Exploiting
the unreasonable effectiveness of
geometry in computing

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1

The Role of Geometry

Geometry is key in **many** scientific fields

- at the crossroad of several sciences
  - observable invariants/symmetries of the world around us
- "mothertongue" of most physical theories
  - from E&M to General Relativity, differential structures and symmetry groups are central
- studied for centuries
  - Cartan, Poincaré, Lie, Hodge, de Rham, Noether…
- mostly differential geometry, though
  - based on differential and integral calculus

Large body of work available on geometry
… alas, discrete counterpart lacking in substance

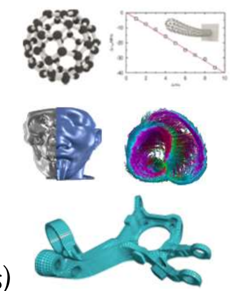
2

2

Continuum vs. Finitude

"Discrete" differential geometry?

- *finite-dimensional counterpart* to continuous theory
  - where we *leverage* differential understanding
- geometry as a guiding principle to **discretization**
  - discretize the geometric principles
    - predictive power guaranteed
  - NOT THE PDES DIRECTLY !!
    - PDEs often hide structures completely



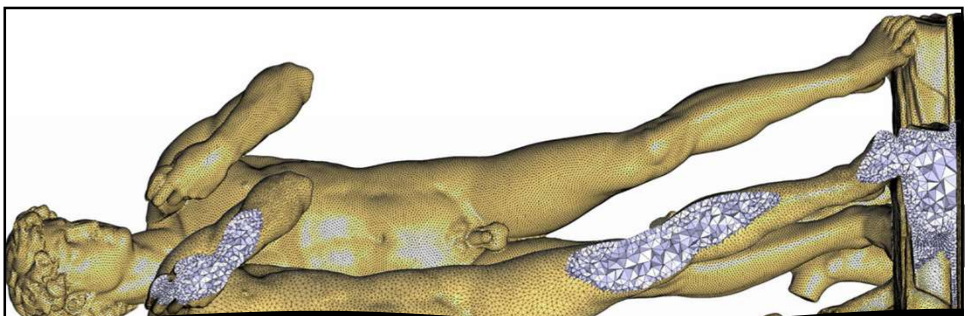
Of both academic and practical interests

- education *(simple discrete analogs)*
- Hollywood *(cool graphics, fast animation)*
- computational science *(new numerical methods)*

Next, four vignettes to illustrate a few aspects…

3

3

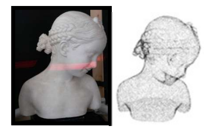


Vignette 1:
Surface Flows

4

4

Surface Denoising



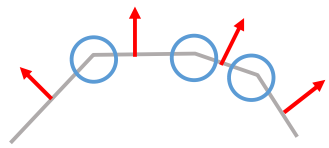
Scanners introduce noise to geometry

- can be smoothed though *non-linear diffusion*

$$\dot{\mathbf{x}} = -\kappa\ \mathbf{n}$$

How to "reproduce" this equation on a PWL surface?

- what's the curvature? normal?
  - not even collocated...
- local polynomial fitting just bad...



What about a geometric way?

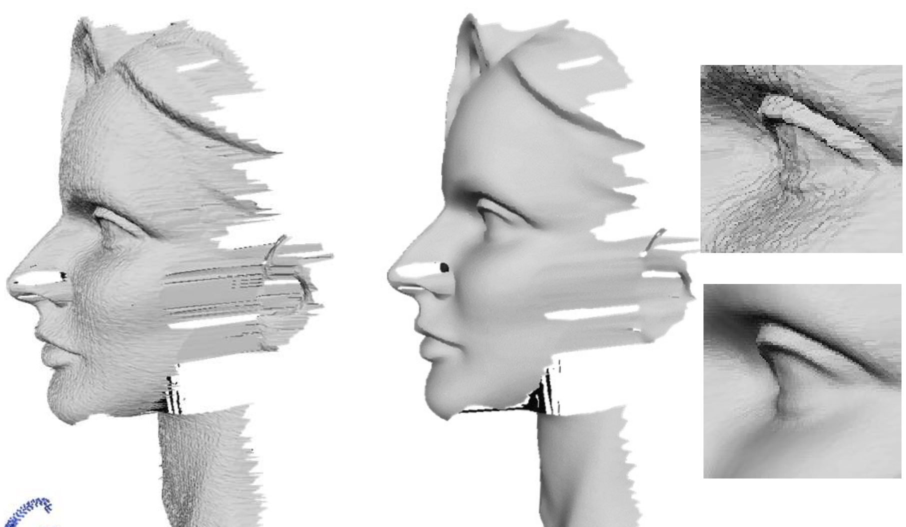
- simply reduce **area** (or length for curves)
  - and area trivial to compute exactly for triangles
- *variational* definition of mean curvature vector
  - L^2-minimization of area known to Darboux in '99

