1st Hellenic Forum for Science Technology and Innovation

National Center for Scientific Research – Demokritos, July 17-19, 2013

Harvard – Dept. of Physics and
School of Engineering and Applied Sciences
1991 – present

University of Crete – 1997-98 (Physics Dept.)

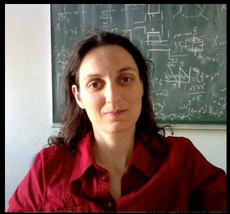
University of Ioannina – 2002-04 (Materials Science Dept.)

Foundation for Research and Technology Hellas (FORTH)
Affiliated Member – 1998 - present

Paul Maragakis (PhD: University of Crete)
now: D.E. Shaw Research, New York

Ioannis Remediakis (PhD: University of Crete)
now: Department of Materials Science and Technology, University of Crete (Assistant Professor)

Maria Fyta (PhD: University of Crete)
now: Institute of Computational Physics, University of Stuttgart (Junior Professor)



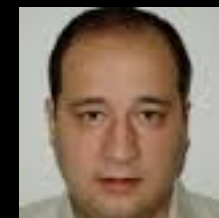
Argyrios Tsolakidis (PhD: University of Thessaloniki)
now: Shell Oil, The Netherlands

George Papamokos (PhD: University of Ioannina)
now: Forschungszentrum Jülich, Institute for Advanced Simulation

Dionisios Margetis (PhD: Harvard University)
now: Department of Mathematics,
University of Maryland (Professor)

Dimitrios Kontaxakis (PhD: University of Thessaloniki)
now: FlowKit Ltd, Lausanne, Switzerland

Costas Papaloukas (PhD: University of Ioannina)
now: Department of Biotechnology,
University of Ioannina (Assistant Professor)



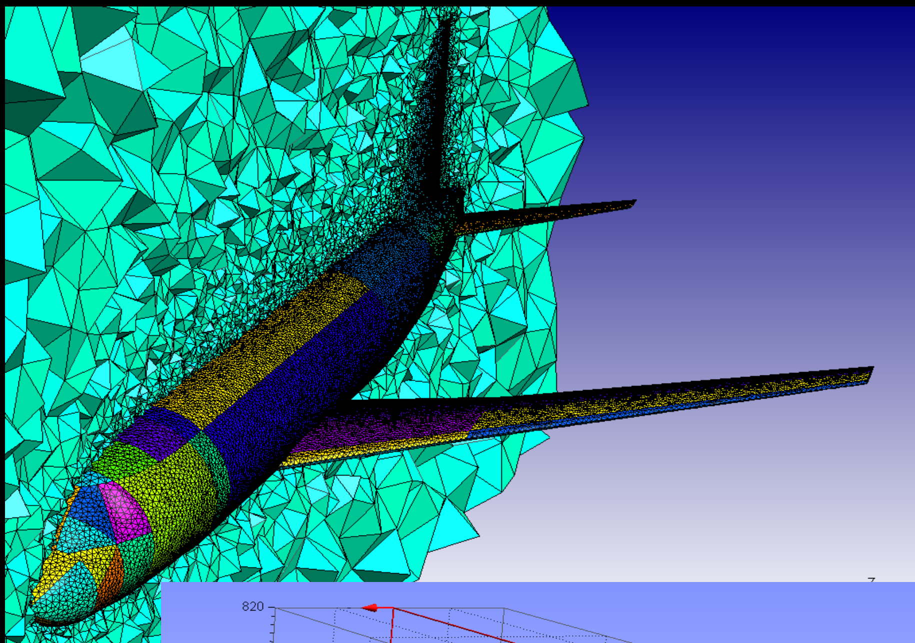
George Tritsaris (PhD: University of Patras)
now: Harvard SEAS - postdoc

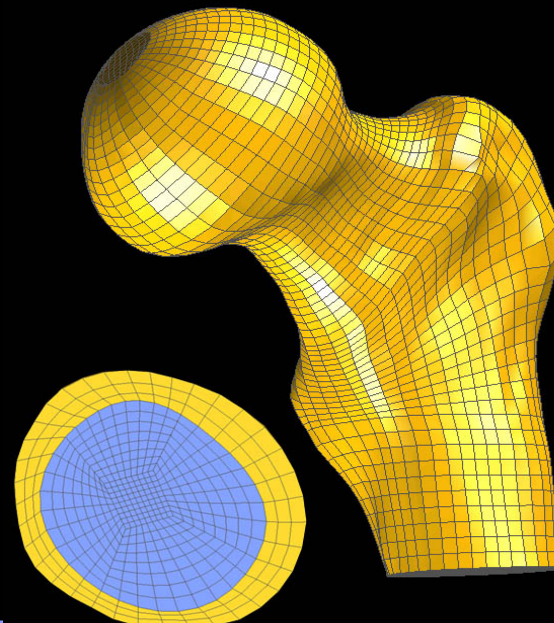
Predicting and Interpreting Complex Phenomena through Multiscale Modeling

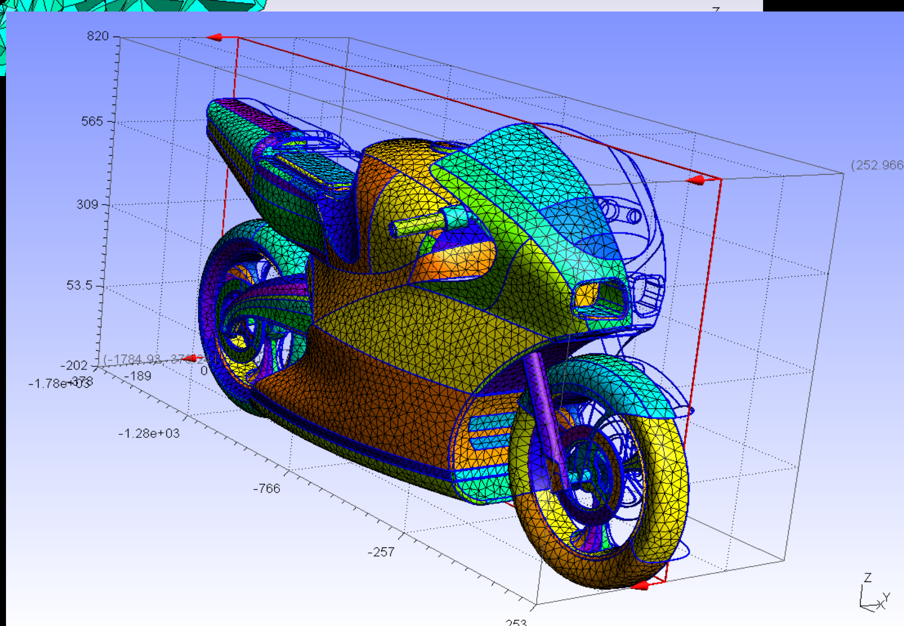
Two examples (challenges - opportunities):
- predictions for new materials (OPV’s)
- hemodynamics simulations for coronary artery disease

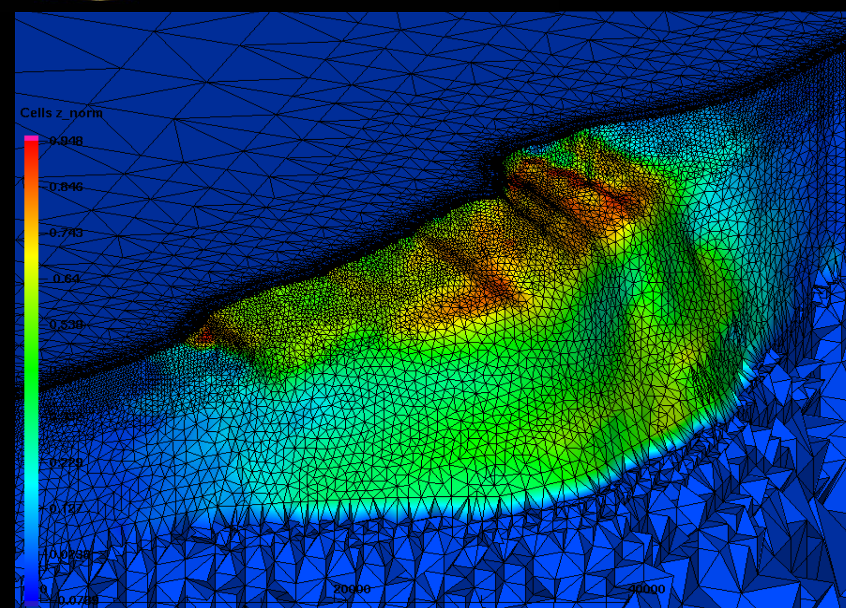
Broader picture: modeling and simulation

