INTERNATIONAL CONFERENCE ON EMERGING TECHNOLOGIES TO COMBAT THE COVID-19 PANDEMIC

1 December 2020, Guangzhou, China (Hybrid event)

Leveraging 4th Industrial Revolution (4IR) Technologies in the Fight Against COVID-19

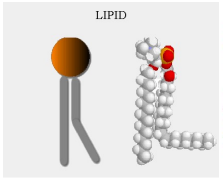
Xue-Feng Yuan CPhys FInstP FRSC

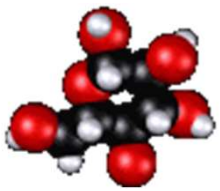
The Asia-Pacific Regional Innovation Knowledge Network for 4th Industrial Revolution Technologies (APRIKNET-4IR)

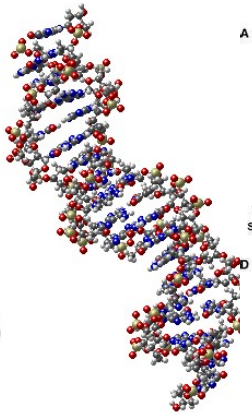
Guangzhou University, P. R. China

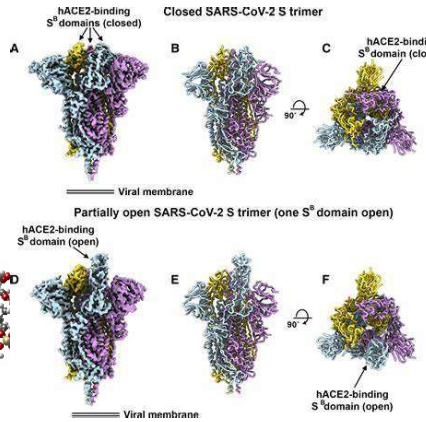
Email: xuefeng.yuan@gzhu.edu.cn

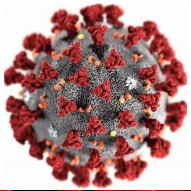
Molecules → Complex Systems

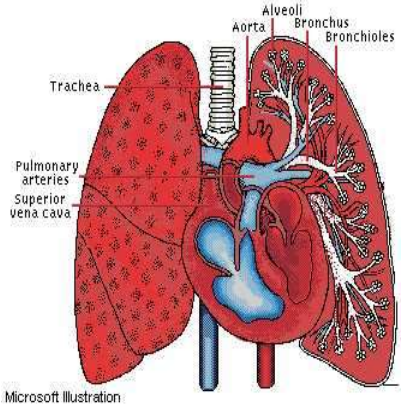


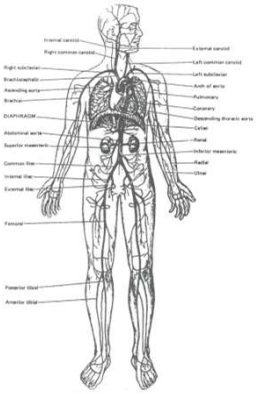




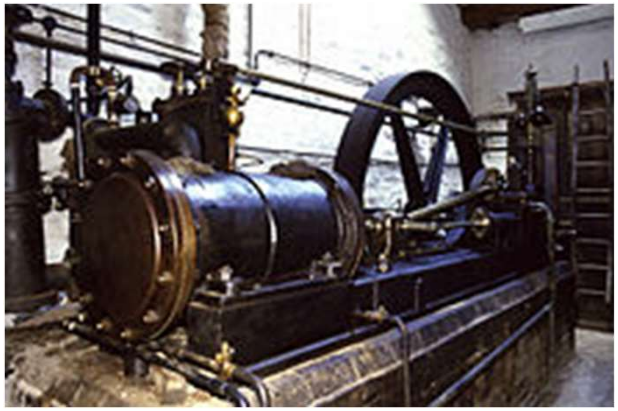








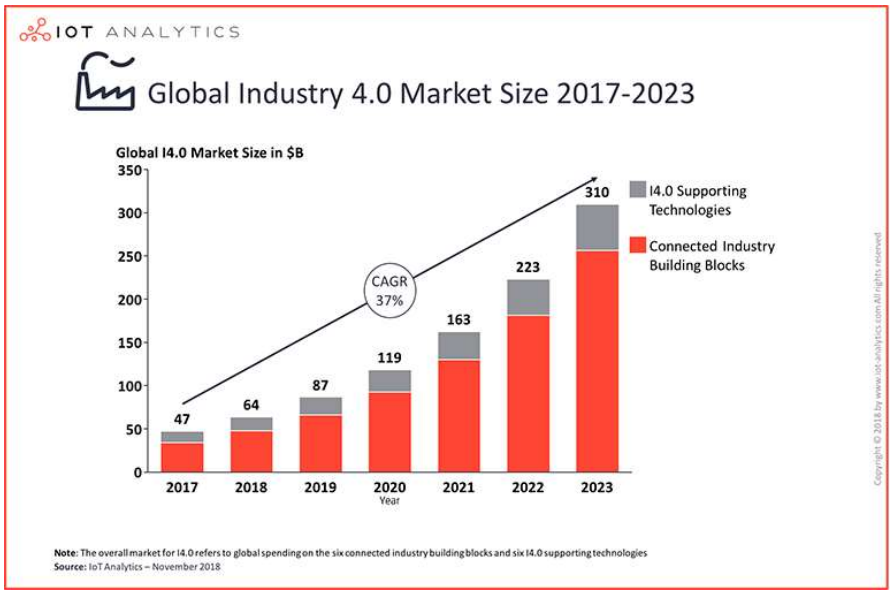
The 4th Industrial Revolution Driven by Innovation