$$\kappa\mathbf{n} \sim \nabla\mathcal{A}$$

5

5

Real-life Example



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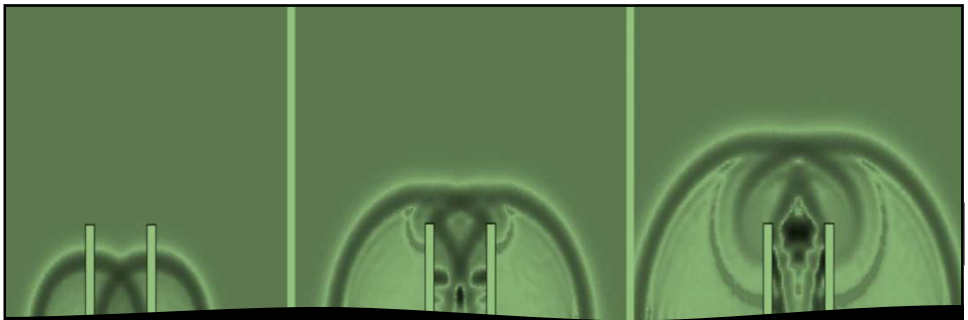


Vignette 2:
Calculus on Meshes

7

October 29, 1675

Leibnitz wrote:

Utile erit scribit ∫ pro Omnia

A revolution ensued
- from discrete, to differential modeling
- easy to manipulate with pen & paper

Fast-forward three centuries: advent of computers…
- computers deal with sets of finite numbers
- need for **discretization**
  - differential equations are not usable as is

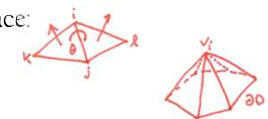
Strange cycle…

8

Discrete Differential Modeling

Discrete, yet differential quantities:

- they "live" at special places, as distributions
  - again, think of a piecewise linear surface:
    - mean curvature at edges only
    - Gaussian curvature at vertices only



- they can be handled through **integration**
  - integration calls for k-forms (antisymmetric tensors)
    - you've heard of it before: $\int f(x)\,dx$
  - not often used for computations, though…

Need framework *linking* discrete & continuous worlds…

Exterior Calculus

Foundation of calculus on smooth manifolds

- historically, purpose was to extend div, curl, grad
  - Poincaré, Cartan, Lie, …
- building blocks: *differential forms* (antisymmetric tensors)
  - objects begging to be integrated (k-forms over k-D sets)
  - not obscured by coordinate-system dependent notations
    - in fact, often correspond to measurements (e.g., flux)
  - Hodge decomposition, modern diff. geometry, …
    - untangles topology and metric
- only a few basic operators are needed
  - $\mathbf{d}$, $\star$, $\wedge$, $\flat/\sharp$, i_X, $\mathcal{L}_X$ (see [Abraham, Marsden, Ratiu], ch. 6-7)

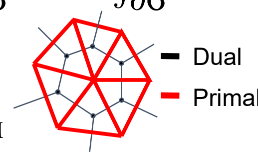
Discrete Exterior Calculus

Foundations: discrete differential forms

- mesh as computational structure
  - chains as proxies for domains

  - store k-forms as integrated values over simplices
    - cochains extends point sampling to "simplex sampling"
- basic operators: d (exterior derivative) and ⋆ (Hodge star) through heavy use of **adjointness**
  - d through Stokes
    - d is a topological operator, hence **exact**
    - exact link to (co)homology [Munkres]
  - simplest Hodge duality via **mesh duality**
    - exploits Delaunay/Voronoi duality – or FEEM

$$\int_\sigma d\omega = \int_{\partial\sigma} \omega$$



11

Discrete De Rham Sequence

Discrete calculus through linear algebra:

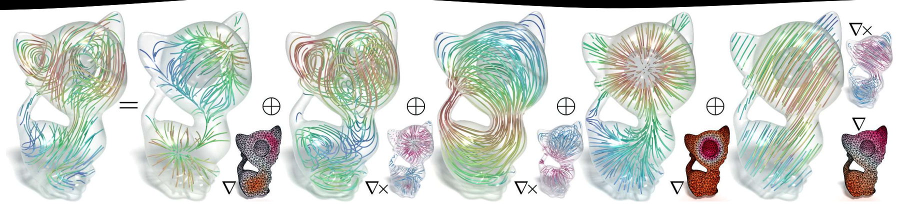
point-based scalar field	∇ →	*edge-based* **vector field**	$\nabla\times$ →	*face-based* **vector field**	$\nabla\cdot$ →	*cell-based* scalar field
↕ ★		↕ ★		↕ ★		↕ ★
cell-based scalar field	← $\nabla\cdot$	*face-based* **vector field**	← $\nabla\times$	*edge-based* **vector field**	← ∇	*point-based* scalar field

- simple exercise in matrix assembly
- discrete Hodge theory particularly simple
  - cohomology, harmonic forms, etc…
- Whitney basis fcts extending FE picture [Arnold]
- can be made higher-order (through subdivision-based Whitney bases) or even spectral bases

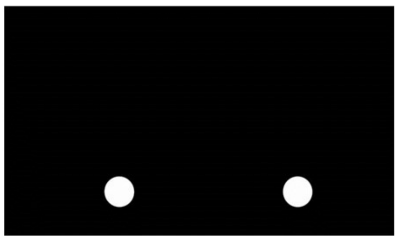
12

12

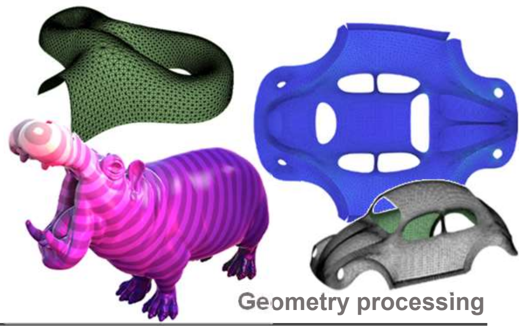
Lots of Applications



Hodge-Morrey-Friedrichs decomposition

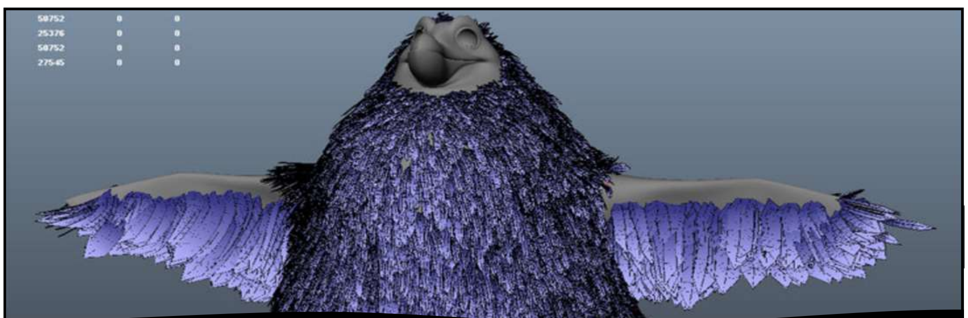


Navier-Stokes simulation



Geometry processing

13



Vignette 3:

Grooming and Cartan's Development

14

14

How Do You Grow Hair?

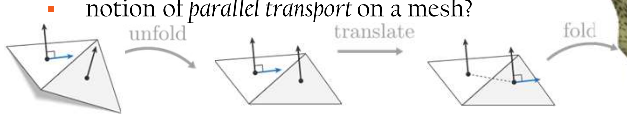
15

15

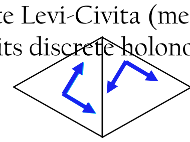
Vector Field Processing

How to design tangent {vector|<u>direction</u>|frame} fields?

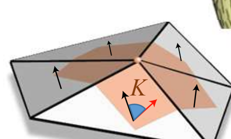
- need to control smoothness, and singularities…
- geometry to the rescue: use of **connection o**
  - notion of *parallel transport* on a mesh?