Computation is pervasive in real world





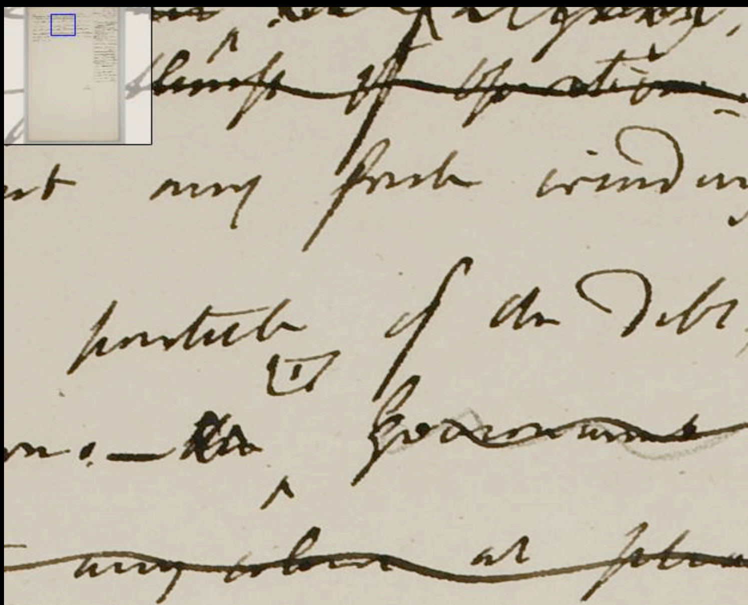




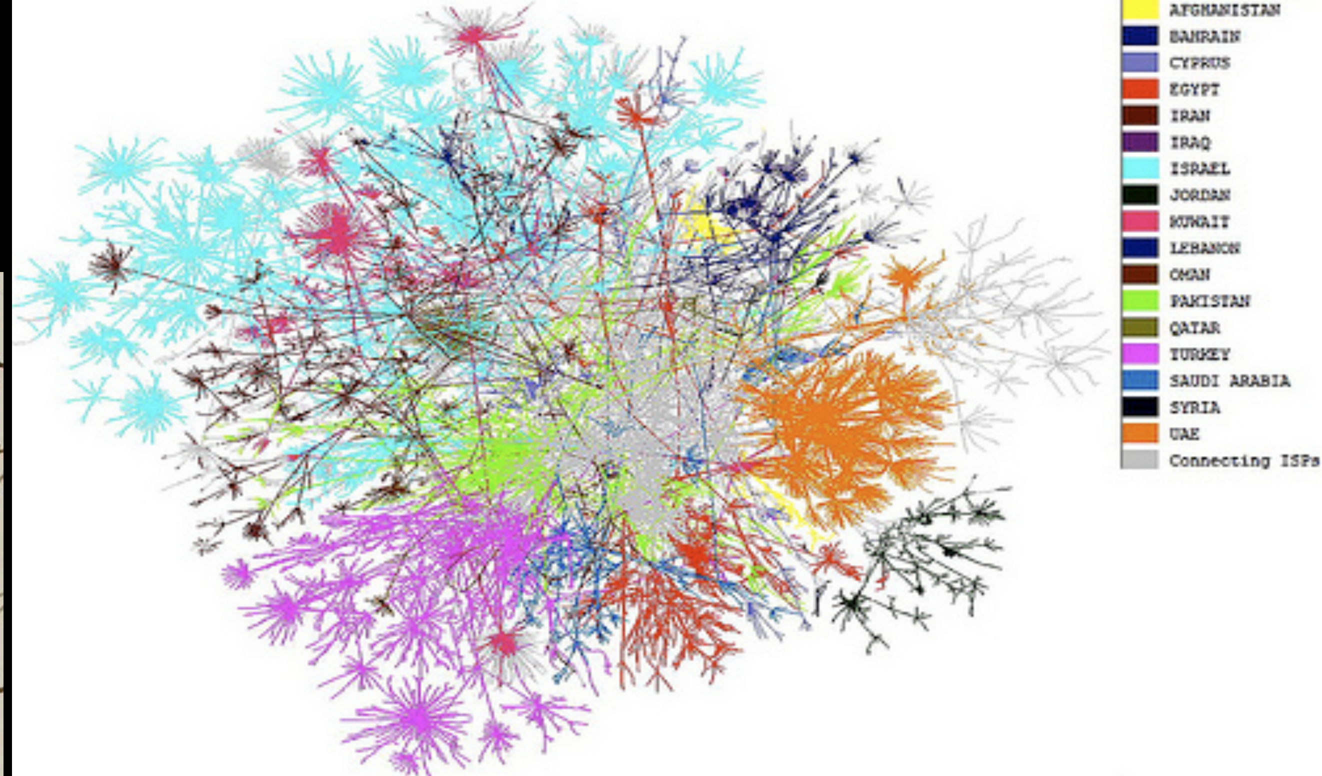
The country that
out-*computes*
will be the one that
out-*competes*.

U.S. Council on Competitiveness, 2004

Greece CAN *out*-compute
- talent
- resources

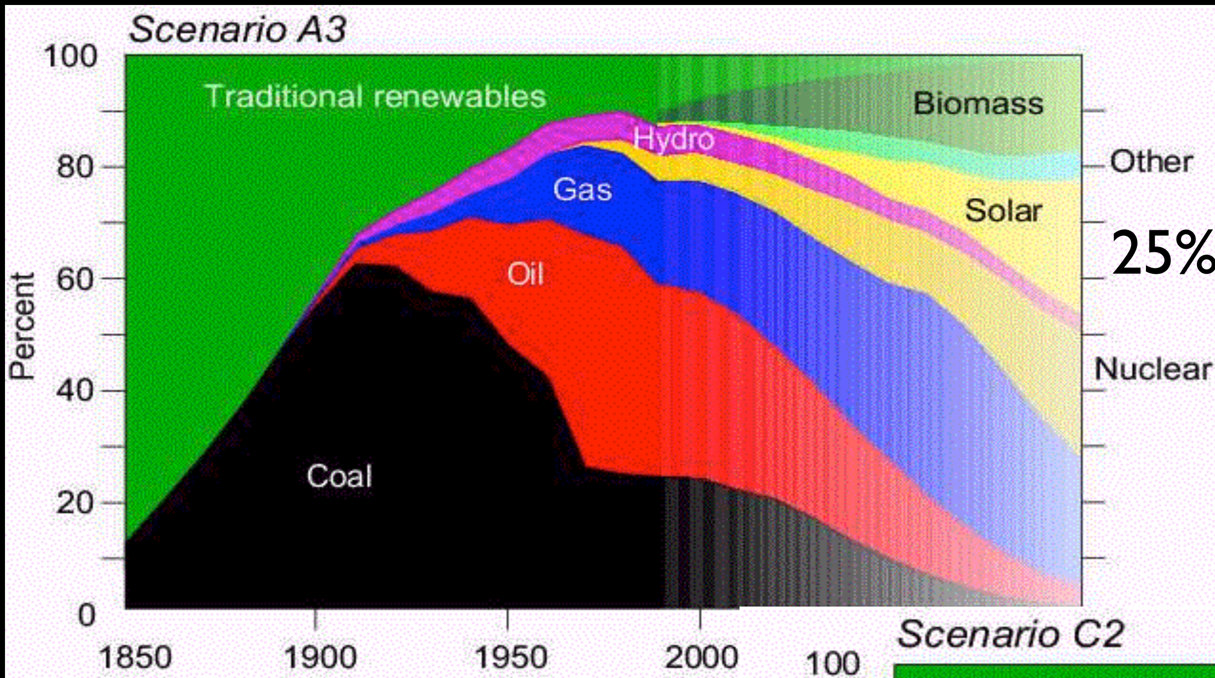


arts / humanities



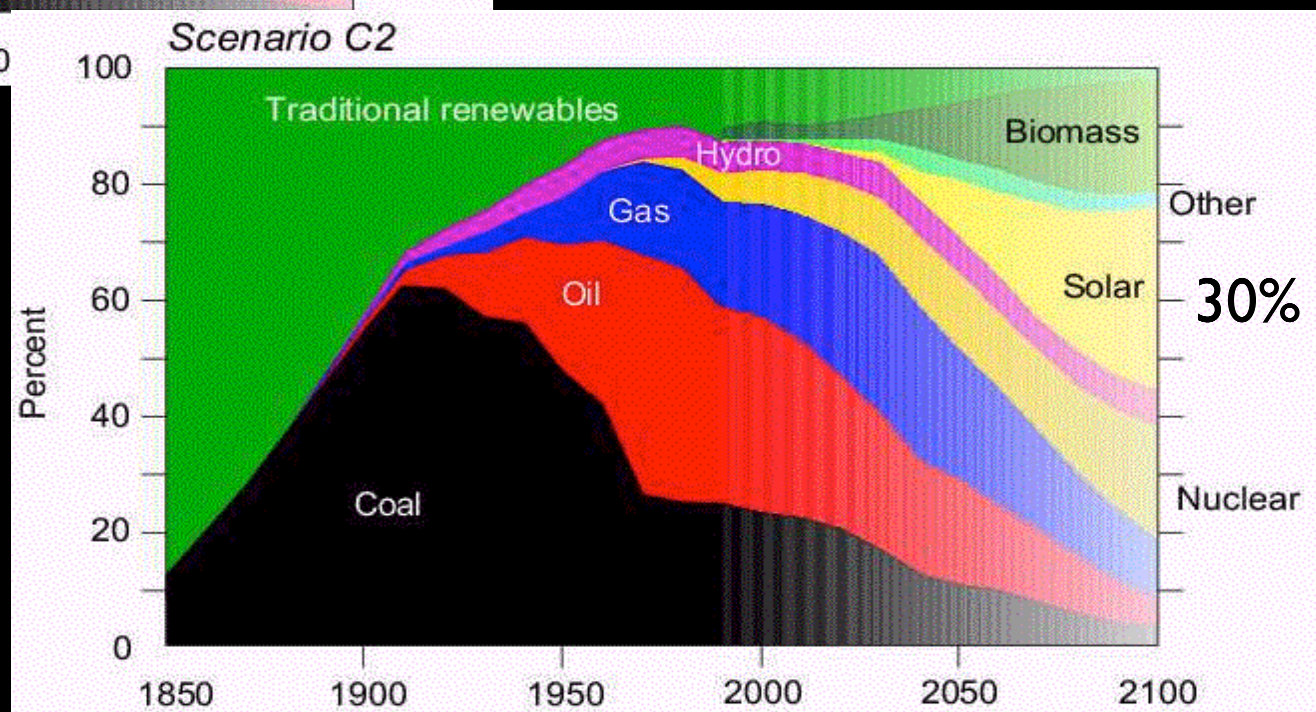
social / political sciences

The challenge of sustainable energy



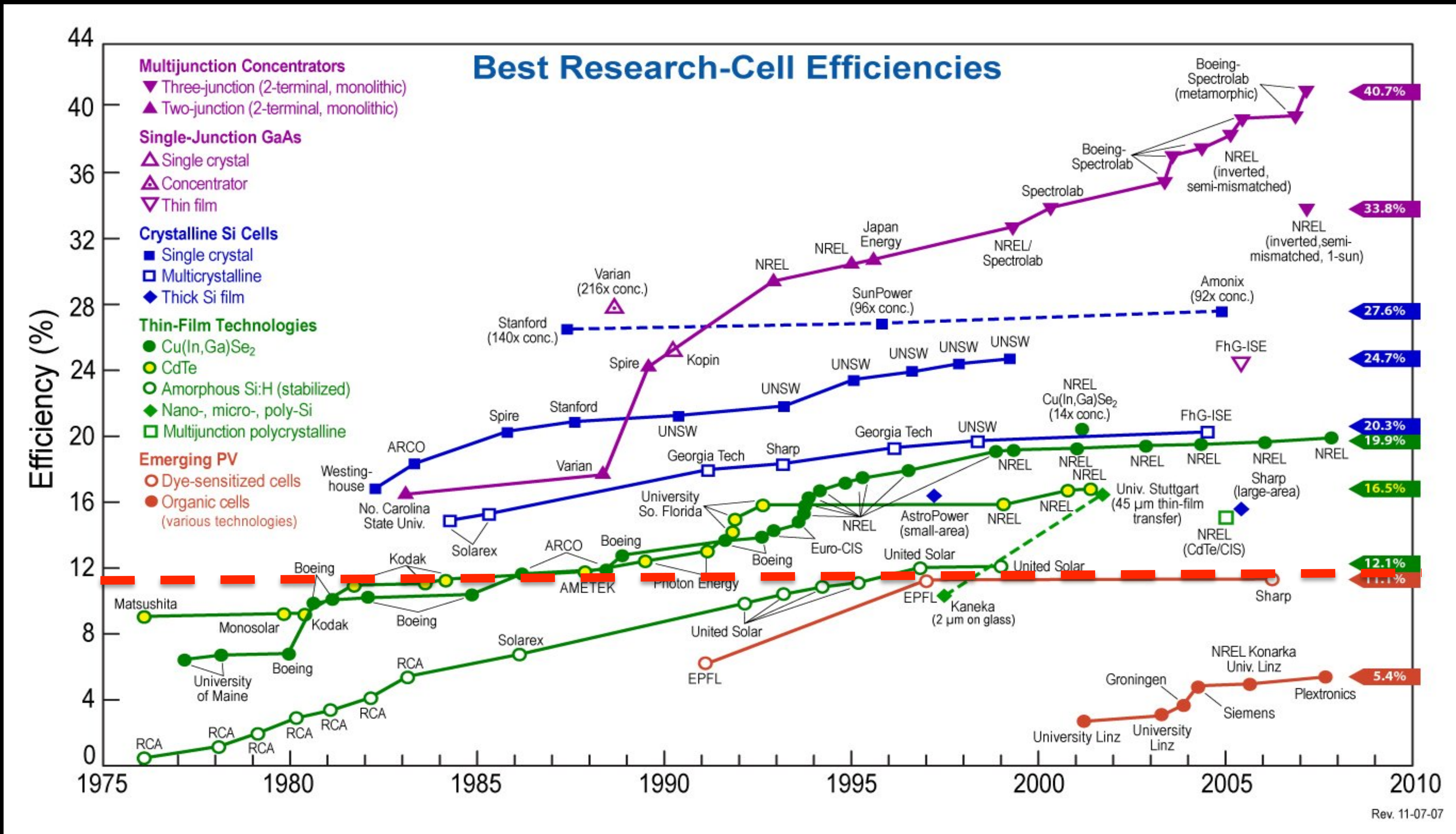
Time and resources running out

Materials Genome Initiative (2012-13)



