Practices and Perils in Multiphysics Simulations

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Enabling the Interface between Statistics and Engineering
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1. What is a multiphysics simulation?

    motivation through some examples

2. Why do we need multiple scales?
3. How is coupling typically done?
4. Uncertainties, instabilities, limitations?

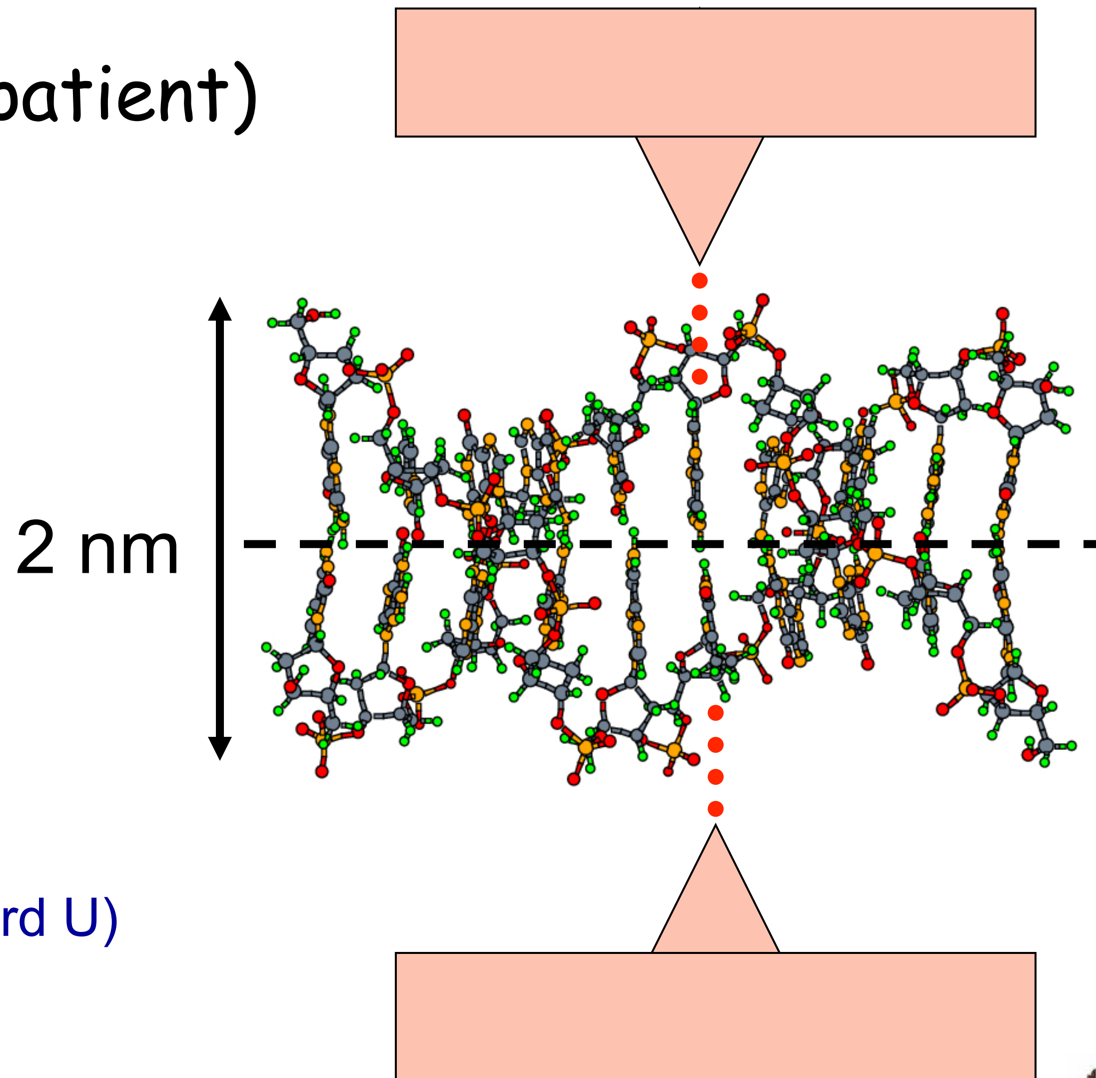
Stress corrosion cracking (SCC):
metal alloys: change from ductile to brittle behavior induced by chemical impurities

brittle fracture in "hostile" environment (moisture)

Aloha Airlines (1988)

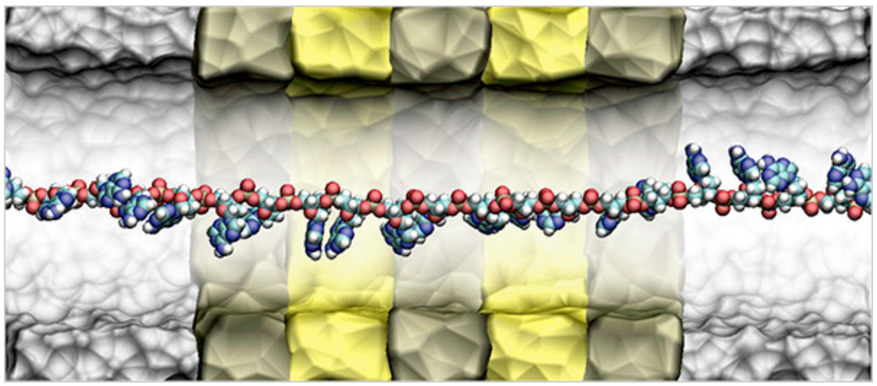
Southwest Airlines (2011)

Ultrafast sequencing of DNA:
use electronic signals to detect
base-pair sequence
(~10 kb/sec, ~1 k$/patient)