The 1st Industrial Revolution: Steam engines

The 2nd Industrial Revolution: Large scale manufacturing

The 3rd Industrial Revolution: Industrial automation



The 4th Industrial Revolution

- Industry 4.0
- China Manufacturing 2025
- Industrial IoT +
- AI +
- 5G +
- HPC + …

An Integrated Cyber Physical System for Intelligent Manufacturing

Physical Platform
Analytical and Measurement to reveal systems dynamics at various time and length scales, Distrubuted Manufacturing Systems

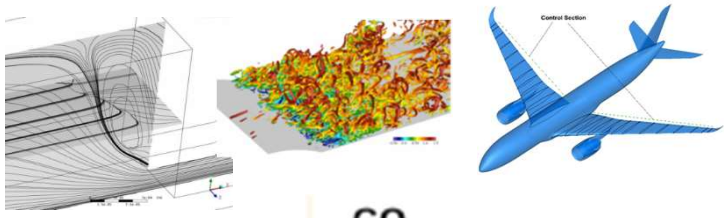
FULLY INTEGRATED Cloud HPC +AI PLATFORM

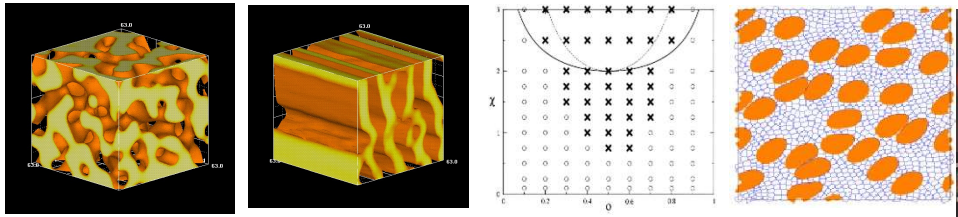
Simulation Platform
Modularized simulation tools for multiple scale modelling of complex systems with molecular, mesoscopic and continuum dynamics

Big Data + AI Platform
Data and text mining, Machine Learning, seamless data flow of various types between physical and simulation platform and big data analytics tools

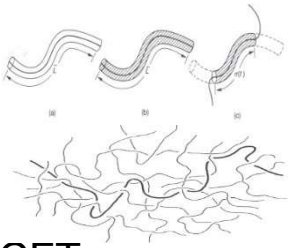
An Integrated Multiple Scale Simulation Platform

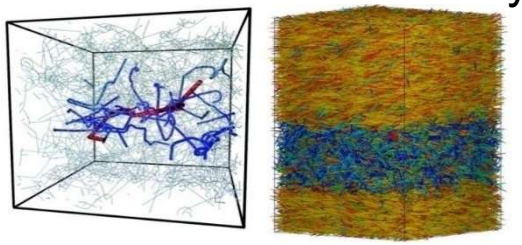
Immersed Boundary Method
Two-fluid Model
Microscopic kinetic models + LBM.
Lagrangian-Eulerian-Stochastic Method





Two-fluid Model (SCFT+Reptation)
Stochastic Entanglement Dynamics
Lattice Boltzmann Methods (LBM)
Smooth Particle Hydrodynamics (SPH)

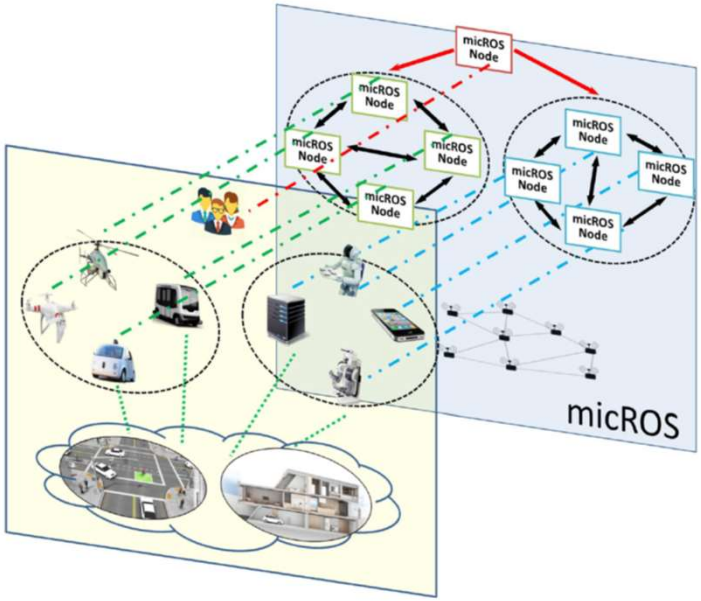




Theoretical approach: SCFT
Kinetics of signalling and metabolic pathways
Coarse-grained Monte Carlo (MC) and Molecular Dynamics (MD) and Non-equilibrium MD
Car-Parrinello MD, Quantum MC

