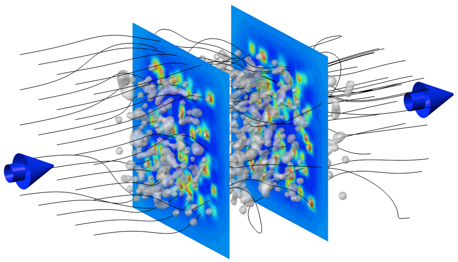
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Institut für Baustoffe
Institute for Building Materials

Fluid Dynamics in Manifolds Using Lattice Kinetic Theory



Miller Mendoza Jiménez

Collaborations: Jens-Daniel Debus, Hans J. Herrmann, Sauro Succi, Jose D. Muñoz C.

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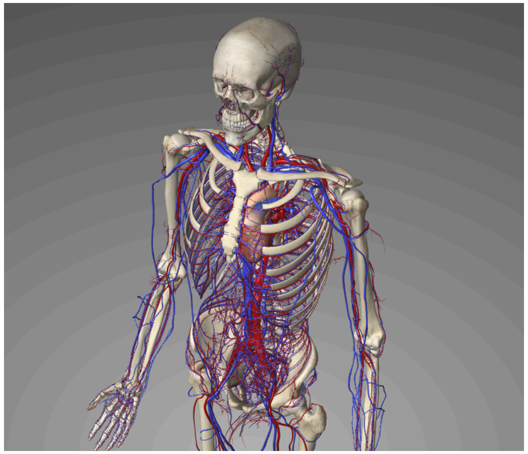
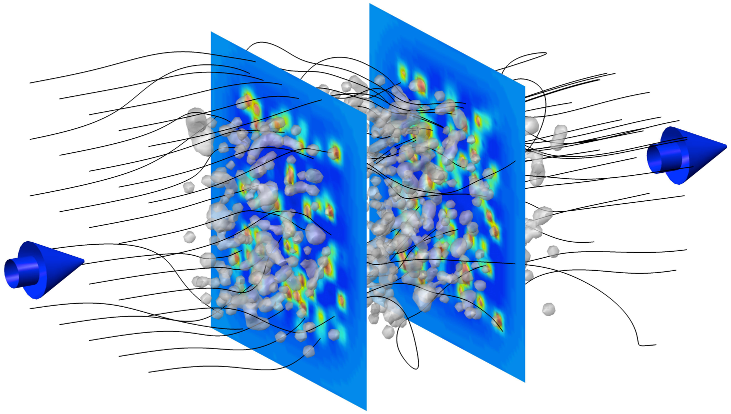
Fluid Dynamics Examples

