PASC NETWORK

Life Sciences Across Scales

Yves Barral, ETHZ - Bastien Chopard, U.of Geneve - Vassily Hatzimanikatis, EPFL - Luisa Iruela-Arispe, ISREC - Petros Koumoutsakos, ETHZ - Rolf Krause, USI - Michele Parrinello, USI – Igor Pivkin, USI - Alfio Quarteroni, EPFL - Matteo dal Peraro, EPFL - Ursula Roethlisberger, EPFL - Olaf Schenk, USI - Gisou van der Groot, EPFL - Viola Vogel, ETHZ - .....

Modeling and Technology

- **No aircraft** is flown without having been designed with complex, mechanistic simulations

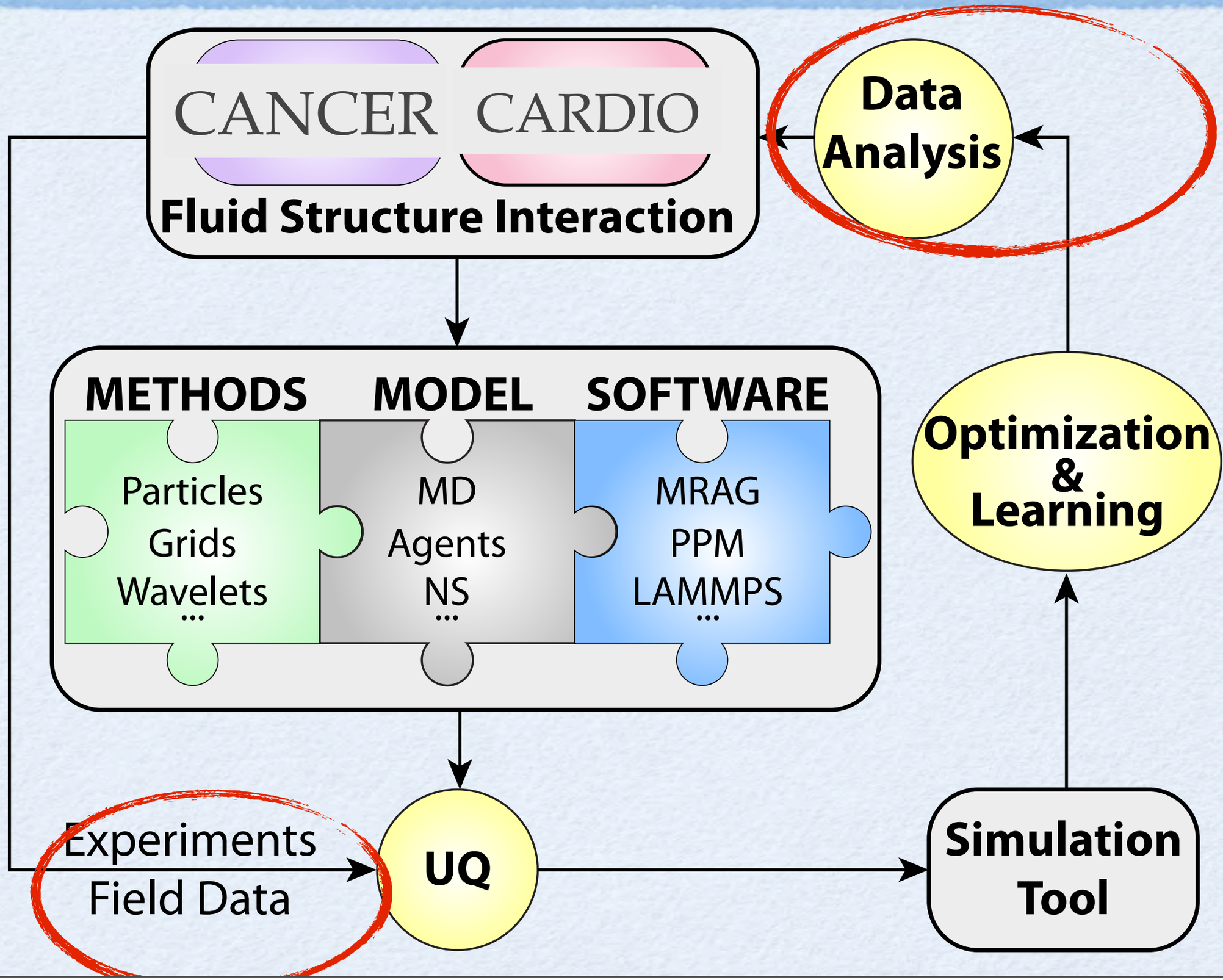
Modeling and Medicine

- Heuristics and Data
- Models ?

