilities of cage-based deformation methods. As a result, there is a large body of research on cage-based deformation. In this report, we provide a comprehensive overview of the current state of the art in cage-based deformation of 3D geometry. We discuss current methods in terms of deformation quality, practicality, and precomputation demands. In addition, we highlight potential future research directions that overcome current issues and extend the set of practical applications. In conjunction with this survey, we publish an application to unify the most relevant deformation methods. Our report is intended for computer graphics researchers, developers of interactive geometry modeling applications, and 3D modeling and character animation artists.

7.1.6 BallMerge: High-quality Fast Surface Reconstruction via Voronoi Balls

Participants: Pooran Memari.

In collaboration with Amal Dev Parakkat (Telecom, IP-Paris), Stefan Ohrhallinger and Michael Wimmer (TU Wien) and Elmar Eisemann (TU Delft).

This work [28] introduces a Delaunay-based algorithm for reconstructing the underlying surface of a given set of unstructured points in 3D. The implementation is very simple, and it is designed to work in a parameter-free manner. The solution builds upon the fact that in the continuous case, a closed surface separates the set of maximal empty balls (medial balls) into an interior and exterior. Based on discrete input samples, our reconstructed surface consists of the interface between Voronoi balls, which approximate the interior and exterior medial balls. An initial set of Voronoi balls is iteratively processed, merging Voronoi-ball pairs if they fulfil an overlapping error criterion. Our complete open-source reconstruction pipeline performs up to two quick linear-time passes on the Delaunay complex to output the surface, making it an order of magnitude faster than the state of the art while being competitive in memory usage and often superior in quality. We propose two variants (local and global), which are carefully designed to target two different reconstruction scenarios for watertight surfaces from accurate or noisy samples, as well as real-world scanned data sets, exhibiting noise, outliers, and large areas of missing data. The results of the global variant are, by definition, watertight, suitable for numerical analysis and various applications (e.g., 3D printing). Compared to classical Delaunay-based reconstruction techniques, our method is highly stable and robust to noise and outliers, evidenced via various experiments, including on real-world data with challenges such as scan shadows, outliers, and noise, even without additional preprocessing. The code for this work has been released as a package in the open-source Computational Geometry Algorithms Library (CGAL).

7.1.7 DynBioSketch: A tool for sketching dynamic visual summaries in biology, and its application to infection phenomena

Participants: Pooran Memari.

In collaboration with Pauline Olivier, Tara Butler, Pascal Guehl, Renaud Chabrier and Marie-Paule Cani (LIX, Ecole Polytechnique) and Jean-Luc Coll (Institute for Advanced Biosciences, Grenoble Alpes University).

Having simple methods of illustration is essential to scientific thinking. To complement the abstract sketches regularly used in cell biology, we propose DynBioSketch [26], an easy-to-use digital modeling and animation tool, enabling biologists to resort to less simplified representations when necessary without having to call professional artists. DynBioSketch is an interactive sketching system dedicated to the design and communication of biological phenomena at the cellular scale that can be illustrated in a few minutes of animation. Our model integrates 3D modeling, pattern-based design of 3D shape distributions, and sketch-based animation. These elements can be combined to create complex scenarios such as the infection phenomenon on which we focus, allowing a narrative design adapted to communication between researchers or educational applications in biology. Our results, along with a user study conducted with biology researchers, highlight the potential of DynBioSketch in enabling the direct design of dynamic visual summaries that convey relevant information, as shown in our infection case study. By bridging the gap between abstract representations used by experts and more illustrative depictions, DynBioSketch opens a new avenue for communicating biological concepts.

7.1.8 Ricci flow-based brain surface covariance descriptors for diagnosing Alzheimer's disease

Participants: Pooran Memari.

In collaboration with Fatemeh Ahmadi, Mohamad-Ebrahim Shiri, Behroz Bidabad, Maral Sedaghat (Math department of Amirkabir University of Technology).

Automated feature extraction from MRI brain scans and diagnosis of Alzheimer's disease are ongoing challenges. With advances in 3D imaging technology, 3D data acquisition is becoming more viable and efficient than its 2D counterpart. Rather than using feature-based vectors, in this work [17], for the first time, we suggest a pipeline to extract novel covariance-based descriptors from the cortical surface using the Ricci energy optimization. The covariance descriptors are components of the nonlinear manifold of symmetric positive-definite matrices, thus we focus on using the Gaussian radial basis function to apply manifold-based classification to the 3D shape problem. Applying this novel signature to the analysis of abnormal cortical brain morphometry allows for diagnosing Alzheimer's disease. Experimental studies performed on about two hundred 3D MRI brain models, gathered from Alzheimer's Disease Neuroimaging Initiative (ADNI) dataset demonstrate the effectiveness of our descriptors in achieving remarkable classification accuracy.

7.1.9

Participants: Pooran Memari.

In collaboration with Charline Grenier and Basile Sauvage (Strasbourg University).

In this work [35], we present an interactive tool to control the parameters of the procedural model introduced by Grenier et al. [2022]. Procedural textures generate large, detailed textures with minimal memory usage, but can be difficult to control. Our tool simplifies this by allowing users to adjust noise through spectral parameters and color maps through ink volumes and color adjacency. Using a constrained optimal transport framework, colors are treated as cells in a weighted Voronoi diagram, while noise acts as a probability measure. Ink volumes are enforced as hard constraints, enabling intuitive and efficient control over color relationships in procedural textures.

7.1.10 Versatile Curve Design by Level Set with Quadratic Convergence

Participants: Jiong Chen.

In collaboration with Xiaohu Zhang, Shuang Wu, Hujun Bao and Jin Huang (Zhejiang University), and Yao Jin (Zhejiang Sci-Tech University).