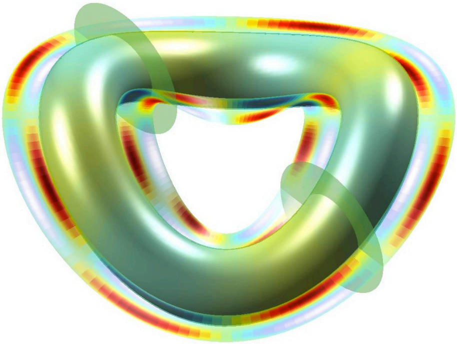
Vessels



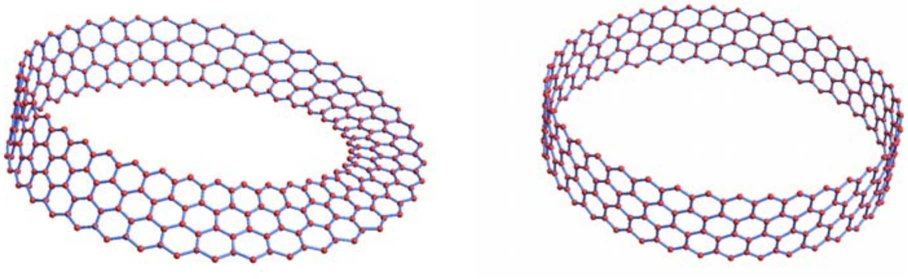
Generalized curved spaces



Curved boundary conditions

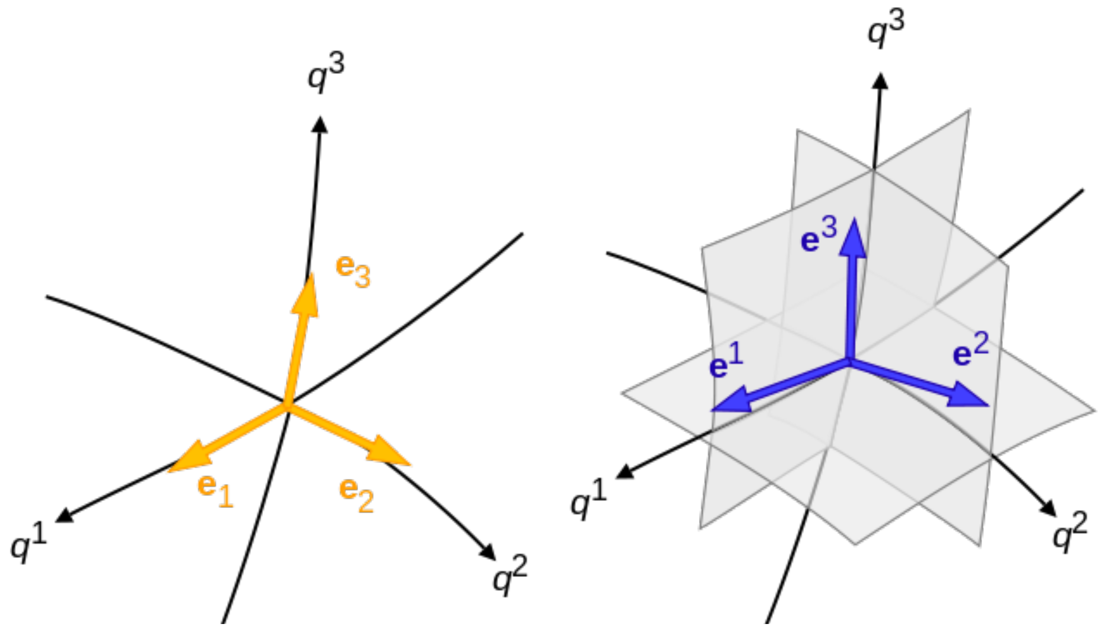


Graphene Semiconductor
Möbius band



Key: Working with contravariant components of vectors

$$\vec{v} = v^i \vec{e}_i = v_i \vec{e}^{\,i}$$



$$\vec{v}^{\,2} = v^j v^i \vec{e}_i \cdot \vec{e}_j = v^j v^i g_{ij}$$

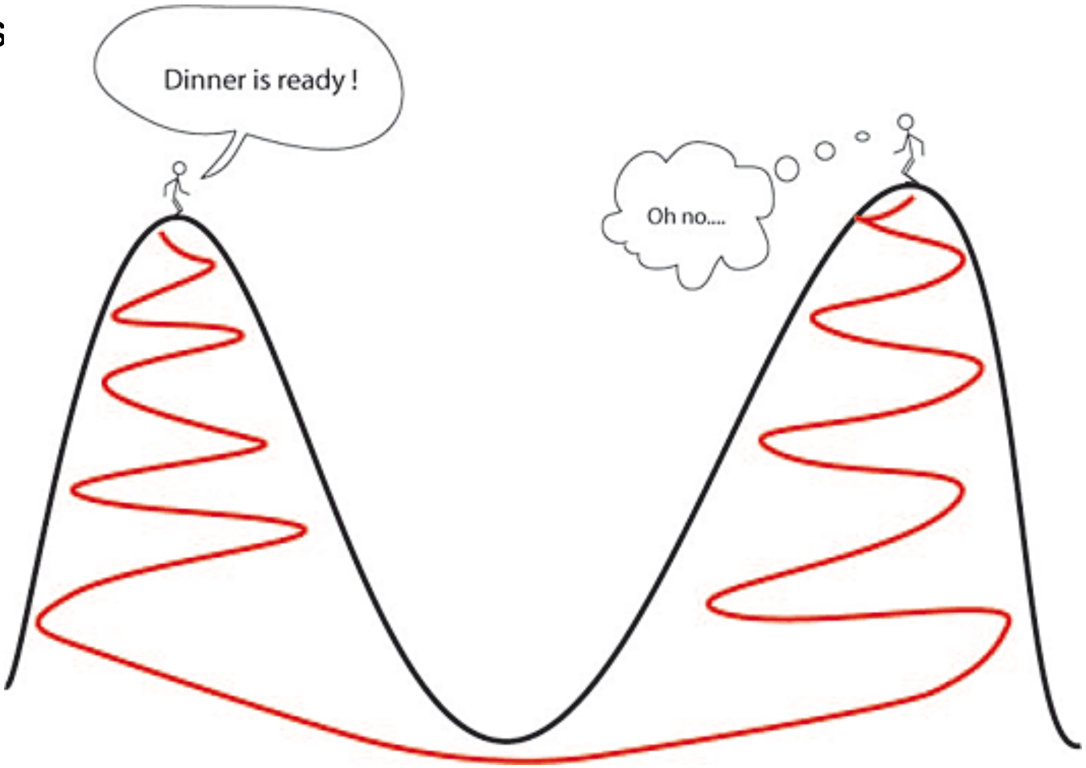
Metric tensor

Measure of the distance

Two infinitesimally separated points

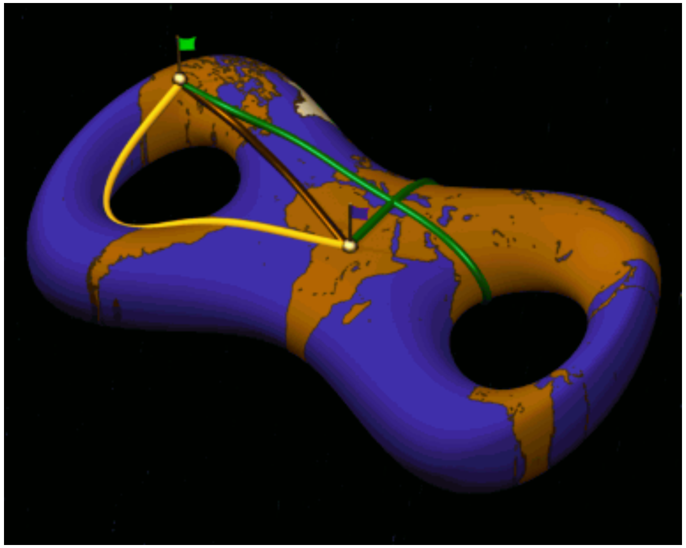
$$ds^2 = g_{ij} dx^i dx^j$$

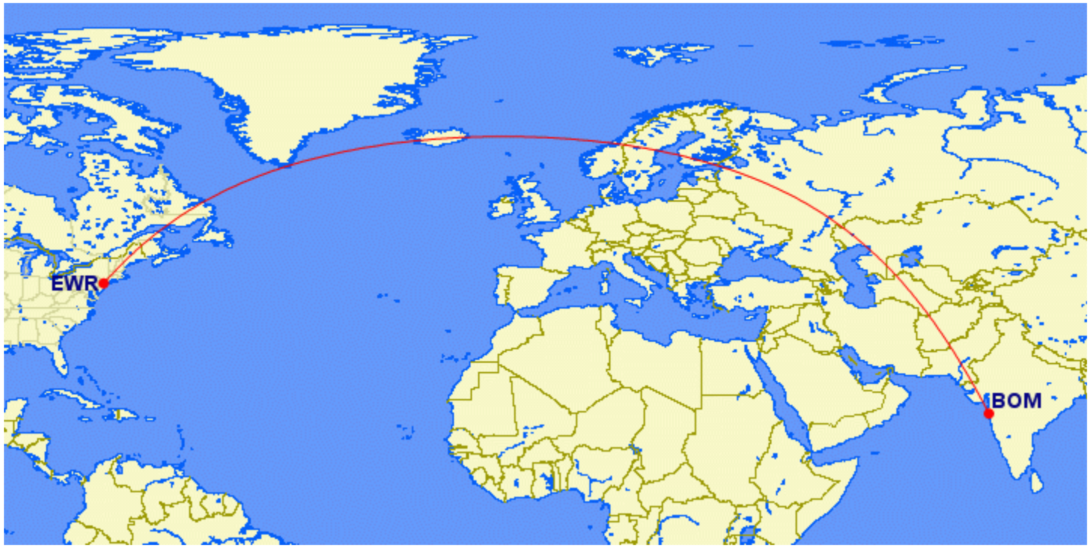
$$\Delta s = \int_{\Omega} \sqrt{g_{ij} \frac{dx^i}{d\lambda} \frac{dx^j}{d\lambda}} d\lambda$$



Two separated points, λ is an arbitrary parameter, and Ω is the trajectory joining them.

Geodesics: Shortest path





Geodesic equation:

$$\delta(\Delta s) = \delta \int_\Omega \sqrt{g_{ij} \frac{dx^i}{d\lambda} \frac{dx^j}{d\lambda}} d\lambda = 0$$

$$\frac{d^2 x^i}{d\lambda^2} = -\Gamma^i_{kl} \frac{dx^k}{d\lambda} \frac{dx^l}{d\lambda}$$

For a particle:

Geodesic equation contains inertial forces:

$$\frac{dp^i}{dt} = -\Gamma^i_{kl} p^k p^l + F^i_{ext}$$

Boltzmann Equation in Manifolds

Taking into account that particles move along geodesics:

$$\partial_t f + \xi^i \partial_i f - \Gamma^i_{jk} \xi^j \xi^k \partial_{\xi^i} f = \mathcal{C}(f)$$

Add a forcing term

BGK:
$\mathcal{C} = -(1/\tau)(f - f^{\mathrm{eq}})$