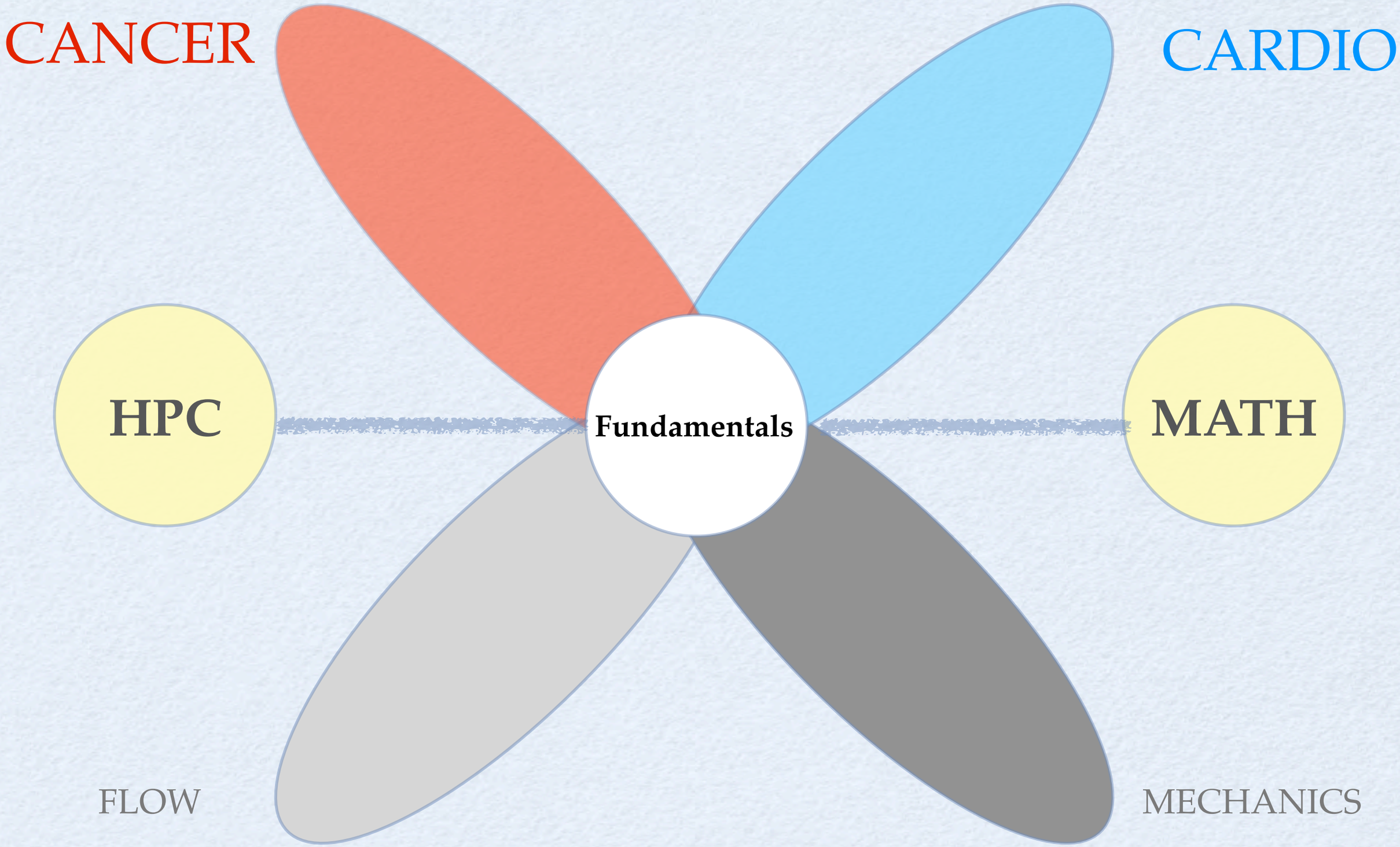
Dreamstime.com


DISEASE
CANCER
Blood
CARDIO
~6M deaths a year
~7.6M deaths a year

SIMULATIONS - DATA - OPTIMIZATION

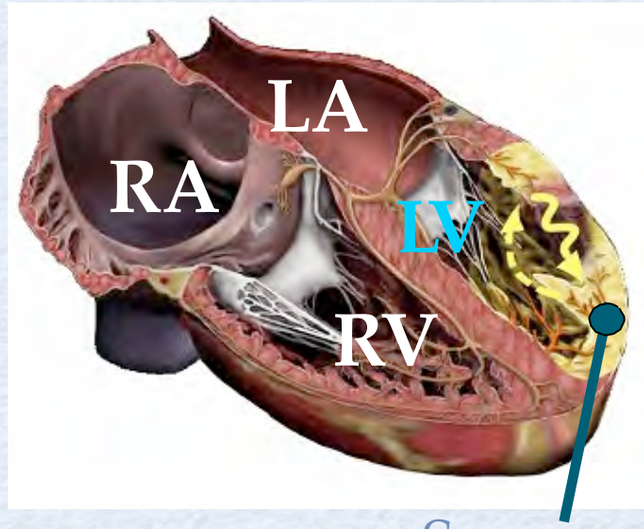


LSAS

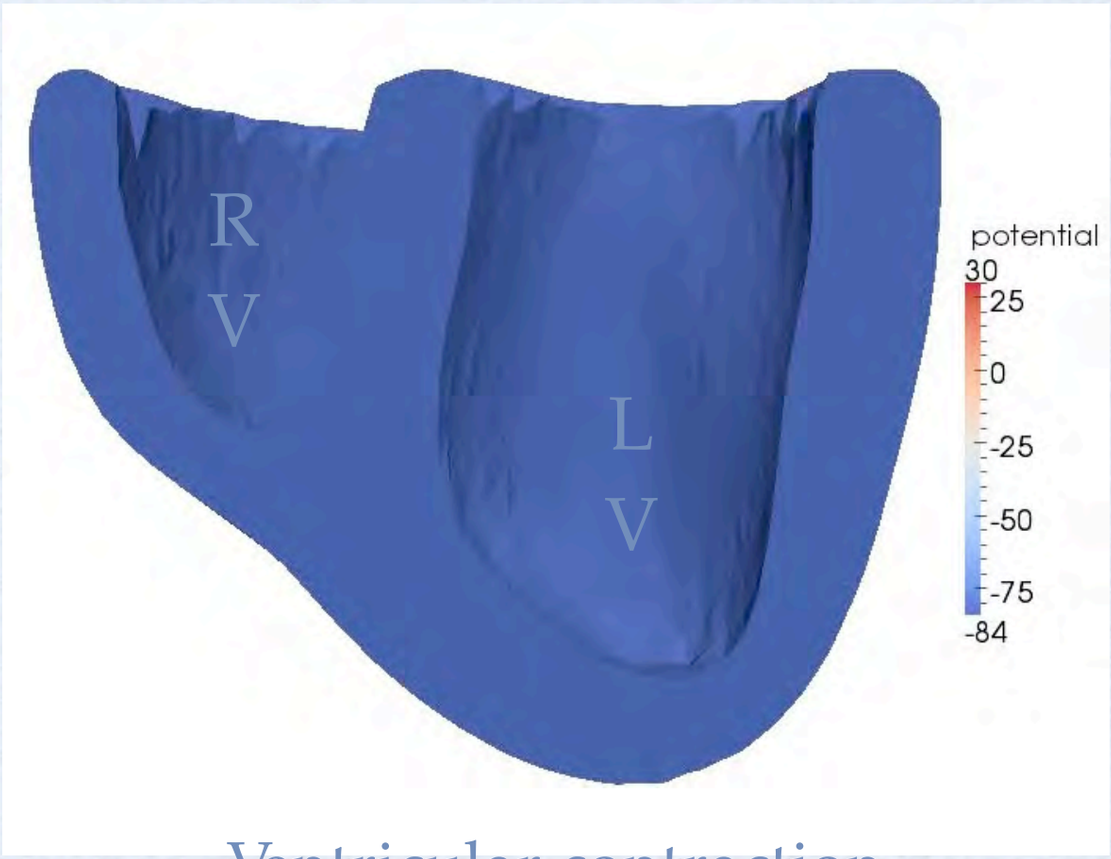


CARDIO: Physiopathological aspects

- Resynchronization
- Hypertrophies (concentric, eccentric)
- Myocardial scarring and heterogeneities (influence on the ventricular **flow** dynamics, **tissue** elastic properties and reduced **conductivity**)



Scar Tissue

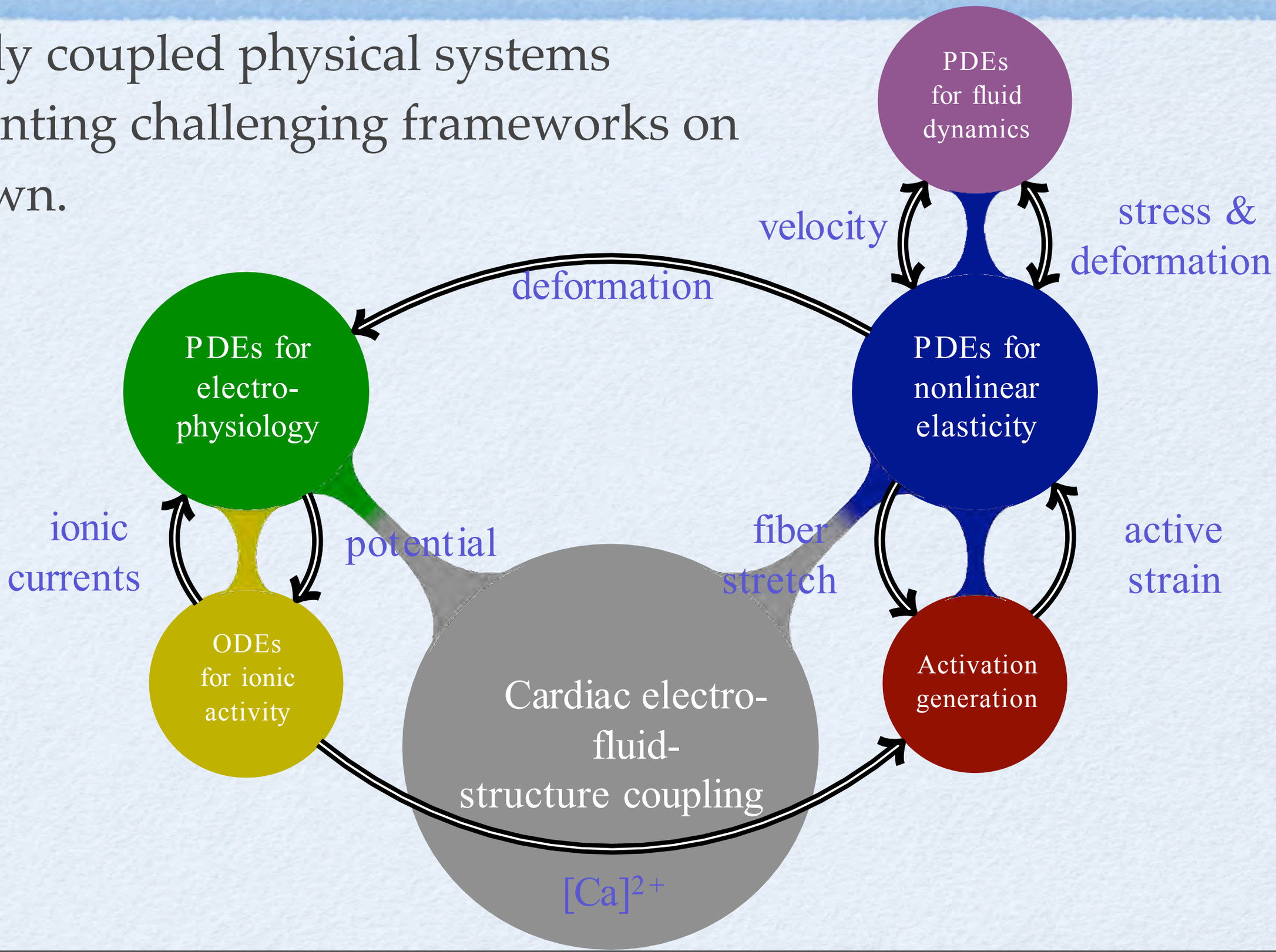


Ventricular contraction

- Altered patterns of **electrical signals** may originate arrhythmias, yielding an ineffective **mechanical** contraction and poor **fluid** ejection volume.