Report of Intergovernmental Panel on Climate Change

2007 Nobel Peace Prize (shared with A. Gore)

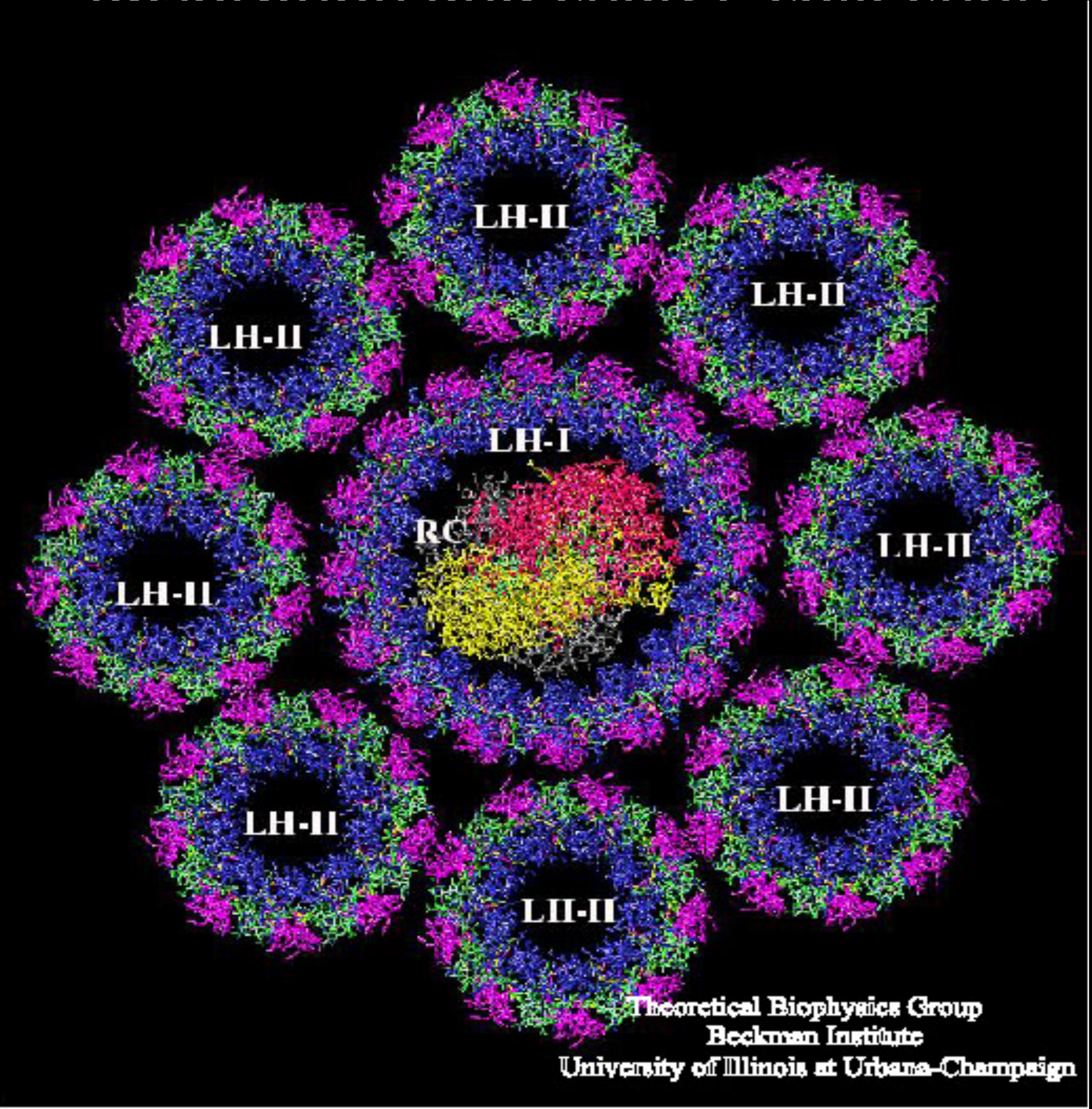


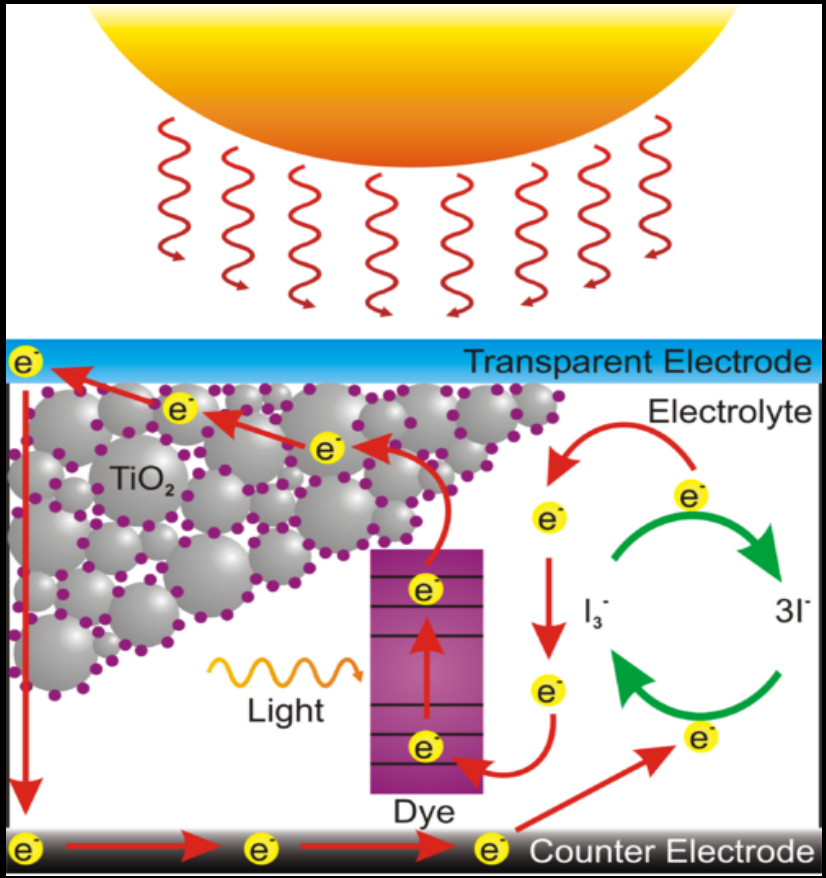
Best Research-Cell Efficiencies
Efficiency (%)
Multijunction Concentrators
Three-junction (2-terminal, monolithic)
Two-junction (2-terminal, monolithic)
Single-Junction GaAs
Single crystal
Concentrator
Thin film
Crystalline Si Cells
Single crystal
Multicrystalline
Thick Si film
Thin-Film Technologies
Cu(In,Ga)Se2
CdTe
Amorphous Si:H (stabilized)
Nano-, micro-, poly-Si
Multijunction polycrystalline
Emerging PV
Dye-sensitized cells
Organic cells (various technologies)
40.7%
33.8%
27.6%
24.7%
20.3%
19.9%
16.5%
12.1%
11.1%
5.4%
Boeing-Spectrolab (metamorphic)
NREL (inverted, semi-mismatched)
NREL (inverted,semi-mismatched, 1-sun)
Amonix (92x conc.)
SunPower (96x conc.)
Stanford (140x conc.)
Varian (216x conc.)
NREL Cu(In,Ga)Se2 (14x conc.)
Univ. Stuttgart (45 µm thin-film transfer)
AstroPower (small-area)
Kaneka (2 µm on glass)
NREL (CdTe/CIS)
Sharp (large-area)
NREL Konarka Univ. Linz
Rev. 11-07-07

The dye-sensitized (3rd generation) solar cell

The Principle: Separate light-absorption and charge collection

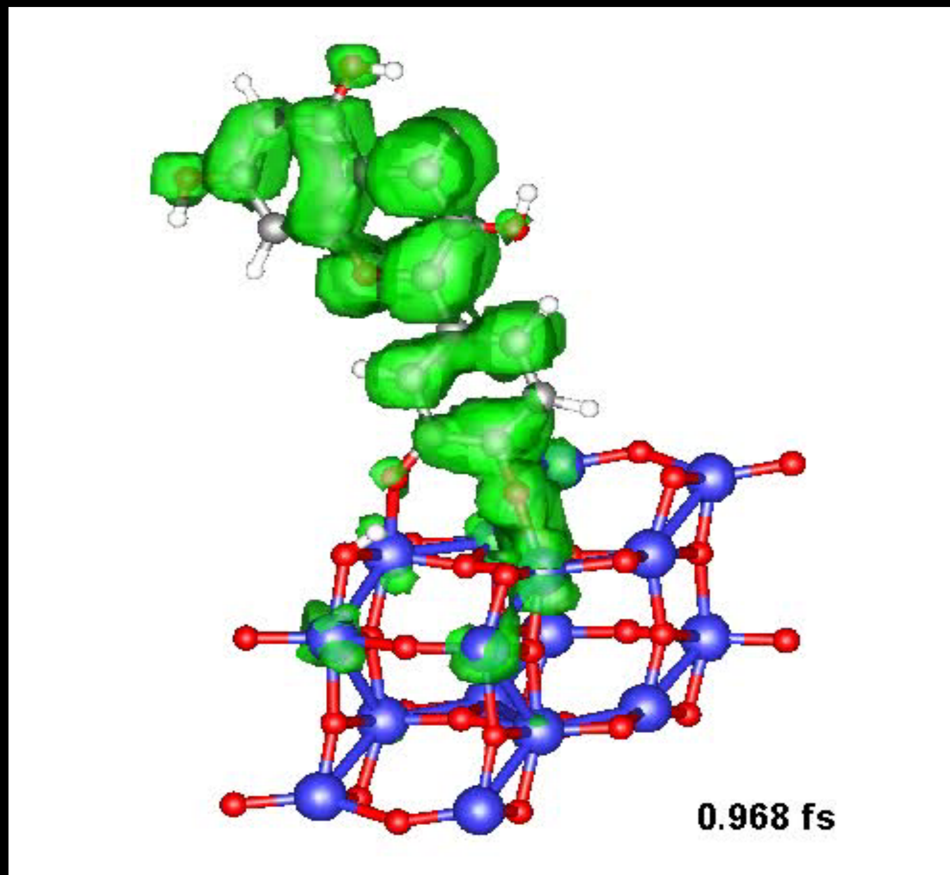
Typical plant: ~0.1%
Crop plants: ~1%
Sugarcane: ~8%