This is also the case for the Boltzmann equation in curvilinear coordinates (polar, cylindrical and spherical coordinates).

In thermodynamic equilibrium

$$f^{\mathrm{eq}} = \frac{\sqrt{g}\rho}{(2\pi\theta)^{3/2}} \exp\left[-\frac{1}{2\theta} g_{ij}(\xi^i - u^i)(\xi^j - u^j)\right]$$

P. J. Love and D. Cianci, Phil. Trans., of the Royal Soc. A 369, 2362 (2011).

Anisotropic Gaussian Shape:
Hermite polynomials expansion possible !!

ξ^i	: Microscopic Velocity
u^i	: Macroscopic Velocity
θ	: Normalized Temperature

Expansion and Lattice Configuration

$$f^{\mathrm{eq}} = \frac{\sqrt{g}\rho}{(2\pi\theta)^{3/2}} \exp\left[-\frac{1}{2\theta} g_{ij}(\xi^i - u^i)(\xi^j - u^j)\right]$$

$$f(x^i, \xi^i, t) = w(\xi) \sum_{n=0}^{\infty} \frac{1}{n!} a_{(n)}(x^i, t) H_{(n)}(\xi^i)$$

$$w(\xi) = \frac{1}{(2\pi)^{3/2}} \exp(-\xi^2/2)$$

$$a_{(n)} = \int f H_{(n)}(\xi) d\xi$$

Expansion and Lattice Configuration

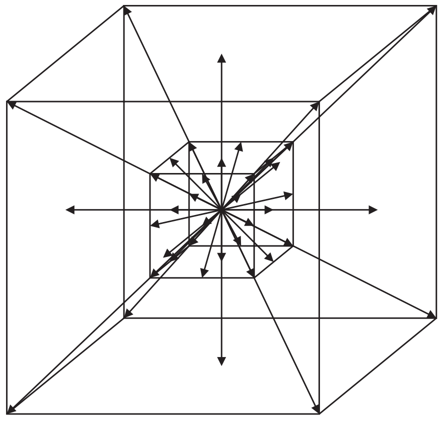
$$f(x^i, \xi^i, t) = w(\xi) \sum_{n=0}^{\infty} \frac{1}{n!} a_{(n)}(x^i, t) H_{(n)}(\xi^i)$$

To ensure Hydrodynamics: First four moments of the equilibrium distribution.

$$\rho = \int f d\xi \quad , \quad \rho u^i = \int f \xi^i d\xi \quad ,$$

$$\rho\theta g^{ij} + \rho u^i u^j = \int f \xi^i \xi^j d\xi \quad ,$$

$$\rho\theta(u^i g^{jk} + u^j g^{ik} + u^k g^{ij}) + \rho u^i u^j u^k = \int f \xi^i \xi^j \xi^k d\xi.$$



D3Q41

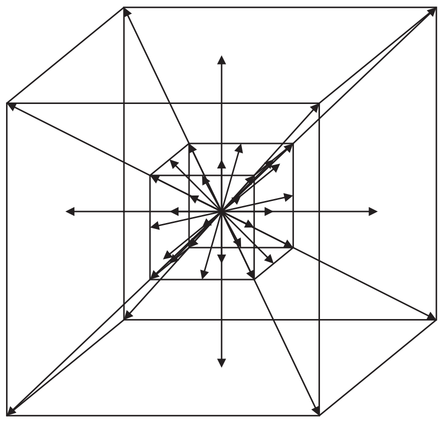
Christoffel Symbols and Boltzmann Equation

$$\partial_t f + \xi^i \partial_i f - \Gamma^i_{jk} \xi^j \xi^k \partial_{\xi^i} f = \mathcal{C}(f)$$