In this work [33], we present an efficient and versatile approach to curve design based on an implicit representation known as the level set. While previous works have explored the use of the level set to generate curves with minimal length, they typically have limitations in accommodating additional conditions for rich and robust control. To address these challenges, we formulate curve editing with constraints like smoothness, interpolation, tangent control, etc., via a level set based variational problem by constraining the values or derivatives of the level set function. However, the widely used gradient flow strategy converges very slowly for this complicated variational problem compared to the classical geodesic one. Thus, we propose to solve it via Newton's method enhanced by local Hessian correction and a trust-region strategy. As a result, our method not only enables versatile control, but also excels in terms of performance due to nearly quadratic convergence and almost linear complexity in each iteration via narrow band acceleration. In practice, these advantages effectively benefit various applications, such as interactive curve manipulation, boundary smoothing for surface segmentation and path planning with obstacles as demonstrated.

7.2 Geometry for simulation

7.2.1 Hybrid LBM-FVM Solver for Two-phase Flow Simulation

Participants: Mathieu Desbrun.

In collaboration with Wei Li and Xiaopei Liu (Shanghaitech University)

In this work [25], we introduce a hybrid LBM-FVM solver for two-phase fluid flow simulations in which interface dynamics is modeled by a conservative phase-field equation. Integrating fluid equations over time is achieved through a velocity-based lattice Boltzmann solver which is improved by a central-moment multiple-relaxation-time collision model to reach higher accuracy. For interface evolution, we propose a finite-volume-based numerical treatment for the integration of the phase-field equation: we show that the second-order isotropic centered stencils for diffusive and separation fluxes combined with the WENO-5 stencils for advective fluxes achieve similar and sometimes even higher accuracy than the state-of-the-art double-distribution function LBM methods as well as the DUGKS-based method, while requiring less computations and a smaller amount of memory. Benchmark tests (such as the 2D diagonal translation of a circular interface), along with quantitative evaluations on more complex tests (such as the rising bubble and Rayleigh-Taylor instability simulations) allowing comparisons with prior numerical methods and/or experimental data, are presented to validate the advantage of our hybrid solver. Moreover, 3D simulations (including a dam break simulation) are also compared to the time-lapse photography of physical experiments in order to allow for more qualitative evaluations.

7.2.2 Kinetic Simulation of Turbulent Multifluid Flows

Participants: Mathieu Desbrun.

In collaboration with Wei Li (Tencent)

Despite its visual appeal, the simulation of separated multiphase flows (i.e., streams of fluids separated by interfaces) faces numerous challenges in accurately reproducing complex behaviors such as guggling, wetting, or bubbling. These difficulties are especially pronounced for high Reynolds numbers and large density variations between fluids, most likely explaining why they have received comparatively little attention in Computer Graphics compared to single- or two-phase flows. In this work [24], we present a full LBM solver for multifluid simulation. We derive a conservative phase field model with which the spatial presence of each fluid or phase is encoded to allow for the simulation of miscible, immiscible and even partially-miscible fluids, while the temporal evolution of the phases is performed using a D3Q7 lattice-Boltzmann discretization. The velocity field, handled through the recent high-order moment-encoded LBM (HOME-LBM) framework to minimize its memory footprint, is simulated via a velocity-based distribution stored on a D3Q27 or D3Q19 discretization to offer accuracy and stability to large density ratios even in turbulent scenarios, while coupling with the phases through pressure, viscosity, and interfacial forces is achieved by leveraging the diffuse encoding of interfaces. The resulting solver addresses a number of limitations of kinetic methods in both computational fluid dynamics and computer graphics: it offers a fast, accurate, and low-memory fluid solver enabling efficient turbulent multiphase simulations free of the typical oscillatory pressure behavior near boundaries. We present several numerical benchmarks, examples and comparisons of multiphase flows to demonstrate our solver's visual complexity, accuracy, and realism.

7.2.3 Lightning-fast Method of Fundamental Solutions

Participants: Jiong Chen, Mathieu Desbrun.

In collaboration with Florian Schaefer (Georgia Tech)

The method of fundamental solutions (MFS) and its associated boundary element method (BEM) have gained popularity in computer graphics due to the reduced dimensionality they offer: for three-dimensional linear problems, they only require variables on the domain boundary to solve and evaluate the solution throughout space, making them a valuable tool in a wide variety of applications. However, MFS and BEM have poor computational scalability and huge memory requirements for large-scale problems, limiting their applicability and efficiency in practice. By leveraging connections with Gaussian Processes and exploiting the sparse structure of the inverses of boundary integral matrices, we introduce in this work [20] a variational preconditioner that can be computed via a sparse inverse-Cholesky factorization in a massively parallel manner. We show that applying our preconditioner to the Preconditioned Conjugate Gradient algorithm greatly improves the efficiency of MFS or BEM solves, up to four orders of magnitude in our series of tests.

7.2.4 TwisterForge: Controllable and Efficient Animation of Virtual Tornadoes

Participants: Jiong Chen.

In collaboration with James Gain (University of Cape Town), Jean-Marc Chomaz and Marie-Paule Cani (LIX, Ecole Polytechnique)

In this work [44], we introduce a layered approach for creating and animating realistic virtual tornadoes in computer graphics. The method centers on two types of cureves: a 3D curve to intitialize the tornado's core as a vortex filament and 2D profile curves to control the surrounding funnel shape. The core evolves dynamically subject to the Biot-Savart law, bending and twisting driven by its initial curvature, while the funnel profile represents the Stokes stream function and dictates the radial and axial air motion around the core. These two components, together, capture the rotation, sliding, and uplift of the tornado's air volume. Our method achieves visually plausible animations of tornadoes, capable of interacting with uneven terrain, destroying infrastructure, and transporting debris, offering a controllable and realistic solution for visual effects and interactive applications.

7.2.5 Volcanic Skies: coupling explosive eruptions with atmospheric simulation to create consistent skyscapes

Participants: Jiong Chen.

