Q: Can a computer save you from heart attack?

A: maybe …

Why?

How?

Efthimios (Tim) Kaxiras
Physics & SEAS
February 9, 2014

WASHINGTON - Tim Russert, NBC News' Washington bureau chief and the moderator of "Meet the Press," died after suffering a heart attack at the bureau. He was 58.

"asymptomatic coronary artery disease",

"well-controlled with medication and exercise"

"performed well on a stress test in late April"

Komla Dumor was a highly acclaimed journalist who presented Focus on Africa on BBC World News, as well as being one of the lead presenters for World News' European morning segment.
To the great shock and sadness of the BBC and its audience around the world, Komla died suddenly from heart attack in January 2014 at age 41.

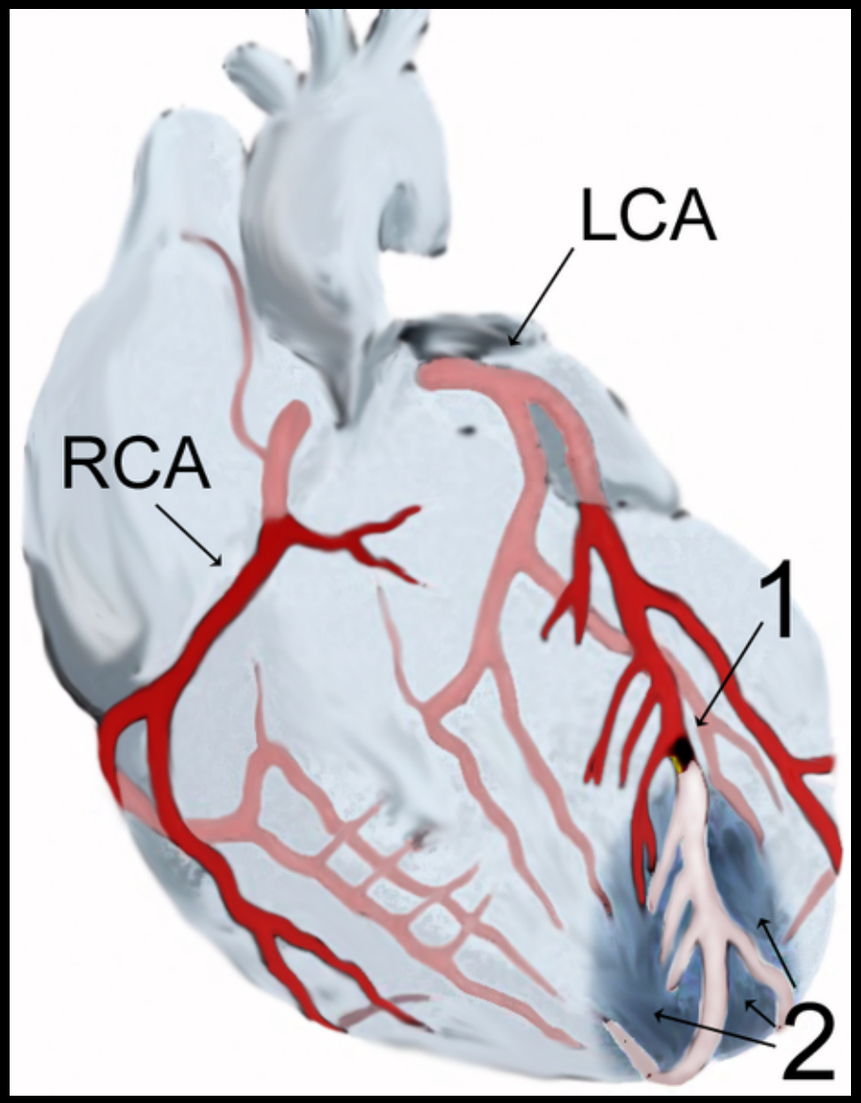
Cardiovascular Disease

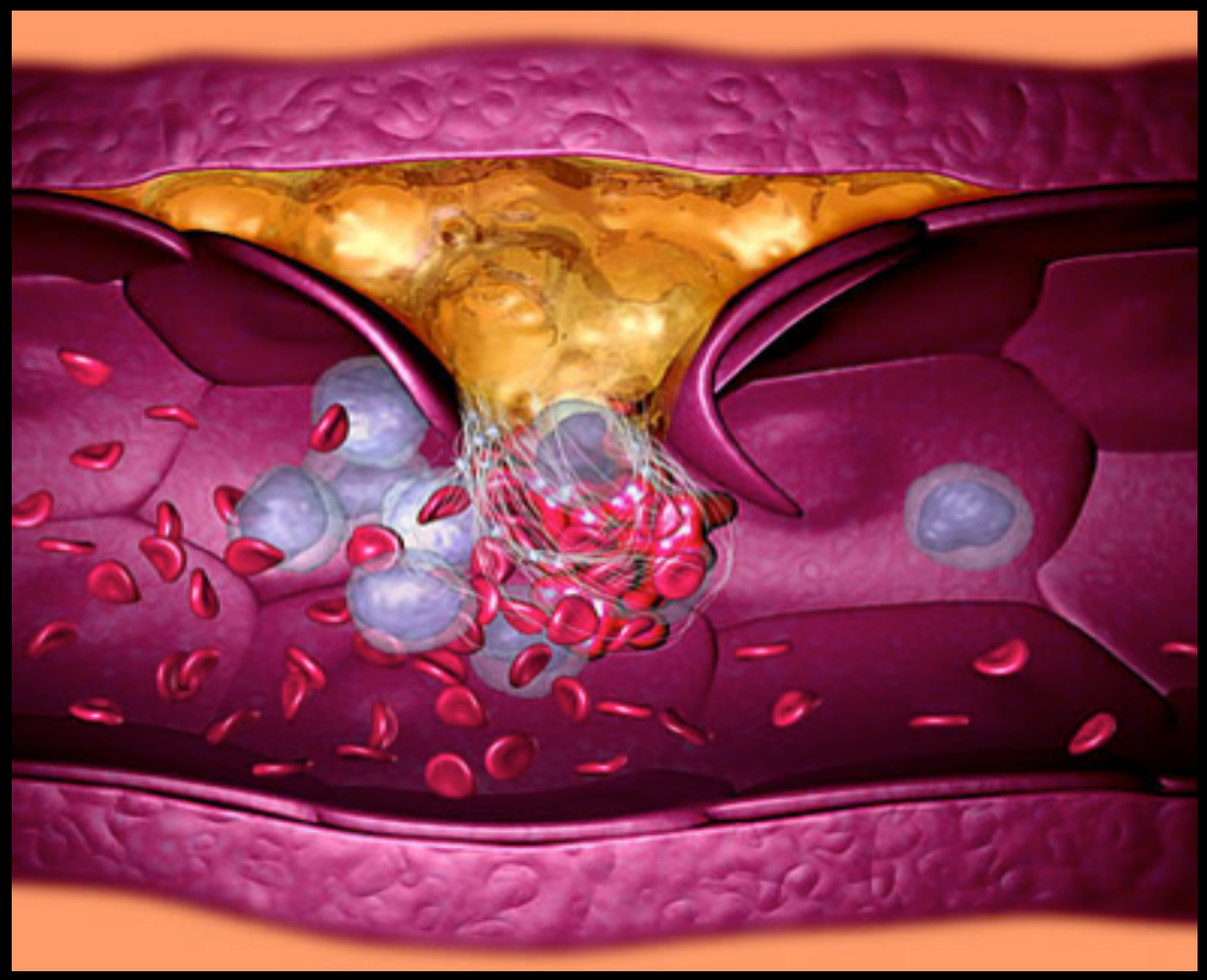
Leading cause of death in the western world

about 1 in 3 deaths in the US alone (700,000 deaths)