Length
10^{-3} m
10^{-9} m
10^{-9} sec
Time
10^{3} sec

“AI+HPC+5G” based Digital Twins Technologies for Intelligent Manufacturing




Heavy-load Robot


7-axis Collaborative Robot


High-altitude Electrical Maintenance Robot


Robotic Welding Workstation


Patrol Robot


Mobile Collaborative Robot


Footwear Adhesive Application Robot

Applications

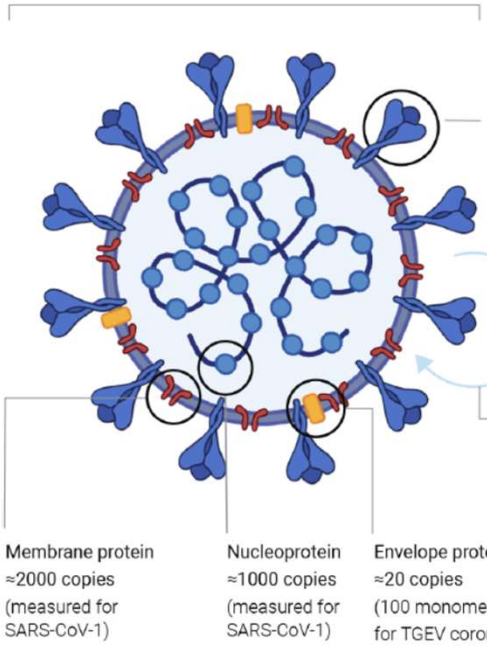
- Intelligent Industrial Robots
- Intelligent Unmanned Aerial Vehicles (UAV)
- Intelligent Unmanned Ground Vehicles (UGV)

SARS-CoV-2 (COVID-19) by the Numbers

Bar-On *et al.* eLife 2020;9:e57309

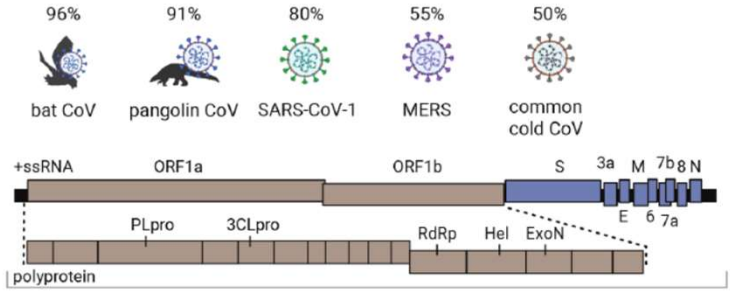
Size & Content

Diameter: ≈100 nm
Volume: ~10^6 nm^3 = 10^{-3} fL
Mass: ~10^3 MDa ≈ 1 fg



Genome

Nucleotide identity to SARS-CoV-2



Length: ≈30kb; β-coronavirus with 10-14 ORFs (24-27 proteins)

Evolution rate: ~10^{-3} nt^{-1} yr^{-1} (measured for SARS-CoV-1)
Mutation rate: ~10^{-6} nt^{-1} $cycle^{-1}$ (measured for MHV coronavirus)

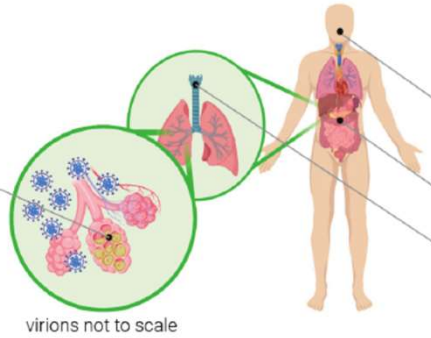
Replication Timescales

(in tissue-culture)
Virion entry into cell: ~10 min (measured for SARS-CoV-1)
Eclipse period: ~10 hrs (time to make intracellular virions)
Burst size: ~10^3 virions (measured for MHV coronavirus)

The basic production number R_0=2~4

Host Cells

(tentative list; number of cells per person)
Type I & II pneumocytes (~10^{11} cells)
Alveolar macrophage (~10^{10} cells)
Mucous cell in nasal cavity (~10^9 cells)
Host cell volume: ~10^3 μm^3 = 10^3 fL