J. Golovchenko *et al.* (Harvard U)
C. Decker *et al.* (Delft U)

I.B.M. Joins Pursuit of $1,000 Personal Genome



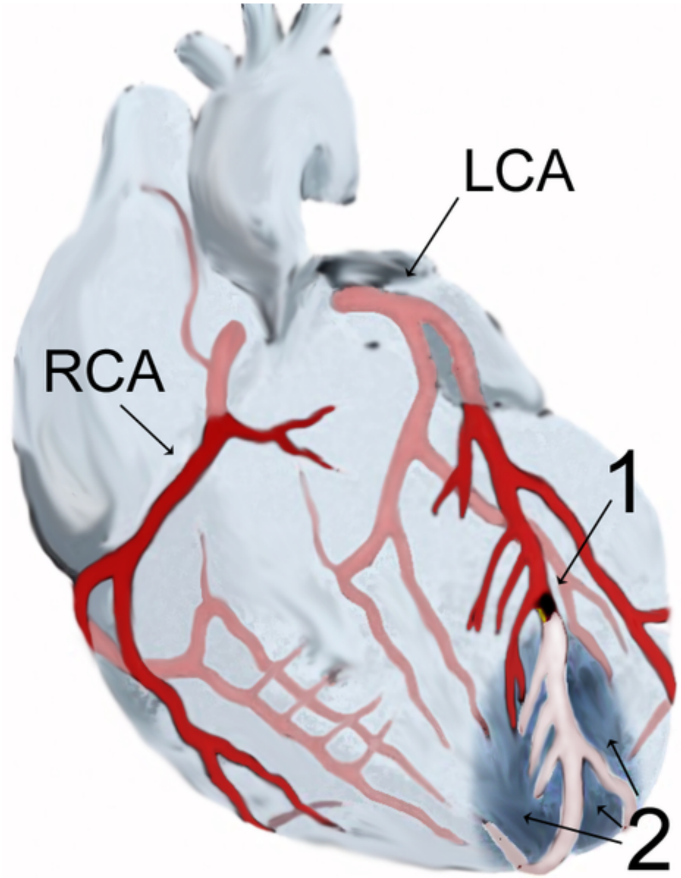
J. Michael Loughran

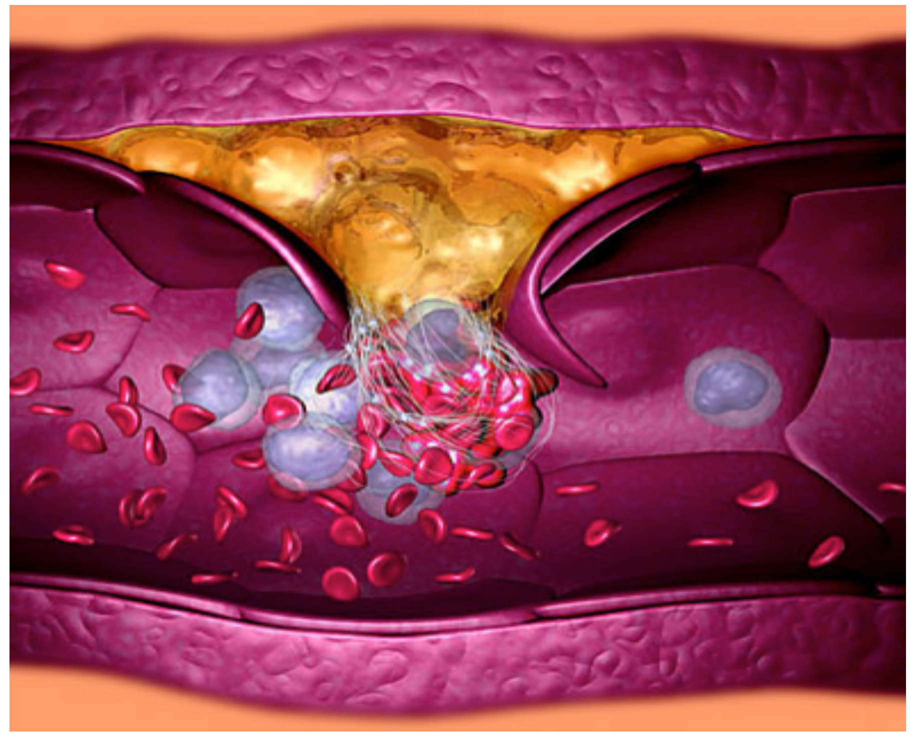
GENETICS An I.B.M. simulation of the “DNA transistor” it hopes will sequence genomes by reading DNA pulled through an atomic-size hole.

By JOHN MARKOFF
Published: October 5, 2009

One of the oldest names in computing is joining the race to sequence the genome for $1,000. On Tuesday, I.B.M. plans to give technical details of its effort to reach and surpass that goal, ultimately bringing the cost to as low as $100, making a personal genome cheaper than a

Acute Myocardial Infarction (heart attack)





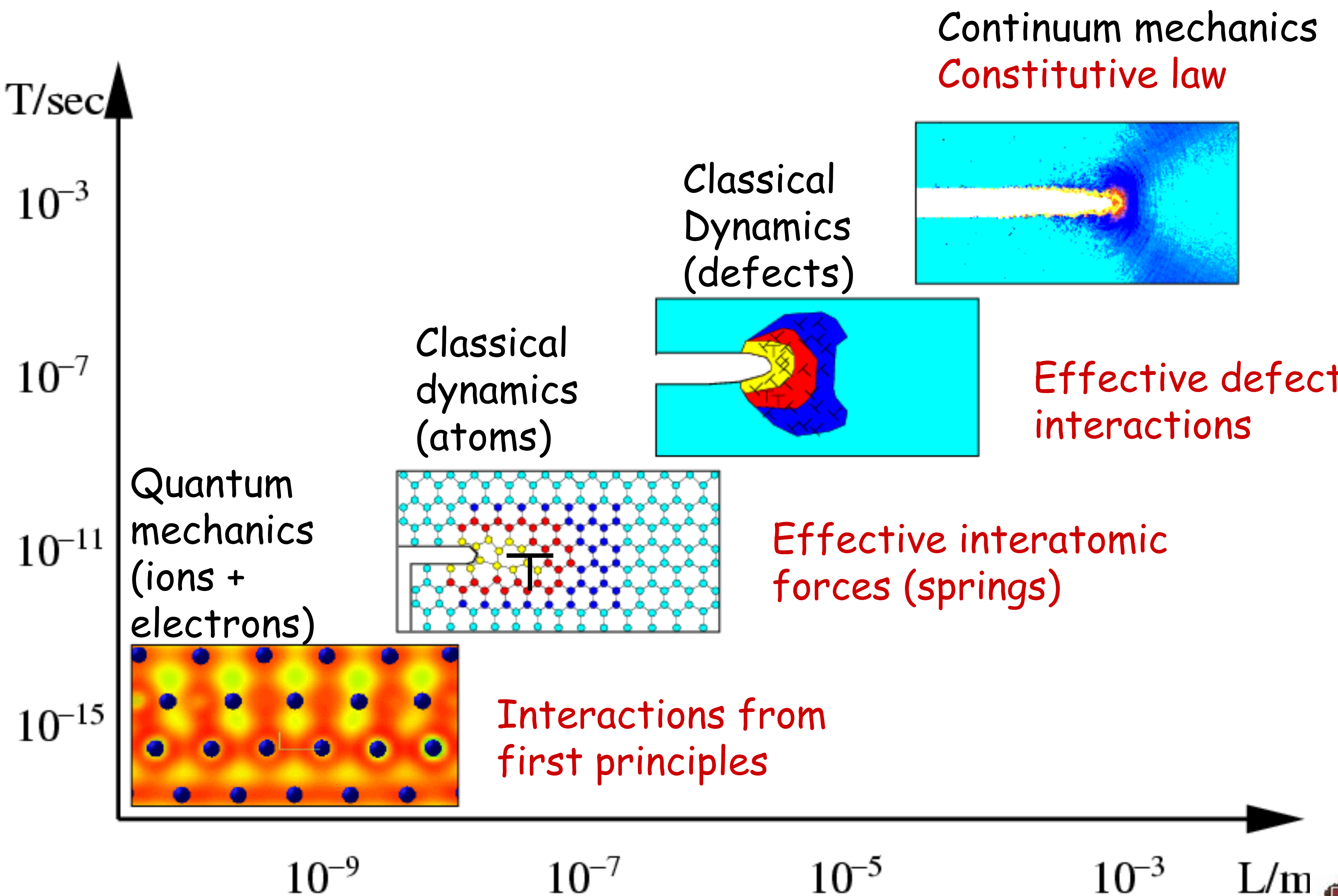
Deaths in USA: out of ~2.5 M per year total,

