Multiscale Hemodynamics: Using Computation to Diagnose and Predict Heart Disease

IACS Seminar, September 13, 2013

Based on PhD Thesis of Amanda P. Randles

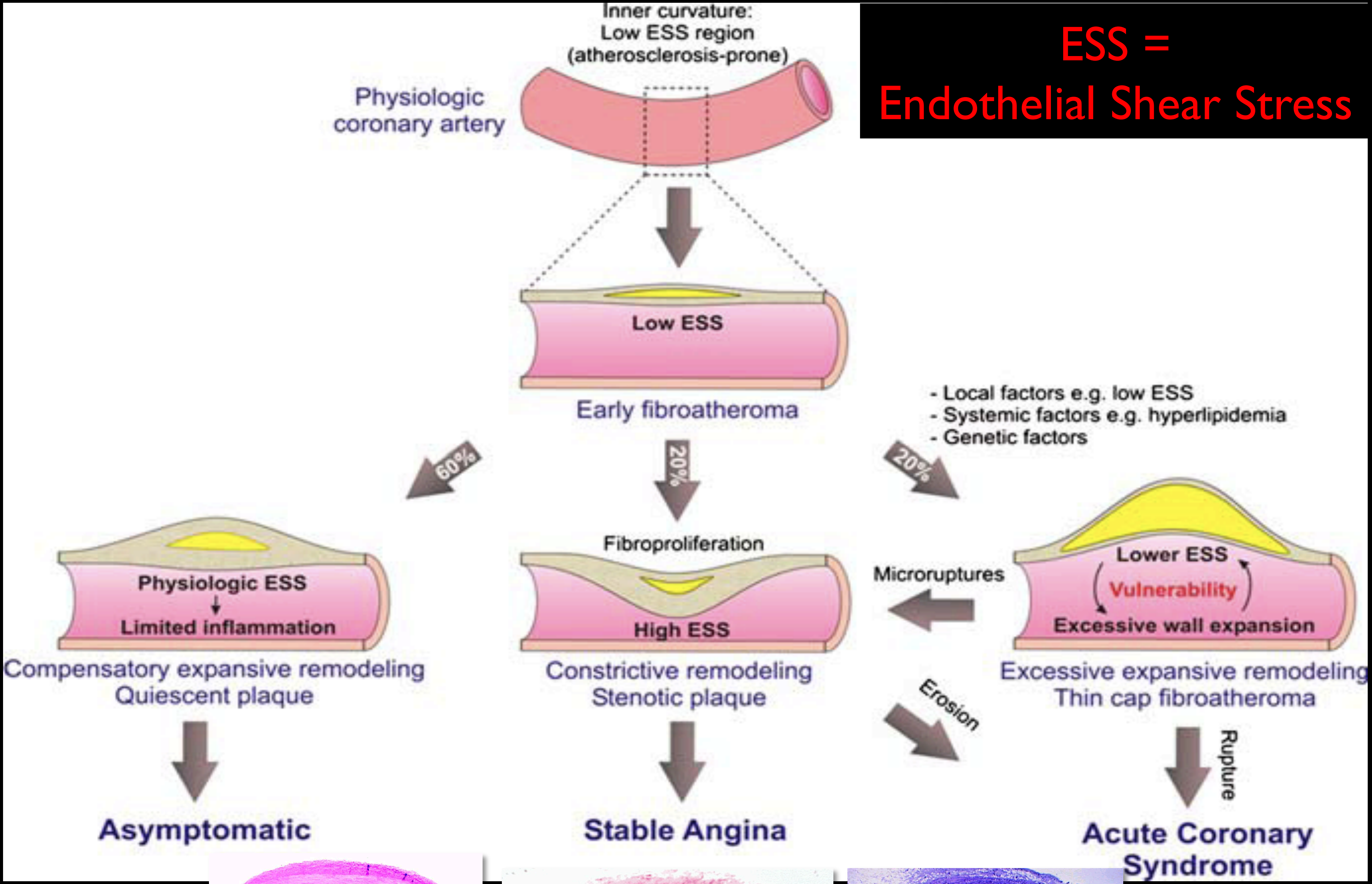
Cardiovascular Disease

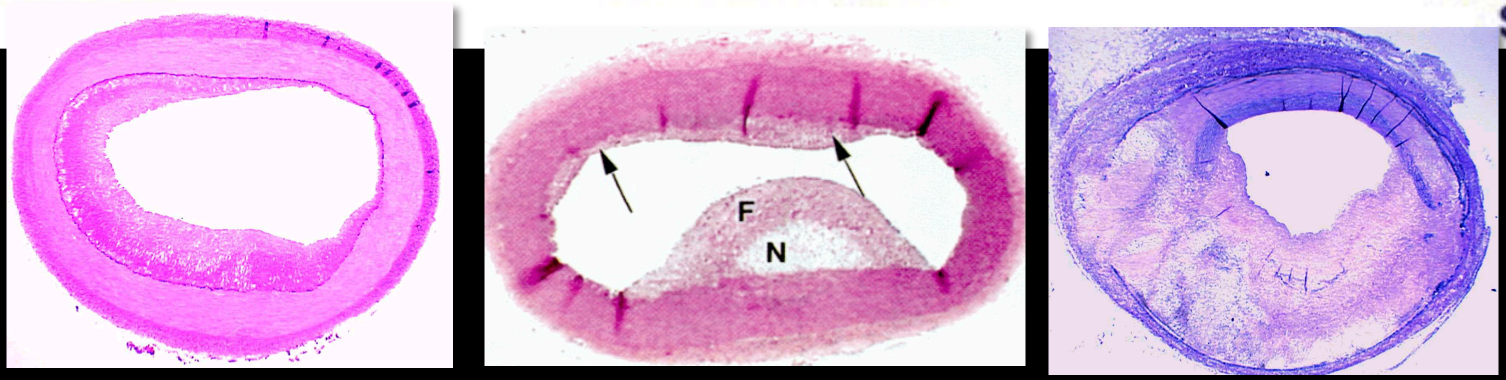
- Leading cause of death in the western world
- 1 in ~3 deaths in the US alone
- 50% of instances occur without prior symptoms

Roger et al. Circulation, 2012

Formation and evolution of plaques

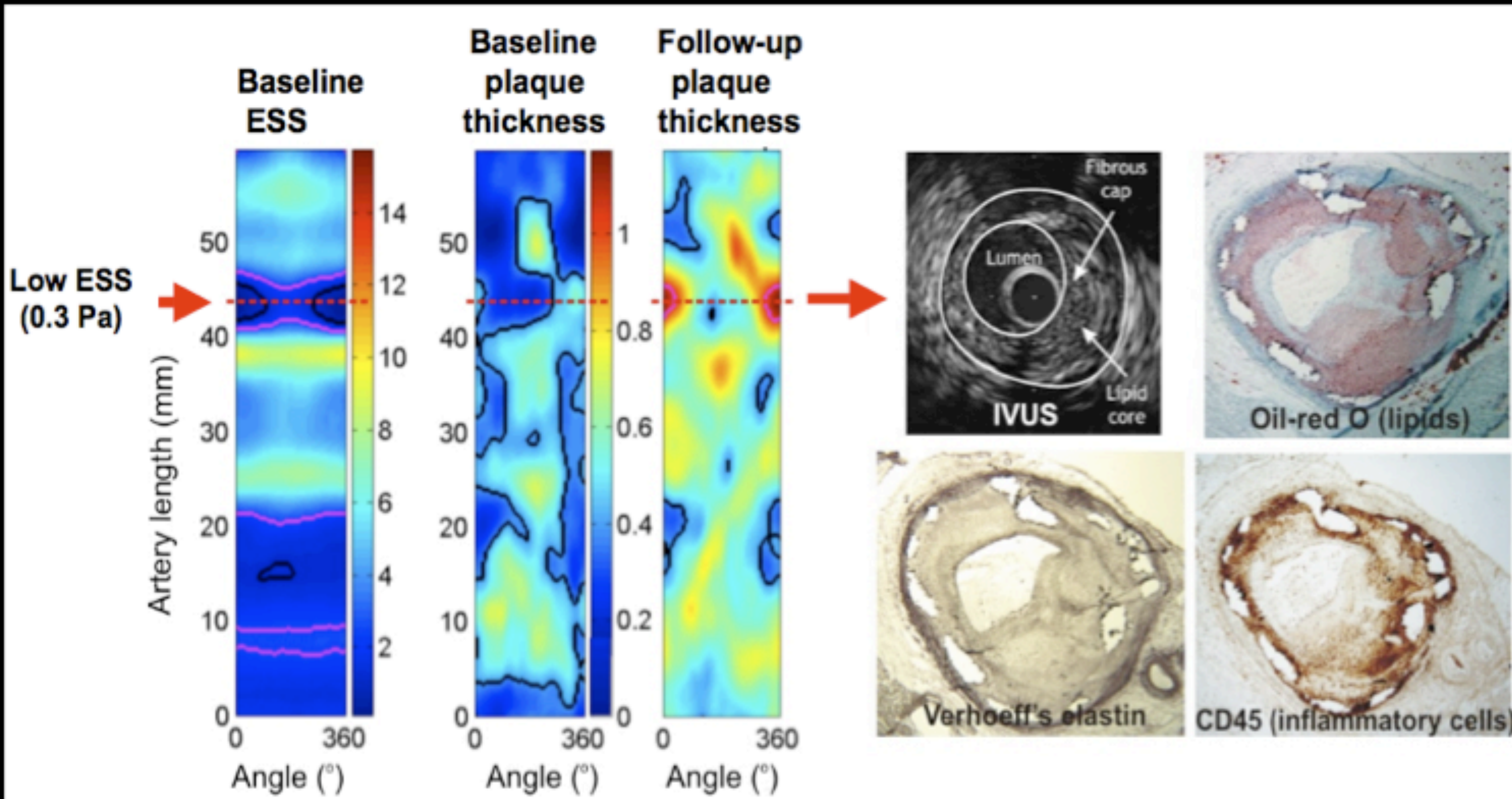
ESS =
Endothelial Shear Stress





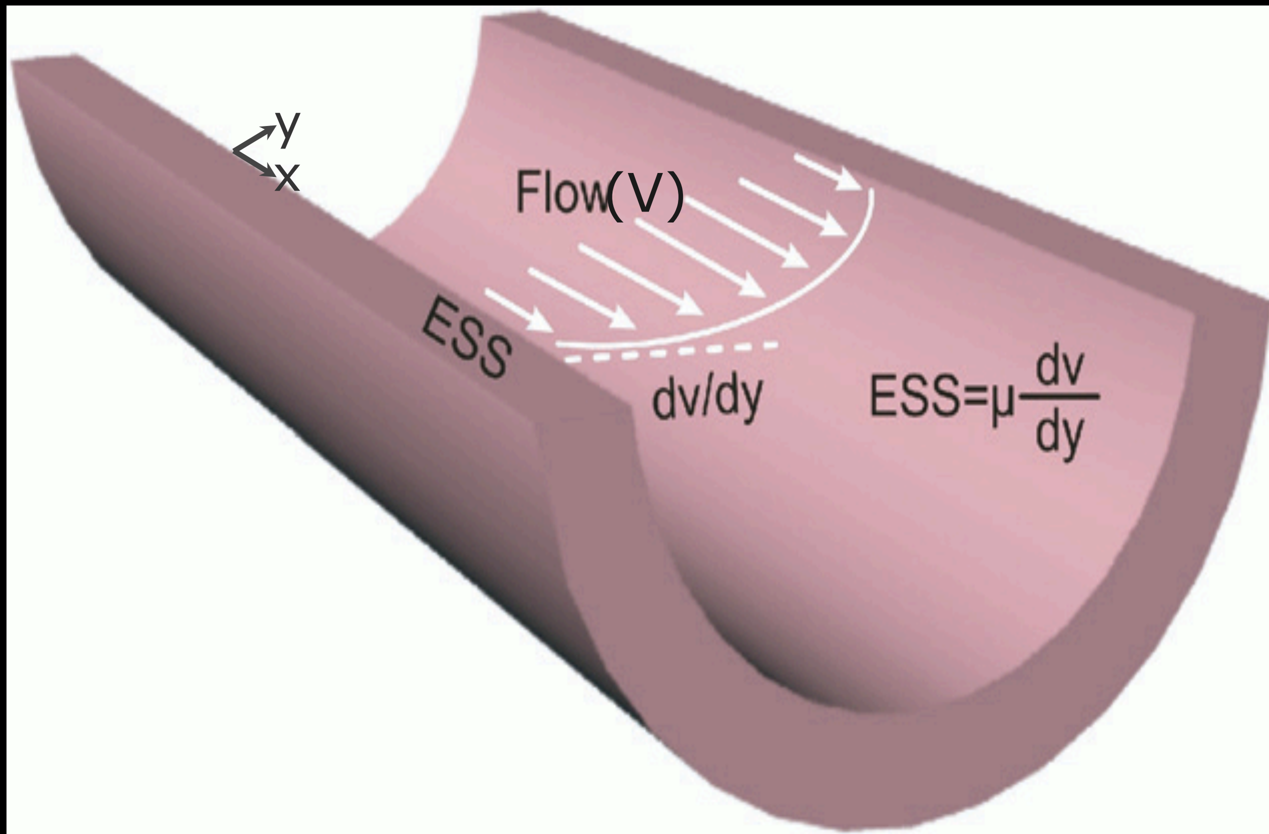
Vascular Remodeling

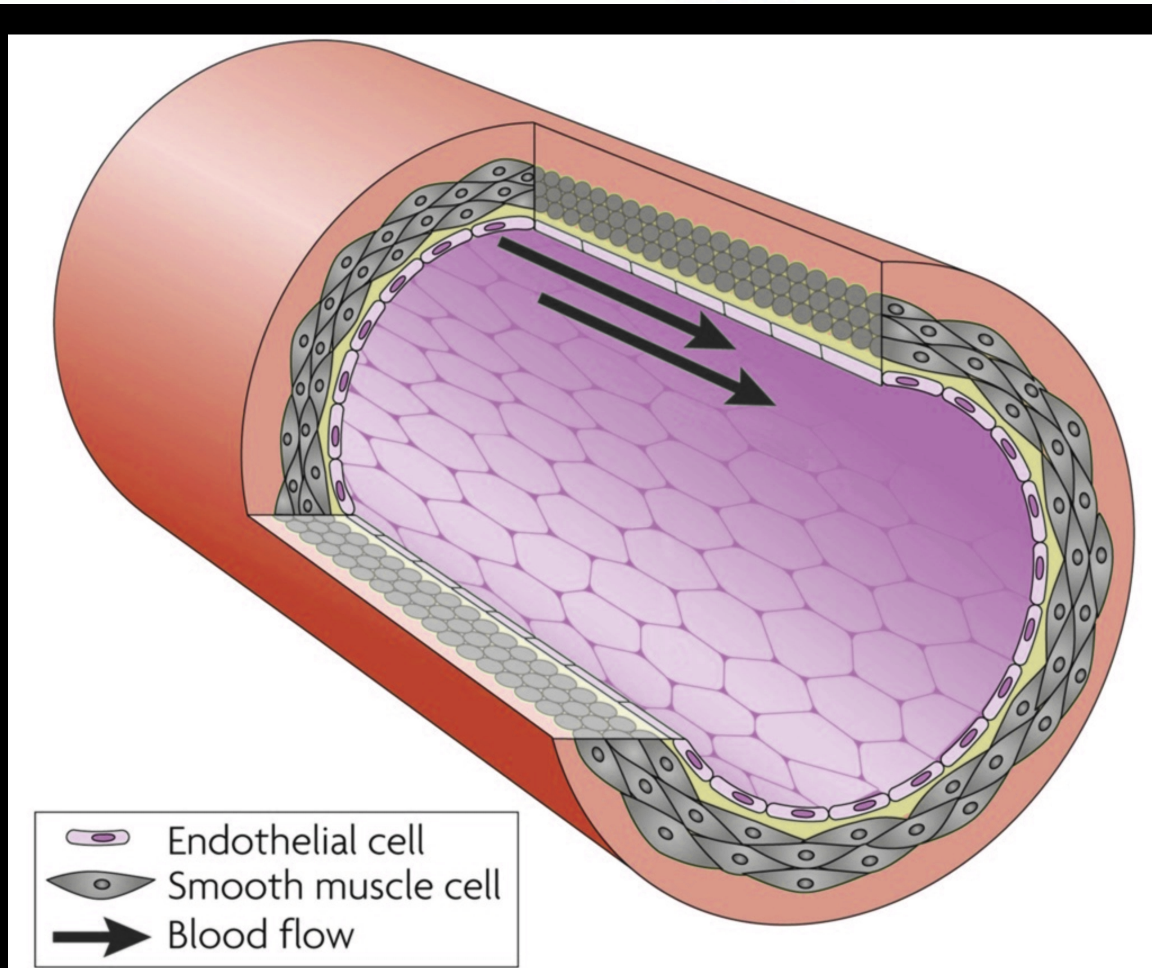
Role of Endothelial Shear Stress (ESS)

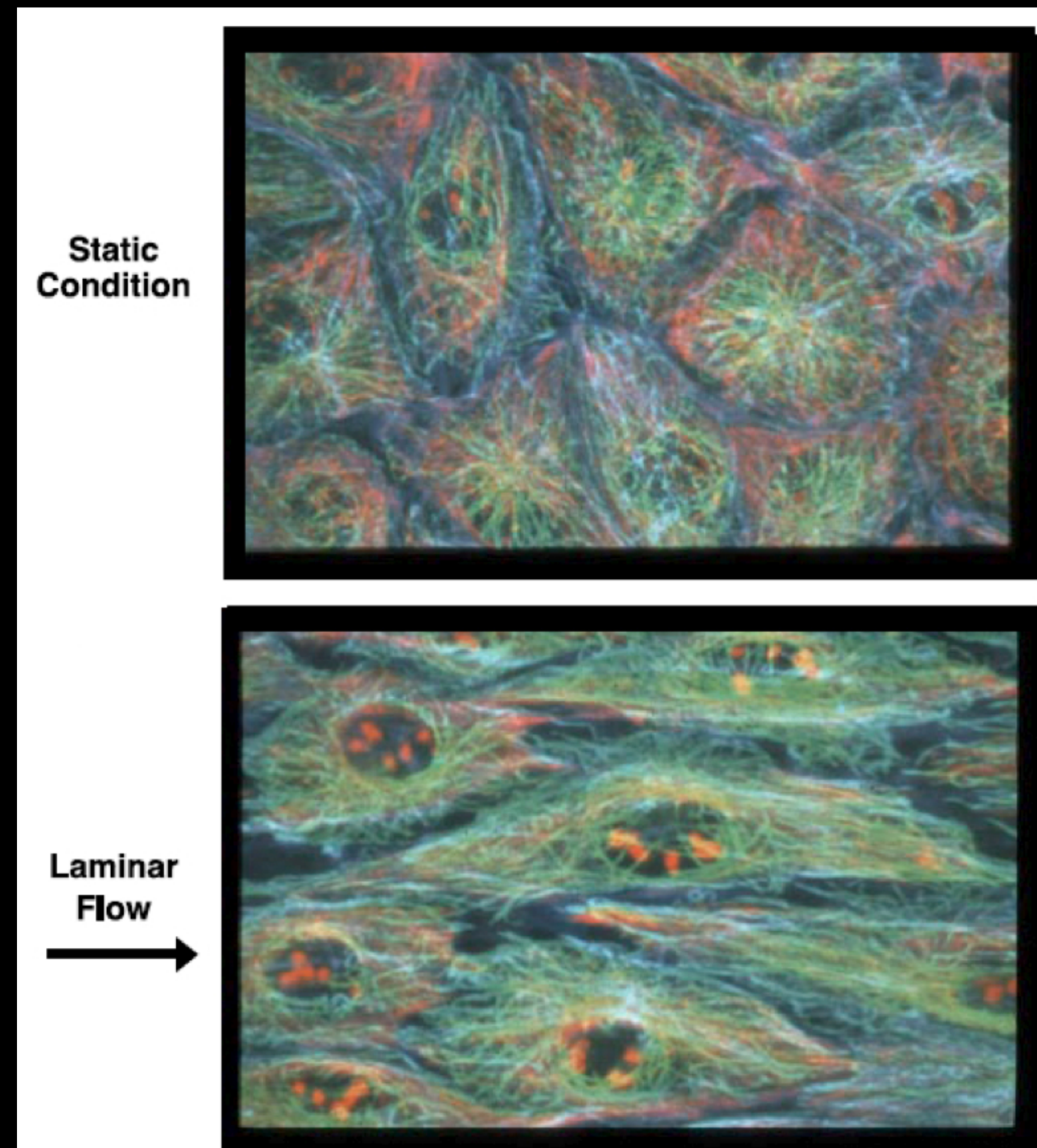


Currently, the only way to assess a patient's endothelial shear stress is through simulation

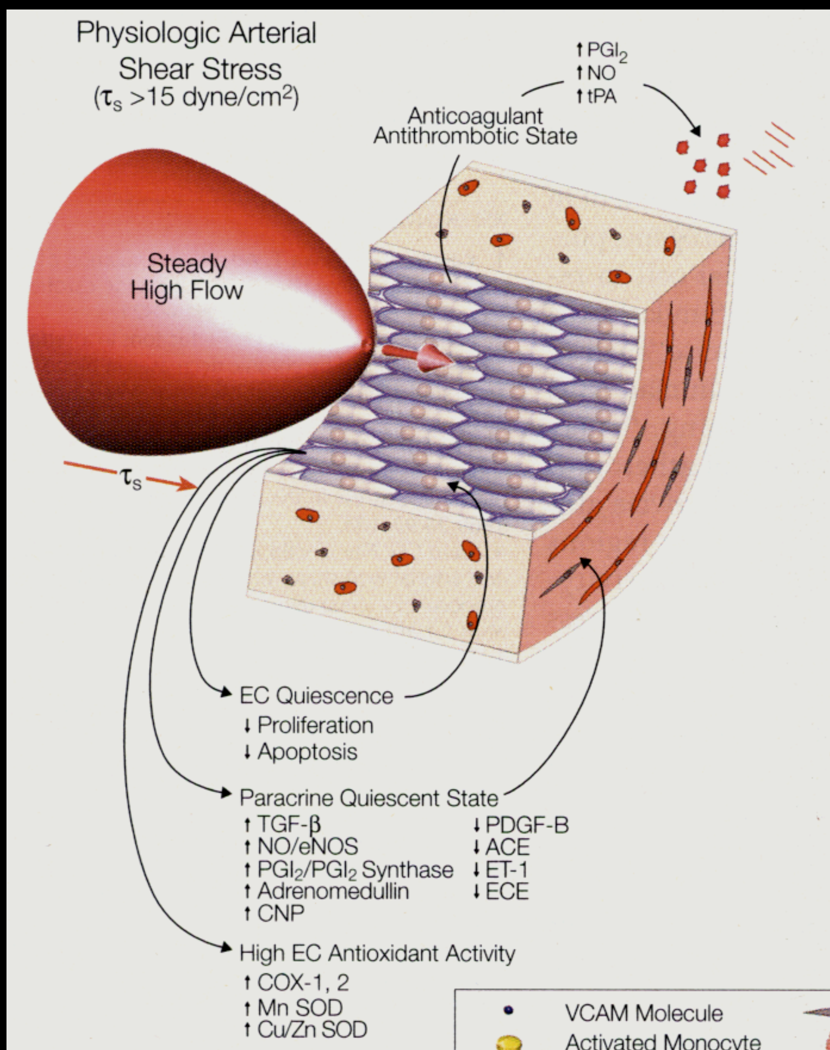
How does the flow reshape the endothelium?