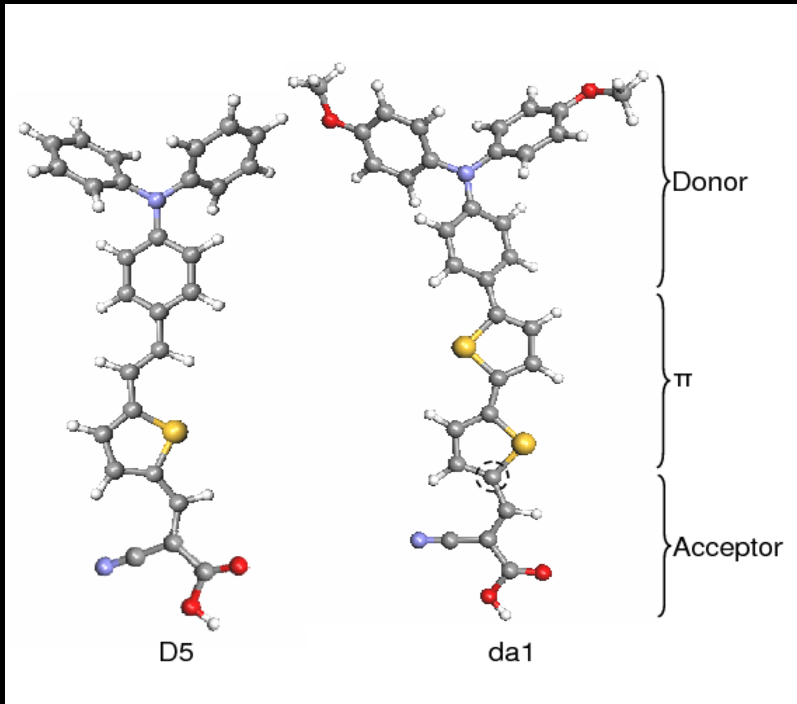


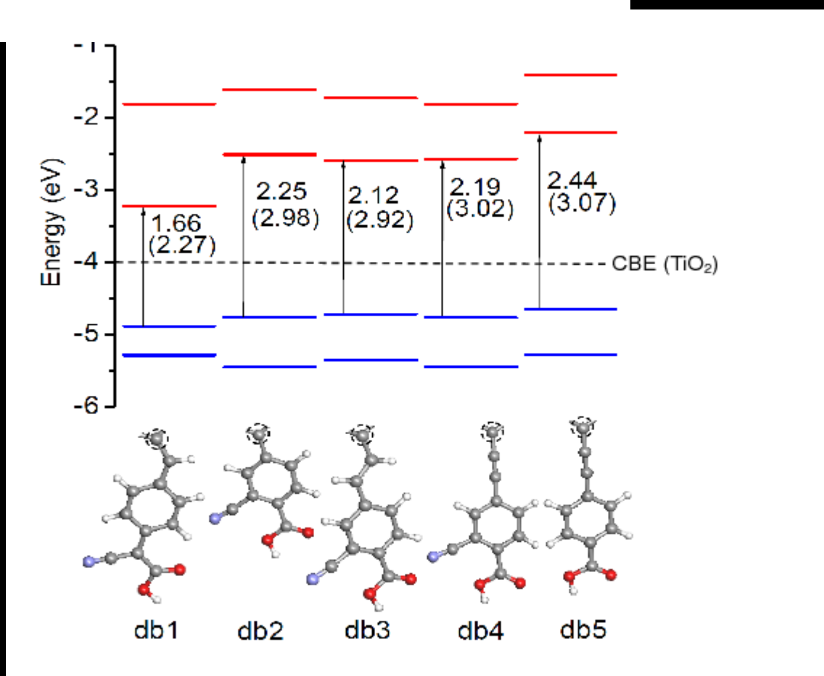
O'Regan & Graetzel, Nature (1991)

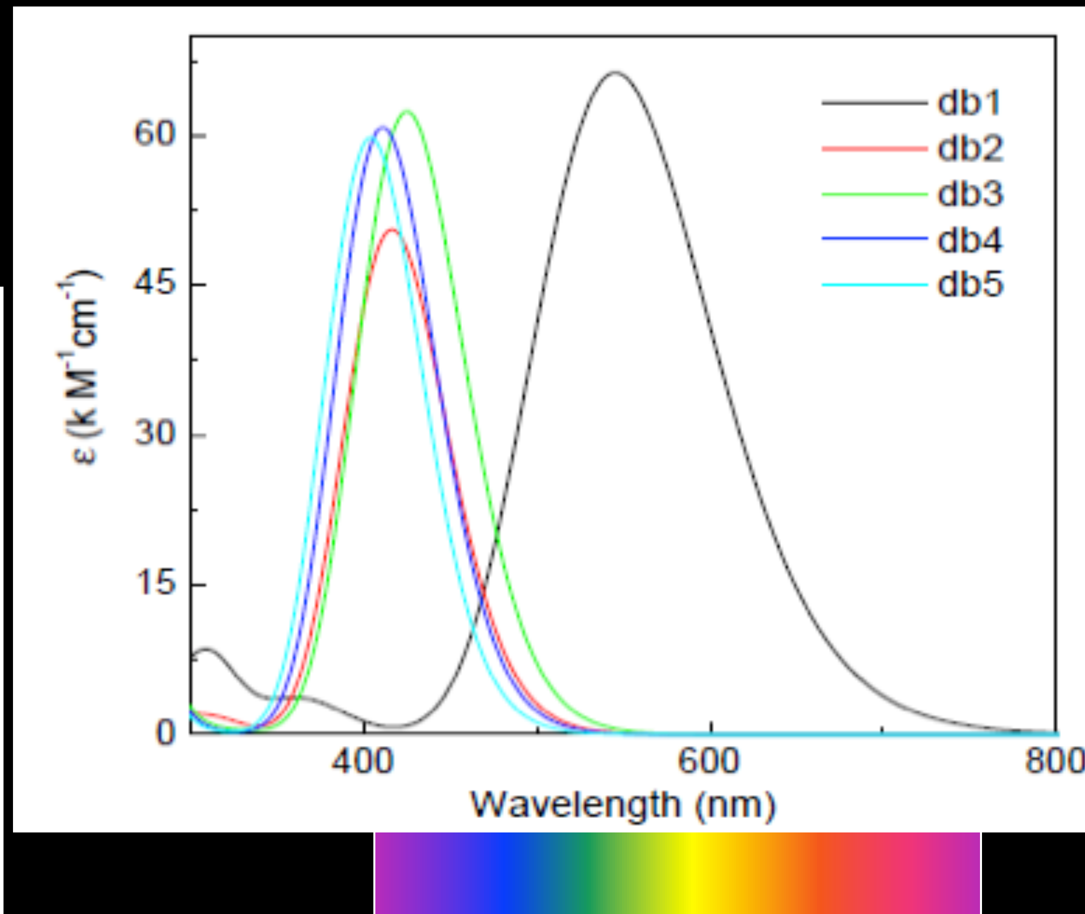
Electron motion in PV device: solve the time-dependent Schodinger equation



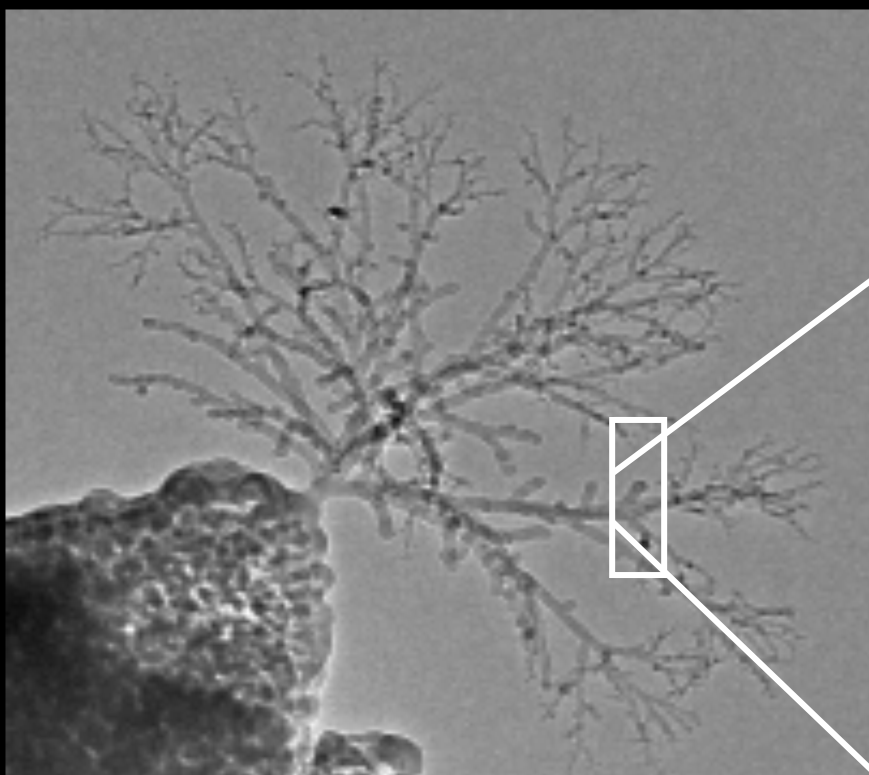
“Designer” dyes: Predict properties of new dyes (not yet tried in experiments)

