Simulations of real complex systems: computational science comes of age

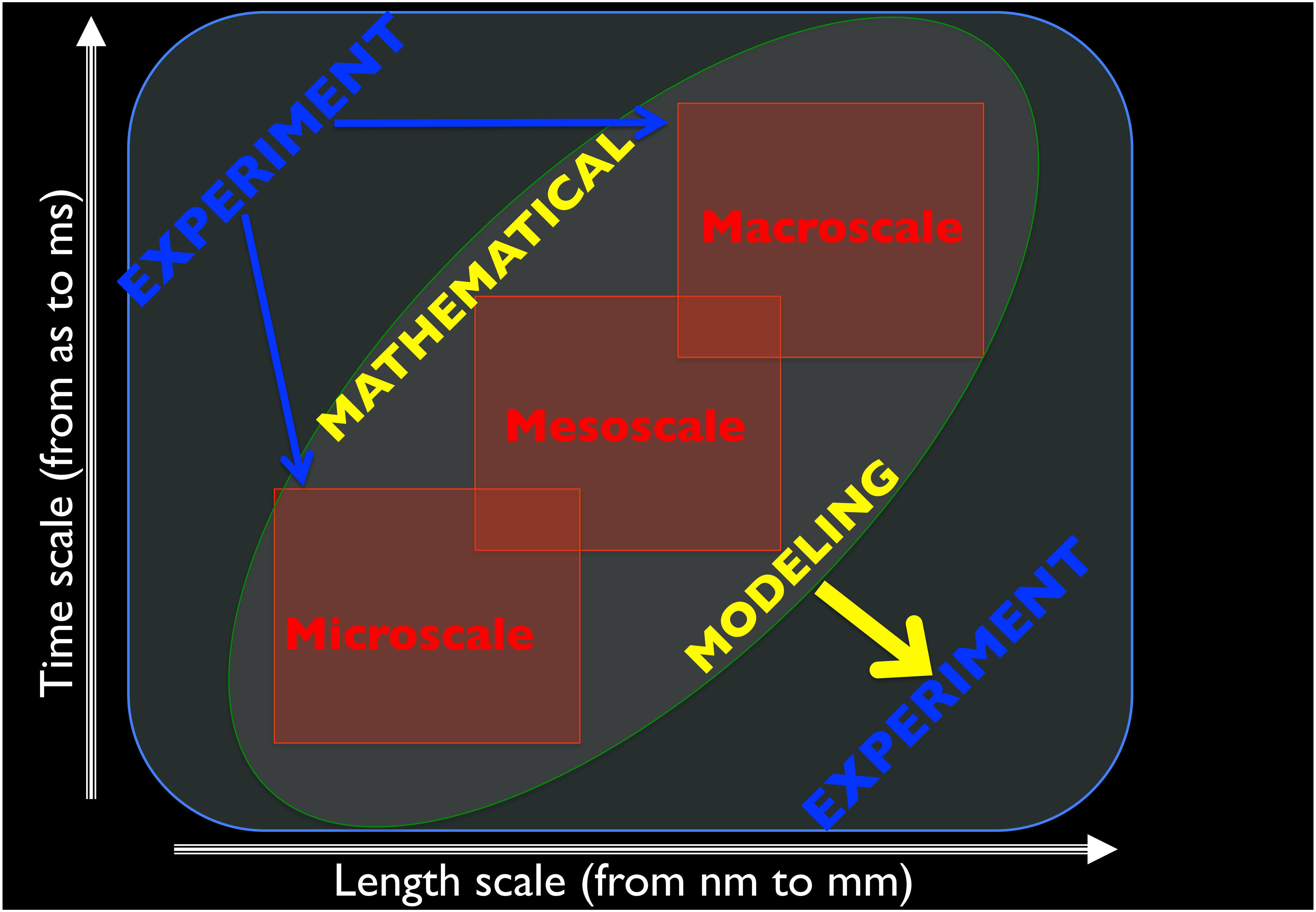
PICS Inaugural Symposium
UPenn - October 10, 2013

Multiscale models for complex physical systems

The Nobel Prize in Chemistry 2013
Martin Karplus, Michael Levitt and Arieh Warshel

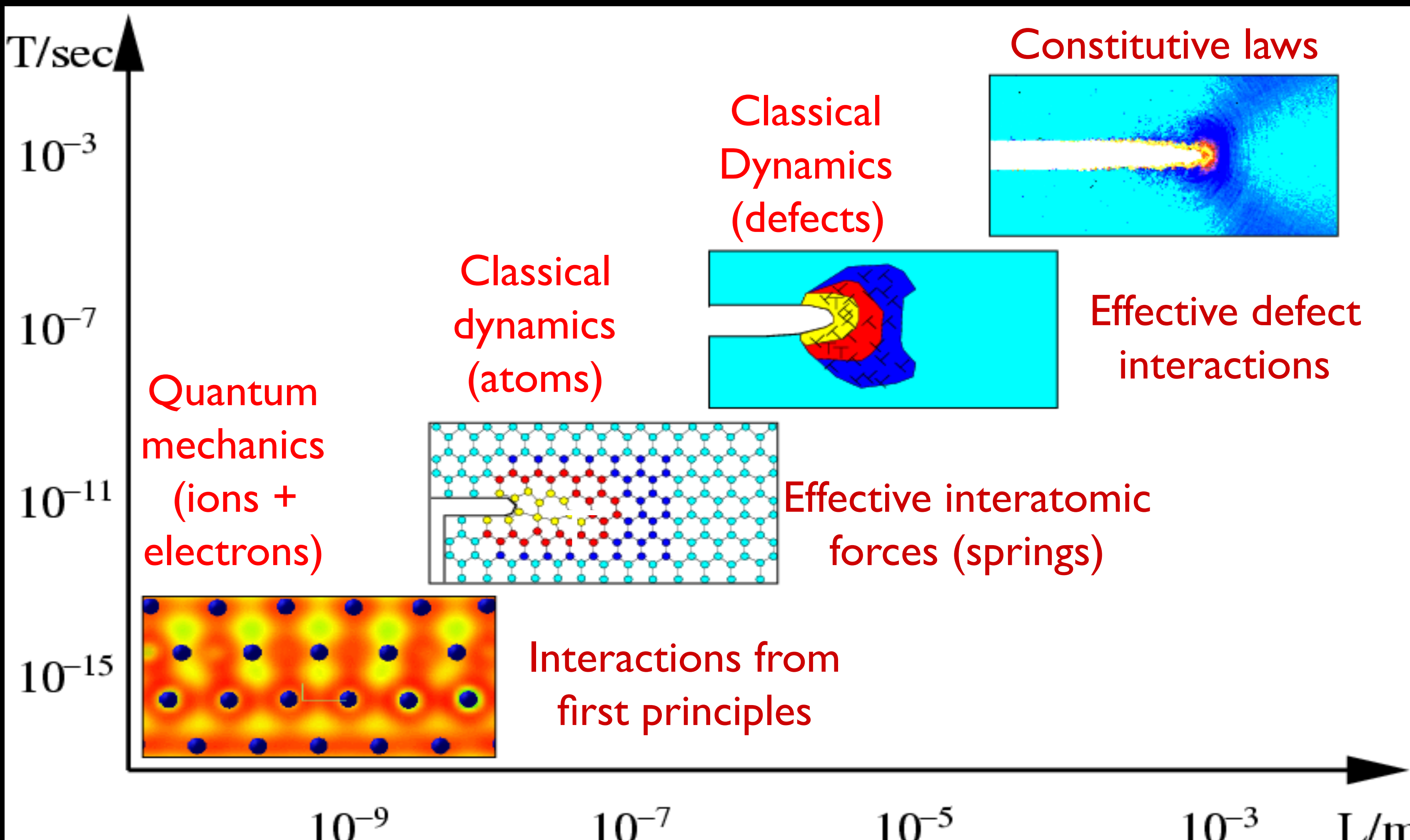
"for the development of multiscale models for complex chemical systems"
October 9, 2013

PICS – October 10, 2013



EXPERIMENT
MATHEMATICAL
Macroscale
Mesoscale
Microscale
MODELING
EXPERIMENT
Time scale (from as to ms)
Length scale (from nm to mm)

Multiple length/time scales: brittle fracture (corrosion)



Density Functional Theory

Many-body:

$$\left(\hat{H} - E\right)\psi\left(\mathbf{r}_1\sigma_1, \mathbf{r}_2, \sigma_2, \ldots\right) = 0$$

: Unsolvable

Hohenberg & Kohn (PRB, 1964):

$$E\left[V(\mathbf{r})\right] = \min_{\rho(\mathbf{r})} E'\left[V(\mathbf{r}); \rho(\mathbf{r})\right]$$

Kohn & Sham (PRB, 1965):

$$E'\left[V(\mathbf{r}); \rho(\mathbf{r})\right] =$$

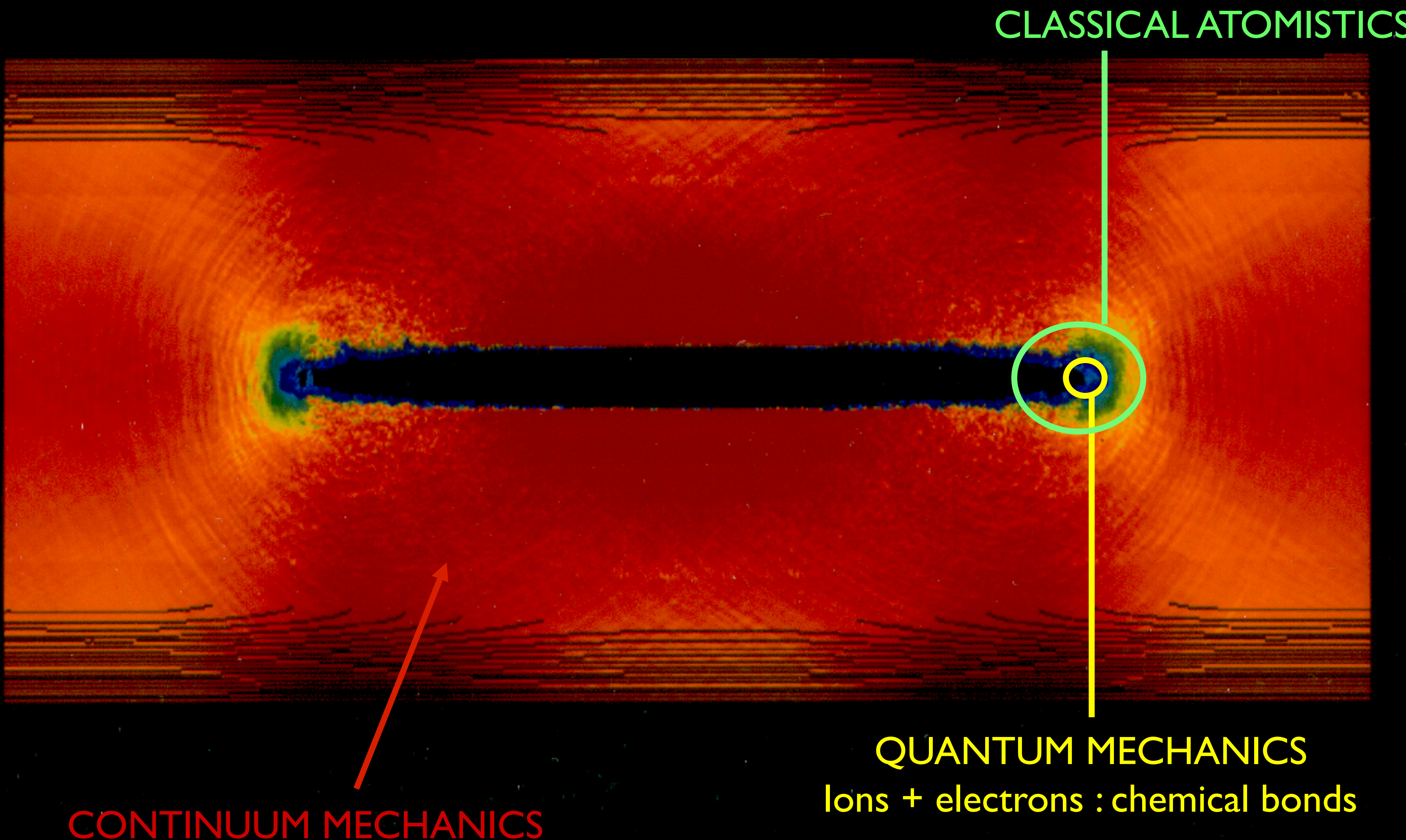
$$T_s[\rho] + E_{\mathrm{Hart}}[\rho] + \int \rho(\mathbf{r})V(\mathbf{r})d\mathbf{r} + E_{\mathrm{xc}}[\rho]$$

$$\left(\hat{H}_{\mathrm{KS}} - \epsilon_i\right)\psi_i(\mathbf{r}) = 0$$

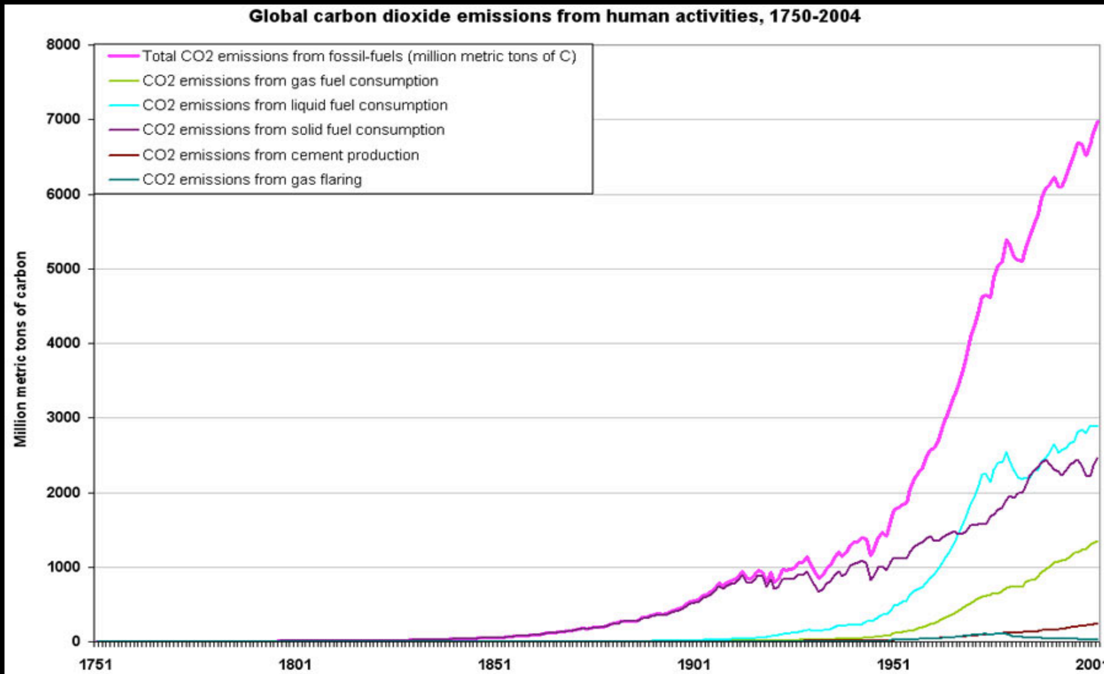
Kohn, Pople
Nobel Prize in
Chemistry, 1998