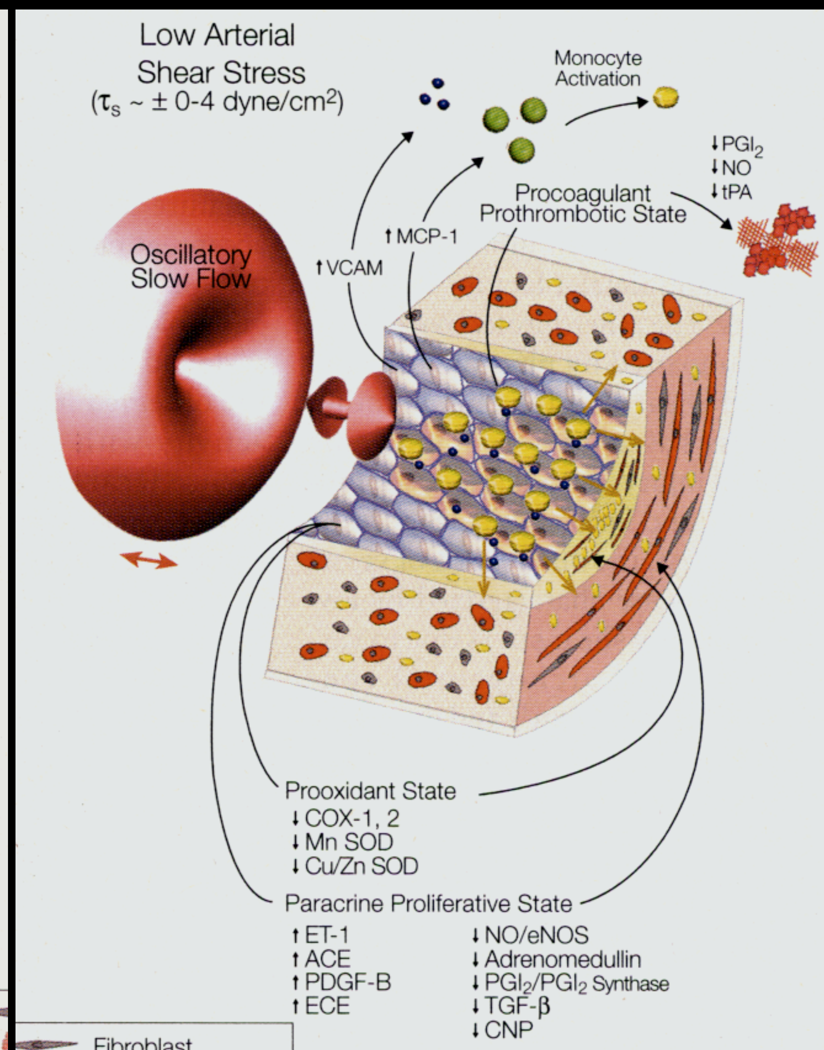


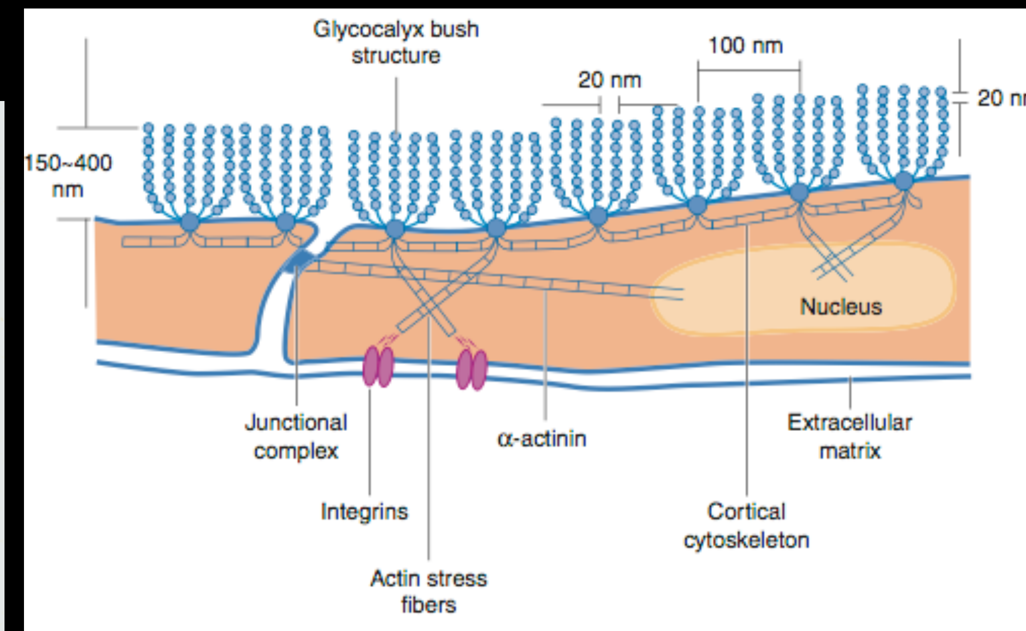


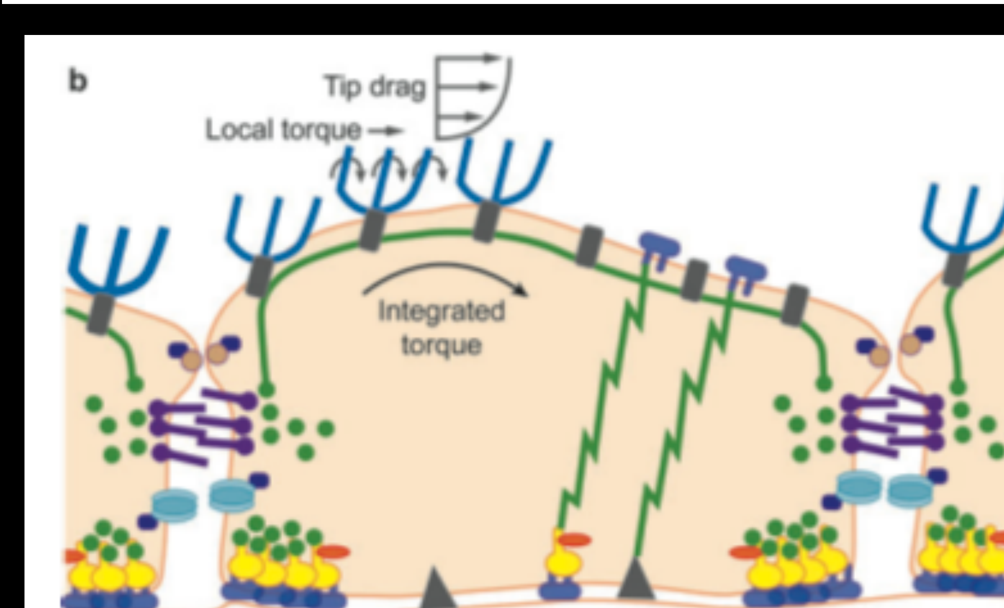


Mechanosensing and transduction









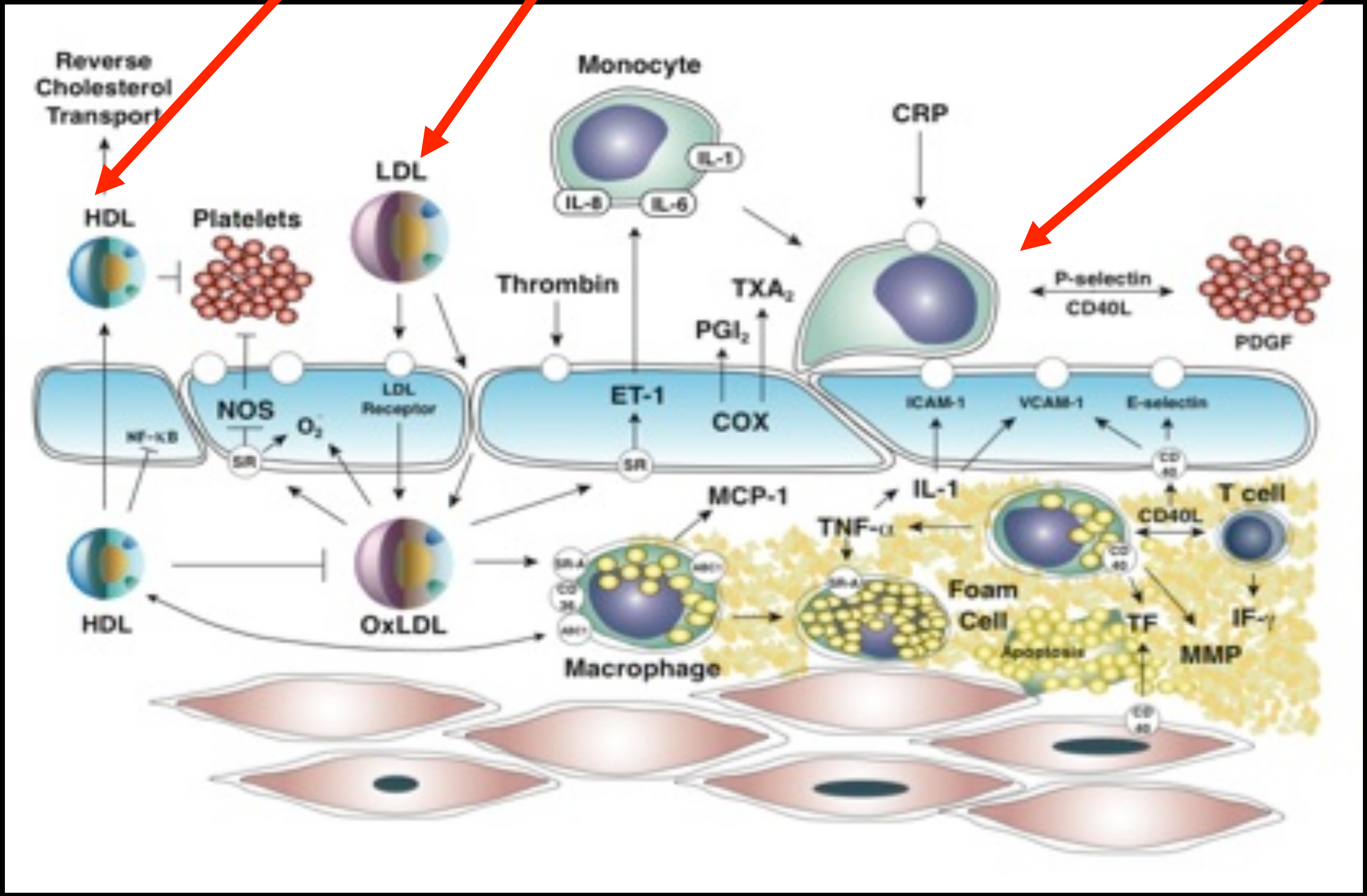
Vasculoprotective

Vascular adhesion of lipoproteins & inflammatory cells

Inflammatory response & Feedback

Cholesterol (HDL, LDL)

White blood cells



Endothelium

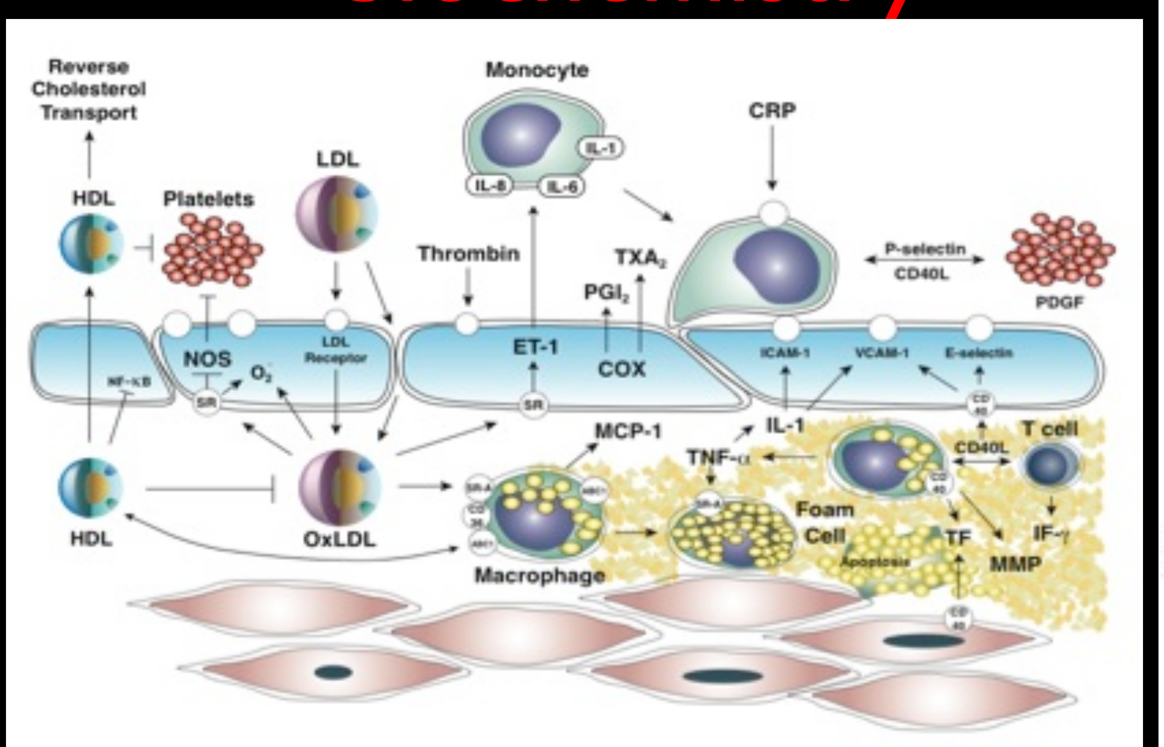
Muscle tissue

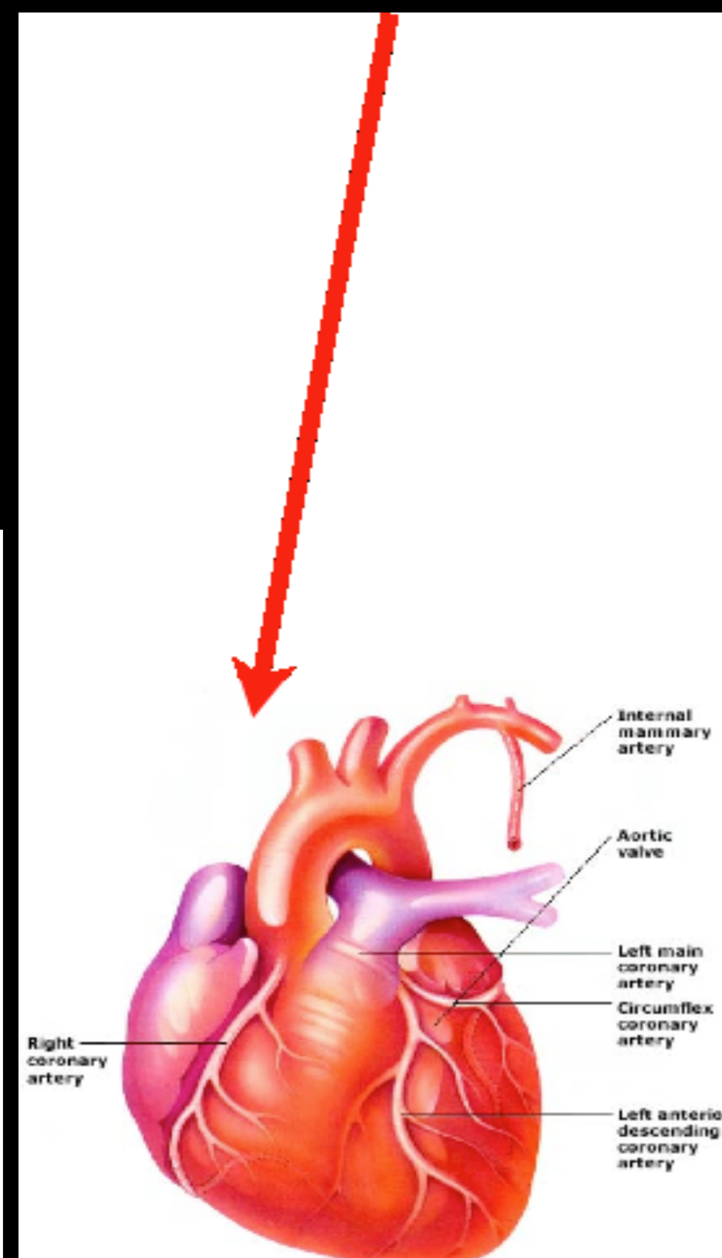
Grand Challenge: Multiscale Hemodynamics

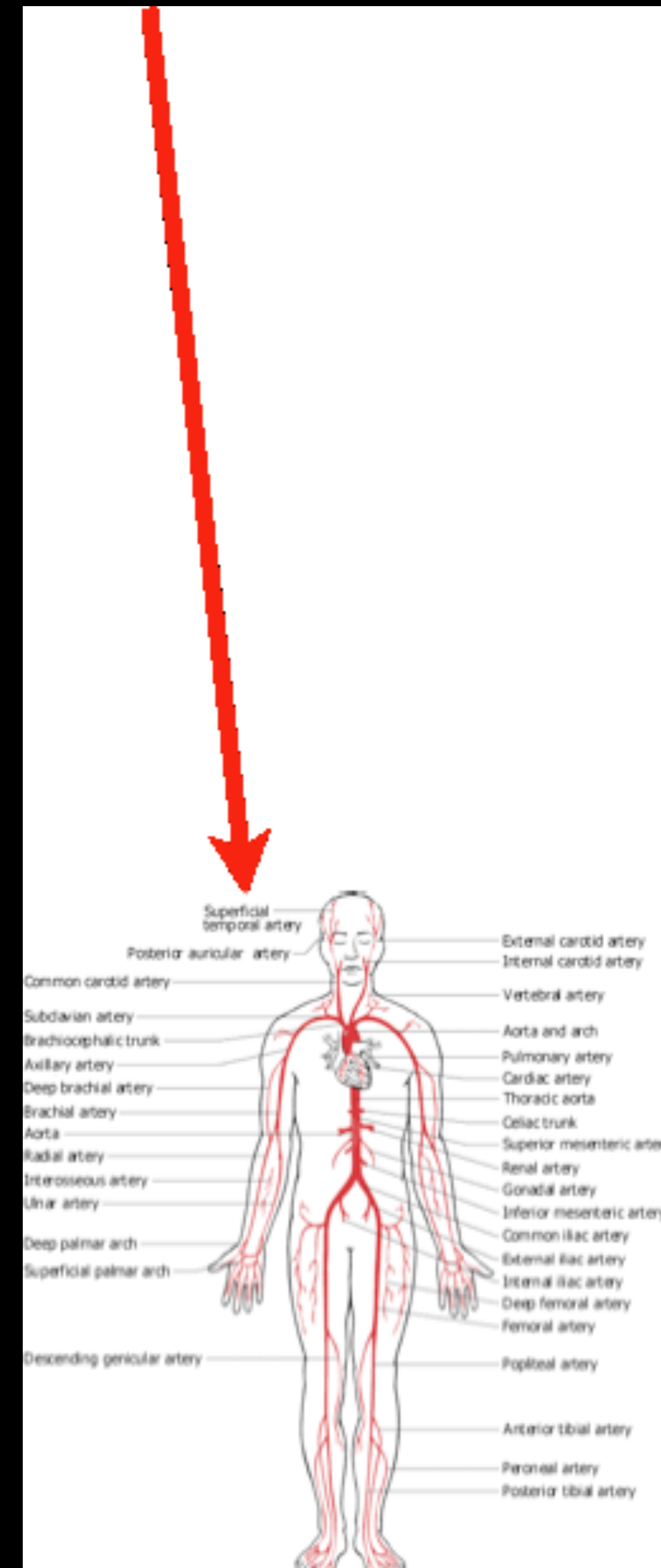
m scale – BC's

cm-mm scale – geometry/ fluid dynamics

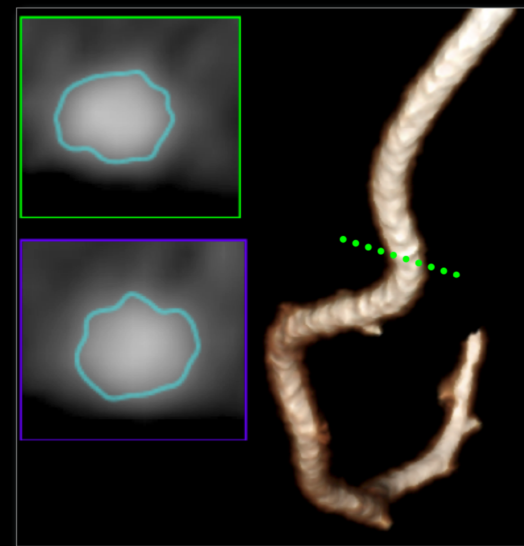
μm-nm scale – biochemistry



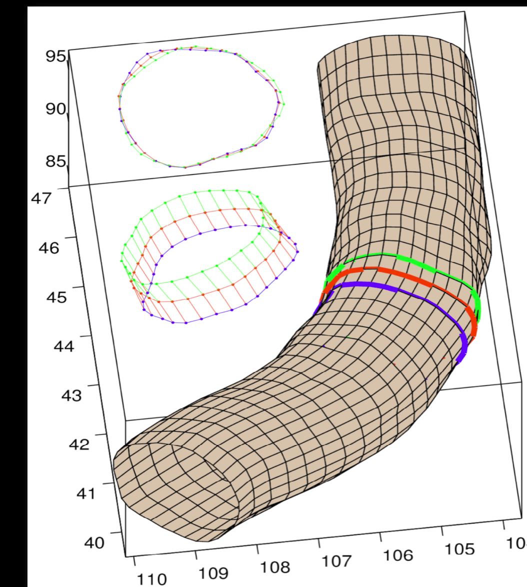




Patient Data

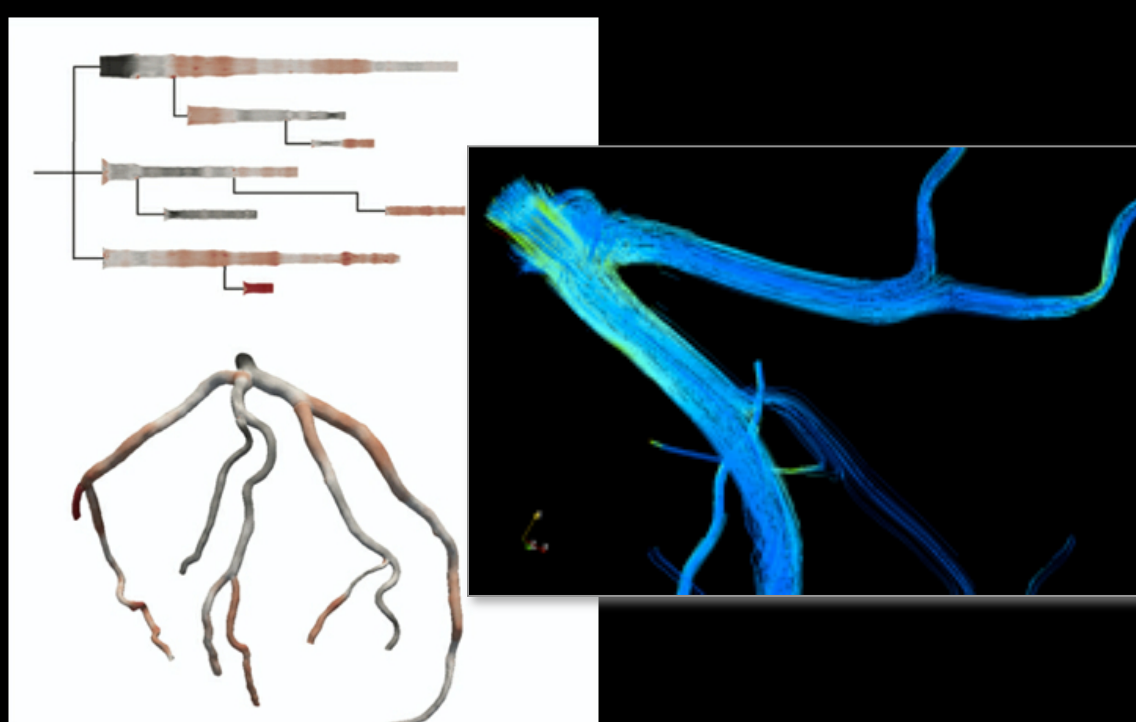


Data Segmentation



HPC Data Preparation

Parallel Code: MUPHY & HARVEY

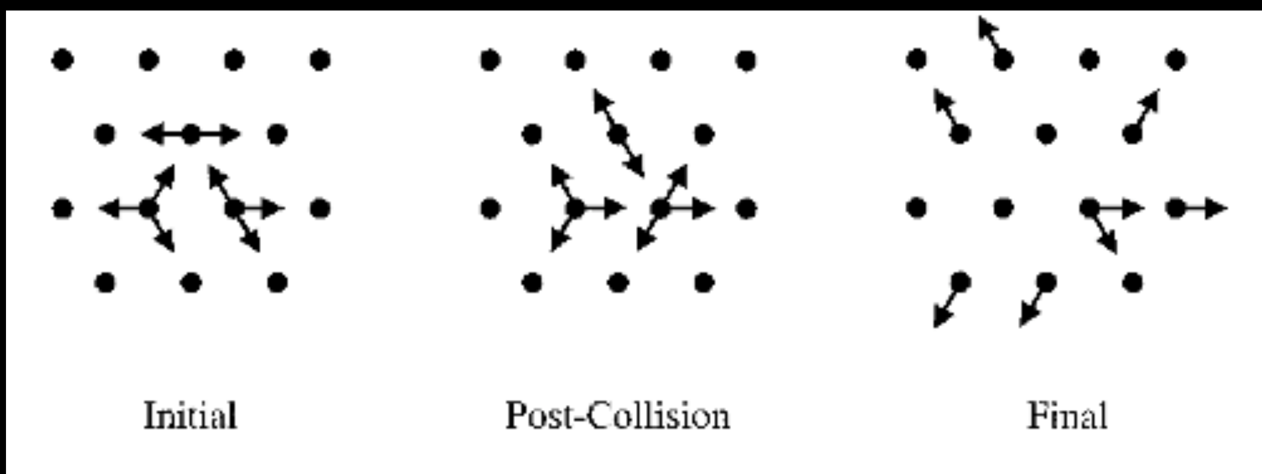


Borkin et al. IEEE Transactions on Visualization and Computer Graphics, 2011

Output visualization

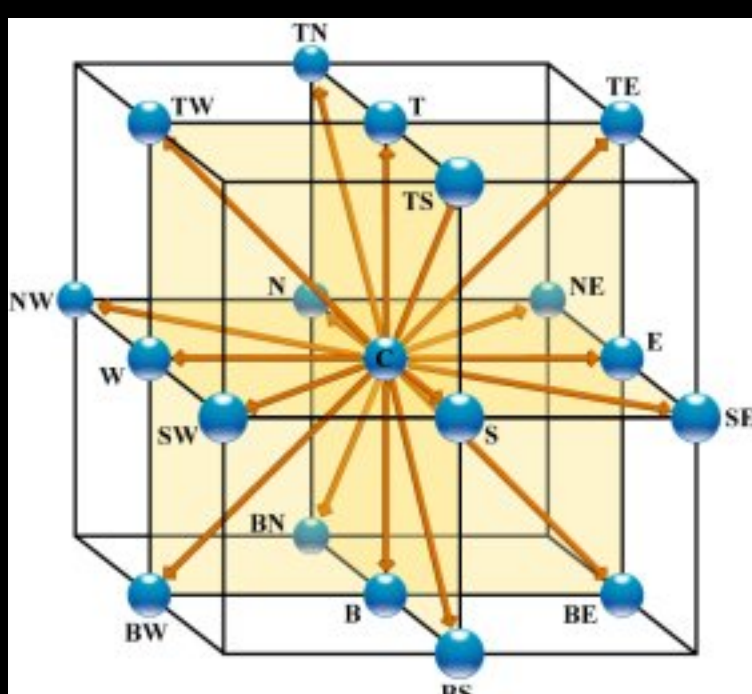
Fluid dynamics by cellular automata : Lattice Boltzmann Equation (LBE)

