Nematic colloids for photonic systems with *FreeFem*++

Iztok Bajc

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MARIE CURIE ACTIONS

Outline

- **Nematic liquid crystals**
- **Colloidal particles**
- **Methods/computations**
- **Photonic systems**

Modeling requirements in 3D!

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Most well-known application of liquid crystals?

Applications of liquid crystals

- **LCD** (Liquid Crystal Displays).

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- **Eye protecting filters** for welding helmets (Balder)

- **Polarizing glasses for 3D vision**

Liquid crystals have unique ***optical*** properties.

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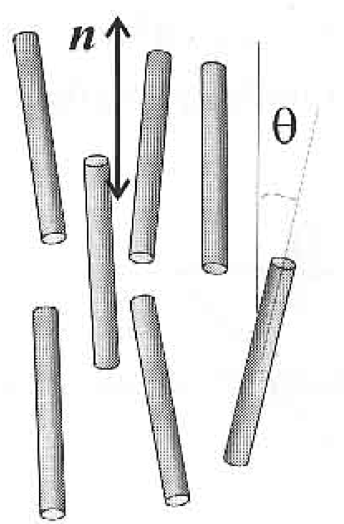

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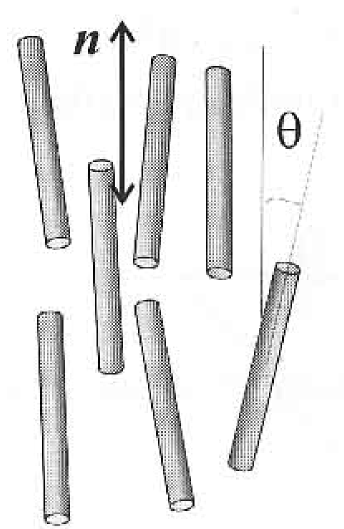

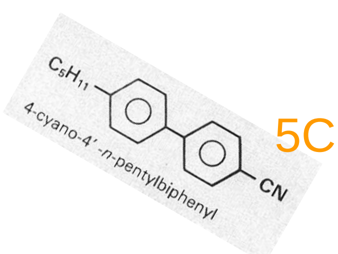

5CB

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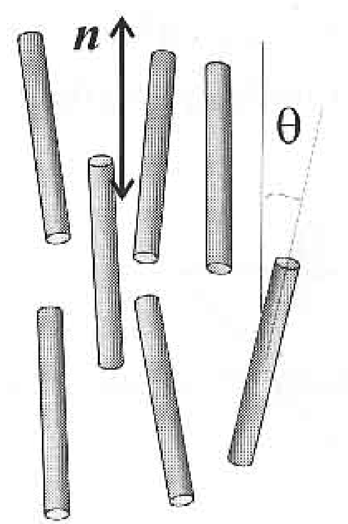

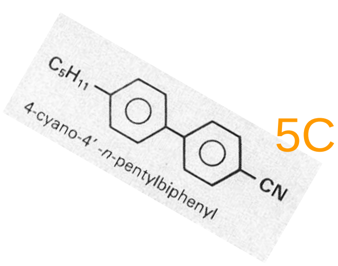

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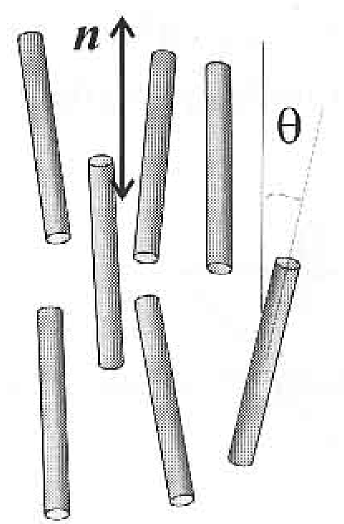

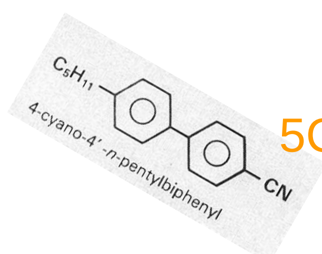

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Low enough temperature

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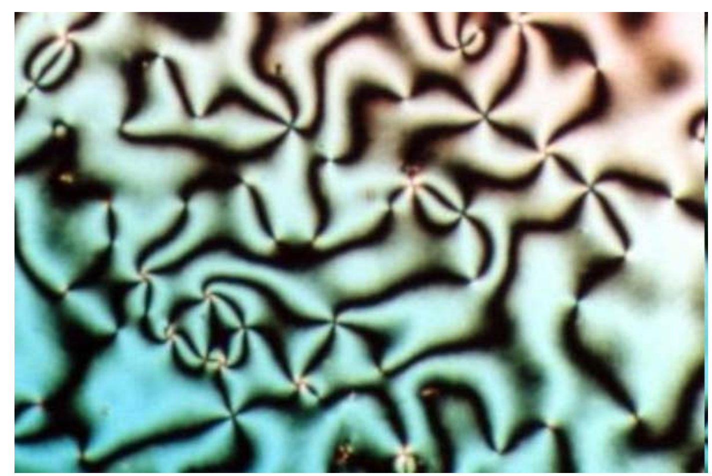

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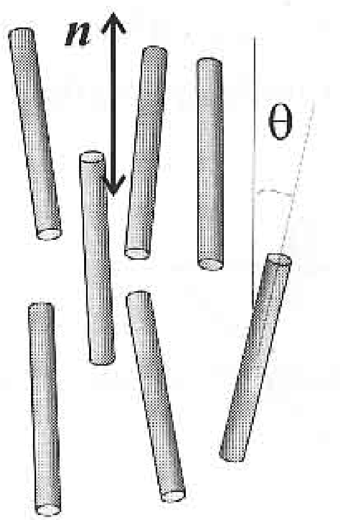

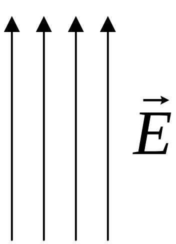

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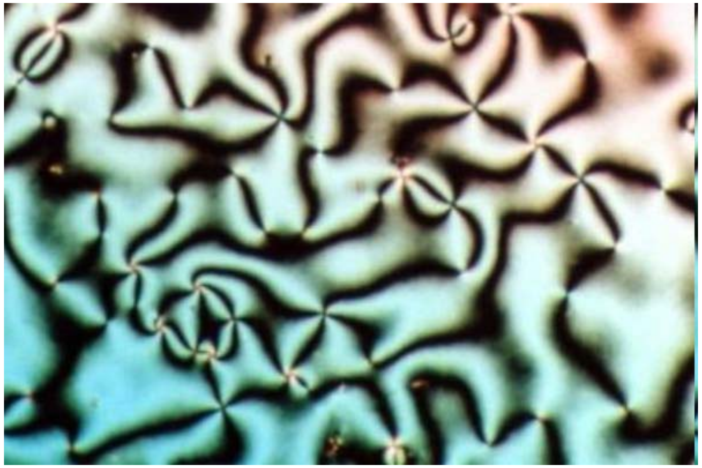
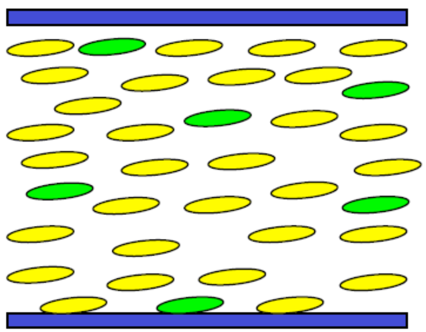
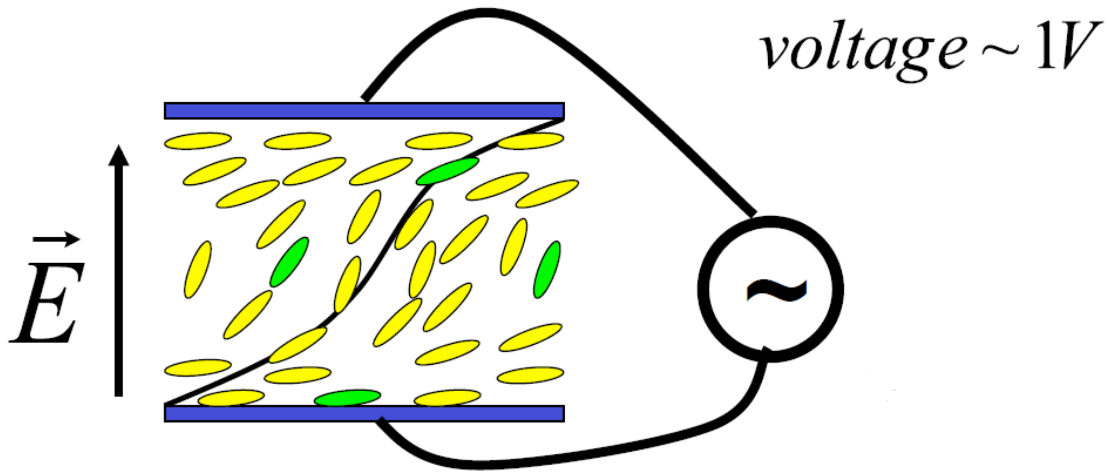


Basic example of nematic structure

Thin cell (~microns):





Description of nematic liquid crystals

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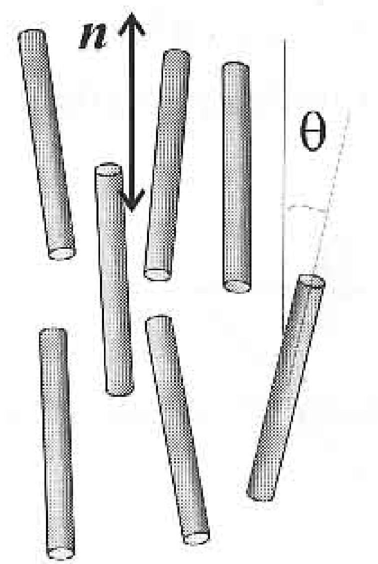
$$\boxed{\vec{n}(\vec{r})}$$

$$|\vec{n}| = 1$$



Points in preferenced orientation.