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

UNPREDICTABLE

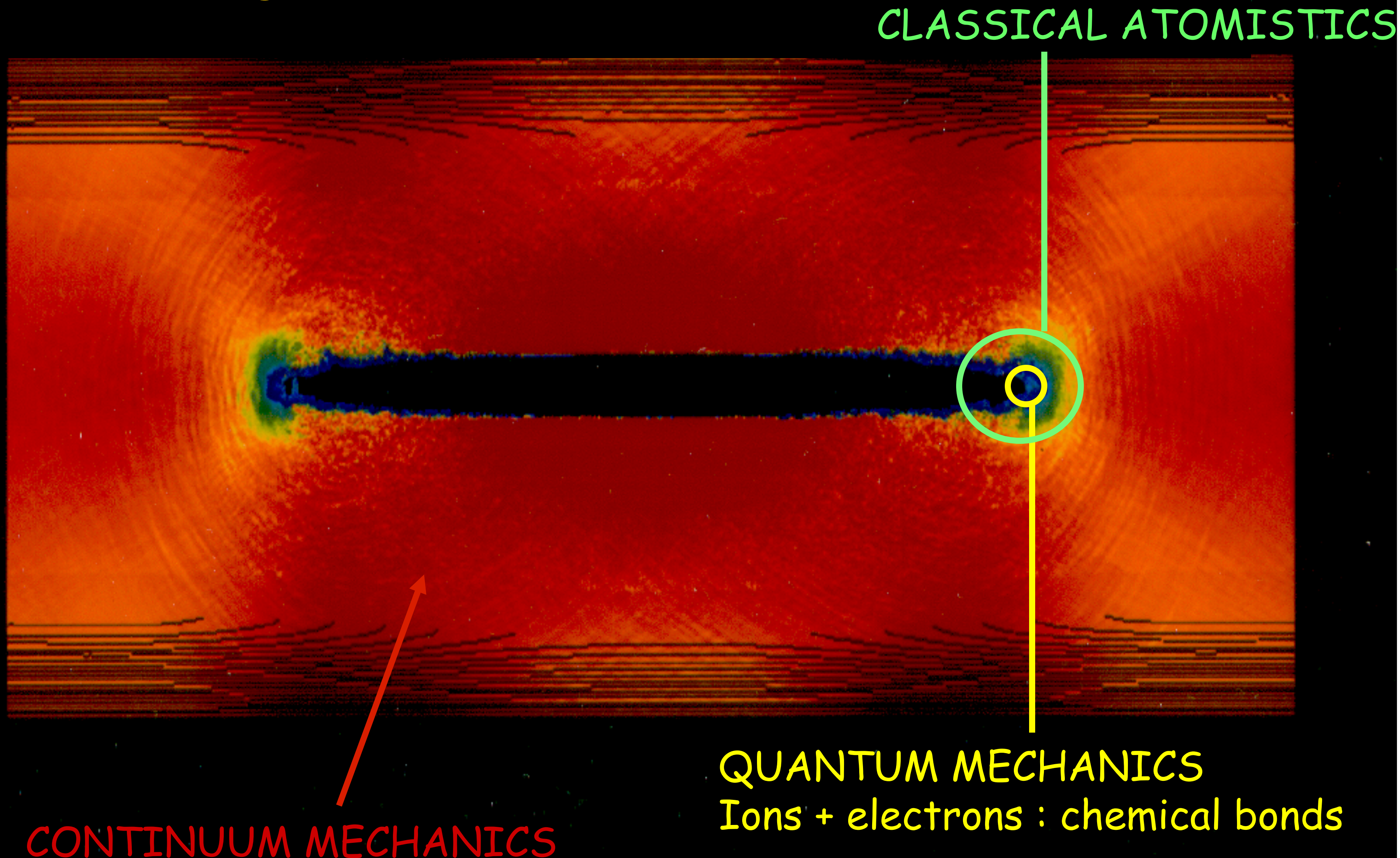
- 25% cancer (all types)

Multiple length scales: crack propagation



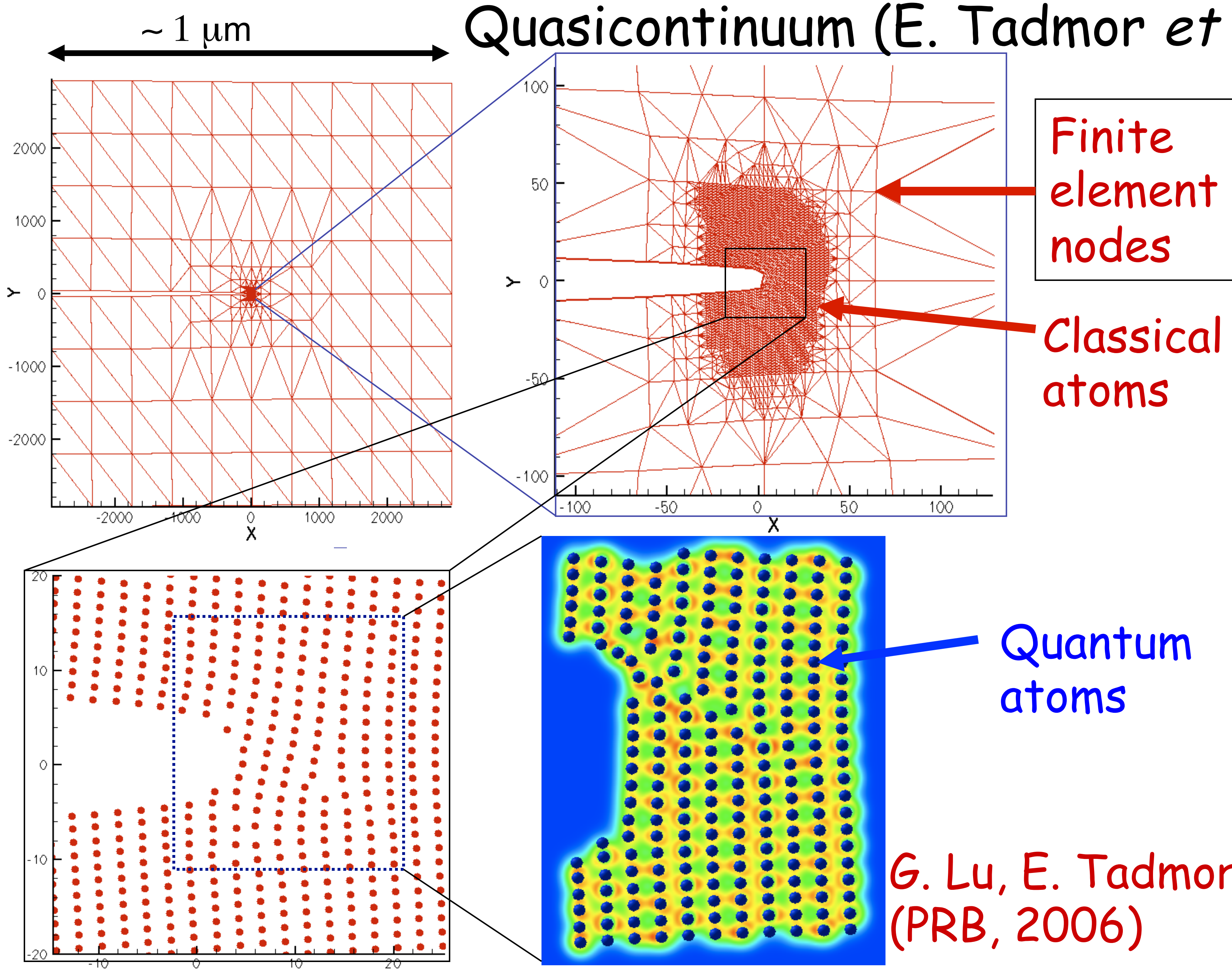
Brittle fracture of silicon

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



Easy case to model because of covalent bonds

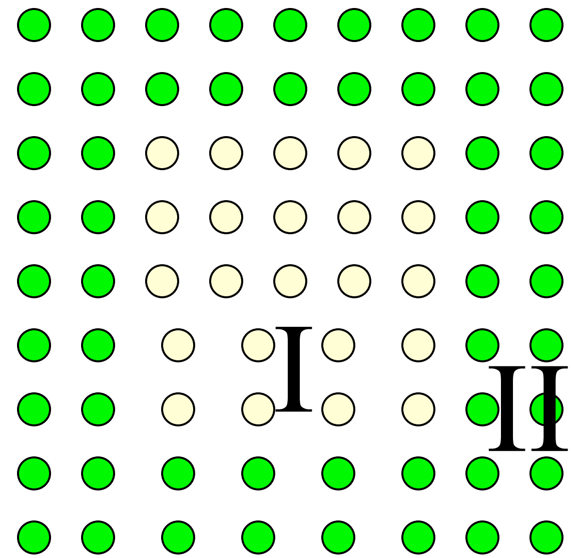
Quasicontinuum (E. Tadmor *et al.*)