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



Bhatnagar-Gross-Krook algorithm

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



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

Fluid dynamics :

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

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

|

Advantages of Lattice Boltzmann

- Simple, time-explicit, robust, and accurate algorithm
- Straight forward handling of extremely complex geometries
- Recovers Navier-Stokes equations
- Data locality (helps parallel implementation)
- Computational simplicity (cubic grid)

Accuracy of flow patterns for real, patient-specific geometries

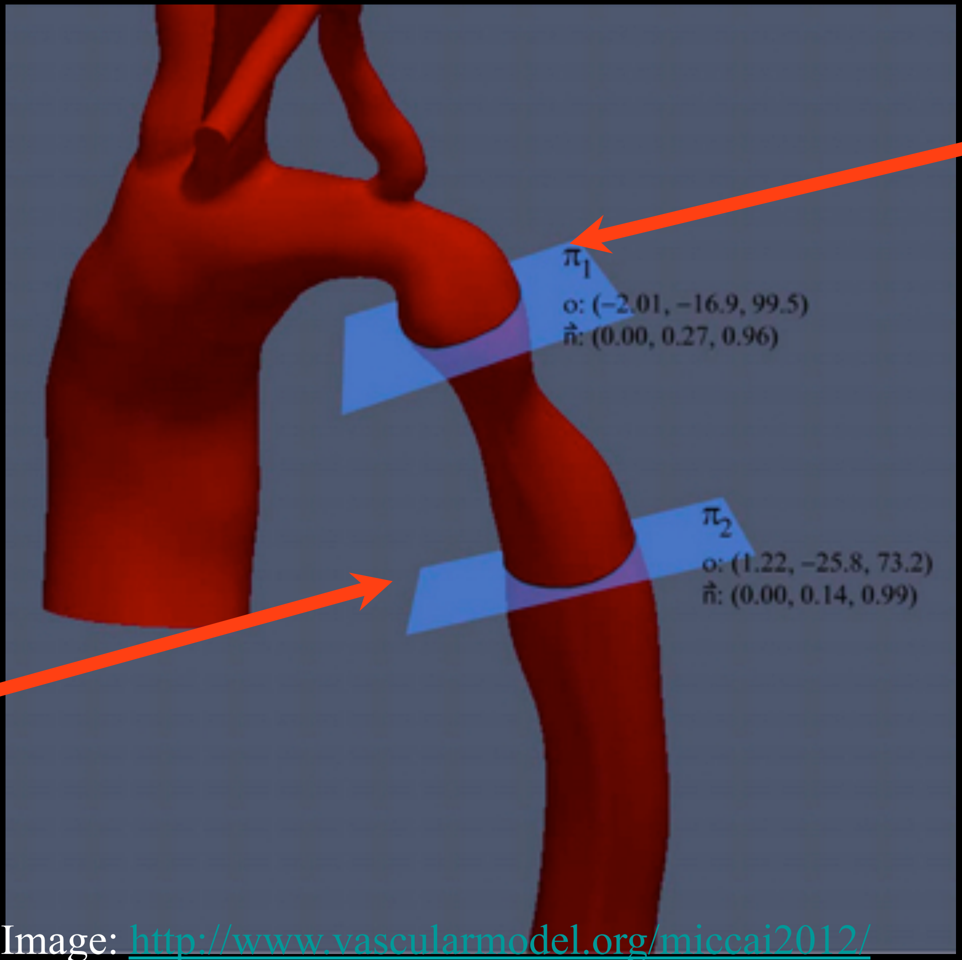
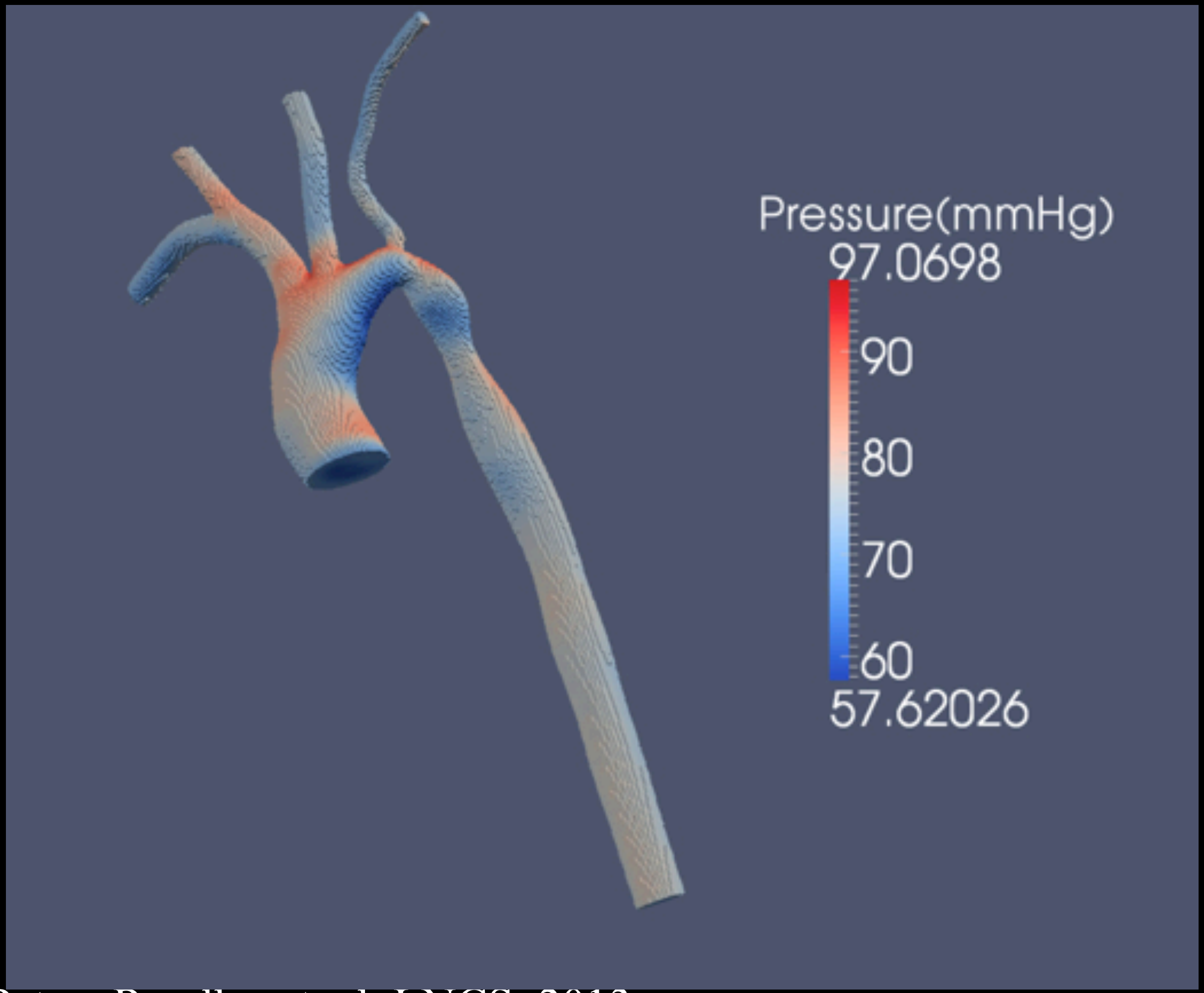


Image: http://www.vascularmodel.org/miccai2012/

STACOM Computational Fluid Dynamics Challenge

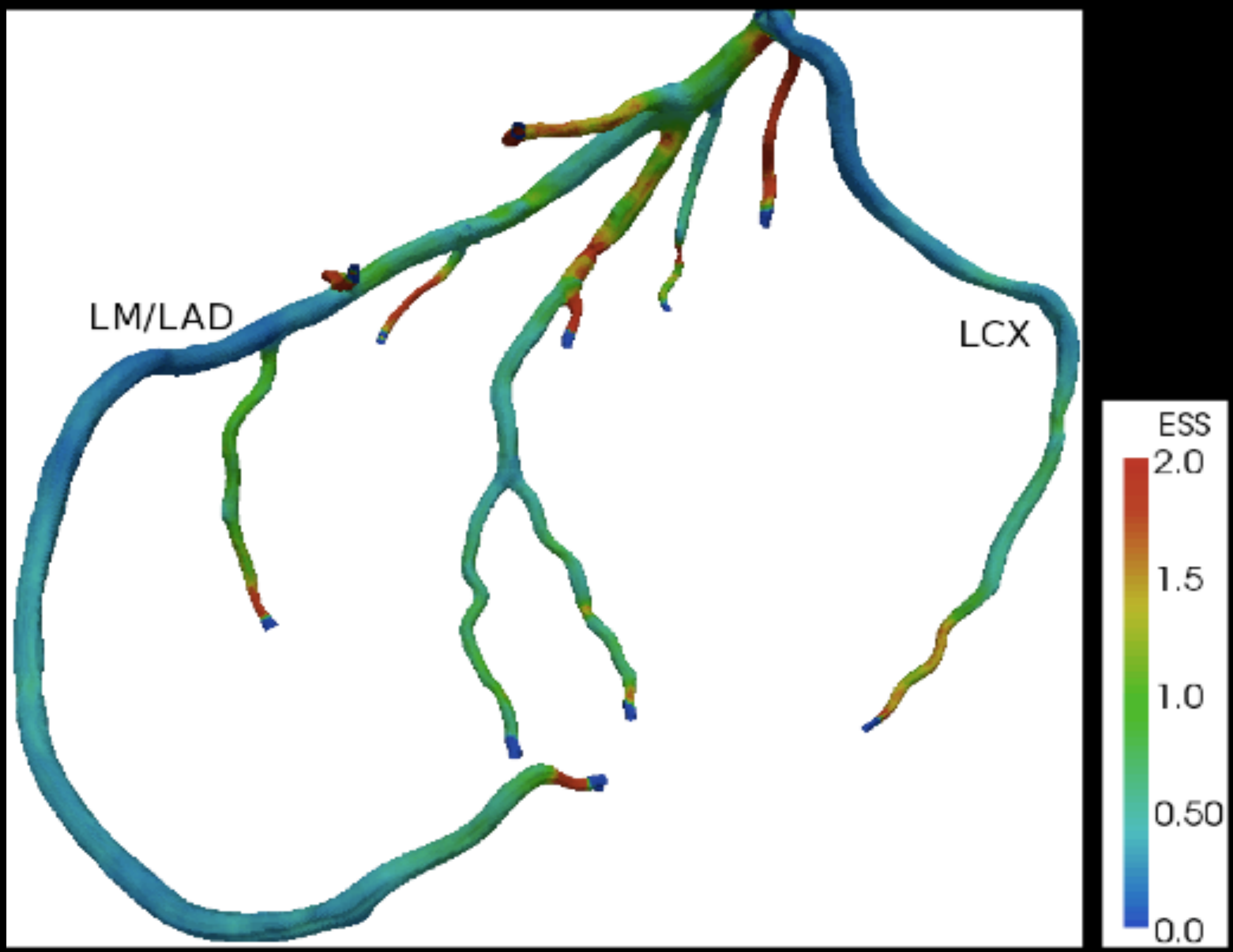
Comparison with *in vivo* measurements



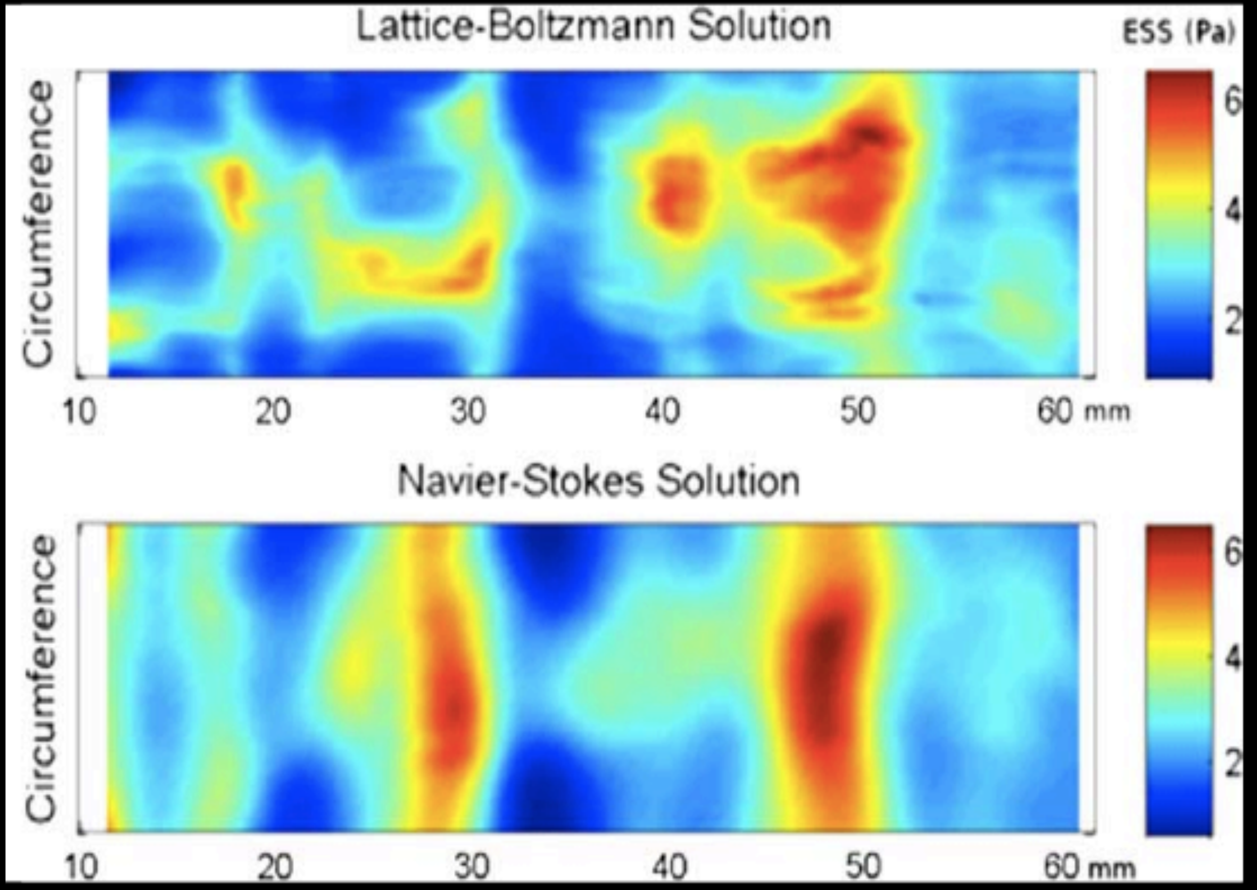
Peters Randles et. al. LNCS, 2013

- Convergence of pressure at 20 microns
- 2 mmHg change between diastole and systole
- Mean pressure difference of 9.2 mmHg
- Best mean pressure drop in the competition

ESS calculation in patient-specific arterial tree

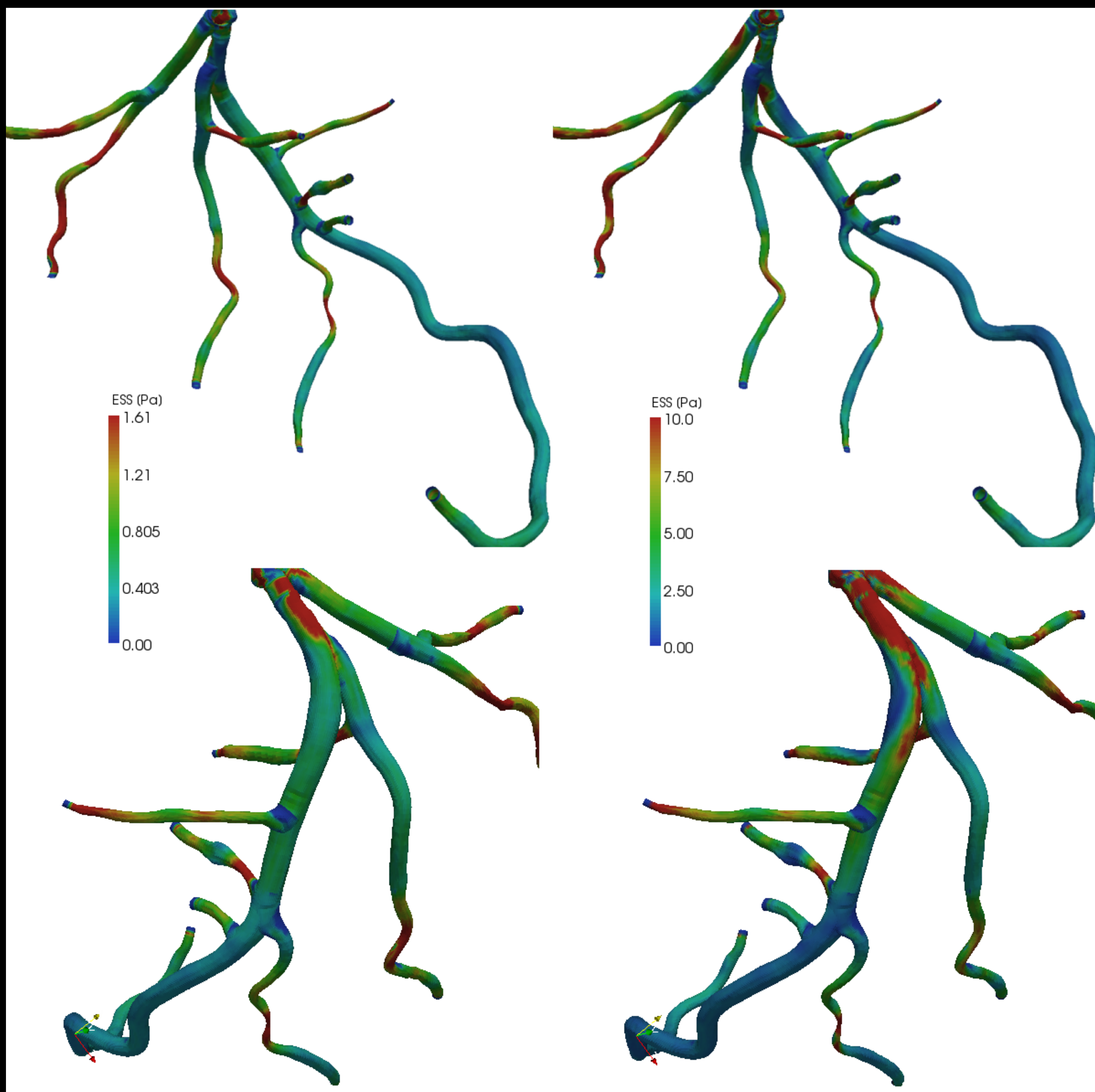


Validation



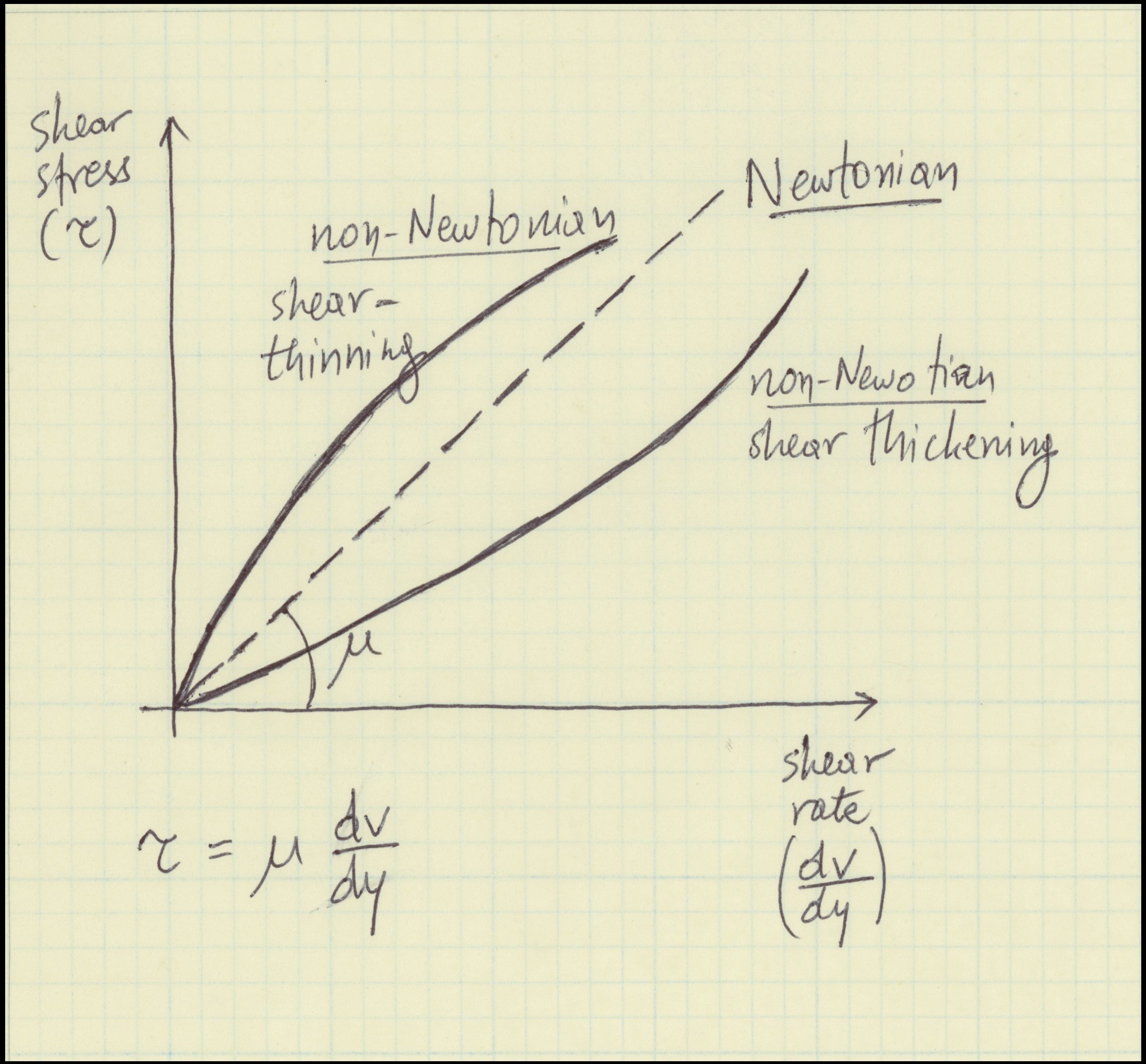
3D ESS maps at different flow conditions