about 50% of instances occur without prior symptoms

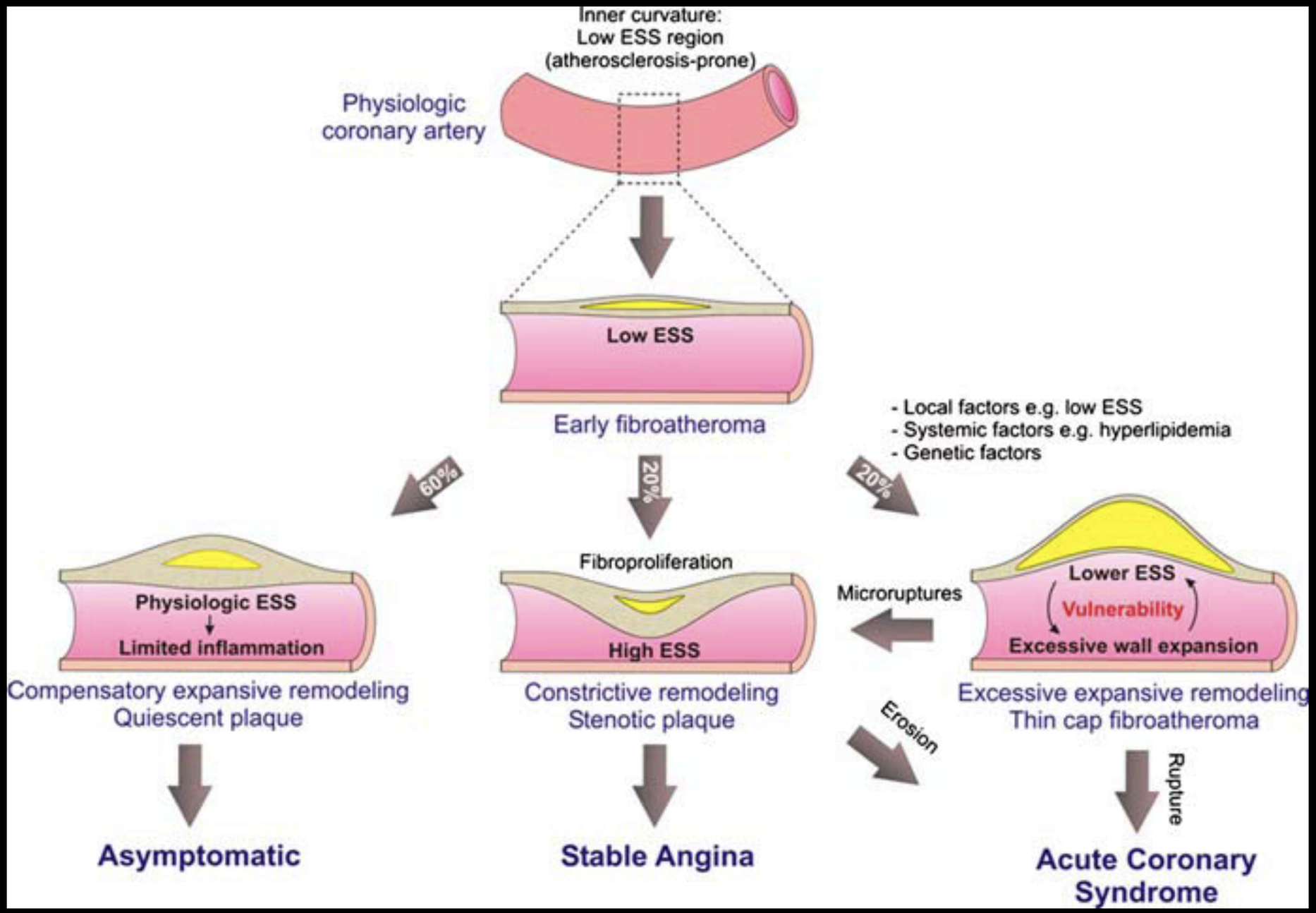
Acute Myocardial Infarction (heart attack)





Formation and evolution of plaques:

"If you are over 16 and you eat, you have placque in your arteries" (C. Feldman, B&W Hospital)