G. Lu, E. Tadmor, EK (PRB, 2006)

Coupling Formalism

Wesolowski and Warshel *J.Phys.Chem.* (1993)



$$E_{tot}\left[\mathrm{I}+\mathrm{II}\right]=E\left[\mathrm{I}\right]+E\left[\mathrm{II}\right]+E^{\mathrm{int}}\left[\mathrm{I},\mathrm{II}\right]$$

DFT *EAM*

$$E^{\mathrm{int}}\left[\mathrm{I},\mathrm{II}\right]\equiv E\left[\mathrm{I}+\mathrm{II}\right]-E\left[\mathrm{I}\right]-E\left[\mathrm{II}\right]\approx$$

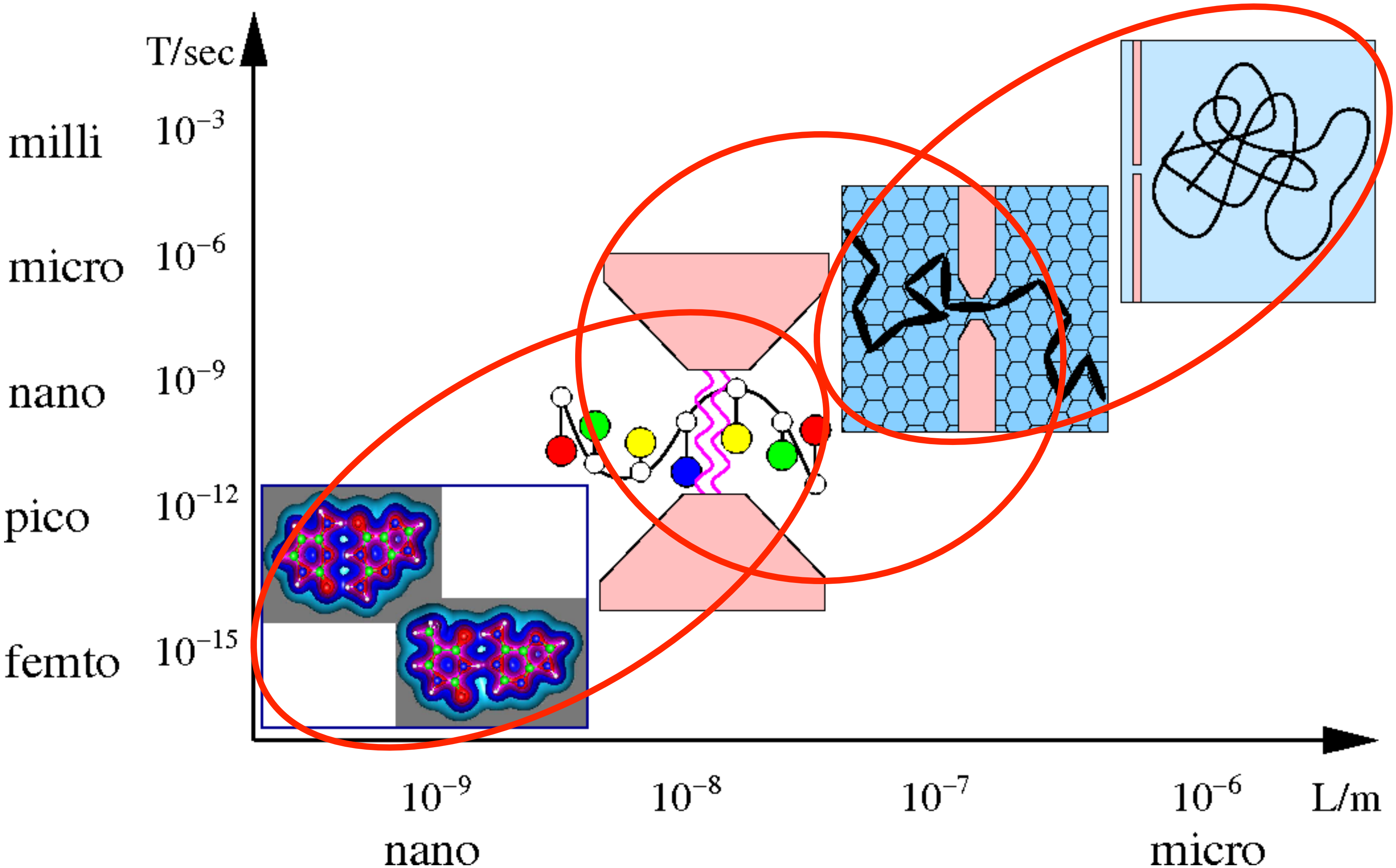
$$E^{EAM}\left[\mathrm{I}+\mathrm{II}\right]-E^{EAM}\left[\mathrm{I}\right]-E^{EAM}\left[\mathrm{II}\right]\Rightarrow$$

$$E_{tot}[\mathrm{I}+\mathrm{II}]=E^{DFT}[\mathrm{I}]+\left(E^{EAM}[\mathrm{I}+\mathrm{II}]-E^{EAM}[\mathrm{I}]\right)$$

For dynamics: only terms on the boundary due to coupling

- forces inside I : purely DFT
- forces inside II : purely EAM
- forces on boundary: EAM+DFT
  - (can improve accuracy by force matching schemes)

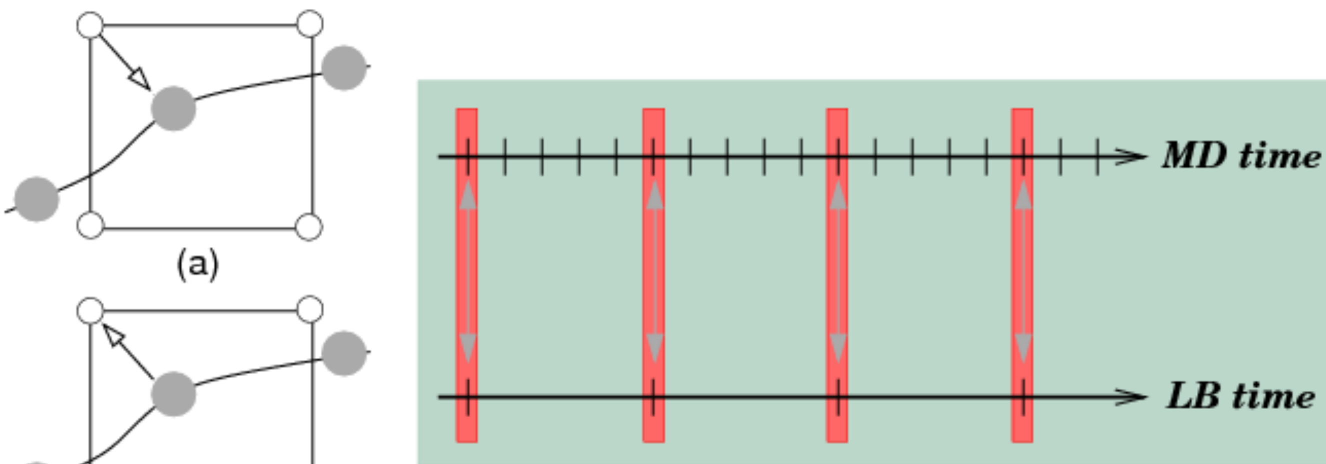
Multiple length/time scales: DNA translocation and electronic detection