To ensure Hydrodynamics: Expansion up to third order Hermite polynomials.

$$F^i \partial_{\xi^i} f = w \sum_{n=1}^{\infty} \frac{a_{(n-1)} F^i}{(n-1)!} H^i_{(n)}$$

$$F^i = -\Gamma^i_{jk} \xi^j \xi^k$$



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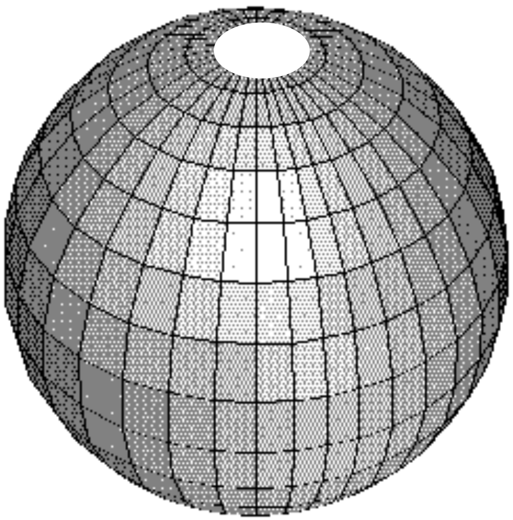
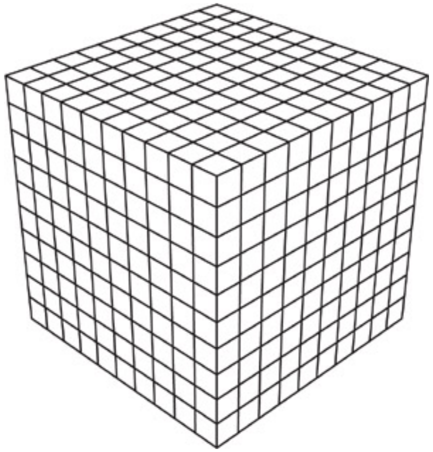
Boundary Conditions

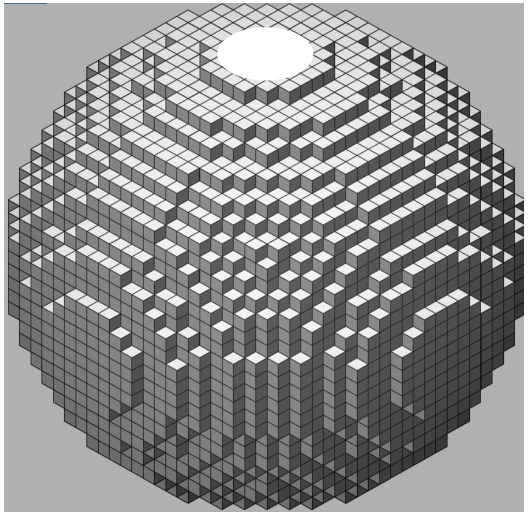


Real geometry

Contravariant coordinates transformation.



Brute force approximation of a sphere



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Curved Spaces and Curvilinear Coordinates

$$R = g^{ij} R_{ij}$$

$$R_{ik} = \frac{\partial \Gamma^l_{ik}}{\partial x^l} - \frac{\partial \Gamma^l_{il}}{\partial x^k} + \Gamma^l_{ik}\Gamma^m_{lm} - \Gamma^m_{il}\Gamma^l_{km}$$

Ricci scalar or Curvature Scalar

Ricci curvature tensor

Curved spaces, e.g. 2D surface of a sphere:

$$R \neq 0$$

Spherical and cylindrical coordinates represent flat spaces. One can demonstrate:

$$R = 0$$

Some Advantages

- Lattice Boltzmann computations in curved spaces and/or curvilinear (cylindrical, polar, etc.) coordinates.
- Curved spaces in Cartesian grids due to the contravariant components.
- The instabilities due to inertial forces are automatically included.
- Low relativistic flow through intrinsically curved spaces, e.g. interstellar media.
- Metric tensor and Christoffel symbols can vary with time. Modeling of elastic pipes, vessels, and flow within deformable membranes.
- “Exact” representation of the geometry of complex boundaries by using contravariant coordinates.

Some Disadvantages

- Unable to model topological singularities: Sphere poles, or regions where the metric tensor has determinant equal zero.

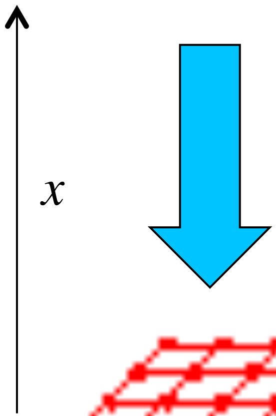
- Implementation of boundary conditions when the metric tensor is not diagonal: This depends on the chosen coordinates system.

- Boundary conditions for higher order lattices are always a bit more complicated than for standard lattices.