Multiphysics in Cardiac Modeling

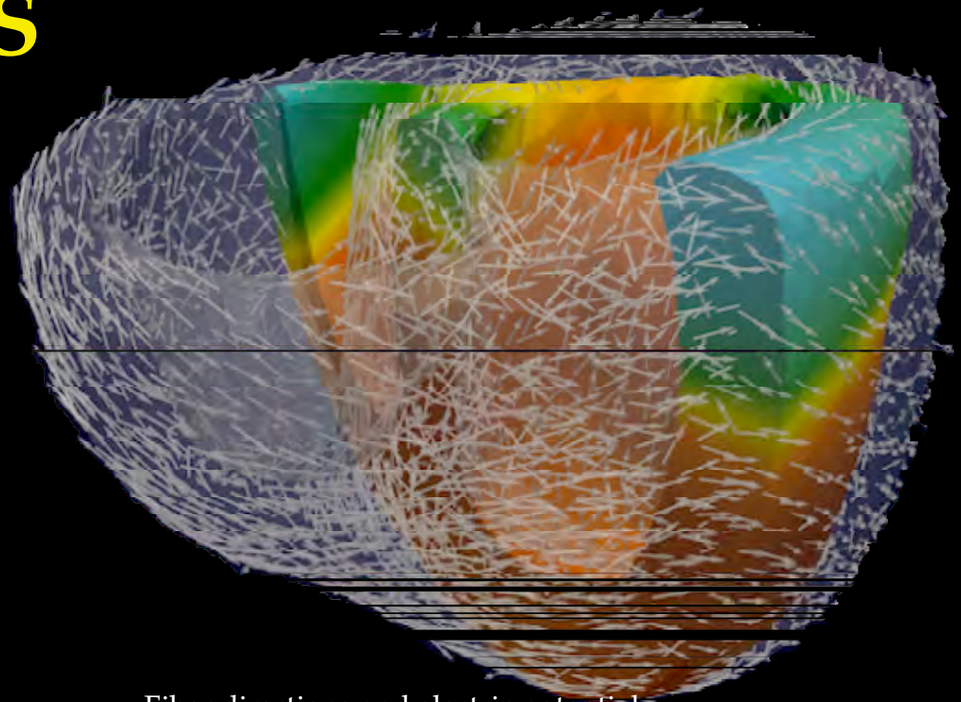
Strongly coupled physical systems representing challenging frameworks on their own.



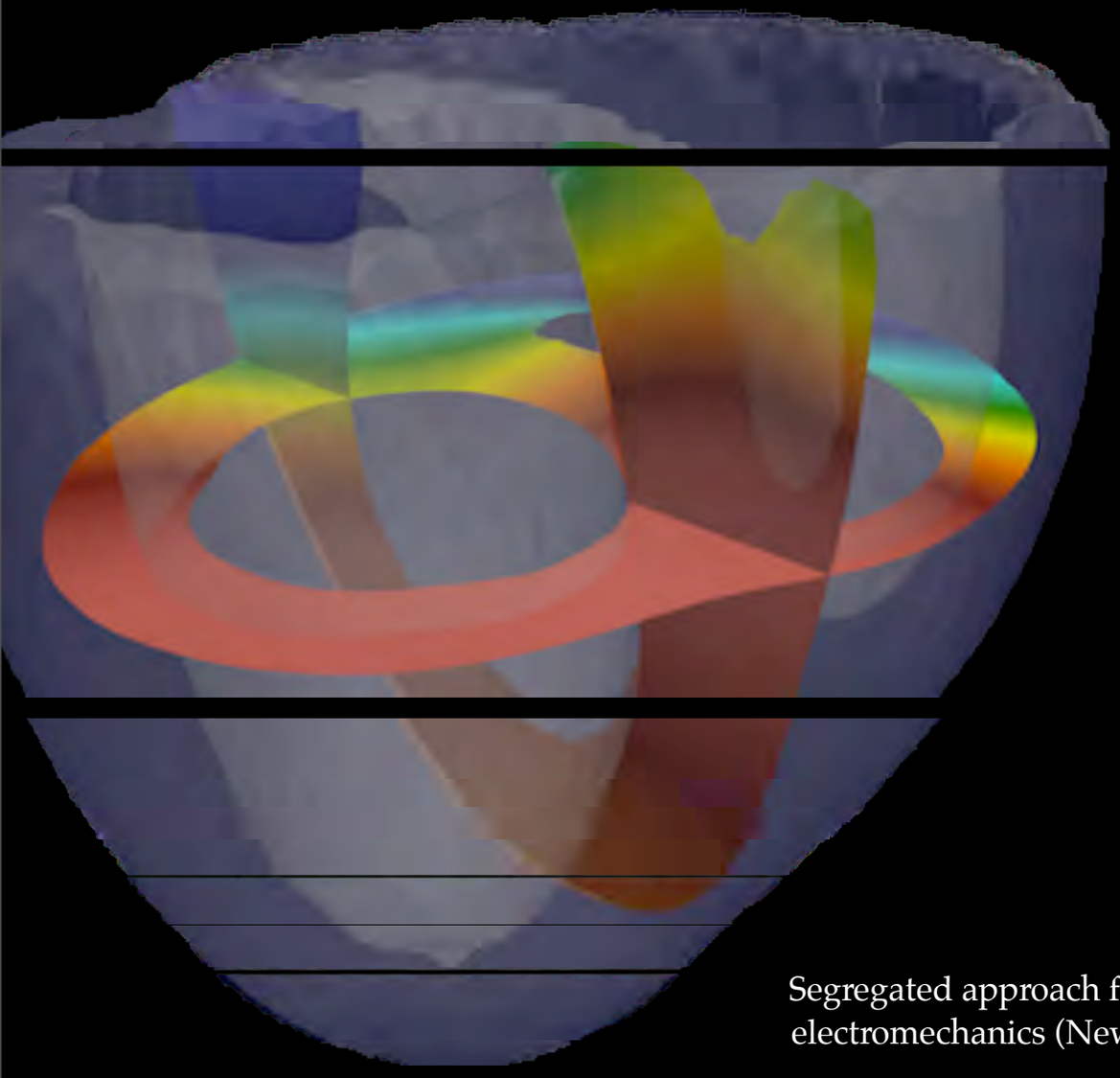
CARDIAC ELECTROMECHANICS

MODELS

- Orthotropic hyperelastic passive material
- Thermodynamically consistent anisotropic activation mechanism
- Bidomain equations for electrophysiology