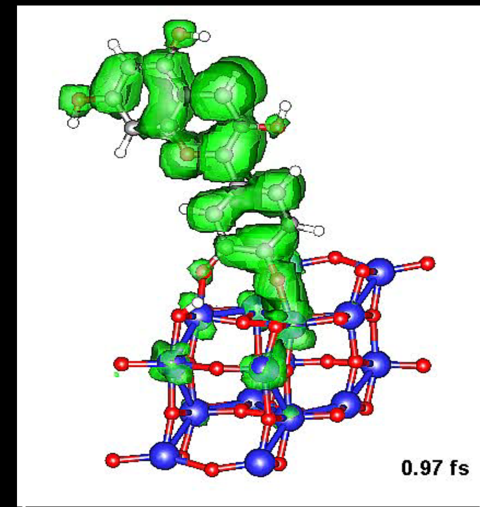


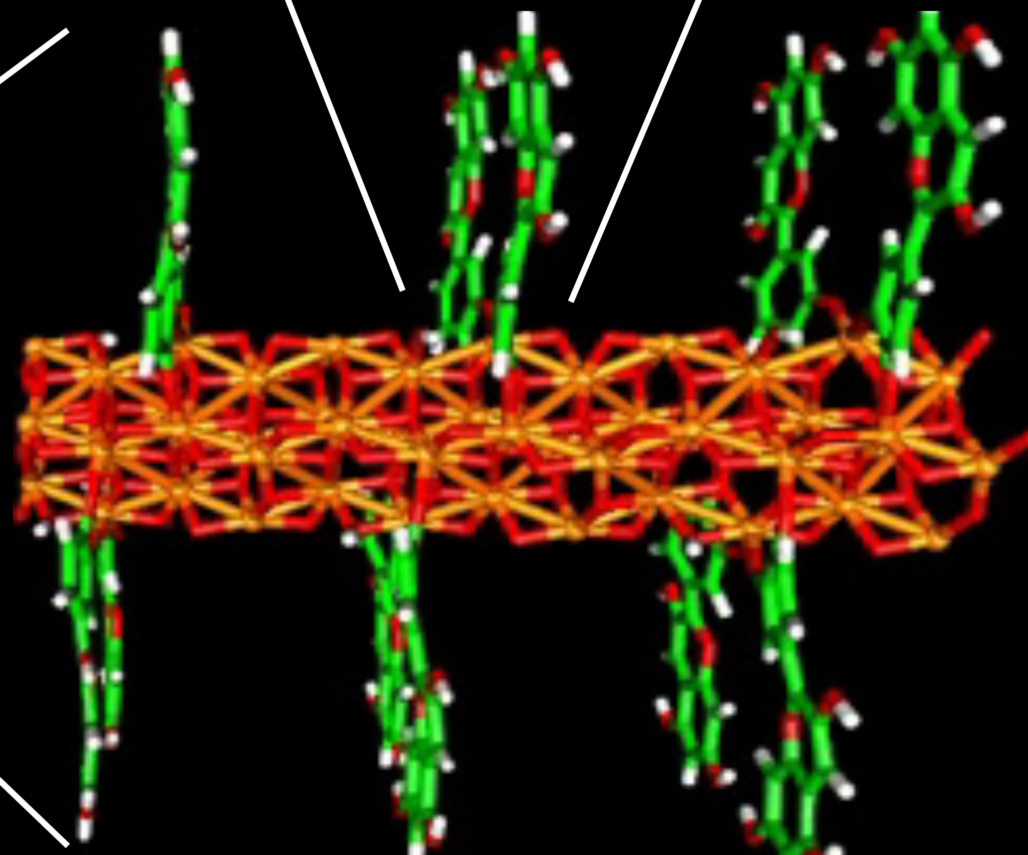




Artificial Nano Tree
(based on QM simulations)

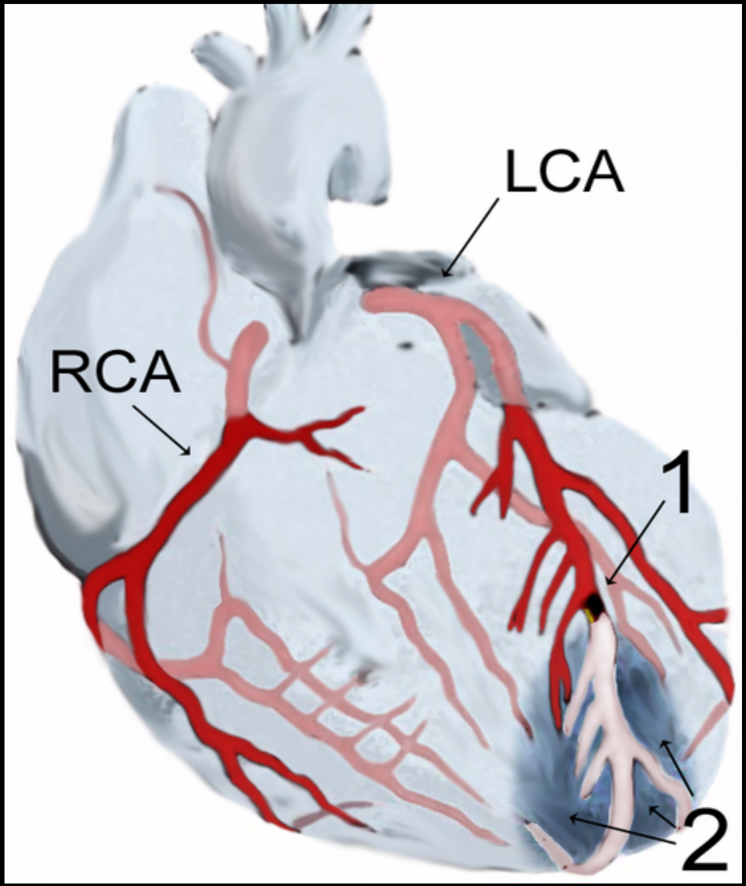


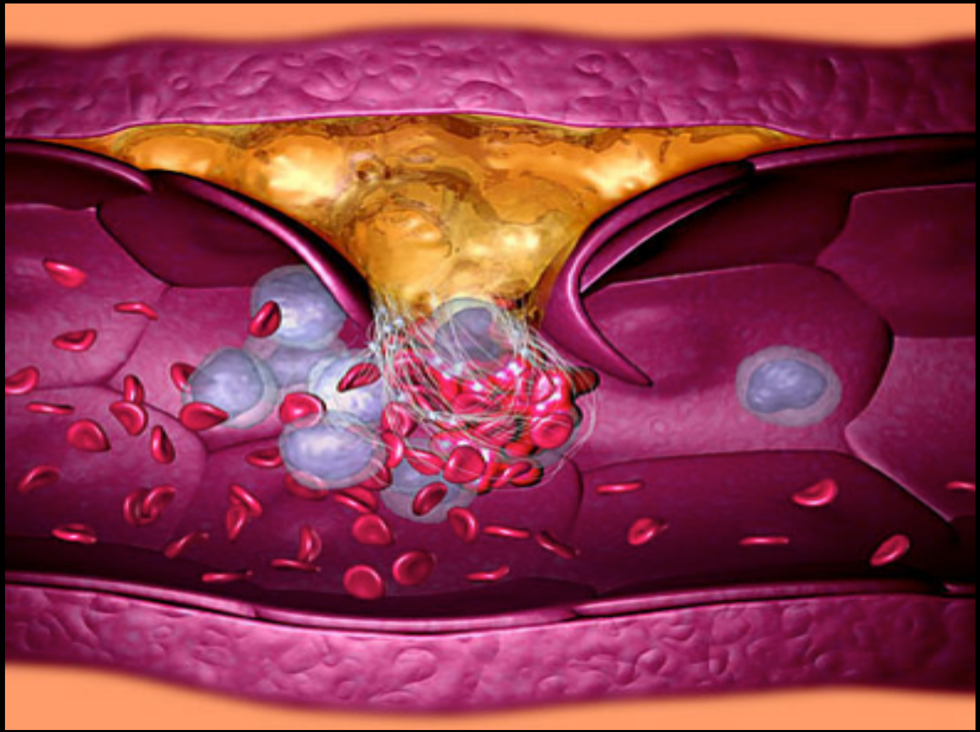




Flexible materials – deposit on any surface

Acute Myocardial Infarction (heart attack)





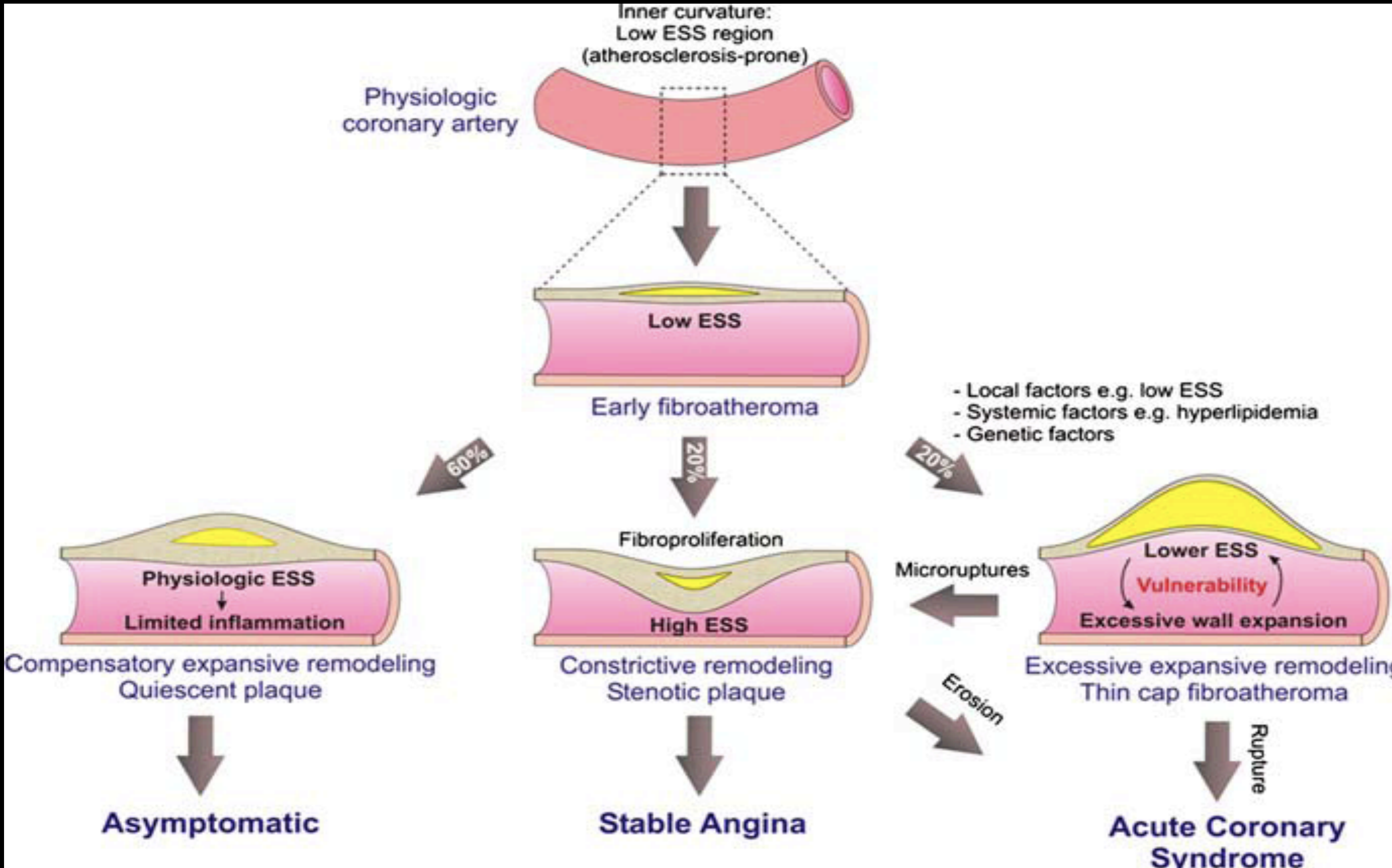
Deaths in USA: out of ~2.5 M per year total,

- 35% blood flow obstruction (80% heart, 20% brain)