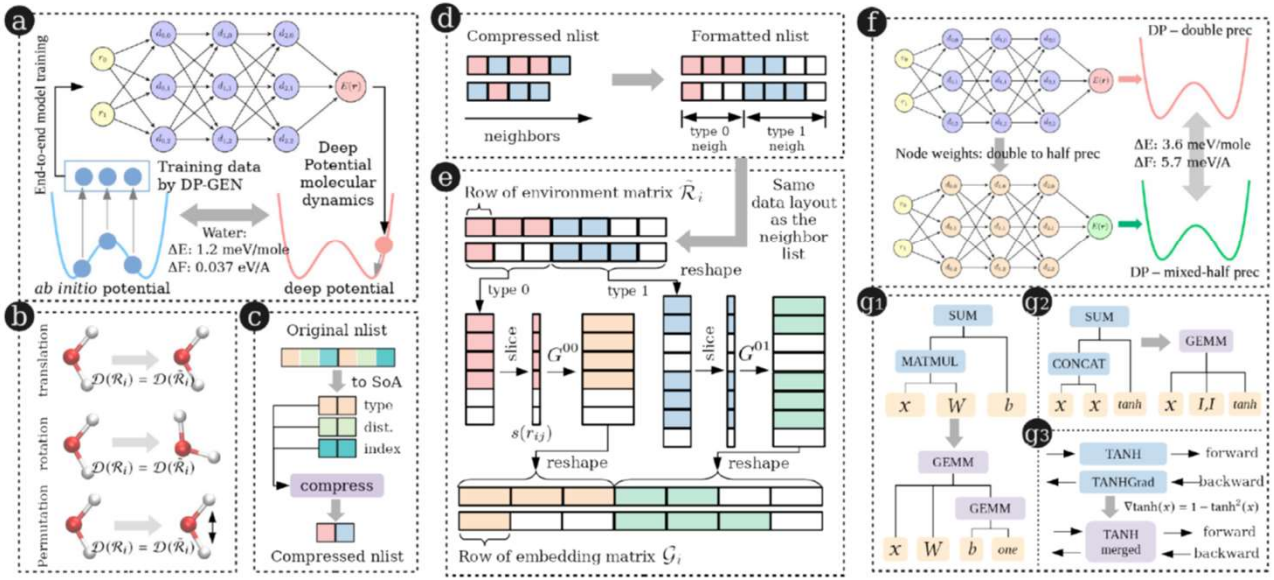
Concentration

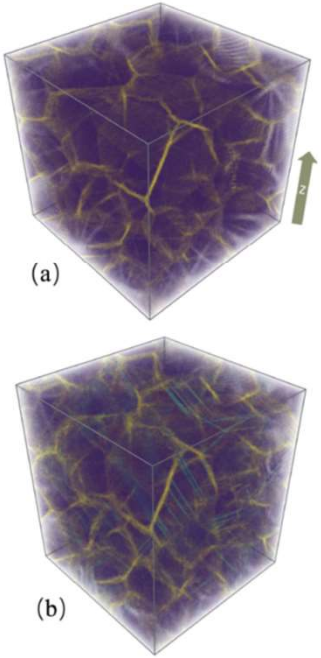
(maximal observed values following diagnosis)
Nasopharynx: 10^6-10^9 RNAs/swab
Throat: 10^4-10^8 RNAs/swab
Stool: 10^4-10^8 RNAs/g
Sputum: 10^6-10^{11} RNAs/mL
RNA counts can markedly overestimate infectious virions

Pushing the Limit of Molecular Dynamics with *Ab Initio* Accuracy to 100 Million Atoms with Machine Learning

W. Jia *et.al*, SC20, November 9-19, 2020

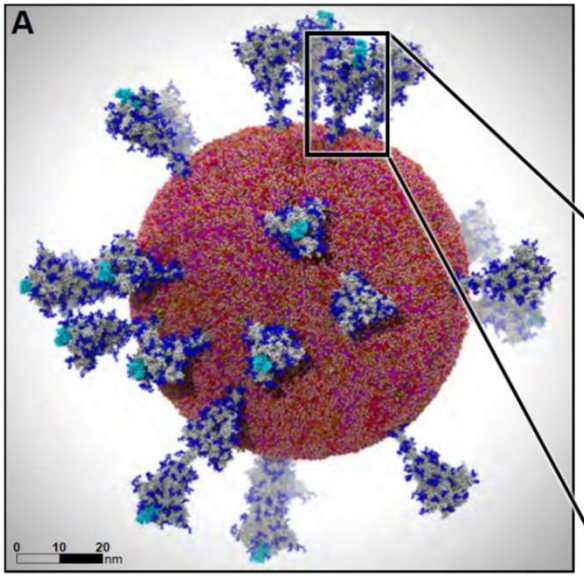
Work	Year	Pot.	System	#atoms	#CPU cores	#GPUs	Machine	Peak[FLOPS]	TtS [s/step/atom]
Qbox [12]	2006	DFT	Mo	1K	262K	–	BlueGene/L	207T	2.8×10^{-1}
LS3DF [14]	2008	LS-DFT	ZnTeO	16K	131K	–	BlueGene/P	108T	1.8×10^{-2}
RSDFT [46]	2011	DFT	Si	107K	442K	–	K-computer	3.1P	2.6×10^{0}
DFT-FE [13]	2019	DFT	Mg	11K	159K	22.8K	Summit	46P	6.5×10^{-2}
CONQUEST [17]	2020	LS-DFT	Si	1M	200K	–	K-computer	?	4.0×10^{-3}
Simple-NN [47]*	2019	BP	SiO_2	14K	80	–	Unknown‡	?	3.6×10^{-5}
Singraber el.al. [48]*	2019	BP	H_2O	9K	512	–	VSC†	?	1.3×10^{-6}
Baseline [45]**	2018	DP	H_2O	25K	1	1	Summit	–	5.6×10^{-5}
This work (double)	2020	DP	H_2O	679M	27.3K	27.3K	Summit	80P	3.0×10^{-10}
This work (mixed-half)	2020	DP	H_2O	679M	27.3K	27.3K	Summit	212P	1.1×10^{-10}
This work (double)	2020	DP	Cu	127M	27.3K	27.3K	Summit	91P	8.1×10^{-10}
This work (mixed-half)	2020	DP	Cu	127M	27.3K	27.3K	Summit	275P	2.7×10^{-10}