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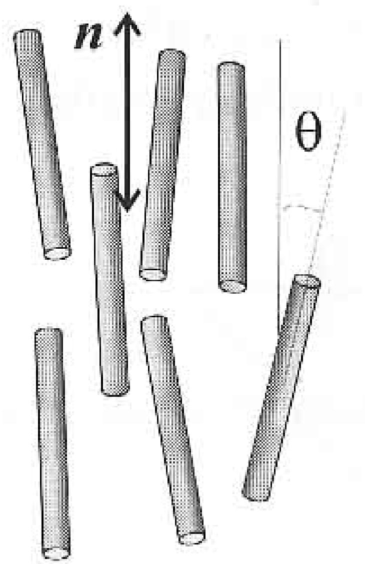

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$$-\frac{1}{2} \leq S \leq 1$$

Quantifies the *degree of order* of the director orientation:

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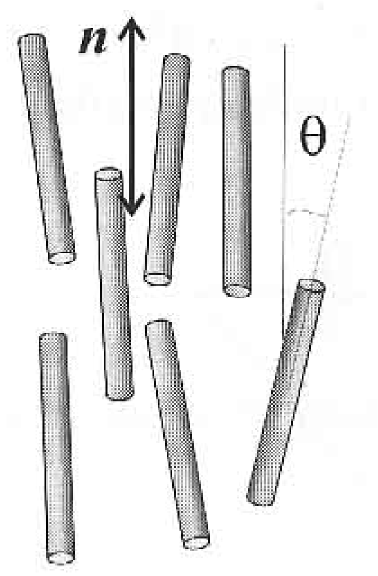

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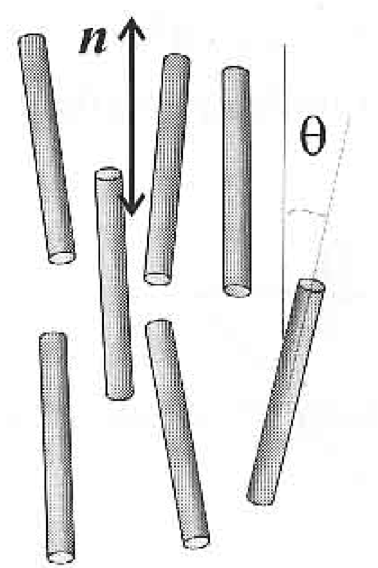

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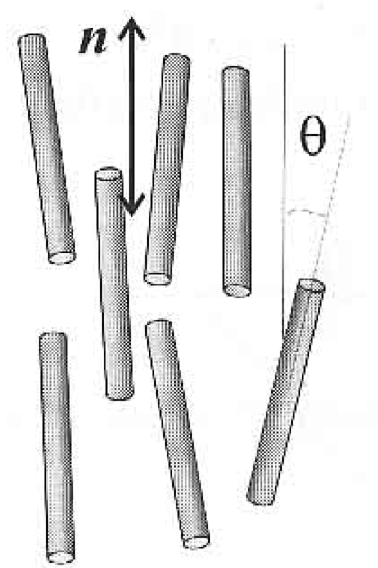

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S=0.53 → *a typical* intermediate bulk value (for 5CB)

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Alternative description with Q-tensor field

New quantity: **tensor order parameter** $Q(\vec{r})$:

$$\boxed{Q = \frac{S}{2}\left(3\vec{n}\otimes\vec{n} - I\right) + \frac{P}{2}\left(\vec{e}_1\otimes\vec{e}_1 - \vec{e}_2\otimes\vec{e}_2\right)}$$

S its largest eigenvalue and $\vec{n}$ its corrispondent eigenvector.

- Q **traceless**: $Q_{11} + Q_{22} + Q_{33} = 0 \longrightarrow \boxed{Q_{33} = -Q_{11} - Q_{22}}$
- Q **symmetric**: $\boxed{Q_{ij} = Q_{ji}}$

$\longrightarrow$ Only *5 independent components* of Q are required.

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Uniaxial approximation

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L – elastic constants

A, B, C – material constants

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Surface energy

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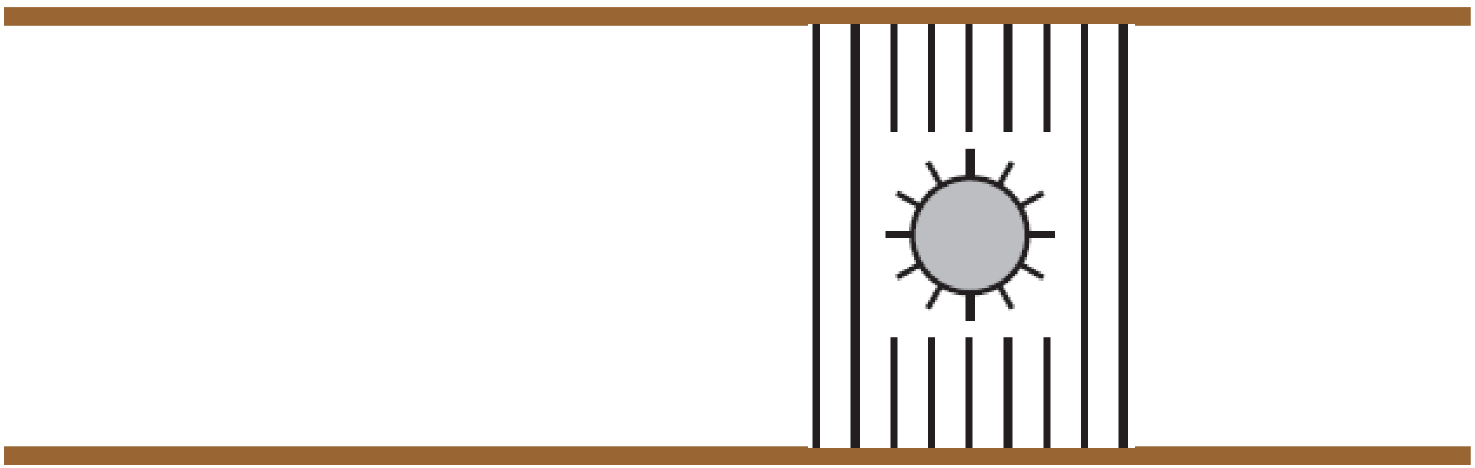
- **Colloidal particles**
- **Methods/computations**
- **Photonic systems**

One colloidal particle



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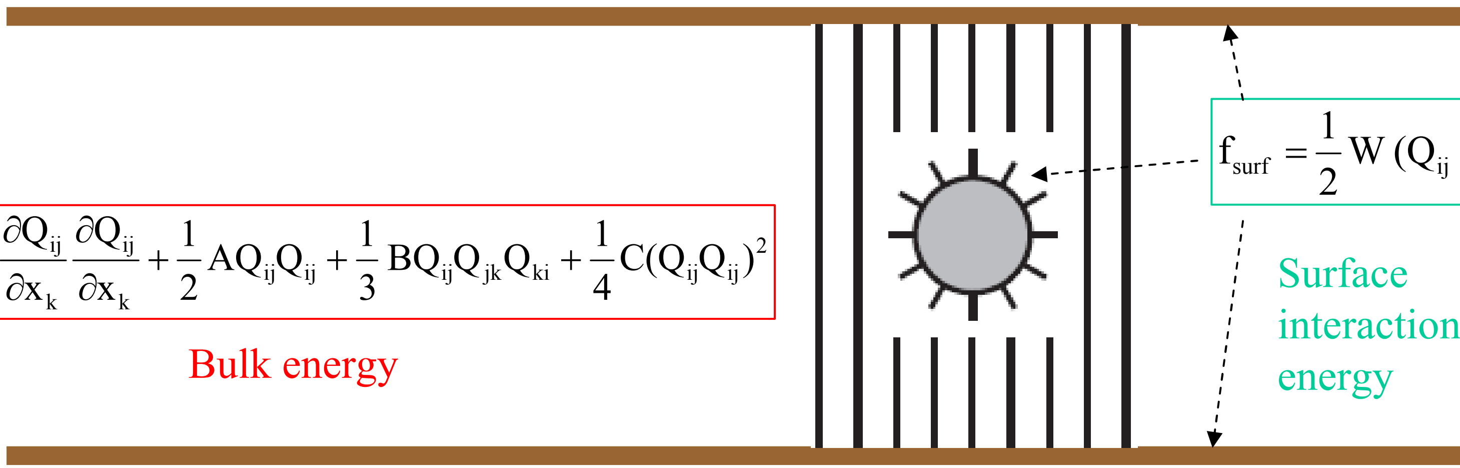

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Surface interaction energy

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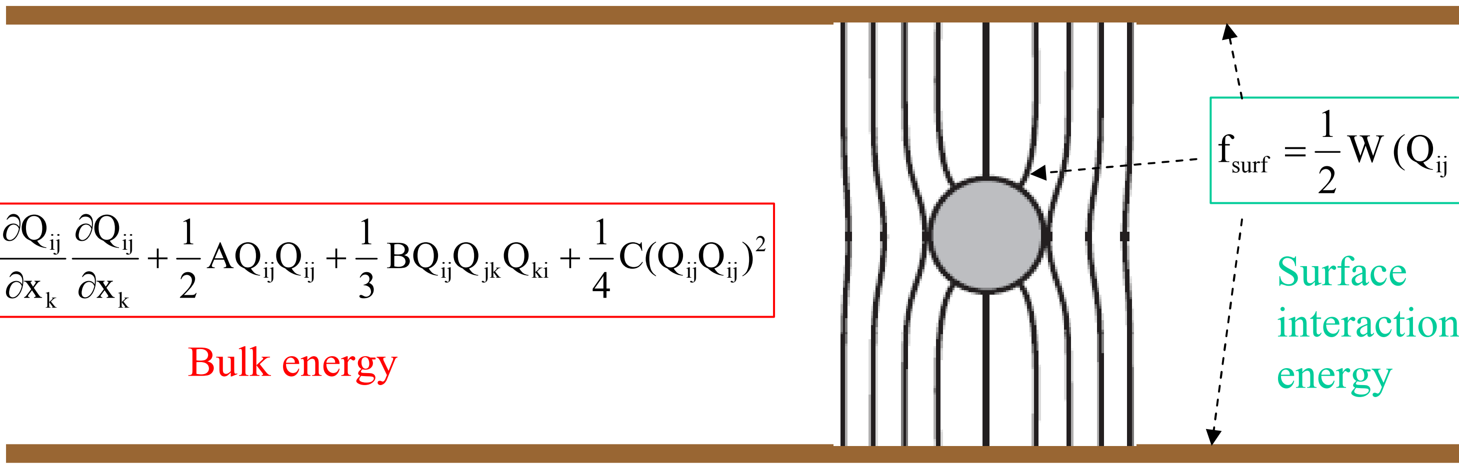

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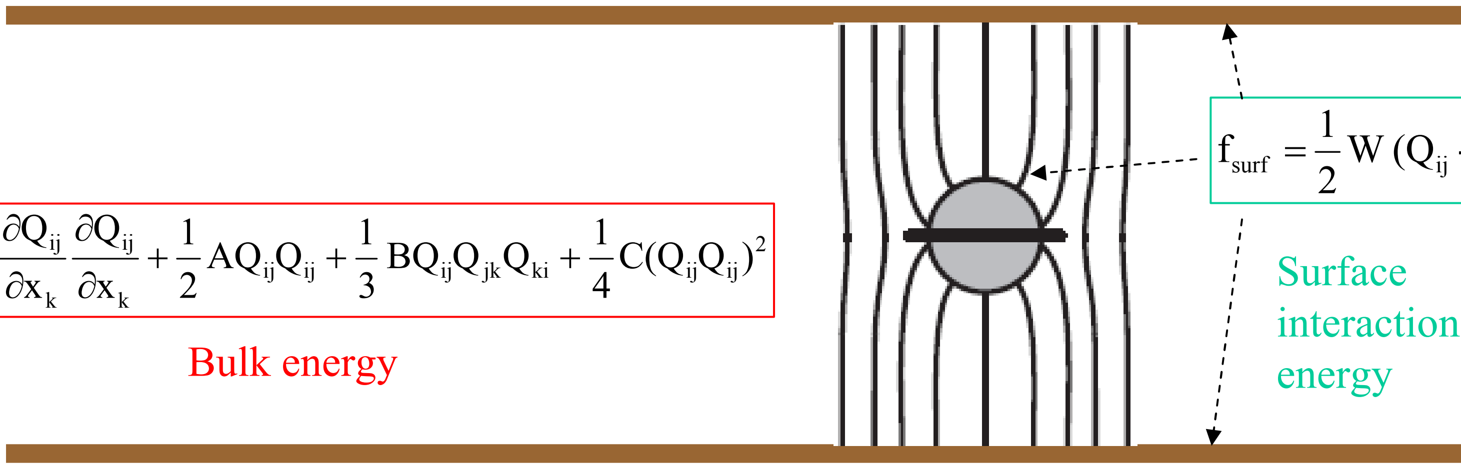