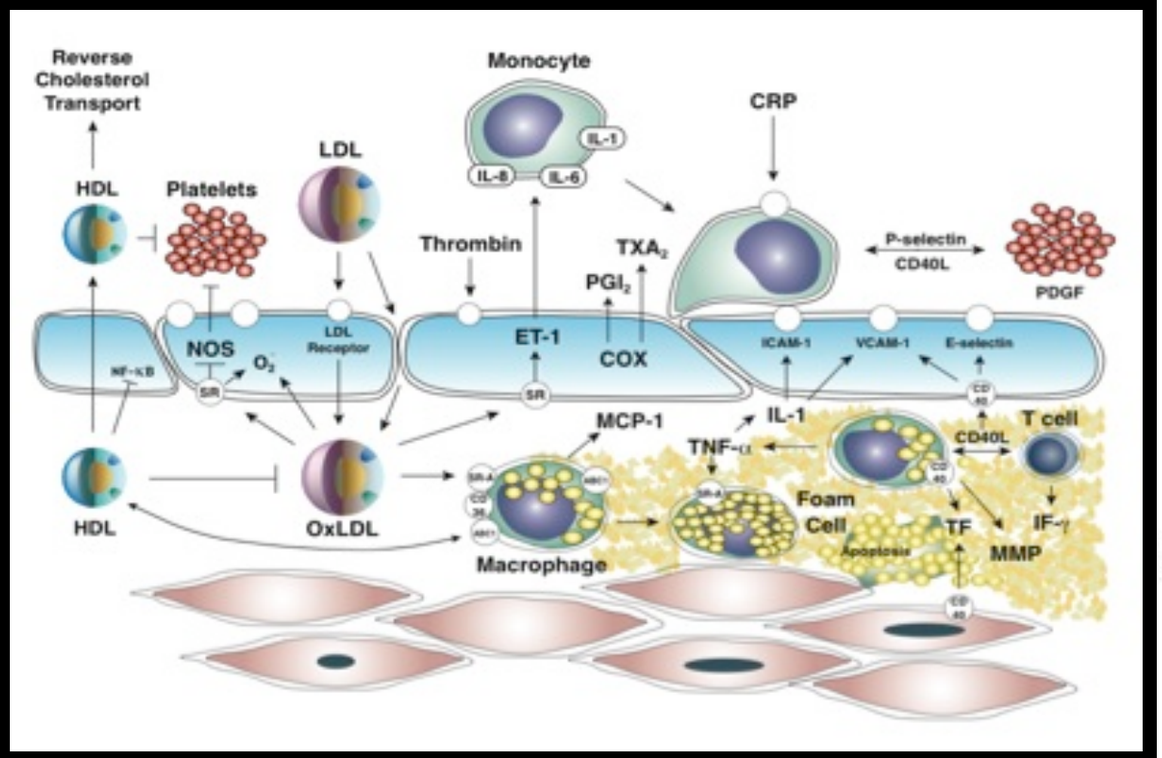


ESS = Endothelial Shear Stress,

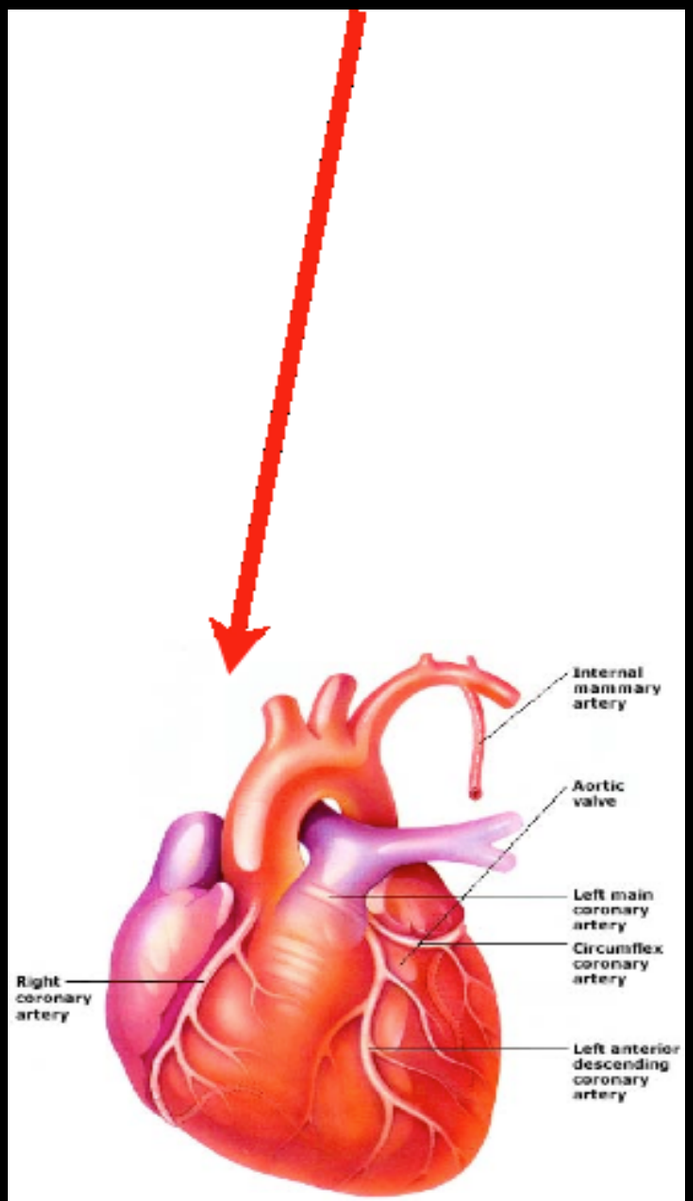
ACCESSIBLE ONLY BY SIMULATION

Grand Challenge: Multiscale Hemodynamics

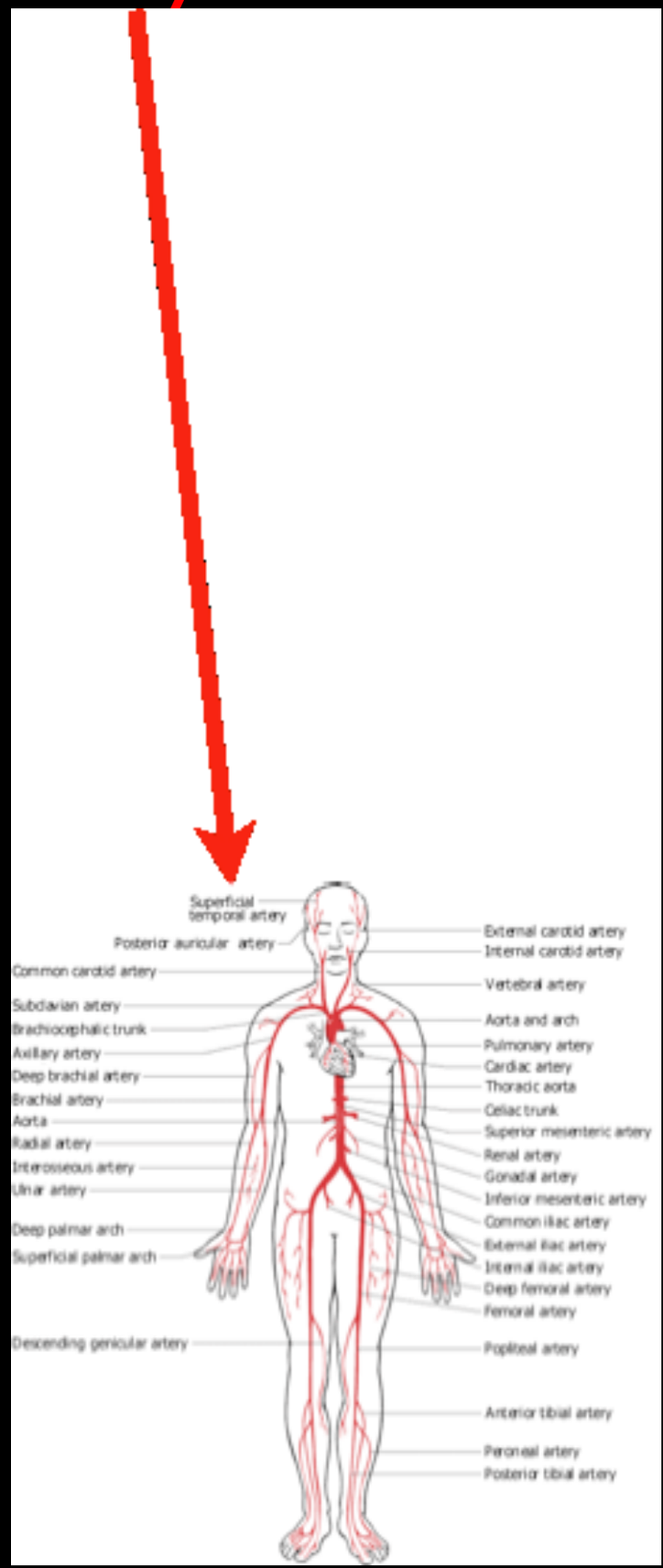
μm-nm scale – biochemistry



cm-mm scale – geometry/ fluid dynamics

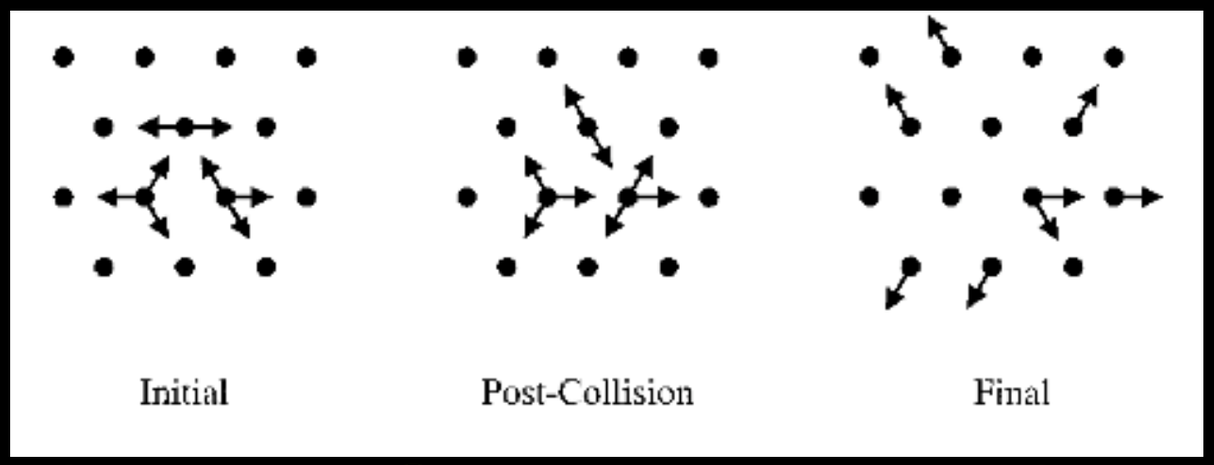


m scale – boundary conditions



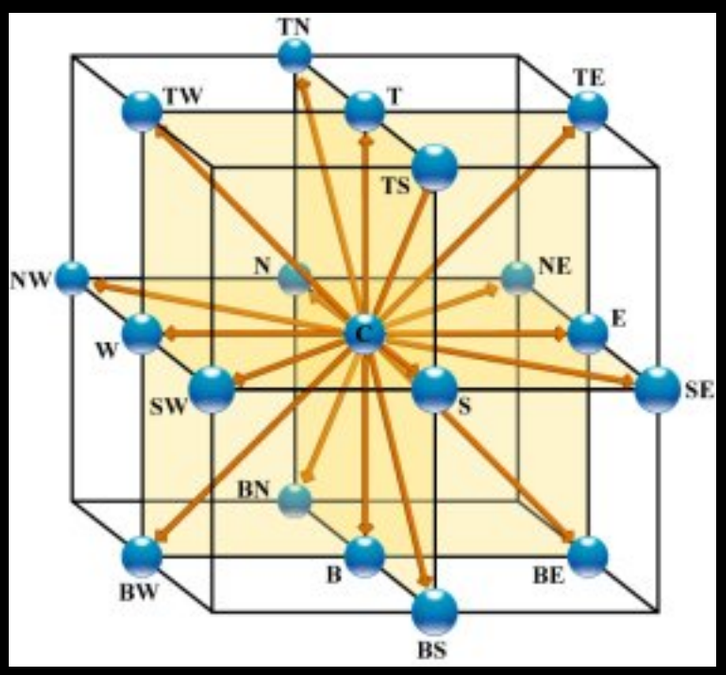
Fluid dynamics by cellular automata : Lattice Boltzmann Equation (LBE)

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



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

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)