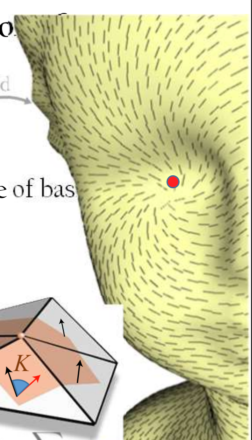


  - code for it? just store an angle per edge (change of bas
  - discrete Levi-Civita (metric) connection
  - … and its discrete holonomy



simple rotation of coordinate frame





$$K = 2\pi - \sum_a \gamma_a$$

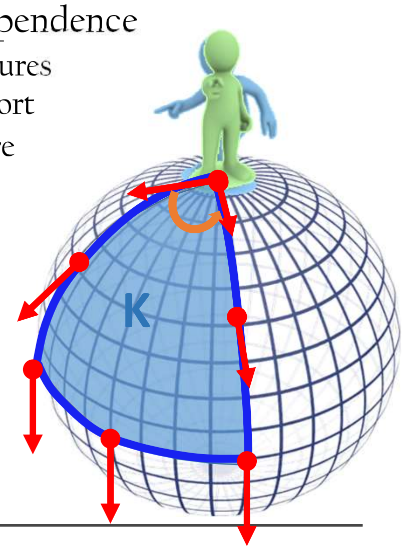
16

16

[Holonomy for our Planet]

Holonomy: measure of path-dependence

- for a (contractible) loop, measures angle difference after transport
- represents integrated curvature
  - integral of Gaussian curvature for canonical Levi-Civita



17

Vector Field Processing

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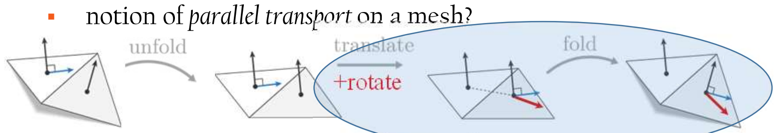
- need to control smoothness, and singularities…
- geometry to the rescue: use of **connection one-forms**
  - notion of *parallel transport* on a mesh?



  - code for it? just store an angle per edge
  - discrete Levi-Civita (metric) connection, & discrete holonomy
- extension to an arbitrary principal connection?
  - add adjustment rotation during the translation…
  - *integrated* connection 1-form
    - see Discrete Exterior Calculus

18

18

Discrete Trivial Connection

We can encode *adjustment* to Levi-Civita…

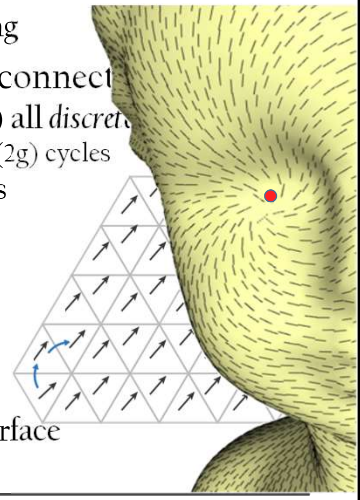
- one rotation angle per edge crossing

to cancel holonomy of Levi-Civita connect…

- forcing zero holonomy on (almost) all *discret…*
  - contractible (V) & noncontractible (2g) cycles
- *except* for a few chosen singularities
  - Poincaré-Hopf theorem
- and get smallest adjustments!
  - L2-minimum of adjustment vector for "straightest" solution

Now, path-independent transport!

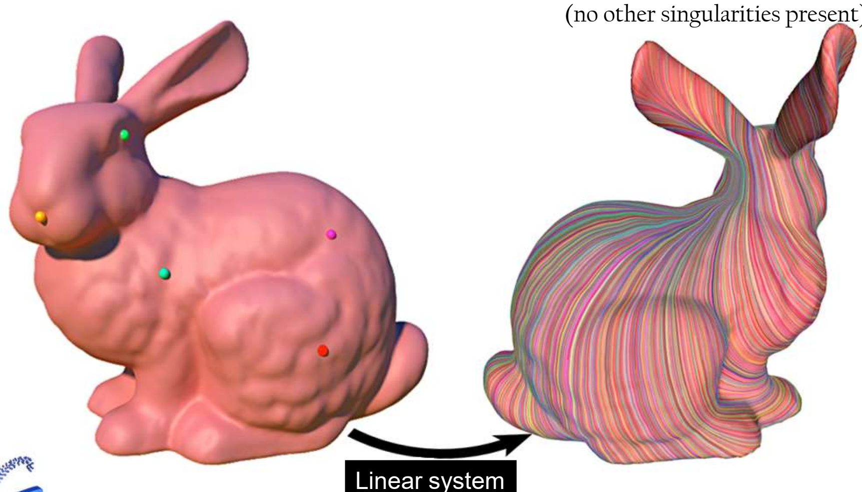
- creating discrete vector field on surface