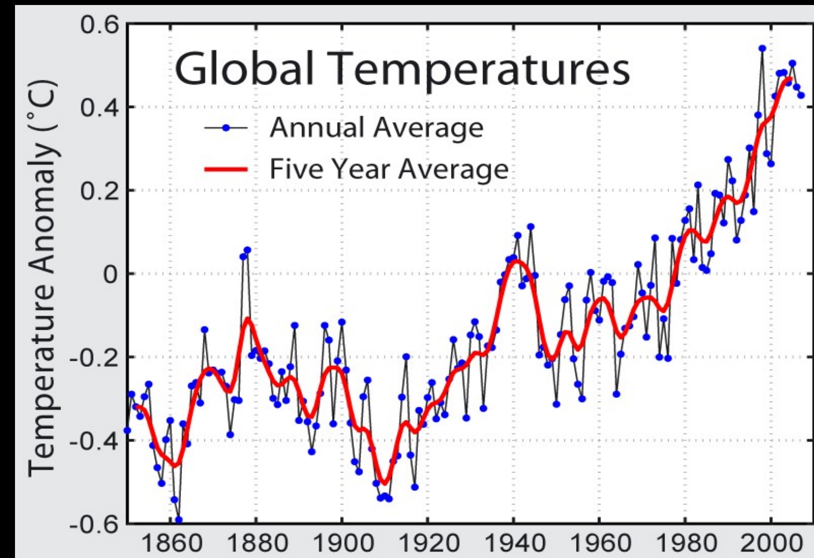
Brittle fracture of silicon

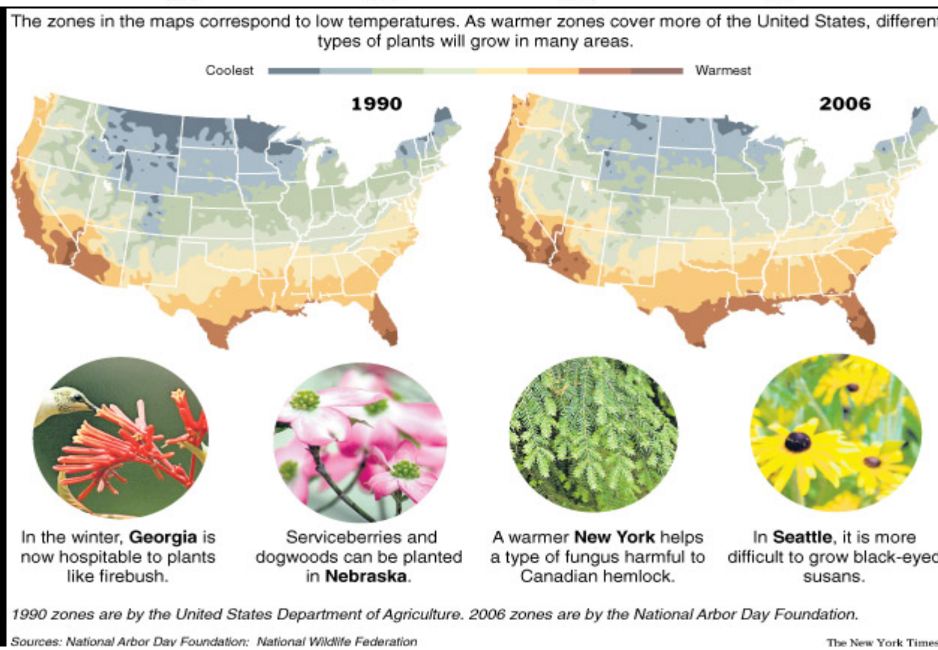
Abraham, Broughton, Bernstein, Kaxiras, PRB (1998)



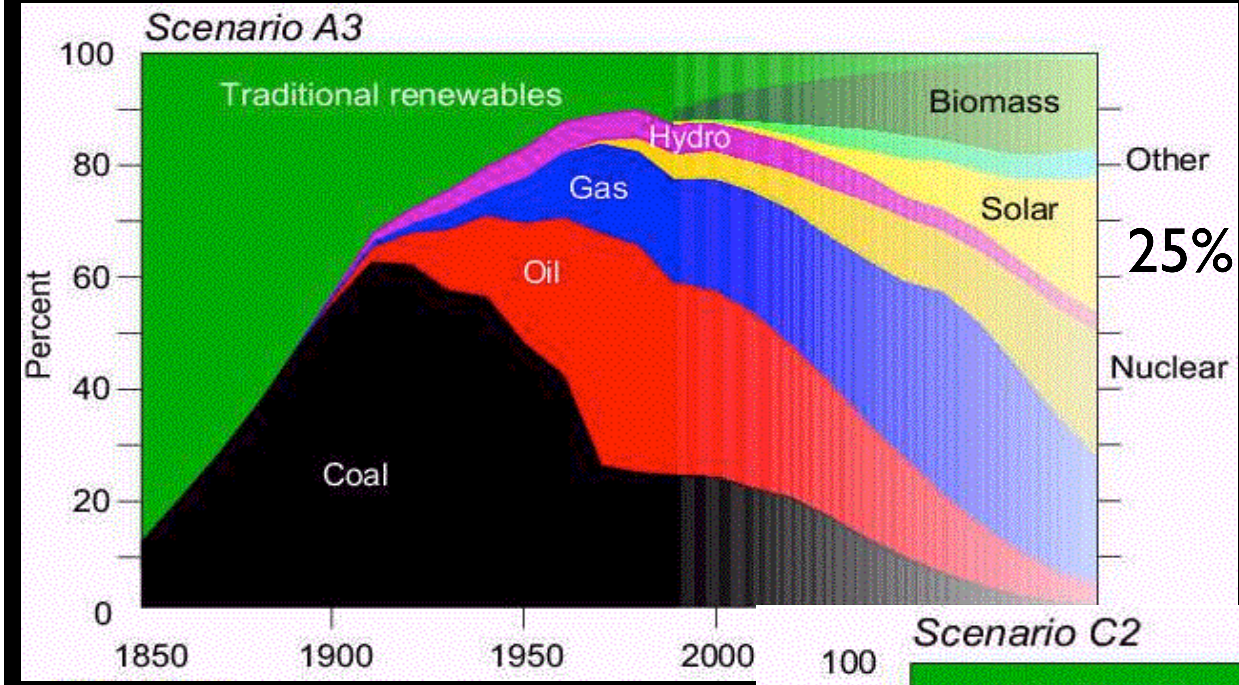
The need for alternative energy sources



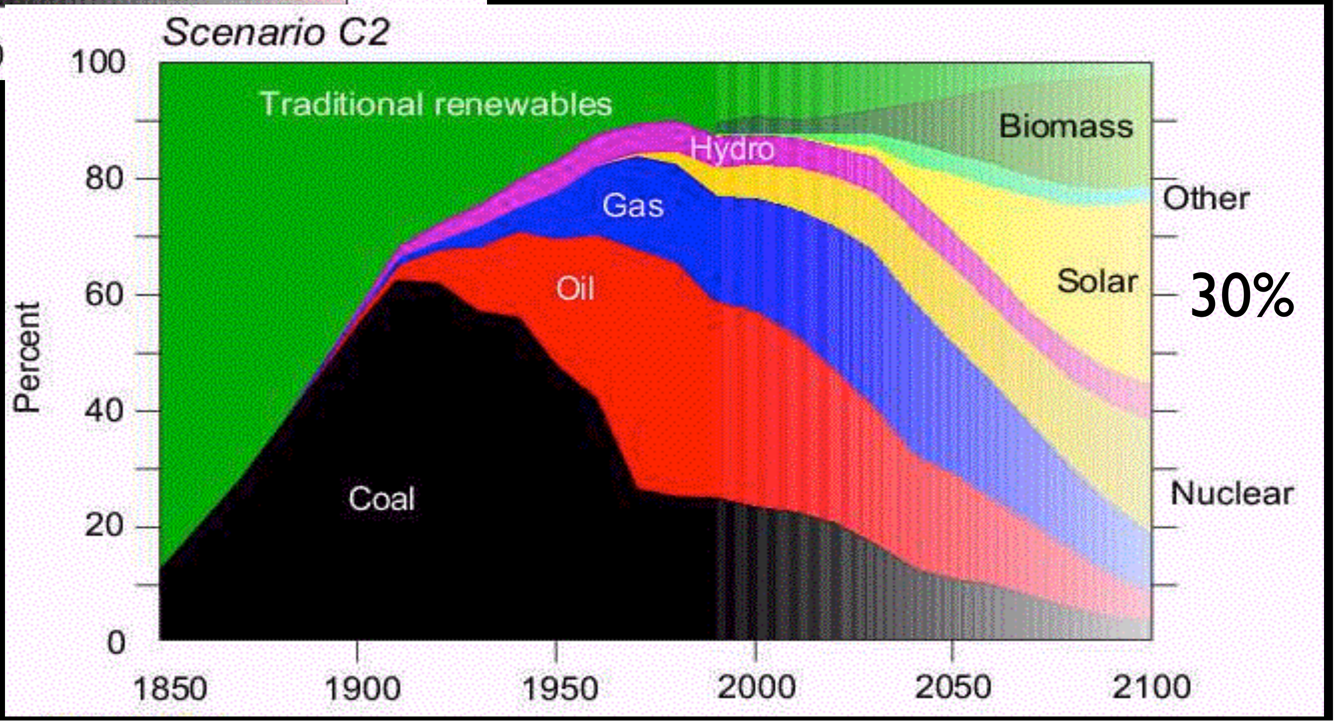




The challenge of sustainable energy

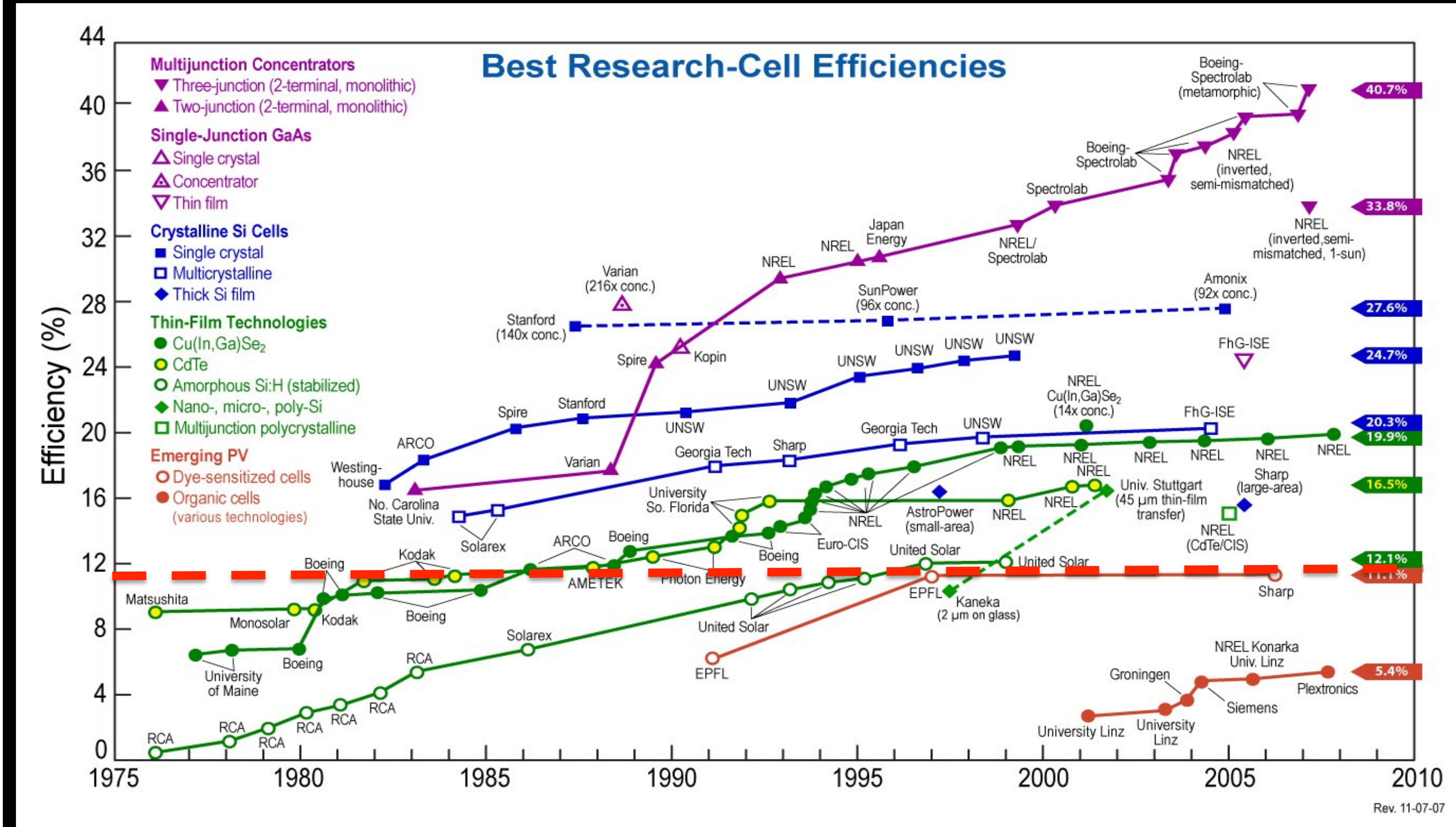


Time and resources running out



Report of Intergovernmental Panel on Climate Change

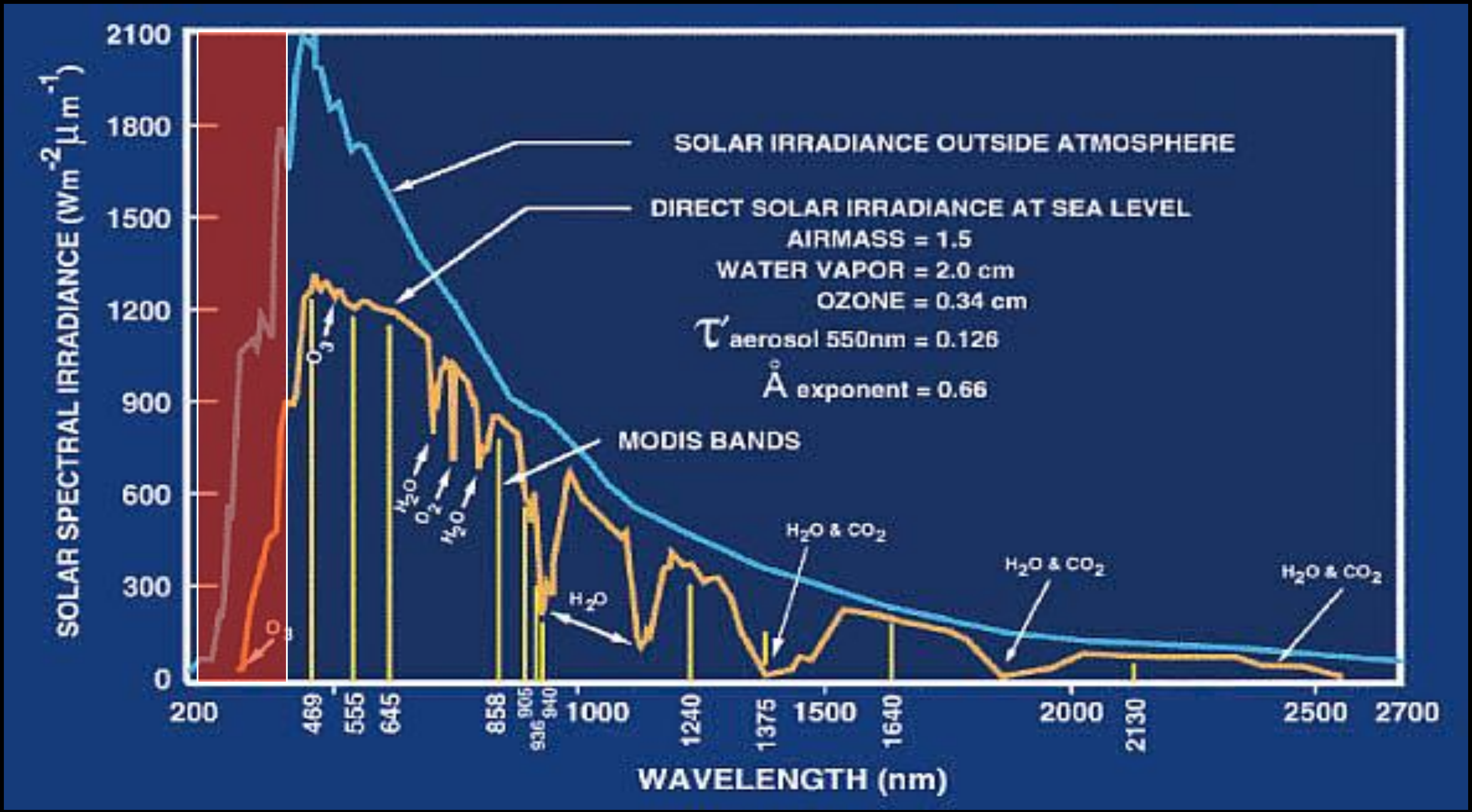
2007 Nobel Peace Prize (shared with A. Gore)