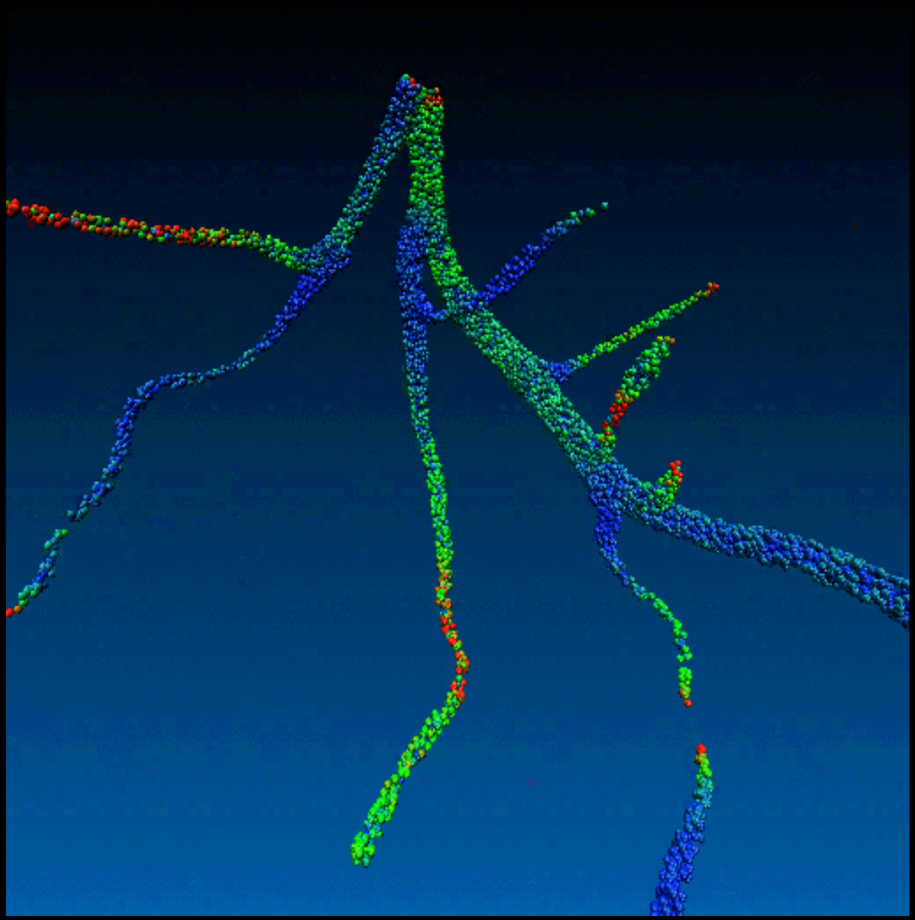
Low flow High flow



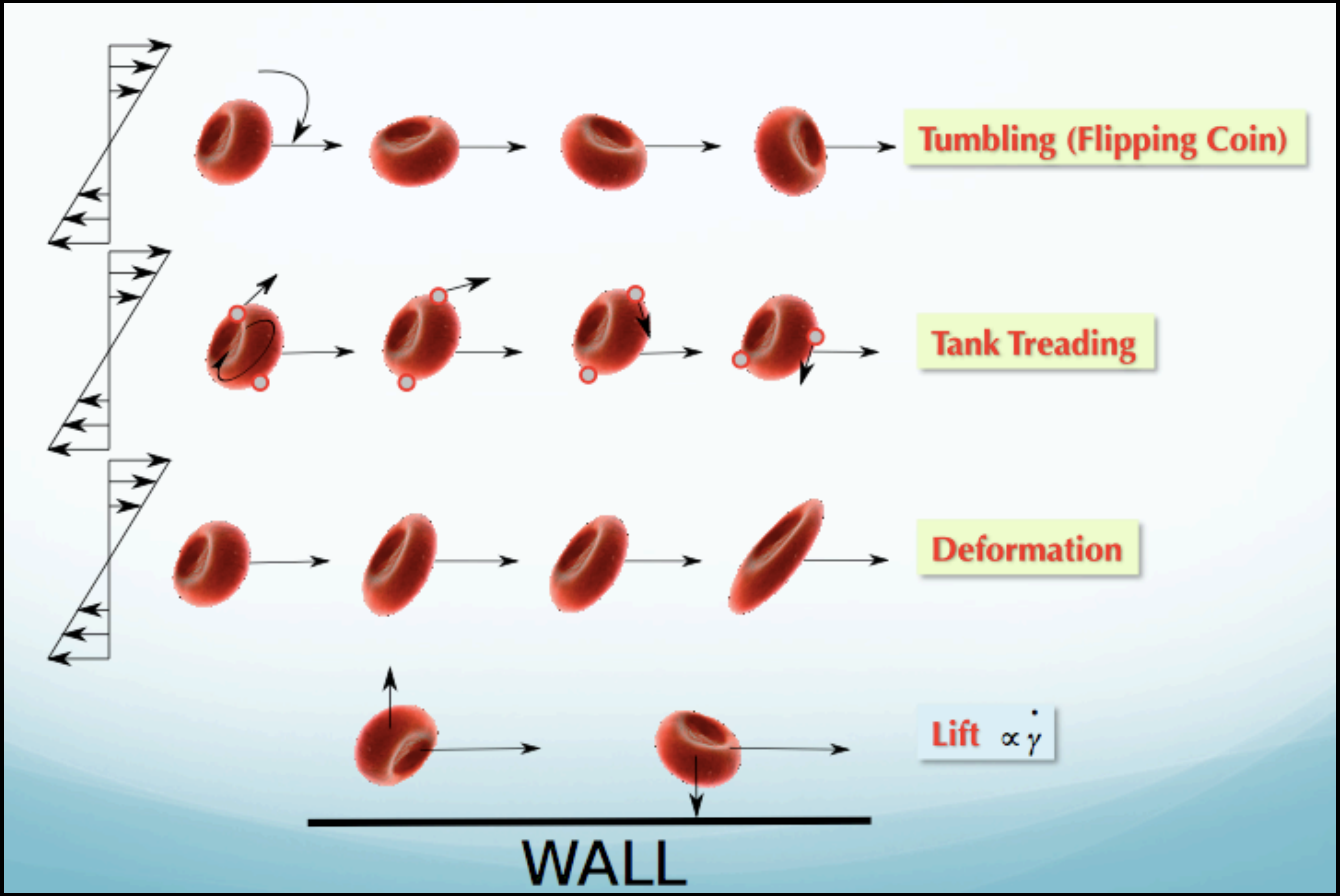
Full heart beat (1 sec, ~ 10^6 simulation steps)

Challenge: non-Newtonian nature of blood





Red Blood Cell in Motion



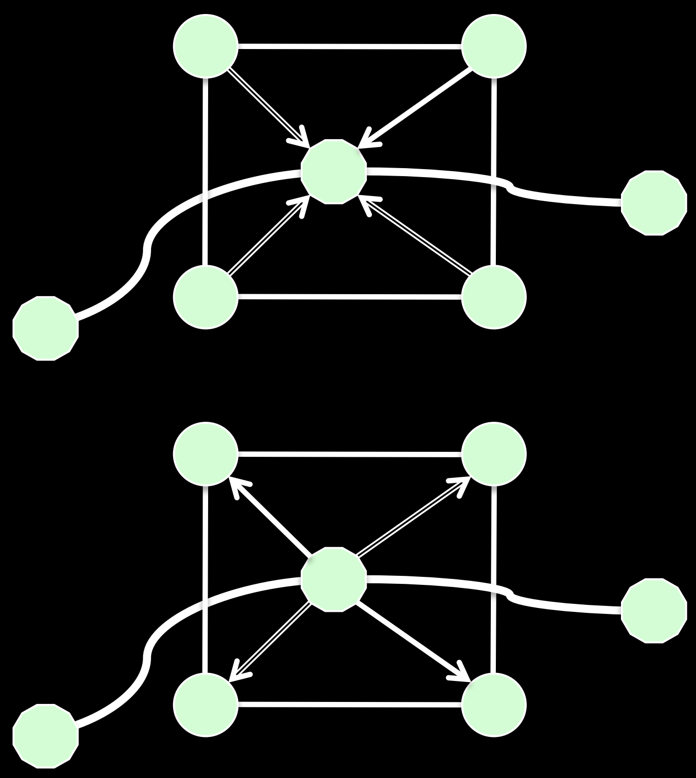
Coupling of particle and fluid (continuum) scales

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

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

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

Momentum exchange (Newton's law)

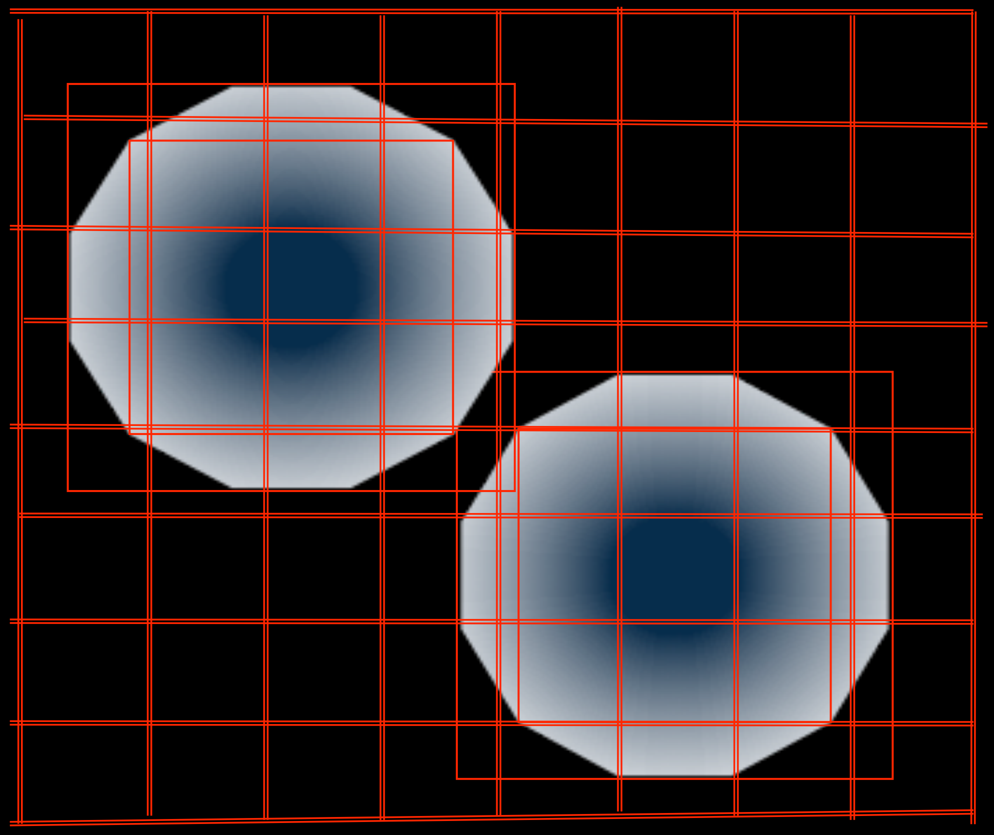


Definition of particles (cells, proteins, …)

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

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

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



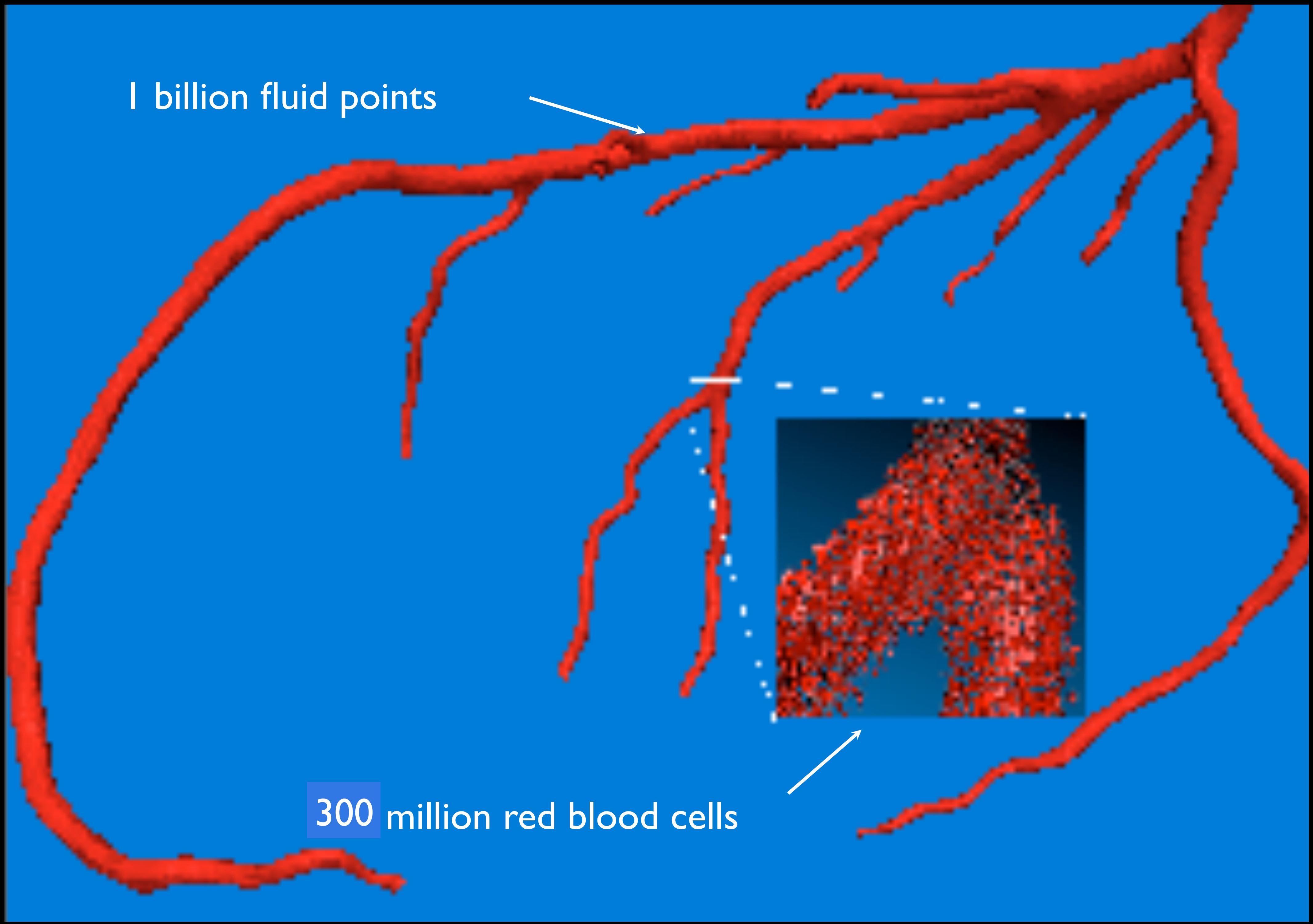
$$\varphi(x,R) = -\gamma\left(V - u(x)\right)\tilde{\delta}_\xi(x-R)$$

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

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

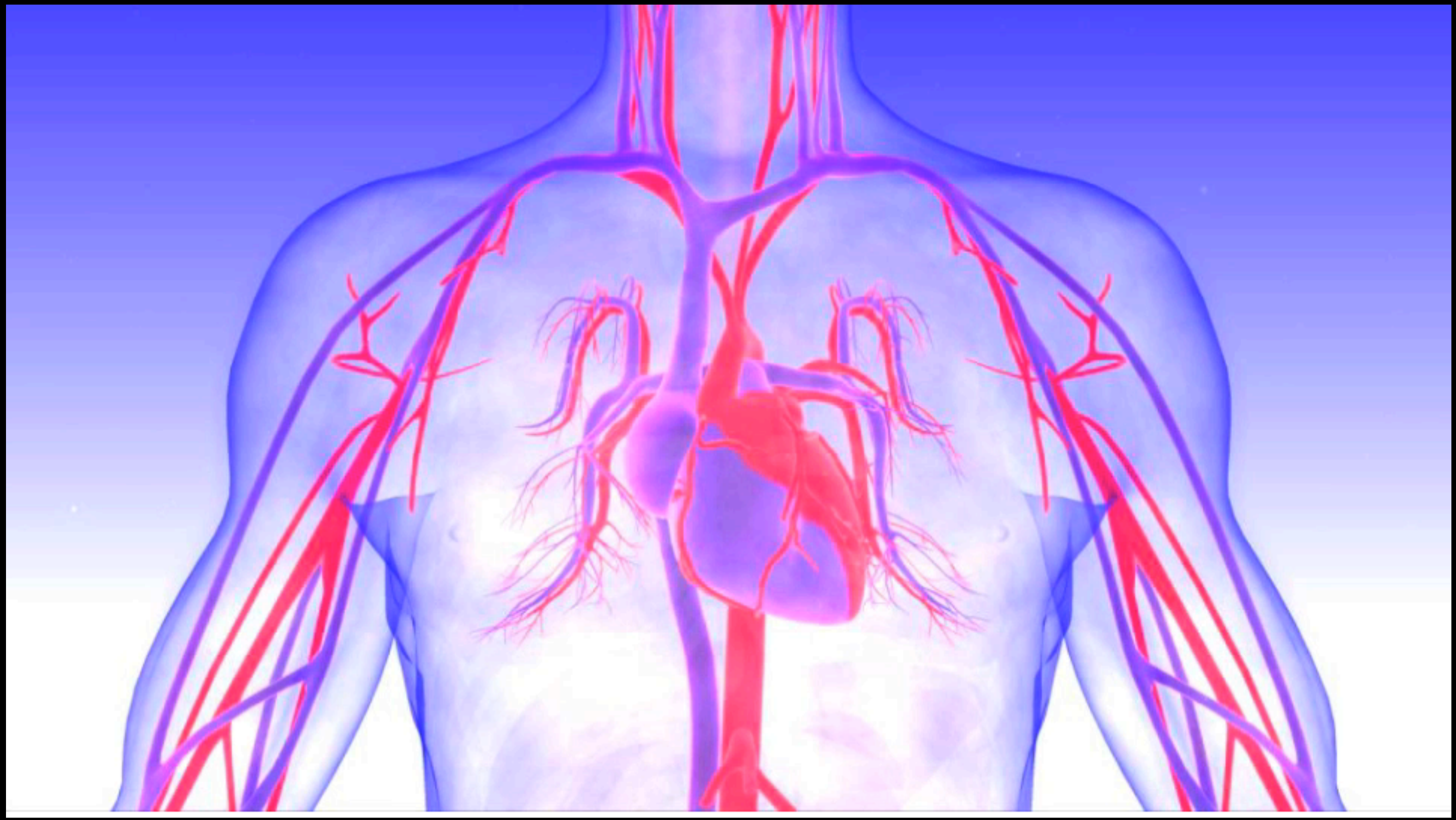
$$\Delta f_p = -\frac{w_p}{c^2} c_p \cdot \sum_R \varphi$$

Full artery simulation: computationally demanding



Peters, et al. Supercomputing, 2010

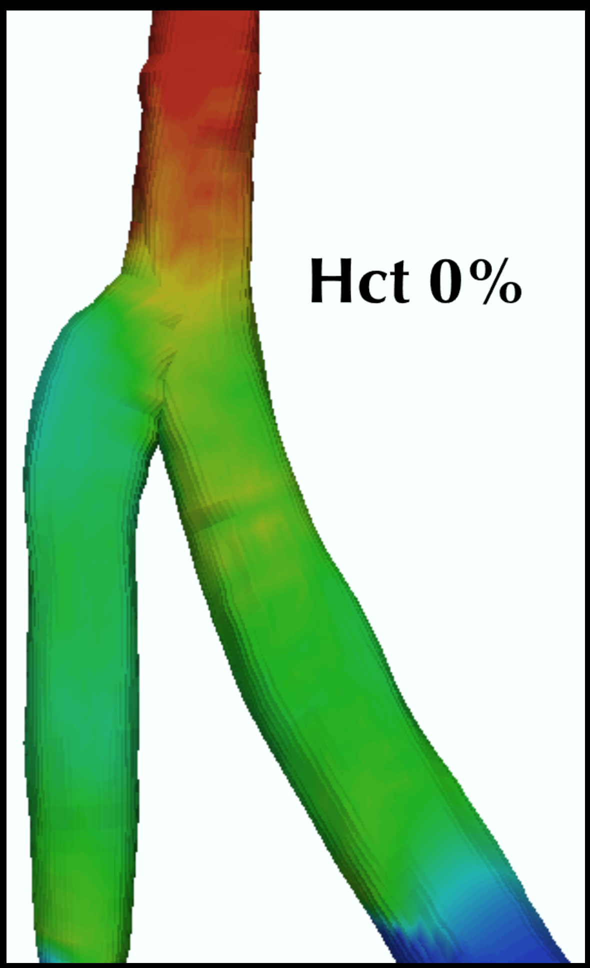
Full heartbeat simulation

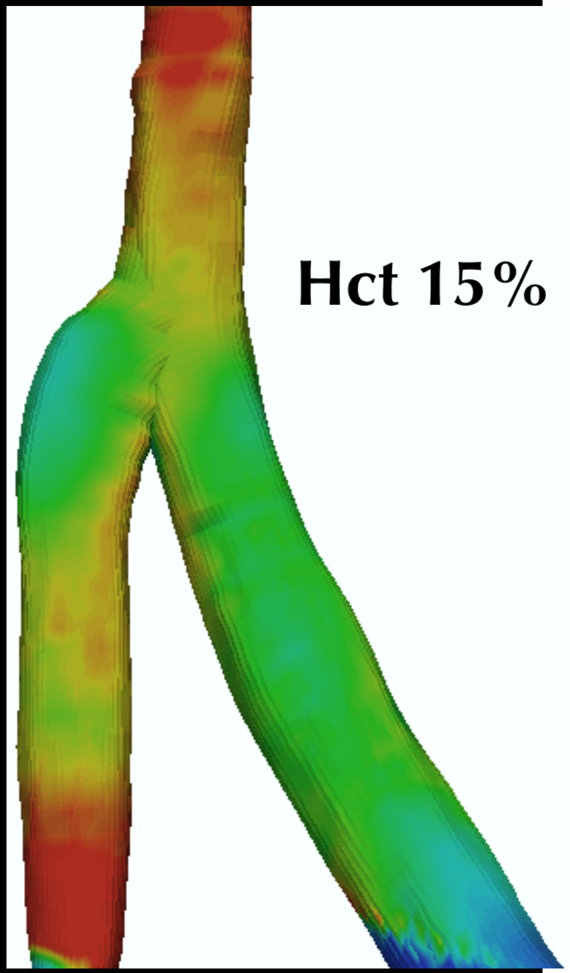


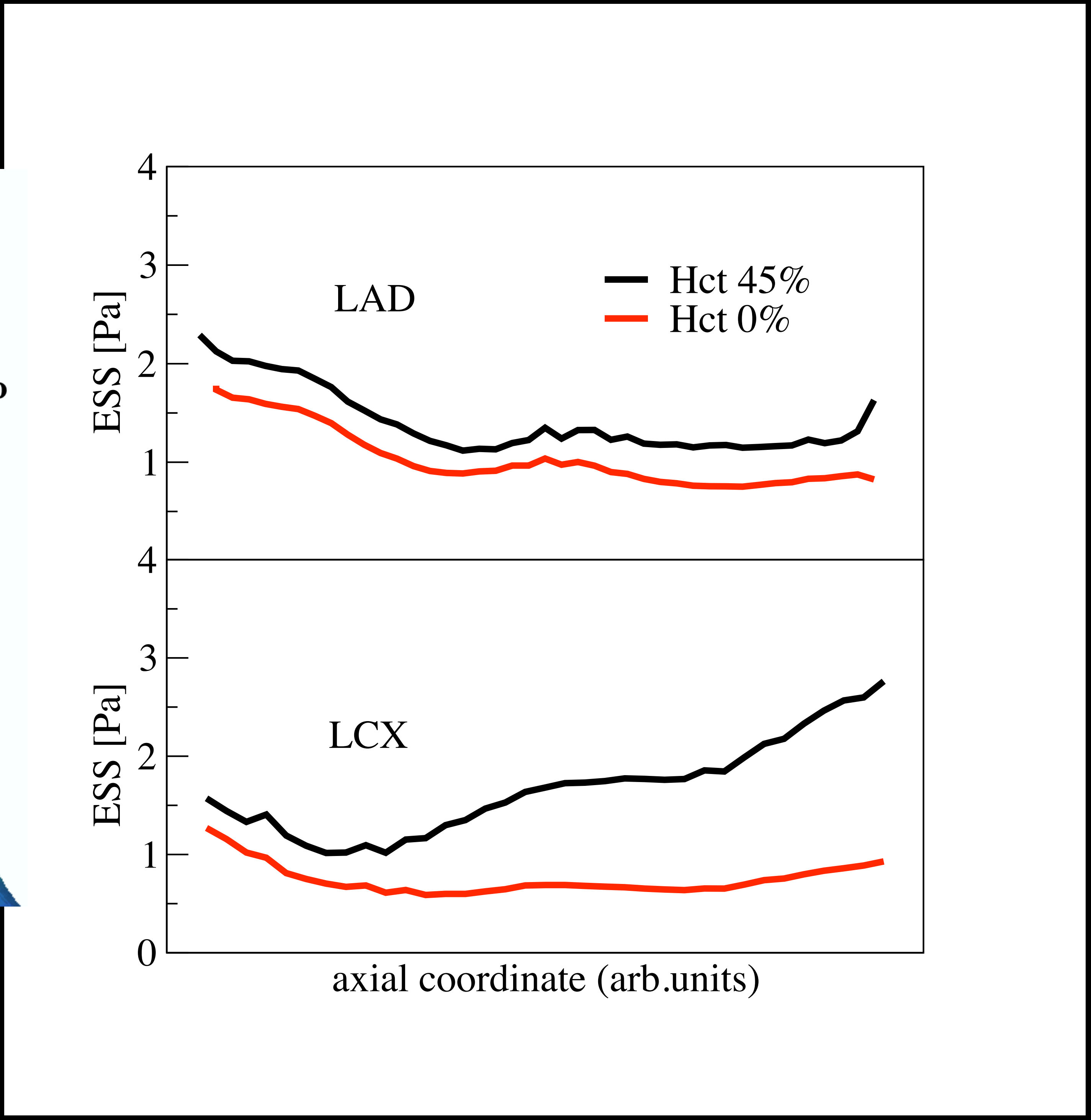
- Average of 0.7 seconds
- 300 million RBC's
- 294,912 processors
- Simulation took:
    - 6 hours
    - 2,000,000 compute hours