19

Growing Hair on a Bunny…

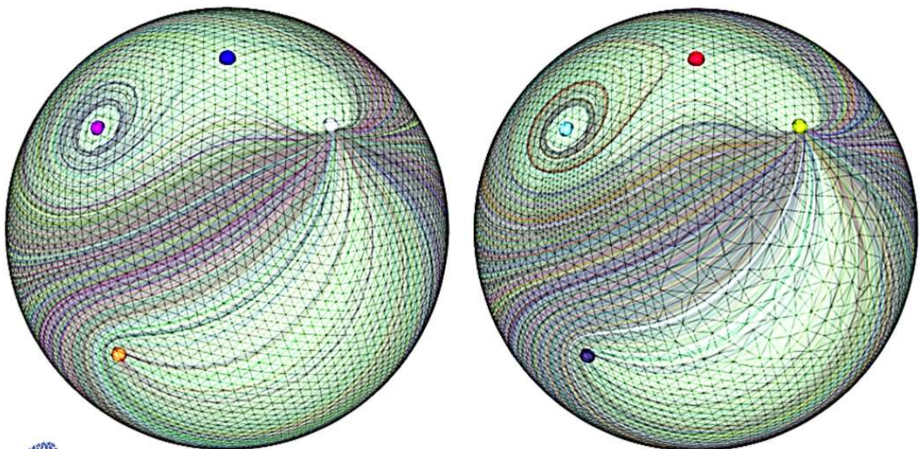
Resulting trivial connection
(no other singularities present)



20

20

Robustness to Meshing Too!



21

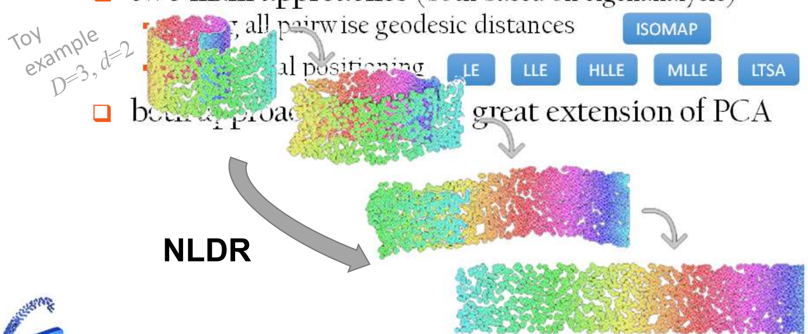
Recent Use

22

Connections for Data Science?

Dimensionality Reduction:
mapping data from $\mathbb{R}^D$ to $\mathbb{R}^d$, with $d \ll D$

- i.e., finding a *Euclidean embedding* in low dimension
  - in a "most isometric" way (*try to preserve pairwise distances*)
- two main approaches (both based on eigenanalysis)
  - all pairwise geodesic distances ISOMAP
  - al positioning LE LLE HLLE MLLE LTSA
- great extension of PCA

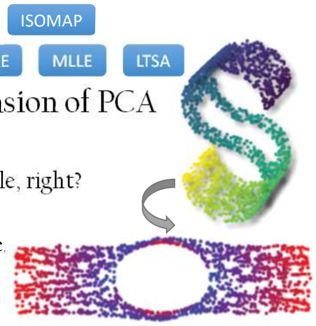


23

Connections for Data Science?

Dimensionality Reduction:
mapping data from $\mathbb{R}^D$ to $\mathbb{R}^d$, with $d \ll D$

- i.e., finding a *Euclidean embedding* in low dimension
  - in a "most isometric" way (e.g., *try to preserve pairwise differences*)
- two main approaches (both based on eigenanalysis)
  - using all pairwise geodesic distances ISOMAP
  - using local positioning LE LLE HLLE MLLE LTSA
- both approaches hailed as great extension of PCA
  - although they both have pros and cons
    - planar pointsets *should* be trivial to handle, right?
    - pointsets on a developable surfaces too
    - not robust to irregular sampling or noise
    - or even holes!