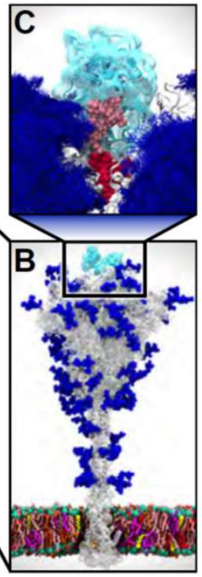


AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics

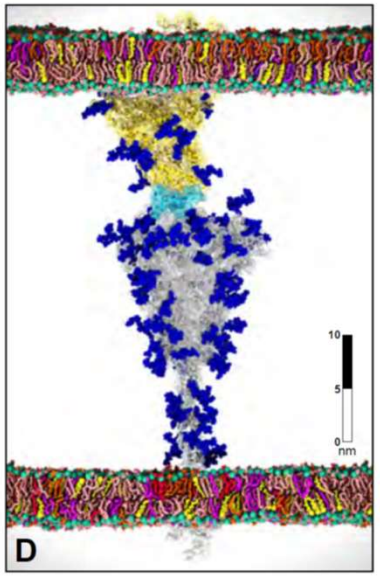
L. Casalino *et.al*, bioRxiv preprint doi: https://doi.org/10.1101/2020.11.19.390187

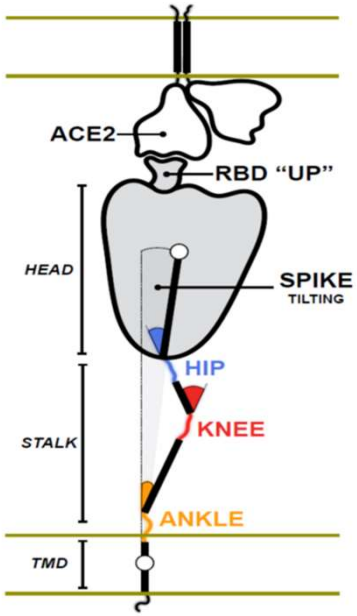


SARS-CoV-2 viral envelope (305 M atoms)

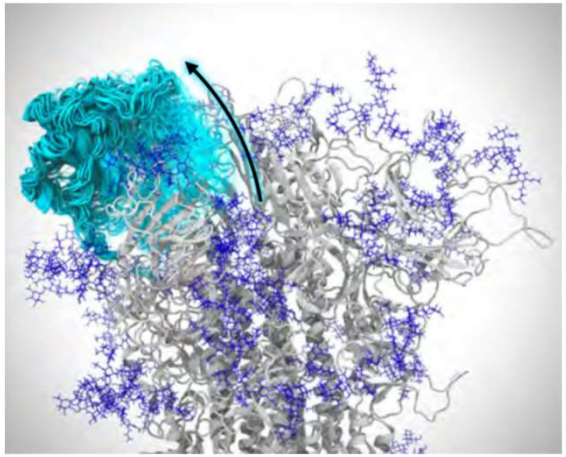


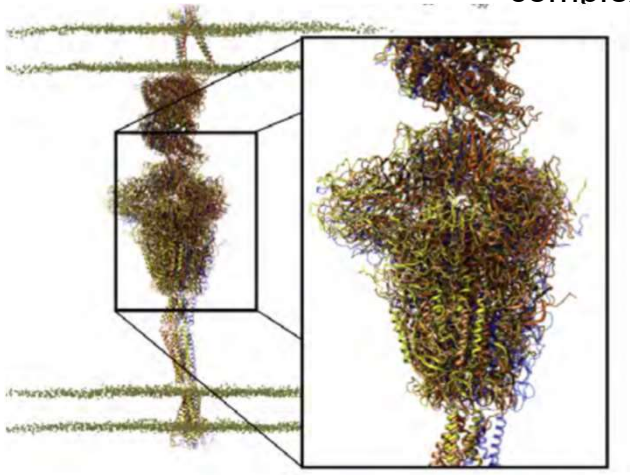
The glycosylated spike protein

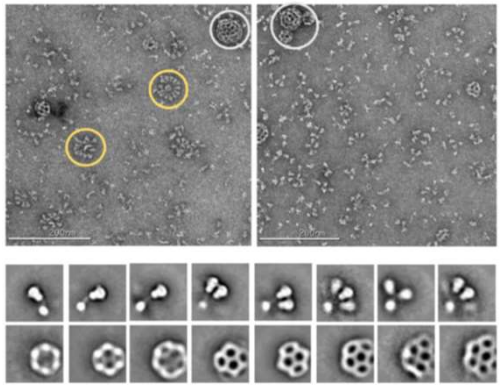




Two-parallel-membrane system of the spike-ACE2 complex (8.5M atoms)