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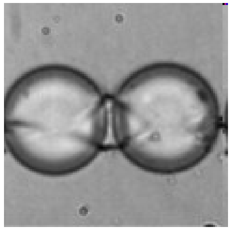

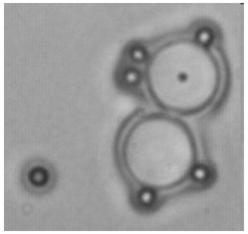

Photos: I. Muševič group,
PRE, PRL, Science, 2006-2010

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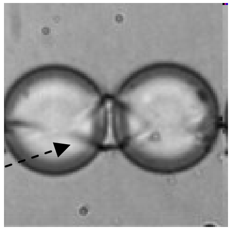

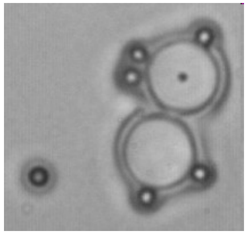

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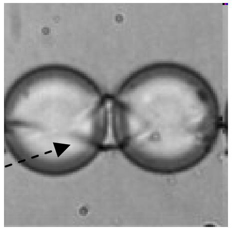
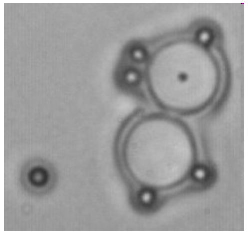
Strong **attractive forces**





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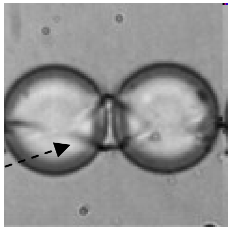

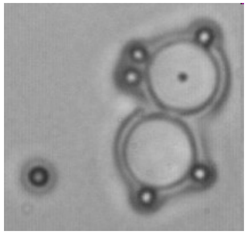

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Colloidal **structures**
- crystals in nematic.

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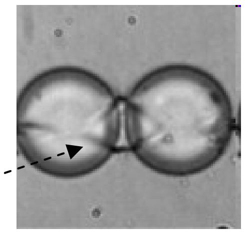

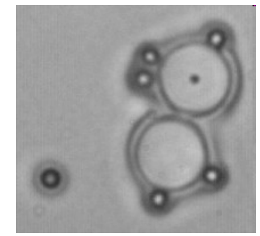

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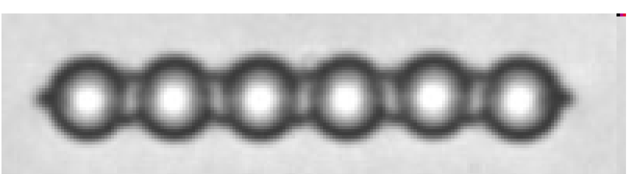

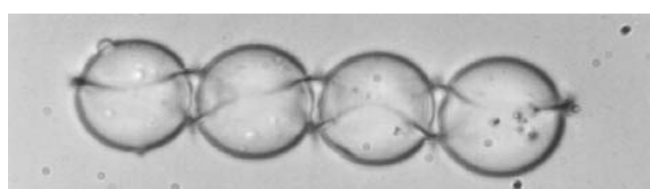

1D structures

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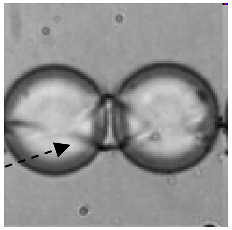

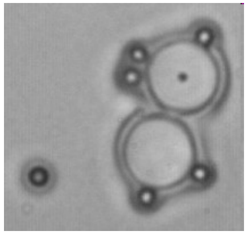

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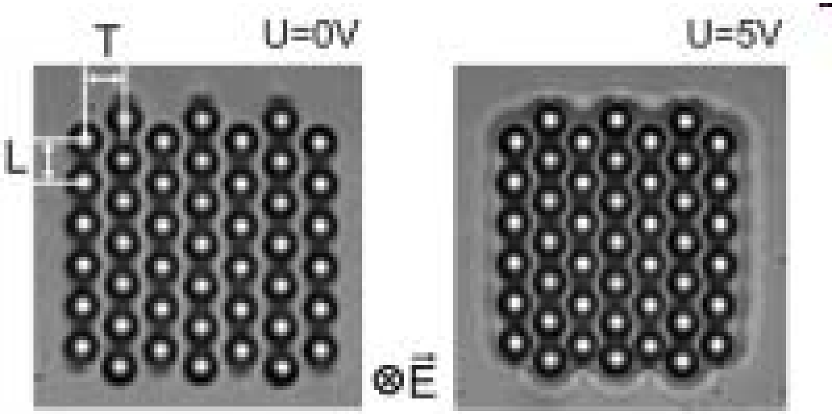
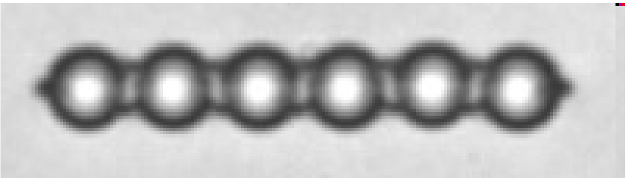
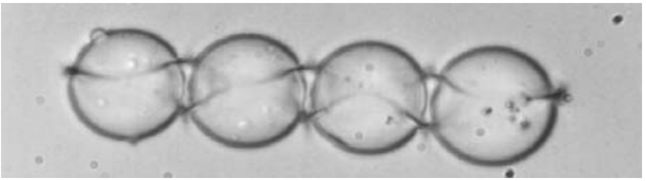


Colloidal **structures**
- crystals in nematic.

2D structures - crystals





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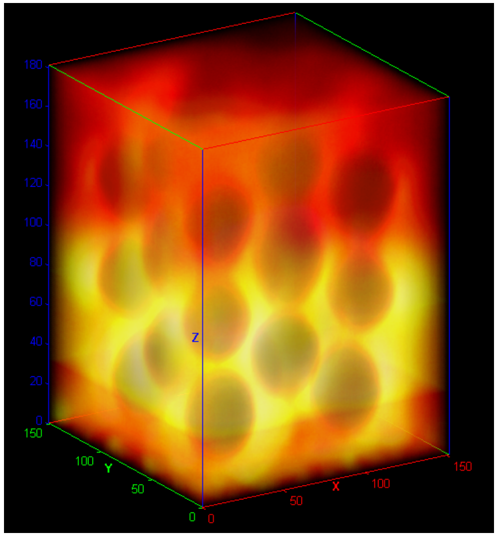
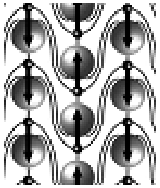
Final aim

Large 3D structures - crystals:

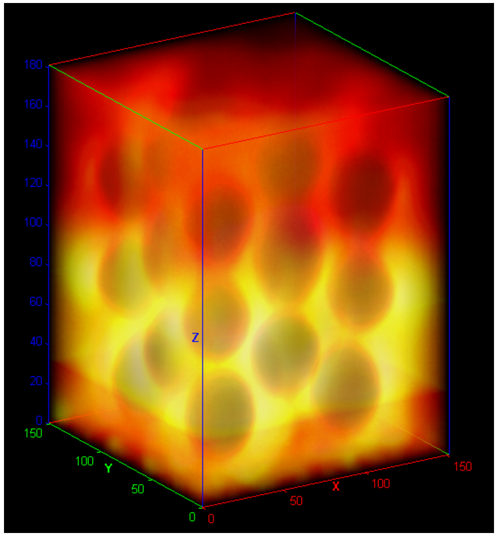


3×3×3 dipolar crystal.
Experiment by Andriy Nych, 2010 (*to be published*).

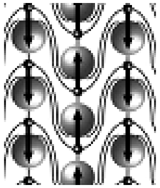


Large 3D structures - crystals:

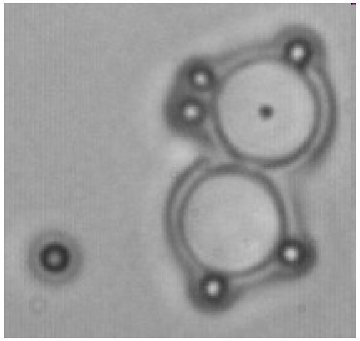
Final aim



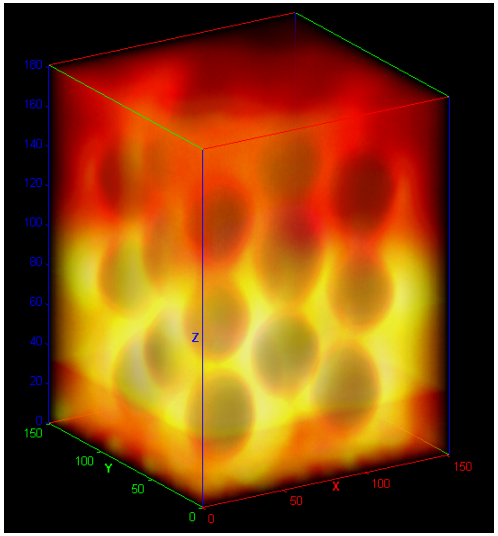
3×3×3 dipolar crystal.
Experiment by Andriy Nych, 2010 (*to be published*).



In the meanwhile:



Large 3D structures - crystals:



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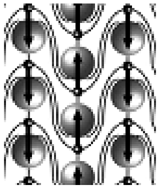
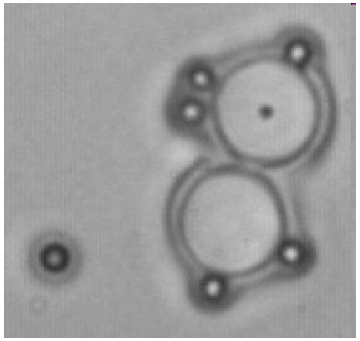
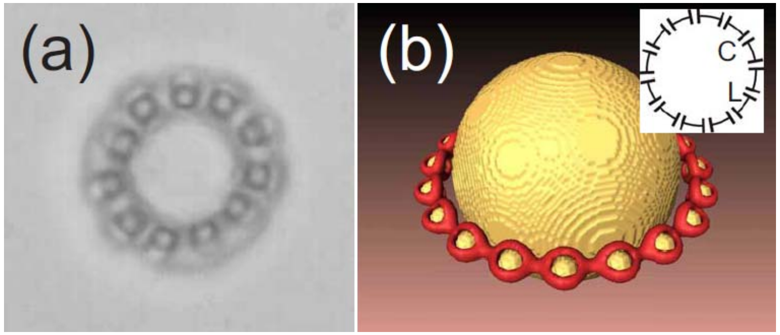
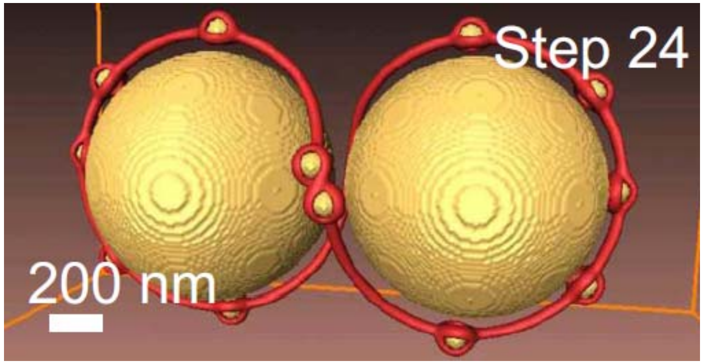