Peters, et al. Supercomputing, 2010

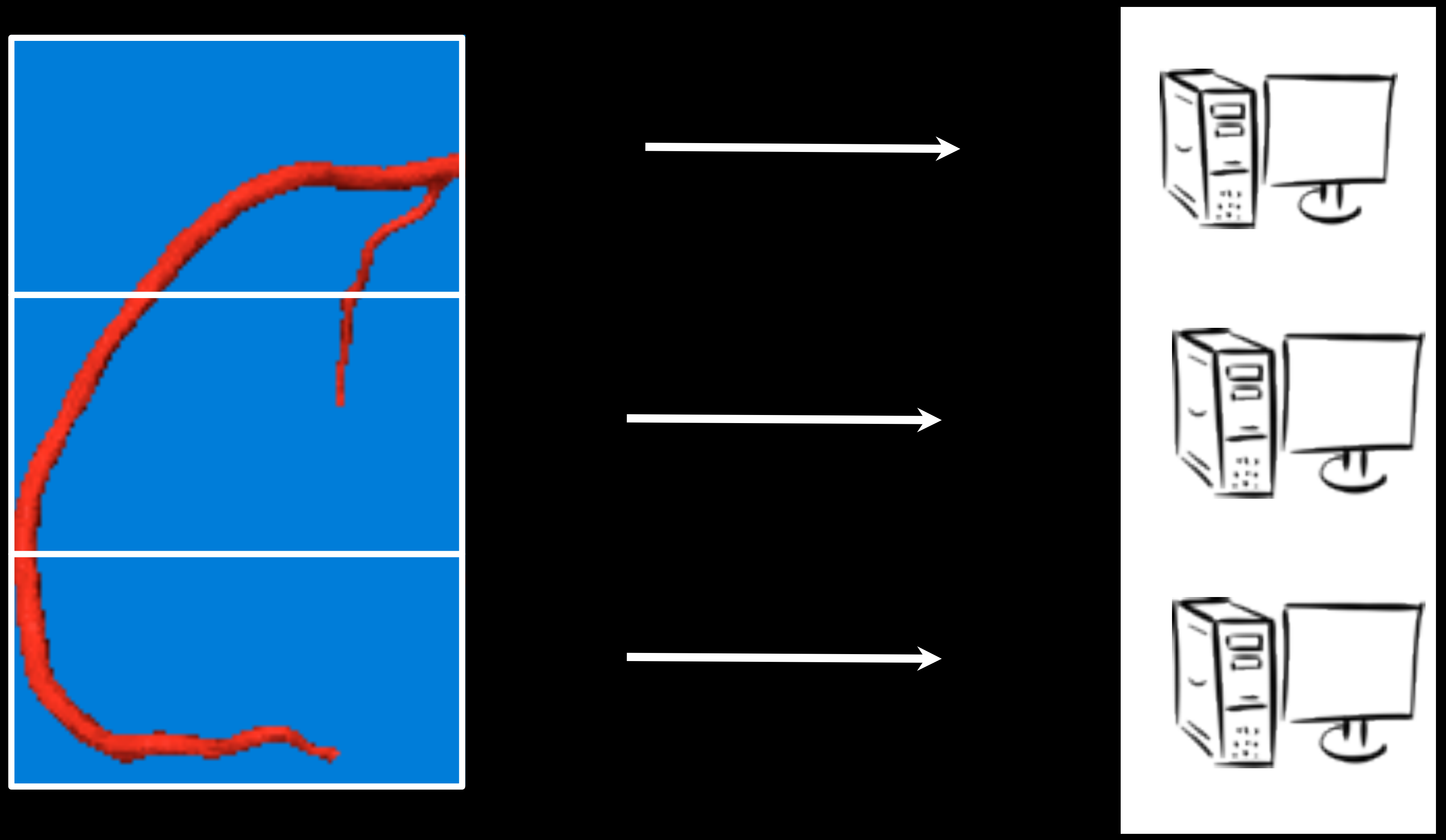
Effect of particle motion on ESS:



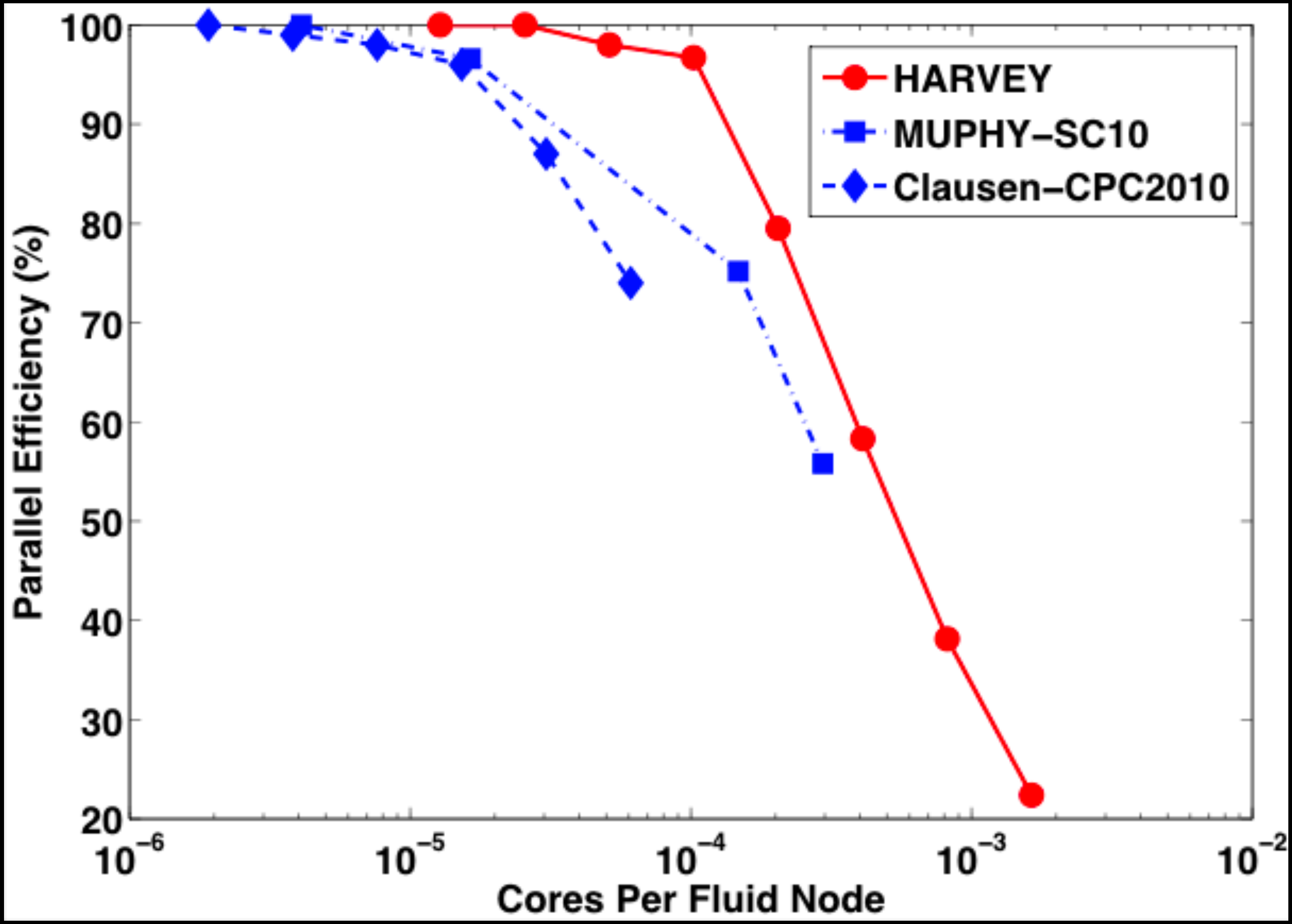




So far: spatial decomposition



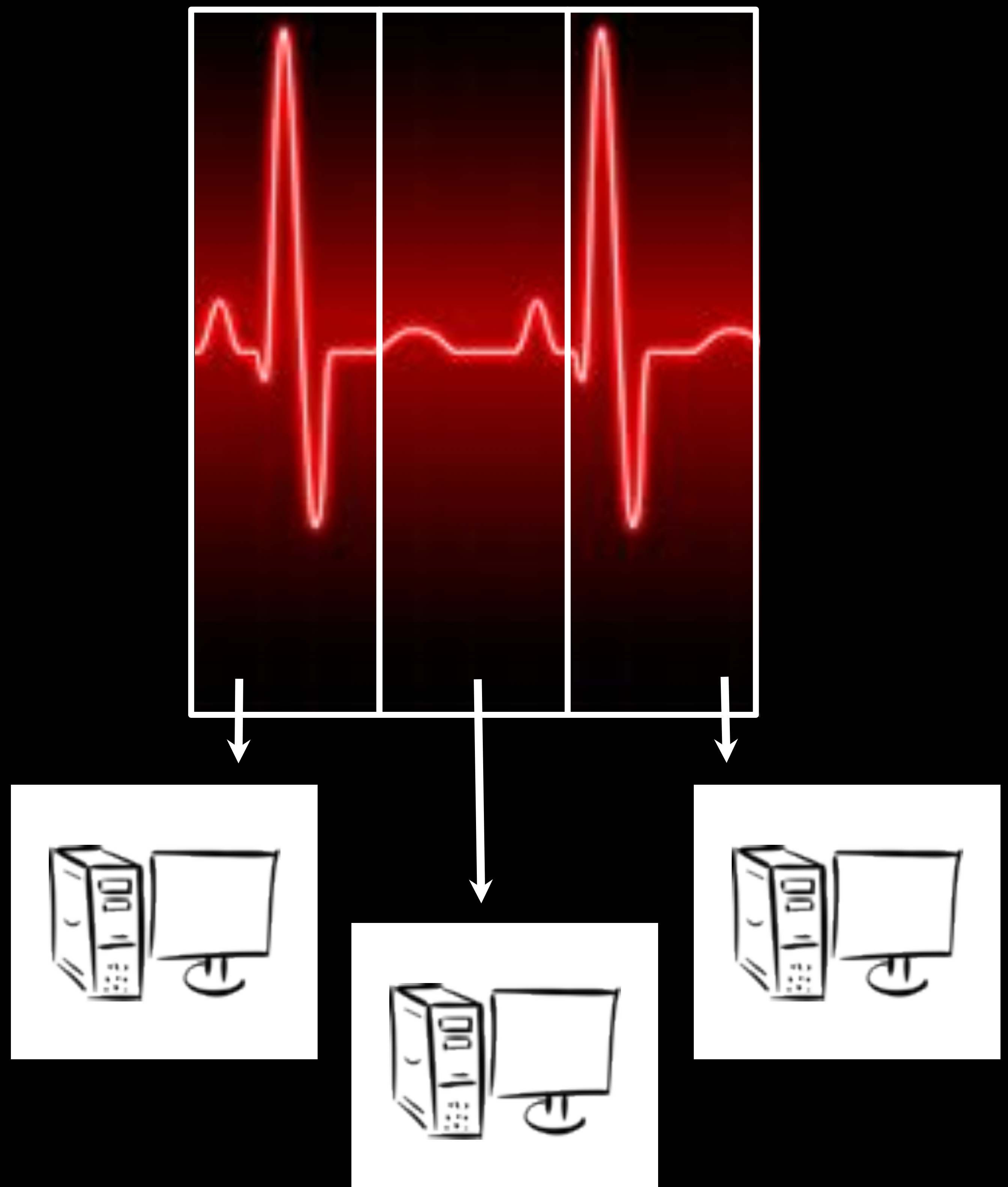
Spatial Scaling Limit

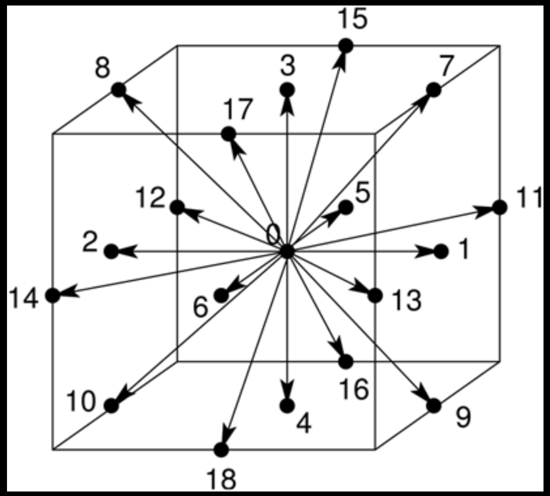


Peters Randles, et al. Supercomputing, 2013 (submitted)

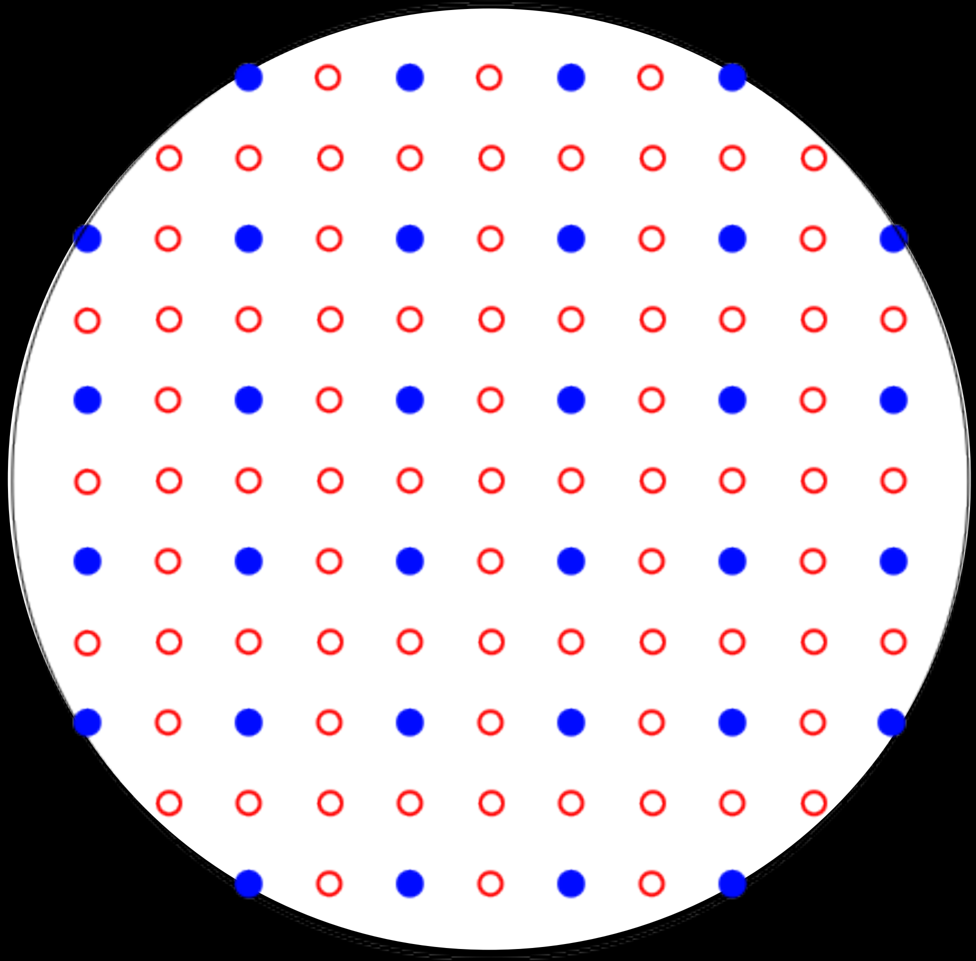
Peters Randles, et. al. IPDPS 2013
Peters, et al. Supercomputing, 2010
Clausen, et al. Computer Physics Communications, 2010

Goal: reduce wallclock time by parallel-in-time simulations



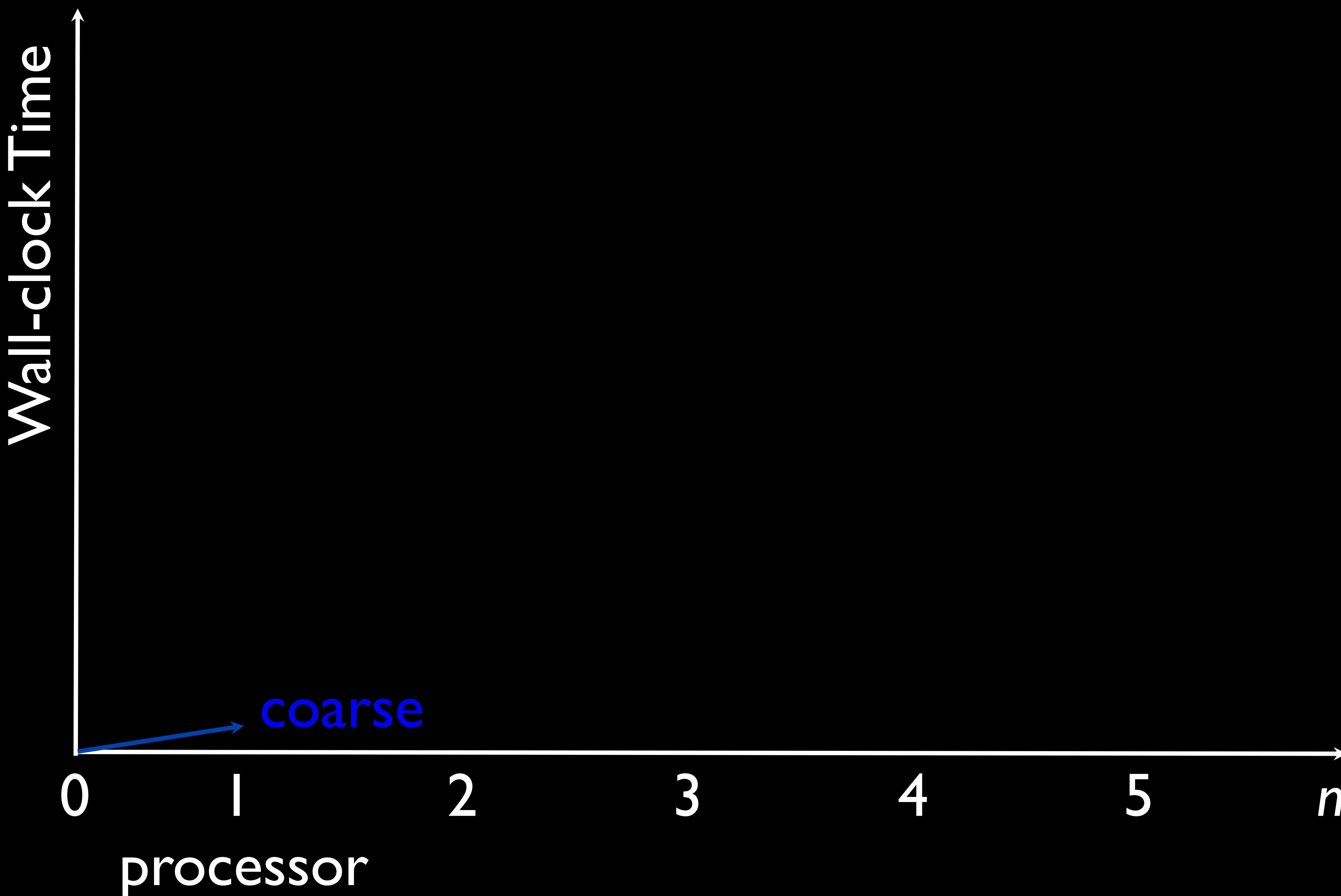


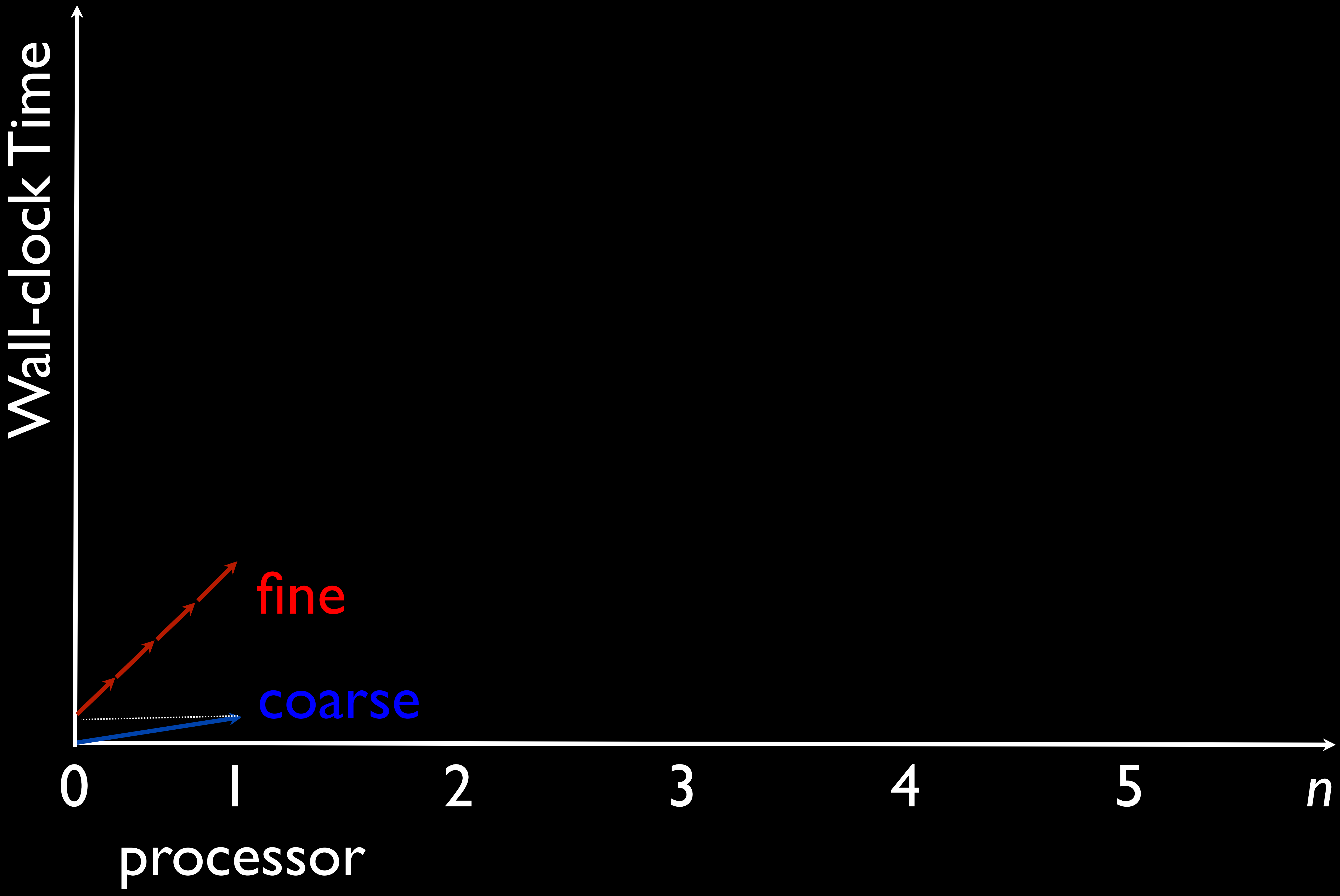
Parareal simulation for Lattice Boltzmann Equation