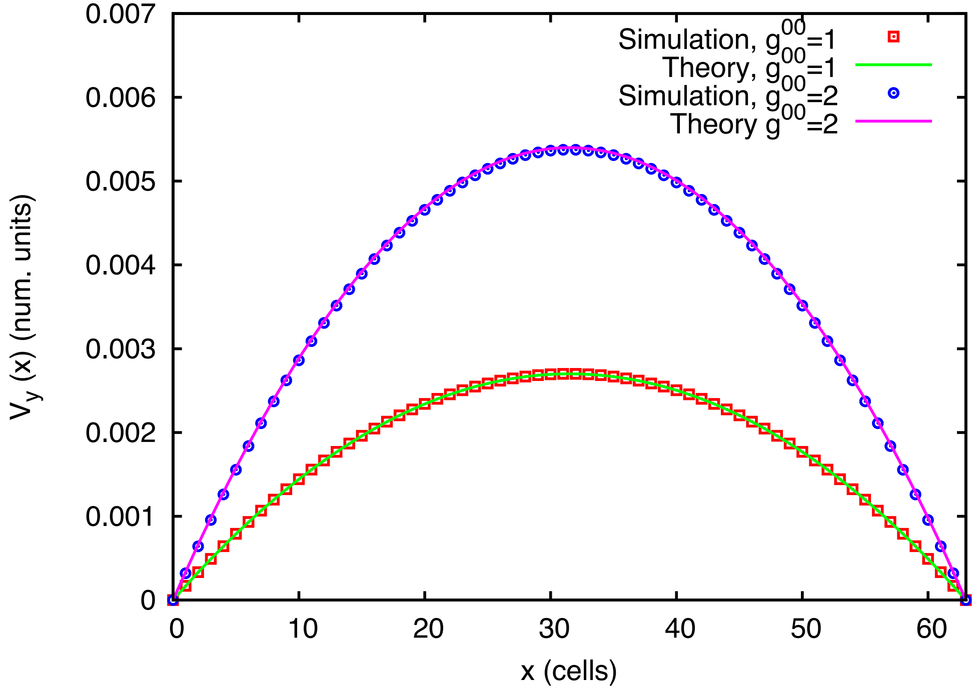
Some Applications

Stretching. Poiseuille Flow

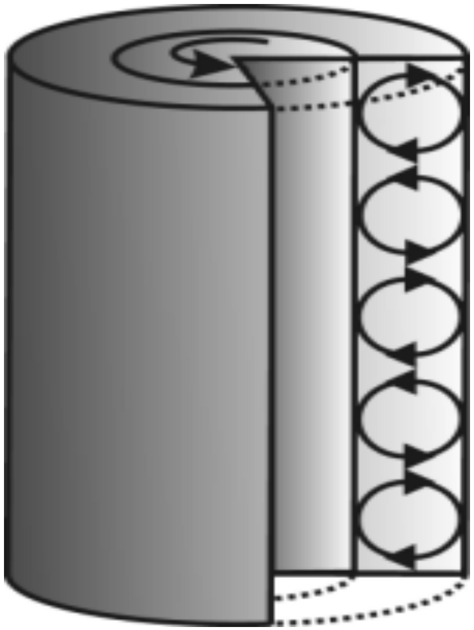
$$g_{ik} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

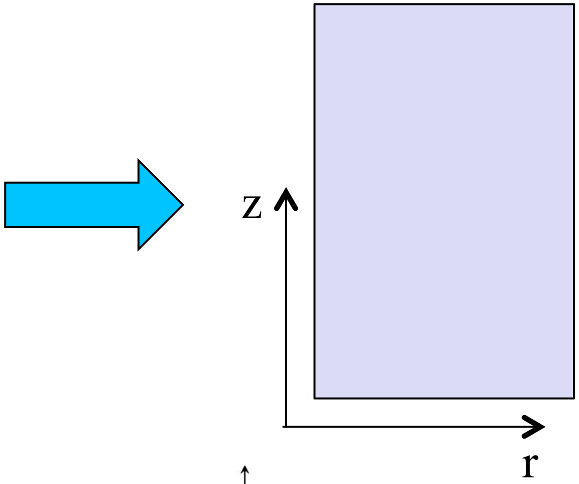


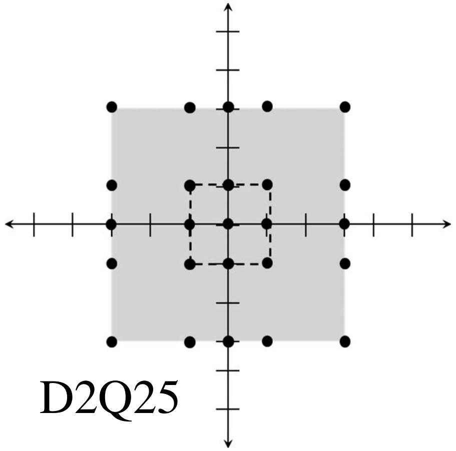
$$g_{ik} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