Final aim →

In the meanwhile:





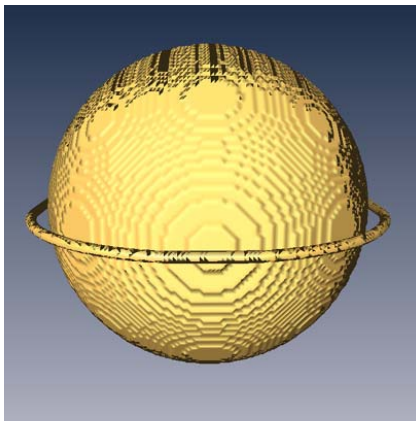


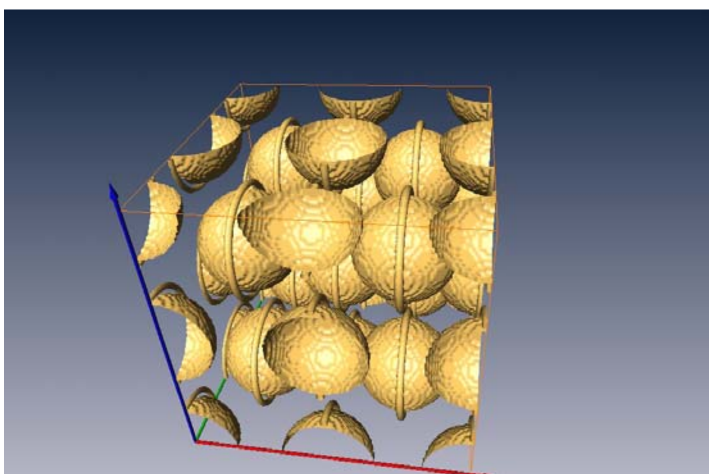
Škarabot, Ravnik et al., PRE, 2008.

Outline

- **Nematic liquid crystals**
- **Colloidal particles**
- **Methods/computations**
- **Photonic systems**

Some already made simulations

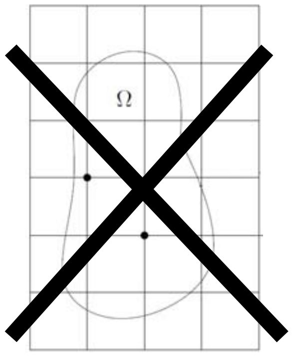




M. Ravnik, S. Žumer, **Soft Matter**, 2009.

Computational requirements

Use of <u>uniform grid</u> becomes **impracticable** (time/memory) for *larger systems* or *localized resolutions*.



↓

<u>Nonuniform grid</u> required, for ex. with the **finite element method (FEM)**.

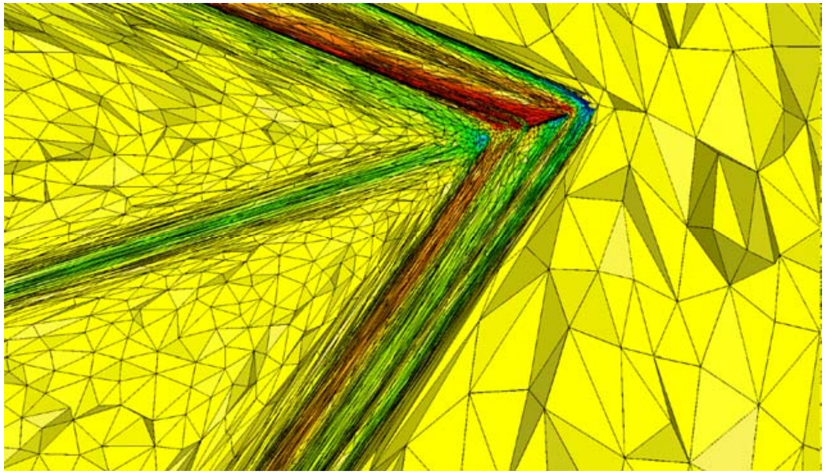
Strategy: ***<u>mesh adaptivity</u>***

→ *less* degrees of freedom (so less memory/time)

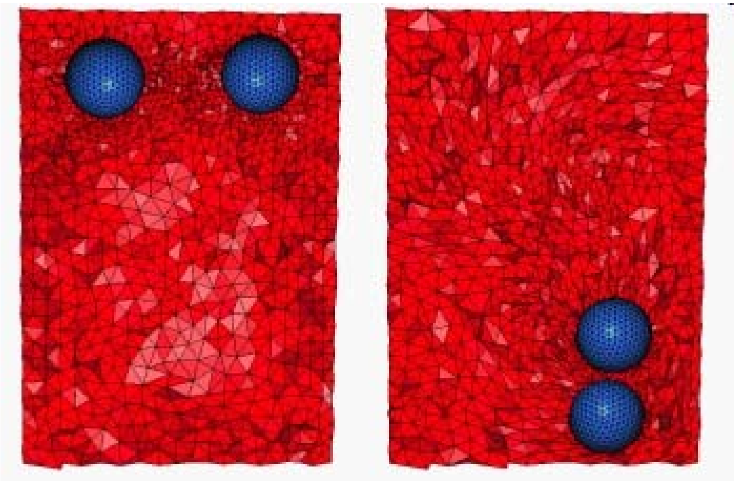
→ *more details* given *only* where needed (*e.g.* around defects)

A priori *Metric based*

New modeling requirements



Mesh adaptivity in 3D, preferably with **anisotropic metric**.



Moving objects (due to nematic elastic forces).

Parallel processing (computer clusters).

Meshes by *Cécile Dobrzynski*, Institut de Mathématiques de Bordeaux.

Newton iteration of tensor fields

Newton iteration of tensor fields

$F(Q)$ min: $\boxed{\delta F(Q) = F'(Q)\delta Q = 0}$ ***Euler-Lagrange equations***

Newton iteration of tensor fields

$F(Q)$ min: $\boxed{\delta F(Q) = F'(Q)\delta Q = 0}$ ***Euler-Lagrange equations***

$$\delta F(Q) = \delta \int_\Omega f(Q, \nabla Q) dV$$

$$= \int_\Omega \left(\frac{\partial f}{\partial Q} - \frac{\partial}{\partial \vec{r}} \frac{\partial f}{\partial(\nabla Q)} \right) \delta Q dV + \int_{\partial\Omega} \frac{\partial f}{\partial(\nabla Q)} \cdot \vec{v} \delta Q dV$$

$$= \int_\Omega L \nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left(A Q_{ij} + B Q_{ik} Q_{kj} + C Q_{ik} Q_{kl} Q_{lj} \right) \varphi_{ij} dV - W \int_{\partial\Omega} \left(Q_{ij} - Q_{ij}{}^0 \right) \varphi_{ij} dA$$

Newton iteration of tensor fields

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$$L \nabla \mathrm{Q}_{\mathrm{ij}} \cdot \vec{v} = -\mathrm{W} (\mathrm{Q}_{\mathrm{ij}} - \mathrm{Q}_{\mathrm{ij}}{}^{0})$$

$$= \int_{\Omega} L \nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left(A Q_{ij} + B Q_{ik} Q_{kj} + C Q_{ik} Q_{kl} Q_{lj} \right) \varphi_{ij} dV - W \int_{\partial\Omega} \left(Q_{ij} - Q_{ij}{}^{0} \right) \varphi_{ij} dA$$

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$$L\nabla Q_{ij} \cdot \vec{v} = -W(Q_{ij} - Q_{ij}{}^{0})$$

$$= \int_{\Omega} L\nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left(AQ_{ij} + BQ_{ik}Q_{kj} + CQ_{ik}Q_{kl}Q_{lj} \right) \varphi_{ij} dV - W \int_{\partial\Omega} \left(Q_{ij} - Q_{ij}{}^{0} \right) \varphi_{ij} dA$$

$$\boxed{F''(Q_k) v_k \varphi = -F'(Q_k)\varphi}$$

Newton iteration equation

(φ - *test functions*)

$$Q_{k+1} = Q_k + v_k$$

(next iteration step)

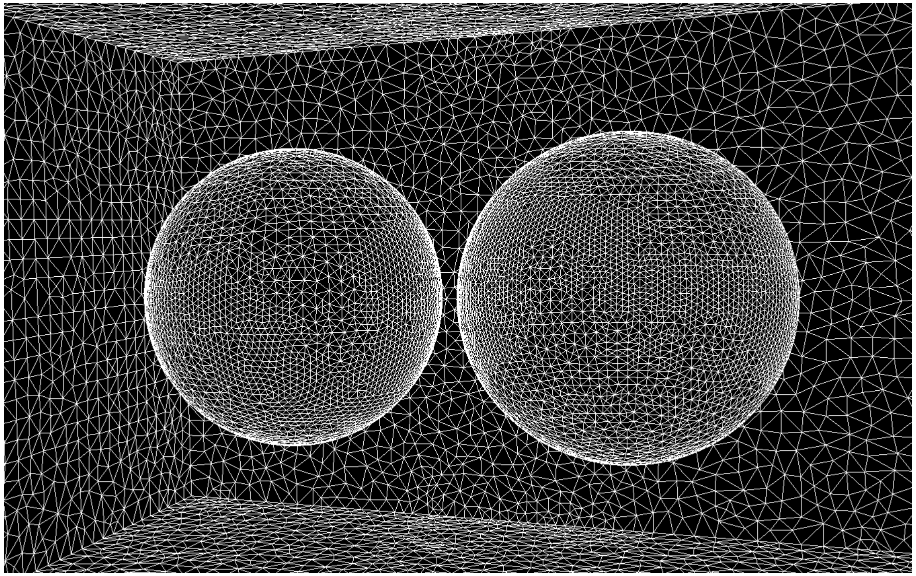
Outline

- **Nematic liquid crystals**
- **Colloidal particles**
- **Methods/computations**
- **Photonic systems**

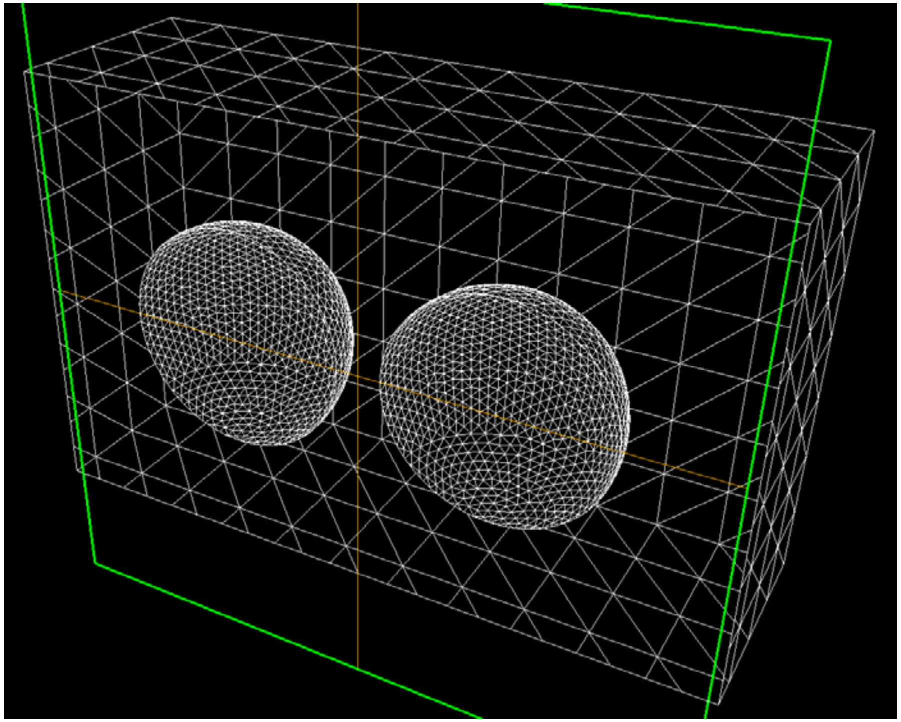
1. Two particles (dimer)