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)
Boeing-Spectrolab
NREL (inverted, semi-mismatched)
NREL (inverted,semi-mismatched, 1-sun)
Spectrolab
NREL/Spectrolab
Japan Energy
NREL
Varian (216x conc.)
Stanford (140x conc.)
SunPower (96x conc.)
Amonix (92x conc.)
FhG-ISE
Spire
Kopin
Varian
UNSW
Stanford
ARCO
Westing-house
No. Carolina State Univ.
Solarex
Georgia Tech
Sharp
NREL Cu(In,Ga)Se2 (14x conc.)
University So. Florida
AstroPower (small-area)
Univ. Stuttgart (45 μm thin-film transfer)
Sharp (large-area)
NREL (CdTe/CIS)
Euro-CIS
Boeing
United Solar
Kodak
ARCO
AMETEK
Photon Energy
Matsushita
Monosolar
University of Maine
RCA
EPFL
Kaneka (2 μm on glass)
Sharp
NREL Konarka Univ. Linz
Groningen
Siemens
Plextronics
University Linz
Rev. 11-07-07

Light absorption by hybrid cells

The Problem: materials for carrier transport with large band gaps

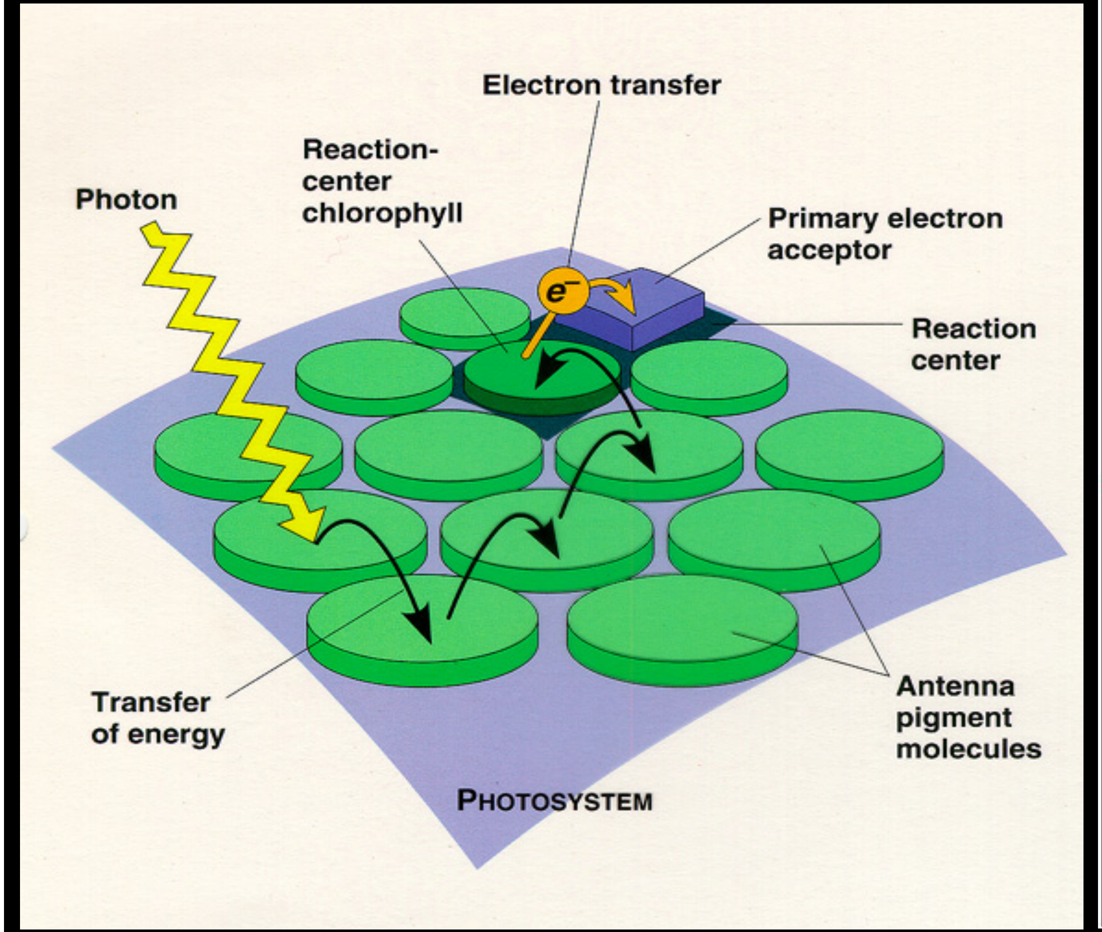
TiO_2 gap = 3.2 eV (200 nm < λ < 400 nm)

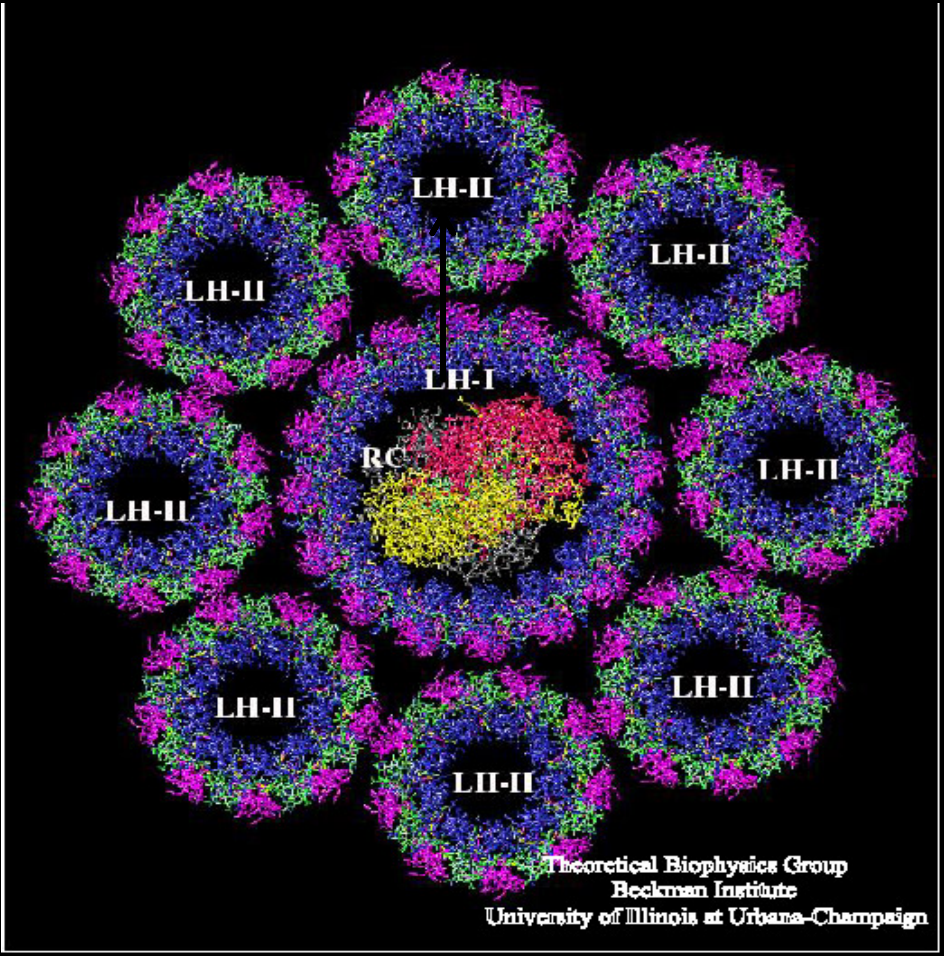


solar spectrum

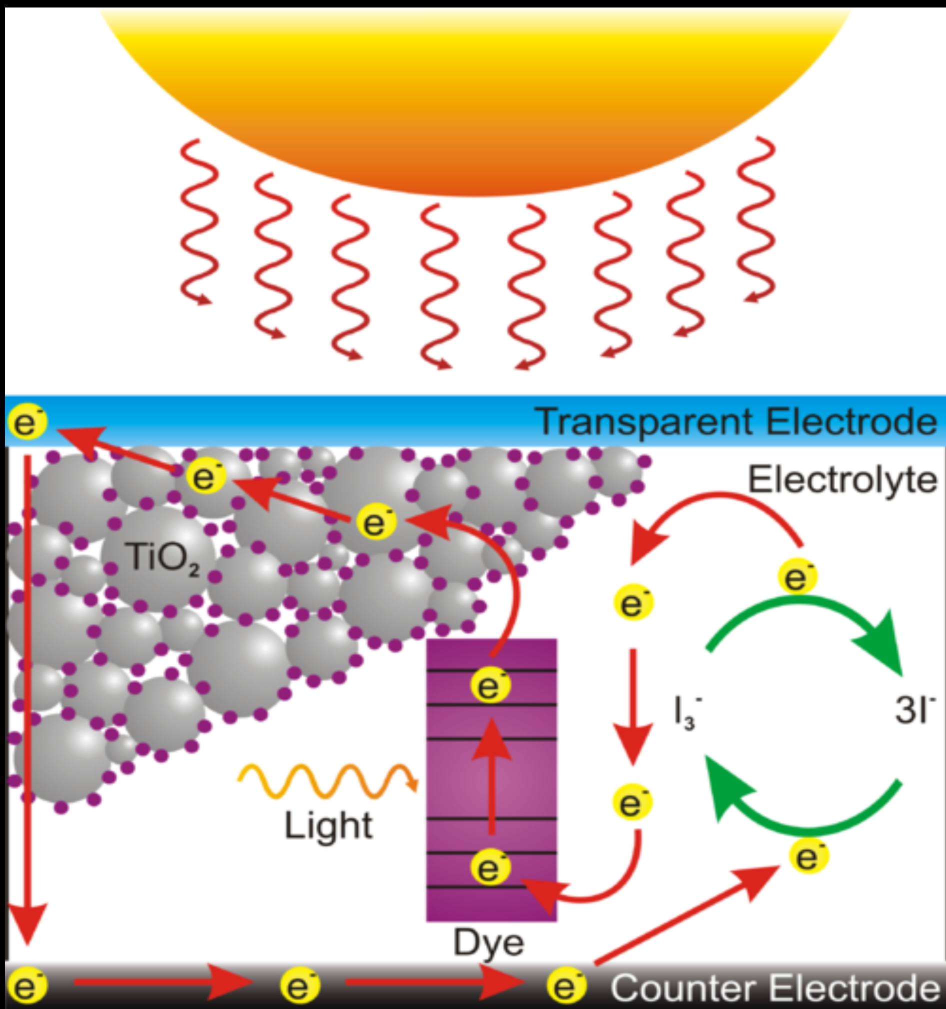
The dye-sensitized (3rd generation) solar cell

The Principle: Separate light-absorption and charge collection processes





The dye-sensitized solar cell (DSSC)
O'Regan & Graetzel, Nature (1991)



Major issues:

- stability
- efficiency

  Incident Photon to Current Efficiency

$$IPCE(\lambda) = LHE(\lambda) \times \Phi(inj) \times \eta(c)$$

LHE = Light Harvesting Efficiency

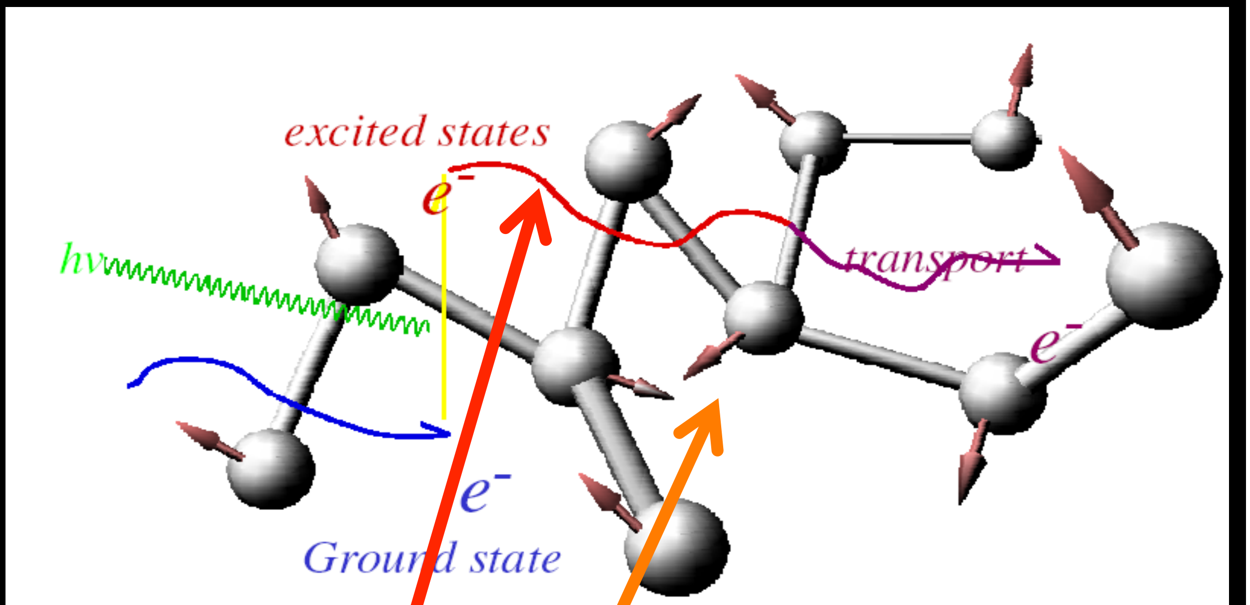
$\Phi(inj)$ = electron injection efficiency

$\eta(c)$ = charge collection efficiency

Main issue: coupled electron-ion dynamics

Previous work:

-Schroedinger eq. with model Hamiltonian
Thoss, Miller, Stock, JCP (2000);
Rego& Batista, JACS (2003);…
-semiempirical Hamiltonian (tight-binding)
Allen et al., JMO (2003);…
-ground state DFT + TDDFT
Prezhdo et al., PRL (2005); JACS (2007)…



self-consistent TDDFT with atomic motion

Meng & Kaxiras, J. Chem. Phys. (2008).