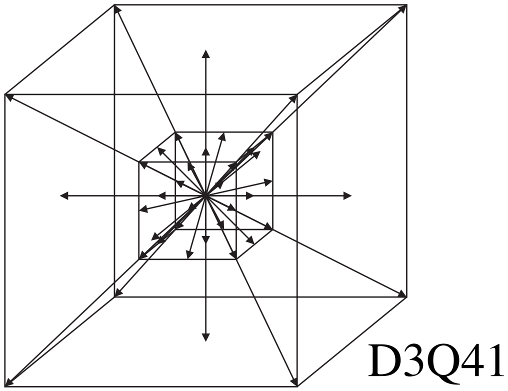


A solution in curvilinear coordinates: Taylor-Couette Instability



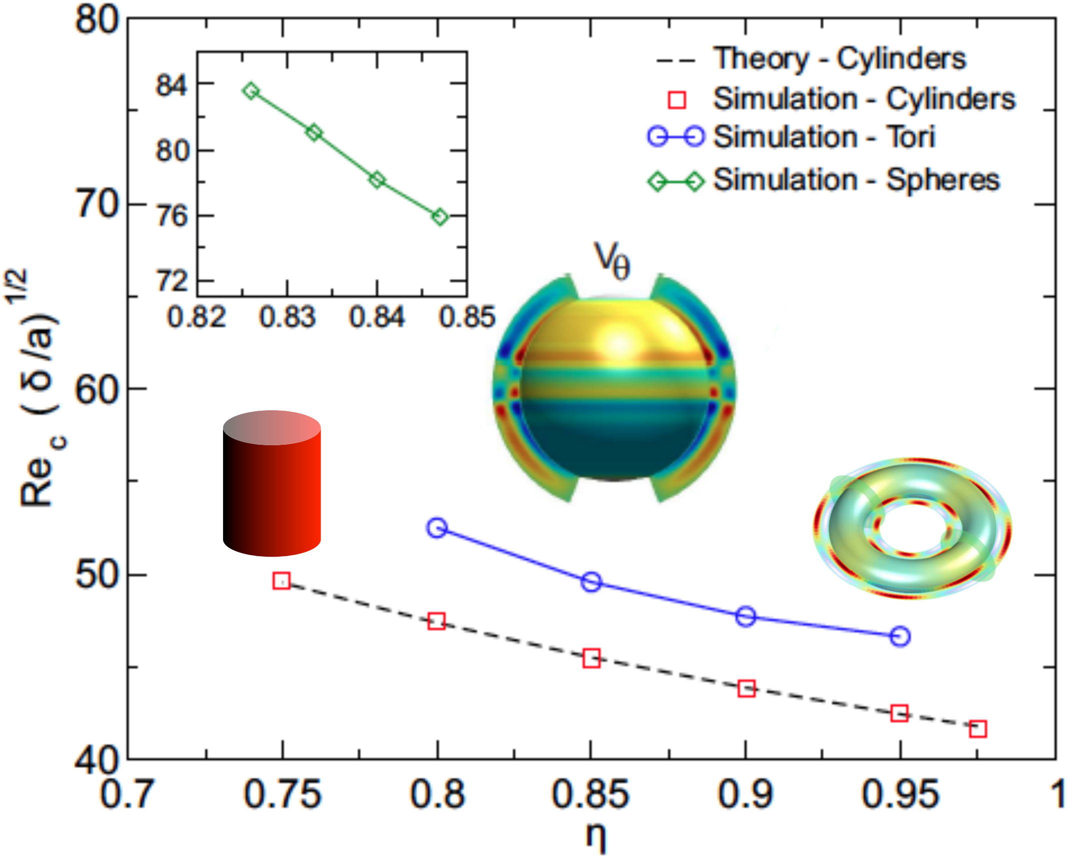


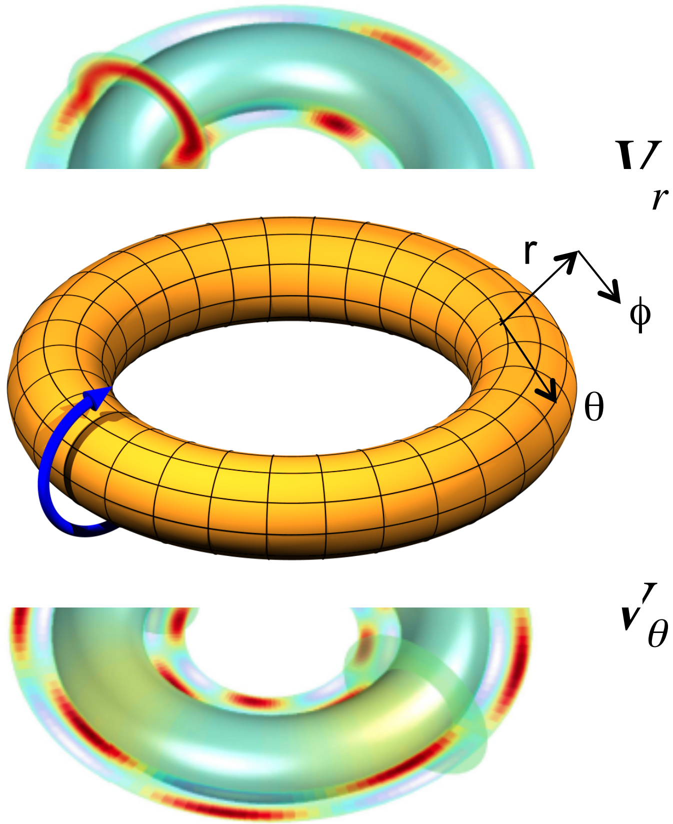




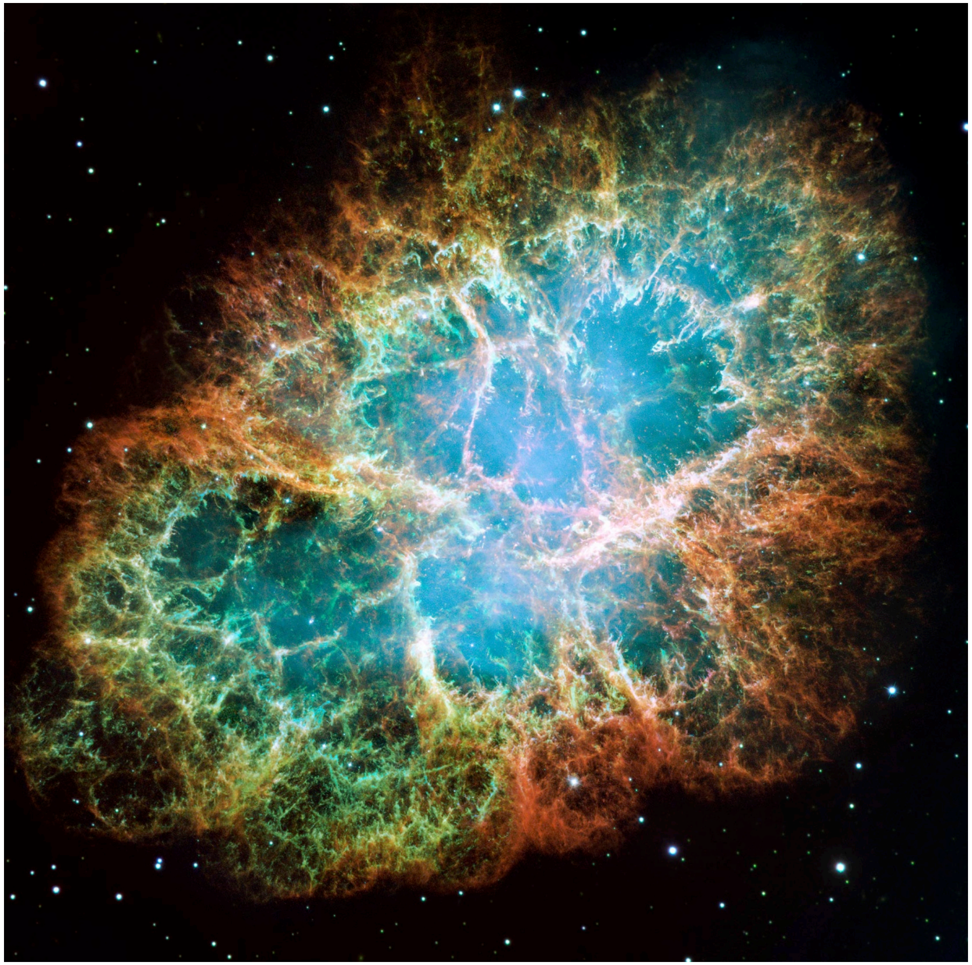
Validation and New Results