<u>Two-scale approach to DNA translocation</u>

– ***Molecular Dynamics*** for DNA:
course-grained molecules (~30 bp/bead)

– ***Lattice Boltzmann Equation*** for the solvent:
- advantages in describing arbitrary shapes
- fluid dynamics in particle language

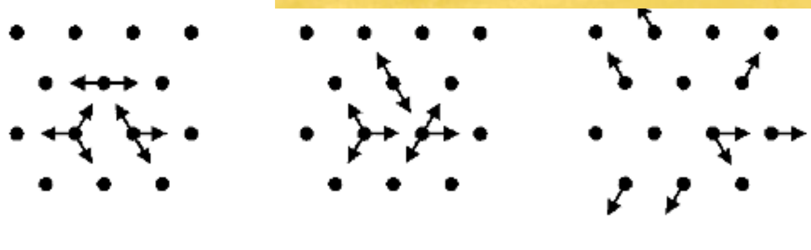


(b) (c)

spatial temporal

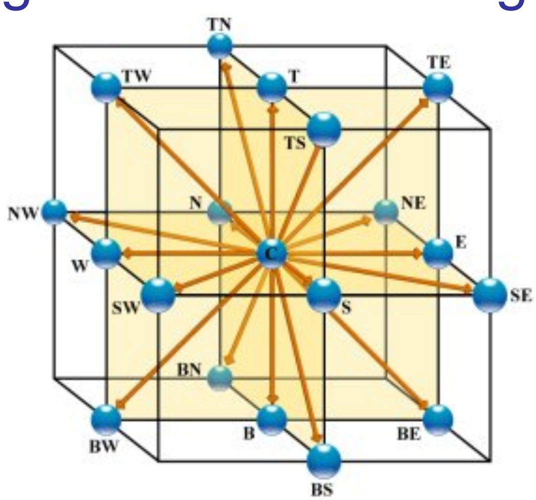
Fluid dynamics by cellular automata : Lattice Boltzmann Equation (LBE)

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



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

Bhatnagar-Gross-Krook algorithm



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

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

Molecular (Langevin) Dynamics (MD)

DNA with N beads at positions r_p with velocities υ_p :

$$m\frac{d\vec{\upsilon}_i}{dt} = \vec{F}_i^c + \vec{F}_i^f + \vec{F}_i^r + \lambda_i \partial_{\vec{r}_i}\sigma$$

bead-bead interactions

Solute-solvent interactions

random force

constraint force

$$\sigma = |\vec{r}_{i+1} - \vec{r}_i|^2 - r_0^2 = 0$$

implemented by SHAKE algorithm

Coupling LB to MD: $$\vec{F}_i^f = -m\gamma(\vec{u}_i - \vec{\upsilon}_i)$$

υ : bead velocity

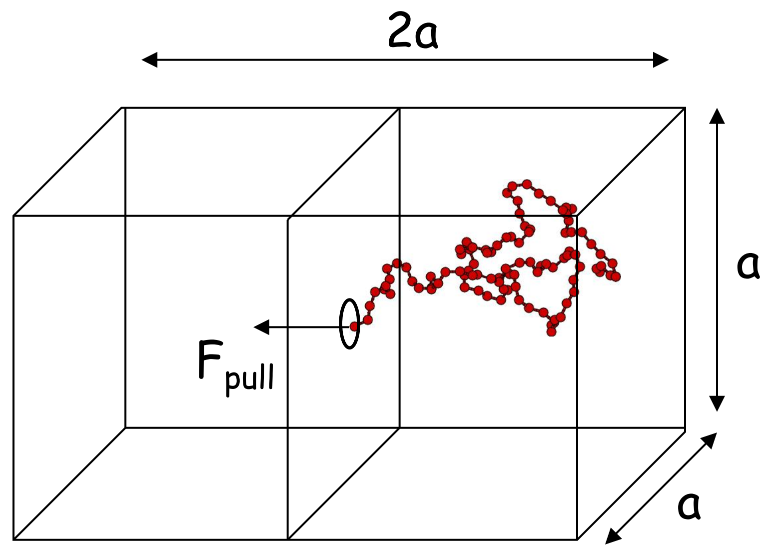
u : fluid velocity

Coupling MD to LB: $$G_p(\vec{r},t) = w_p \beta \sum_{i \in D(\vec{r})} [\vec{F}_i^f + \vec{F}_i^r] \cdot \vec{c}_i$$

M. Fyta, S. Melchionna, E. Kaxiras, S. Succi, *Multiscale Model. Sim.* (2006)

Details of simulation

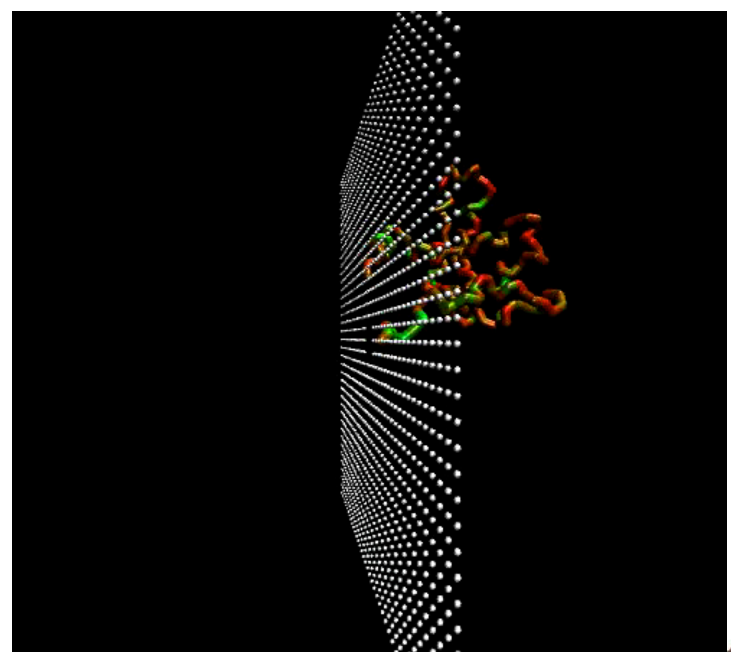
- 3D box of (2a x a x a) size
- hole size = 6 nm
- lattice spacing Δx = 3 nm



- F_{pull} =0.02, kT =10^{-4}
- Fast translocation regime :