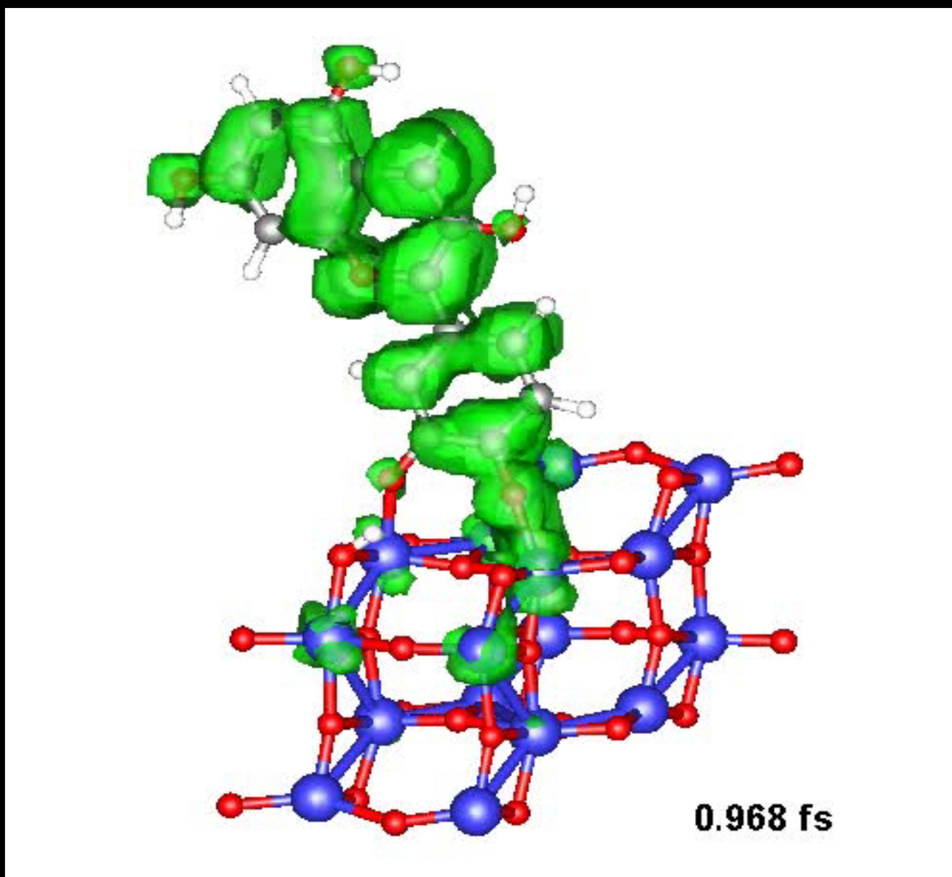
10^{-18} s 10^{-15} s Transport: 10^{-12} s

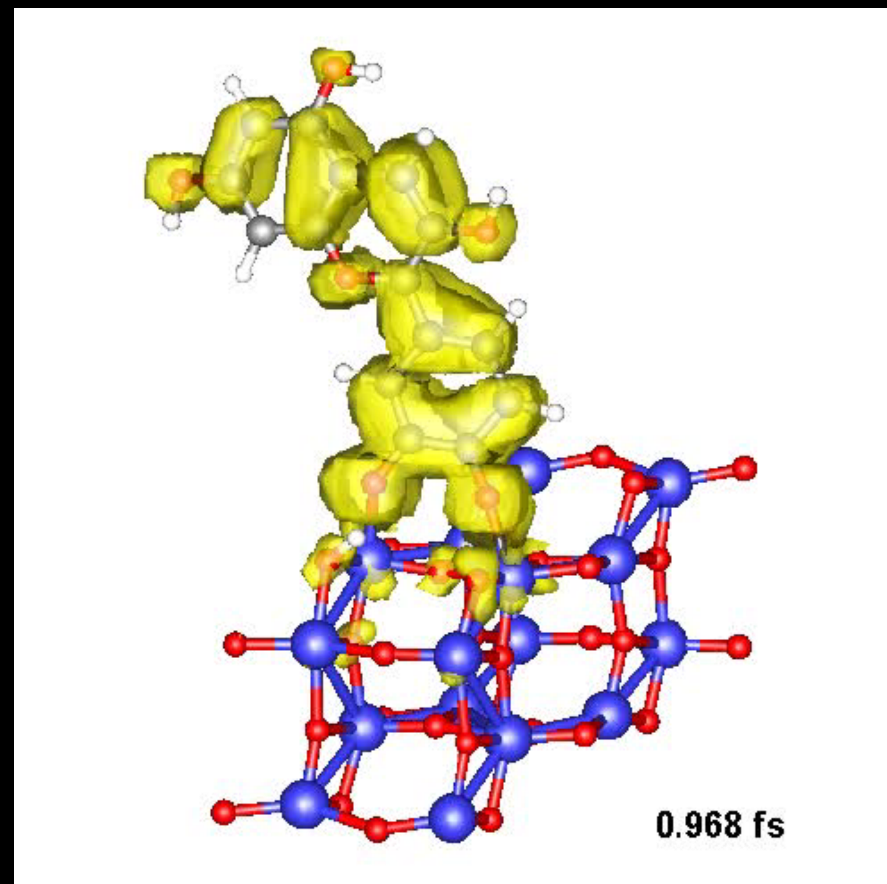
Coupled electron-ion dynamics

$$
\begin{cases}
i\hbar\frac{\partial\phi_j(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} + v_{ext}(\mathbf{r},t) + \int\frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' - \sum_I \frac{Z_I}{|\mathbf{r}-\mathbf{R}^{cl}_I|} + v_{xc}[\rho](\mathbf{r},t)\right]\phi_j(\mathbf{r},t) \\
M_J\frac{d^2\mathbf{R}^{cl}_J(t)}{dt^2} = -\nabla_{\mathbf{R}^{cl}_J}\left[V^J_{ext}(\mathbf{R}^{cl}_J,t) - \int\frac{Z_J\rho(\mathbf{r},t)}{|\mathbf{R}^{cl}_J-\mathbf{r}|}d\mathbf{r} + \sum_{I\neq J}\frac{Z_J Z_I}{|\mathbf{R}^{cl}_J-\mathbf{R}^{cl}_I|}\right]
\end{cases}
$$

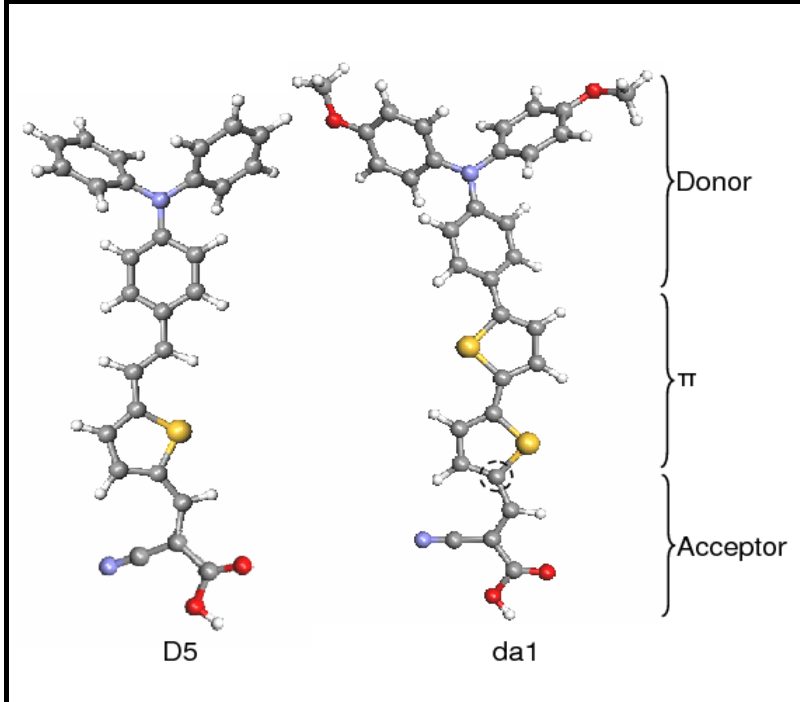
Propagation of electrons in time (TDSE) + Ehrenfest dynamics for ions

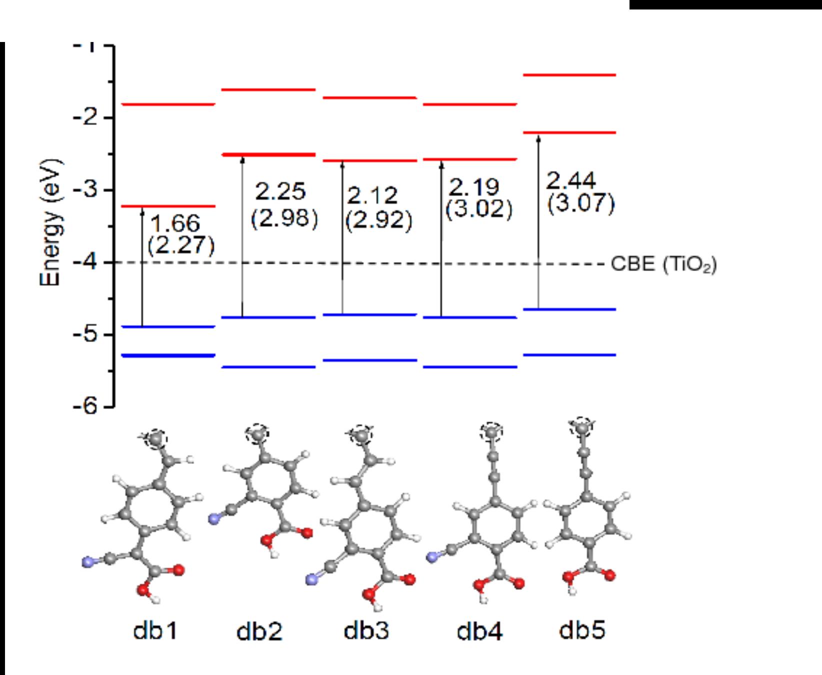
Electron and hole motion in DSSC

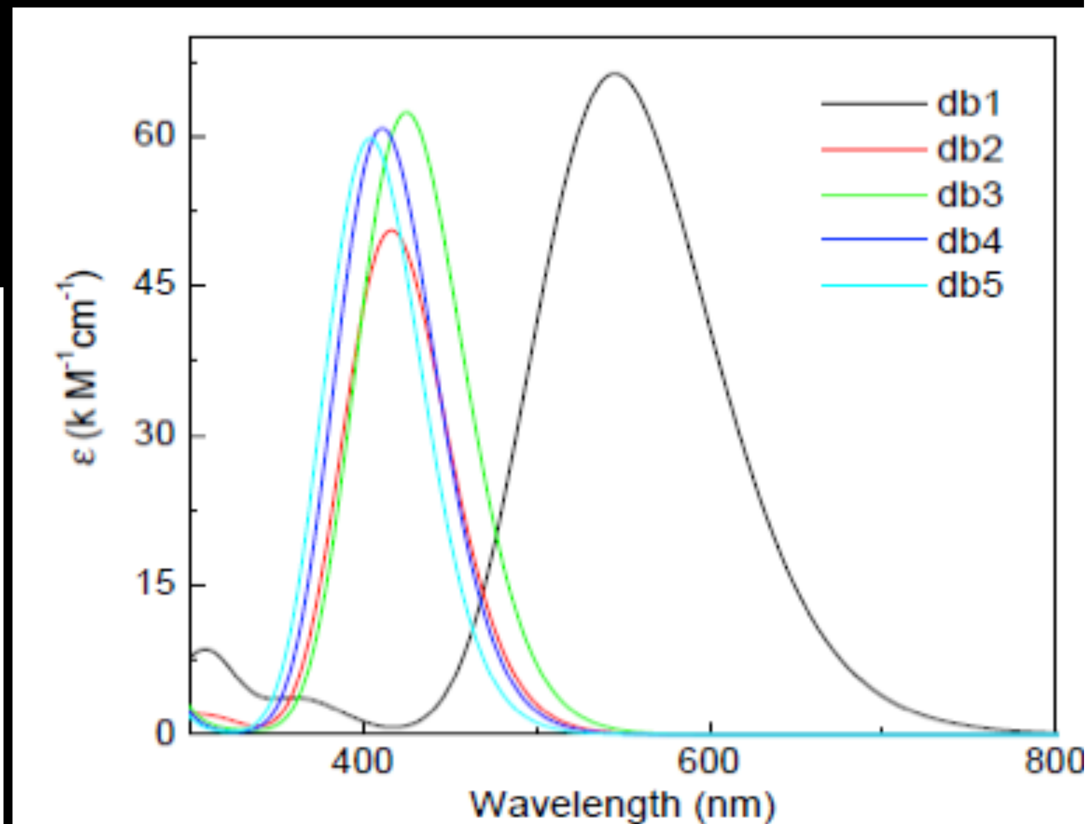




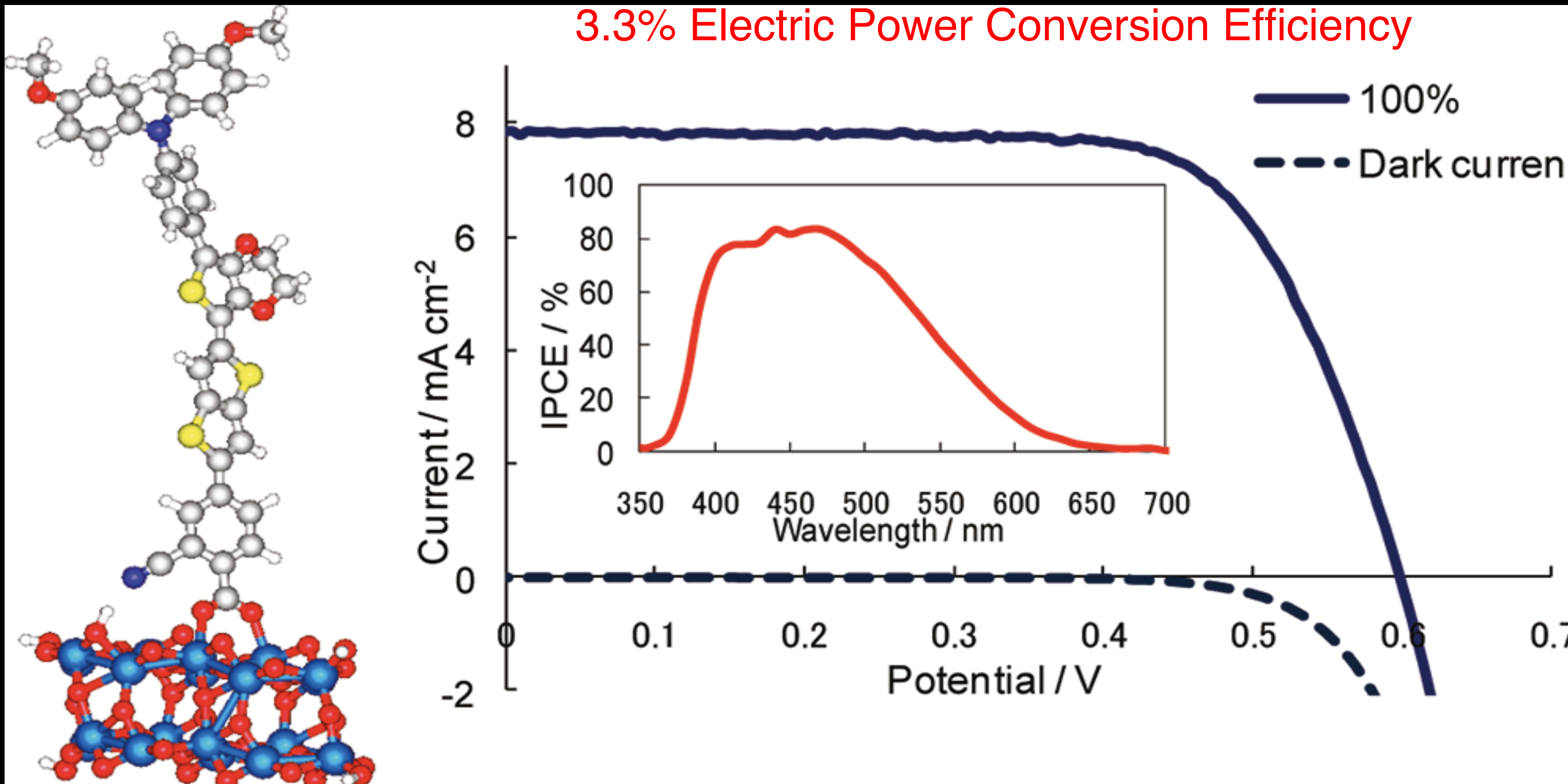
“Designer” dyes: Predict properties of new dyes (not yet tried in experiments)







84% Incident Photon to Current Efficiency,
3.3% Electric Power Conversion Efficiency