24

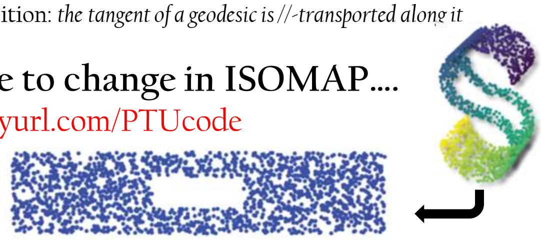
Connection-based ISOMAP

Key idea: Parallel transport to find geodesic distances

- use *intrinsic neighborhoods* to estimate tangent spaces
- define *metric connection* between tangent spaces
  - rotation of a tangent space frame to get to a parallel one nearby
- geodesic distances easy to evaluate (instead of Dijkstra's)
  - through Cartan's development (unfold path in tangent space)
    - intuition: *the tangent of a geodesic is //-transported along it*

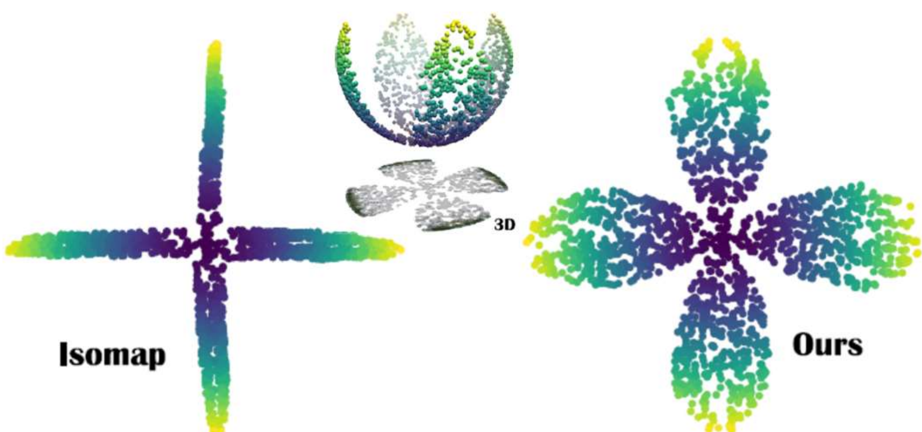
6 lines of code to change in ISOMAP….

- https://tinyurl.com/PTUcode



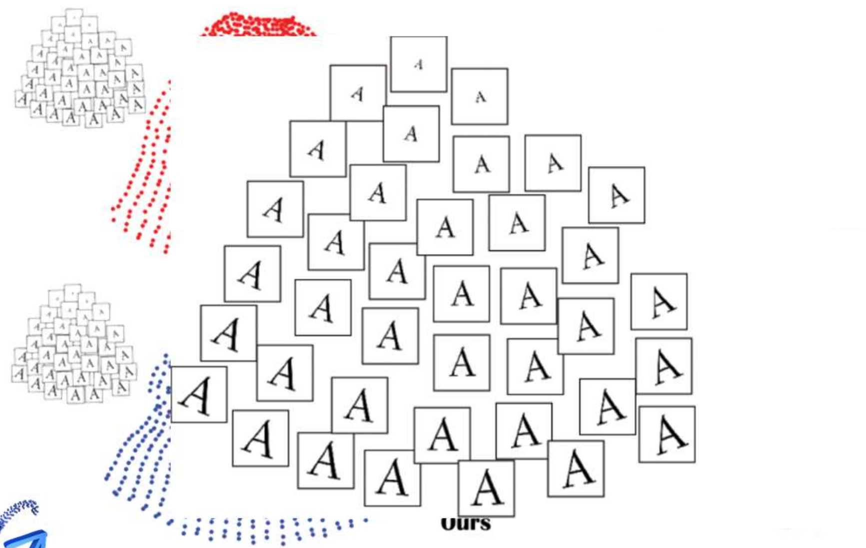
25

Result on 3D Data

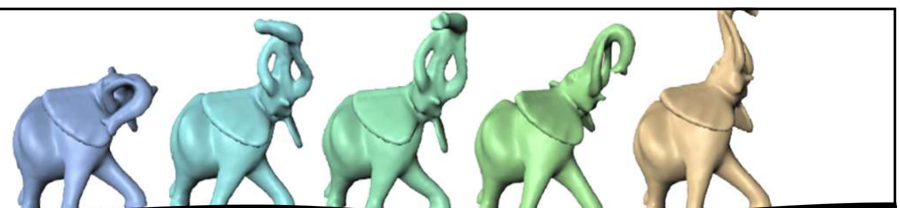


26

On «Real» Data (letter A rotated/scaled)