[translocation time << DNA relaxation time]

$$\frac{F_{pull}R}{kT} >> 50$$

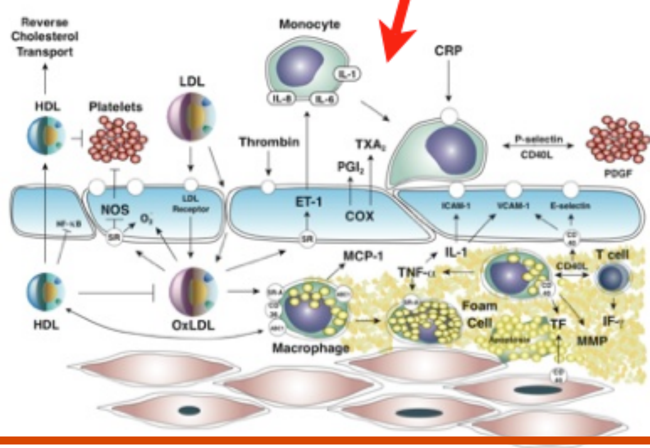


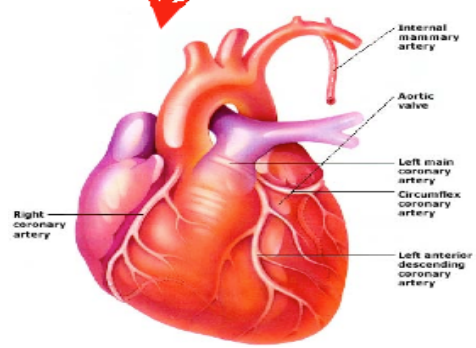
Grand Challenge: Multiscale Hemodynamics

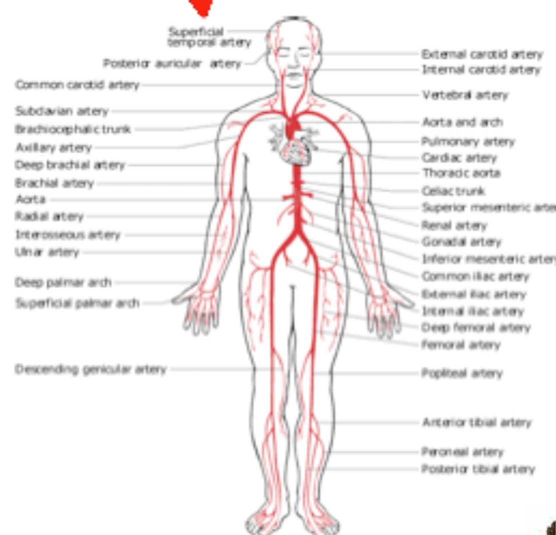
Arterial tree
10^{1} – 10^{-2} m

Organs/arteries
10^{-2} – 10^{-4} m

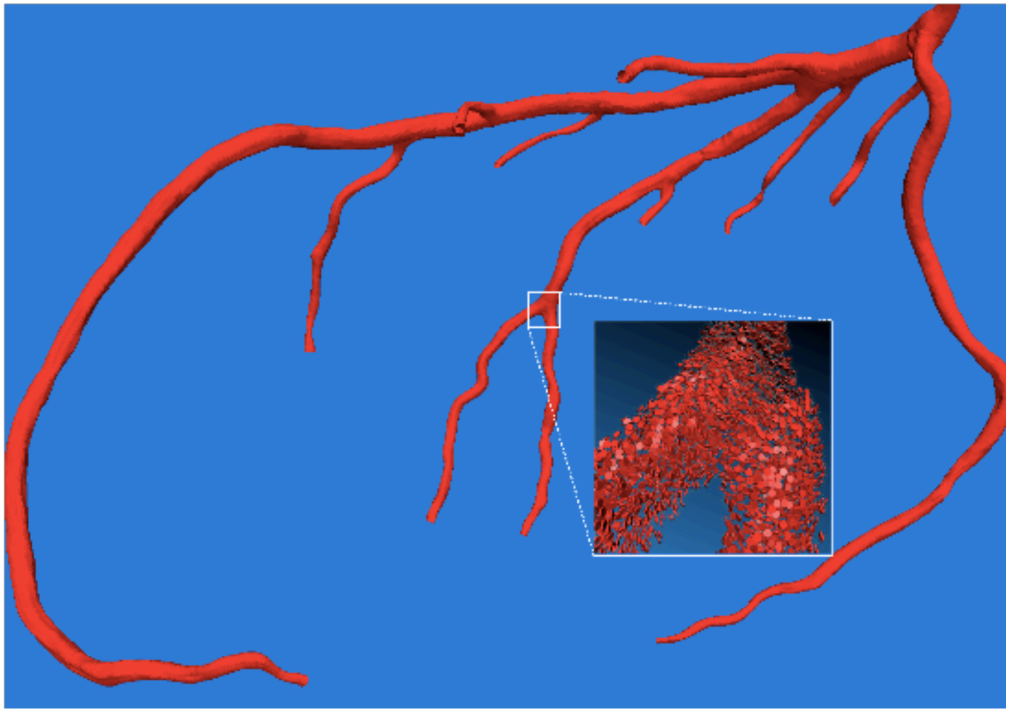
Cellular/molecular
10^{-5} – 10^{-9} m





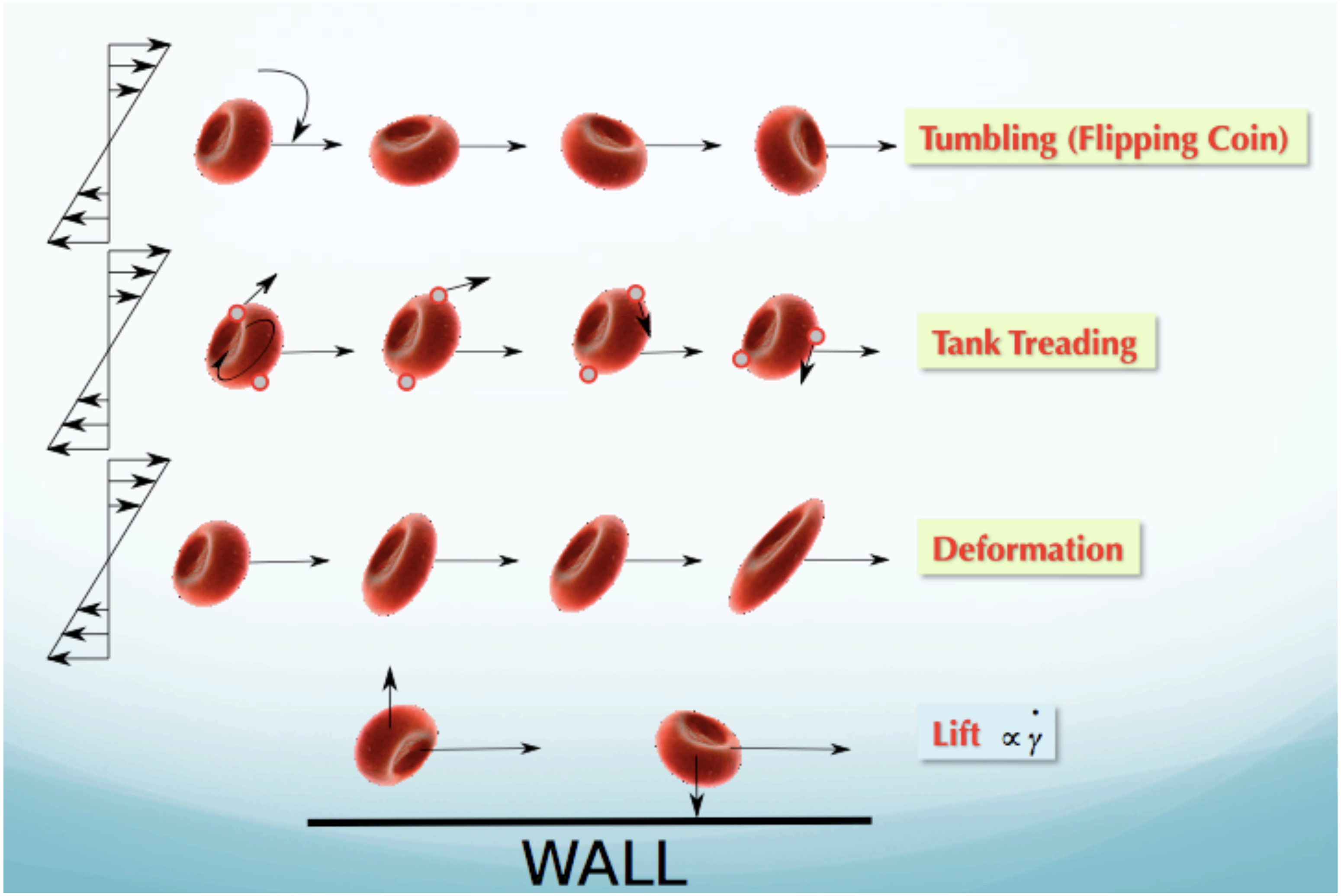


Two-scale Hemodynamics



Physics: dynamics of deformable objects (RBC's) within fluid motion, in complex vessel geometry (arterial branch)