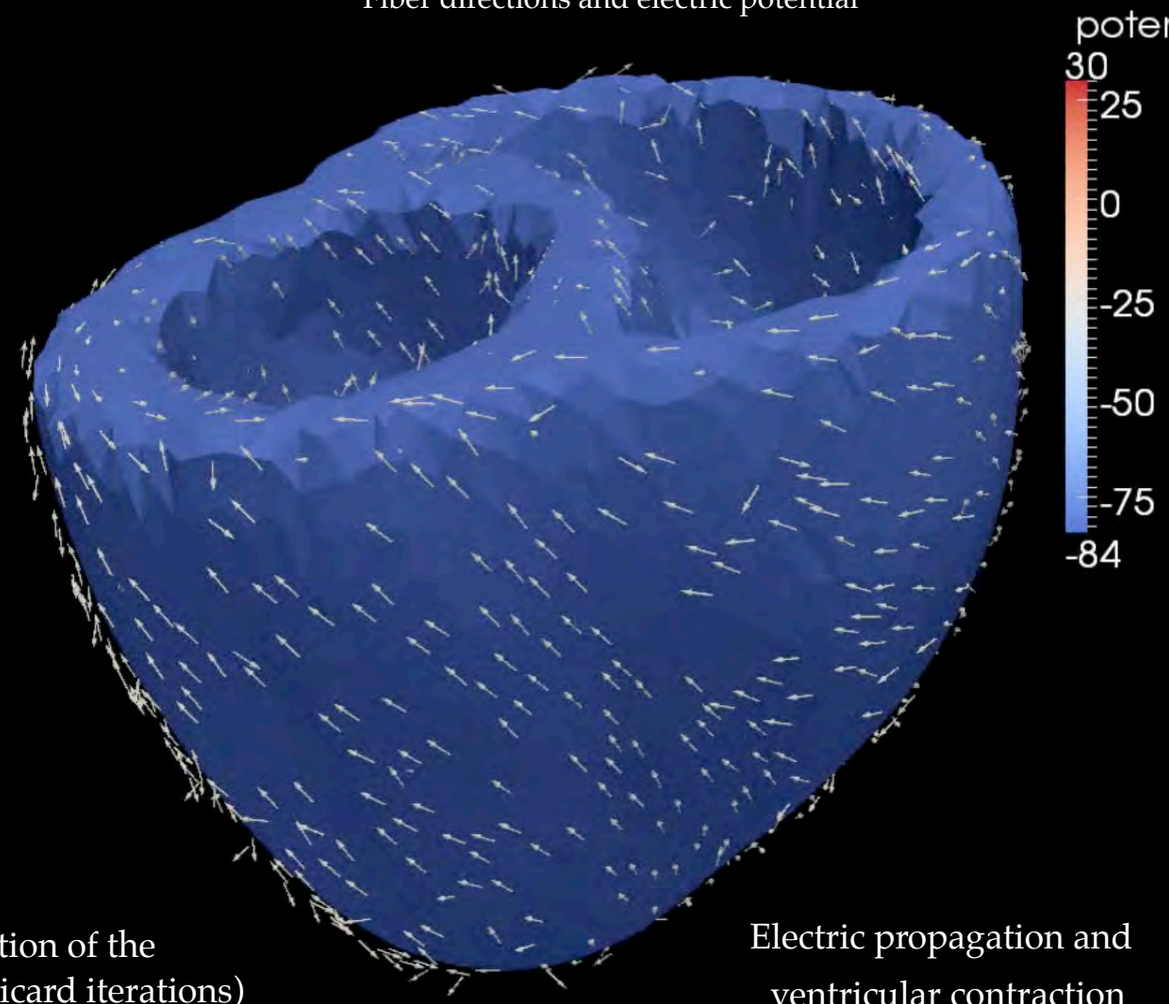
Fiber directions and electric potential



Ventricular pressure profile

Coupling:

Segregated approach for the solution of the electromechanics (Newton and Picard iterations)