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

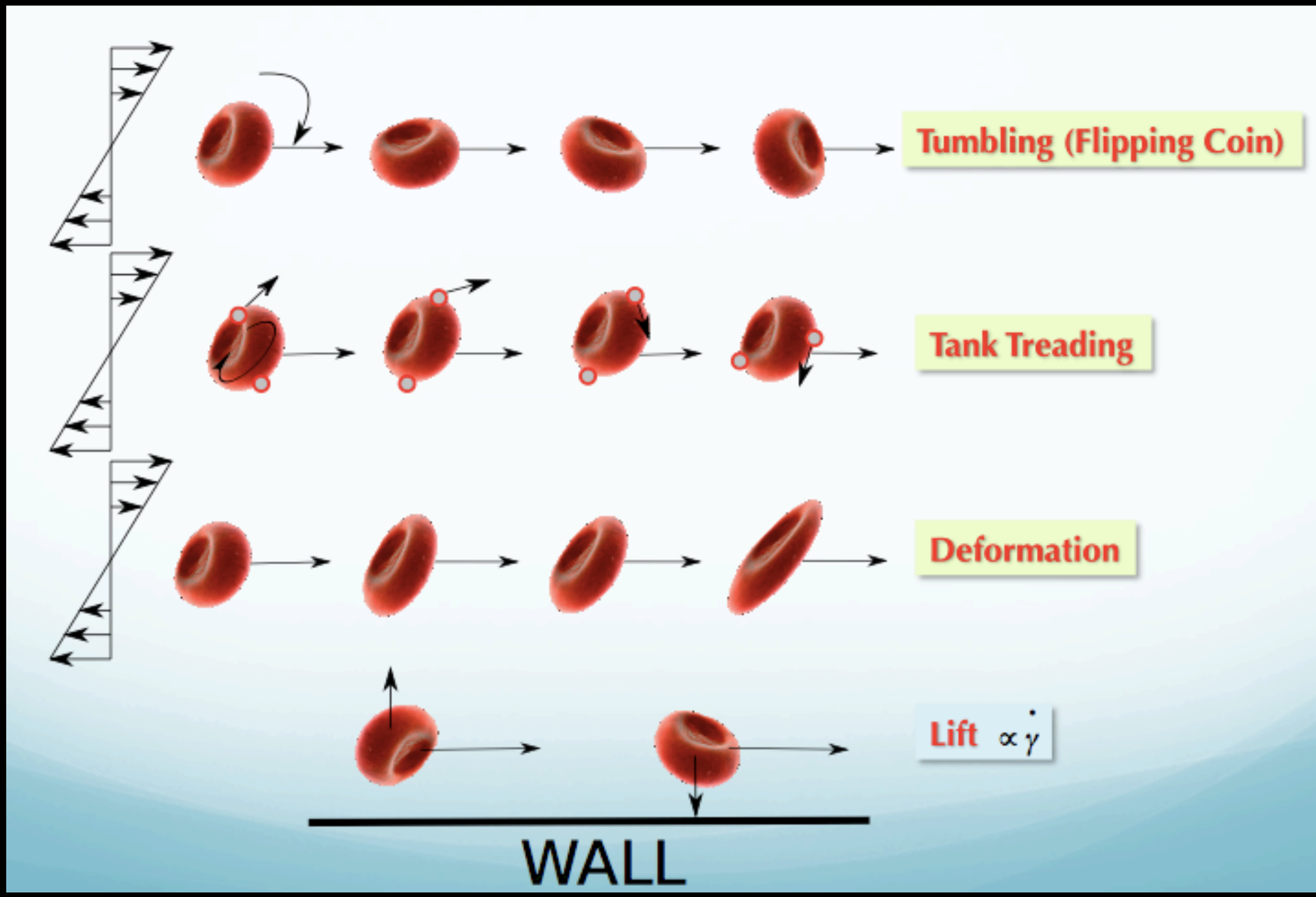
Stress Tensor

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

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

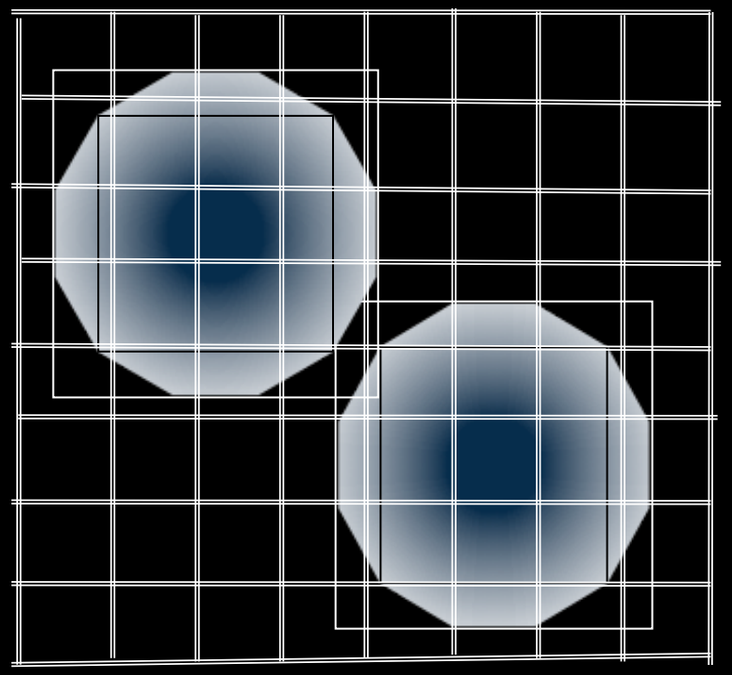


Definition of “particles” (cells, proteins, …)

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

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

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



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

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

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

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

Equations of motion:

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

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

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

Brenner *et al.* (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

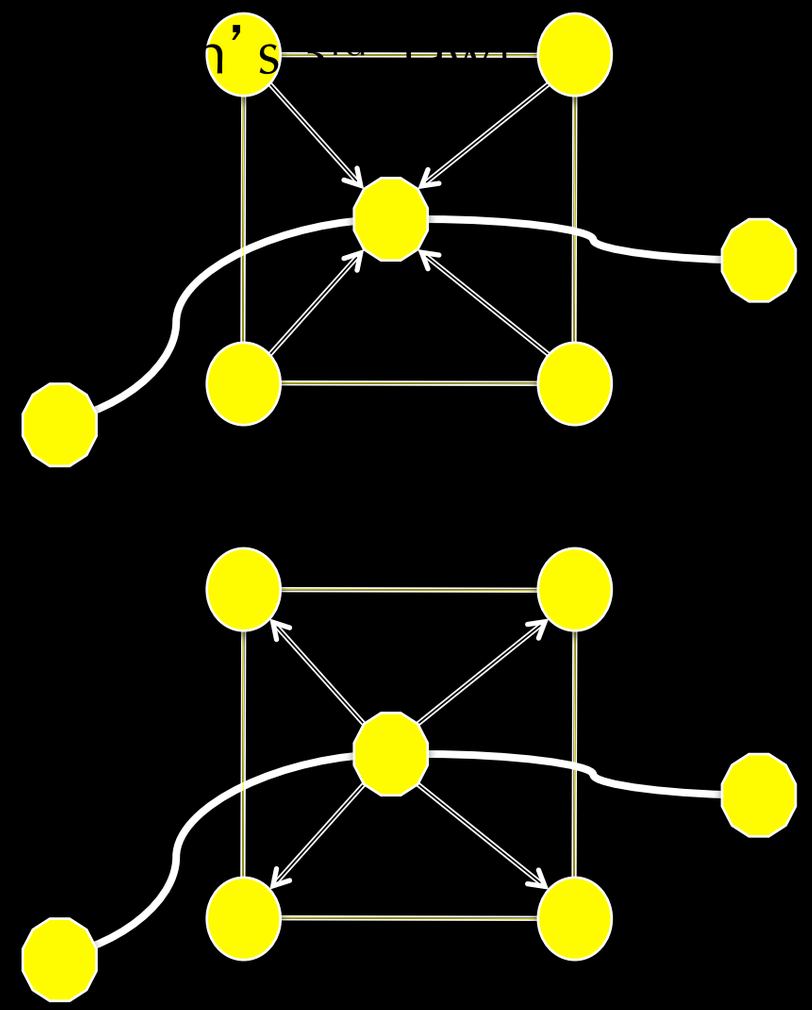
$O(N^3)$ complexity!

Fluid-particle coupling:

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

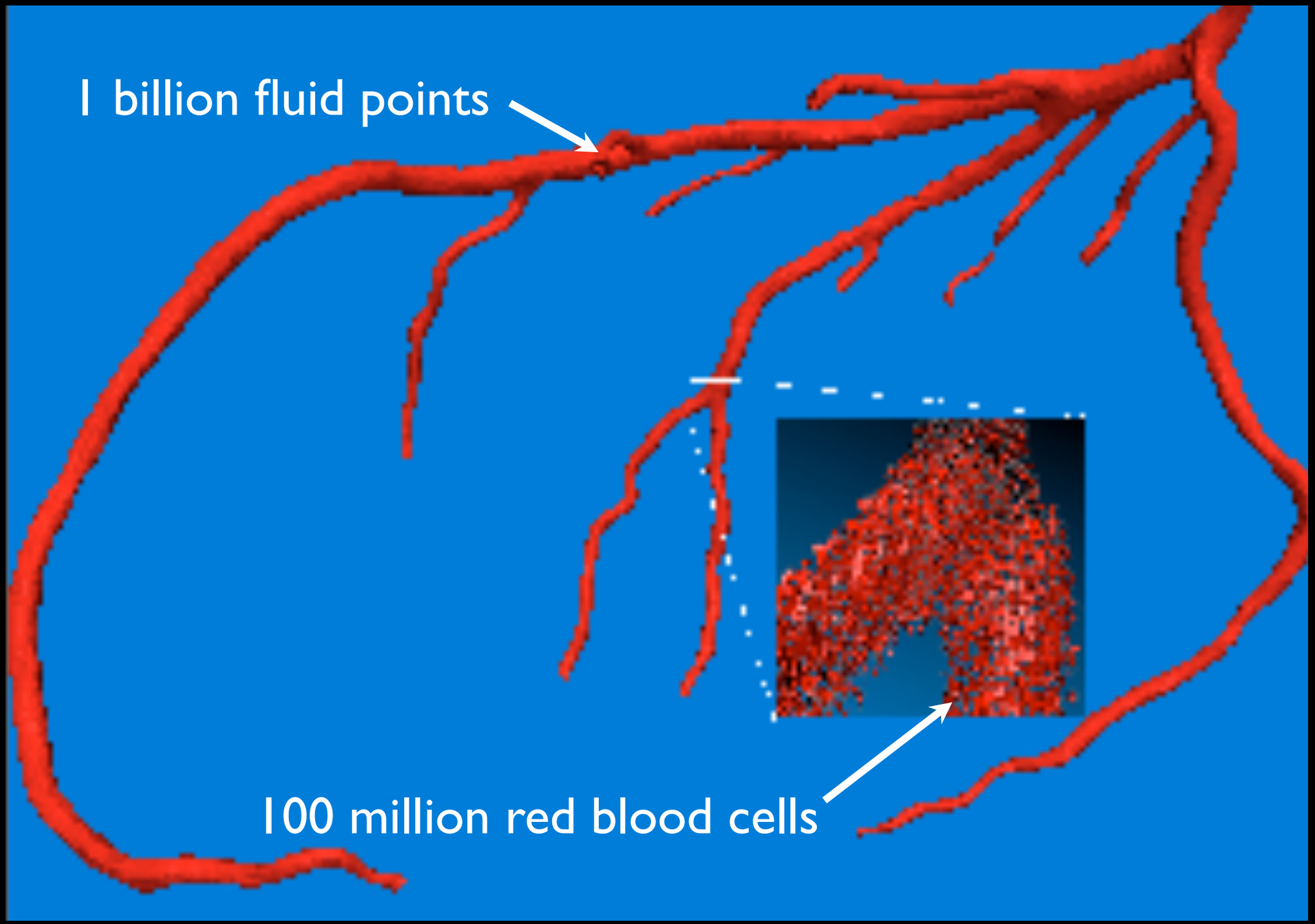
$$\frac{d}{dt}V = \frac{1}{M}(F + F^H)$$

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

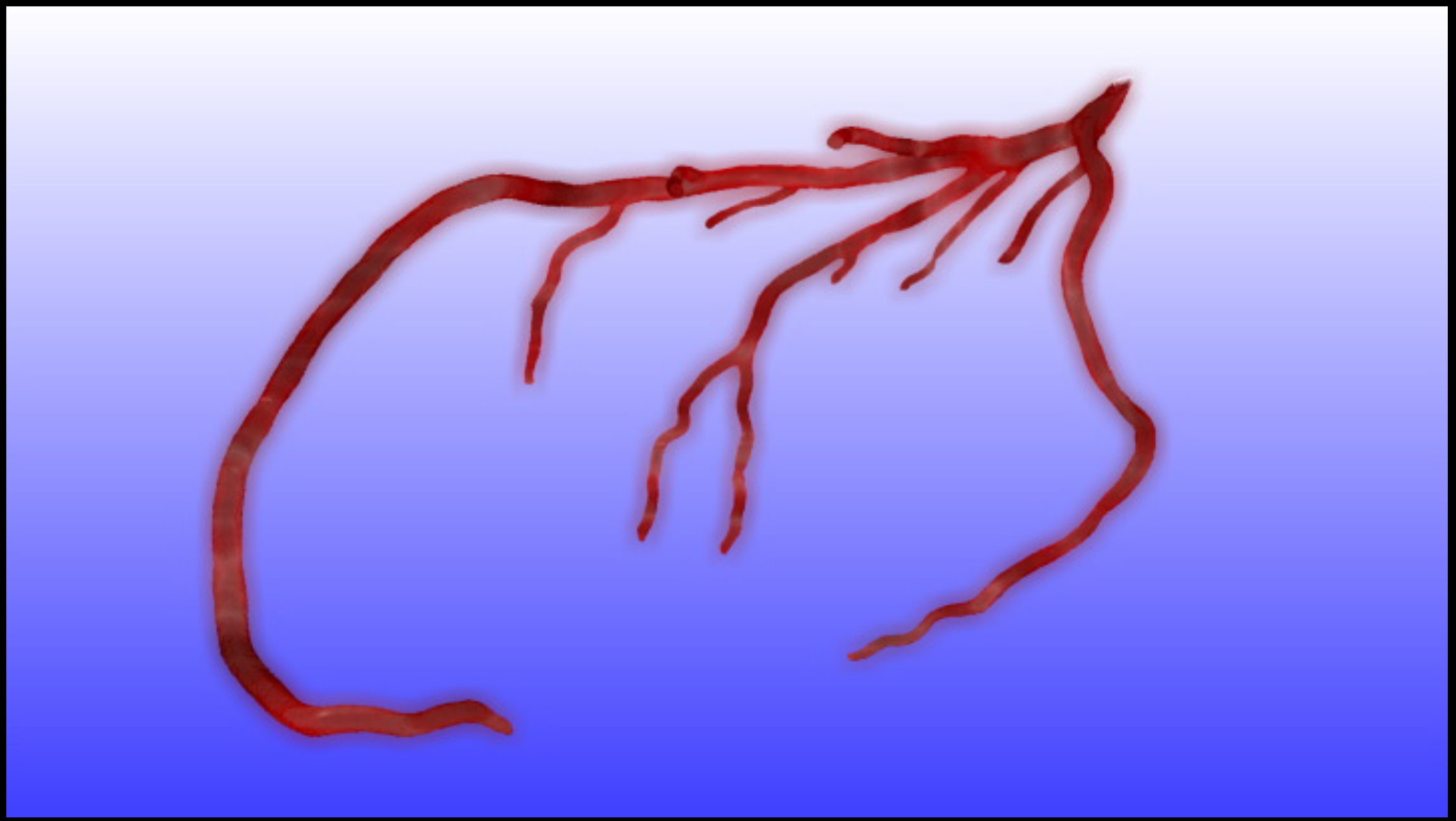


QUIZ TIME!

Full artery simulation: real patient data



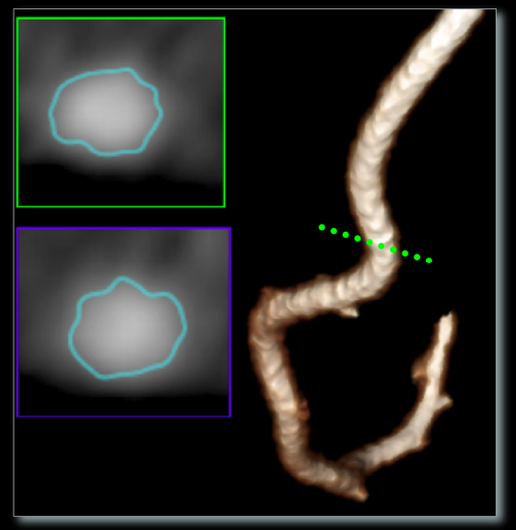
A. Peters, *et al.* Supercomputing, 2010



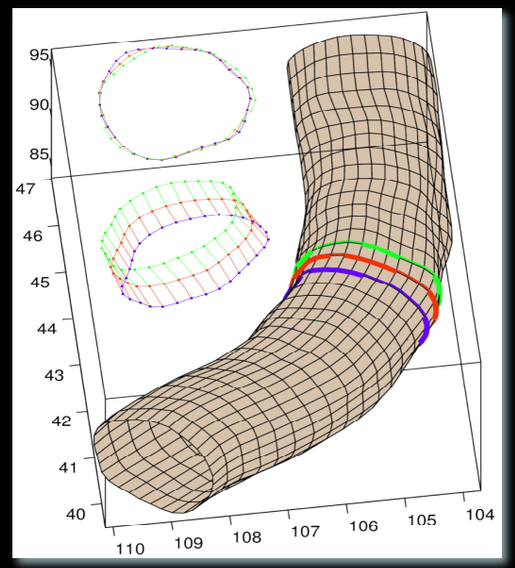
A. Peters, *et al.*
Supercomputing, 2010

Hemodynamics pipeline:

Patient Data



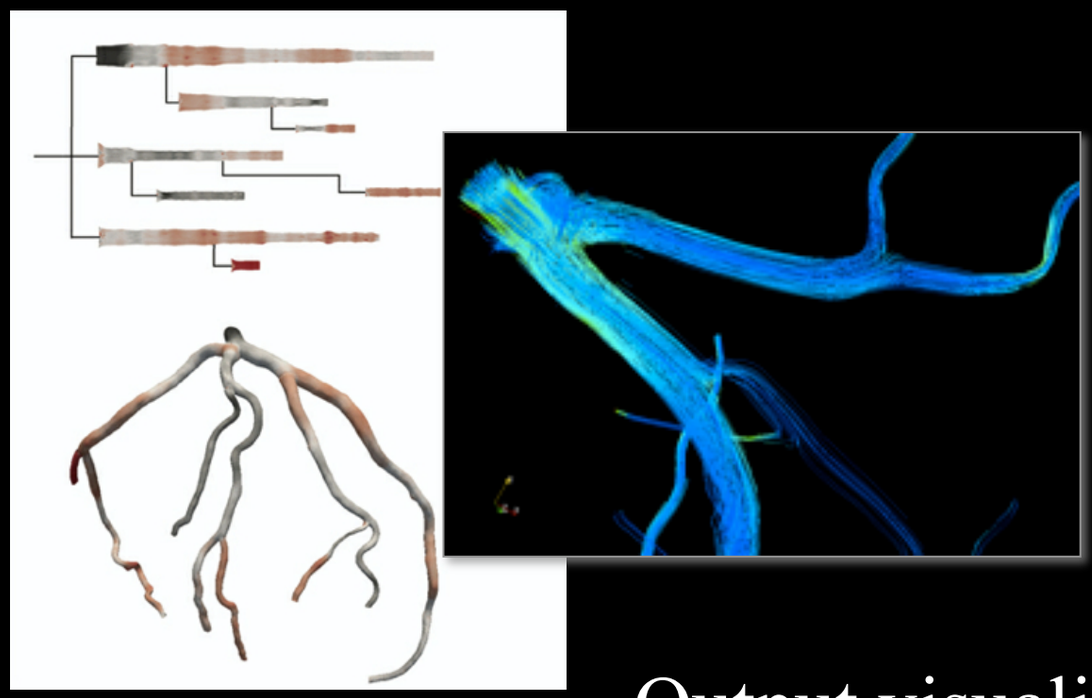
Data Segmentation



HPC Data Preparation

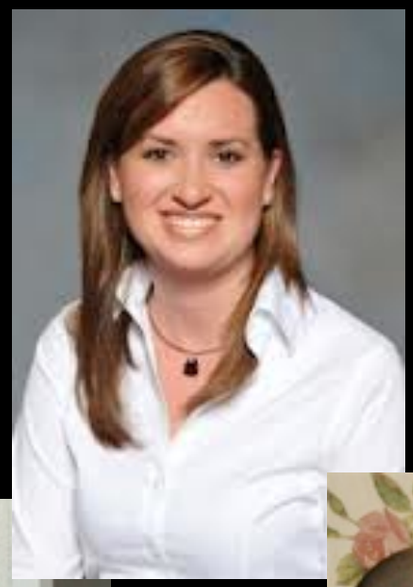
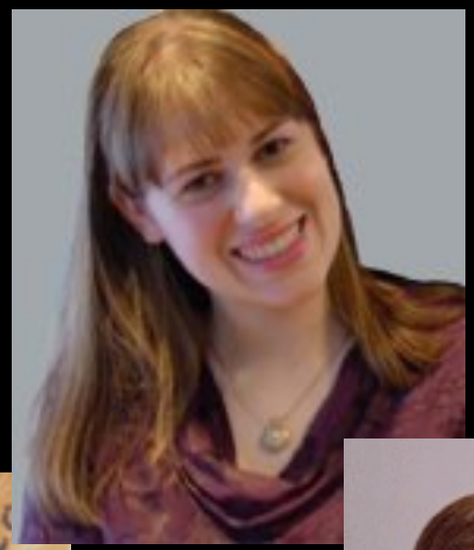
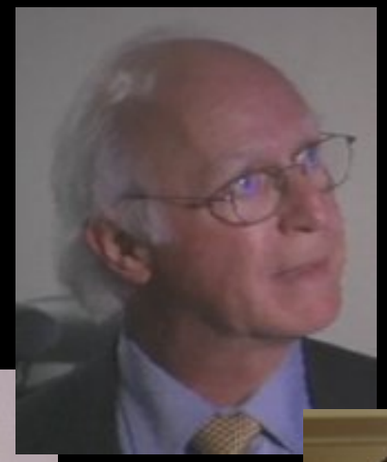
Parallel Code: MUPHY & HARVEY

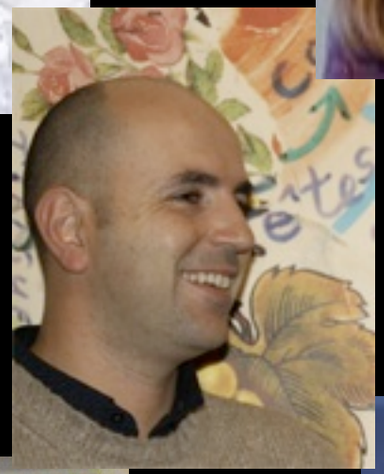
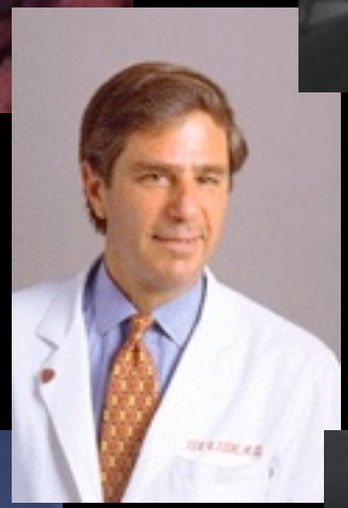
Output visualization