Red Blood Cell in Motion

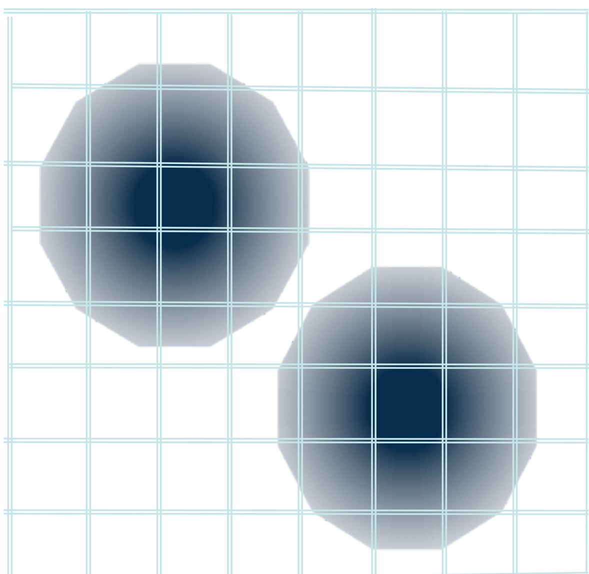


Definition of particles (cells, proteins, …)

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

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

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



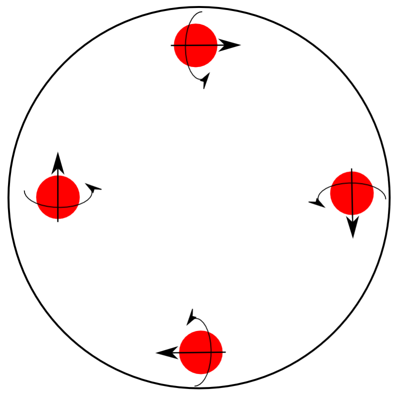
$$\varphi(x,R) = -\gamma\big(V - u(x)\big)\tilde{\delta}_\xi(x-R)$$

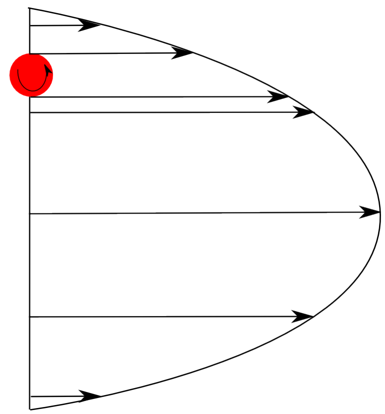
$$F^H = \sum_x \varphi = -\gamma\big(V - \tilde{u}\big)$$

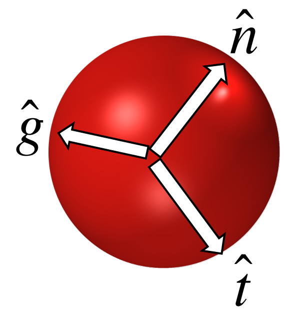
$$\tilde{u} = u * \tilde{\delta}_\xi$$

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

Rotating particles







$$Q=\begin{pmatrix} n_x & t_x & g_x \\ n_y & t_y & g_y \\ n_z & t_z & g_z \end{pmatrix}$$

$$\tau(x,R) = -\gamma_R\left(\Omega-\omega(x)\right)\tilde{\delta}_\xi(x-R)$$

$$T^H = \sum_x \tau = -\gamma_R\left(\Omega-\tilde{\omega}\right)$$

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

$$\Delta f_p = -\frac{w_p}{c^2} c_p \cdot \sum_R \left(\varphi - \partial\tilde{\delta}_\xi \times \tau\right)$$

Particle dynamics:

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

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

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

Brenner et al '72

Γ Grand Resistance matrix

Δ Shear Resistance matrix

E Strain tensor

u Fluid velocity

$\omega = \frac{1}{2} \partial \times u$ Fluid vorticity

Γ and Δ depend on the whole configuration

Pair-wise superposition $O(N^3)$ complexity!

Brady & Bossis '89

movies

Multiscale Hemmodynamics on the JUGENE - Juelich IBM BlueGene/P

(#5 in the world - 2010 Top 10 List, largest number of cores in the world)

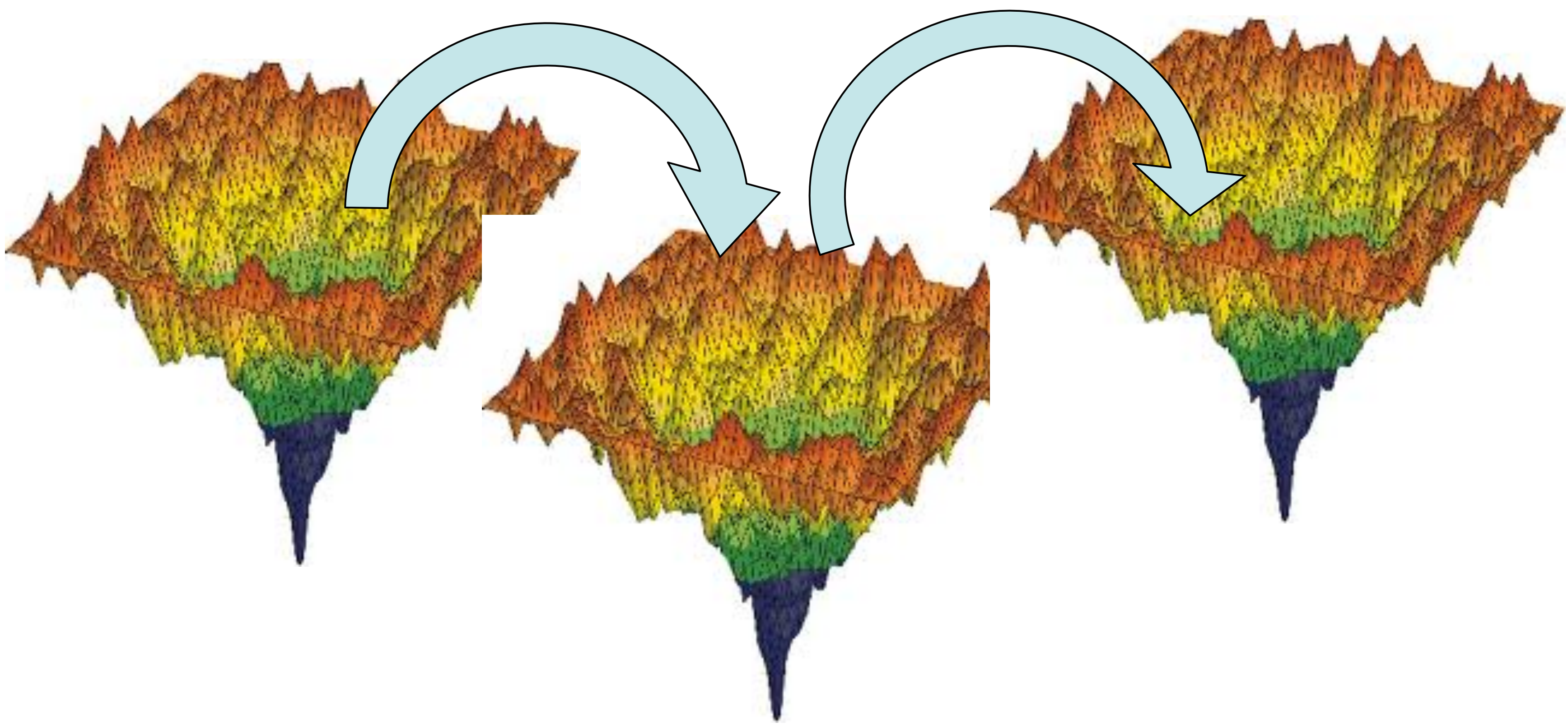
- 72 racks of BlueGene/P
- 294,912 cores
- Peak Performance: 1 PFs
- Memory: 2 Gb/core