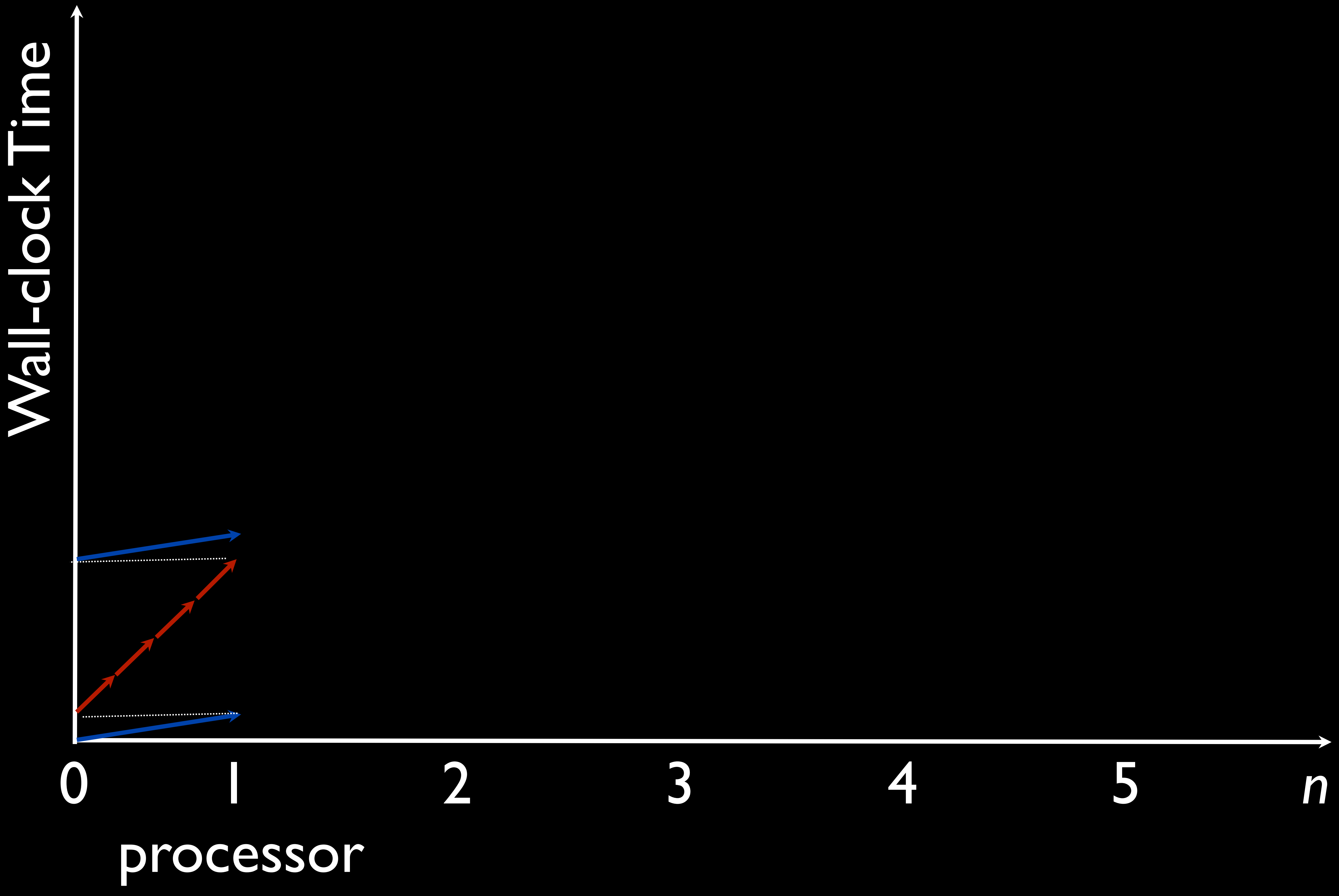


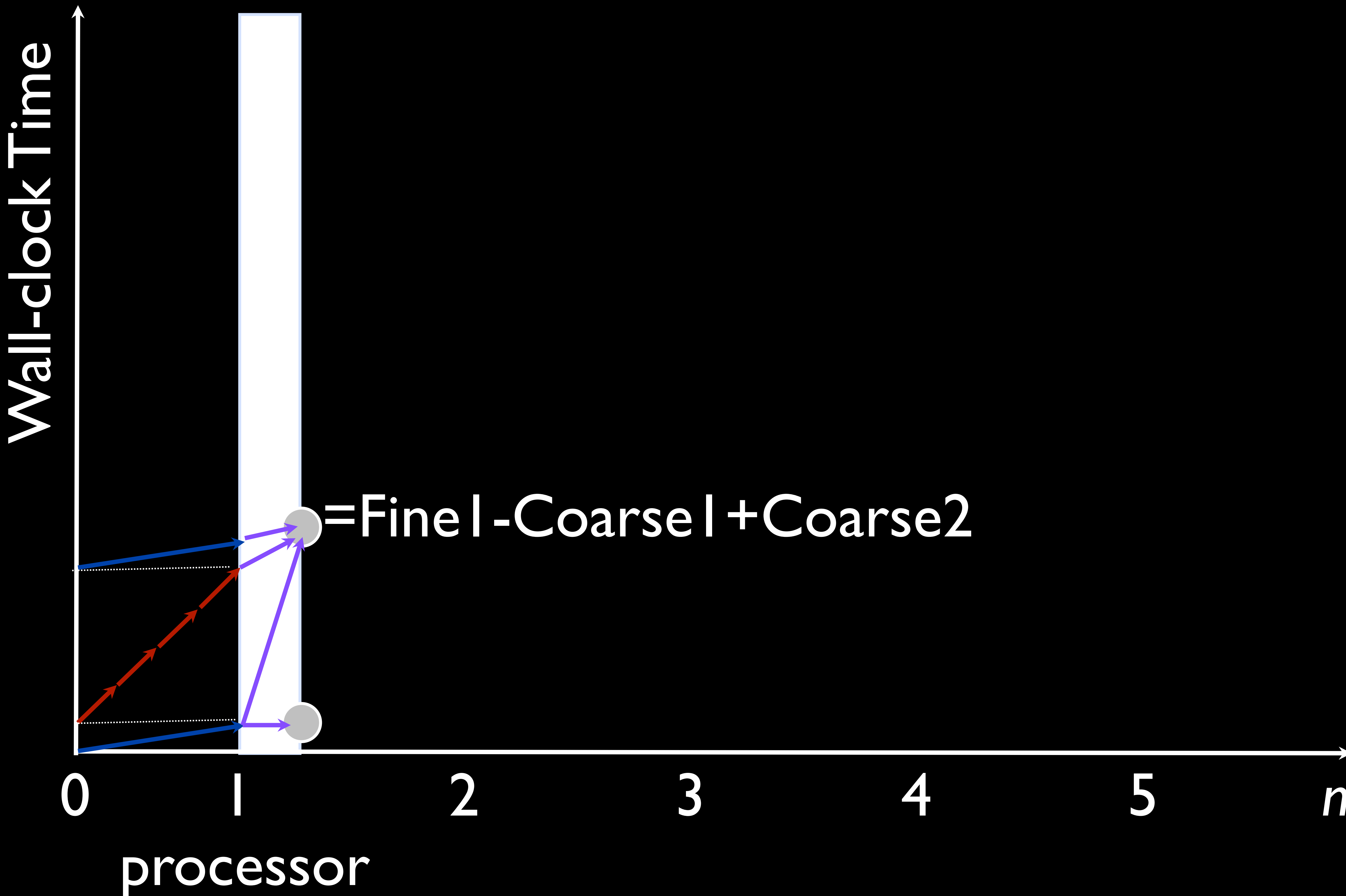
Grid Refinement

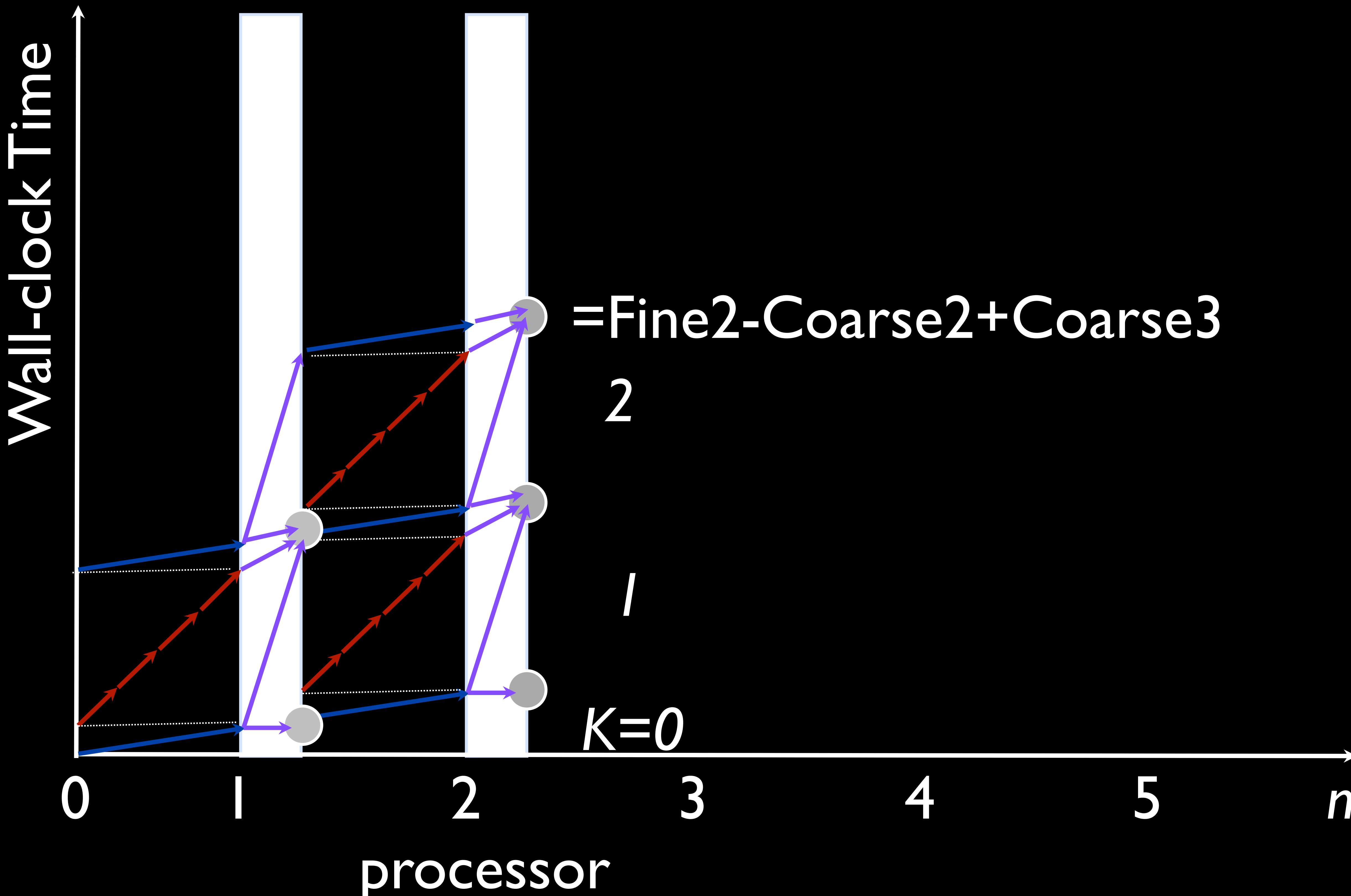
- Address stability and accuracy concerns
- Coarsening and extrapolating schemes
- Careful coupling between fine and coarse solver


Wall-clock Time
coarse
0
1
2
3
4
5
n
processor

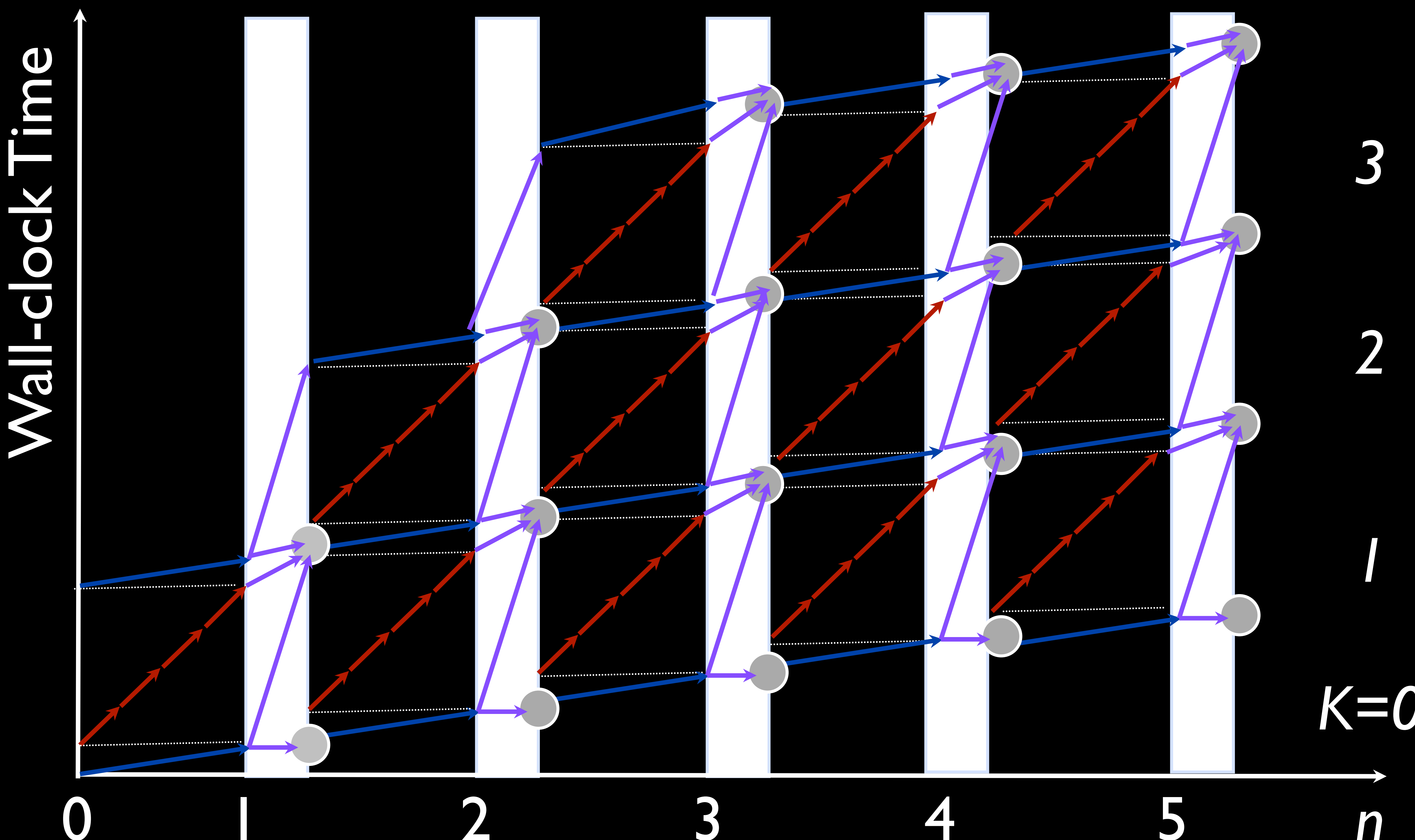

Wall-clock Time
fine
coarse
0
1
2
3
4
5
n
processor


Wall-clock Time
0
1
2
3
4
5
n
processor


Wall-clock Time
=Fine1-Coarse1+Coarse2
0
1
2
3
4
5
n
processor

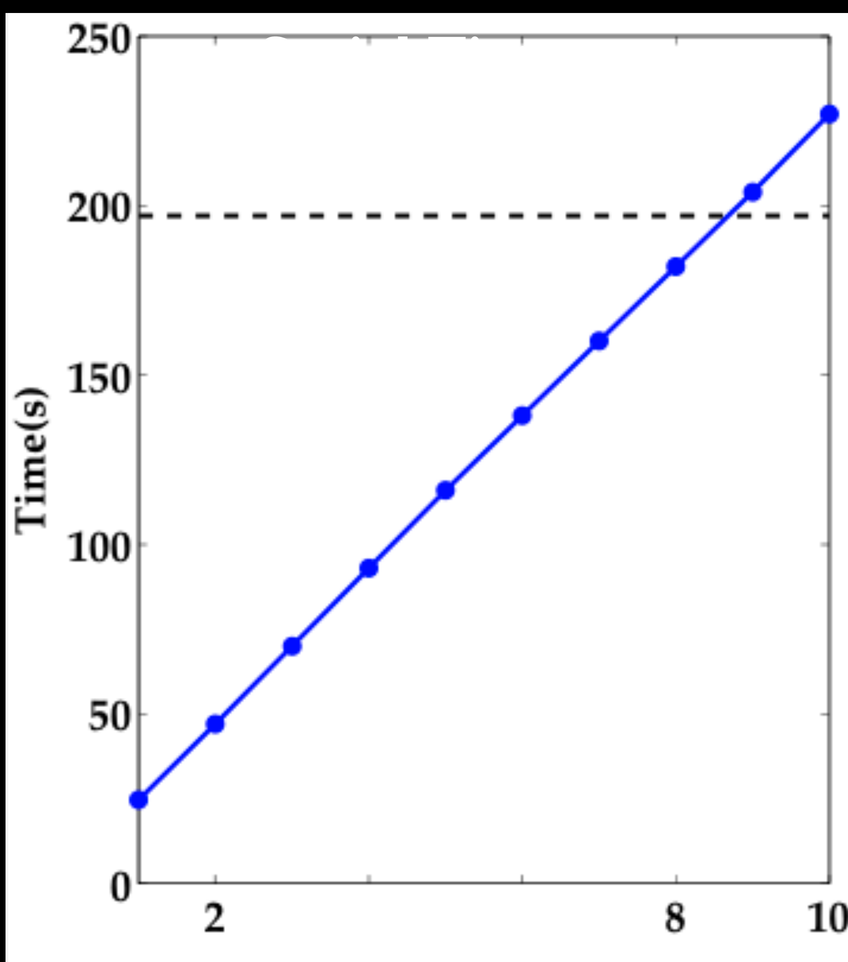


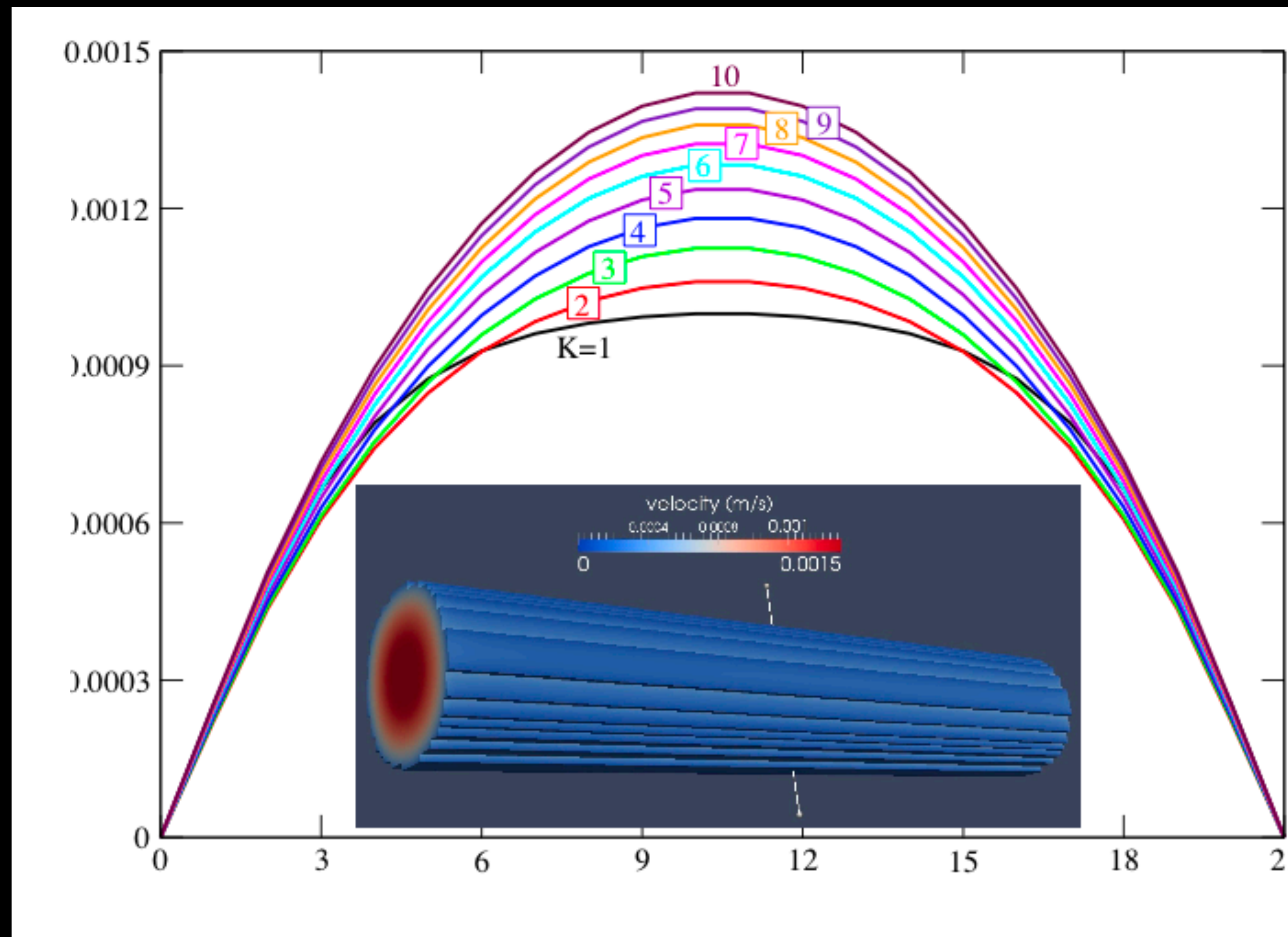
Wall-clock Time
=Fine2-Coarse2+Coarse3
2
1
K=0
0
1
2
3
4
5
n
processor