In collaboration with Cilliers Pretorius and James Gain (University of Cape Town), Maud Lastic, Damien Rohmer and Marie-Paule Cani (LIX, Ecole Polytechnique), and Guillaume Cordonnier (Inria).

Explosive volcanic eruptions rank among the most terrifying natural phenomena, and are thus frequently depicted in films, games, and other media, usually with a bespoke once-off solution. In this work [29], we introduce the first general-purpose model for bi-directional interaction between the atmosphere and a volcano plume. In line with recent interactive volcano models, we approximate the plume dynamics with Lagrangian disks and spheres and the atmosphere with sparse layers of 2D Eulerian grids, enabling us to focus on the transfer of physical quantities such as temperature, ash, moisture, and wind velocity between these sub-models. We subsequently generate volumetric animations by noise-based procedural upsampling keyed to aspects of advection, convection, moisture, and ash content to generate a fully-realized volcanic skyscape. Our model captures most of the visually salient features emerging from volcano-sky interaction, such as windswept plumes, enmeshed cap, bell and skirt clouds, shockwave effects, ash rain, and sheathes of lightning visible in the dark.

7.3 Geometry for dynamical systems

7.3.1 ADAPT: Multimodal Learning for Detecting Physiological Changes under Missing Modalities

Participants: Julie Mordacq, Steve Oudot.

In collaboration with Vicky Kalogeiton (Vista, LIX), Leo Milecki and Maria Vakalopoulou (Centrale Supelec).

Multimodality has recently gained attention in the medical domain, where imaging or video modalities may be integrated with biomedical signals or health records. Yet, two challenges remain: balancing the contributions of modalities, especially in cases with a limited amount of data available, and tackling missing modalities. To address both issues, in this work [40] we introduce the AnchoreD multimodAl Physiological Transformer (ADAPT), a multimodal, scalable framework with two key components: (i) aligning all modalities in the space of the strongest, richest modality (called anchor) to learn a joint embedding space, and (ii) a Masked Multimodal Transformer, leveraging both inter- and intra-modality correlations while handling missing modalities. We focus on detecting physiological changes in two real-life scenarios: stress in individuals induced by specific triggers and fighter pilots' loss of consciousness induced by g-forces. We validate the generalizability of ADAPT through extensive experiments on two datasets for these tasks, where we set the new state of the art while demonstrating its robustness across various modality scenarios and its high potential for real-life applications.

7.3.2 Multimodal Learning for Detecting Stress under Missing Modalities

Participants: Julie Mordacq, Steve Oudot.

In collaboration with Vicky Kalogeiton (Vista, LIX), Leo Milecki and Maria Vakalopoulou (Centrale Supelec).

Dealing with missing modalities is critical for many real-life applications. In this work [48], we propose a scalable framework for detecting stress induced by specific triggers in multimodal data with missing modalities. Our method has two key components: (i) aligning all modalities in the space of the strongest modality (the video) for learning a joint embedding space and (ii) a Masked Multimodal Transformer, leveraging inter- and intra-modality correlations while handling missing modalities. We validate our method through experiments on the StressID dataset, where we set the new state of the art while demonstrating its robustness across various modality scenarios and its high potential for real-life applications.

7.4 Geometry for data science

7.4.1 On the bottleneck stability of rank decompositions of multi-parameter persistence modules

Participants: Steve Oudot.

In collaboration with Magnus botnan (Vrije Universiteit Amsterdam), Steffen Oppermann (NTNU) and Luis Scoccola (University of Oxford).

A significant part of modern topological data analysis is concerned with the design and study of algebraic invariants of poset representations—often referred to as persistence modules. One such invariant is the minimal rank decomposition, which encodes the ranks of all the structure morphisms of the persistence module by a single ordered pair of rectangle-decomposable modules, interpreted as a signed barcode. This signed barcode generalizes the concept of persistence barcode from one-parameter persistence to any number of parameters, raising the question of its bottleneck stability. We show in this work [19] that the minimal rank decomposition is not stable under the natural notion of signed bottleneck matching between signed barcodes. We remedy this by turning our focus to the rank exact decomposition, a related signed barcode induced by the minimal projective resolution of the module relative to the so-called rank exact structure, which we prove to be bottleneck stable under signed matchings. As part of our proof, we obtain two intermediate results of independent interest: we compute the global dimension of the rank exact structure on the category of finitely presentable multi-parameter persistence modules, and we prove a bottleneck stability result for hook-decomposable modules. We also give a bound for the size of the rank exact decomposition that is polynomial in the size of the usual minimal projective resolution, we prove a universality result for the dissimilarity function induced by the notion of signed matching, and we compute, in the two-parameter case, the global dimension of a different exact structure related to the upsets of the indexing poset. This set of results combines concepts from topological data analysis and from the representation theory of posets, and we believe is relevant to both areas.

7.4.2 Signed Barcodes for Multi-parameter Persistence via Rank Decompositions and Rank-Exact Resolutions

Participants: Steve Oudot.

In collaboration with Magnus botnan (Vrije Universiteit Amsterdam) and Steffen Oppermann (NTNU).

In this work [18], we introduce the signed barcode, a new visual representation of the global structure of the rank invariant of a multi-parameter persistence module or, more generally, of a poset representation. Like its unsigned counterpart in one-parameter persistence, the signed barcode decomposes the rank invariant as a $\mathbb{Z}$-linear combination of rank invariants of indicator modules supported on segments in the poset. We develop the theory behind these decompositions, both for the usual rank invariant and for its generalizations, showing under what conditions they exist and are unique. We also show that, like its unsigned counterpart, the signed barcode reflects in part the algebraic structure of the module: specifically, it derives from the terms in the minimal rank-exact resolution of the module, i.e., its minimal projective resolution relative to the class of short exact sequences on which the rank invariant is additive. To complete the picture, we show some experimental results that illustrate the contribution of the signed barcode in the exploration of multi-parameter persistence modules.