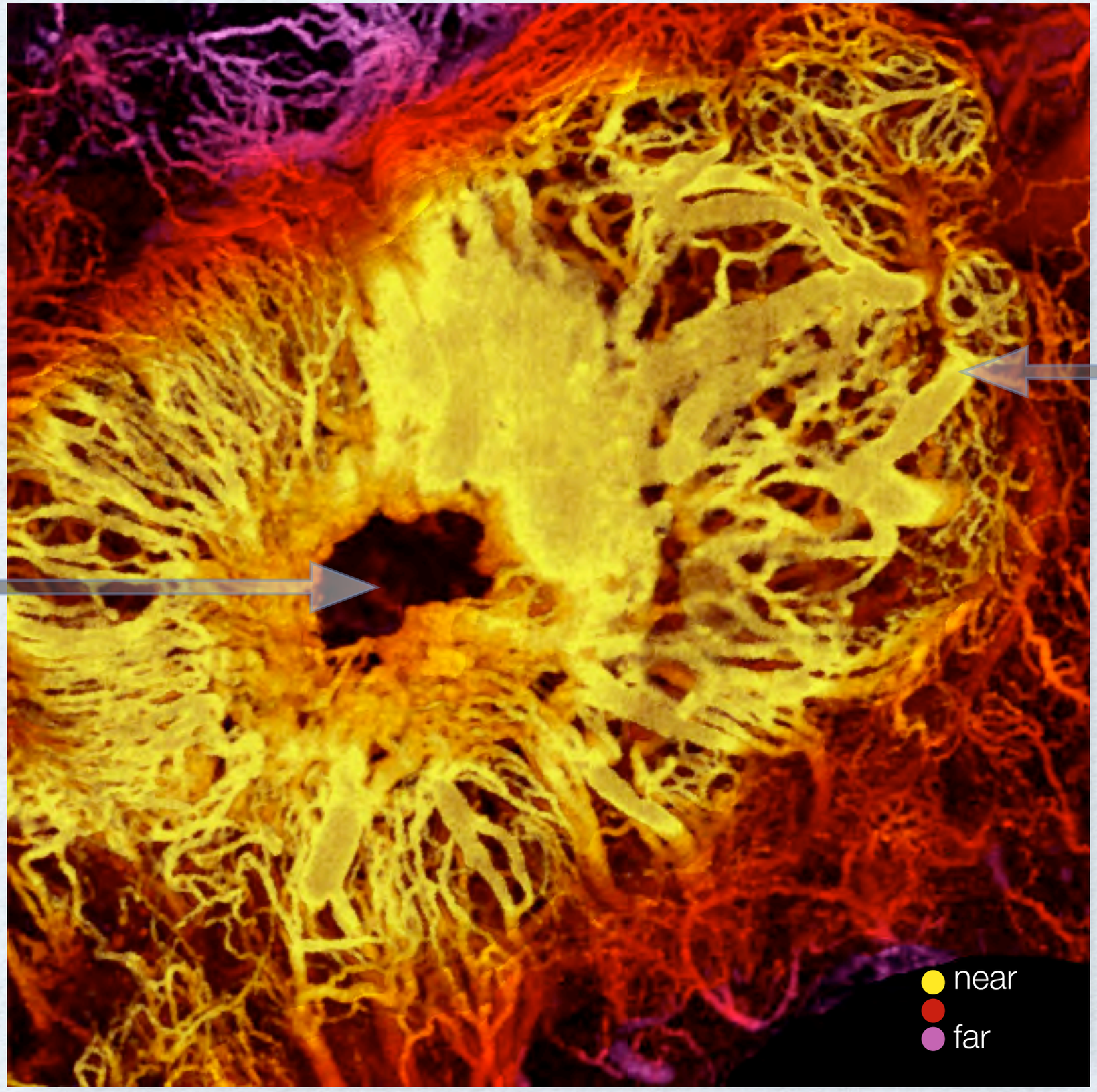


Electric propagation and ventricular contraction

ruizbaier@lifev-cmcs

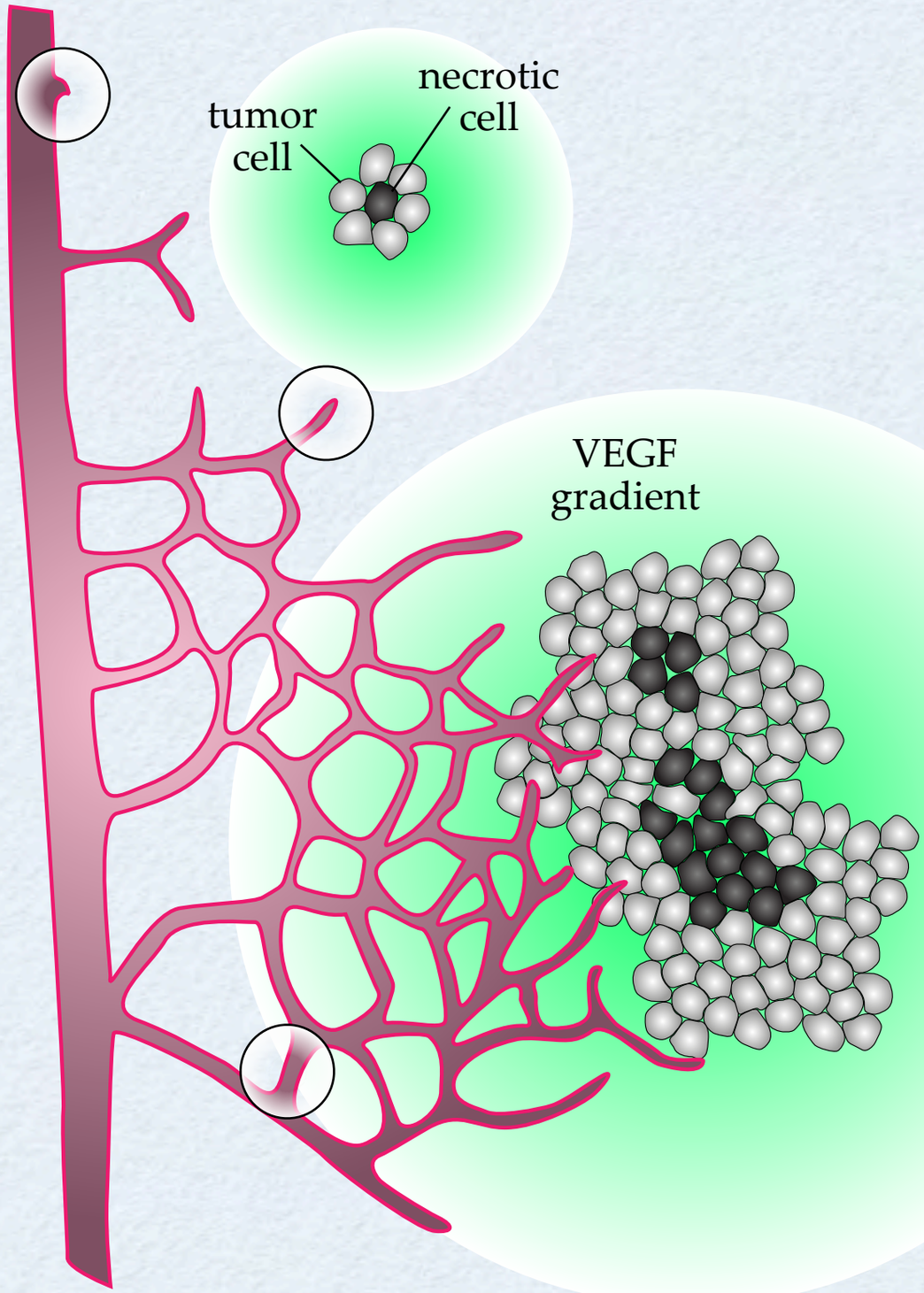
CANCER: Genetics meets Physics meets HPC