Wall-clock Time
3
2
1
K=0
0
1
2
3
4
5
n

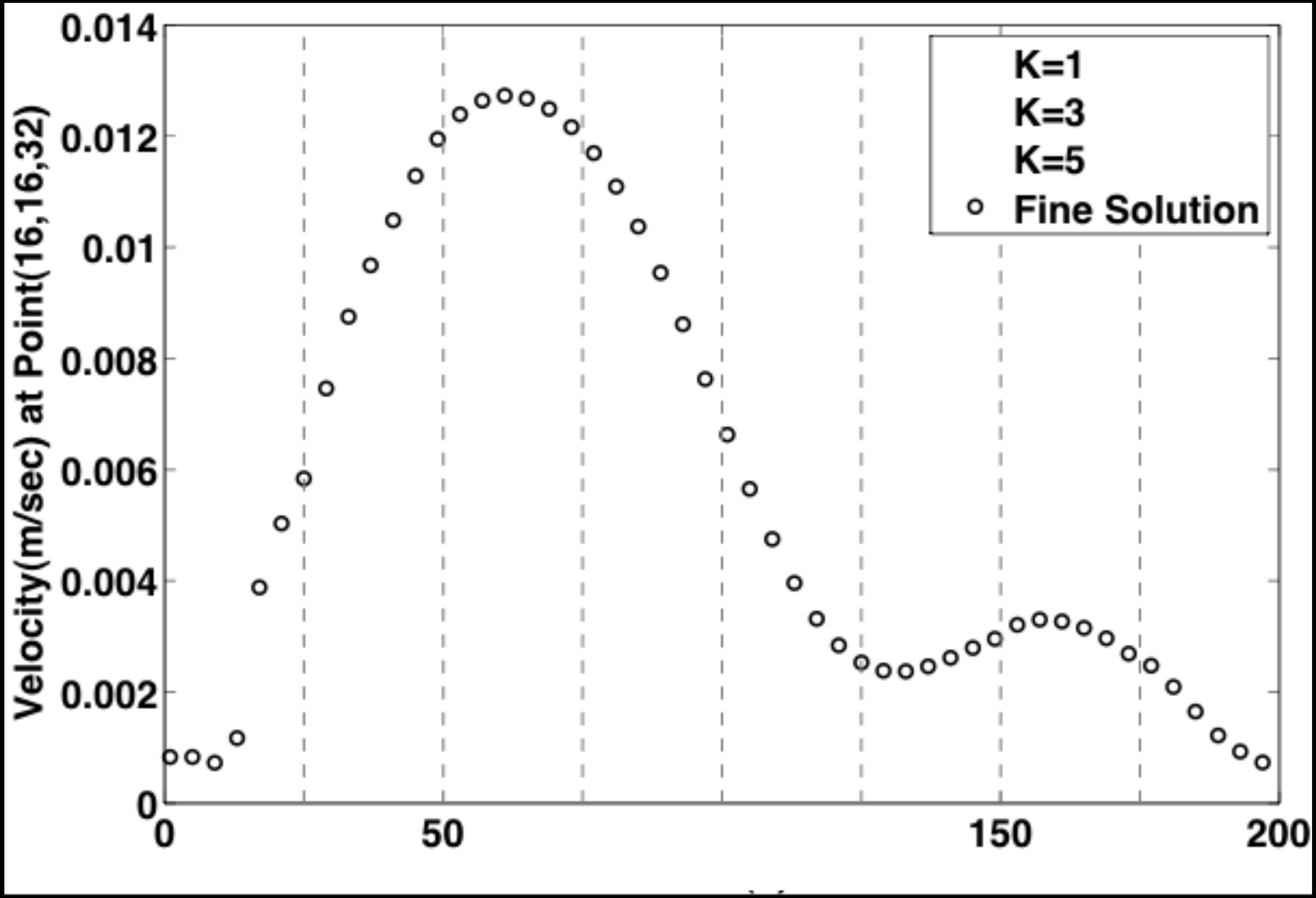
Runtime vs. Accuracy





Peters Randles et al., Journal of Computational Physics, 2013 (submitted)

Time Dependent Phenomena



Peters Randles, et al. Supercomputing, 2013 (submitted)

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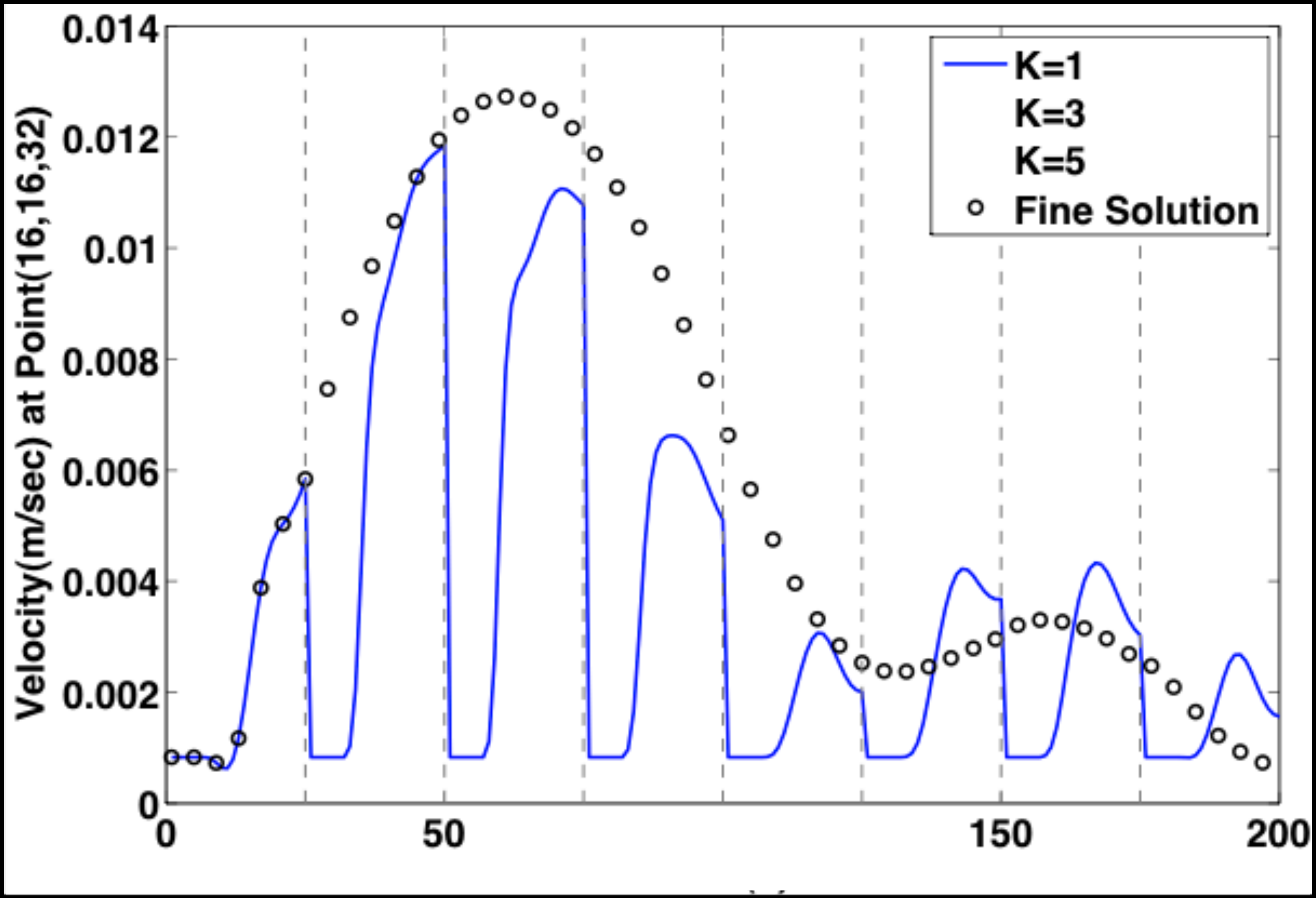

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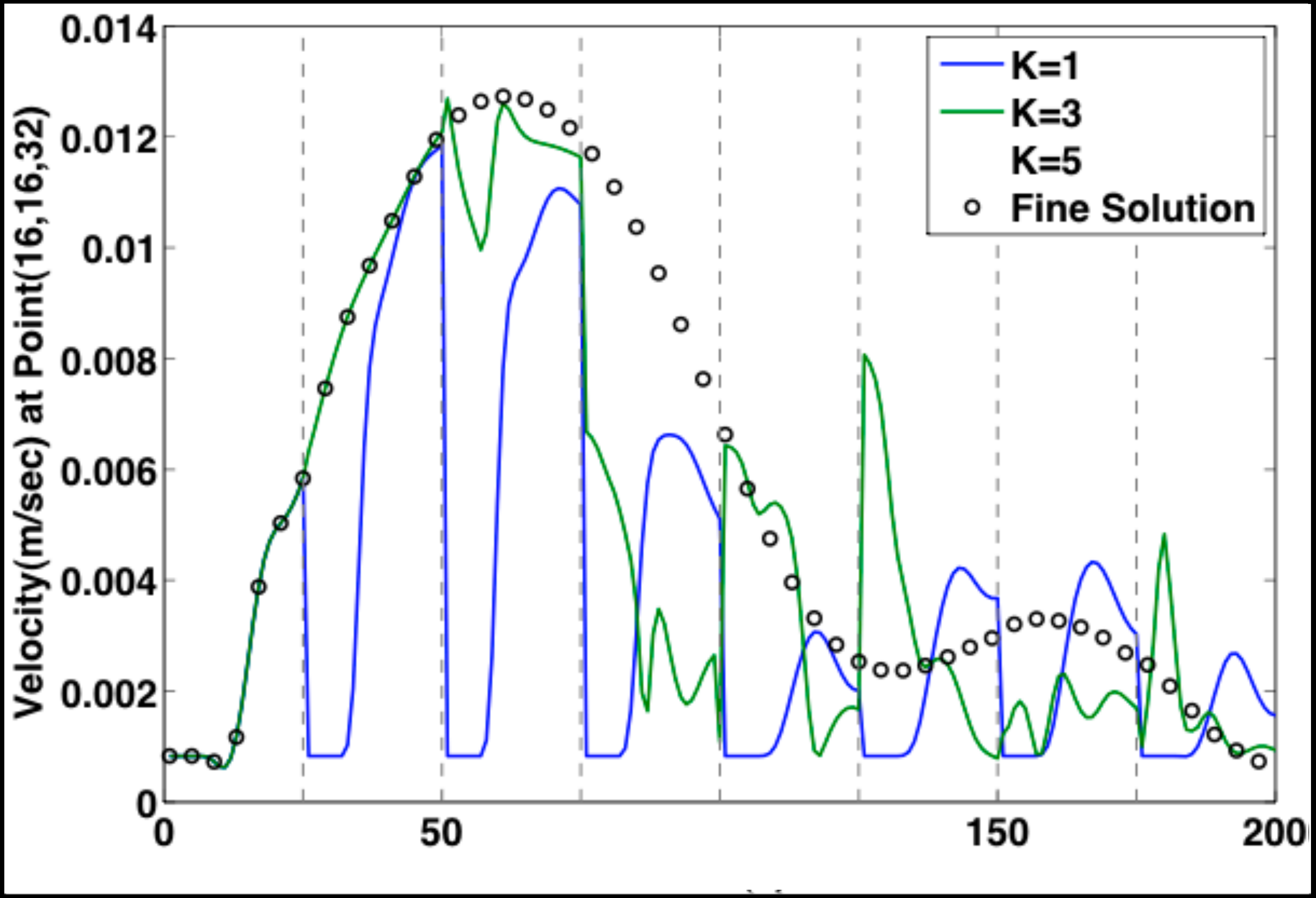
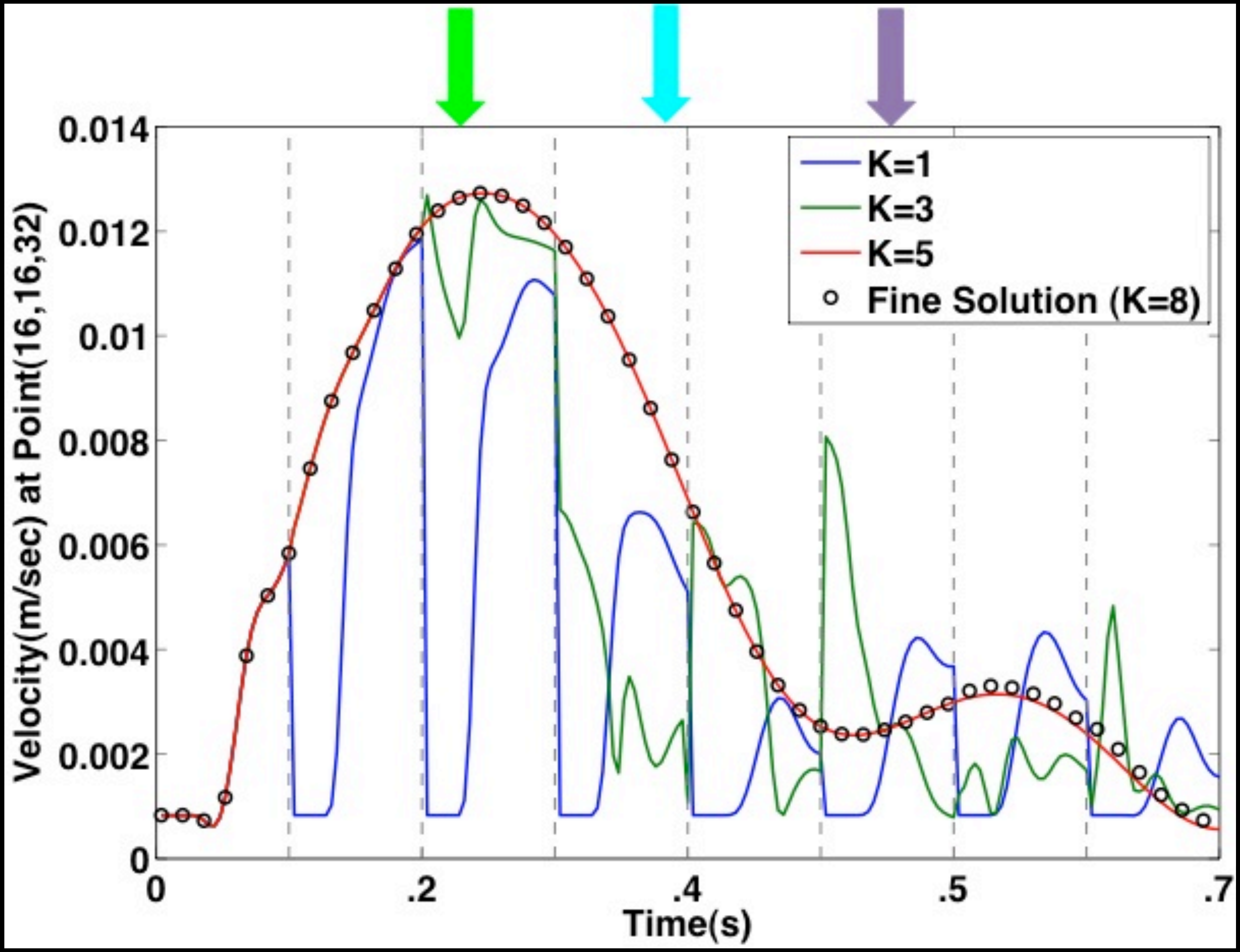


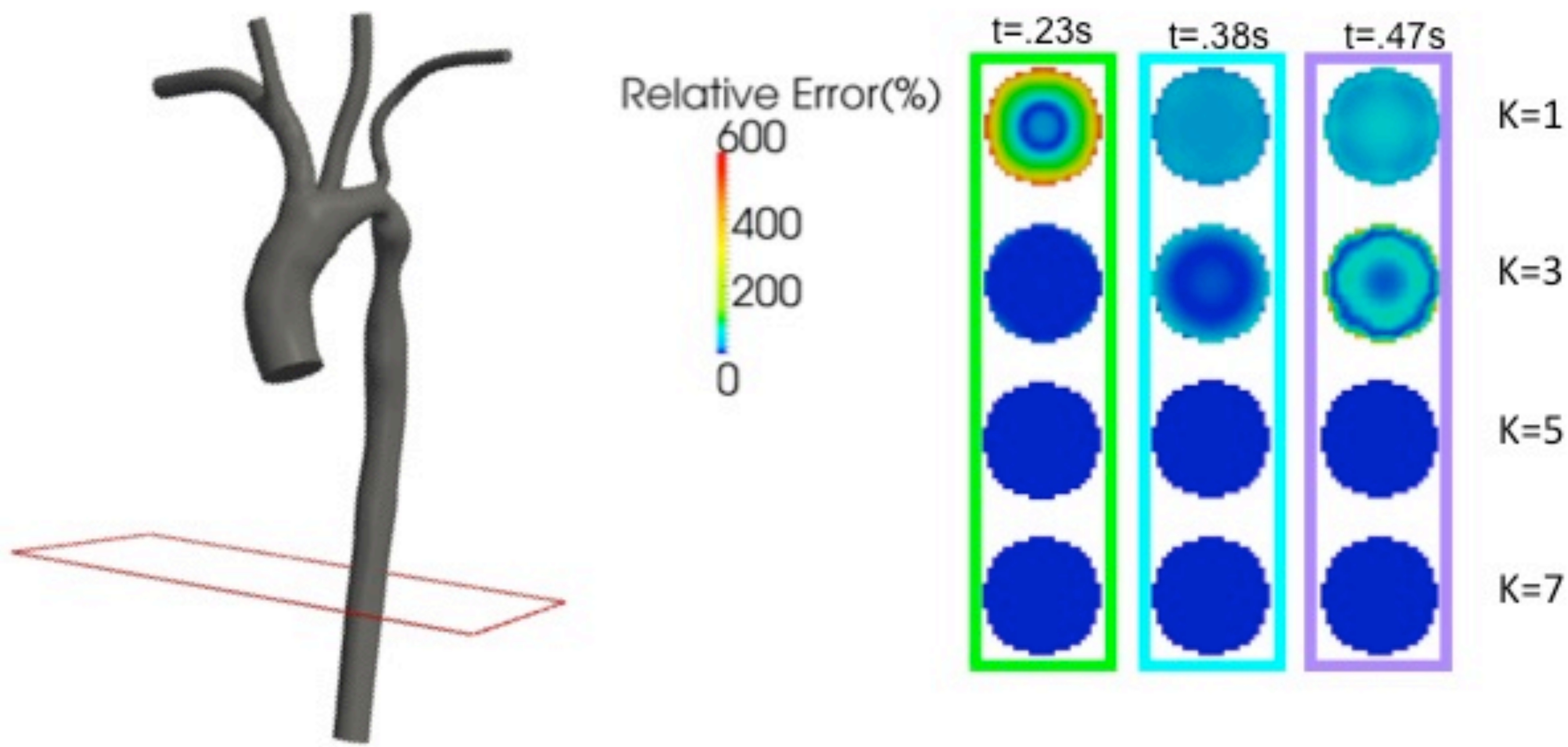
Peters Randles, et al. Supercomputing, 2013 (submitted)

Time Dependent Phenomena



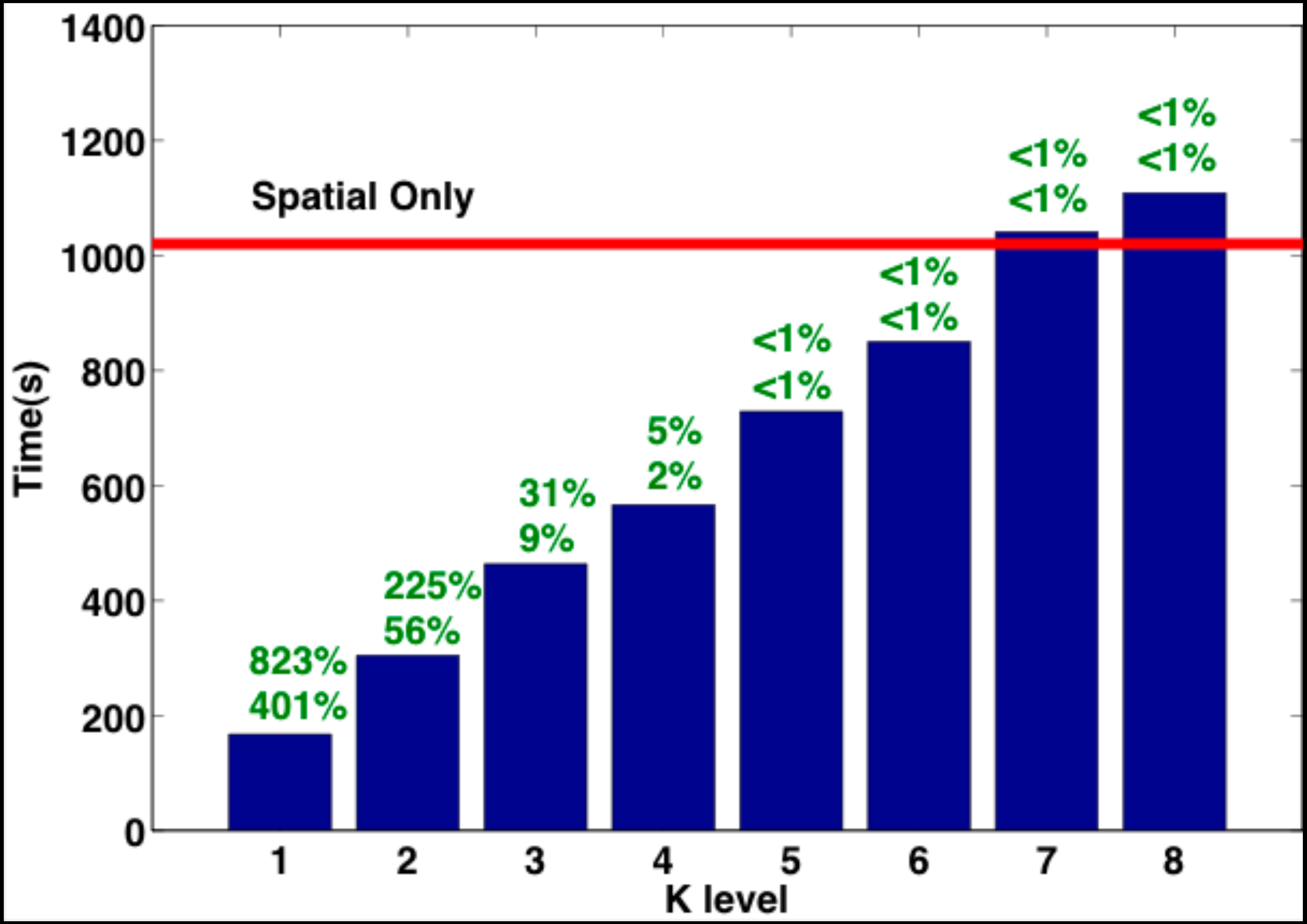
Peters Randles, et al. Supercomputing, 2013 (submitted)

Relative Error



Peters Randles, et al. Supercomputing, 2013 (submitted)

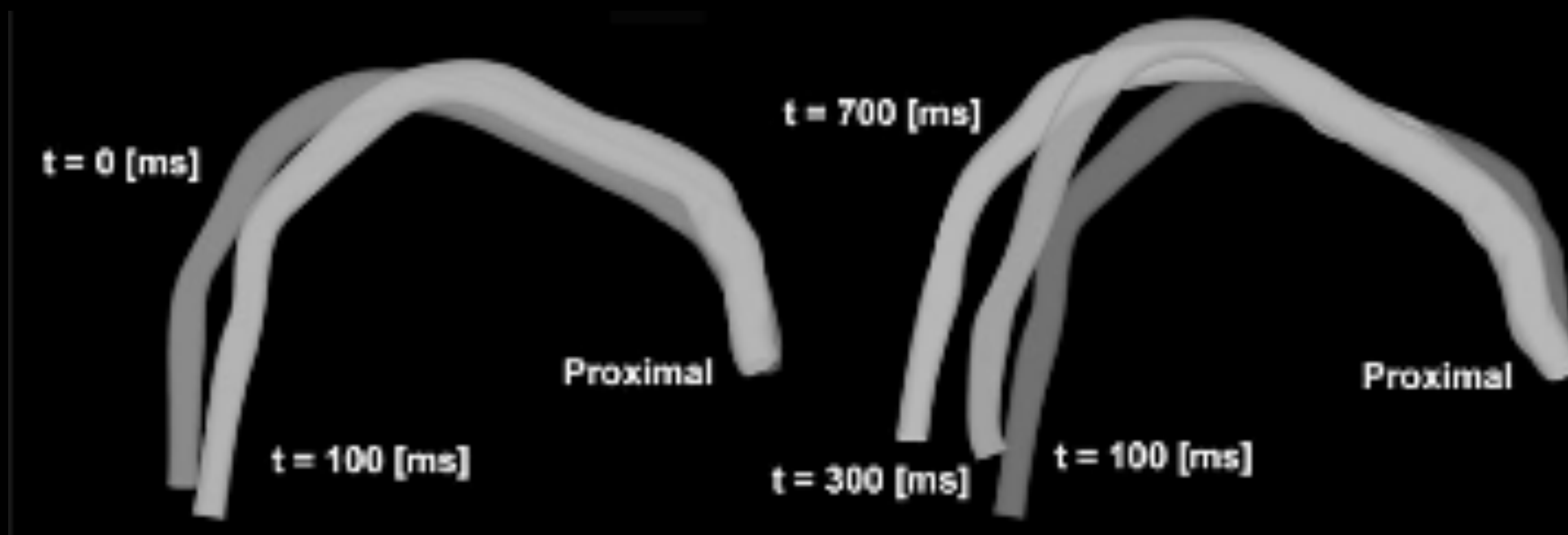
Time-to-Solution



Peters Randles, et al. Supercomputing, 2013 (submitted)