UNPREDICTABLE

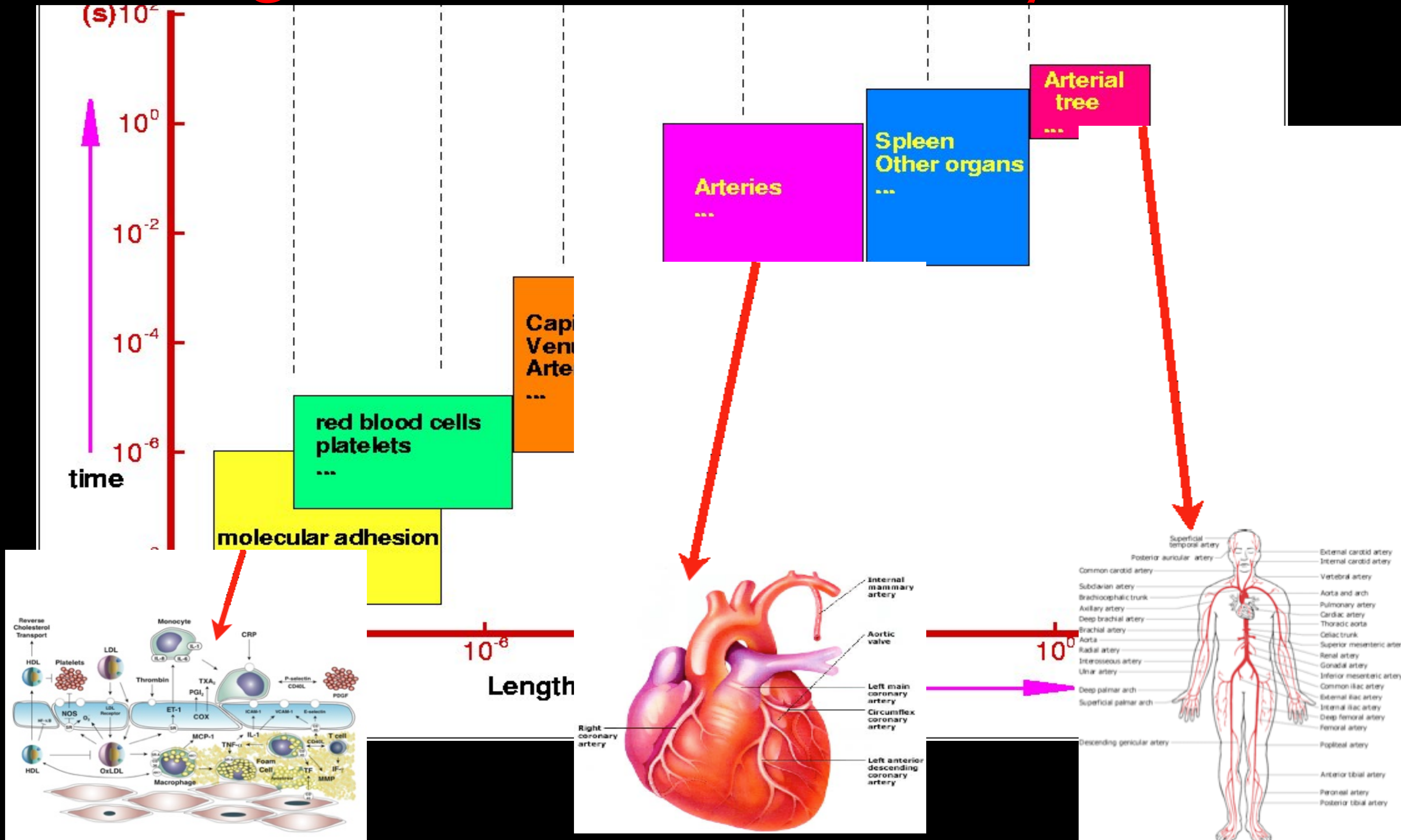
- 25% cancer (all types)

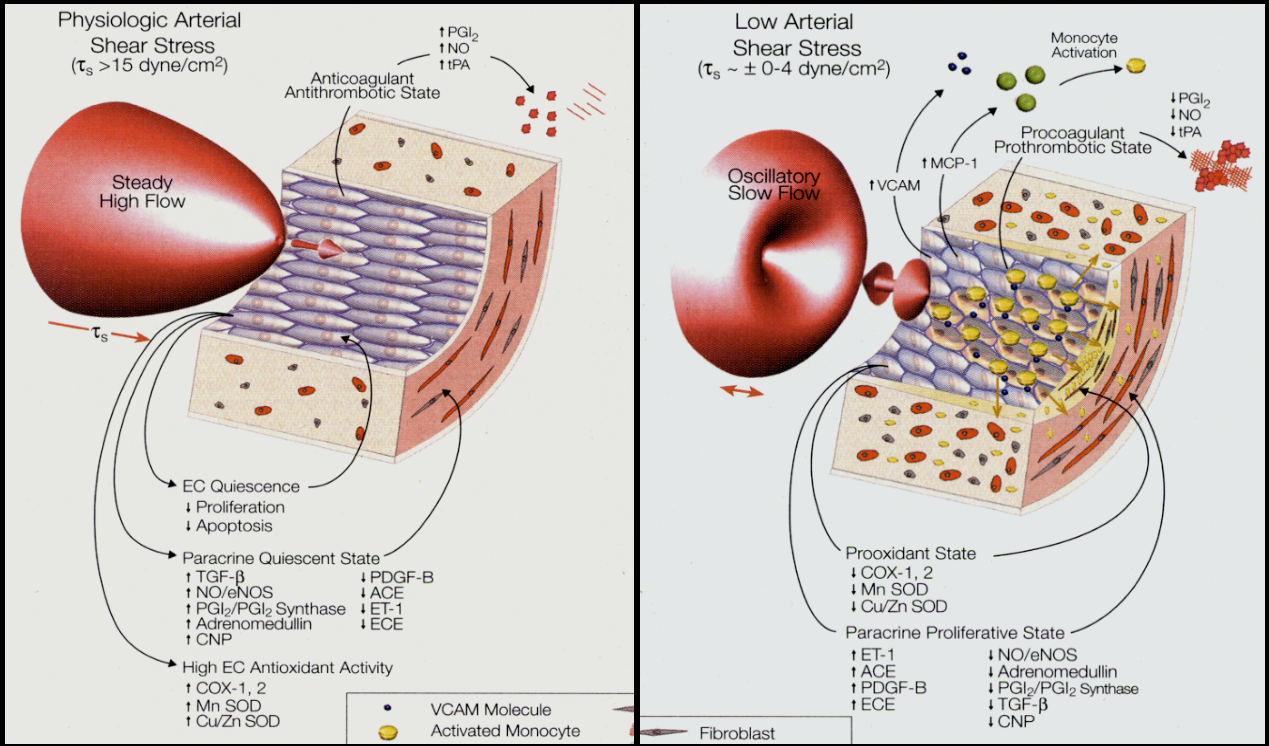
Formation and evolution of plaques



ESS = Endothelial Shear Stress, ACCESSIBLE ONLY BY SIMULATION

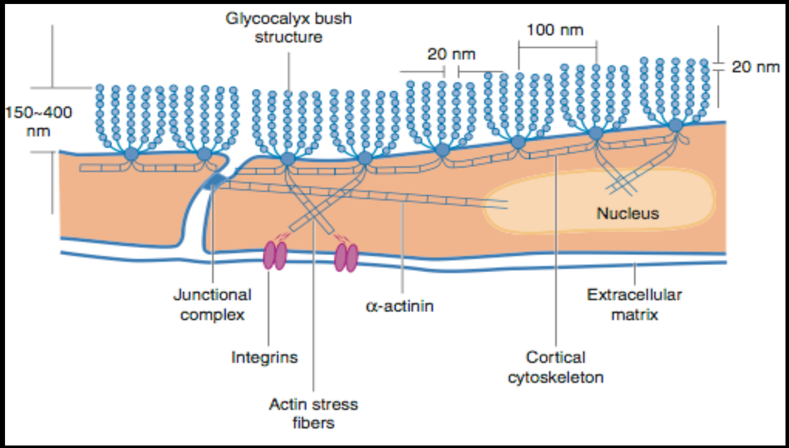
Challenge: Multi-scale hemodynamics

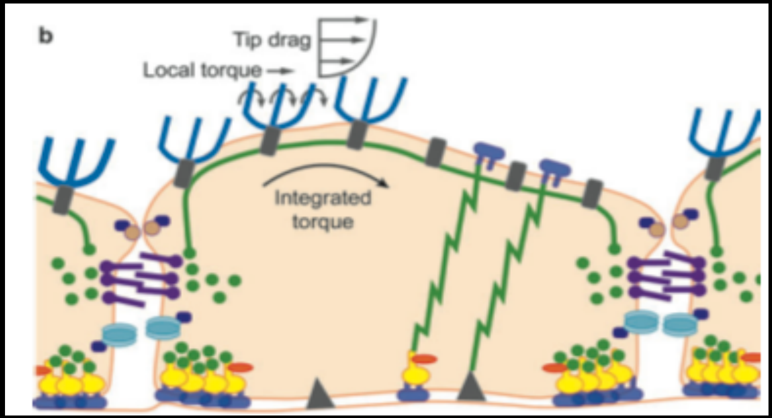




Vasculoprotective

Vascular adhesion of lipoproteins & inflammatory cells



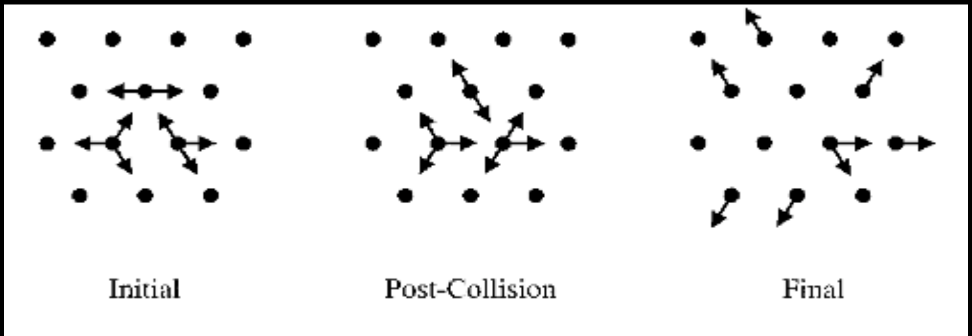


CT scan data

smoothing

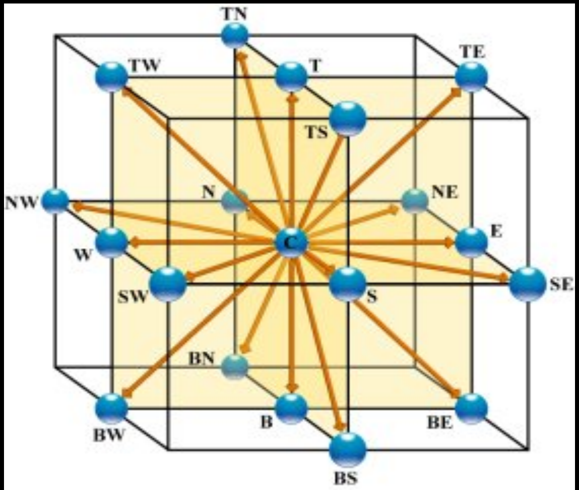
Fluid dynamics by cellular automata : Lattice Boltzmann Equation (LBE)

$$f_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = f_i(\vec{x},t) - \omega\Delta t(f_i - f_i^{eq})(\vec{x},t)$$



$$f_i^{eq} \propto \rho w_i \left[1 + \frac{\vec{c}_i \cdot \vec{u}}{c^2} + \frac{(\vec{c}_i \cdot \vec{u})^2 - c^2 u^2}{2c^4}\right]$$

Bhatnagar-Gross-Krook algorithm



Reproduces the physics of fluid dynamics (Navier-Stokes equation)

Fluid properties :