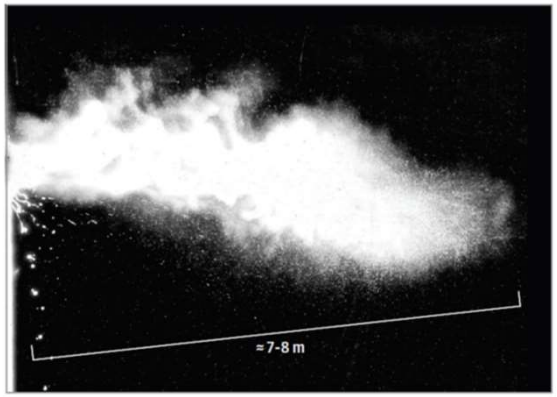


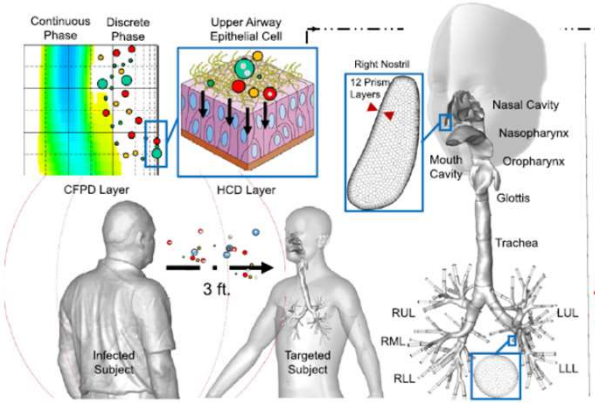


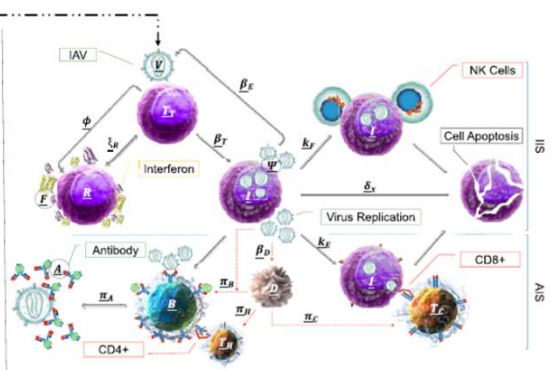


S. Bangaru *et al.*, *Science* 10.1126/science.abe1502 (2020)

Multiple Scale Respiratory Dynamics





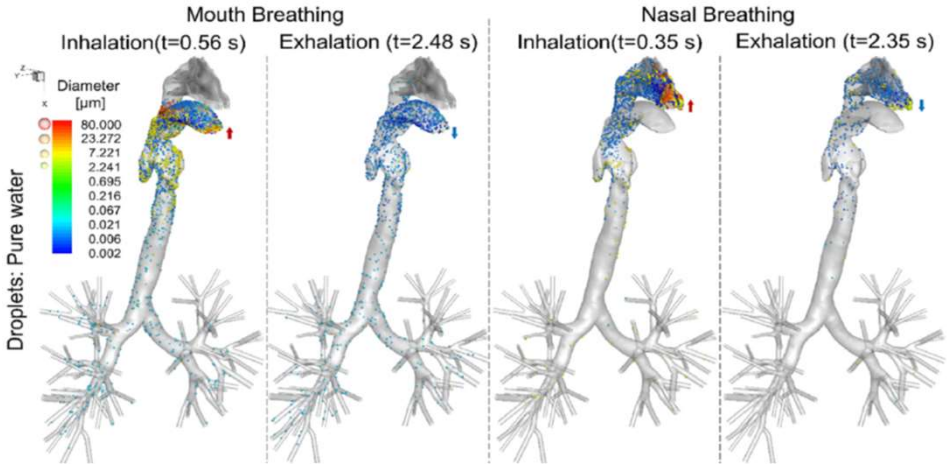


L. Bourouiba, JAMA Insights, E3(2020). A. Haghnegahdar *et.al*, J. Aerosol Sci, 134, 34(2019)

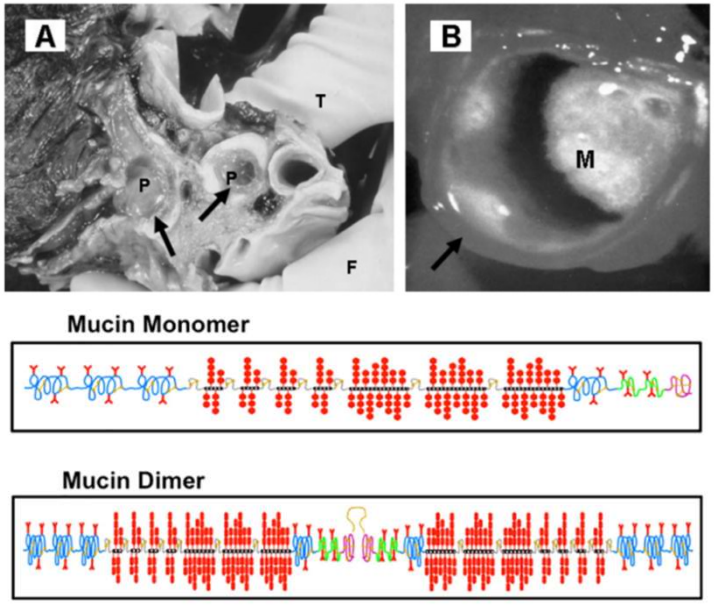
Vessels	Generation/Number	Diameter (mm)	Cum. Volume (ml)	Average velocity (cm/s)	Reynolds number
Trachea	0/1	18	31	393	4350
Segmental bronchus	4/16	4.5	51	392	1110
Bronchi	8/256	1.86	66	144	164
Bronchioles	13/8190	0.82	106	23.1	11
Resp. bronchiole	$17/131\times10^{3}$	0.54	217	3.33	1.1
Alveolar duct	$20/1.05\times10^{6}$	0.45	510	0.60	0.17
Alveolar sac	$23/8.39\times10^{6}$	0.41	1675	0.09	--