7.4.3 Intrinsic Interleaving Distance for Merge Trees

Participants: Steve Oudot.

In collaboration with Ellen Gasparovic (Union College), Elizabeth Munch (Michigan State University), Katharine Turner (Australian National University), Bei Wang (University of Utah) and Yusu Wang (University of California).

A merge tree is a type of graph-based topological summary that tracks the evolution of connected components in the sublevel sets of scalar functions. Merge trees enjoy widespread applications in data analysis and scientific visualization. In this work [21], we consider the problem of comparing two merge trees via the notion of interleaving distance in the metric space setting. We investigate several theoretical properties of such a metric. In particular, we show that the interleaving distance is intrinsic on the space of labeled merge trees and provide an algorithm to construct metric 1-centers for collections of labeled merge trees. We further prove that the intrinsic property of the interleaving distance also holds for the space of unlabeled merge trees. Our results provide practical recipes for performing statistics on merge trees.

7.4.4 On the stability of multigraded Betti numbers and Hilbert functions

Participants: Steve Oudot.

In collaboration with Luis Scoccola (University of Oxford).

Multigraded Betti numbers are one of the simplest invariants of multiparameter persistence modules. This invariant is useful in theory—it completely determines the Hilbert function of the module and the isomorphism type of the free modules in its minimal free resolution—as well as in practice—it is easy to visualize, and it is one of the main outputs of current multiparameter persistent homology software, such as RIVET. However, to the best of our knowledge, no stability result with respect to the interleaving distance has been established for this invariant so far, and this potential lack of stability limits its practical applications. In this work [27] we prove a stability result for multigraded Betti numbers, using an efficiently computable bottleneck-type dissimilarity function we introduce. Our notion of matching is inspired by recent work on signed barcodes and allows matching bars of the same module in homological degrees of different parity, in addition to matchings bars of different modules in homological degrees of the same parity. Our stability result is a combination of Hilbert's syzygy theorem, Bjerkevik's bottleneck stability for free modules, and a novel stability result for projective resolutions. We also prove, in the two-parameter case, a 1-Wasserstein stability result for Hilbert functions with respect to the 1-presentation distance of Bjerkevik and Lesnick.

7.4.5 Efficient computation of topological integral transforms

Participants: Steve Oudot.

In collaboration with Vadim Lebovici (University of Oxford) and Hugo Passe (École Normale Supérieure de Lyon).

Topological integral transforms have found many applications in shape analysis, from prediction of clinical outcomes in brain cancer to analysis of barley seeds. Using Euler characteristic as a measure, these objects record rich geometric information on weighted polytopal complexes. While some implementations exist, they only enable discretized representations of the transforms, and they do not handle weighted complexes (such as for instance images). Moreover, recent hybrid transforms lack an implementation. In this work [37], we introduce eucalc, a novel implementation of three topological integral transforms - the Euler characteristic transform, the Radon transform, and hybrid transforms - for weighted cubical complexes. Leveraging piecewise linear Morse theory and Euler calculus, the algorithms significantly reduce computational complexity by focusing on critical points. Our software provides exact representations of transforms, handles both binary and grayscale images, and supports multi-core processing. It is publicly available as a C++ library with a Python wrapper. We present mathematical foundations, implementation details, and experimental evaluations, demonstrating eucalc's efficiency.

7.4.6 Differentiability and Optimization of Multiparameter Persistent Homology

Participants: Steve Oudot.

In collaboration with Luis Scoccola (University of Oxford), Siddharth Setlur (ETH Zürich), David Loiseaux and Mathieu Carrière (Datashape, Inria Sophia-Antipolis).

Real-valued functions on geometric data—such as node attributes on a graph—can be optimized using descriptors from persistent homology, allowing the user to incorporate topological terms in the loss function. When optimizing a single real-valued function (the one-parameter setting), there is a canonical choice of descriptor for persistent homology: the barcode. The operation mapping a real-valued function to its barcode is differentiable almost everywhere, and the convergence of gradient descent for losses using barcodes is relatively well understood. When optimizing a vector-valued function (the multiparameter setting), there is no unique choice of descriptor for multiparameter persistent homology, and many distinct descriptors have been proposed. This calls for the development of a general framework for differentiability and optimization that applies to a wide range of multiparameter homological descriptors. In this work [41] we develop such a framework and show that it encompasses well-known descriptors of different flavors, such as signed barcodes and the multiparameter persistence landscape. We complement the theory with numerical experiments supporting the idea that optimizing multiparameter homological descriptors can lead to improved performances compared to optimizing one-parameter descriptors, even when using the simplest and most efficiently computable multiparameter descriptors.

7.4.7 Fine-tuning 3D foundation models for geometric object retrieval

Participants: Maks Ovsjanikov.

In collaboration with Jarne van den Herrewegen, Tom Tourwé, and Francis Wyffels (from Oqton AI; and AI and Robotics Lab, IDLab-AIRO, Ghent University-imec, Belgium).

This work [23] introduces fine-tuning strategies for 3D foundation models to enhance geometric object retrieval. Foundation models like ULIP-2 (Xue et al., 2023) have advanced 3D deep learning by leveraging large-scale data and multi-modal architectures, combining 2D image and text branches to enhance representation learning. Despite their success in tasks like shape classification, their 3D encoders and adaptability to new downstream tasks remain underexplored, particularly for applications like 3D object retrieval. This paper addresses this gap, demonstrating strong 3D-to-3D retrieval performance across seven datasets, rivaling state-of-the-art view-based methods. It evaluates pre-trained and fine-tuned models, comparing supervised and self-supervised fine-tuning, and introduces a crucial methodology to stabilize transfer learning from 3D foundation models.

7.4.8 DeBaRA: Denoising-Based 3D Room Arrangement Generation

Participants: Léopold Maillard, Maks Ovsjanikov.