Fluid density

$$\rho(\vec{x},t) = \sum_i f_i(\vec{x},t)$$

Momentum (flow)

$$\rho(\vec{x},t)\vec{u}(\vec{x},t) = \sum_i f_i(\vec{x},t)\vec{c}_i$$

Stress Tensor

$$\overleftrightarrow{\sigma}(\vec{x},t) = \frac{\nu\omega}{c_s^2}\sum_i \vec{c}_i\vec{c}_i\left[f_i - f_i^{eq}\right](\vec{x},t)$$

Wall Stress

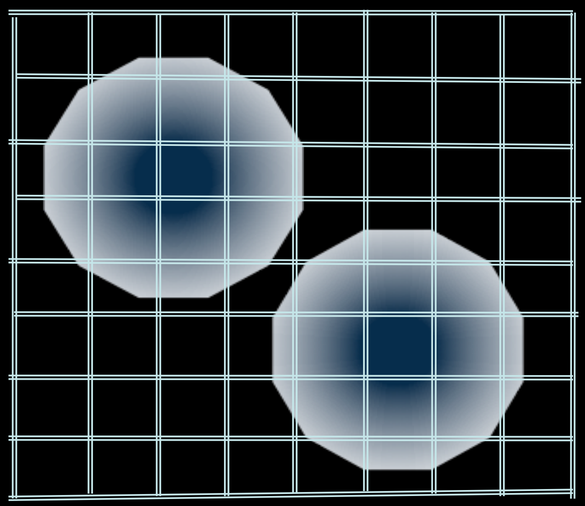
$$S(\vec{x}_w,t) = \sqrt{\left(\overleftrightarrow{\sigma} : \overleftrightarrow{\sigma}\right)\left(\vec{x}_w,t\right)}$$

Definition of "particles" (cells, proteins, …)

$$\tilde{\delta}_\xi(x-R) = \prod_{\alpha=x,y,z} \tilde{\delta}_\xi(x_\alpha - R_\alpha)$$

$$\sum_x \tilde{\delta}_\xi(x-R) = 1$$

$$\tilde{\delta}_\xi(a) = \begin{cases} \frac{1}{2\xi}\left(1+\cos\left(\frac{\pi|a|}{\xi}\right)\right) & 0 \le |a| \le \xi \\ 0 & \xi \le |a| \end{cases}$$



$$\varphi(x,R) = -\gamma\left(V - u(x)\right)\tilde{\delta}_\xi(x-R)$$

$$F^H = \sum_x \varphi = -\gamma\left(V - \tilde{u}\right)$$

$$\tilde{u} = u * \tilde{\delta}_\xi$$

$$\Delta f_p = -\frac{w_p}{c^2} c_p \cdot \sum_R \varphi$$

Equations of motion:

$$\Xi \frac{d\Psi}{dt} \equiv \begin{pmatrix} M\frac{dV}{dt} \\ I\frac{d\Omega}{dt} \end{pmatrix} = \begin{pmatrix} F + F^H \\ T + T^H \end{pmatrix} \equiv \Phi + \Phi^H$$

$$\Phi^H_{6\times1} = \Gamma_{6\times6}\Psi^*_{6\times1} + \Delta_{6\times3\times3} : E_{3\times3}$$

$$\Psi^* \equiv \begin{pmatrix} V - u \\ \Omega - \omega \end{pmatrix}$$

Brenner et al '72

Γ	Grand Resistance matrix
Δ	Shear Resistance matrix
E	Strain tensor
u	Fluid velocity @center
$\omega = \frac{1}{2}\partial \times u$	Fluid vorticity @center

Γ and Δ depend on the whole configuration

Pair-wise superposition

$O(N^3)$ complexity!

Brady & Bossis '89

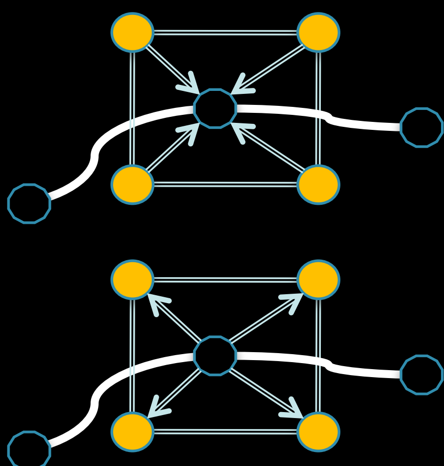
Fluid-particle coupling:

$$(\partial_t + v \cdot \partial_x) f = -\omega(f - f^{eq}) - \frac{1}{M} \sum_R F^H \cdot \partial_v f$$

$$\frac{d}{dt} V = \frac{1}{M} (F + F^H)$$

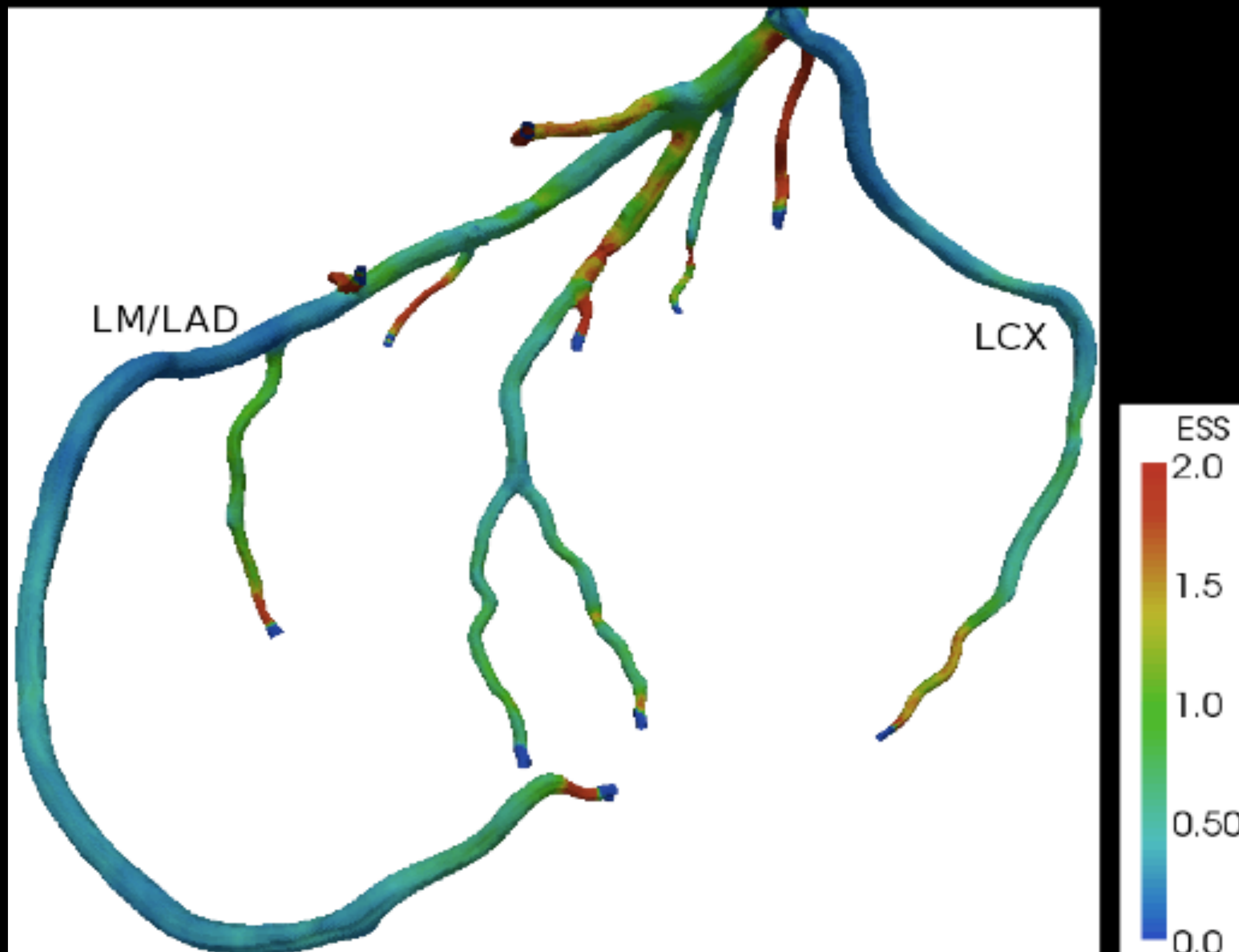
$$F^H = -\gamma \left[V - u(x, \{R, V\}) \right] \delta(x - R)$$

Momentum exchange
(Newton’ s restitution law)



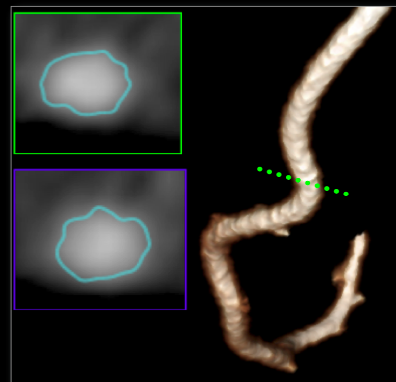

computing in SCIENCE & ENGINEERING
Multiscale Simulation of Nanobiological Flows
MARIA FYTA AND EFTHIMIOS KAXIRAS
Harvard University
SIMONE MELCHIONNA
University of Rome
SAURO SUCCI
National Research Council, Italy

ESS Calculation in patient-specific arterial tree

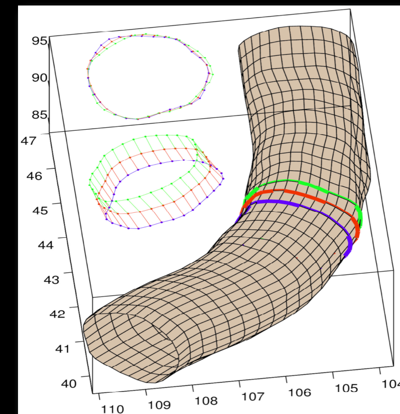


A practical tool for patient-specific diagnosis and intervention (a bit more work to do ...)