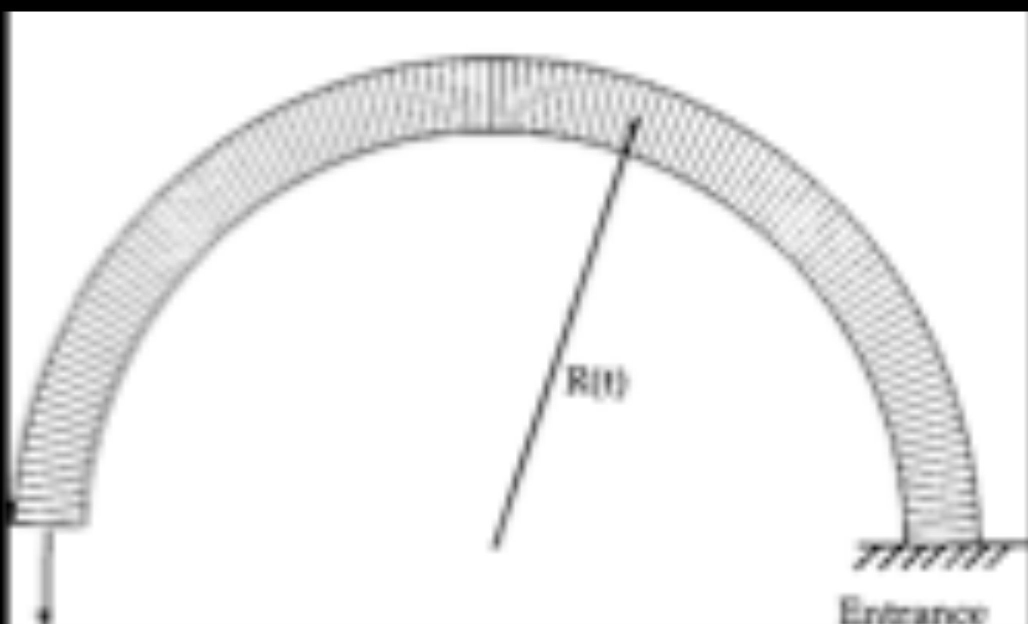
32,768 Cores of the IBM Blue Gene/P

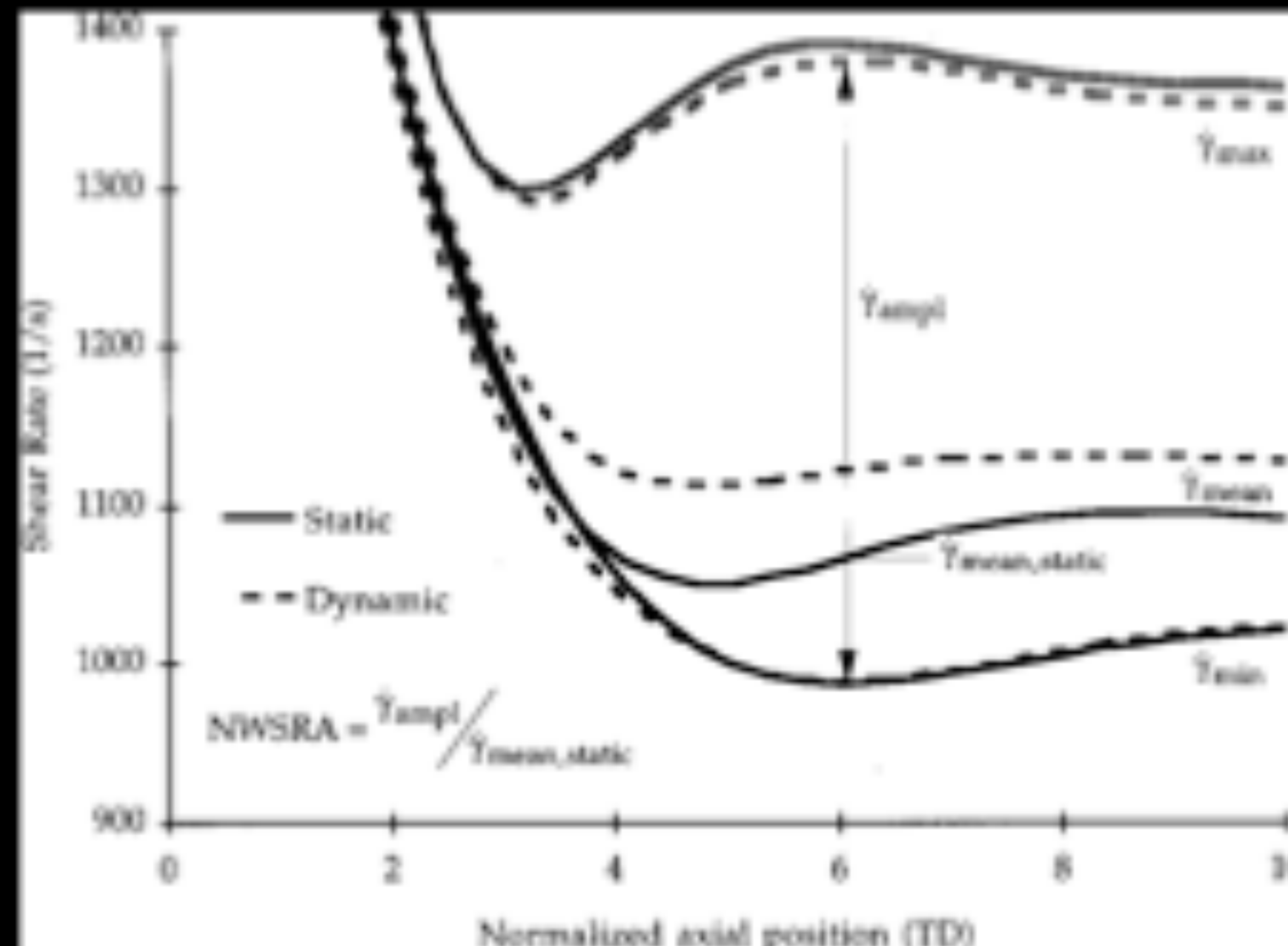
Curvature Change Over One Heartbeat



Torri et al. Annals of Biomedical Engineering, 2010
Santamarina *et al.* Annals of Biomedical Engineering, 1998

Wall Shear Rate Impact

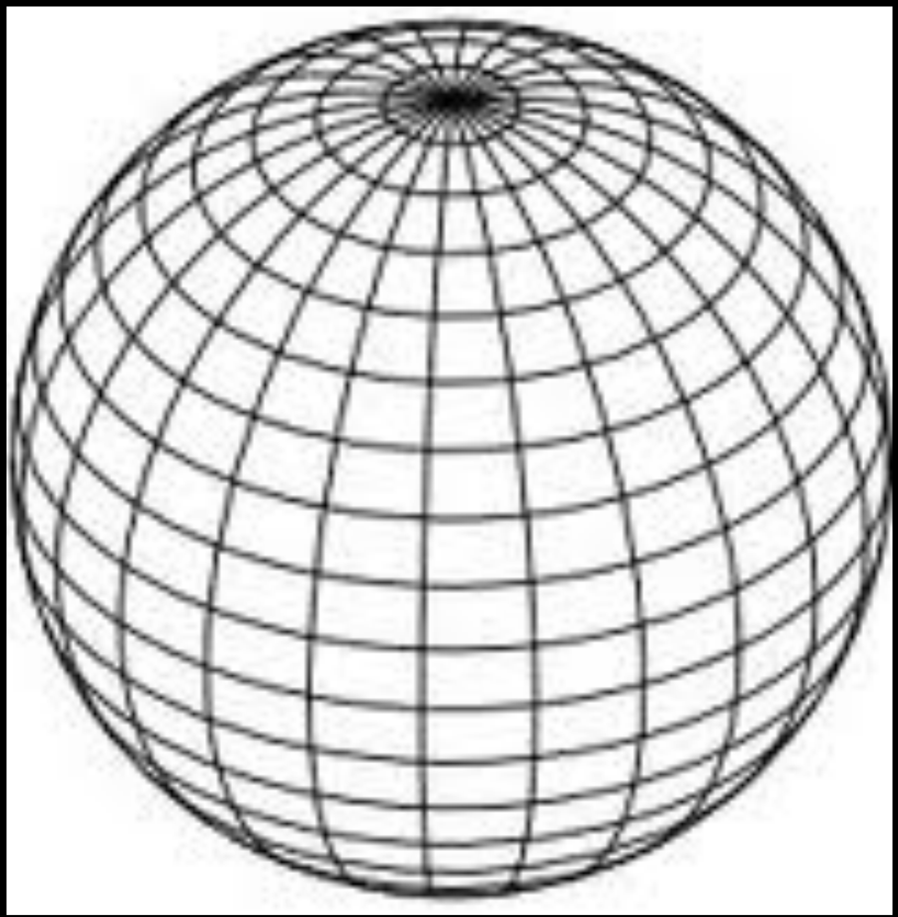




Santamarina *et al.* Annals of Biomedical Engineering, 1998

Wall Shear Rate varied as much as 52%

Fluid modeling on a moving mesh



- General relativity formulation
- Bernstein model for the expanding universe
- Lattice Boltzmann implementation

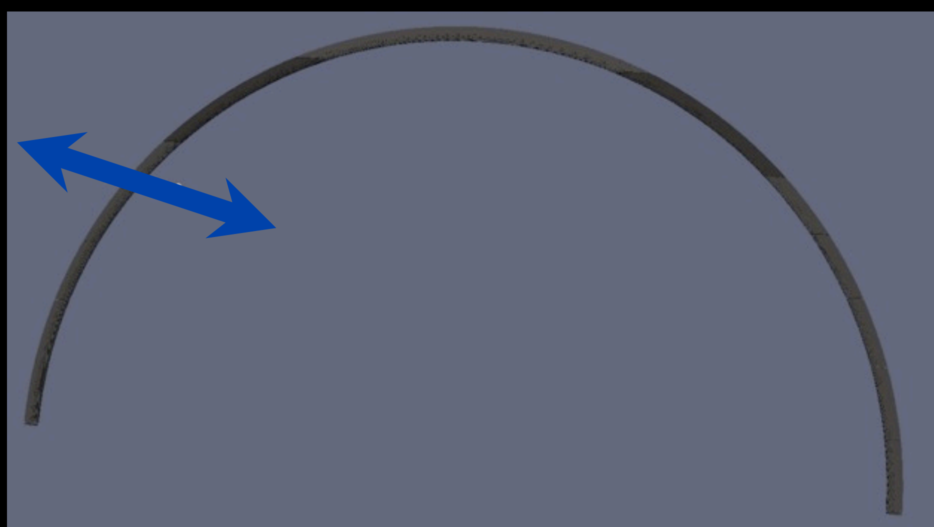
Force Term

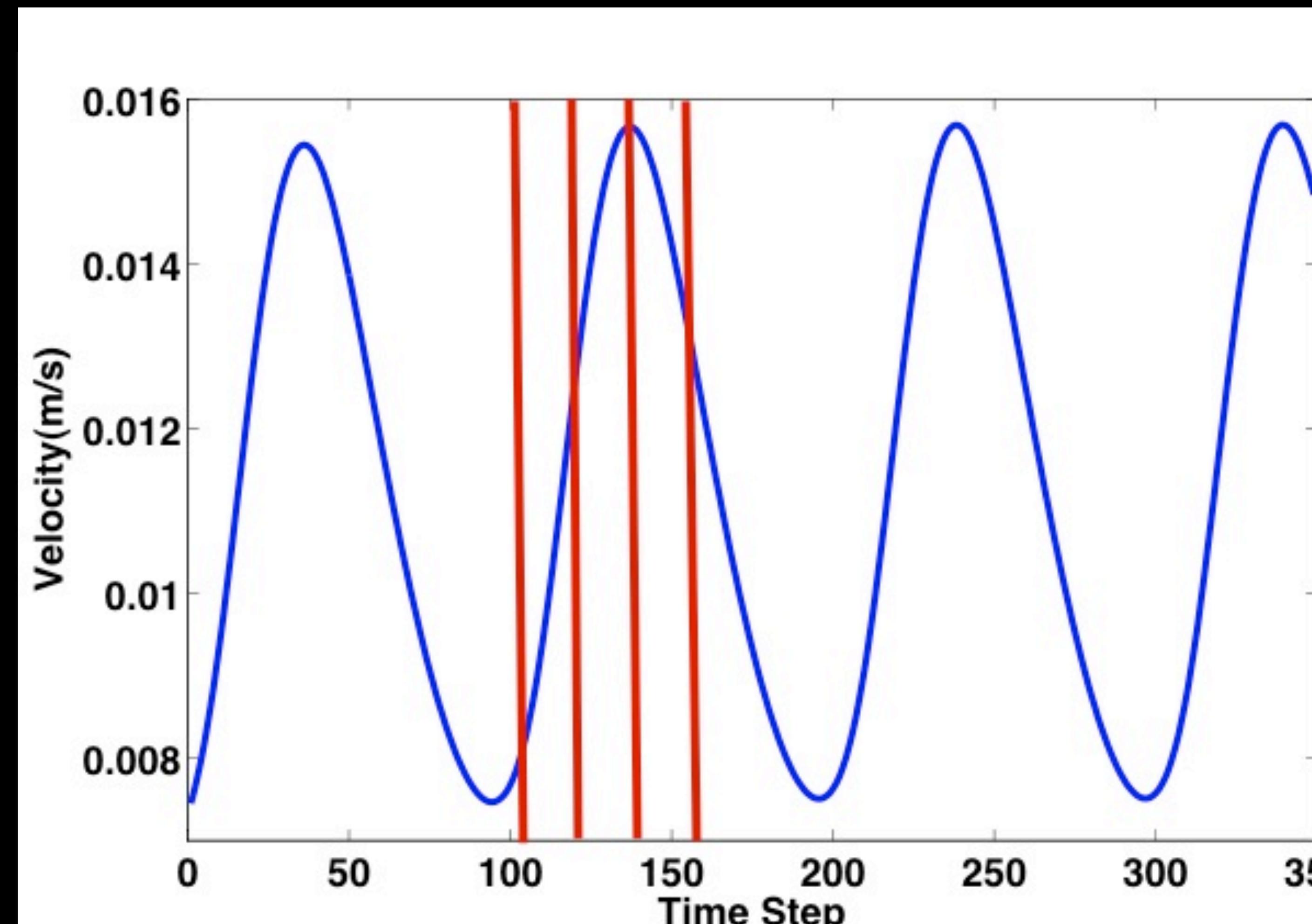
$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = f_i(\vec{x}, t) - \omega \Delta t (f_i - f_i^{eq})(\vec{x}, t) + \vec{g} \cdot \partial v f$$

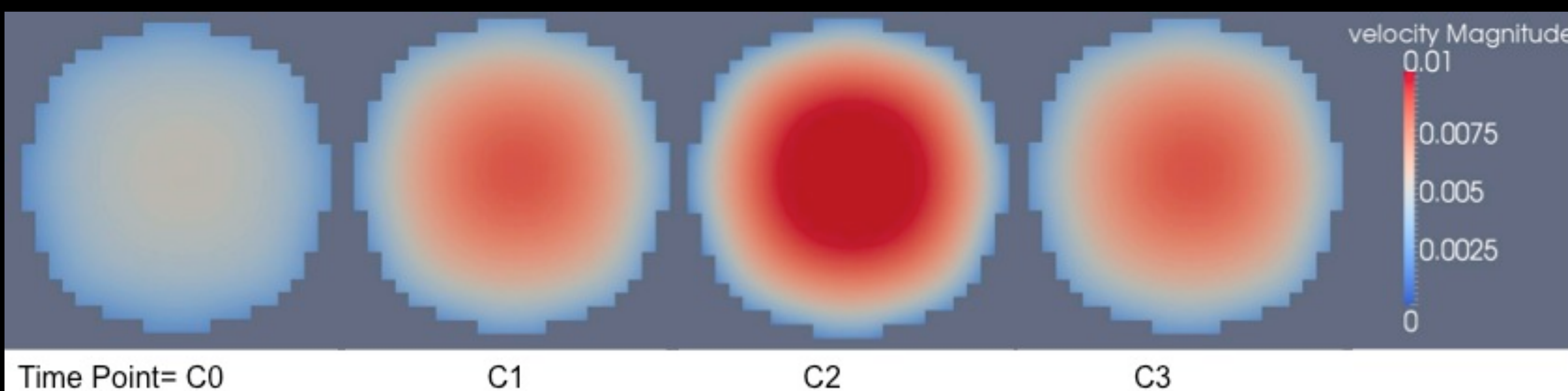
External Force

Deformational Force in Continuum Space: $\vec{g} = -\frac{\dot{R}}{R} \vec{v}$

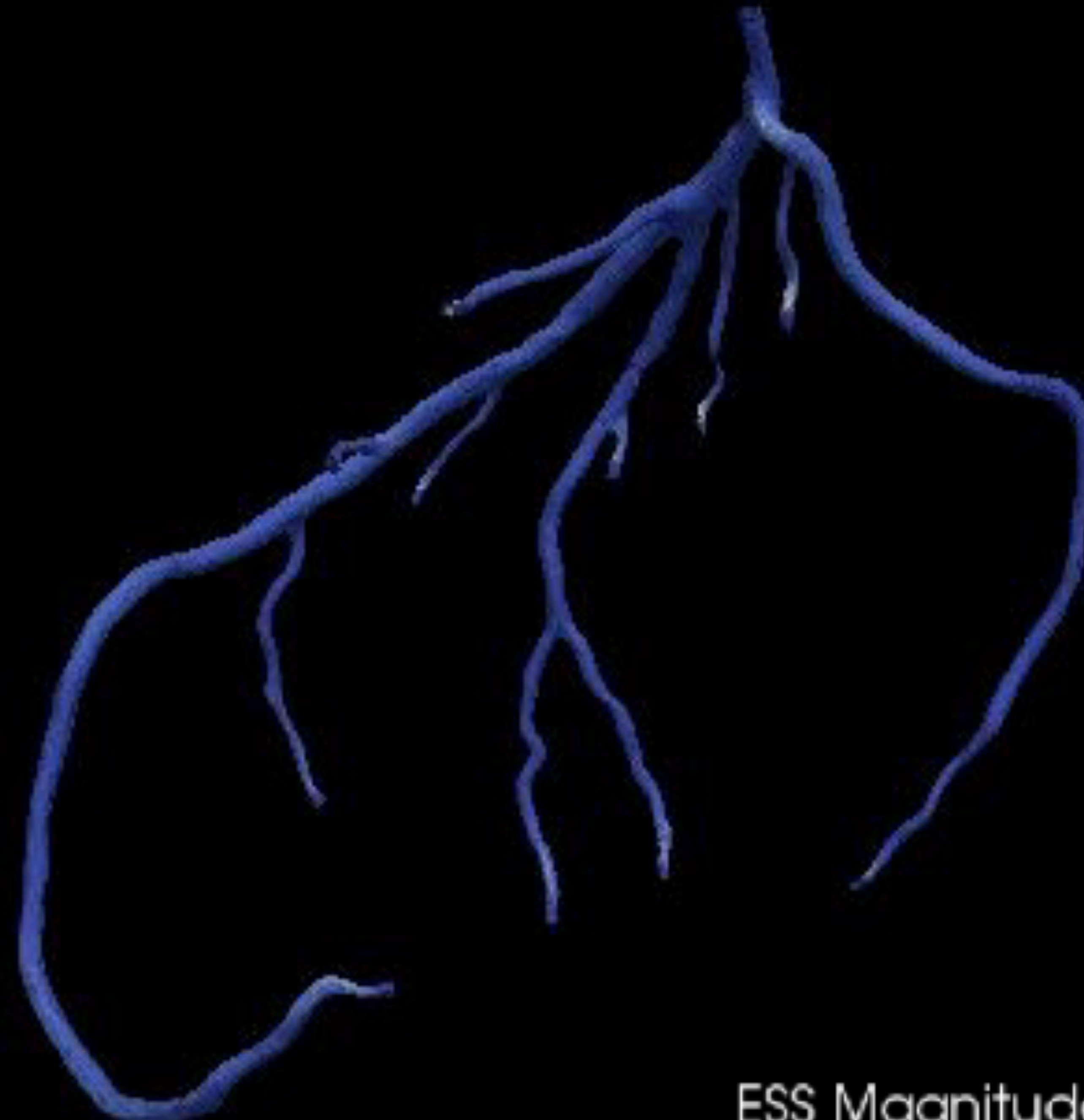
Sinusoidal Expansion



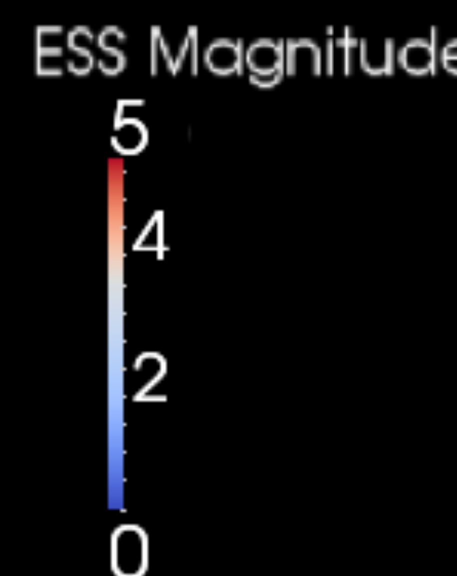




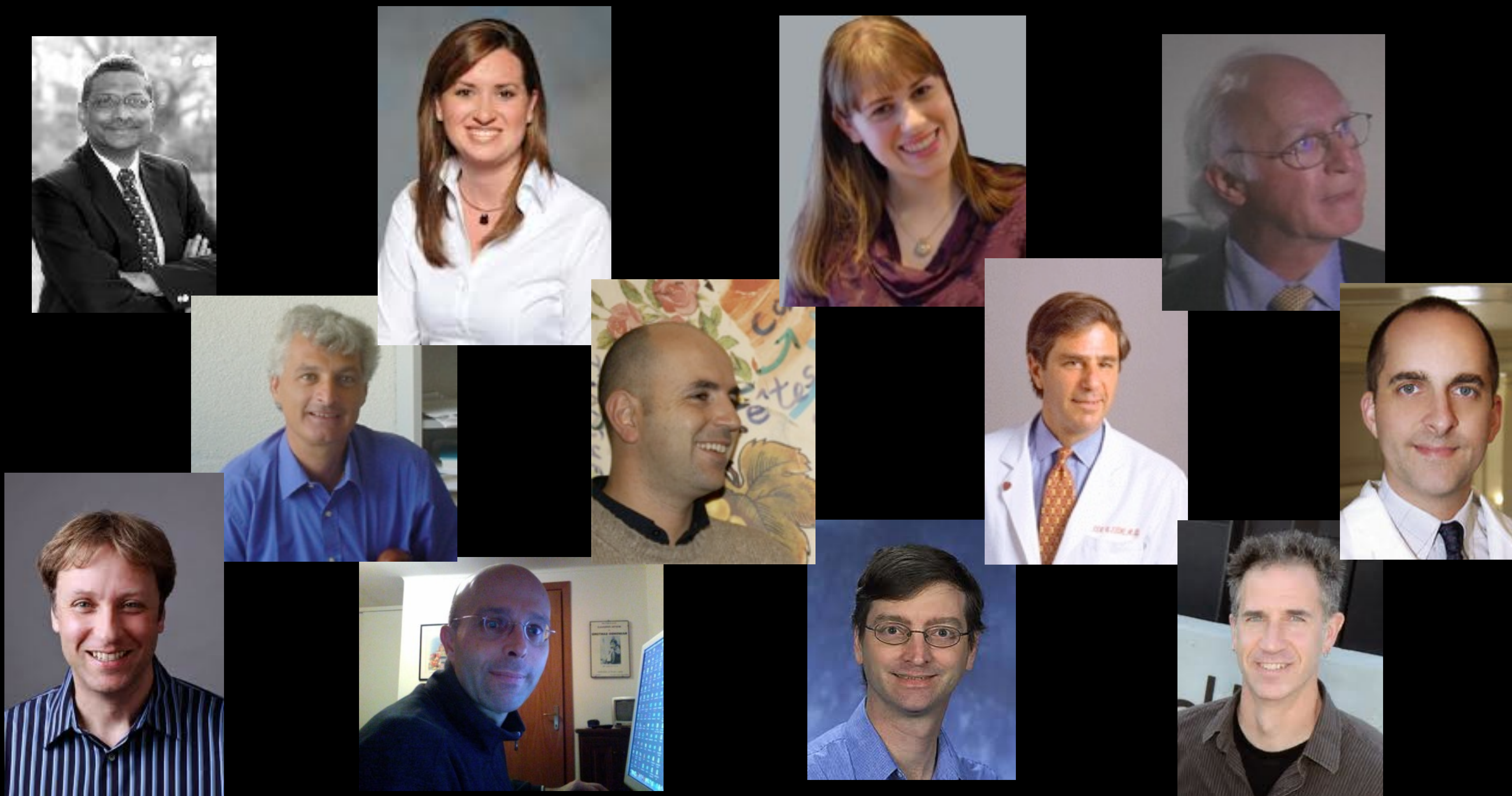
Static



With deformational force



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