tumor location



[2] B. Vakoc et. al., Nature Medicine, 2009

angiogenesis: a multi-scale process



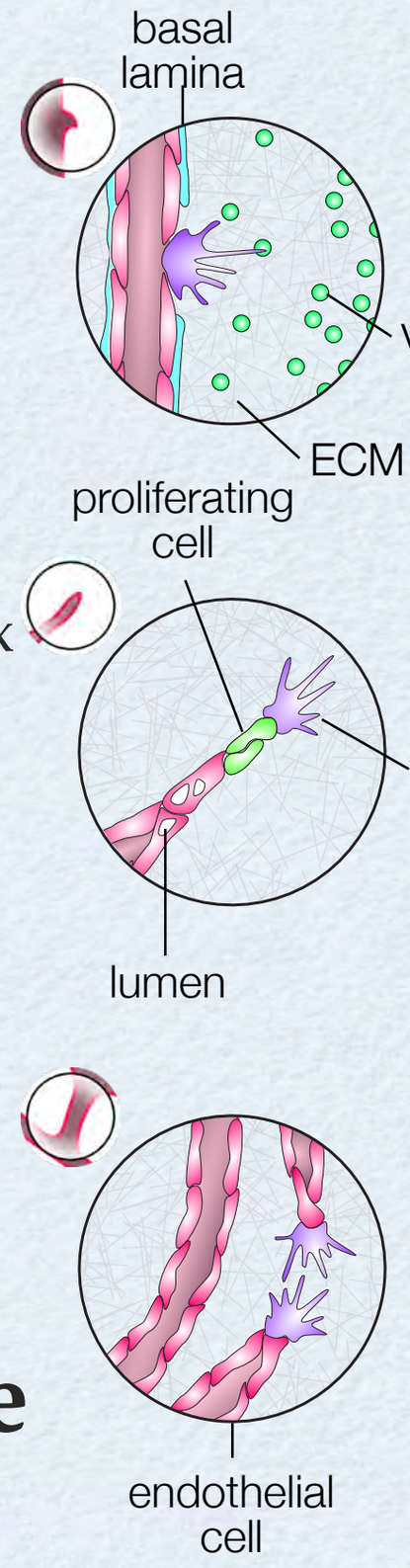
growth factors

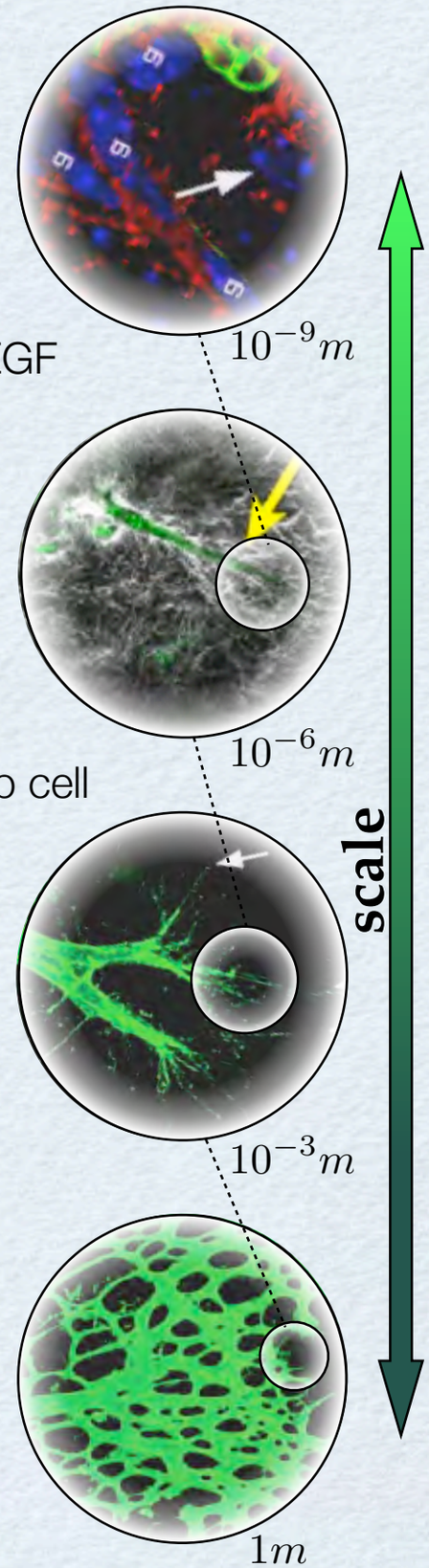
ECM

Extracellular Matrix

tip cell

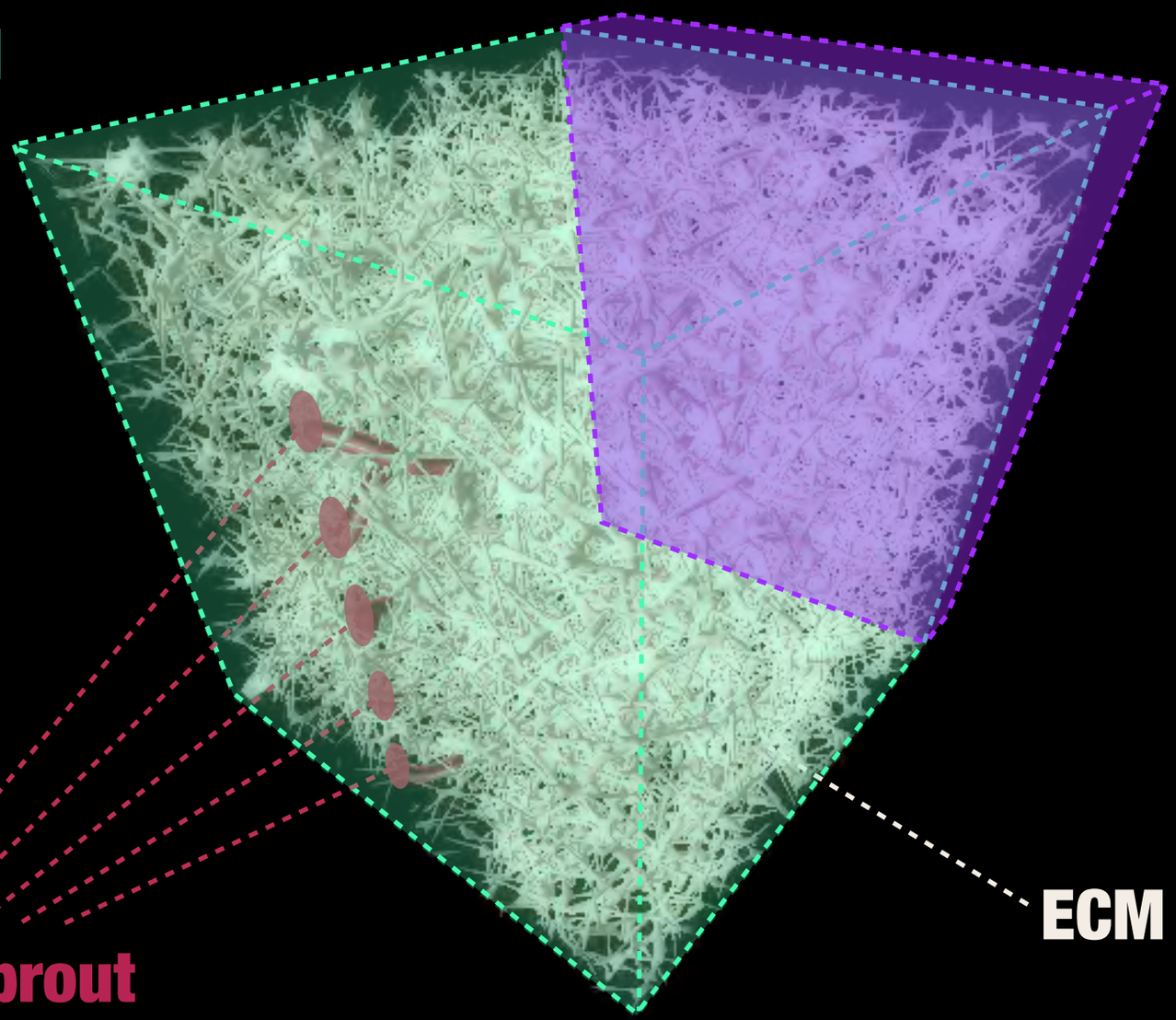
vasculature





[3] H. Gerhardt et al., J. Cell Biol., 2003

computational domain



tumor releasing VEGF (not shown)

initial sprout location

ECM fibers

SOFTWARE meets METHODS

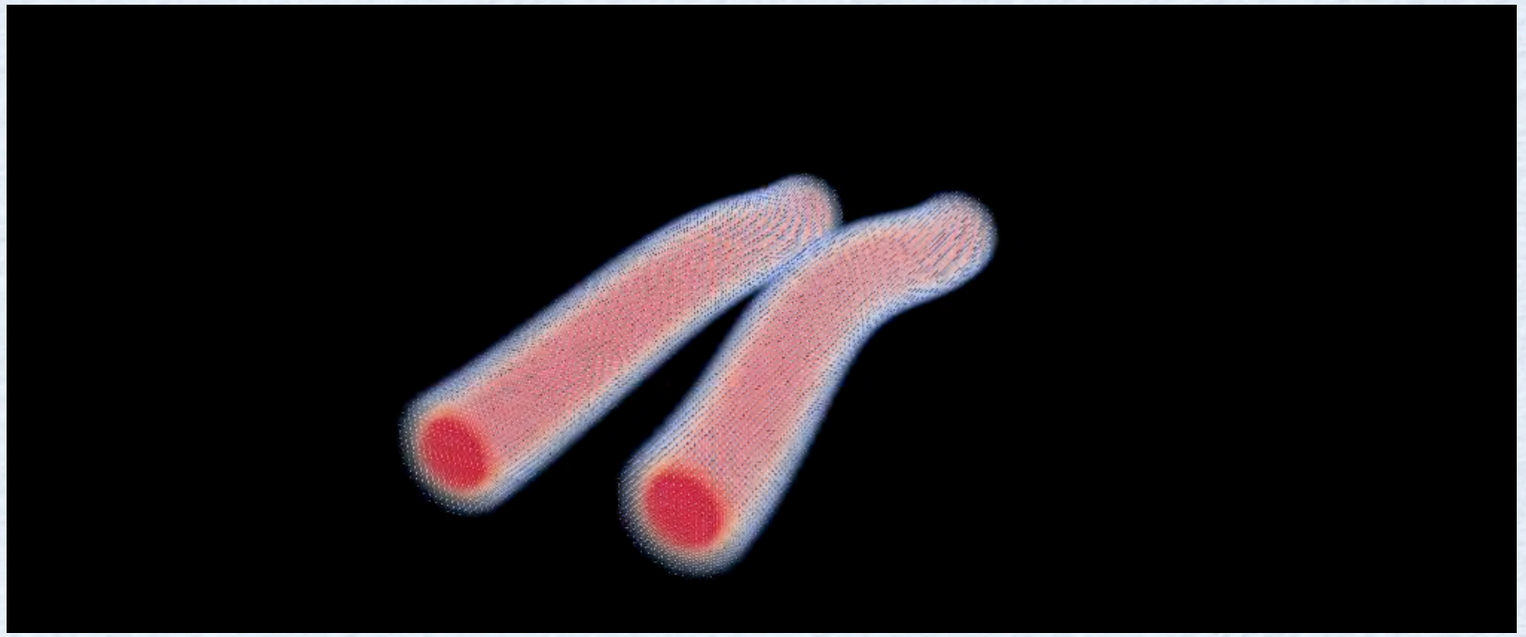
- Software tools(e.g. MAPPER http://www.mapper-project.eu) for developing multiscale, multiphysics and multicode simulations on HPC resources.