In collaboration with Nicolas Sereyjol-Garros, and Tom Durand (Dassault Systèmes).

This work [46] presents a novel denoising-based approach for generating 3D room arrangements. Generating realistic and diverse layouts of furnished indoor 3D scenes is challenging due to complex object interactions, limited data, and spatial constraints. DeBaRA, a score-based model, addresses this by enabling precise, controllable arrangement generation with 3D spatial awareness. It supports applications like scene synthesis, completion, and re-arrangement, and incorporates a Self Score Evaluation procedure for better integration with external LLMs. Experiments show DeBaRA significantly outperforms state-of-the-art methods.

7.4.9 Smoothed Graph Contrastive Learning via Seamless Proximity Integration

Participants: Maysam Behmanesh, Maks Ovsjanikov.

This work [34] introduces a smoothed graph contrastive learning (SGCL) technique for unsupervised representation learning on graphs, while leveraging proximity integration. Standard graph contrastive learning (GCL) aligns node representations by classifying node pairs as positives or negatives, typically treating all negatives equally in the contrastive loss. The Smoothed Graph Contrastive Learning model (SGCL) improves this by leveraging the geometric structure of augmented graphs to include proximity information for positive and negative pairs, regularizing the learning process. SGCL uses three smoothing techniques to adjust penalties in the contrastive loss and employs a batch-generating strategy to efficiently train on large-scale graphs. Extensive experiments show SGCL outperforms recent baselines in unsupervised settings across various benchmarks.

7.4.10 To Supervise or Not to Supervise: Understanding and Addressing the Key Challenges of Point Cloud Transfer Learning

Participants: Souhail Hadgi, Maks Ovsjanikov.

In collaboration with Lei Li (Technical University of Munich).

This work [36] examines the challenges of point cloud transfer learning and proposes solutions. Classical transfer learning has significantly advanced 2D image analysis but has seen limited applicability in 3D data processing. While contrastive learning has gained prominence for point cloud transfer learning, existing methods have been studied only in limited scenarios, with little understanding of when and why they are effective. This work conducts the first in-depth investigation of supervised and contrastive pre-training strategies for 3D tasks, showing that layer-wise feature analysis reveals insights into the utility of trained networks. Based on these findings, a geometric regularization strategy is proposed to enhance the transferability of supervised pre-training, addressing key challenges in point cloud transfer learning.

7.4.11 Self-Supervised Dual Contouring

Participants: Ramana Sundararaman, Roman Klokov, Maks Ovsjanikov.

This work [42] introduces a self-supervised dual contouring framework. Learning-based isosurface extraction methods offer robust alternatives to axiomatic techniques but often rely on supervised training with axiomatically computed ground truths, inheriting their biases. To address this, Self-Supervised Dual Contouring (SDC) introduces a self-supervised training scheme for the Neural Dual Contouring framework. SDC employs novel self-supervised loss functions to optimize mesh vertices by enforcing consistency with distances to the generated mesh. SDC surpasses data-driven methods in capturing intricate details and handling input irregularities. Additionally, the self-supervised objective regularizes Deep Implicit Networks (DINs), improving the quality of implicit functions and detail preservation across input modalities. SDC also enhances single-view reconstruction by enabling joint training of the predicted SDF and output mesh.

7.4.12 Back to 3D: Few-Shot 3D Keypoint Detection with Back-Projected 2D Features

Participants: Maks Ovsjanikov.

In collaboration with Thomas Wimmer and Peter Wonka (from Technical University of Munich and KAUST).

This work [43] focuses on few-shot 3D keypoint detection using back-projected 2D features. Specifically, in this work, we propose to explore 2D foundation models for the task of keypoint detection on 3D shapes. A unique characteristic of keypoint detection is that it requires semantic and geometric awareness while demanding high localization accuracy. To address this problem, we propose, first, to back-project features from large pre-trained 2D vision models onto 3D shapes and employ them for this task. We show that we obtain robust 3D features that contain rich semantic information and analyze multiple candidate features stemming from different 2D foundation models. Second, we employ a keypoint candidate optimization module which aims to match the average observed distribution of keypoints on the shape and is guided by the back-projected features. The resulting approach achieves a new state of the art for few-shot keypoint detection on the KeyPointNet dataset, almost doubling the performance of the previous best methods.

7.4.13 Unsupervised Representation Learning for Diverse Deformable Shape Collections

Participants: Souhaib Attaiki, Maks Ovsjanikov.

In collaboration with Sara Hahner and Jochen Garcke (Fraunhofer SCAI, Sankt Augustin, Germany, and Institute for Numerical Simulation, University of Bonn, Germany).

This work [45] explores unsupervised learning methods for diverse deformable shape collections. Namely, we introduce a novel learning-based method for encoding and manipulating 3D surface meshes. Our method is specifically designed to create an interpretable embedding space for deformable shape collections. Unlike previous 3D mesh autoencoders that require meshes to be in a 1-to-1 correspondence, our approach is trained on diverse meshes in an unsupervised manner. Central to our method is a spectral pooling technique that establishes a universal latent space, breaking free from traditional constraints of mesh connectivity and shape categories. The entire process consists of two stages. In the first stage, we employ the functional map paradigm to extract point-to-point (p2p) maps between a collection of shapes in an unsupervised manner. These p2p maps are then utilized to construct a common latent space, which ensures straightforward interpretation and independence from mesh connectivity and shape category. Through extensive experiments, we demonstrate that our method achieves excellent reconstructions and produces more realistic and smoother interpolations than baseline approaches.

7.4.14 RIVQ-VAE: Discrete Rotation-Invariant 3D Representation Learning

Participants: Maks Ovsjanikov.

In collaboration with Mariem Mezghanni and Malika Boulkenafed (Dassault Systèmes).