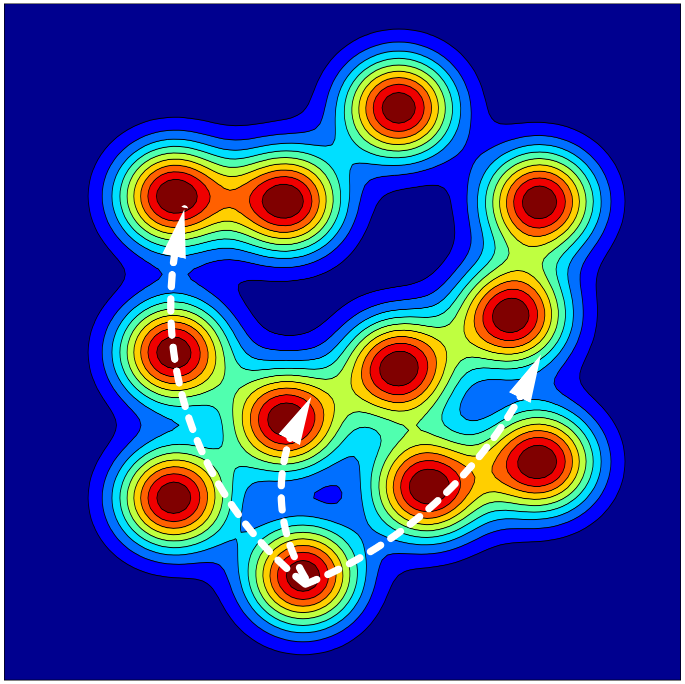
Uncertainties, instabilities, limitations:

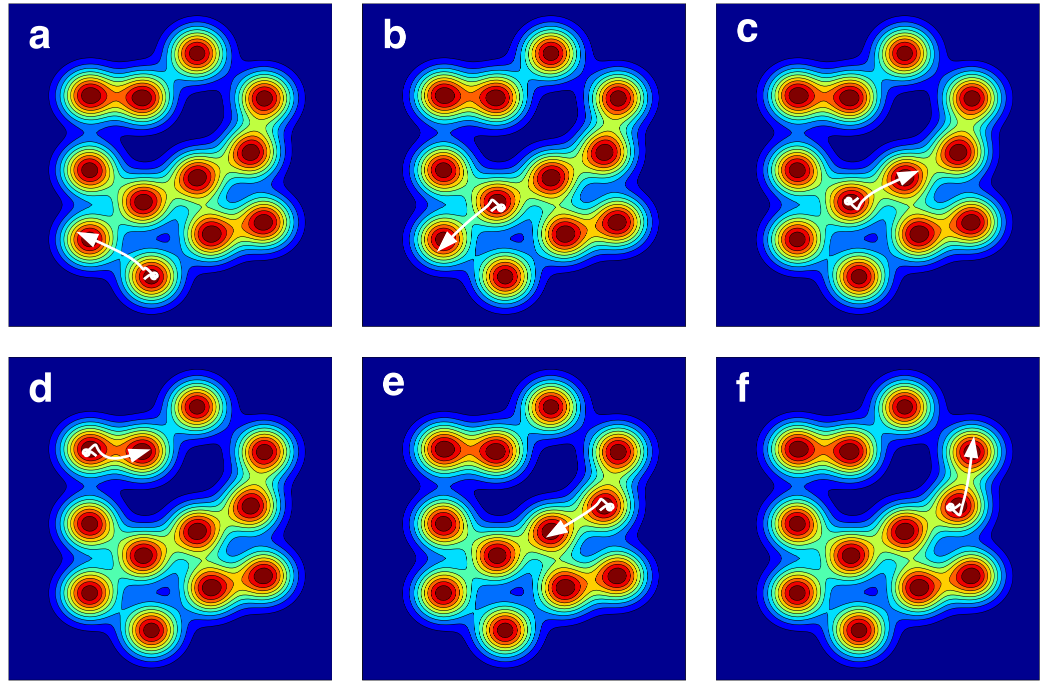
- Spatial integration:
  - QM important, but problems:
    - 90% of computational cost (~100 atoms)
    - source of code instabilities
      (simulation does not always converge)
    - not easily parallelizable
      (orthogonal wave-functions)
    - inherent limitations – "ghost forces"
      (long-range nature of wave-functions)

  - Classical regions coupling:
    - loss of information physically important
      (entropy, thermal properties)

- Time-scale problem:
  - controlled by smallest time-step
  - [e.g. QM leads to fs (10^{-15} sec)]
  - simple/general coarse-graining methods ?






a
b
c
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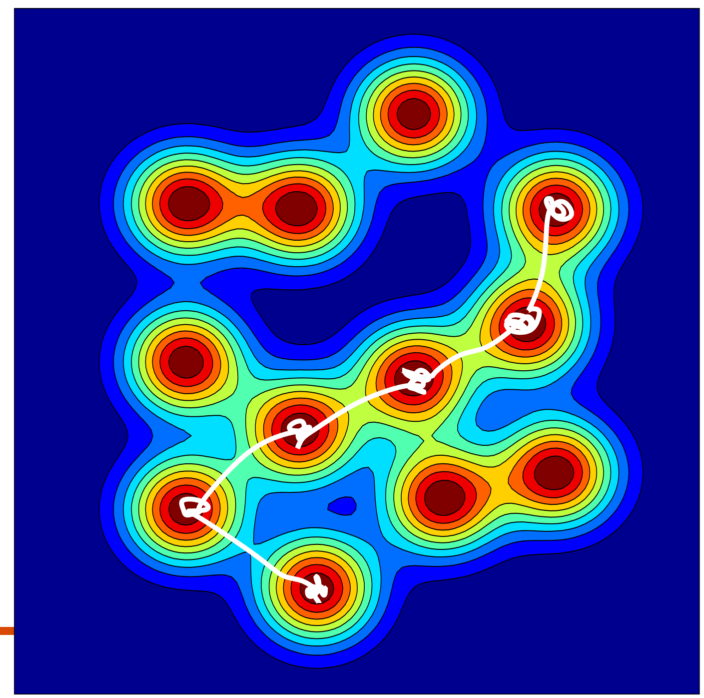

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