27



Vignette 4:
Discrete Mechanics

28

28

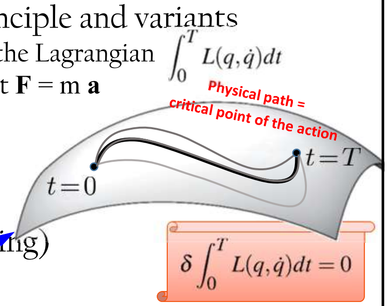
Variational Nature of Mechanics

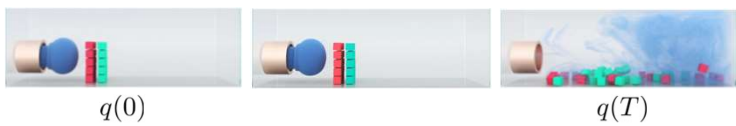
The basic structure of mechanics is geometric

- Hamilton's stationary action principle and variants
  - motion extremizes the integral of the Lagrangian $\int_0^T L(q,\dot{q})dt$
  - Euler-Lagrange eqs are nothing but **F** = m **a**
    - but change an IVP into a BVP

Numerical solvers?

- leverage geometric properties!
- just discretize paths (time stepping)





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- Hamilton's stationary action principle and variants
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  - Euler-Lagrange eqs are nothing but **F** = m **a**
    - but change an IVP into a BVP

Numerical solvers?

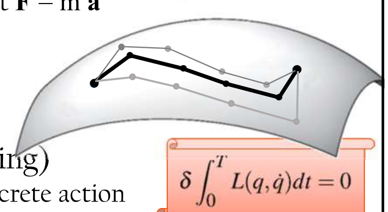
- leverage geometric properties!
- just discretize paths (time stepping)
  - and use quadrature to evaluate discrete action

solve DEL (a time integrator)

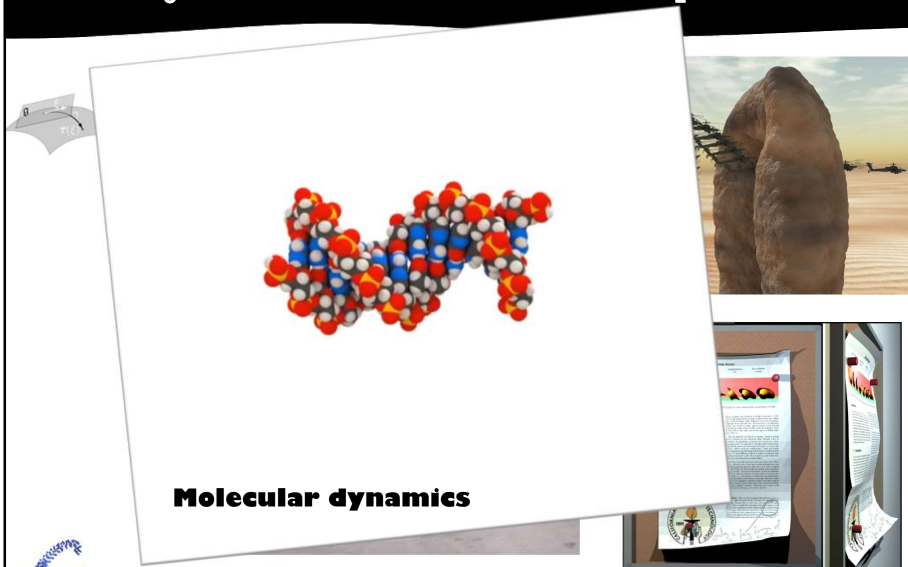
$L_d(q_k, q_{k+1}) = \int_{t_k}^{t_{k+1}} L(q,\dot{q})dt$

$(q_{k-1}, q_k) \rightarrow q_{k+1}$

- make for better numerics
  - preserves symplecticity
  - conserves energy remarkably well
  - preserves symmetries through (discrete) Noether's theorem