3D geometry:

Interior

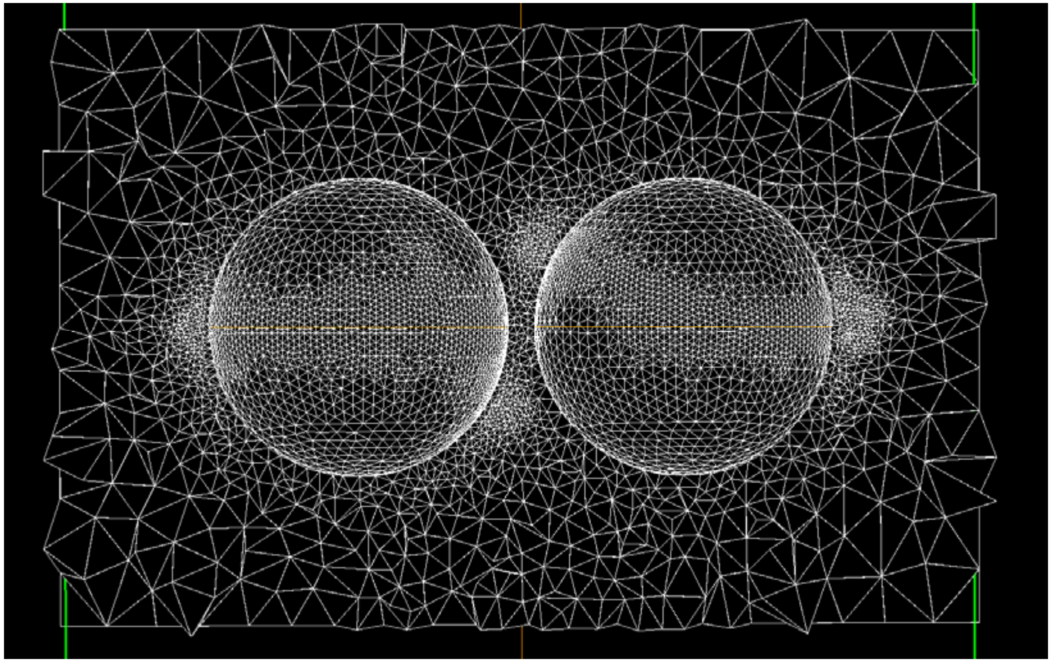


Profile cross section



- **Particle diameter**: 1 um
- Boundary condition: **strong radial** (energy density *W=1e-2* J/m^2).

- **Cell dimensions**: side: 2×2×3.15 [um].
  Floor, bottom, walls: **strong vertical BC**
- Inbetween particles and box: **nematic liquid crystal** (**5CB**).

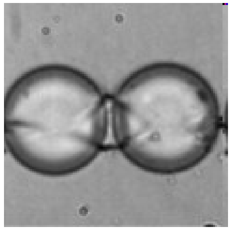


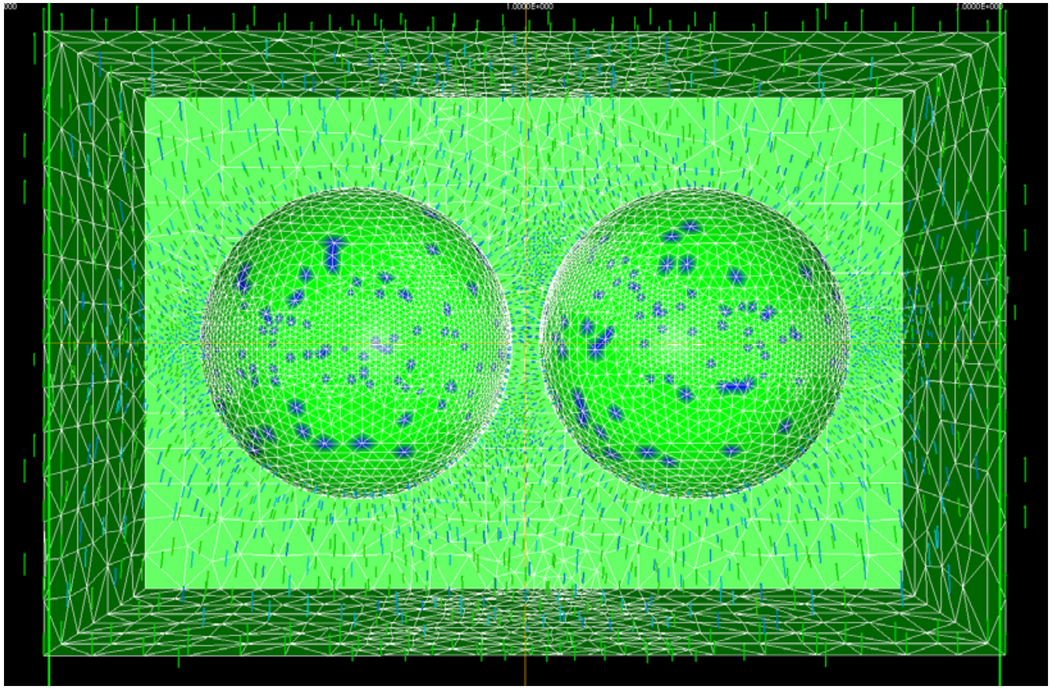
Tetrahedral mesh (cross section)

~ **90.000** mesh points**.**

- **Mesh adaptivity** used: <u>metric based</u>.
- At the moment <u>isotropic</u> adaptivity
- but **anisotropic** being setting up.

(prooved to be globally quasi-optimal)





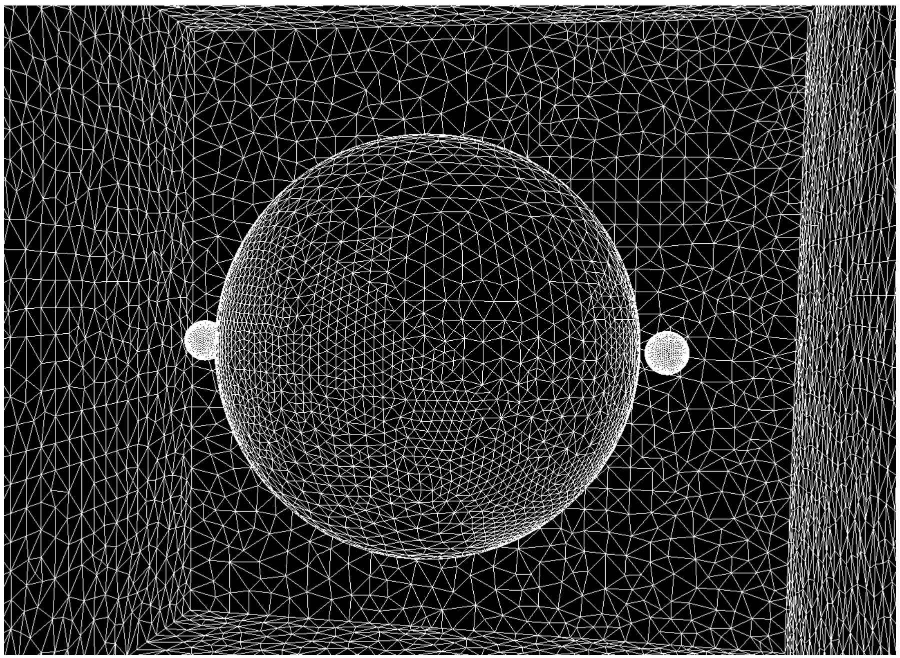
Director field (cross section)

- Code written in *FreeFem++*: ~ 2000 lines.

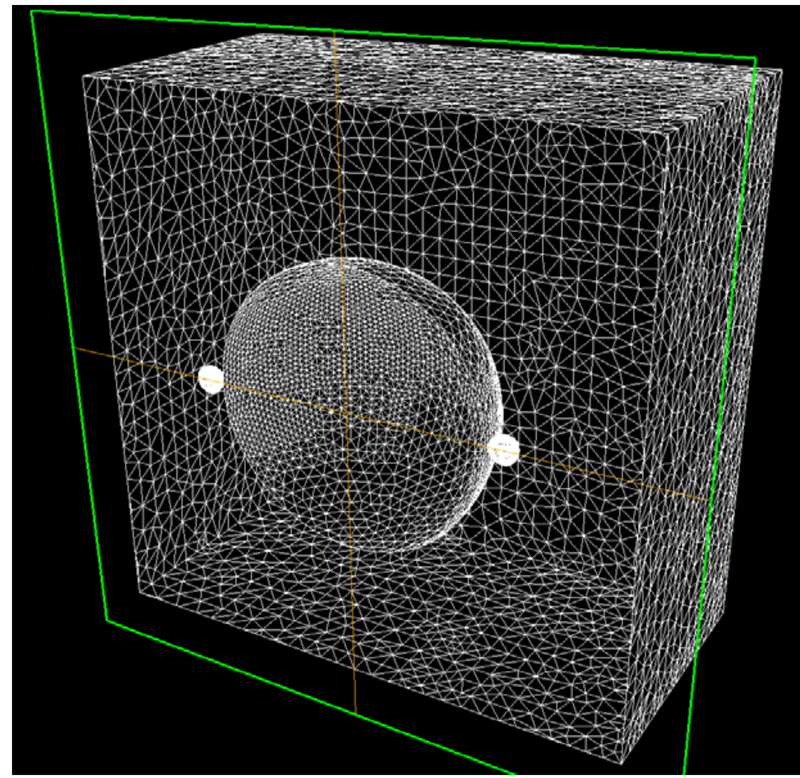
2. One large + two small particles

3D geometry:

Interior

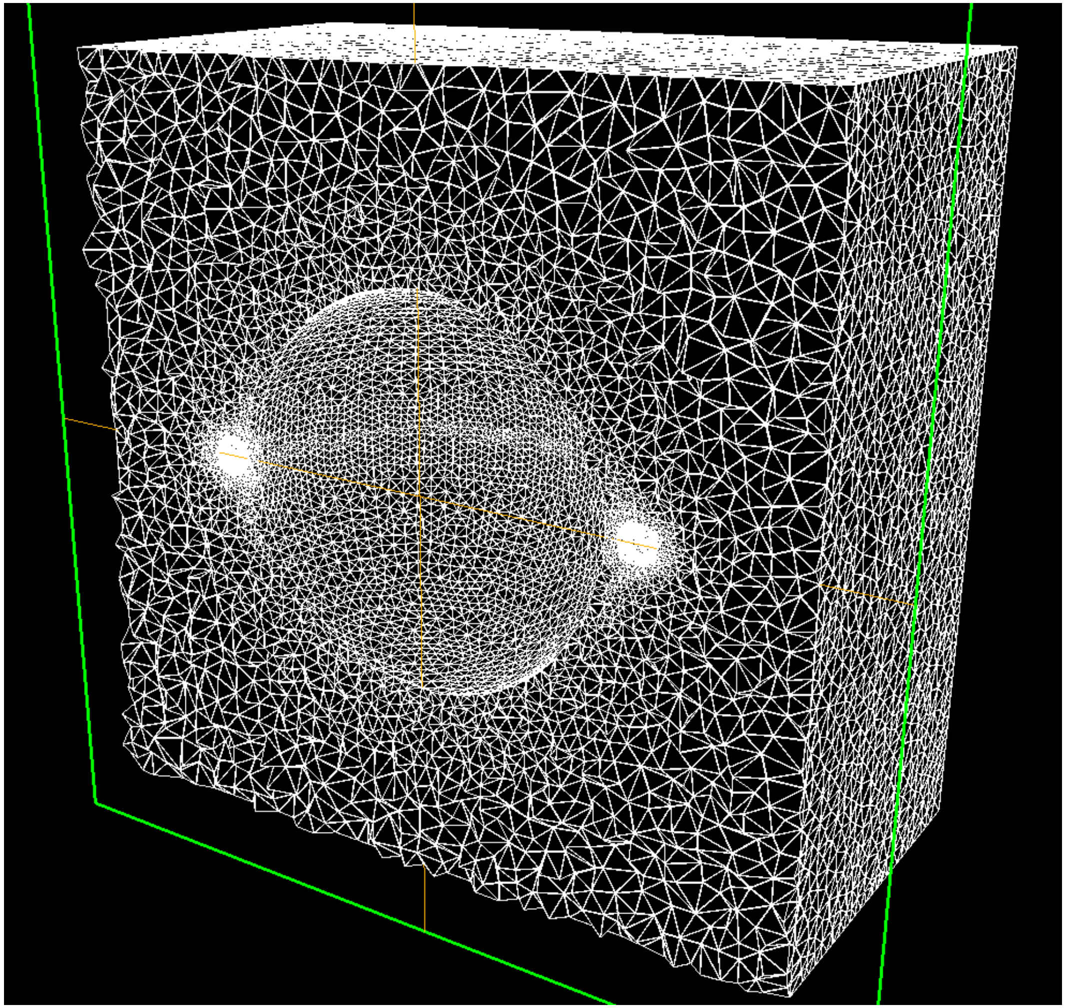


Cross section

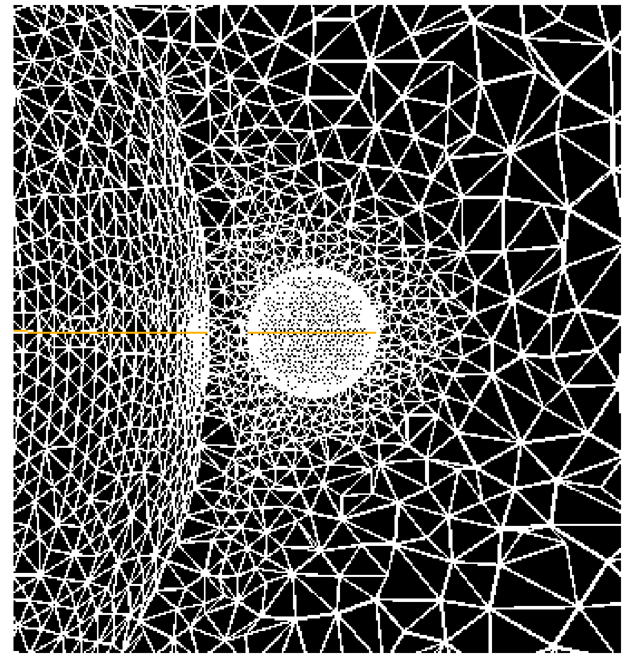


- **1 large particle**: 1 um
- **2 small particles**: 0,1 um
- Boundary conditions: **strong radial** (energy density *W=1e-2* J/m^2).
- **Cubical simulation cell**: side = 2 um. Floor, bottom, walls: **strong vertical BC.**
- Inbetween particle and box: **nematic liquid crystal** (**5CB**).

2. **Tetrahedral mesh** – profile cross section



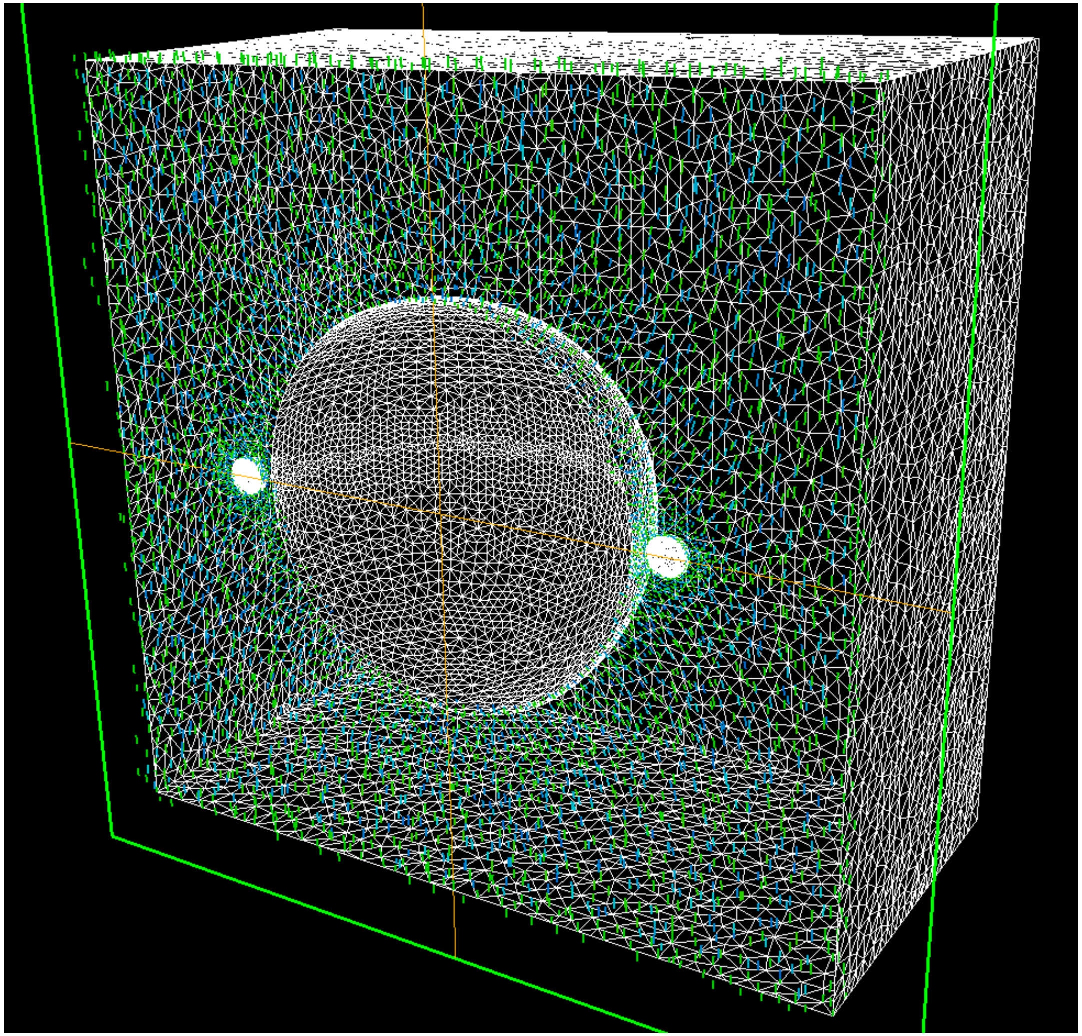
~ **170.000** mesh points.