Borkin et al. IEEE Transactions on Visualization and Computer Graphics, 2011

Multiscale Hemodynamics Team



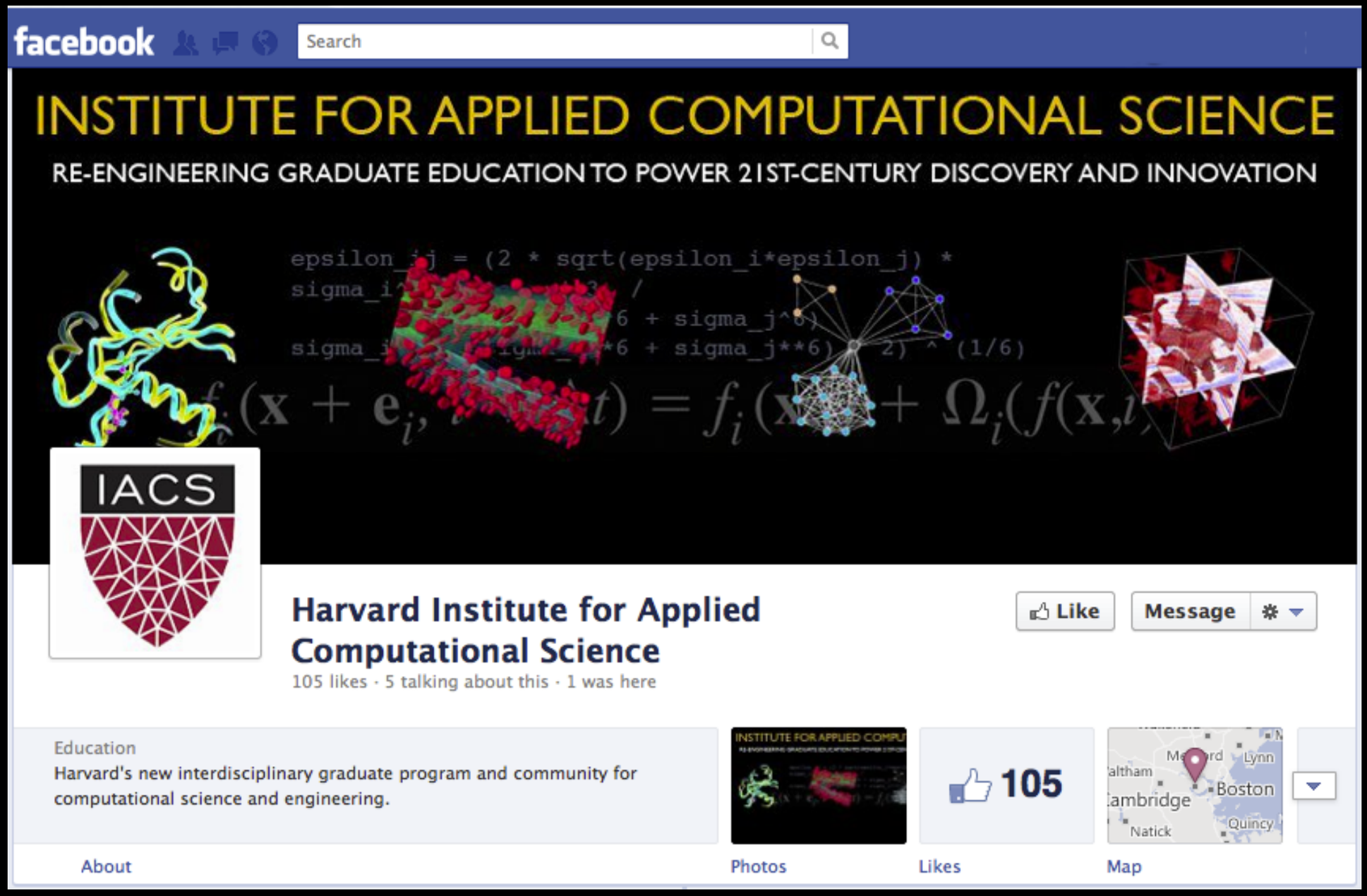

Massimo Bernaschi - Michelle Borkin - Mauro Bisson - Ahmet Coskun - Charles Feldman - William Gropp - Jeff Hammond - Joseph Insley - Vivek Kale - Efthimios Kaxiras - Jonas Latt - Simone Melchionna - Dimitris Mitsouras - Amanda Peters - Hanspeter Pfister - Frank Rybicki - Joy Sircar - Michael Steigner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

Educating the next generation of computational scientists and engineers

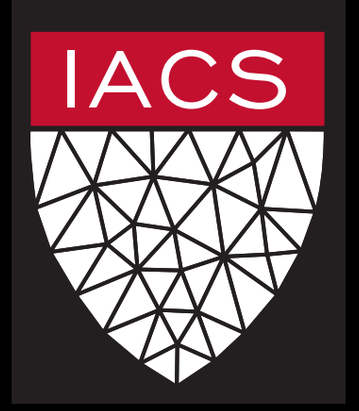
The country that out-*computes* will be the one that out-*competes*.

U.S. Council on Competitiveness, 2004

Dean Cherry Murray
E. Kaxiras – Founding Director (2010-2013)
H. Pfister – Faculty Director (2013-)



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



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
- New CORE COURSES (AM 205-207, CS 205-207) + Electives

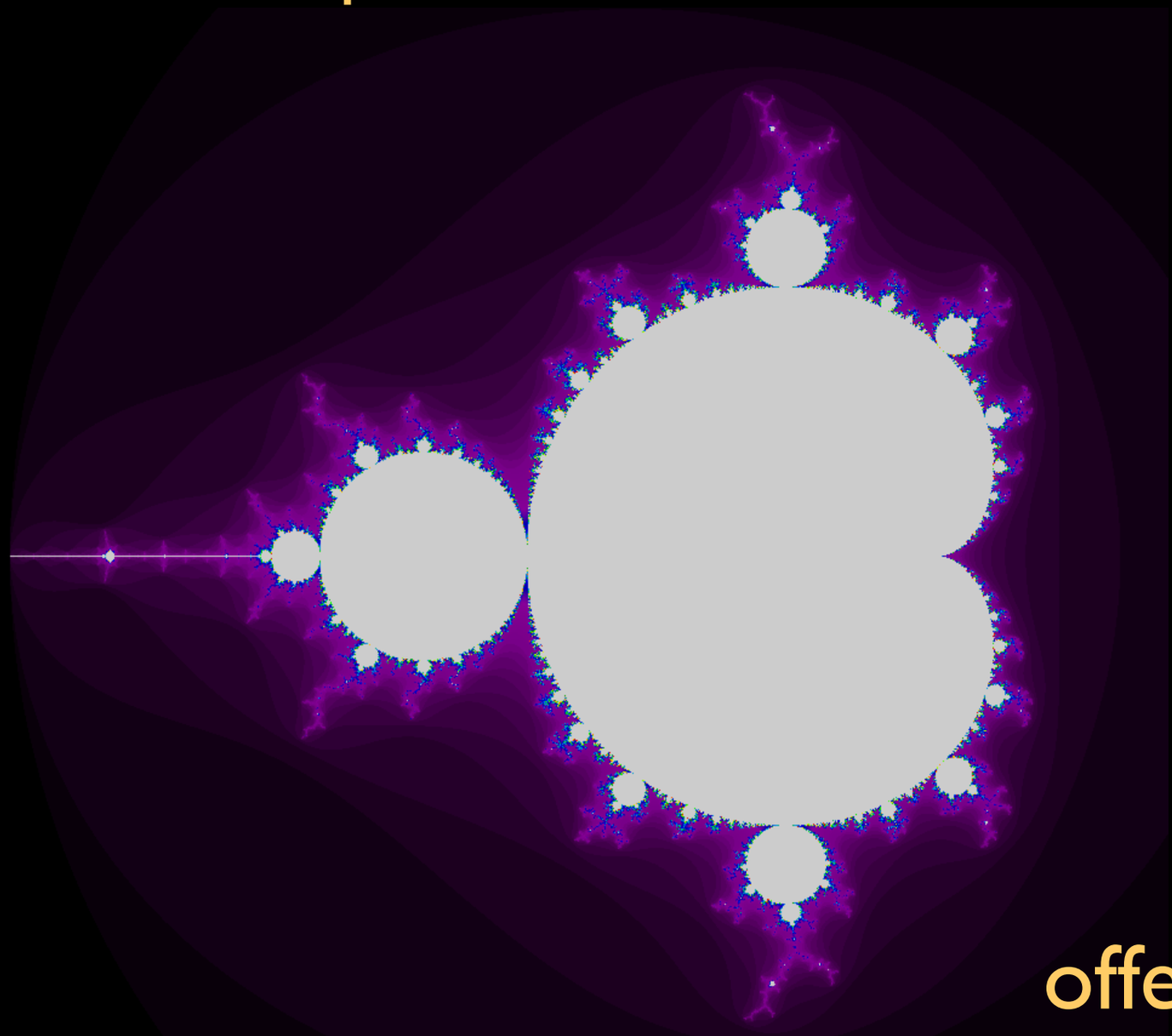
core courses

AM205 Advanced Scientific Computing: Numerical Methods

offered in fall

core courses

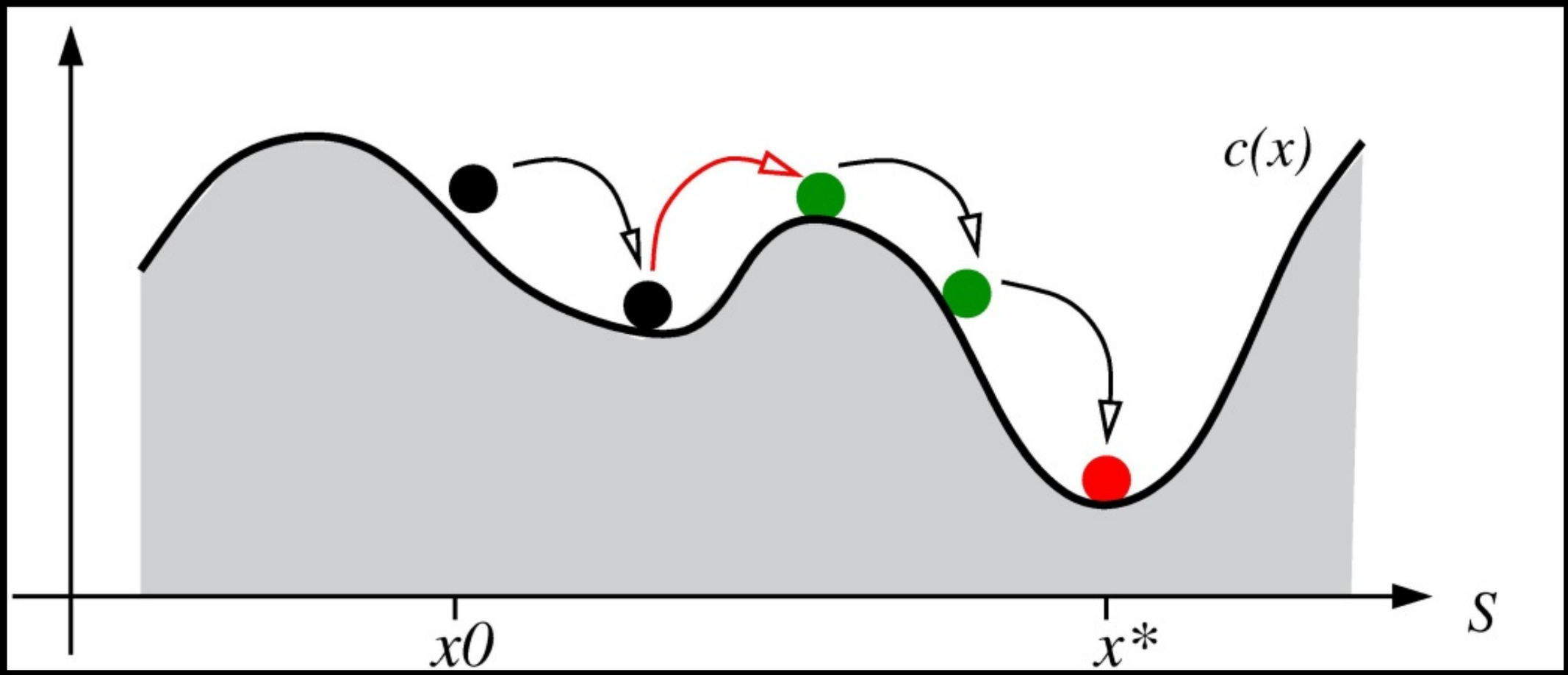
CS205 Computing Foundations for Computational Science