- Multi/Many core Integration Across Scales

PARTICLES : Lagrangian, Conservation and Other Laws

SPH, Vortex Methods

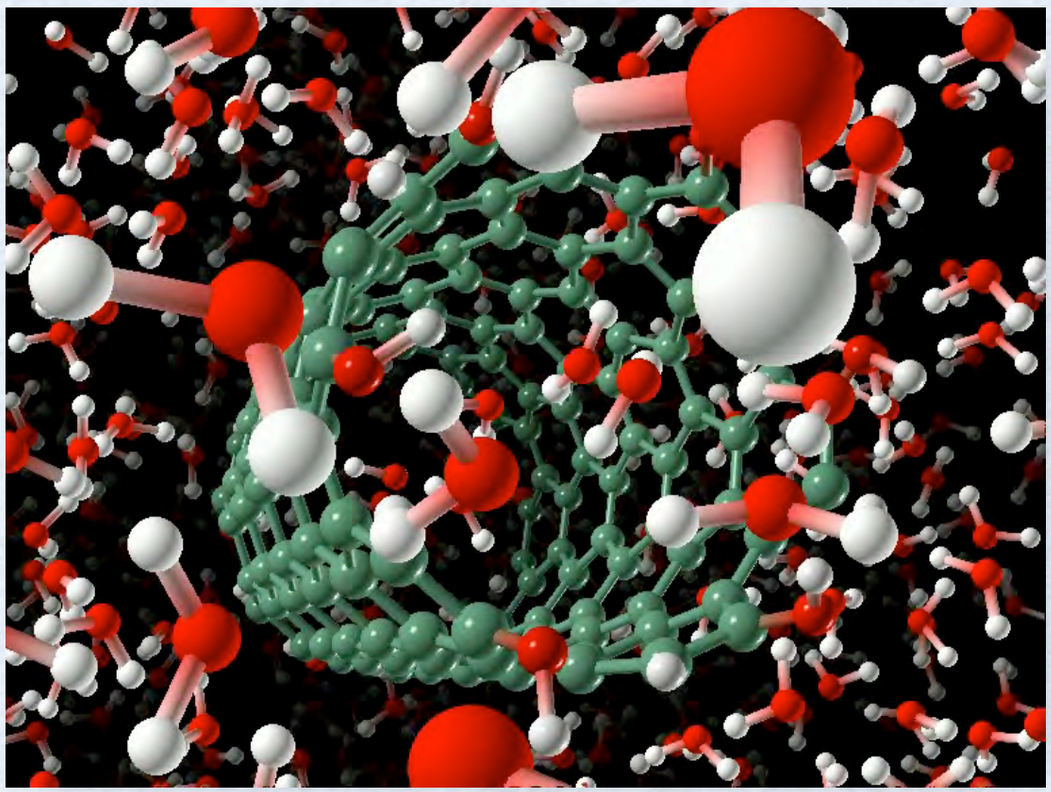
$$\rho_p \frac{D\mathbf{u_p}}{Dt} = (\nabla \cdot \sigma)_p$$



$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

$$m\frac{d\mathbf{u_p}}{dt} = F_p$$

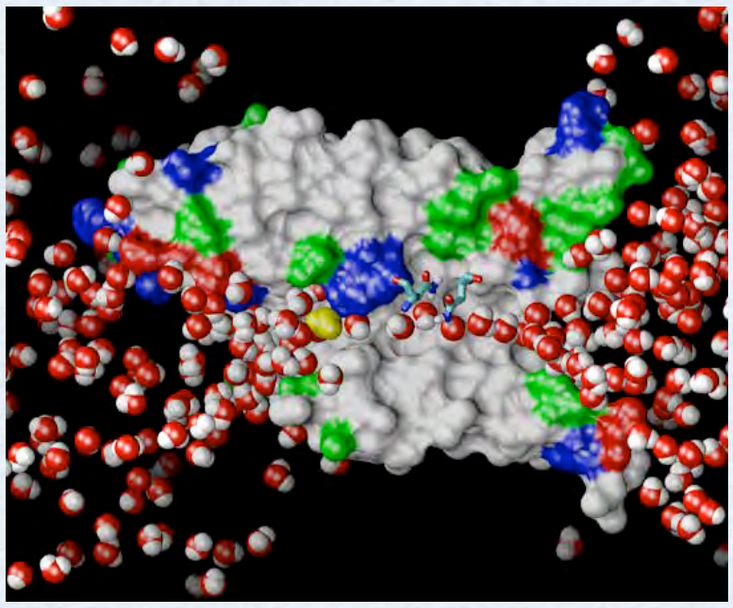
MD, DPD, CGMD



PARTICLES across scales

Molecular Dynamics

-9



Transport in aquaporins
Schulten Lab, UIUC

Vortex Methods

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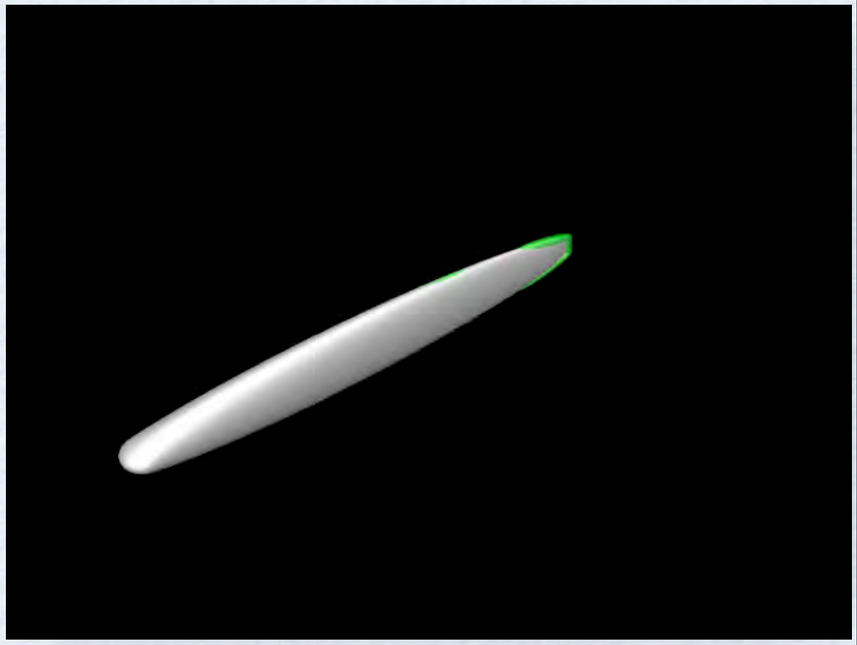
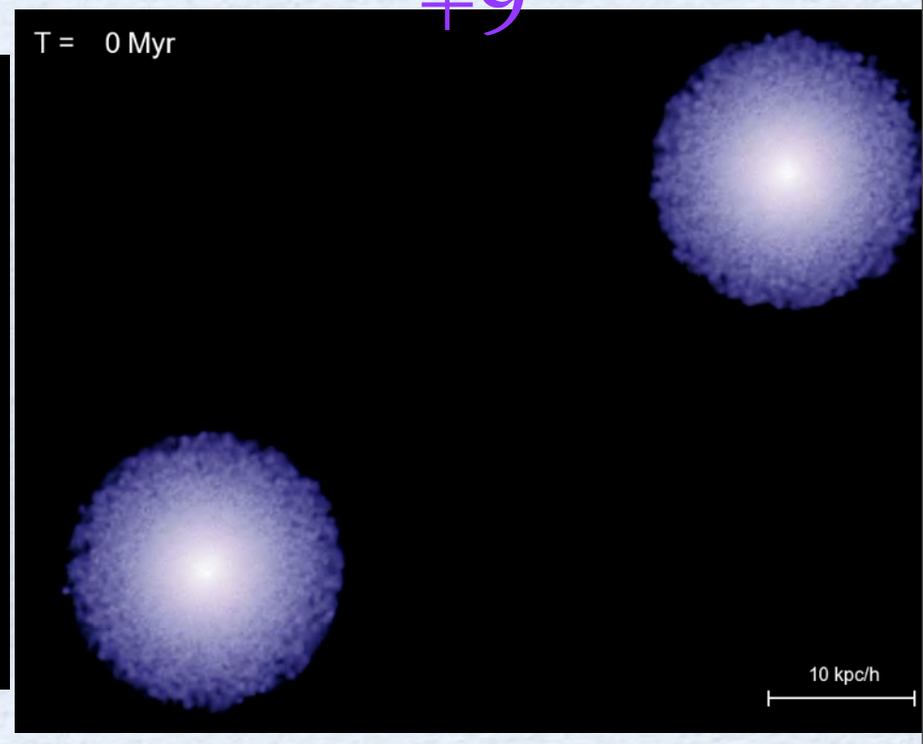