Very Successful Developments

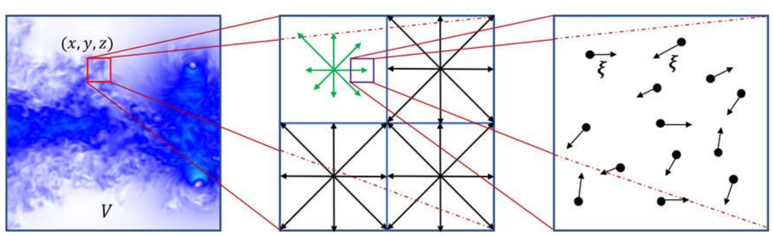


31

31

Boltzmann Discretization

Introducing a <u>mesoscopic</u> description of fluid



Macroscopic view	**Mesoscopic view**	**Microscopic view**
Navier-Stokes equations	Boltzmann equation	Molecular dynamics

32

32

Boltzmann Discretization

Introducing a mesoscopic description of fluid

- based on a statistical-mechanics (a.k.a. kinetic) model
  - use a **particle distribution function** $f(\boldsymbol{x}, \boldsymbol{v}, t)$
    - probability for a particle to be at $\boldsymbol{x}$ at time t with a velocity $\boldsymbol{v}$
  - Boltzmann transport equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f = \Omega(f) + \boldsymbol{F} \cdot \nabla_{\boldsymbol{v}} f$$

    - ~~amounts to (near) incompressible Navier-Stokes~~
      - ar… st sa… xw… mann distribution

streaming — particles going straight

collision — particles collide

forcing — particles pushed around

Macroscopic quantities simple to recover!

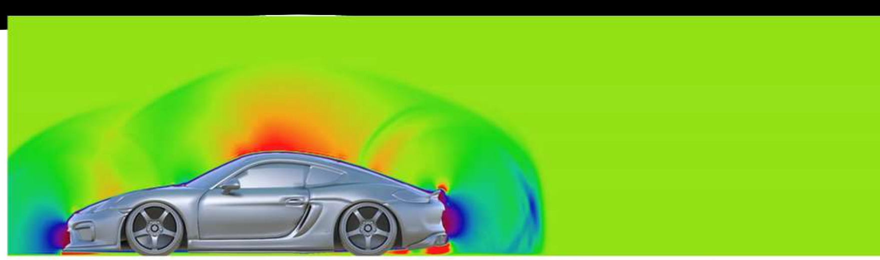
$$\rho(\boldsymbol{x}, t) = \int f d\boldsymbol{v} \qquad \rho\boldsymbol{u}(\boldsymbol{x}, t) = \int \boldsymbol{v} f d\boldsymbol{v}$$

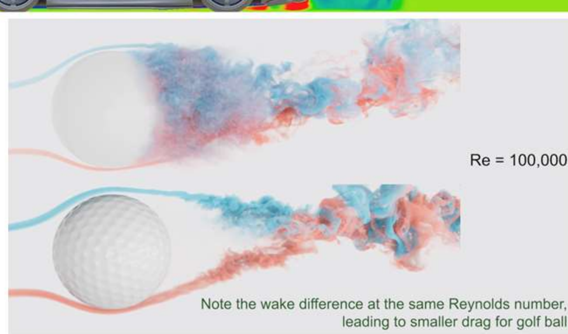
note: "$\boldsymbol{u}$=0" ≠ no motion!

33

33

Turbulence, Guggling, Bubbling

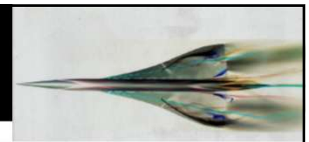




34

34

Concorde Test



35

35

Wrapping Up

DDG useful for computing in high & low dims

- **computing through the lens of geometry**
  - geometry-powered numerics
- blurring the line between discrete & differential treatments
- non-linearity dealt with more systematically
  - exploiting connections, in particular

But… it requires quite a bit of knowledge!

- math, physics, linear algebra, etc…
  - to the young people out there: learn it while you can
- even machine learning recently
  - space-time upsampling for flows, for instance
- and creativity too

Trained with a very different flow!

36

Acknowledgements

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- Fernando de Goes
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- Jerry Marsden
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37

QUESTIONS?

38

38