offered in fall

core courses

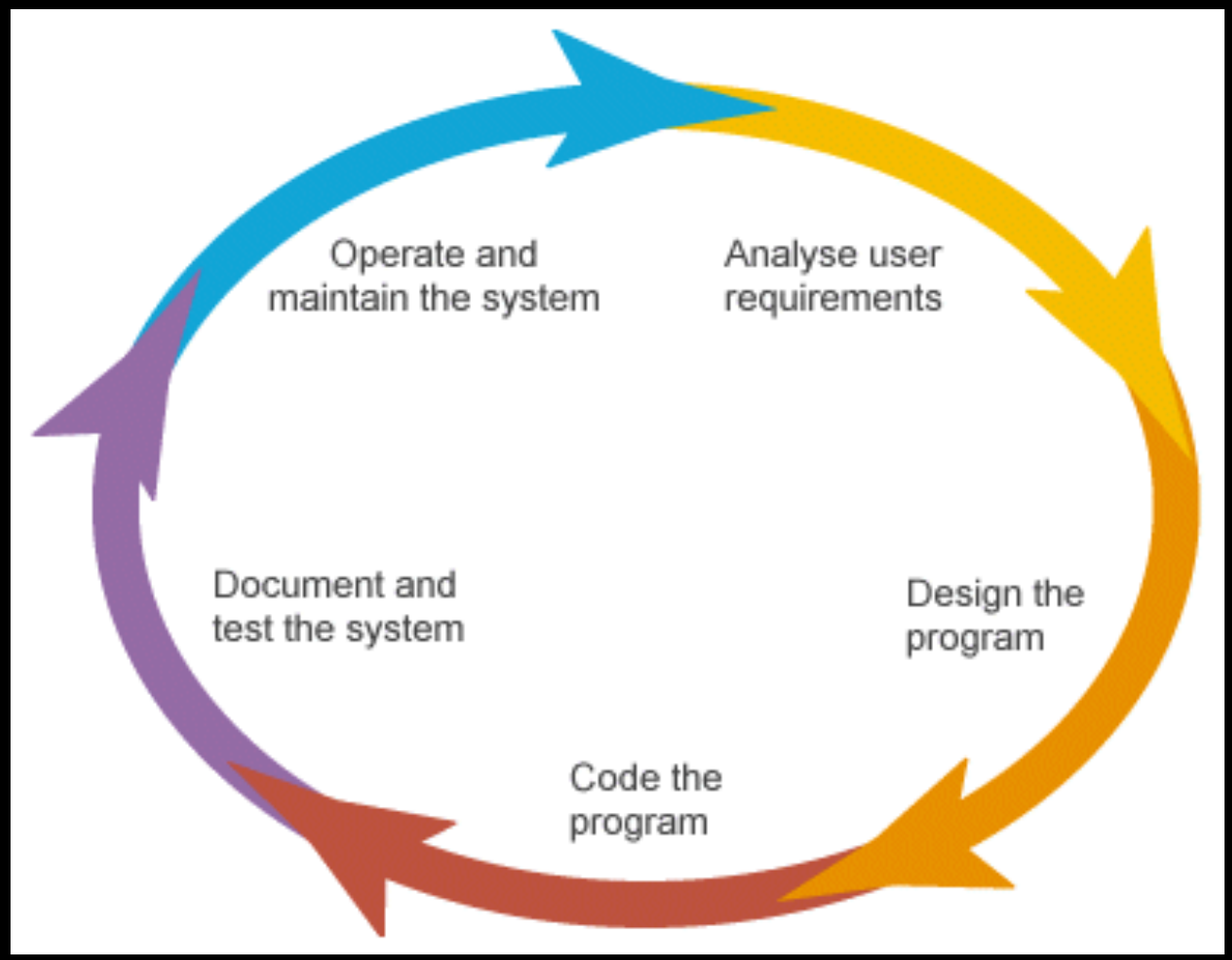
AM207 Advanced Scientific Computing:
Stochastic Optimization Methods



offered in spring

core courses

CS207 Systems Design for Computational Science

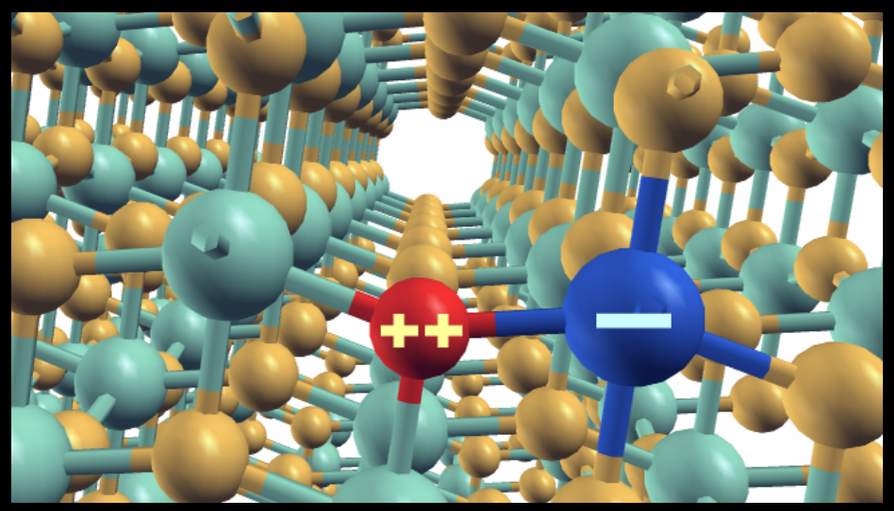


offered in spring

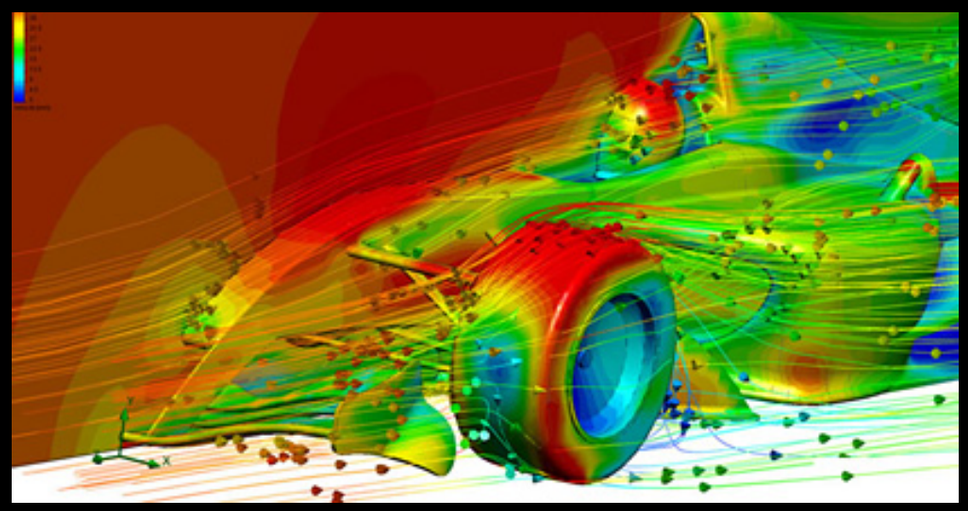
electives

CS 109 / AC 209 Data Science

AC 274 Computational Design of Materials



AC 275 Computational Fluid Dynamics



January Symposium: Computing at Exascale (January 2013)

HARVARD
School of Engineering and Applied Sciences

Graduate program so far

Institute for Applied Computational Science

- January 2013: ~150 applicants

  40 admits, 24 enrolled (60% yield)

- January 2014: ~160 applicants

  50 admits (25-30 to enroll)

- Core Course enrollments: 40 – 80 students,

  (~25% undergrads)

- June 2014: Assessment review