Vortex Dynamics
Koumoutsakos Lab, ETHZ

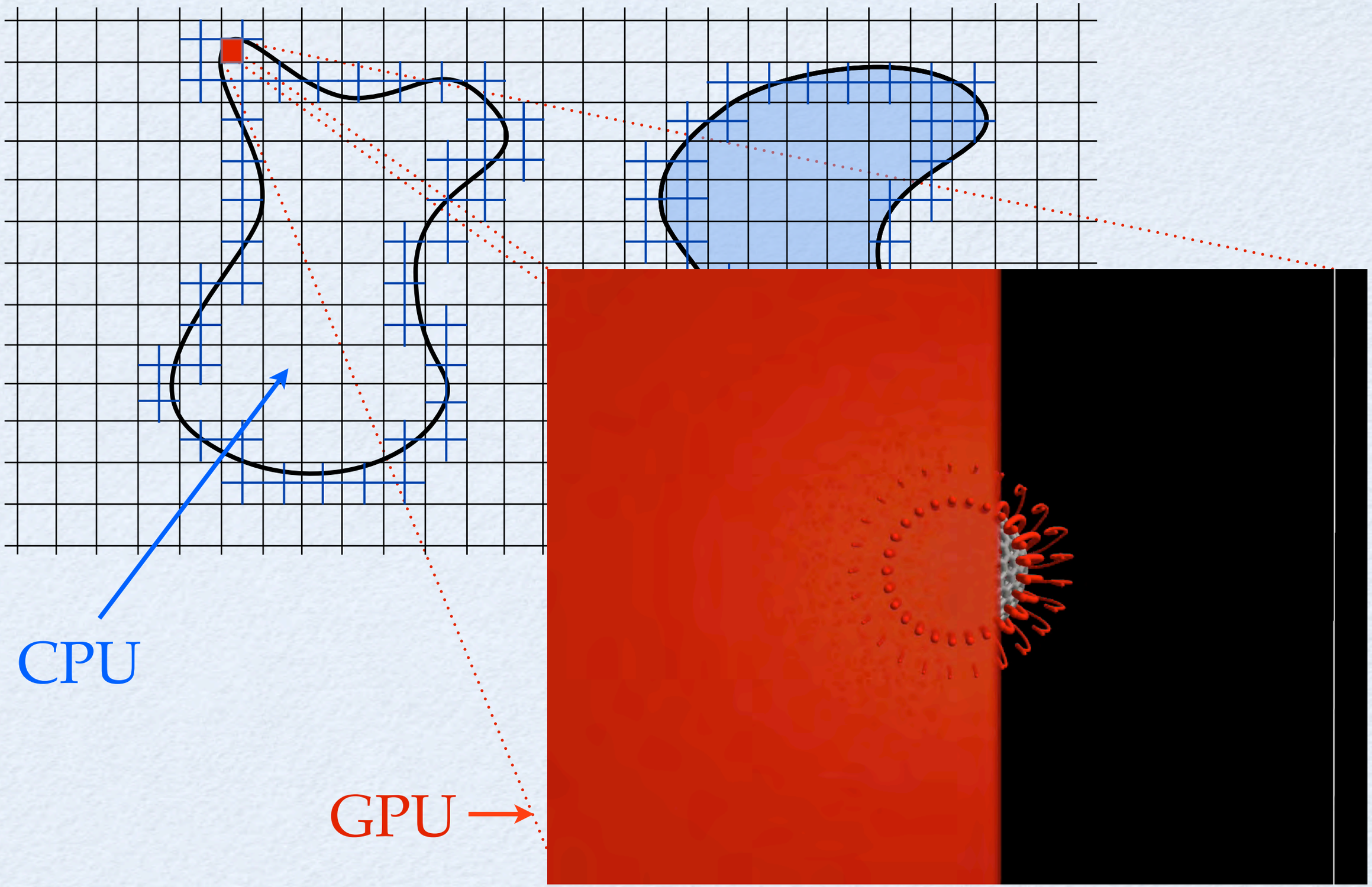
Smoothed Particle Hydrodynamics

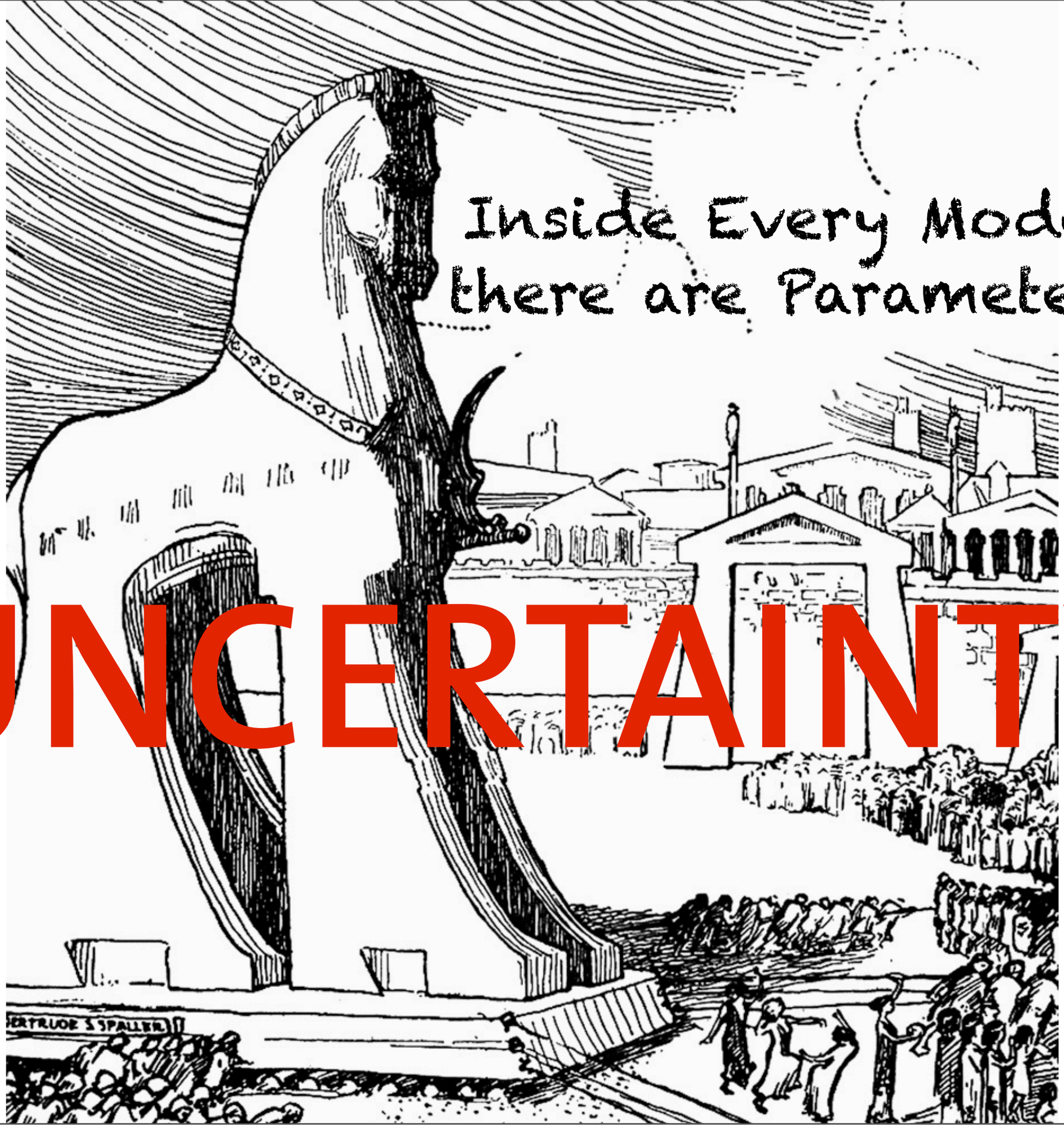
+9



Growth of Black Holes
Springel, MPI - Hernquist, Harvard

MULTI-PHYSICS/SCALE/CORES




Inside Every Model
there are Parameters
UNCERTAINTY
GERTRUDE S SPALLER

LSAS

- Common Elements

- **Multiscale-Multiphyics Modeling + Multi/Many Core architectures**

- **DATA : Uncertainty Quantification + Optimization**

PLAN

- Workshops bridging Applications and Methods
- Proposals in PASC
  - Develop CODE Integration (e.g. particles)
  - Multiscale Platforms (e.g. MAPPER)
  - Methodological Interfaces

How to build a ship ?

When you want to build a ship,
then do not drum the men together
in order to procure wood,
to give instructions or to distribute work;
but teach them longing for the wide
endless sea

Antoine de Saint-Exypery