This work [47] presents RIVQ-VAE, a framework for discrete rotation-invariant 3D representation learning. Building local surface representations for 3D shapes has gained attention in 3D vision, structuring complex shapes into sequences of simpler local geometries. Inspired by 2D discrete representation learning, recent methods use regular grids with discrete codes from a learnable codebook. However, these methods overlook local rigid self-similarities and orientation ambiguities, requiring large codebooks to capture variability in geometry and pose. To address this, a novel generative model is proposed, embedding local geometries in a rotation- and translation-invariant manner. This compact approach reduces redundancies, enabling the codebook to represent a wider range of structures. Careful architecture design ensures meaningful shape recovery and global consistency, with experiments showing significant performance improvements over baselines.

7.4.15 Deformation Recovery: Localized Learning for Detail-Preserving Deformations

Participants: Ramana Sundararaman, Maks Ovsjanikov.

In collaboration with Nicolas Donati (Ansys, France), Simone Melzi (University of Milano-Bicocca, Italy), Etienne Corman (Université de Lorraine, CNRS, Inria).

This work [31] proposes a novel data-driven approach for designing high-quality shape deformations using a coarse localized input signal, eliminating the need for global shape encoding. Observing that detail-preserving deformations can often be estimated without global context, we represent deformations using Jacobians in a one-ring neighborhood as input to a neural network. A series of MLPs with feature smoothing learns the Jacobian for detail-preserving deformations, and embeddings are recovered through a standard Poisson solve. This localized approach makes each point a training example, enabling lightweight supervision. Trained on a shape class, the method generalizes across object categories and supports tasks like refining shape correspondence, unsupervised deformation and mapping, and shape editing.

7.4.16 Memory-Scalable and Simplified Functional Map Learning

Participants: Robin Magnet, Maks Ovsjanikov.

This work [49] propose a memory-scalable and efficient functional map learning pipeline. Deep functional maps have become a leading framework for non-rigid shape matching, with recent advancements promoting consistency between functional and pointwise maps to improve accuracy. However, these methods rely on large dense matrices from soft pointwise maps, limiting efficiency and scalability. To address this, we propose a new method that avoids storing pointwise maps by leveraging the functional map structure. Additionally, we introduce a differentiable map refinement layer adapted from an axiomatic refinement algorithm, which can be used during training to enforce consistency between refined and initial maps. This approach is simpler, more efficient, and numerically stable, achieving near state-of-the-art results in challenging scenarios.

8 Bilateral contracts and grants with industry

8.1 Bilateral contracts with industry

8.1.1 Contract with Sanofi Inc.

Participants: Maks Ovsjanikov.

Title: Machine learning approaches for cryo-EM

Partner Institution(s): Sanofi Inc.

Date/Duration: 2023-2024

Additionnal info/keywords: Cryogenic electron microscopy (cryo-EM) allows the structure determination of antibody fragments bound to pharmaceutically relevant targets to accelerate drug discovery. The process of cryo-EM data analysis is time consuming and requires user input. To accelerate the rate of structure solution by cryo-EM, this project investigates machine learning approachesto fit and model the atomic coordinates of antibody fragments into the cryo-EM density.

The project funds one post-doctoral researcher for 2 years, jointly between Sanofi Inc., and Ecole Polytechnique (the employer of Maks Ovsjanikov).

8.1.2 Contract with DASSAULT SYSTEMES

Participants: Maks Ovsjanikov.

Title: Generative Models for the Guided Synthesis of Complex and Functional 3D Scenes

Partner Institution(s): DASSAULT SYSTEMES

Date/Duration: 2023-2026

Additionnal info/keywords: This thesis focuses on machine learning applied to 3D computer vision, specifically addressing challenges related to the automatic synthesis of 3D environments.

The project funds one PhD student for 3 years.

8.1.3 MEDITWIN with DASSAULT SYSTEMES

Participants: Maks Ovsjanikov, Mathieu Desbrun.

Title: MEDITWIN: Virtual human twins for medical applications

Partner Institution(s): DASSAULT SYSTEMES

Date/Duration: 2023-2028

Additionnal info/keywords: In the context of IPCEI on Health called MEDITWIN, Geomerix has started working on geometric measure theory and reduced models (Desbrun) and non-rigid registration (Ovsjanikov), with one student and two postdocs to be hired soon.

9 Partnerships and cooperations

9.1 International research visitors

9.1.1 Visits of international scientists

Other international visits to the team

Diana Marin

Status: PhD

Institution of origin: TU Wien

Country: Austria

Dates: End of January – April 2024

Context of the visit: Research collaboration leading to a publication in ACM Siggraph Asia

Mobility program/type of mobility: Research stay, under the supervision of Pooran Memari

9.1.2 Visits to international teams

Sabbatical programme

- Maks Ovsjanikov Visiting Researcher, Google DeepMind, Paris.

9.2 European initiatives

9.2.1 Horizon Europe

ERC Consolidator grant VEGA

Participants: Maks Ovsjanikov.

Title: VEGA: Universal Geometric Transfer Learning

Partner Institution(s):
- European Research Concil (ERC)

Date/Duration: 2024-2028

Additionnal info/keywords: In this project, we propose to develop a theoretical and practical framework for transfer learning with geometric 3D data. Most existing learning-based approaches, aimed at analyzing 3D data, are based on training neural networks from scratch for each data modality and application. Our main goal will be to develop universally-applicable methods by combining powerful pre-trainable modules with effective multi-scale analysis and fine-tuning, given minimal task-specific data. The overall key to our study will be analyzing rigorous ways, both theoretically and in practice, in which solutions can be transferred and adapted across problems, semantic categories and geometric data types.

9.3 National initiatives

Contrat de recherche Inria - SHOM

Participants: Steve Oudot.