Cylinders   Spheres   Tori





Randomly Curved Space: Campylotic Medium



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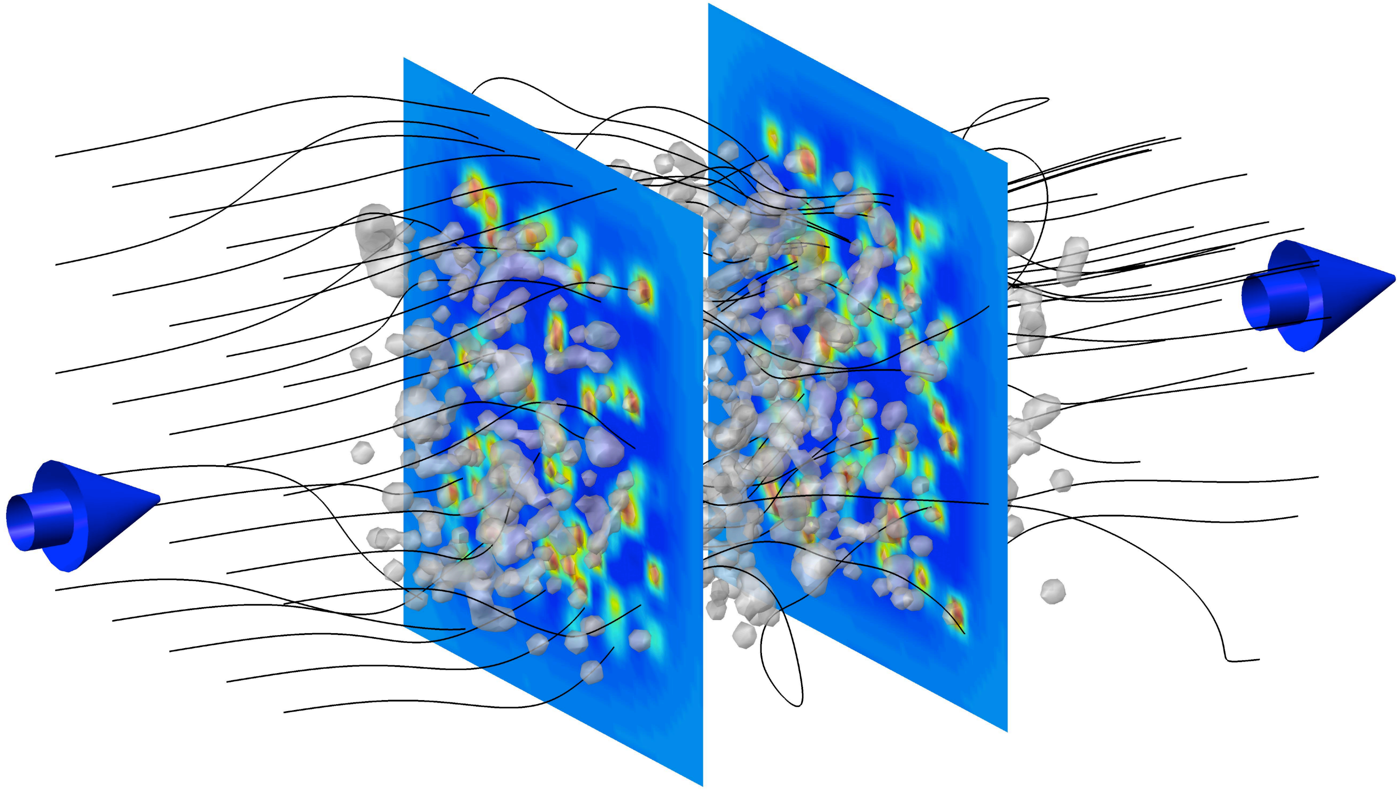
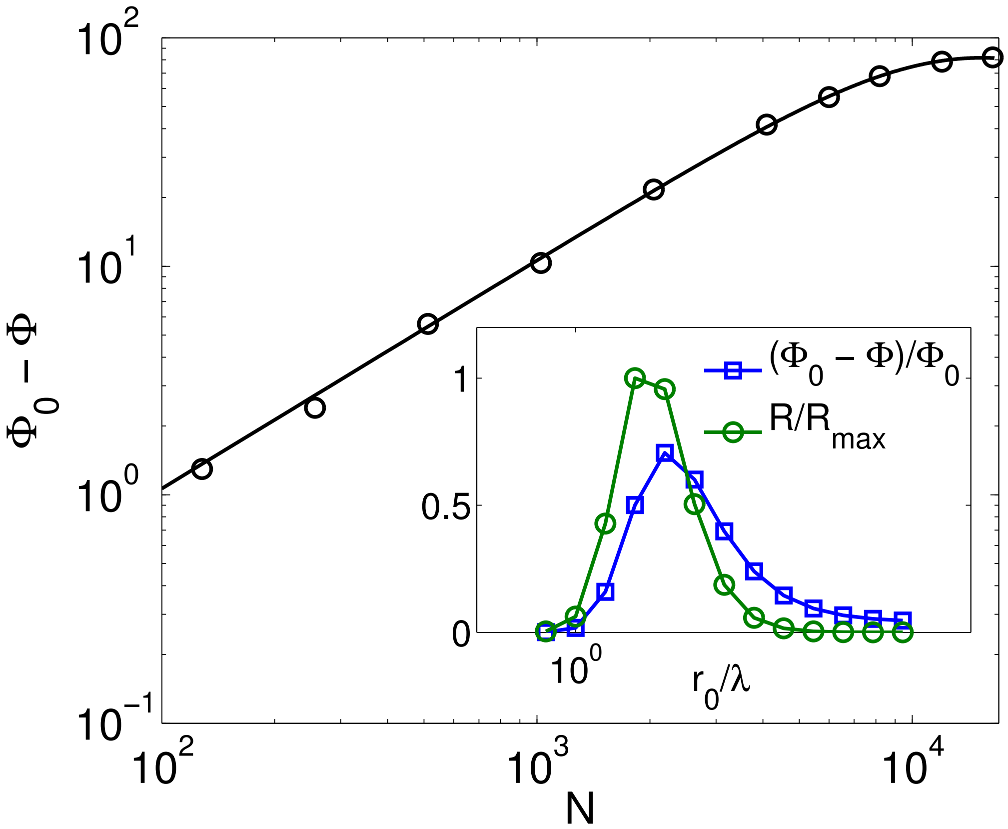
Genuinely Campylotic Medium (Randomly curved space)