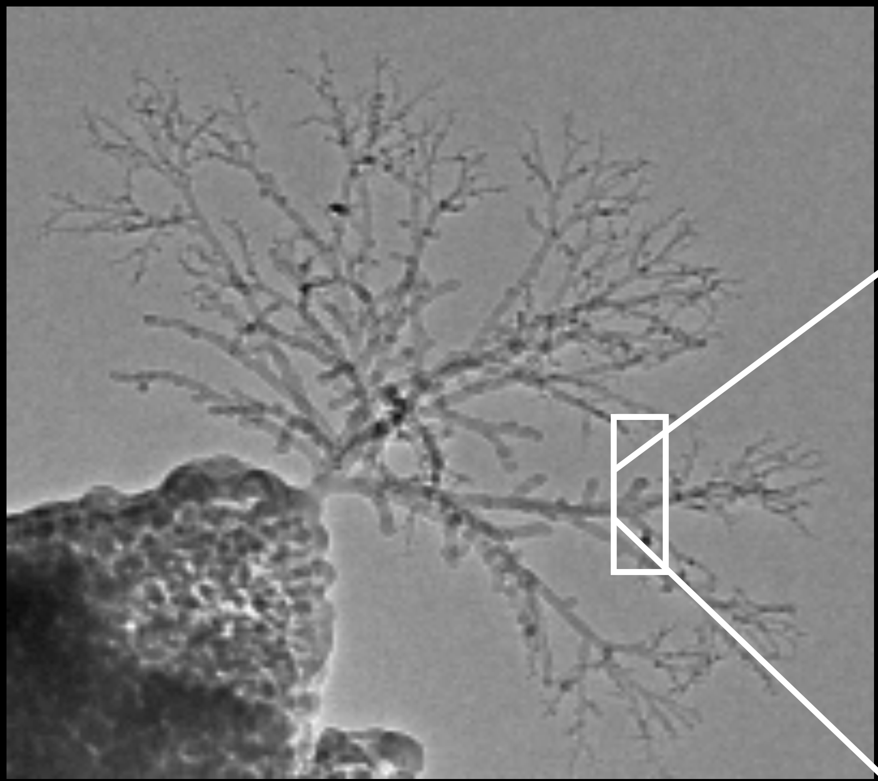


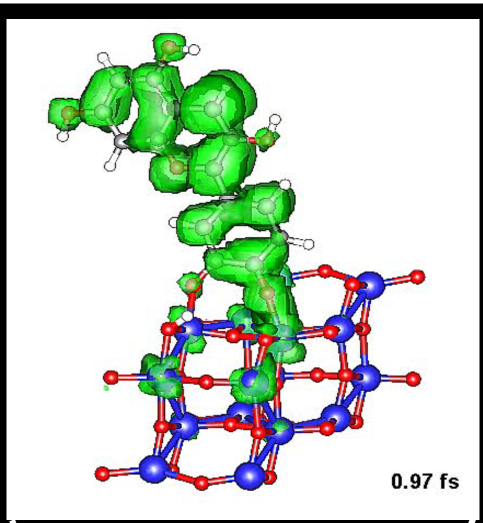
D-π-A Dye System Containing Cyano-Benzoic Acid as Anchoring Group for Dye-Sensitized Solar Cells

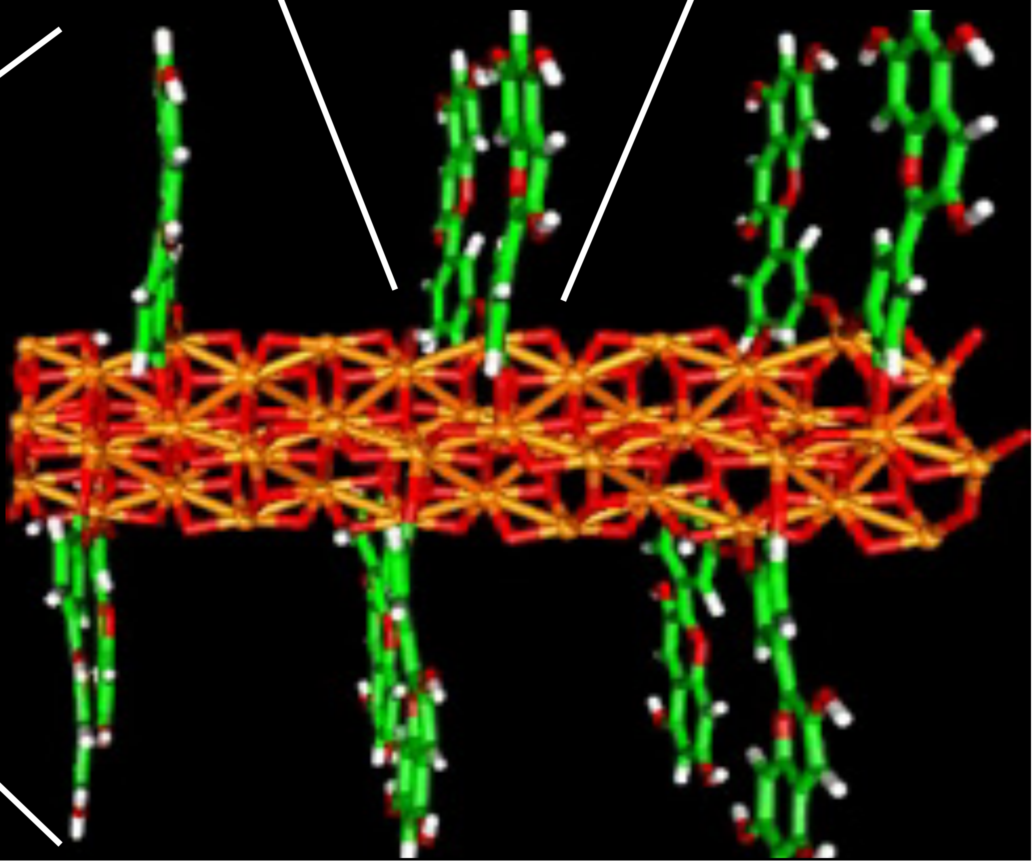
Masataka Katono, Takeru Bessho, Sheng Meng, Robin Humphry-Baker, Guido Rothenberger, Shaik M. Zakeeruddin, Efthimios Kaxiras, and Michael Gratzel

Langmuir 2011, **27**, 14248–14252

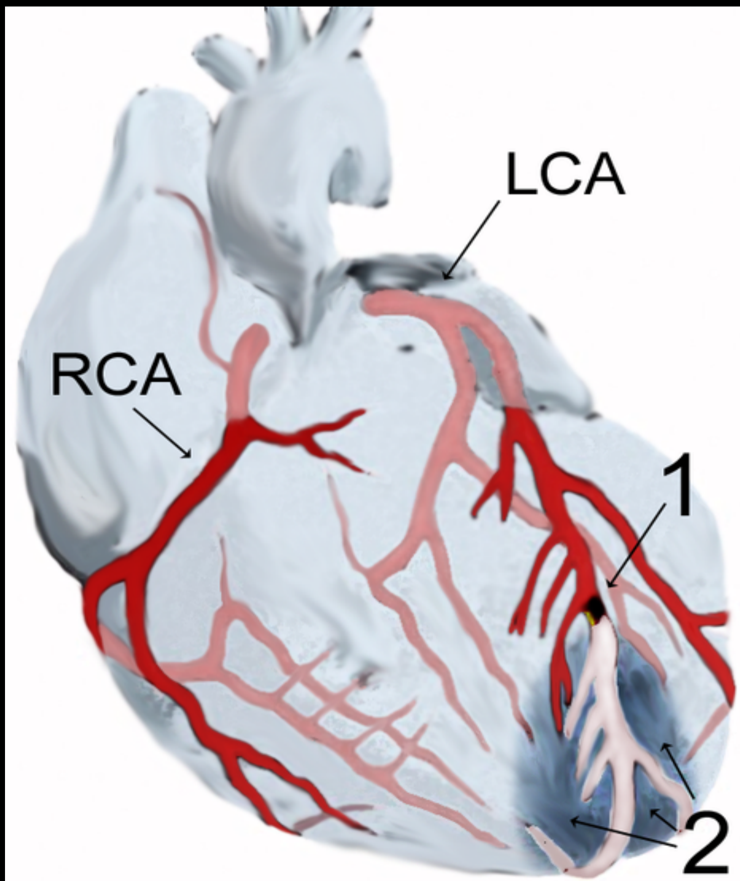
Artificial Nano Tree
(based on QM simulations)

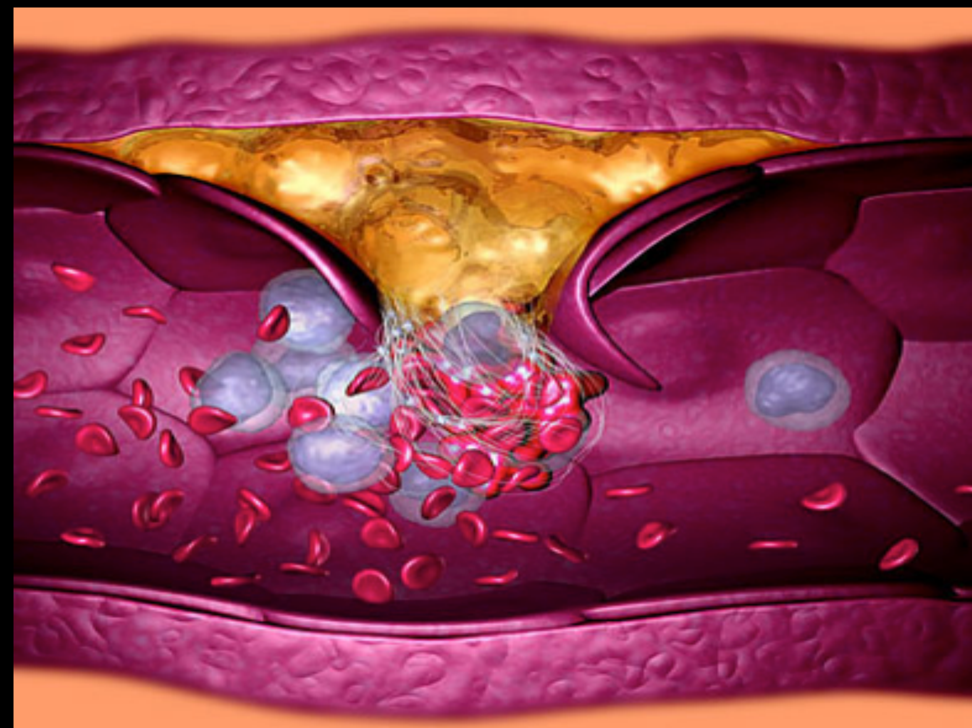






Acute Myocardial Infarction (heart attack)





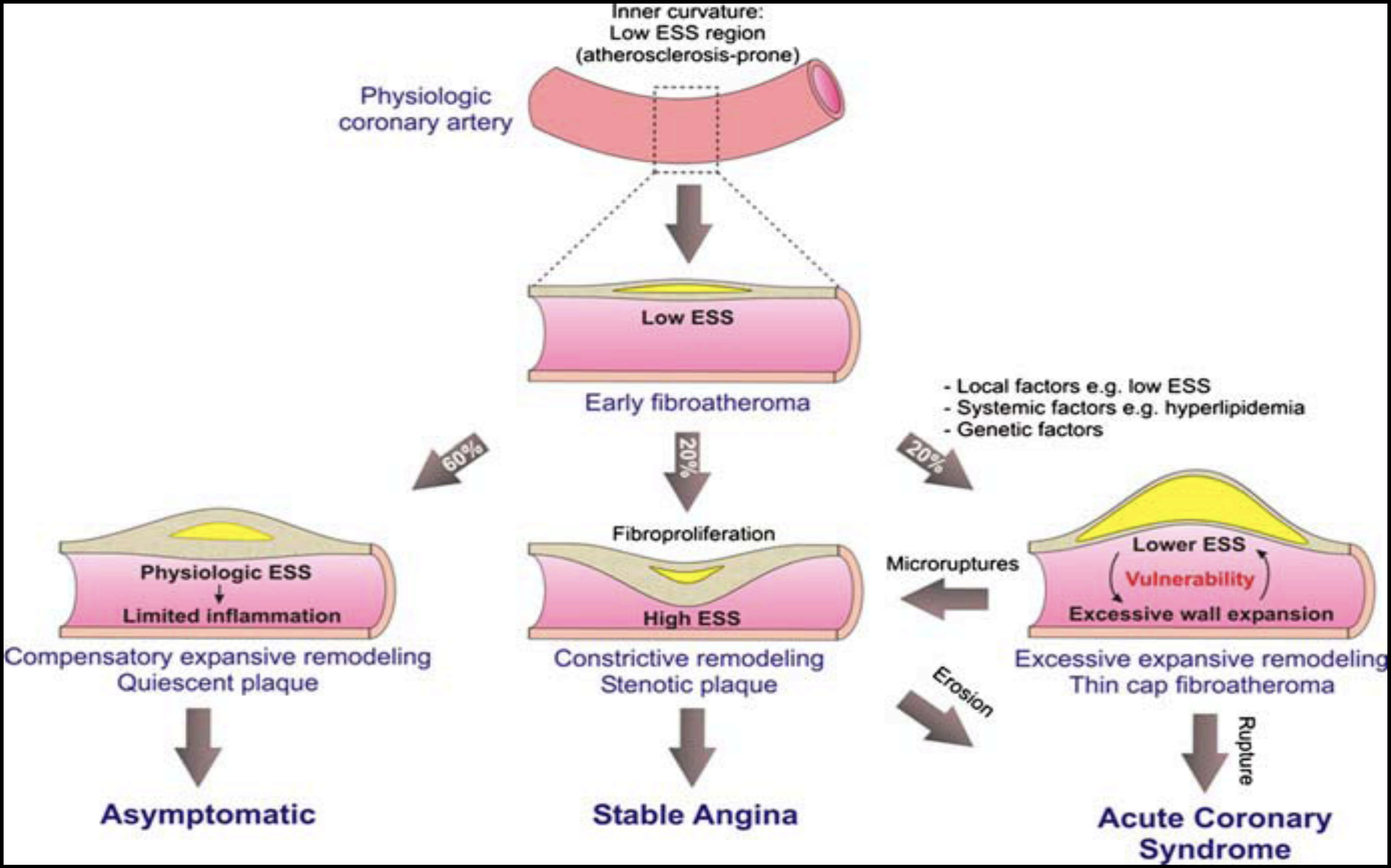
Deaths in USA: out of ~2.5 M per year total,

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

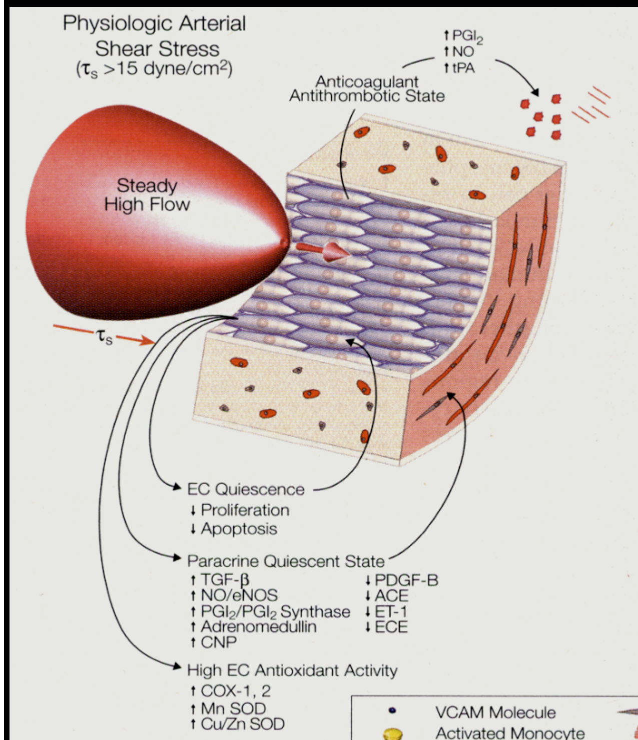
UNPREDICTABLE

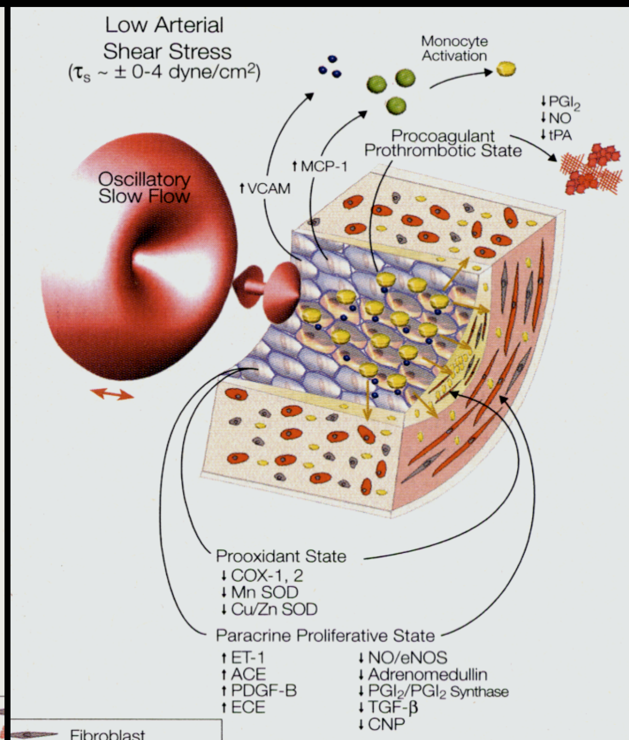
- 25% cancer (all types)