From Medical Images to Digital Models

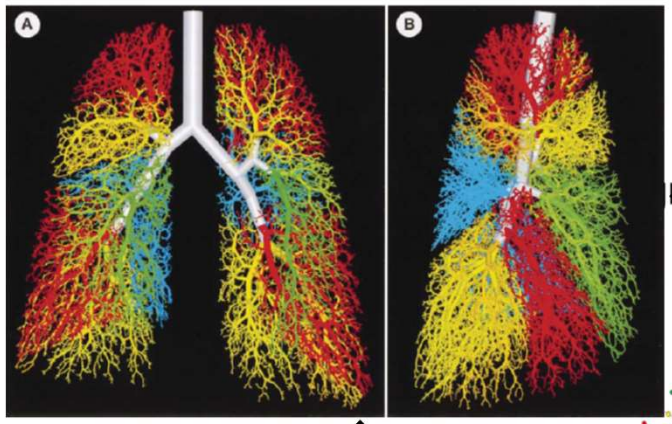
W. Li, *et. al*, AI image screening for SARS-CoV-2, pulmonary nods, & multi-type pneumonia

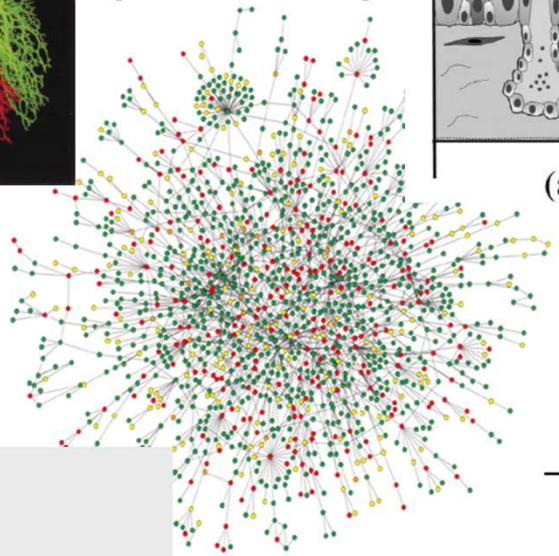


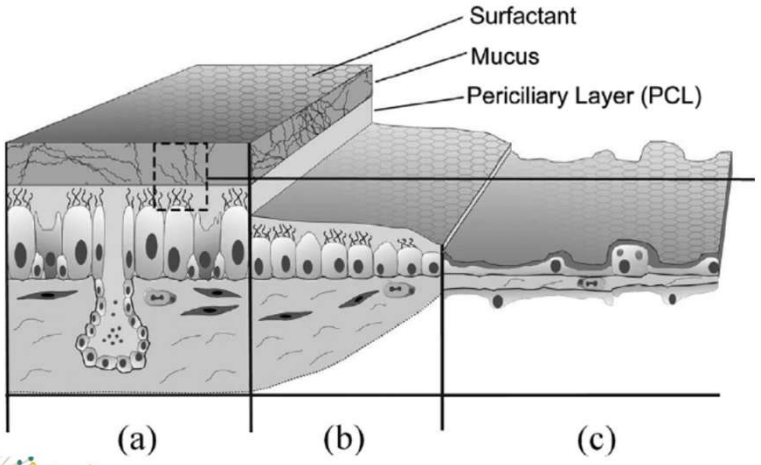
A. Haghnegahdar *et.al*, J. Aerosol Sci, 134, 34(2019)

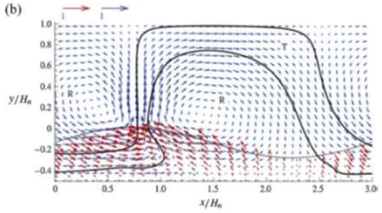


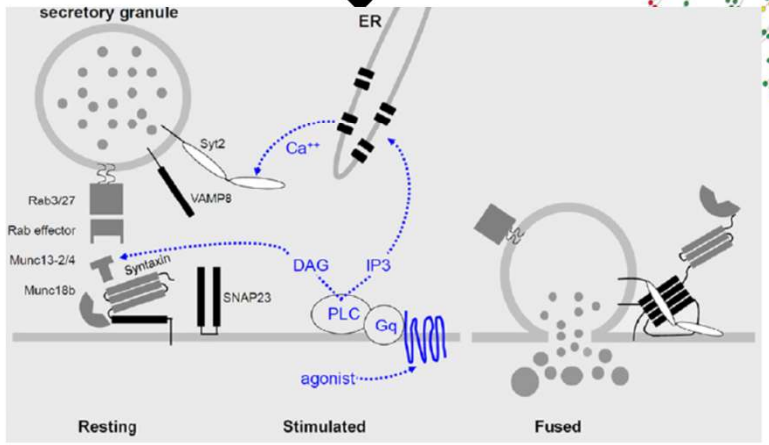
Multiple Scale Simulation from Molecular to Organ Level