$$g_{ij} = \delta_{ij}(1 - a_0 \sum_{n=1}^{N} \exp(-r_n/r_0))$$

Curvature Disordered Media



Φ_0 : Flux in absence of impurities

Φ : Flux

N : Number of impurities

r_0 : Range of curvature perturbation

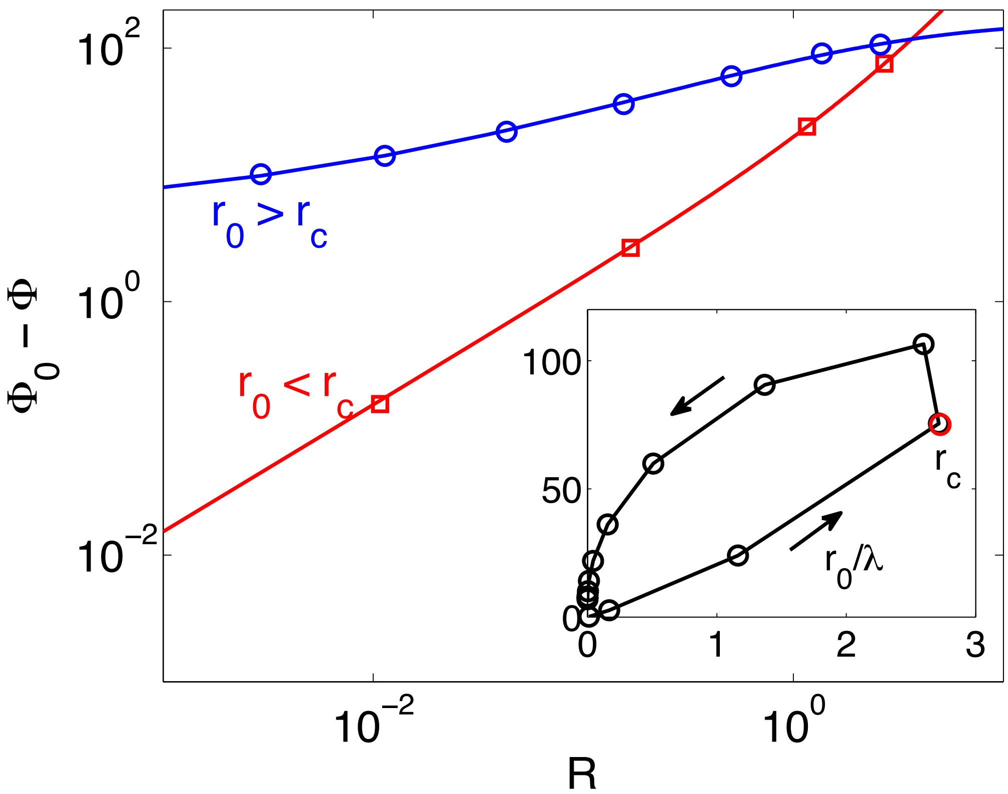
$\lambda : V^{1/3} / N$

R_{ik} : Ricci or curvature tensor

R : Ricci or curvature scalar

$$R = g^{ij} R_{ij} \qquad R_{ik} = \frac{\partial \Gamma^l_{ik}}{\partial x^l} - \frac{\partial \Gamma^l_{il}}{\partial x^k} + \Gamma^l_{ik}\Gamma^m_{lm} - \Gamma^m_{il}\Gamma^l_{km}$$

Curvature Disordered Media



Φ_0 : Flux in absence of impurities

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Summary

1. We have developed a lattice Boltzmann model for general manifolds:

   a) Allows to make computations in virtually any curvilinear coordinate system (polar, cylindrical, spherical, etc.) with LBM.

   b) The LB for manifolds can represent very complex geometries "exactly" in a cubic lattice due to the fact that it works in the contravariant coordinate system, and avoiding a stair case approximation for curved boundary conditions.

   c) Non-inertial forces are automatically included via the Christoffel symbols.

2. Wave equations can also be modeled with the contravariant components of the coordinates system.

3. Flow through randomly curved spaces can present very unusual behaviors.

Muchas gracias a todos, especialmente a los organizadores!