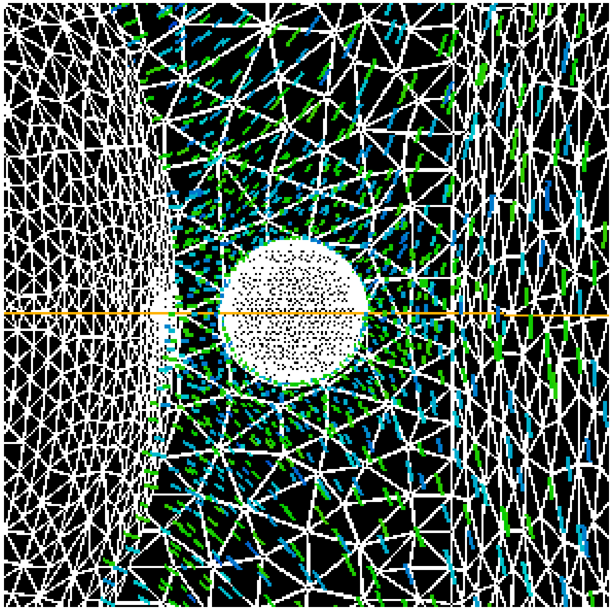


Mesh generator: **TetGen**

Metric**: mshmet**

2. **Director field** – profile cross section





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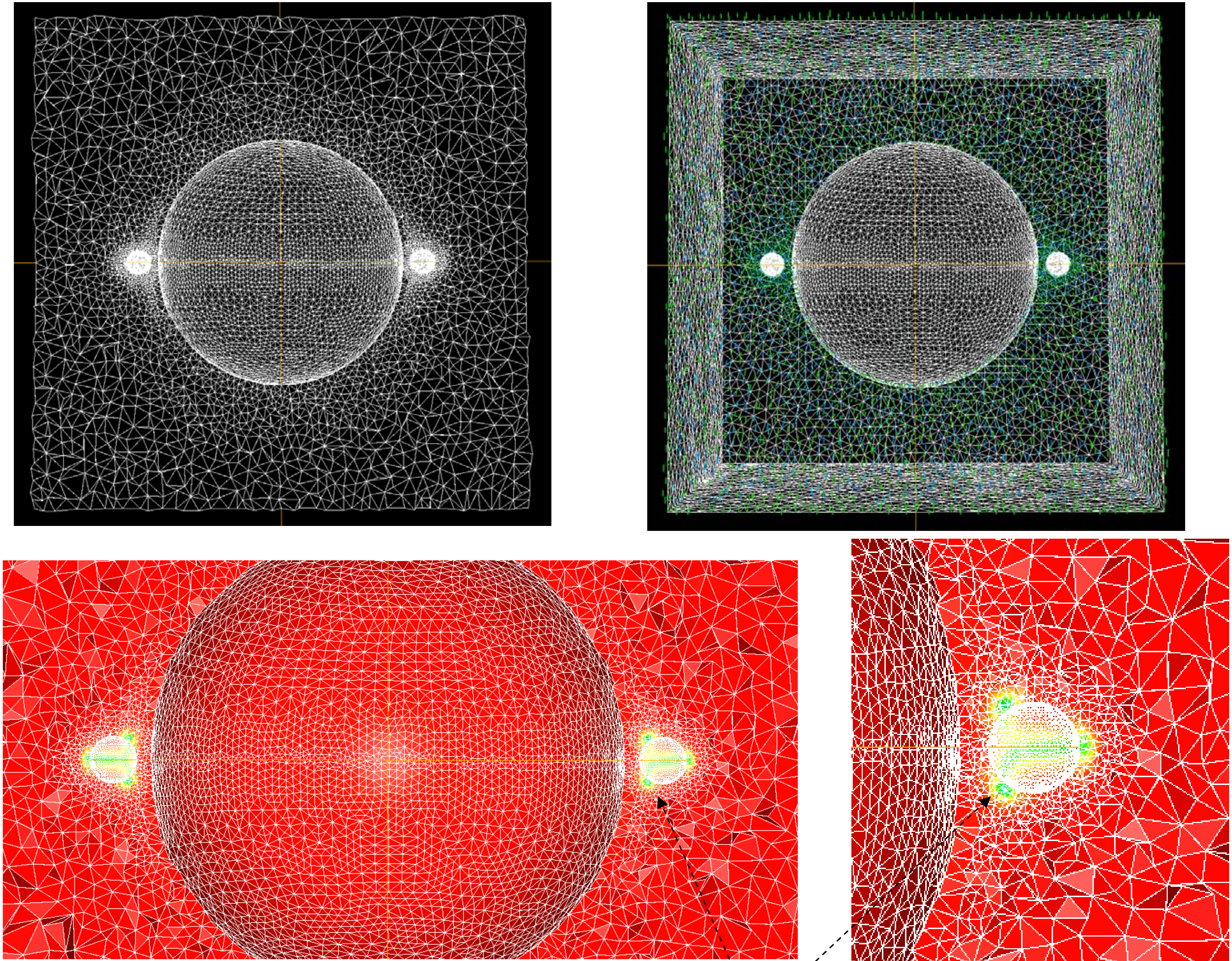
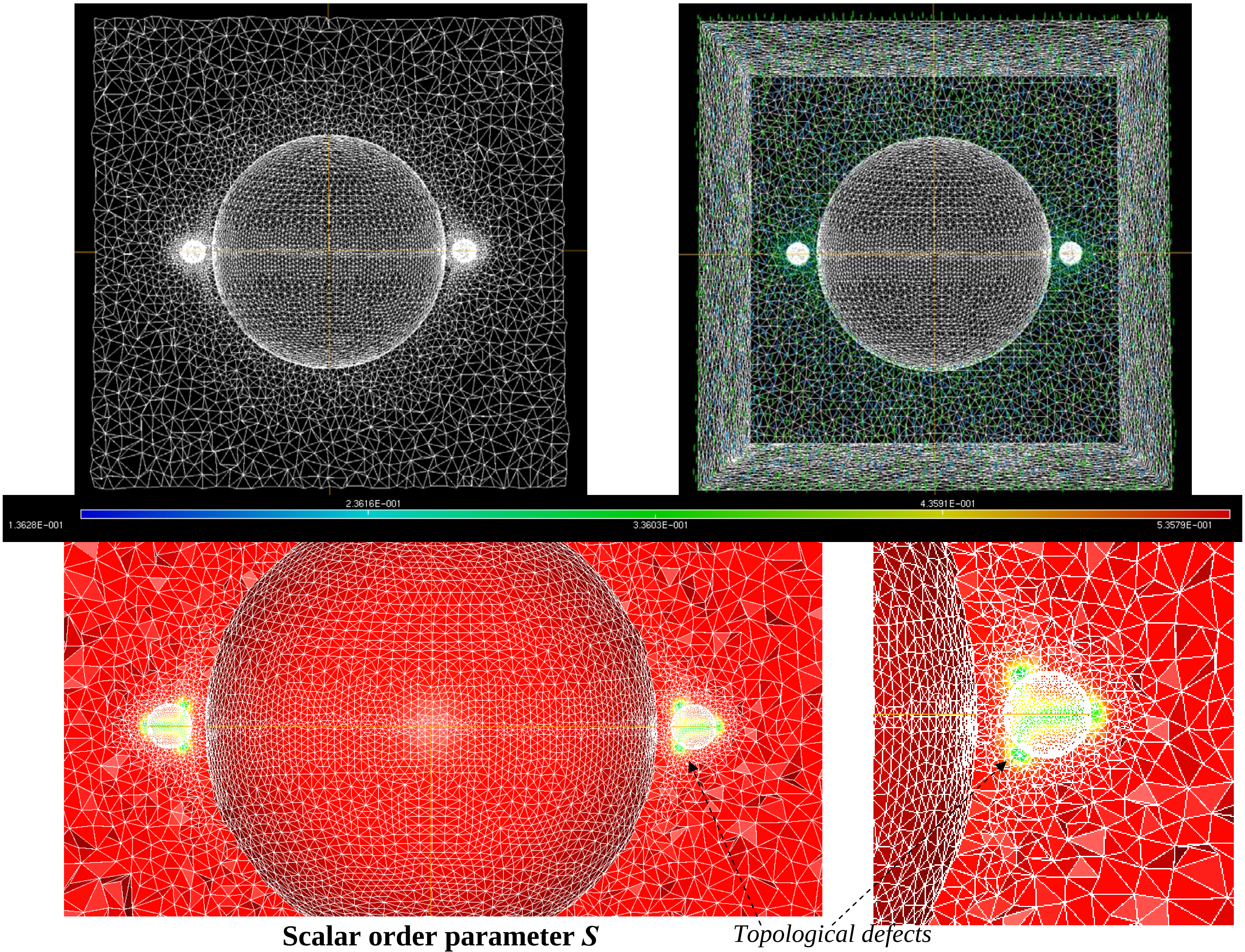


Scalar order parameter *S* *Topological defects*


2.3616E-001
4.3591E-001
1.3628E-001
3.3603E-001
5.3579E-001
Scalar order parameter S
Topological defects

Outline

- **Nematic liquid crystals**
- **Colloidal particles**
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- **Photonic systems**

New potential applications:
metamaterials, microresonators

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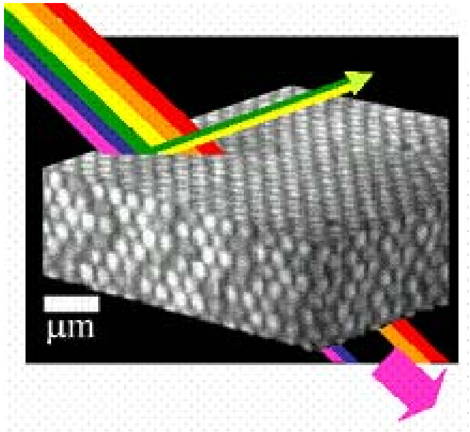
- *Photonic crystals:*



New potential applications: **metamaterials, microresonators**

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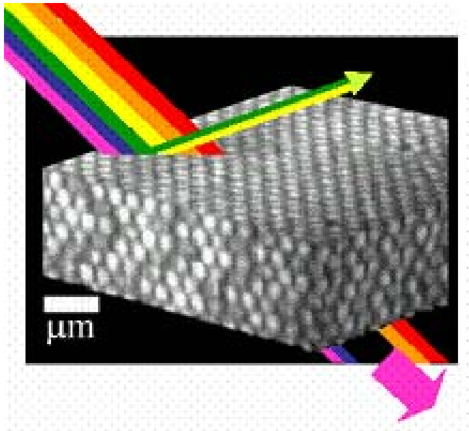
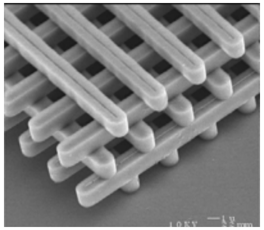
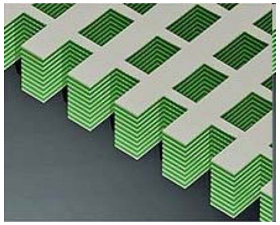


- *Solid state metamaterials:*





New potential applications:
metamaterials, microresonators

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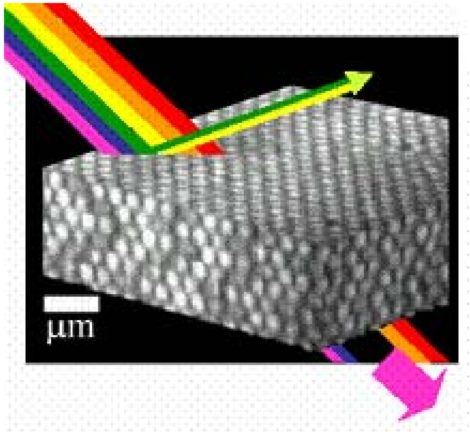

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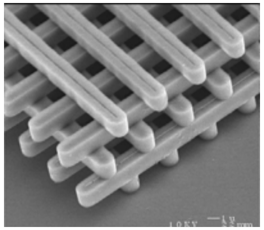

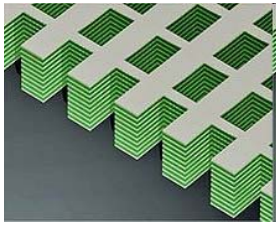

- ***Soft metamaterials?***

New potential applications:
metamaterials, microresonators

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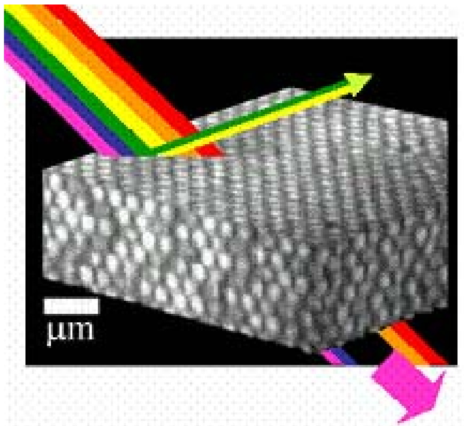

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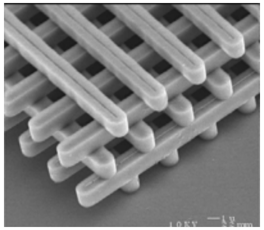

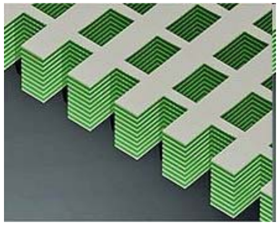

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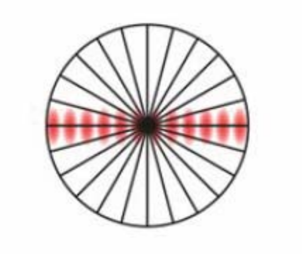
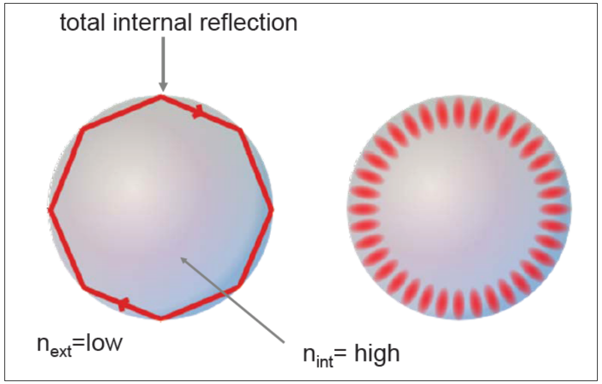


Nematic droplet.



Figures: I. Muševič, CLC Ljubljana Conference, 2010.