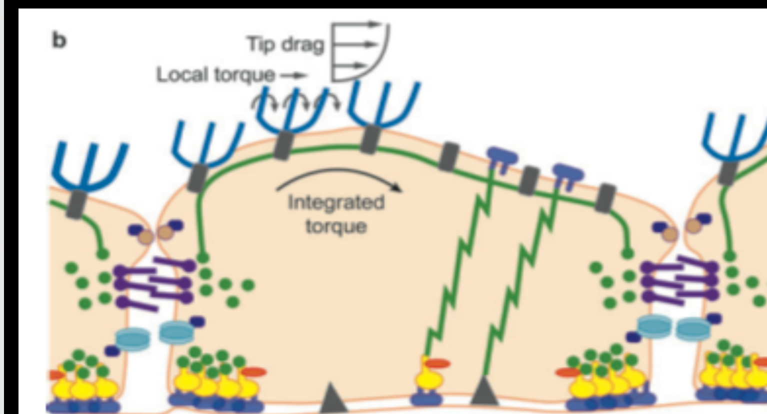
Formation and evolution of plaques



ESS = Endothelial Shear Stress, ACCESSIBLE ONLY BY SIMULATION







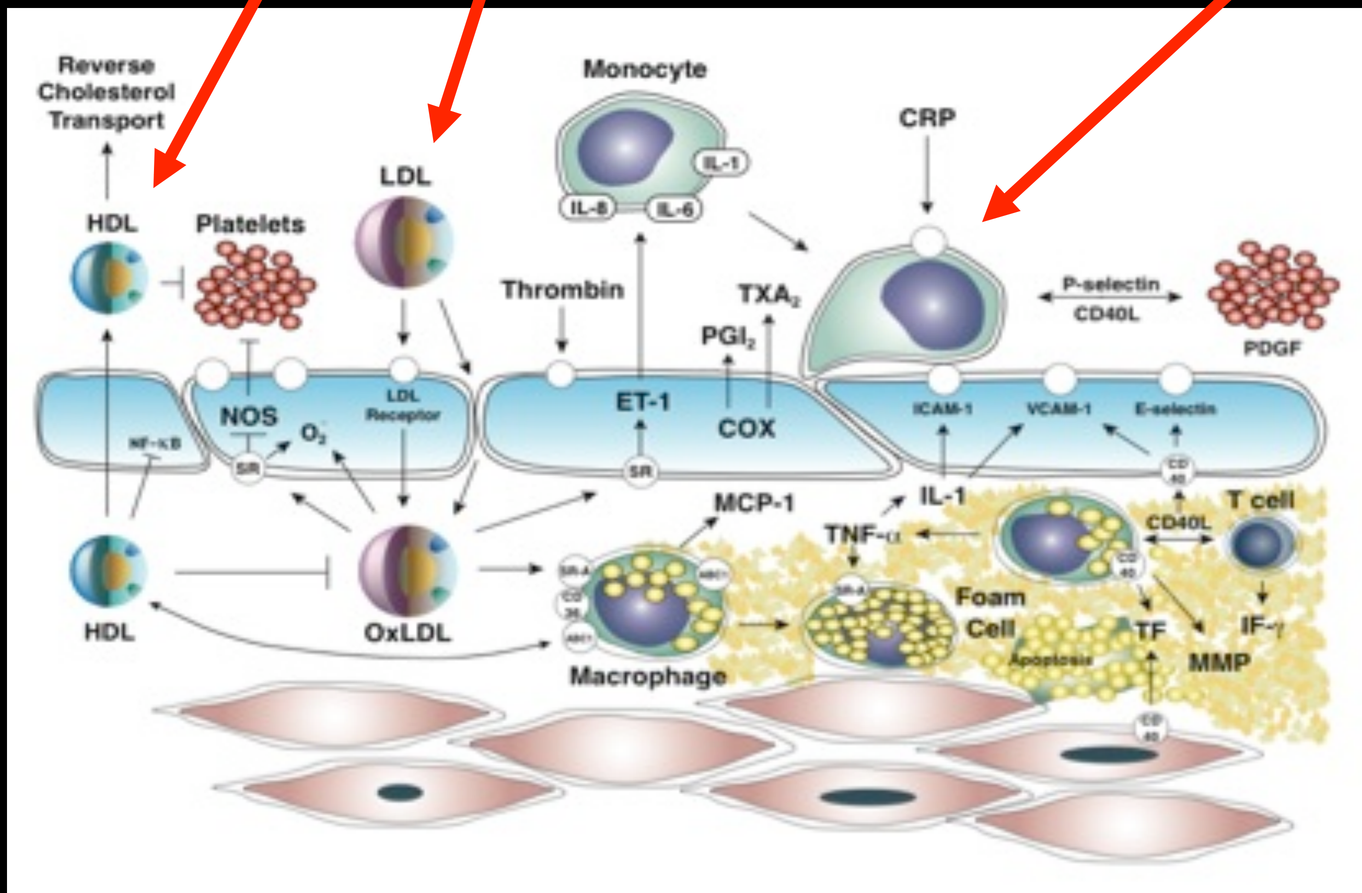
Vasculoprotective

Vascular adhesion of
lipoproteins & inflammatory cells

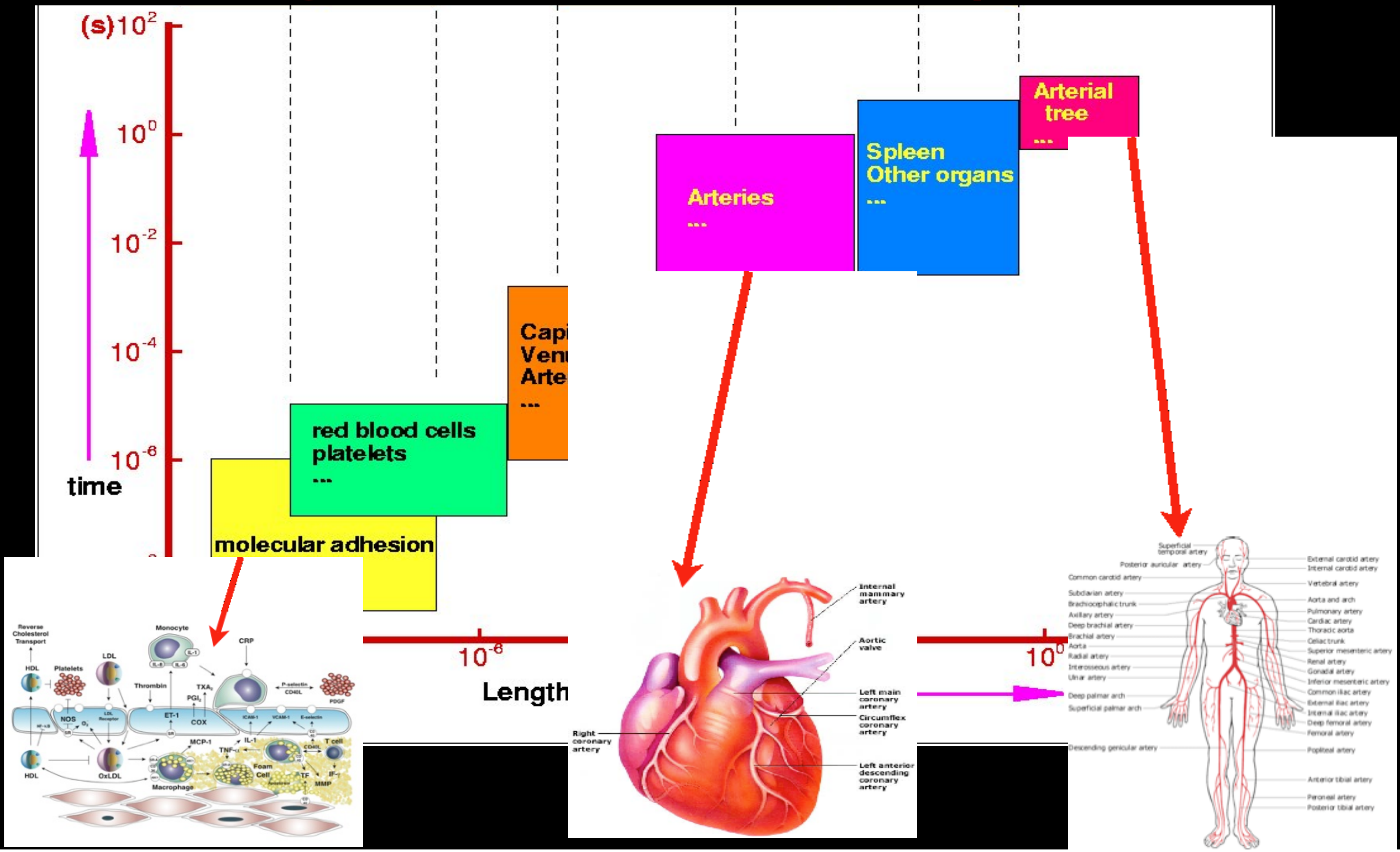
Inflammatory response & Feedback

Cholesterol (HDL, LDL)

White blood cells

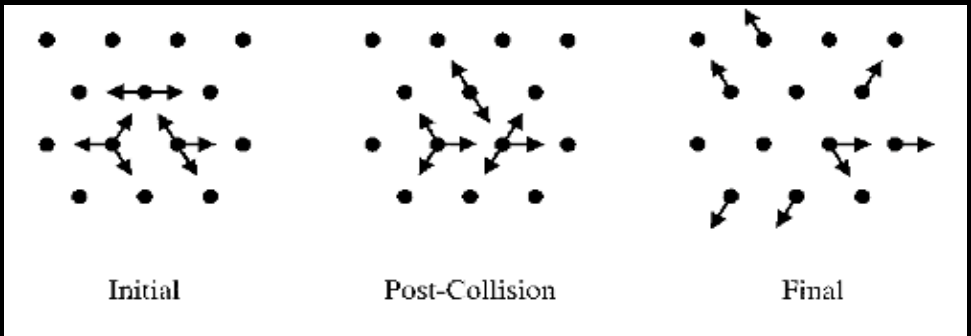


Challenge: Multi-scale hemodynamics



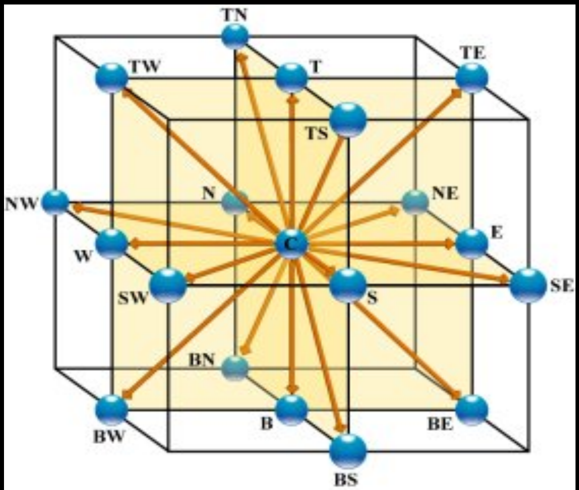
Fluid dynamics by cellular automata : Lattice Boltzmann Equation (LBE)

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



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

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)

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

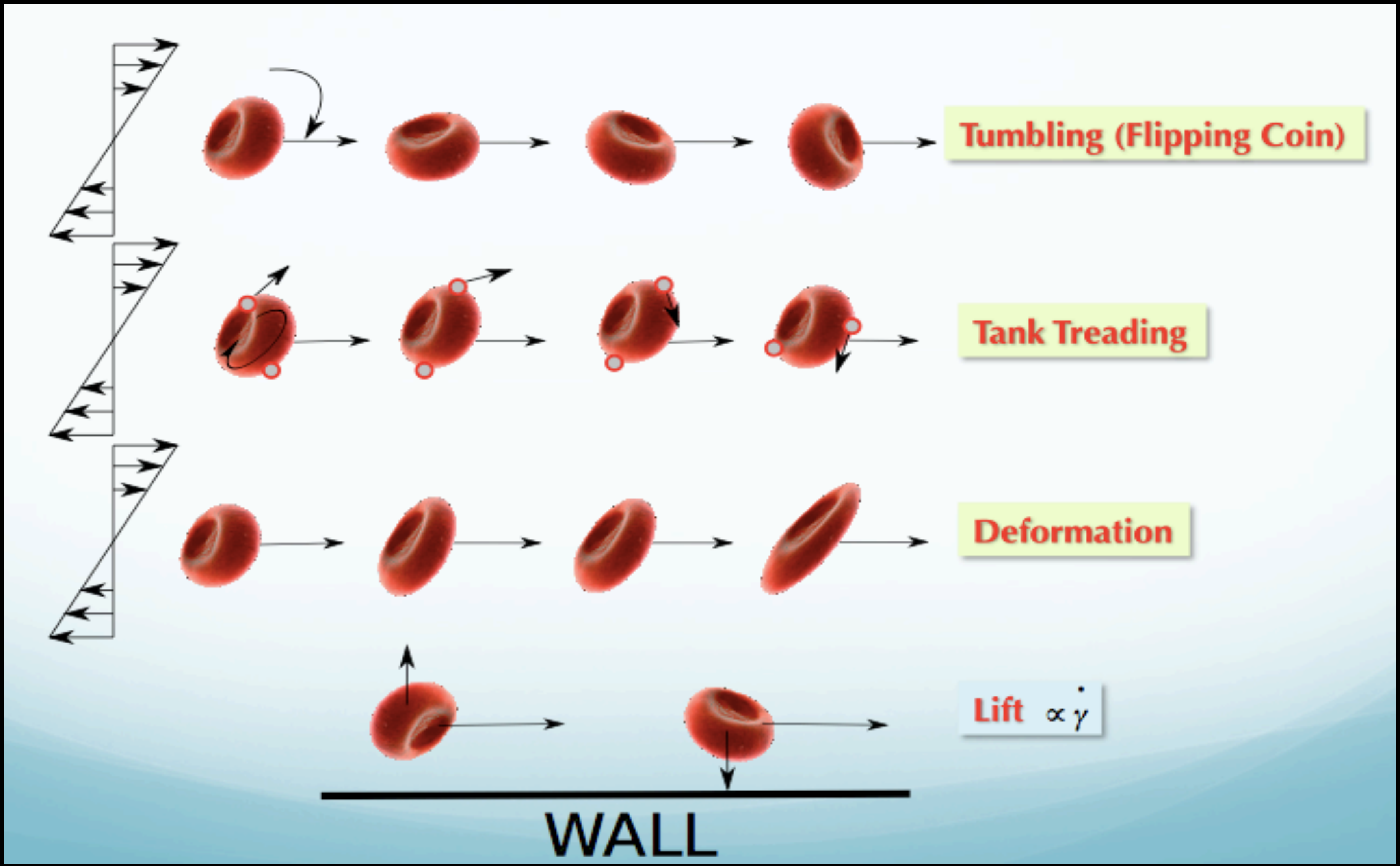
Stress Tensor

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

Wall Stress

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

Red Blood Cell in Motion

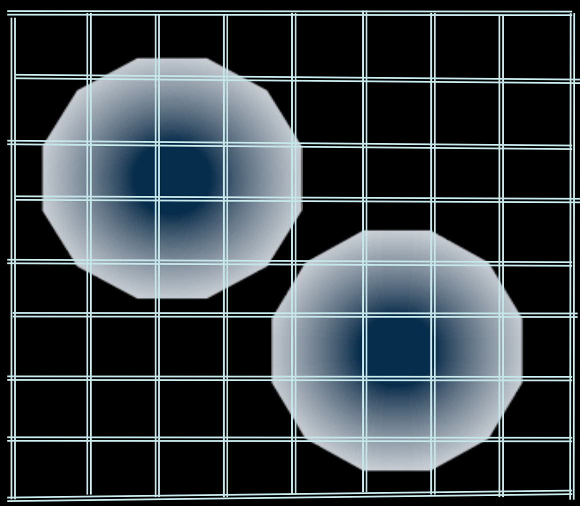


Definition of “particles” (cells, proteins, …)

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

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

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



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

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

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

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

Equations of motion:

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

$$\Phi^H_{6\times 1} = \Gamma_{6\times 6}\Psi^*_{6\times 1} + \Delta_{6\times 3\times 3} : E_{3\times 3}$$

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

Brenner *et al.* (1972) Brady & Bossis (1989)

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!