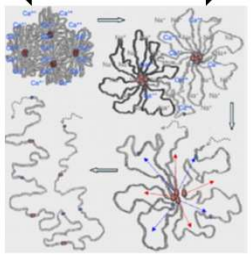


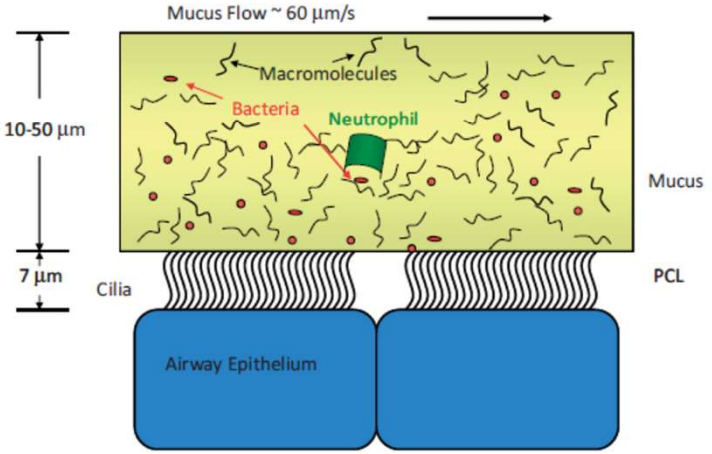






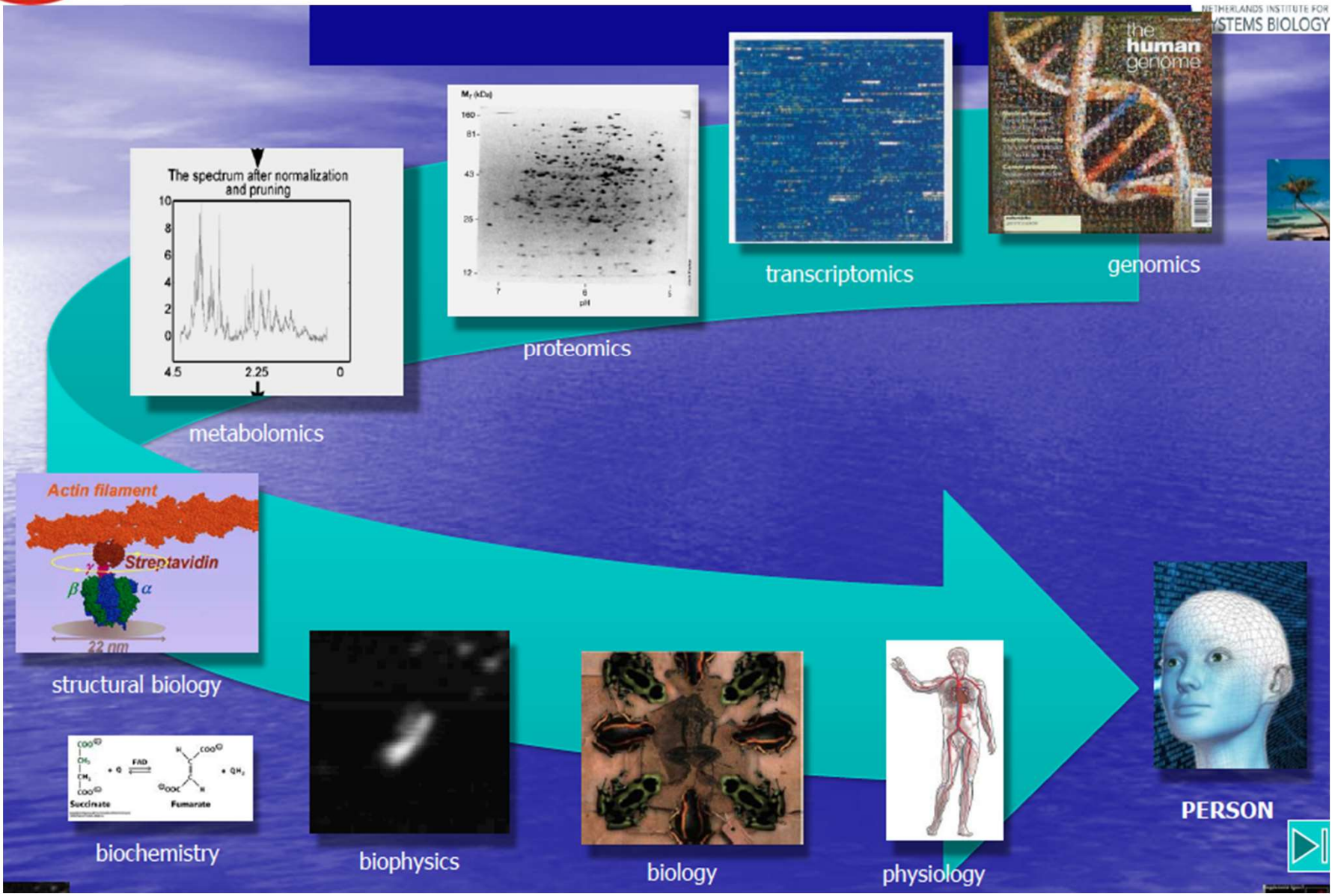






R. Bansil, B.S. Turner, Adv. Drug Delivery Rev. 124 (2018) 3–15

Integration of Biological and Medical Big Data for Development of Digital Twins



Thanks
for your attention!