New potential applications:
metamaterials, microresonators

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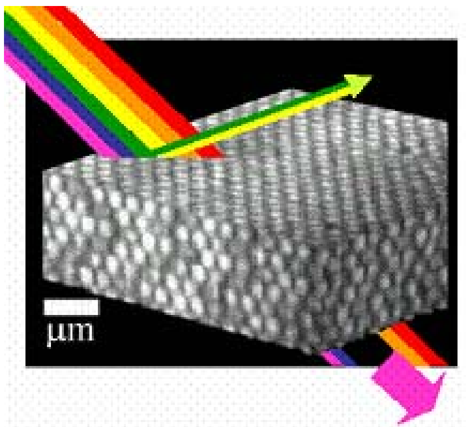

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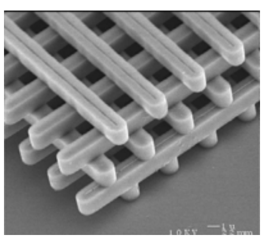

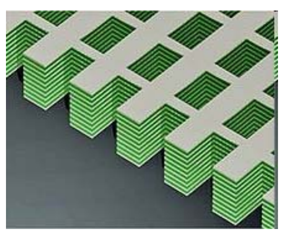

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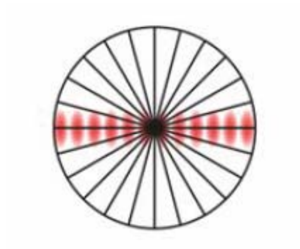

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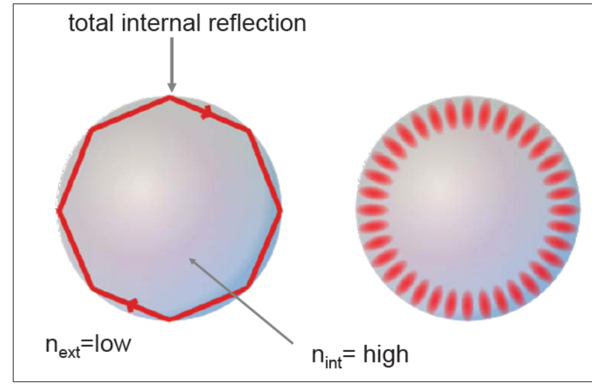

Whispering Gallery Modes (WGM) in a **microresonator.**

Figures: I. Muševič, CLC Ljubljana Conference, 2010.

New potential applications:
metamaterials, microresonators

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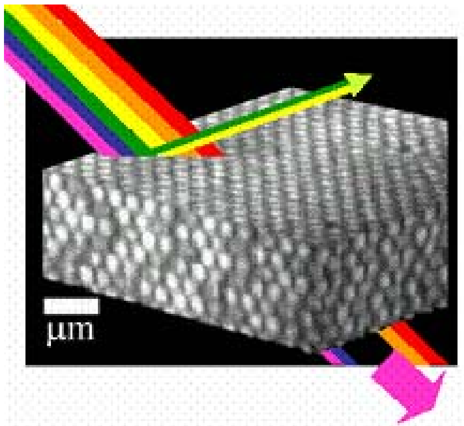

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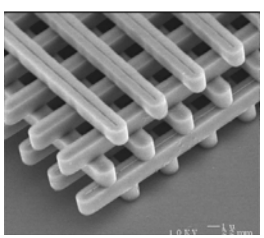

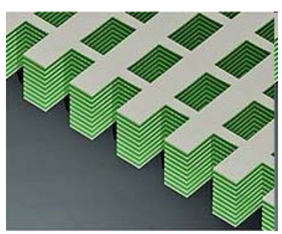

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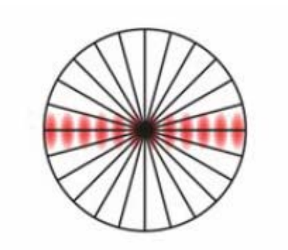
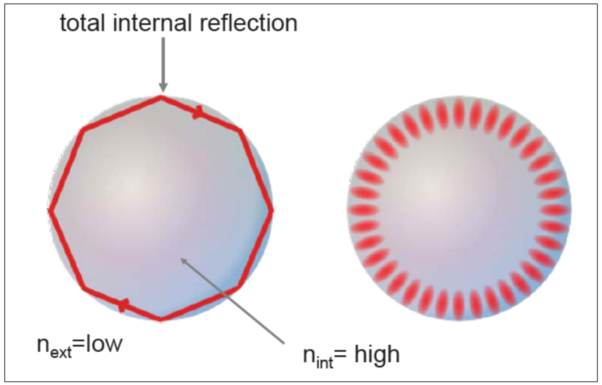
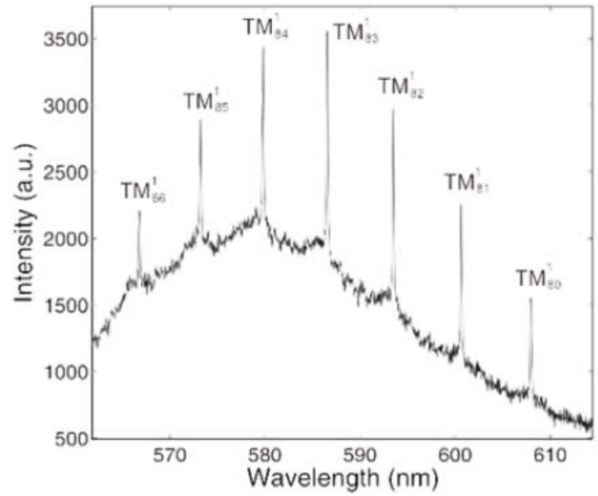


Nematic droplet.



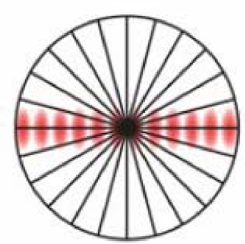
Whispering Gallery Modes (WGM) in a **microresonator.**

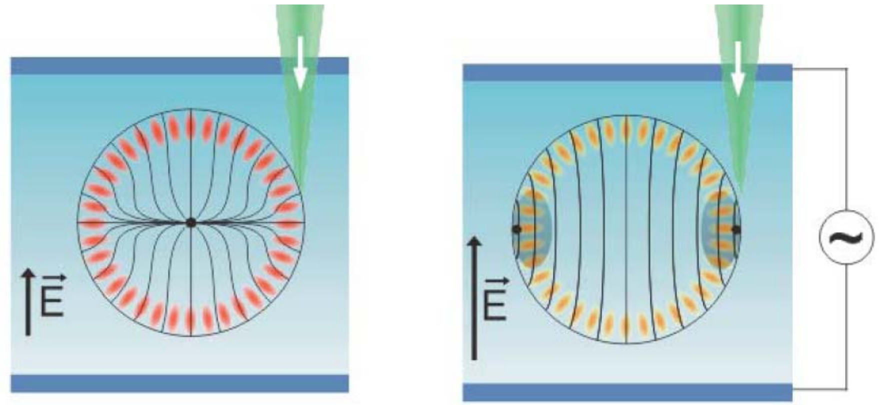


Figures: I. Muševič, CLC Ljubljana Conference, 2010.

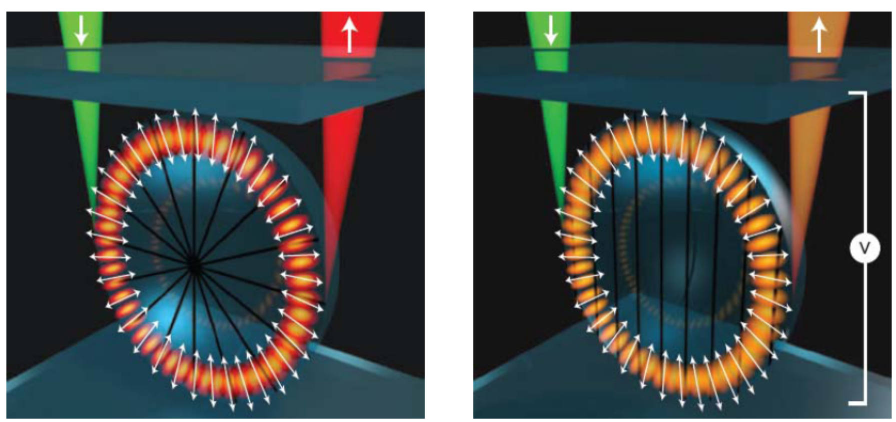
Nematic droplet

$E = 0$





By **tuning** electric field $\longrightarrow$ we **switch** between **optical modes**.



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Computational photonics

• **Detail dimensions** comparable with **wavelength**. → ~~Ray optics **not adequate**.~~

↓

Numerical solution of full Maxwell equations

↓

Time-harmonic expansion

↓

1) Frequency-domain eigenproblems

2) Frequency-domain response

Frequency domain eigenproblems

$$\vec{\nabla}\times\underline{\underline{\varepsilon}}(\vec{r})^{-1}\vec{\nabla}\times\vec{H}=\left(\frac{\omega}{c}\right)^{2}\vec{H}$$

$$\vec{\nabla}\cdot\vec{H}=0$$

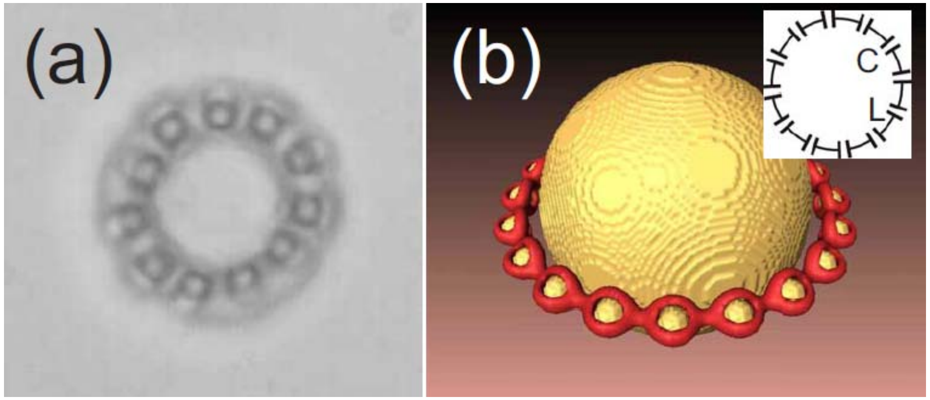
Eigenequation

(+ condition)

- Reduces to a

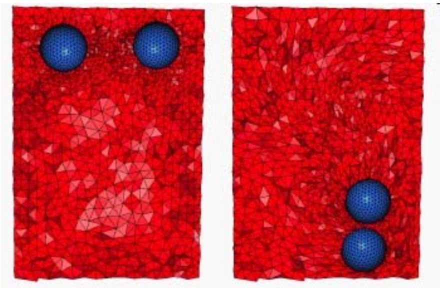
  matrix eigenproblem:

$$\boxed{Ax=\omega^{2}Bx}$$



Škarabot, Ravnik et al., PRE, 2008.

Future work



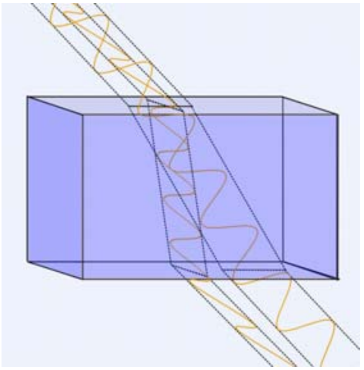
– Movement of particles to stationary positions → movement of mesh.

– Initial mesh and starting guess for general setting of spherical particles (*should be good enough in order to converge*).

– Anisotropic mesh adaptivity (code module **mmg3d**).

– Visualization.

– EM code for solving Maxwell eqns in *nonhomogeneously anisotropic* media.



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