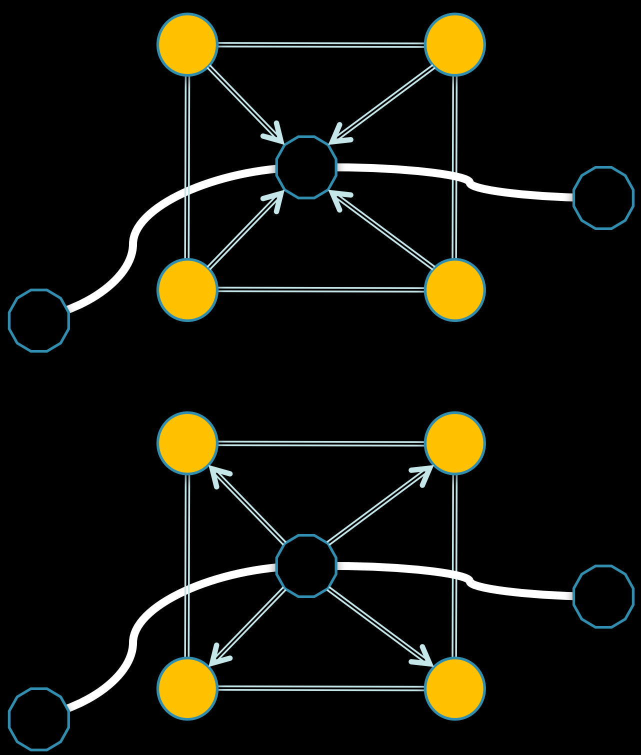
Fluid-particle coupling:

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

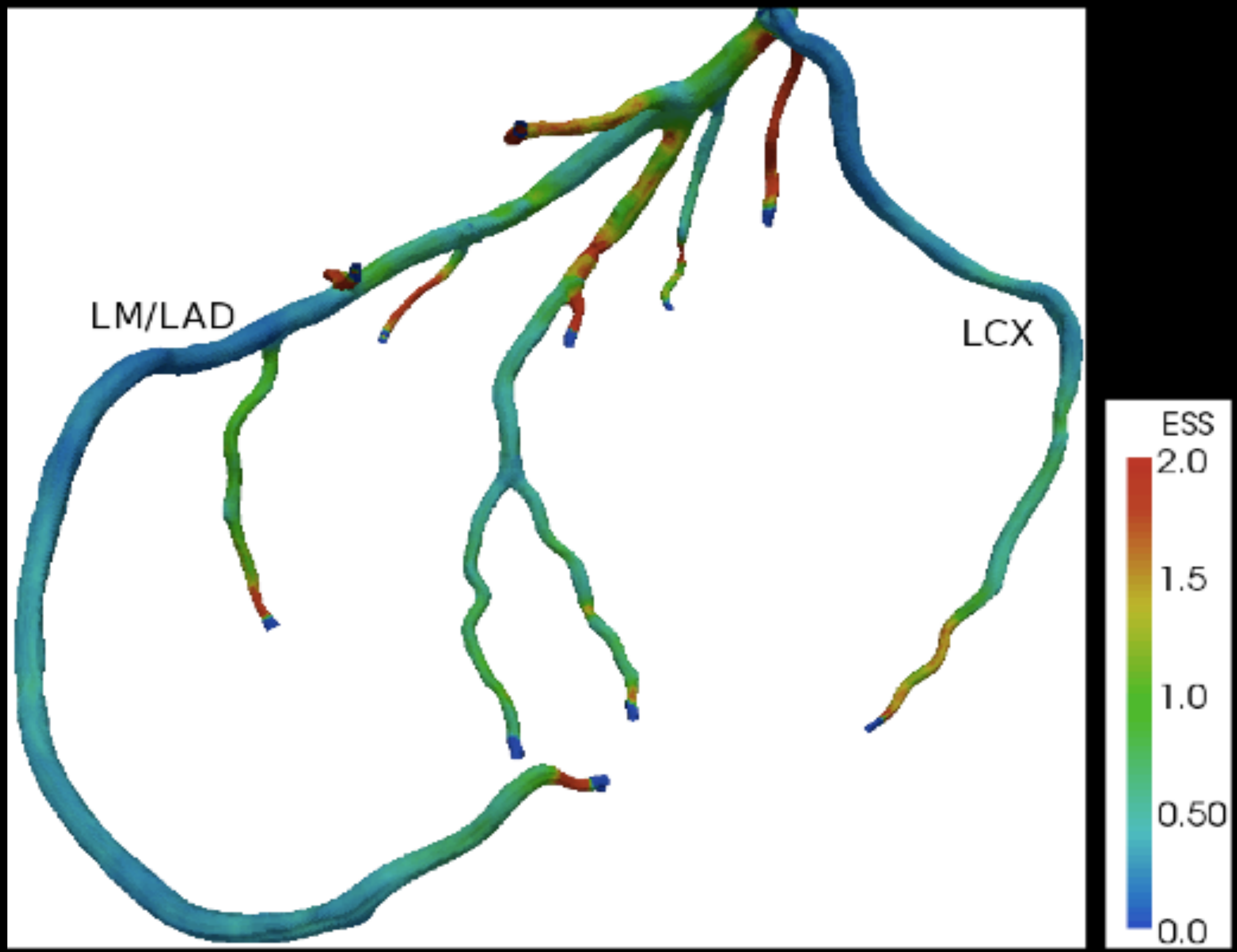
$$\frac{d}{dt} V = \frac{1}{M} (F + F^H)$$

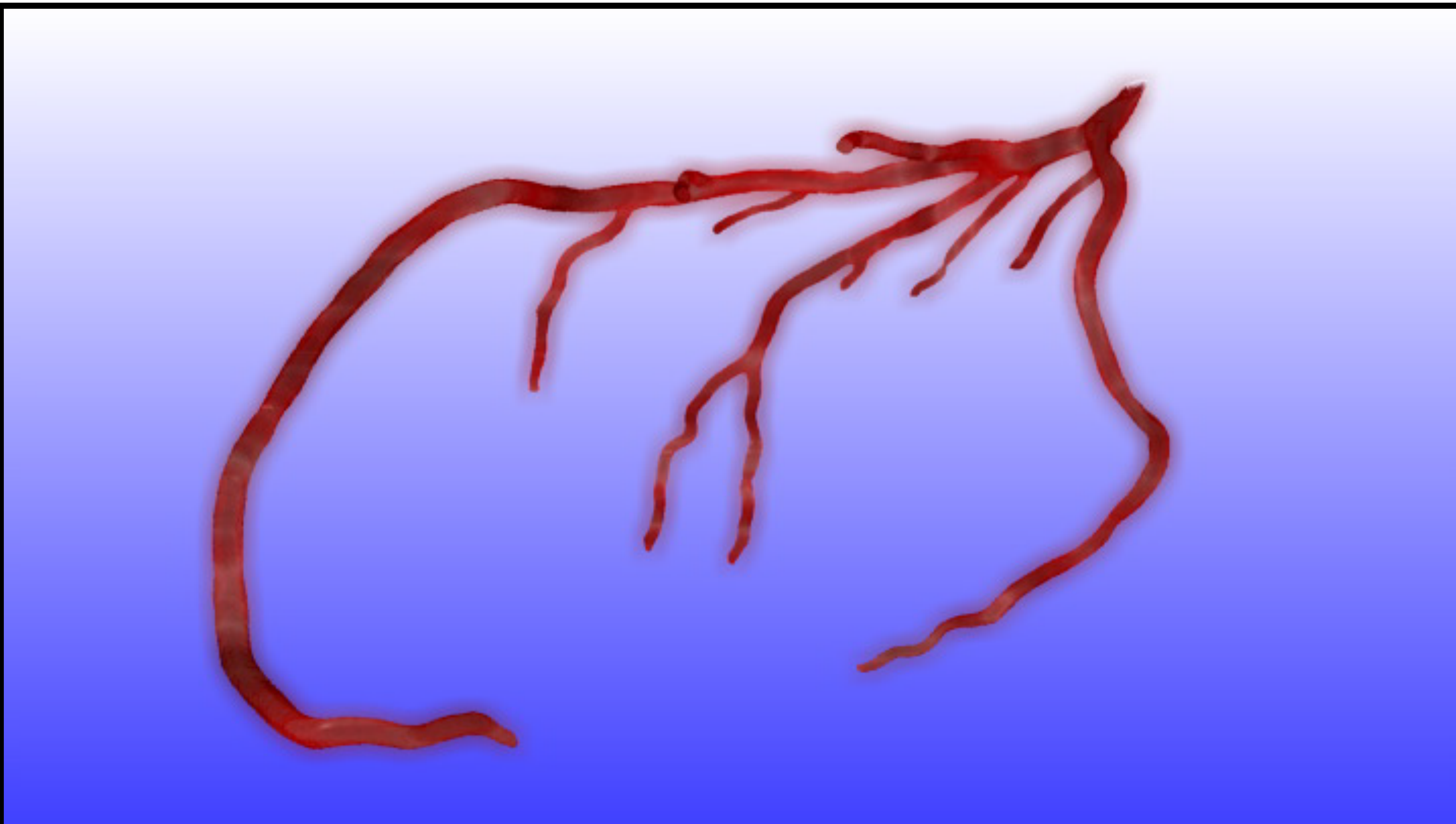
$$F^H = -\gamma \left[V - u(x, \{R, V\}) \right] \delta(x - R)$$

Momentum exchange
(Newton's 3rd law)



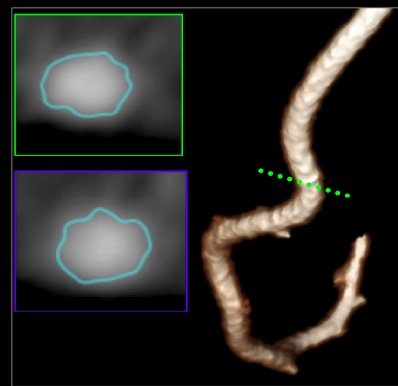
ESS Calculation in patient-specific arterial tree



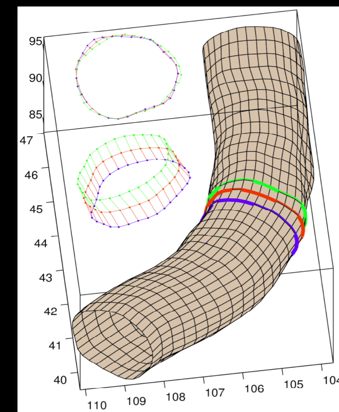


Full arterial tree (10^9 grid points) with RBC's (10^8 cells)

Patient Data

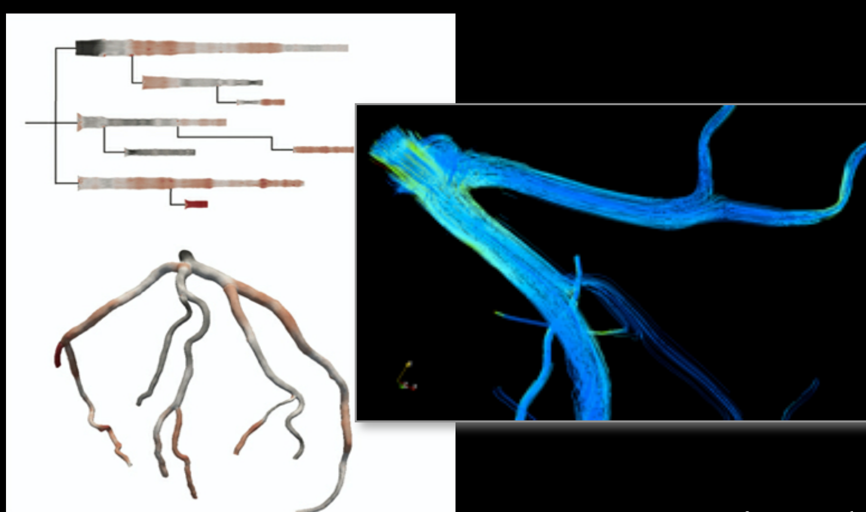


Data Segmentation



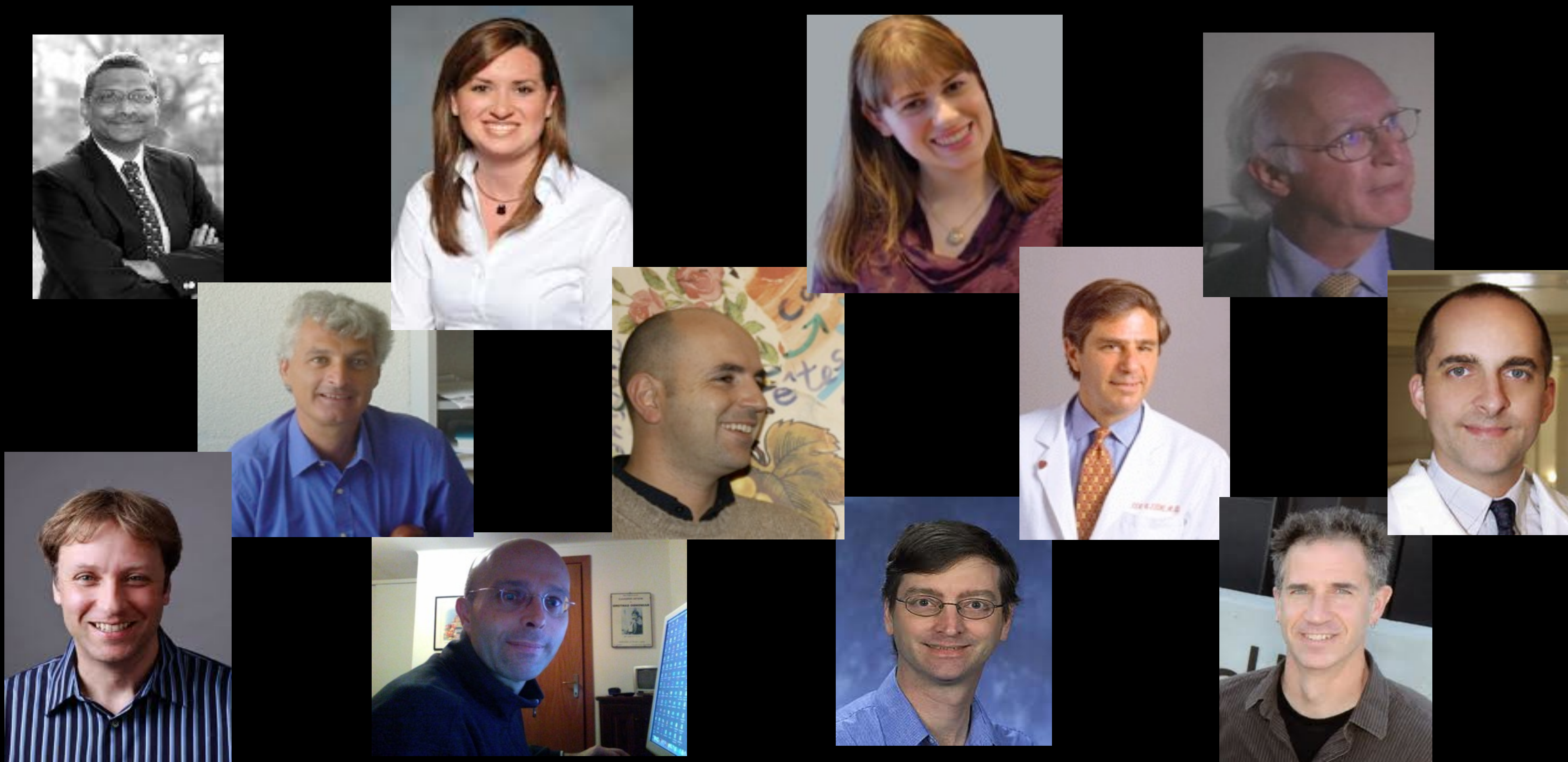
Data Preparation

Parallel Code: MUPHY & HARVEY



Output visualization

Multiscale Hemodynamics Team



Massimo Bernaschi - Michelle Borkin - Mauro Bisson - Ahmet Coskun - Charles Feldman - Bill Gropp - Jeff Hammond - Joseph Insley - Vivek Kale - Efthimios Kaxiras - Jonas Latt - Simone Melchionna - Dimitris Mitsouras - Amanda Peters Randles- Hanspeter Pfister - Frank Rybicki - Joy Sircar - Michael Steigner - Peter Stone - Sauro Succi - Frederick Welt