Title: Traitement de nuage de points bathyémtriques (SMF et Lidar) par l'approche apprentissage automatique

Partner Institution(s):
- Service Hydrographique et Océanographique de la Marine (SHOM), Brest, France

Date/Duration: 2024-2028

Additionnal info/keywords: Ce projet a pour objectif de mieux appréhender, à l'aide de l'apprentissage automatique, la donnée bathymétrique sous forme de nuages de points pour améliorer la description des fonds marins et des zones côtières. Ce sujet est en lien avec le traitement des erreurs ponctuelles de la donnée bathymétrique et également avec l'utilisation de cette donnée pour la génération de modèles numériques de terrain.

AEx PreMediT

Participants: Steve Oudot.

Title: Precision Medicine using Topology

Partner Institution(s):
- CRESS, Hôtel-Dieu, France

Date/Duration: 2022-2025

Additionnal info/keywords: While recent advances in machine learning are opening promising prospects for precision medicine, the sometimes small size, sparsity, or partly categorical nature of the data involved pose some crucial challenges. The goal of PreMediT is to address these challenges by integrating information about the geometric and topological structure of the data into the machine learning pipelines.

ANR AI Chair AIGRETTE

Participants: Maks Osjanikov.

Title: Analyzing Large Scale Geometric Data Collections

Partner Institution(s):
- ANR

Date/Duration: 2020-2024

Additionnal info/keywords: Motivated by the deluge of 3D data using geometric representations (point clouds, triangle, quad meshes, graphs...) that are ill-suited for modern applications, we are developing efficient algorithms and mathematical tools for analyzing diverse geometric data collections.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

General chair, scientific chair

- Mathieu Desbrun (cochairing with Jacques-Olivier Lachaud) for Year of Geometry, funded by the GDR IFM, with its capstone *Geometry and Computing* conference at the CIRM in October 2024.

Member of the organizing committees

- Steve Oudot co-organizer (with Claire Amiot, Thomas Brüstle, Sergio Estrada and Luis Scoccola) of BIRS workshop Representation Theory and Topological Data Analysis (24w5241), April 7-12, Banff, Canada.

10.1.2 Scientific events: selection

Member of the conference program committees

- Pooran Memari for ACM Siggraph 2024
- Pooran Memari for Eurographics 2024
- Steve Oudot for International Symposium on Computational Geometry (SoCG) 2024

10.1.3 Journal

Member of the editorial boards

- Pooran Memari Associate Editor of Computer Graphics Forum (CGF), since April 2021.
- Pooran Memari Associate Editor of Graphical Models Journal, Elsevier, April 2023 – May 2024.
- Mathieu Desbrun Associate Editor of ournal of Geometric Mechanics, AIMS, 2024.
- Maks Ovsjanikov Associate Editor, Transactions on Visualization and Computer Graphics journal, since 2020.
- Steve Oudot Associate Editor of Journal of Computational Geometry.

10.1.4 Invited talks

- Pooran Memari Invited talk at the Geometry & Computing conference, CIRM Luminy, October 2024.
- Mathieu Desbrun, invited talk at the annual GDR IFM meeting in 2024.
- Steve Oudot Invited speaker at the 9th European Congress of Mathematics (9ECM), Seville, July 2024.
- Steve Oudot Plenary speaker at the 21st International Conference on Representations of Algebras (ICRA), Shanghai, August 2024.
- Steve Oudot Invited speaker at the workshop Representation theory - combinatorial aspects and applications to TDA, NTNU, Trondheim, December 2024.
- Steve Oudot Seminar speaker in the Mathematical Institute of the University of Oxford, January 2024.

10.1.5 Research administration

- Maks Ovsjanikov Fellow of ELLIS, senior member of the European society for top AI researchers, since 2023.
- Pooran Memari Member of the Board of the French Chapter of Eurographics (EGFR), since October 2024.
- Pooran Memari Co-responsible for the Interaction, Graphics & Design (IGD) master's program at IP-Paris, since September 2024.
- Steve Oudot member of the Conseil Académique of IP Paris, representing Inria

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- Master: Steve Oudot, Computational Geometry and Topology, 18h eq-TD, M2, MPRI;
- Master: Maks Ovsjanikov, Geometry Processing and Geometric Deep Learning, M2, MVA;
- Master: Steve Oudot, Topological data analysis, 45h eq-TD, M1, École polytechnique, France;
- Master: Mathieu Desbrun, Digital Representation and Analysis of Shapes, M2, École polytechnique, France;
- Master: Mathieu Desbrun, Computer Animation, M2, École polytechnique, France;
- Master: Pooran Memari, Digital Representation and Analysis of Shapes, M2, École polytechnique, France;
- Master: Pooran Memari, Computer Science refresher course at Artificial Intelligence and Advanced Visual Computing Master Program, M2, École polytechnique, France;
- Master: Maks Ovsjanikov, Artificial Intelligence and Advanced Visual Computing, École polytechnique, France;
- Undergrad-Master: Steve Oudot, Algorithms for data analysis in C++, 22.5h eq-TD, L3/M1, École Polytechnique, France.

10.2.2 Supervision

- PhD in progress: Julie Mordacq, Analyse Topologique des Données et Apprentissage Machine pour analyser et prédire des transitions de phase en n-dimensions, Institut Polytechnique de Paris. Started Sept. 2022. Steve Oudot and Vicky Kalogeiton (Vista, LIX).
- PhD in progress: Jingyi Li, Invariants algébriques effectifs pour la persistance multi-paramètre, Institut Polytechnique de Paris. Started Nov. 2023. Steve Oudot.
- PhD: Souhaib Attaiki, LIX. defended: March 2024?. Maks Ovsjanikov.
- PhD in progress: Nasim Bagheri Shouraki, Application of neurocognition to study the effectiveness of geometric tactile 2D patterns in navigation maps and instructions for Visually Impaired Individuals, IP Paris. Start date: October 2024. Pooran Memari and Panos Mavros (Telecom Paris).
- PhD in progress: Theo Braune, École Polytechnique, Palaiseau. Mathieu Desbrun.
- PhD: Diego Gomez, École Polytechnique, Palaiseau. Defended: September 2024?. Maks Ovsjanikov.
- PhD in progress: Souhail Hadgi, École Polytechnique, Palaiseau. Maks Ovsjanikov.