CT Patient Data →



Data Segmentation →

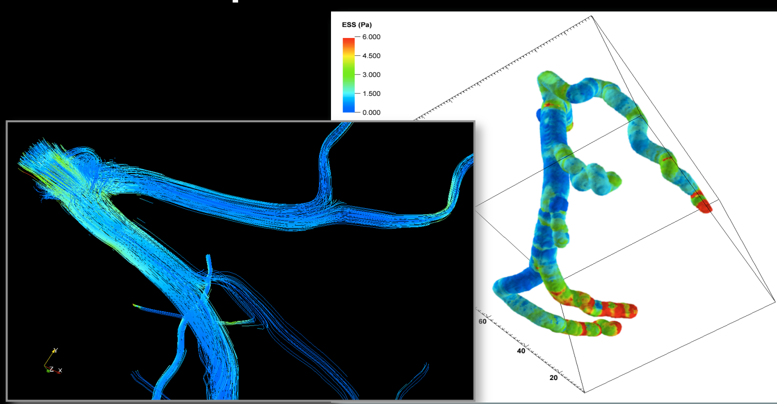


HPC Data Preparation ↓

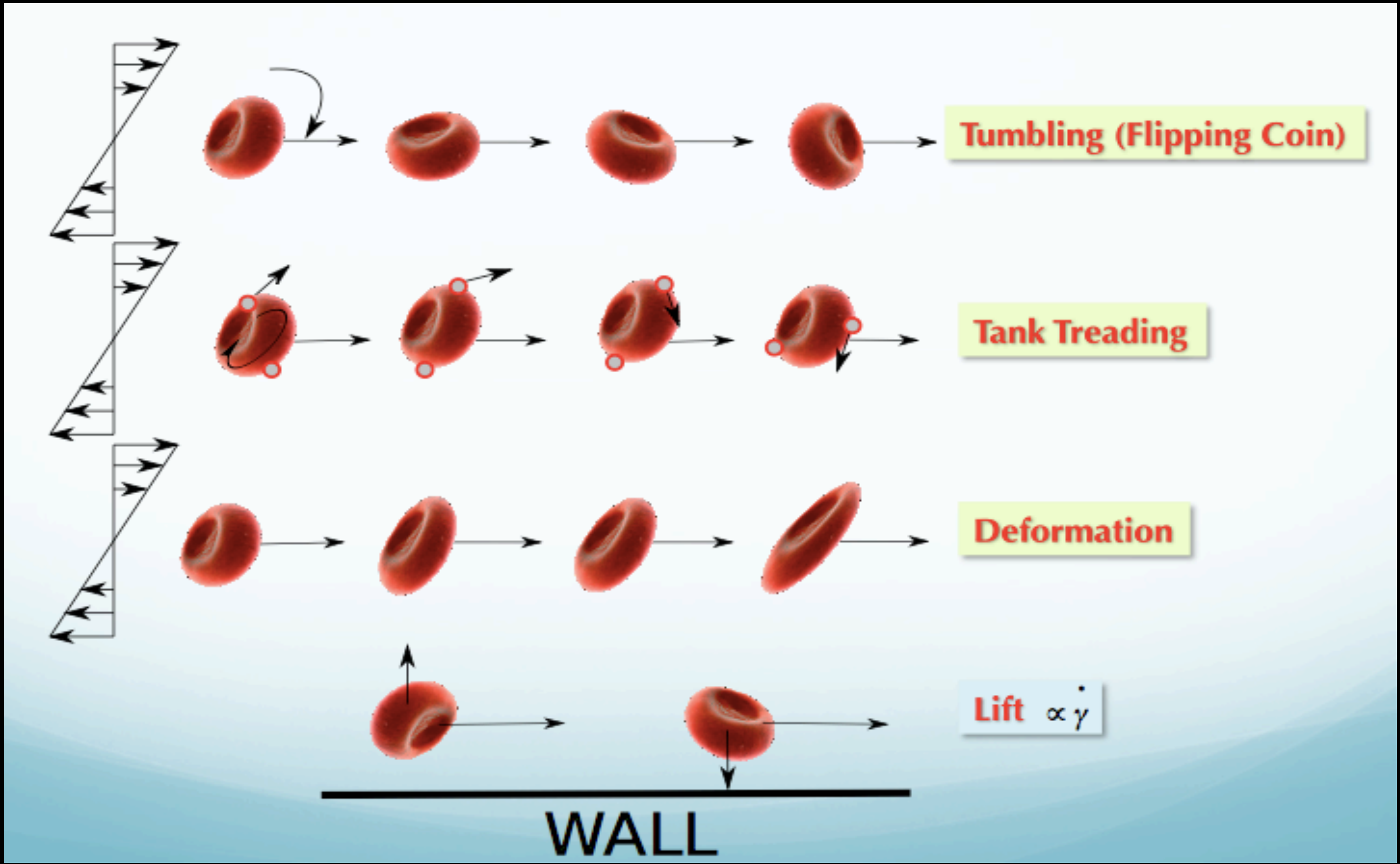
MUPHY

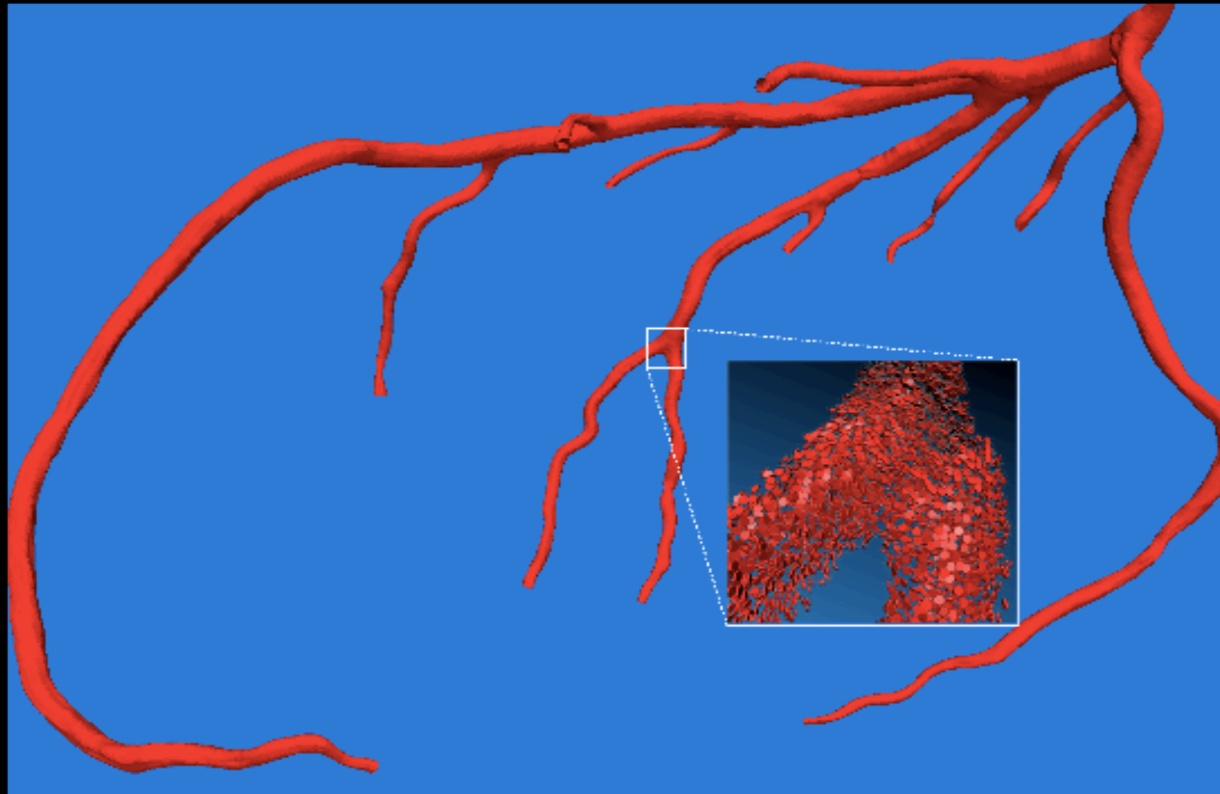
←

Output visualization



Red Blood Cell in Motion





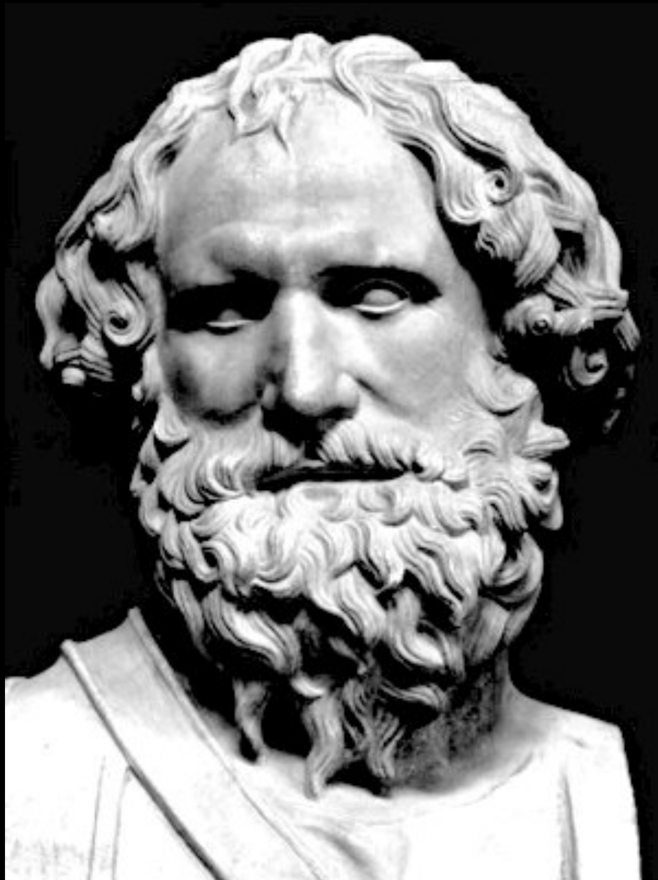
(geometry from cadaver)

MOVIES!

Multiscale Hemodynamics Team:

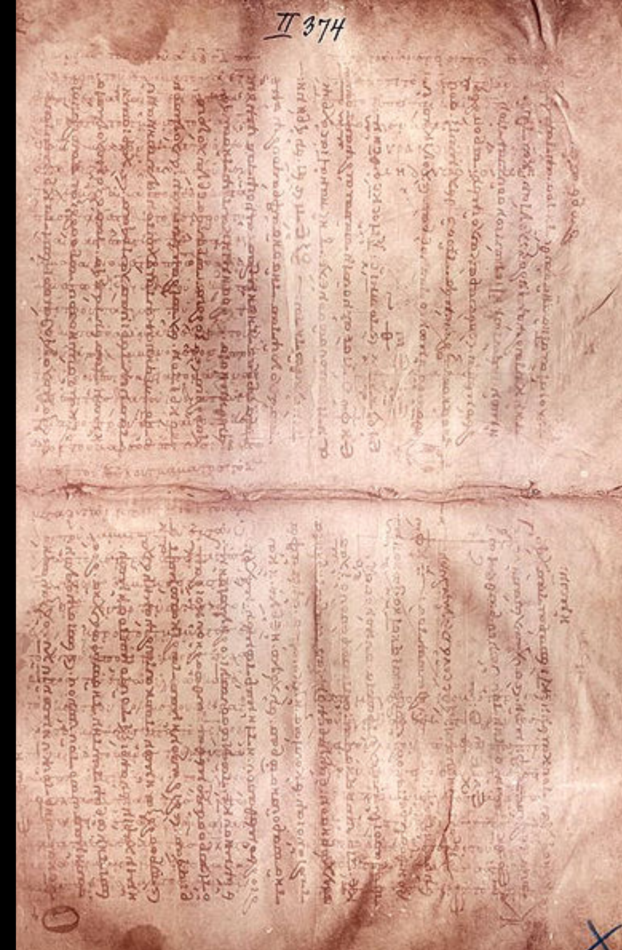
Harvard University (SEAS + B&W-H), Italian CNR, EPFL

Massimo Mernaschi - Amanda Peters - Michelle Borkin - Charles Feldman
Joy Sircar – Simone Melchionna - Peter Stone
Hanspeter Pfister – Sauro Succi - Dimitris Missouras - Franck Rybicki
Ahmet Coskun - Jonas Latt - Michael Steigner - Frederick Welt - Amanda Whitmore



Archimedes (287-212 BC)

Mathematician, physicist, engineer, inventor, astronomer (Wikipedia)



Archimedes' Palimpsest