Computational Science: Education

Course Information

Physical Sciences 12b: Electromagnetism and Statistical Physics from an Analytic, Numerical and Experimental Perspective

Harvard College/GSAS: 82209

Fall 2013-2014

Efthimios Kaxiras

Location: Science Center B
Meeting Time: Tu., Th., 11:30-1
Exam Group: 13,14

This is the second term of a two-semester introductory sequence that uses a combination of analytic and numerical methods to understand physical systems, to analyze experimental data, and to compare data to models. Topics include electrostatics and magnetostatics, electromagnetic fields, optics [all topics illustrated with applications to current technological and societal challenges], and an introduction to the physics of many-body systems and their aggregate properties such as entropy, temperature and pressure. The course is aimed at second year students who have an interest in pursuing a concentration in the sciences and/or engineering. The course structure includes lecture, discussion and laboratory components.

Note: May not be taken for credit by students who have passed Physics 15b or Physics 15c. This course, when taken for a letter grade, meets the General Education requirement for Science of the Physical Universe or the Core area requirement for Science A.

Prerequisite: Physical Sciences 12a

The SEAS graduate program in Computational Science and Engineering (2013-14 inaugural Academic Year)

IACS

Institute for Applied Computational Science

Advisory Board: experts from Industry and National Labs

(IBM, Nvidia, Intel, Microsoft, GoldmanSachs, …
Lawrence Livermore, Los Alamos, …)

Master's programs built around set of learning outcomes

Core and Elective courses

what is a Master's degree in CSE?

- Master of Science (S.M.): total of 8 courses including CSE core courses
- Master of Engineering: total of 16 courses including two semesters of research (Thesis)

- Secondary Field and S.M. are appropriate for Ph.D. students wanting to apply computational methods to a problem in a domain of science, engineering or social science

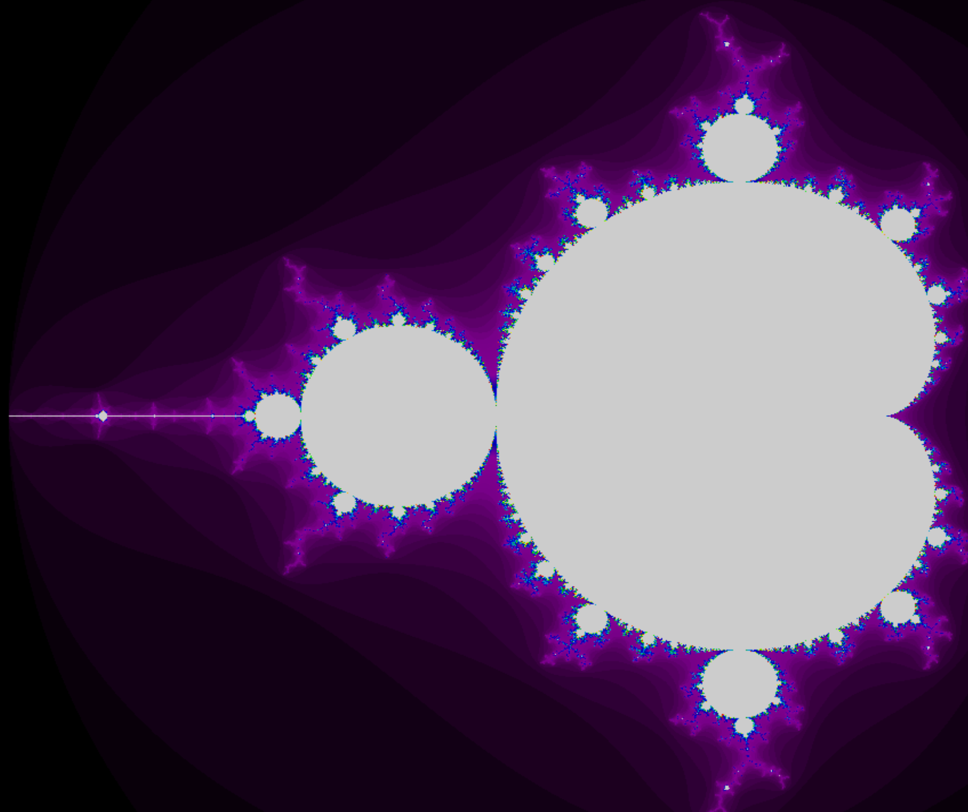
core courses

AM205 Advanced Scientific Computing: Numerical Methods

offered in fall

core courses

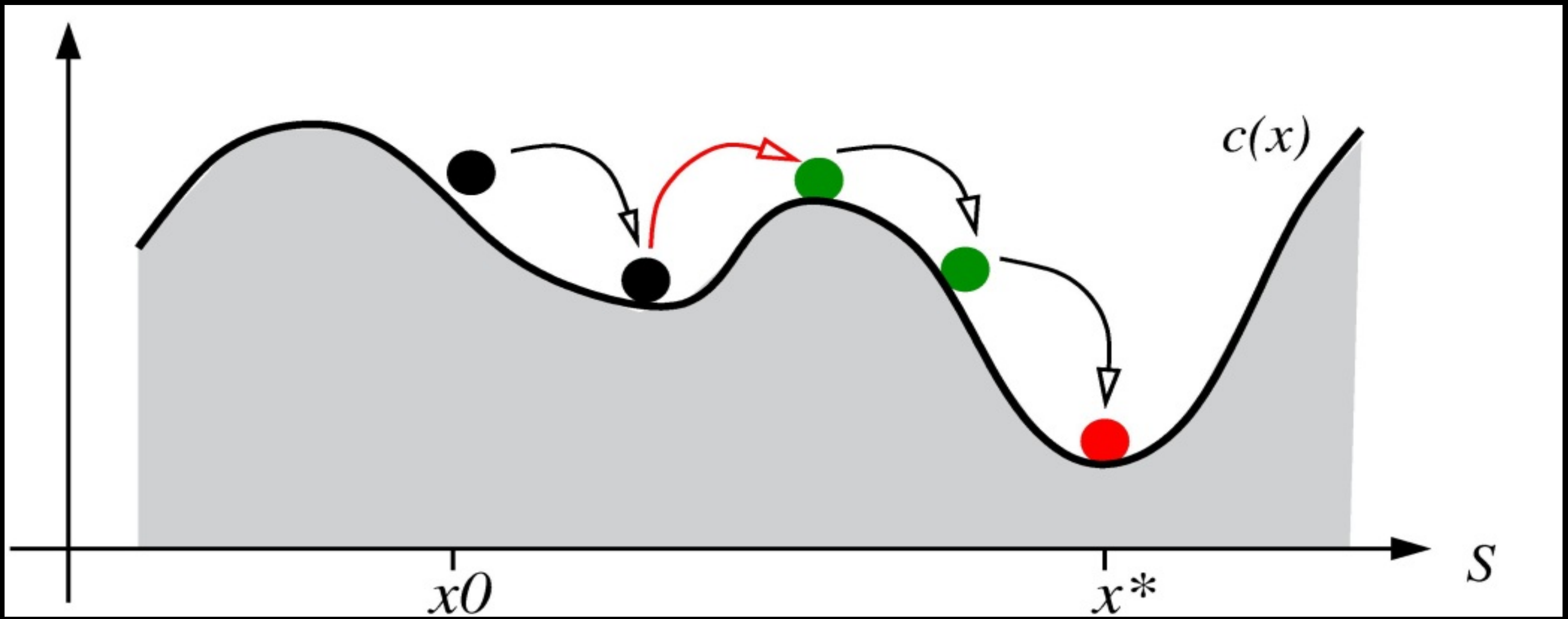
CS205 Computing Foundations for Computational Science



offered in fall

core courses

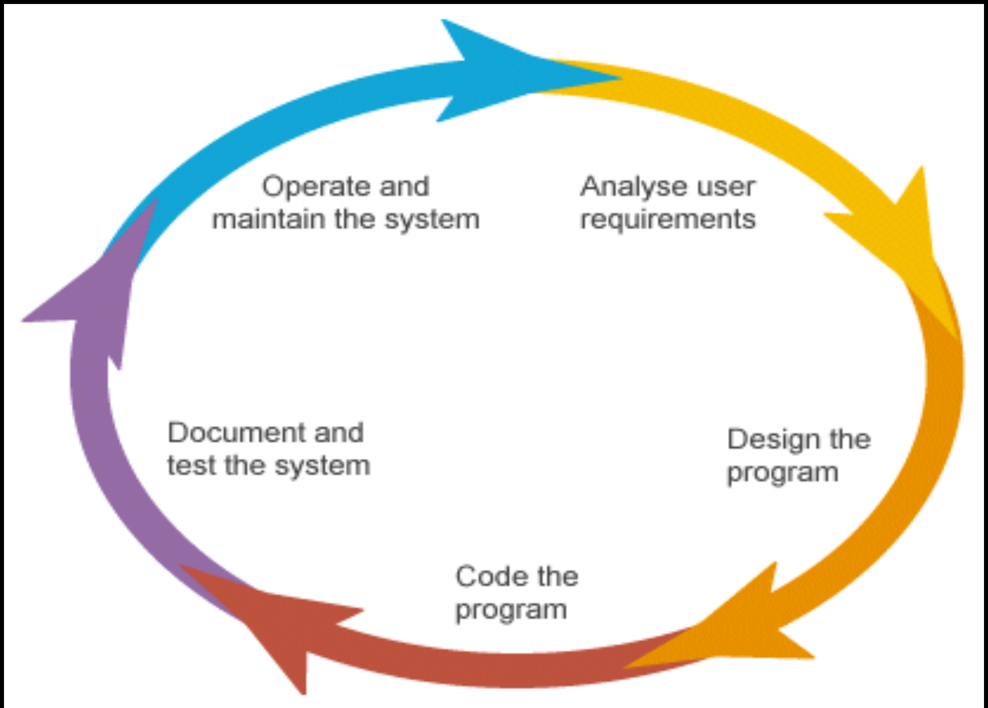
AM207 Advanced Scientific Computing: Stochastic Optimization Methods



offered in spring

core courses

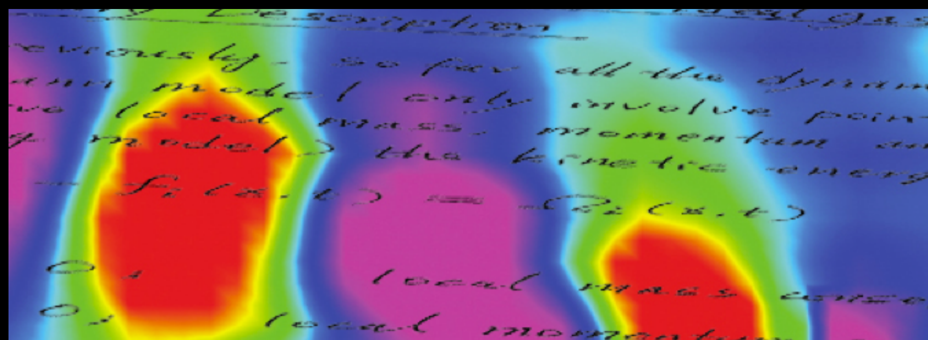
CS207 Systems Design for Computational Science



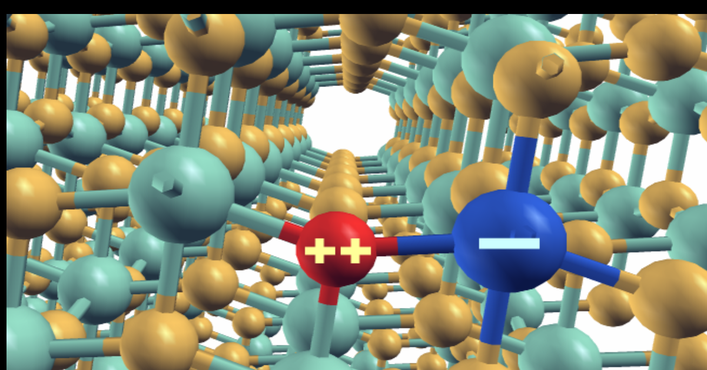
offered in spring

electives

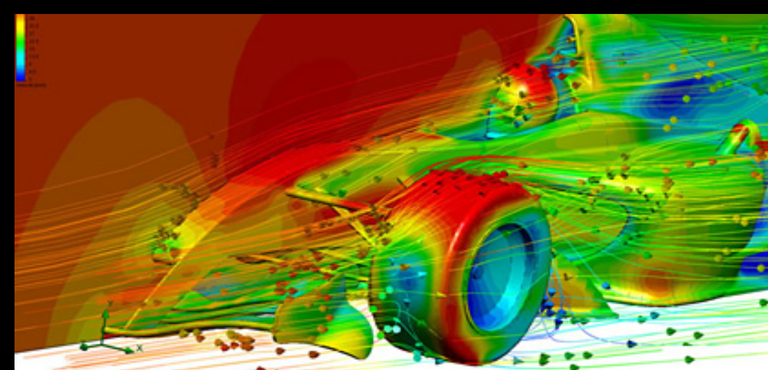
AM272r Kinetic Methods for Fluid: Theory and Applications



AM274 Computational Design of Materials



AM275 Computational Fluid Dynamics



Learning outcomes

1. state-of-the-art modeling and simulation approaches
2. techniques for evaluating and comparing multiple computational approaches
3. skills in collaboration, code implementation and development of robust, reliable software
4. new methods for modeling big data and complex systems
5. how to take advantage of parallel and distributed computing
6. advanced data analysis and visualization methods
7. parallel programming and "parallel thinking"

Congratulations David!
Warm welcome to PICS!
Best wishes for success and growth
(we’re counting on it)!