- PhD: Robin Magnet, LIX. Defended: May 2024?. Maks Ovsjanikov.
- PhD in progress: Leopold Maillard, Dassault Systèmes. Maks Ovsjanikov.
- PhD in progress: Tim Scheller, École Polytechnique, Palaiseau. Maks Ovsjanikov.

10.2.3 Juries

- Mathieu Desbrun reviewer and jury member for Colin Weil-Duflos, Université Savoie Mont-Blanc.
- Pooran Memari Admission Jury for Masters & PhD-Track IGD (Interaction, Graphics & Design), IP-Paris, since 2020.
- Pooran Memari PhD Jury for Clément Chomicki, Université Gustave Eiffel, LIGM UMR8049 (28/11/2024).
- Pooran Memari PhD Jury for Bastien Doignies, Université Lyon 1 (25/11/2024).
- Pooran Memari Recruitment Committee for Assistant Professors at LORIA, Faculty of Sciences and Technologies, University of Lorraine (5/2024).
- Pooran Memari is a member of the Jury d'admission Masters & PhD Track IGD (Interaction, Graphics & Design), IP-Paris (Since 2020).

11 Scientific production

11.1 Major publications

[1] K. Bai, C. Wang, M. Desbrun and X. Liu. 'Predicting high-resolution turbulence details in space and time'. In: *ACM Transactions on Graphics* 40.6 (Dec. 2021), p. 200. DOI: 10.1145/3478513.3480492. URL: https://hal.inria.fr/hal-03551723.

[2] M. B. Botnan, S. Oppermann, S. Oudot and L. Scoccola. 'On the bottleneck stability of rank decompositions of multi-parameter persistence modules'. In: *Advances in Mathematics* 451 (Aug. 2024), p. 109780. DOI: 10.1016/j.aim.2024.109780. URL: https://inria.hal.science/hal-03908009.

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[4] J. Chen, F. Schäfer, J. Huang and M. Desbrun. 'Multiscale Cholesky Preconditioning for Ill-conditioned Problems'. In: *ACM Transactions on Graphics* 40.4 (19th July 2021), Art. 91. DOI: 10.1145/3450626.3459851. URL: https://hal.archives-ouvertes.fr/hal-03277277.

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[9] X. Huang, T. Ritschel, H.-P. Seidel, P. Memari and G. Singh. 'Patternshop: Editing Point Patterns by Image Manipulation'. In: *ACM Transactions on Graphics* 42.4 (26th July 2023), pp. 1–14/53. DOI: 10.1145/3592418. URL: https://hal.science/hal-04235133.

[10] J. Leygonie, S. Y. Oudot and U. Tillmann. 'A Framework for Differential Calculus on Persistence Barcodes'. In: *Foundations of Computational Mathematics* (2021). DOI: 10.1007/s10208-021-09522-y. URL: https://hal.archives-ouvertes.fr/hal-02304300.

[11] W. Li, Y. Ma, X. Liu and M. Desbrun. 'Efficient kinetic simulation of two-phase flows'. In: *ACM Transactions on Graphics* 41.4 (2022), p. 114. DOI: 10.1145/3528223.3530132. URL: https://hal.archives-ouvertes.fr/hal-03828392.

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11.2 Publications of the year

International journals

[17] F. Ahmadi, M.-E. Shiri, B. Bidabad, M. Sedaghat and P. Memari. 'Ricci flow-based brain surface covariance descriptors for diagnosing Alzheimer's disease'. In: *Biomedical Signal Processing and Control* 93 (July 2024), p. 106212. DOI: 10.1016/j.bspc.2024.106212. URL: https://hal.science/hal-04794184 (cit. on p. 20).

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International peer-reviewed conferences

[34] M. Behmanesh and M. Ovsjanikov. 'Smoothed Graph Contrastive Learning via Seamless Proximity Integration'. In: LoG 2024 - Learning on Graphs Conference. Virtual, France, 26th Nov. 2024. URL: https://hal.science/hal-04812977 (cit. on p. 27).

[35] C. Grenier, P. Memari and B. Sauvage. 'Ink-Edit: Interactive color-constrained textures editing'. In: *SA '24: SIGGRAPH Asia 2024 Technical Communications*. Siggraph Asia, technical communications, Tokyo, Japan, décembre 2024. Tokyo, Japan, 19th Nov. 2024. DOI: 10.1145/3681758.3697991. URL: https://hal.science/hal-04792161 (cit. on p. 20).

[36] S. Hadgi, L. Li and M. Ovsjanikov. 'To Supervise or Not to Supervise: Understanding and Addressing the Key Challenges of Point Cloud Transfer Learning'. In: *Lecture Notes in Computer Science*. ECCV 2024 - European Conference on Computer Vision. Vol. LNCS-15136. Computer Vision – ECCV 2024 18th European Conference. MiCo Milano, Italy: Springer Nature Switzerland, 25th Oct. 2025, pp. 146–163. DOI: 10.1007/978-3-031-73229-4_9. URL: https://hal.science/hal-04863811 (cit. on p. 27).

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Conferences without proceedings

[44] J. Chen, J. Gain, J.-M. Chomaz and M.-P. Cani. 'TwisterForge: controllable and efficient animation of virtual tornadoes'. In: MIG 2024 - The 17th Annual ACM SIGGRAPH Conference on Motion, Interaction and Games. Arlington (USA), United States, 2024, pp. 1–11. DOI: 10.1145/3677388.3696335. URL: https://hal.science/hal-04778664 (cit. on p. 22).

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Reports & preprints

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